The structure of CaSO$_4$ nanorods - the precursor of gypsum

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Abstract

The understanding of the gypsum (CaSO$_4$·2H$_2$O) formation pathway from aqueous solutions has been the subject of intensive research in the last couple of years. This interest stems from the fact that gypsum appears to fall into a broader category of crystalline materials whose formation does not follow classical nucleation and growth theories. The pathways involve transitory precursor cluster species, yet the actual structural properties of such clusters are not very well understood. Here, we show how in situ high-energy X-ray diffraction (HEXD) experiments and molecular dynamics (MD) simulations can be combined to derive the structure of small CaSO$_4$ clusters, which are precursors to crystalline gypsum. We fitted several plausible structures to the derived pair distribution functions (PDFs), and explored their dynamic properties using unbiased MD based on both rigid-ion and polarizable force-fields. Determination of the structure and (meta)stability of the primary species is important both from a fundamental and applied perspective; for example, this will allow for improved design of additives for greater control of the nucleation pathway.
In recent years, we have come to appreciate the astounding complexity of the processes leading to the formation of mineral phases from ions in aqueous solutions. The original, and rather naive, ‘textbook’ image of these phenomena, stemming from the adaptation of classical nucleation and growth theories, has increased in complexity due to the discovery of a variety of precursor and intermediate species. These include solute clusters (e.g. prenucleation clusters, PNCs), liquid(-like) phases, as well as amorphous and nanocrystalline solids, among others\textsuperscript{[1–9]}. Such precursor or intermediate species constitute different points along the pathway from dissolved ions to the final solids (e.g. crystals)\textsuperscript{[10]}. Despite a plethora of indirect experimental\textsuperscript{[4]} and modeling-based\textsuperscript{[11]} evidence for the existence of such precursor species there has yet to be any direct structural information derived from experimental observations. Recently, we reported\textsuperscript{[12,13]} that elongated sub-3 nm primary species are the fundamental building units for dihydrated calcium sulfate crystals, i.e. gypsum (\(\text{CaSO}_4 \cdot 2\text{H}_2\text{O}\)). Based on \textit{in situ} and time-resolved small- and wide-angle X-ray scattering data (SAXS/WAXS), we showed that the formation, aggregation, rearrangement and the partial coalescence of these structural units constitutes the actual mechanism behind gypsum crystallization. Nevertheless, from those experiments we were unable to elucidate the nature or the molecular structure of the primary species. To address this issue, we carried out \textit{in situ} high-energy X-ray diffraction experiments and combined these with molecular dynamics simulations. From both \textit{in situ} and \textit{in silico} data we have derived the crystallographic structure of the precursor species. Determination of the actual structure and (meta)stability of the primary species is important both from a fundamental and applied perspective; for example, this will allow for improved design of additives for greater control of the nucleation pathway.

Background-corrected and time-resolved \textit{in situ} diffraction patterns from a 50 mM \(\text{CaSO}_4\) solution at 10 °C are presented in Fig 1A. For the experimental and analysis details please see Supporting Information: Methods. From the very first frame (265 s, see SI: Methods) and during the initial \(~2,000\) s, the measured scattering data contains only an invariant broad diffuse pattern i.e. diffraction peaks were absent. After this induction time, the
diffraction pattern of a crystalline phase gradually started to develop. The crystalline phase coexisted throughout the duration of the measurements with the diffuse pattern (Fig. 1B). Importantly, the as-formed diffuse pattern is significantly different from the scattering patterns obtained from the solvent, i.e. H₂O, and the aqueous solutions containing the various components of the system under consideration (Fig. 1C). Therefore, the diffuse pattern can be attributed to the presence of a disordered phase of CaSO₄ as is demonstrated below. Selected diffraction patterns were converted to pair distribution functions (PDFs, G(r)s) using a numerical inverse Fourier transform, in order to analyze, identify and model the structural changes in real-space. Throughout the reaction, the crystalline material was fitted with a gypsum model structure (Fig. 1D) without any trace of other crystalline CaSO₄ phases (i.e. bassanite or anhydrite). The G(r) resulting from the diffuse scattering shows several interatomic distances common to all calcium sulfate phases (Fig. 1E): S-O at 1.49 Å; Ca-O at ~2.6 Å; shortest (1ˢᵗ neighbour) Ca-Ca and S-S at ~4 Å. With respect to the crystalline forms this disordered phase lacks the longer, i.e. 2ⁿᵈ neighbour, Ca-Ca/Ca-S distance found at ~5-6 Å, although other longer distances are still present. Finally, and most importantly, the PDF plot shows that the structural coherence of the species constituting the diffuse phase does not exceed ~1.5 nm, and thus we can refer to it as a nanophase. Overall, the PDF plots reveal that the species from which the nanophase is built are structurally more complex than simple ions or ion pairs in solution. They have the form of clusters containing at least one single Ca-Ca distance.

The diffuse diffraction patterns shown in Fig. 1A-C are lacking detail, and only show very broad diffraction maxima, which is characteristic of small and thermally labile species in solution. Consequently, one expects that for the primary species a whole family of possible structures can fit to the G(r), rather than one unique solution. Based on our previous small-angle X-ray scattering results, we can narrow down the number of possibilities by constraining the form of such clusters to rod-shaped species with a cross-sectional diameter of ~0.5 nm and a length of several nm[12,13]. Taking into account these constraints, we constructed template clusters, whose structure was further optimized to fit the experimental G(r). Our template clusters were constructed by choosing
a primary motif, which contained at least one single Ca-Ca bond distance, stacking a number of such motifs to obtain a rod, and then optimizing the structure using the randomized simplex method so that the simulated PDF of the structure would match as closely as possible the experimental one. In Fig. 2 we present several possible structures of the primary species, based on the best fits to the $G(r)$ of the nanophase obtained by optimizing the initial template clusters using a DiffPy library$^{[14]}$ (SI: Methods).
Fig. 1. Experimental data that follow the formation of solids in a solution with an initial concentration of 50 mM CaSO$_4$ at 10 °C. (a) time-resolved in situ HEXD pattern in which the first frame corresponds to 265 s and the last to 9,275 s; (b) comparison between the diffraction patterns of the initial nanophase 1 (solid, pink) and the final crystalline product 2 (solid, cyan). This final diffraction pattern is a juxtaposition of the diffraction pattern of the nanophase (dashed, blue) and the second purely crystalline phase 3 (solid, black); (c) comparison between the diffraction patterns of the nanophase and other components of the investigated system; (d) selected PDFs from (a) highlighting the structural difference between the nanophase and the crystalline phase clearly identified as gypsum; (e) comparison of PDFs from the nanophase - N, and other CaSO$_4$ phases: gypsum - G, bassanite - B, and anhydrite - A. The difference in the $G(r)$s for the distance $r \sim 5$-6 Å is highlighted with two black lines. For (b)-(e) offset is introduced for clarity.

The four plausible clusters (Fig. 2; SI for the structural files) were optimized based on the following cross-sectional motifs: I – a simple 2-member square-shaped Ca-SO$_4$-Ca-SO$_4$ unit, where 6 stacks are arranged in an AB pattern and each Ca is coordinated by two in-plane water molecules; II – 3 member triangular Ca-SO$_4$-Ca-SO$_4$-Ca-SO$_4$ units, where 6 such units are stacked into a helix with a torsion of 70.4°; III - analogous to II but with a torsion of 70.7° and each Ca is coordinated by two in-plane water molecules; IV – analogous to I, but with a repetitively stacked (Ca-SO$_4$)$_2$ unit for which the initial positions were taken from a gypsum fragment (which results in a longer length of the cluster). We used a Pearson correlation coefficient ($R$) as a proxy to benchmark the structures based on their simulated $G(r)$s with respect to the experimental one. All the proposed models reproduce almost ideally the experimental $G(r)$s up to $r = 6$ Å ($R > 0.99$), with minor deviations for higher $r < 12$ Å. Our analysis shows that the proposed family of solutions should fulfill three conditions: (1) the clusters are rod-shaped; (2) a single structural unit in the cross-section of the rod does not expand beyond a single Ca-Ca distance, with either of 2 or 3 Ca ions per unit. The diameter of such a cross-sectional unit is ~0.5 nm; (3) the rods are “internally” an anhydrous CaSO$_4$ structure, and bound water is only present at their “surface”; the presence of the coordinated water improves measurably the quality of the fits for $r > 6$ Å (i.e. compare otherwise identical clusters II and III with $R$ of 0.868 vs. 0.960).
Fig. 2. (a) Selected optimized structural models of CaSO$_4$ rod-shaped clusters for the observed nanophase. Upper row: longitudinal view, Lower row: cross-sectional view. Cluster: I – Ca-Ca AB stack hydrated with 6 layers, II – Ca-Ca-Ca helix stack 70.4° anhydrous with 6 layers, III Ca-Ca-Ca helix stack 70.7° hydrated with 6 layers, IV – Ca-Ca AA stack hydrated with 6 layers. See SI for the files containing these models; (b) Experimental PDF from the nanophase compared with the PDFs simulated from the structural models of clusters I-IV; (c) Experimental PDF vs. simulated PDF for structures based on cluster III, in which the number of layers was varied from 2 to 30.

In Fig. 2C we compare the simulated PDFs of clusters similar to type I (with 6 layers) with the experimental data varying the number of layers from 1 to 16. All the clusters considered reproduce the experimental $G(r)$ up to $r = \sim 6$ Å ($R > 0.99$). However, the profile of the PDF is reproduced better for longer clusters with 4 to 16 layers, which is also reflected by the higher $R$-values in comparison with clusters containing 1, 2 or 3-layers for
$r > \sim 6 \text{ Å}$. As the number of layers is further increased the $R$-values for $r > \sim 6$ Å start to marginally decrease again, but they remain relatively high at $R > 0.9$. The values of $R$ suggest that the optimum structure has 4 to 10 layers (length between 1.1 and 3.1 nm), but the clusters could be longer. Nonetheless, taking into account the overall coherence length, which was limited to $\sim 1.5$ nm (Fig. 1E), we can calculate the maximum physical length of a cluster. For anisotropic rod-shaped species, we can use their radius of gyration, $R_g$, as a proxy for the measured isotropic coherence length by using the dimensions of a cylinder of length $L_c$ and radius $R_c$, and the following equation:

$$R_g^2 = R_c^2/2 + L_c^2/12.$$  

The clusters considered have a cross-sectional diameter$^{[12]}$ of $\sim 0.50$ nm, which results in a length that does not exceed 5.2 nm. This in turn is equivalent to a cluster composed of 16 layers at most. Similar trends were found for structures I, III and IV, where the optimal fits are obtained for rods composed of $\sim 4$-12 stacks of structural units, yielding a total length for the rod in the range of $\sim 1.5$ - 3.5 nm depending on the packing of the structural units. The estimate of the length of the clusters obtained from the PDF analysis is in accordance with the earlier SAXS measurements of these species$^{[12,13]}$.

Not only do diffraction data allow us to resolve the possible structures of the observed clusters. They are also useful to evaluate the population of such species with respect to the initial ion concentrations and the final expected gypsum content by calculating the scattering invariants of the crystalline and (SI: Methods). We performed such analysis using diffraction data of gypsum precipitating at 10 ºC from solution containing initially 50 and 100 mM CaSO$_4$. For both conditions, diffraction patterns of an identical nanophase profile were collected, but as expected, the crystallization process progressed faster for the higher initial CaSO$_4$ concentration$^{[13]}$. As shown in Fig. 3, the nanophase constituted $\sim 100\%$ of the initial scattering invariant for the 50 mM solution, and $> 90\%$ for the 100 mM CaSO$_4$. In both cases, by the end of the experiment the nanophase was still persistent and constituted in fact the majority contribution to the invariant at $\sim 82\%$ and $\sim 75\%$ for 50 mM and 100 mM CaSO$_4$ solutions, respectively. Based solely on the HEXD data, it is not possible to determine whether the diffuse pattern originated from solute clusters or from clusters aggregated into larger morphologies.
Using thermodynamic modelling approach (see SI) we evaluated the expected initial speciation, the final composition of the solution at the equilibrium, and the amount of the precipitated solid for the CaSO₄ solution under the as-defined physicochemical conditions (SI: Table 1). Such an approach allowed us to calculate the maximum yield of gypsum (the precipitated solid) that one could obtain from a solution of a given starting concentration of ions (but only including the phases which are in the database). As we compare the final contribution of the amount of the nanophase with respect to the expected amount of gypsum from both solutions, it becomes apparent that the total population of the clusters considerably exceeds what one would expect to find within a crystalline solid, even if we assume that some the clusters could “dwell” in solution (and being equivalent to what the calculation considers to be the free ions or the ion pairs). This in turn translates into the fact that for the both considered conditions the “final” amount of crystalline gypsum is lower than anticipated at the equilibrium, and hence that the processes is not at the equilibrium by the end of the experiments (although the diffraction patterns were not evolving any more). Such an observation can be rationalized if we assume that gypsum single crystals are in fact mesocrystal-like\textsuperscript{[15]} in nature, composed of crystalline domains “glued” together by the disorganized cluster (“bricks-in-the-wall”)\textsuperscript{[16]}, and thus a large proportion of the clusters may co-exist inside the solid together with crystalline gypsum. Such imperfect crystals would mature overtime converting clusters into the crystalline lattice approaching the equilibrium.
Fig. 3. Contribution as a function of time of the nanophase (filled symbols) and gypsum (open symbols) to the total scattering invariant with an initial concentration of 50 mM (black) and 100 mM (pink) CaSO₄ at 10 °C.

To complement the diffraction data, we also attempted to quantify the overall thermodynamic stability of the described above CaSO₄ clusters by using metadynamics simulations with our recently developed force field model and a suite of different collective variables. Although these simulations did not produce unequivocal values for the formation free energy of small clusters (up to 4 formula units), the aggregates did consistently show rod-like shapes (please consult the SI for the further details on the issues in obtaining the reliable thermodynamic properties of the clusters from the simulations). We therefore decided to use unbiased Molecular Dynamics (MD) simulations, with rigid-ion (i.e. classical) and polarizable (i.e. AMOEBA) force fields, to assess the stability of the clusters that gave the best fit to the diffraction data (Fig. 2). The scattering-derived clusters were annealed for 5 ns at 300 K. Independent of the force field used and for all the clusters considered, only cluster I maintained its structure throughout the whole MD simulation (Fig. 4), while the remaining models significantly rearranged. The AMOEBA polarizable force field showed a high degree of instability for the remaining clusters, which tended toward elongated highly distorted structures (e.g. Fig. 4A for
cluster II), while on the other hand, the rigid-ion force field seemed to favour more compact clusters that resembled two cluster I rods side-by-side. This different behaviour can be explained by considering that the rigid-ion force field gives a dissolution free energy for the anhydrous CaSO$_4$ phase$^{[18]}$ that is too endothermic, and therefore the ions tend to form more compact structures where they are in direct contact. A structural comparison between the relaxed geometry of cluster I at the end of the MD simulations shows that there are significant differences between the rigid-ion and polarizable force fields (Fig. 4B, upper). In particular, the former model shows a much more rigid and ordered arrangement of the ions, which form a stack of squares rotated 90 degrees with respect to each other, while the AMOEBA simulations show a more mobile structure where the ions form a stack of distorted squares. Nevertheless, if we consider the overall trajectories of all the atoms in the cluster over a period of 5 ns, then despite this apparent “disordered” structure resulting from the use of the AMOEBA forcefield, this cluster structure matches much better the experimental data than the one from the non-polarizable model (SI: the trajectory files). These differences are evident in the Ca-Ca, Ca-S and S-S pair distribution functions form trajectories obtained from the MD simulations (Fig. 4B and SI: Methods, and SI: trajectory files). In particular, the rigid-ion MD simulations show no strong S-S peaks in the 4 – 4.5 Å and 5.5 - 6 Å regions, or Ca – Ca peaks at 4 – 5 Å (Fig. 4B, lower) that are apparent in the AMOEBA MD simulations and in the experimentally determined cluster I structure. Based on the above results, cluster I seems to be the most likely candidate for the model structure of the CaSO$_4$ clusters that reproduces the recorded scattering pattern. From the MD simulations, it is evident that the terminal parts of the cluster are more mobile, due to having only half of the ionic interactions, which suggests that the core part of the rod is contributing the most to the scattering signal, and therefore the clusters might be slightly longer than the 4-12 stack length that best fits the scattering data. Furthermore, a highly dynamic character is intuitively expected for such small species in solution, yet is practically impossible to implement in our fitting routines used to obtain the rigid structural models in Fig. 2 from the diffraction data. The imposition of constraints results from the fact that we
had to limit the number of degrees of freedom to achieve convergence of the template models. Typically, such constraints are valid assumptions for crystalline structures and are based on symmetry restrictions. Nonetheless, for small clusters such constraints yield merely a valid transitory averaged model (since it fits the experimental PDF), but not necessarily the minimum energy model or any equivalent low-symmetry counterpart structure. Hence, the MD simulations are essential to probe the configuration space from which our cluster I, as defined in Fig. 2, is actually just one of many possibilities. From the MD simulations it is not possible to gauge the actual thermodynamic stability of these clusters, but dynamic models using the AMOEBA force-field strongly support the HEXD and previous SAXS data\textsuperscript{[12]}, which show that CaSO\textsubscript{4} forms rod-shaped structures, upon creation of a supersaturated solution, that are thermodynamically stable/kinetically persistent in solution for sufficiently long time to be observed experimentally. It is very important to also note that at present the solubility of the CaSO\textsubscript{4} phases with the AMOEBA force field is unknown as it was parametrized for the solution phase, and as such it is possible that it may underestimate the stability of the solids. Estimations of the relative stability of a 4 formula structural unit based on cluster I relative to that of a CaSO\textsubscript{4} ion pair using \textit{ab initio} quantum mechanical methods suggest that both species are likely to be similar in free energy (see SI).
Fig. 4. a) Unstable cluster II after 5 ns of an MD simulation using the AMOEBA force field; the cluster shows significant disorder, but it essentially preserves its original elongated shape; b) Comparison between the structures of cluster I as predicted from the rigid-ion classical (left) and AMOEBA polarizable (right) MD simulations. The graphs show the radial pair distribution functions (g(r)s) computed from the whole MD trajectories (see SI for the files) over the course of 5 ns (cyan lines) overlaid with those computed from the static structure of cluster I obtained from the experiments (magenta bars/histograms). The magenta g(r) is generated from the optimized cluster I structure (see Fig. 3), hence the discrete histogram form.

Although our current diffraction and earlier scattering data[12,13], as well as the current MD simulations, clearly point to the presence of small CaSO₄ clusters as a precursor to gypsum and possibly other calcium sulfate crystalline phases[19], it is not clear what their role exactly is. It appears that they might be akin to prenucleation clusters reported for the calcium carbonate system[4,11], though our experimental approach considers de facto supersaturation conditions. Regardless of the classification of the clusters (PNCs sensu lato), their presence and evolution imply that the early stages of gypsum formation from solution are non-classical[1]. Important is also the fact that these primary clusters are numerous and persistent both in aqueous solution as well as later in the solid. Their presence along the crystalline gypsum is consistent with the surface structure factor theory of surface fractal aggregates that we developed recently[16], and the associated SAXS results which showed that the large aggregates of clusters had formed before any crystalline phases were present and
persisted after gypsum crystallization\textsuperscript{[12]}. Most significantly, we recently confirmed using dark field transmission electron microscopy the actual “brick-in-the-wall” (mesocrystalline) character of various natural and synthetic single CaSO\textsubscript{4} crystals\textsuperscript{[20]}. These earlier results, together with the current data, strongly support our conclusion that gypsum crystallizes from the inside of large aggregates of structurally distinct, but flexible, precursor clusters.
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Supporting Information

to

The structure of Ca-SO₄ nanorods - the precursor of gypsum

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Materials & Methods

Synthesis and scattering experiments

CaSO₄ was synthesized by reacting equimolar aqueous solutions (ultrapure deionized water, MilliQ, resistivity >18 MΩ cm) of CaCl₂·2H₂O (pure, Sigma) and Na₂SO₄ (> 99%, Sigma) at final concentrations of 50 and 100 mmol/L at T = 10 °C. Prior to mixing, all solutions were equilibrated in a fridge at the desired reaction temperatures. The compositions of solutions (Table 1), under the assumption that gypsum was the final solid phase, were calculated with PHREEQC[^1] based on the following reaction:

\[
\text{CaCl}_2 + 2\text{H}_2\text{O} + \text{Na}_2\text{SO}_4 \rightarrow \text{CaSO}_4 \cdot 2\text{H}_2\text{O} \downarrow + 2\text{NaCl}
\]

CaSO₄ formation reactions were performed in a 200 mL temperature-stabilized glass reactor. The reaction temperature in the reactor was maintained by means of an active cooling circulator (Huber Ministat 125), and the feedback thermocouple was placed in the reactor. The reacting solutions were continuously stirred at 350 rpm, and circulated through a custom-built PEEK flow-through cell with Kapton capillary (ID 1.5 mm) using a peristaltic pump (Gilson MiniPuls 3, flow ~10 mL/second). Typically, an experiment started with 40 mL of a temperature-stabilized CaCl₂ aqueous solution inside the reactor. This solution was circulated through the capillary cell while scattering patterns were collected continuously as described below. CaSO₄ formation reactions were initiated remotely through the injection of 40 mL of a temperature-stabilized Na₂SO₄ aqueous solution. Injection and mixing (within 30 s) of the two solutions was achieved with the use of a secondary peristaltic pump (Gilson MiniPuls 3) as a remote fast injection system. Depending on the supersaturation, reactions were followed for up to 4 hours.

In order to follow the formation processes in situ, and in a time-resolved manner, the flow-through cell was mounted on a high-energy X-ray diffraction (HEXD) system and the measurements were carried out at
beamline I15 of the Diamond Light Source (UK). The experiments were carried out at a wavelength of 0.16416 Å allowing us to collect scattering in the $q$-range up to ~25 Å$^{-1}$. The $q$-range was calibrated using a CeO$_2$ standard in a 1 mm Kapton capillary. The 2D HEXD patterns were collected using a Perkin Elmer flat panel 1621 EN detector (2048 x 2048 pixels, pixel size 0.2 x 0.2 mm$^2$) in Debye-Scherrer geometry (according to the I15 guidelines) at a time-resolution of 30 s/frame for a series of 5 data frames, after which two detector dark current images (the 6th and the 7th frame) were collected for 30 s. Including the instrumental dead-time, each such series lasted 265 s. Dark current contributions were corrected automatically by the acquisition software. Hence, in our experiments, the time resolution was thus effectively limited to 265 s because the collected frames had to be bundled and averaged to optimize the signal-to-noise, signal-to-background ratios and corrected for the dark current of the CCD detector. Furthermore, various background and reference samples were measured under similar conditions, and included among others, an empty Kapton capillary, a capillary containing pure water and the constituent solutions at T = 10 °C, as well as, powders of solid CaSO$_4$ phases. The as-obtained 2D images were reduced to raw 1D curves using DAWN$^{[2,3]}$. Further processing and correction of raw 1D data curves involved subtraction of background solutions and extraction of characteristic patterns. Due to excluded volume effects, the contributions of solvent to the scattering patterns were smaller than unity and not constant over time. To correct for this effect, we filtered out sharp gypsum peaks in the time resolved data sets, by calculating the minimum over moving window functions and smoothing the resulting set of minima. Then, we fitted a linear combination of background patterns from capillaries with water, constituent solutions and an empty capillary to the peak-filtered data sets. From this approach, we obtained negative contributions of several solutions, which clearly indicated overfitting of the data sets with almost identical patterns of water and the constituent aqueous solutions. This showed us that we could reduce the number of patterns used for background subtraction down to two essential patterns: a capillary with an NaCl solution and an empty capillary. After performing the background subtraction with this reduced set, we observed a decrease of the contribution of the
background coefficient attributed to a capillary with a NaCl solution from 0.85 to 0.75. This in turn suggested an increase in the excluded volume by 10%. Following this approach, we obtained reliable background correction factors and used it to subtract the water/capillary background from all the time-resolved data sets (including those without gypsum diffraction peaks). The diffuse and crystalline scattering patterns were separated from each other by the abovementioned moving minimum window function and the concentration profiles were derived by applying a linear combination fitting method with the derived diffuse and crystalline patterns. After this processing and background subtraction stage the atomic pair distribution functions (PDFs) were obtained by using the PDFgetX3 software package\textsuperscript{[4]}. The background and Compton scattering subtractions were also performed using the same code. Further processing of the data, such as phase identification and fitting of the structural models, principal component analysis (PCA) on the series etc. was performed using custom scripts developed by us in NumPy (Python) and utilizing a dedicated DiffPy library\textsuperscript{[5,6]}. To achieve convergence of the results we introduced several reasonable structural restrictions: (1) the sulfate tetrahedra and water molecules were considered to be internally stiff with a free rotation around Euler angles; (2) model clusters were defined by a network of linked bond-vectors and bond distances were restricted within ±1 Å from the initial average values known from crystalline CaSO\textsubscript{4} phases; (3) to avoid that some atoms get unrealistically close or far from each other we applied a simple potential \( V = \sum (k_c q_i q_j r_{ij}^{-1} + k_{i,j, \text{rep}} r_{ij}^{-12}) \), where \( q_i \) and \( q_j \) are the oxidation number of atoms i and j, \( r_{ij} \) is the distance between atoms i and j, \( k_c \) is a Coulomb constant, and \( k_{i,j, \text{rep}} \) is a repulsive constant optimized to known atom distances.
Classical molecular dynamics simulations were run with the LAMMPS program\textsuperscript{[7]} at 300 K and 1 atm in a cubic simulation cell of approximately 50 Å in side, which contained \~4,130 water molecules and the relevant CaSO\textsubscript{4} cluster. The long-range electrostatics were computed with the Particle Mesh Ewald algorithm with an accuracy of $10^{-5}$ while the bonded and van der Waals interactions were described by our recently developed force field\textsuperscript{[8]} (FF1). The real space cut-off was set to 9 Å with a tapering function applied between 6 and 9 Å. The water was described with the SPC/Fw model\textsuperscript{[9]}, and no tapering was applied to the water-water interactions. The equations of motions were integrated with a 1 fs time-step using the velocity Verlet algorithm, while the temperature was controlled with the Canonical Sampling through Velocity Rescaling algorithm\textsuperscript{[10]}. The cell was constrained to remain cubic throughout the simulations.

All simulations with the AMOEBA polarizable force field\textsuperscript{[11]} were run with the openMM7.1 code\textsuperscript{[12]}. The equations of motion were integrated with the Langevin algorithm using a 0.5 fs time-step, a friction coefficient of 1 ps\textsuperscript{-1} and a temperature of 300 K. The pressure was maintained at 1 atm using an isotropic Monte Carlo barostat\textsuperscript{[13,14]} with a collision frequency of 25 steps. The real space cut-off was set to 10 Å for all non-bonded interactions, while the long-range electrostatic interactions were computed with the Particle Mesh Ewald algorithm, again with an accuracy of $10^{-5}$. Induced dipoles were solved for iteratively at each time-step until an accuracy of $10^{-5}$ was reached. The initial configurations were the same as used in the rigid-ion MD simulations.

The trajectories for cluster I calculated for both force fields are included as a part of this SI: Supporting Files.
Ab initio calculation of cluster stability

Because of the dynamic nature of the clusters, as observed in the atomistic simulation, it is difficult to obtain an accurate estimate of the free energy of species via static quantum mechanical methods. In the present study, we have performed a number of cluster calculations to estimate the stability of CaSO$_4$ ion pair and a four formula unit cluster, with an approximately cubic structure, that was initially extracted from the AMOEBA molecular dynamics with its first solvation shell. All structures were fully optimized at the oB97X-D3/def2-TZVP level of theory using the ORCA 4.1.1 code\textsuperscript{[15]} with Grid4 for the numerical integration of the density. In order to describe the aqueous environment of the species the ion pair and cube cluster were surrounded by 18 and 30 waters of solvation, respectively, in addition to the use of the CPCM continuum solvation model (the radius for Ca was refitted to 1.824 Å to reflect the hydration of the cation, rather than the neutral atom). The aim was to try to ensure that each ion has at least a complete first solvation shell of explicit water. Indeed, during optimization of the ion pair two water molecules relaxed from an initial position in the first solvation shell to become part of the second shell, thus confirming the completion of the first shell. For the cube, all ions remained in the first shell. Given that all Ca ions had three waters coordinated, while the sulfate ions had a mix of 4 and 5 waters of hydration (in addition to bridging waters from Ca), it is possible that extra water could have been accommodated.

Based on the above calculations, the difference in internal energy between the CaSO$_4$ ion pair and (CaSO$_4$)$_4$ cluster was computed to be 55.0 kJ/mol, with the ion pair being more stable. Direct use of the vibrational frequencies to estimate the free energy difference was found to lead to poor results as the energetics are dominated by the zero-point energy of the water molecules surrounding the species. As a result, the free energies were sensitive to the solvation of the water, rather than the CaSO$_4$, which given the single static structure is not representative of the liquid phase. Instead, it is possible to estimate the free energy difference
based on the change in the number of water molecules in the first solvation shell of the ions between the clusters. From the work of Dunitz\textsuperscript{[16]} each molecule of water released during aggregation could contribute up to 29.3 J/K/mol to the entropy of the system, which we have previous used to rationalize the stability of ion pairs in other systems\textsuperscript{[17]}. For the ion pair and cube the optimal first shell water coordination numbers are estimated to be 16 and 32, respectively, which leads to an upper bound to the entropic stabilization of the cube of 69.9 kJ/mol relative to the ion pair. Given the similar magnitude, but opposing signs, of the internal energy and entropy for aggregation of the ion pair to the smallest motif for cluster I we can conclude that formation of such larger structures is feasible, though within the uncertainties of the method it is not currently possible to give an accurate quantitative free energy for the process.
**Supporting Tables**

**Table 1.** Composition of CaSO₄ solutions from PHREEQC\textsuperscript{[1]} modelling.

|                     | 50 mM CaSO₄ | 100 mM CaSO₄ |
|---------------------|-------------|--------------|
| **Initial**         |             |              |
| **composition**     |             |              |
| [Ca\textsuperscript{2+}] = [SO\textsubscript{4}\textsuperscript{2−}] = 35 mM | [Ca\textsuperscript{2+}] = [SO\textsubscript{4}\textsuperscript{2−}] = 69 mM |
| [CaSO₄]* = 15 mM    | [CaSO₄]* = 31 mM |
| **Final**           |             |              |
| **composition**     |             |              |
| [Ca\textsuperscript{2+}] = [SO\textsubscript{4}\textsuperscript{2−}] = 16.3 mM | [Ca\textsuperscript{2+}] = [SO\textsubscript{4}\textsuperscript{2−}] = 20 mM |
| [CaSO₄]* = 3.9 mM   | [CaSO₄]* = 3.9 mM |
| [solid equivalent]  = 29.8 mM | [solid equivalent] = 76.1 mM |

* - dissolved species. The model considers here an ion pair.

**Supporting Files**

Structural files of Ca-SO₄ clusters from Fig. 2 in the main text are included as *cluster_I.cif*, *cluster_II.cif*, *cluster_III.cif* and *cluster_IV.cif*.

Trajectory files from the MD simulations for cluster I from which Fig. 4B in the main text was derived, are included as *cluster_I_classical_trj.xyz* and *cluster_I_amoeba_trj.xyz*.
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SUPPORTING FILES
# Cluster I

# CRYSTAL DATA

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data_VESTA_phase_1

| _chemical_name_common          | '3D'          |
|-------------------------------|---------------|
| _cell_length_a                | 31.00000      |
| _cell_length_b                | 30.00000      |
| _cell_length_c                | 39.00000      |
| _cell_angle_alpha             | 90            |
| _cell_angle_beta              | 90            |
| _cell_angle_gamma             | 90            |
| _space_group_name_H-M_alt     | 'P 1'         |
| _space_group_IT_number        | 1             |

loop

| _space_group_symop_operation_xyz | 'x, y, z' |

loop

| _atom_site_label    | _atom_site_occupancy | _atom_site_fract_x | _atom_site_fract_y | _atom_site_fract_z | _atom_site_adp_type | _atom_site_U_iso_or_equiv | _atom_site_type_symbol |
|---------------------|----------------------|--------------------|--------------------|--------------------|------------------------|--------------------------|------------------------|
| Ca1                 | 1.0                  | 0.432693           | 0.438417           | 0.292682           | Uiso                   | 0.025486                 | Ca                     |
| Ca2                 | 1.0                  | 0.535868           | 0.534654           | 0.302128           | Uiso                   | 0.025486                 | Ca                     |
| Ca3                 | 1.0                  | 0.549820           | 0.439038           | 0.368805           | Uiso                   | 0.025486                 | Ca                     |
| Ca4                 | 1.0                  | 0.436116           | 0.530296           | 0.386790           | Uiso                   | 0.025486                 | Ca                     |
| S1                  | 1.0                  | 0.545146           | 0.437132           | 0.305843           | Uiso                   | 0.025486                 | S                      |
| O1                  | 1.0                  | 0.498238           | 0.431521           | 0.312969           | Uiso                   | 0.025486                 | O                      |
| O2                  | 1.0                  | 0.561588           | 0.476990           | 0.324519           | Uiso                   | 0.025486                 | O                      |
| O3                  | 1.0                  | 0.568908           | 0.396744           | 0.317577           | Uiso                   | 0.025486                 | O                      |
| O4                  | 1.0                  | 0.551849           | 0.443273           | 0.268308           | Uiso                   | 0.025486                 | O                      |
| S2                  | 1.0                  | 0.420822           | 0.529869           | 0.285454           | Uiso                   | 0.025486                 | S                      |
| O5                  | 1.0                  | 0.391868           | 0.493973           | 0.272511           | Uiso                   | 0.025486                 | O                      |
| O6                  | 1.0                  | 0.406220           | 0.544215           | 0.320140           | Uiso                   | 0.025486                 | O                      |
| O7                  | 1.0                  | 0.465839           | 0.512693           | 0.287604           | Uiso                   | 0.025486                 | O                      |
| Atom | U1   | U2   | U3   | Uiso  |
|------|------|------|------|-------|
| O8   | 0.419360 | 0.568595 | 0.261561 | 0.025486 |
| S3   | 0.441400 | 0.438788 | 0.369406 | 0.025486 |
| O9   | 0.405364 | 0.406434 | 0.364965 | 0.025486 |
| O10  | 0.483247 | 0.414360 | 0.397311 | 0.025486 |
| O11  | 0.441106 | 0.471258 | 0.340975 | 0.025486 |
| O12  | 0.565400 | 0.556813 | 0.363471 | 0.025486 |
| O13  | 0.529093 | 0.524363 | 0.365393 | 0.025486 |
| O14  | 0.567526 | 0.582865 | 0.395954 | 0.025486 |
| O15  | 0.606712 | 0.532291 | 0.358421 | 0.025486 |
| O16  | 0.558269 | 0.587733 | 0.334114 | 0.025486 |
| O17  | 0.437625 | 0.358336 | 0.295396 | 0.025486 |
| H1   | 0.437271 | 0.339620 | 0.315360 | 0.025486 |
| H2   | 0.440347 | 0.339289 | 0.275375 | 0.025486 |
| O18  | 0.345165 | 0.428011 | 0.280680 | 0.025486 |
| H3   | 0.322581 | 0.420535 | 0.296509 | 0.025486 |
| H4   | 0.332200 | 0.431665 | 0.258503 | 0.025486 |
| O19  | 0.539159 | 0.612895 | 0.279938 | 0.025486 |
| H5   | 0.535069 | 0.640797 | 0.291543 | 0.025486 |
| H6   | 0.545716 | 0.619423 | 0.256410 | 0.025486 |
| O20  | 0.619903 | 0.516588 | 0.289466 | 0.025486 |
| H7   | 0.643223 | 0.518746 | 0.305577 | 0.025486 |
| H8   | 0.631829 | 0.506844 | 0.268022 | 0.025486 |
| O21  | 0.532124 | 0.357378 | 0.369348 | 0.025486 |
| H9   | 0.530004 | 0.333333 | 0.385503 | 0.025486 |
| H10  | 0.524998 | 0.345656 | 0.347155 | 0.025486 |
| O22  | 0.635953 | 0.438970 | 0.354974 | 0.025486 |
| H11  | 0.659032 | 0.443858 | 0.370951 | 0.025486 |
| H12  | 0.648675 | 0.433963 | 0.332865 | 0.025486 |
| O23  | 0.369710 | 0.524076 | 0.384822 | 0.025486 |
| H13  | 0.347301 | 0.520876 | 0.401633 | 0.025486 |
| H14  | 0.356250 | 0.524128 | 0.362653 | 0.025486 |
| O24  | 0.444060 | 0.613907 | 0.377128 | 0.025486 |
| H15  | 0.441719 | 0.632838 | 0.396886 | 0.025486 |
| H16  | 0.449100 | 0.632715 | 0.357620 | 0.025486 |
| Ca5  | 0.432693 | 0.438417 | 0.461796 | 0.025486 |
| Ca6  | 0.535868 | 0.534654 | 0.471242 | 0.025486 |
| Ca7  | 0.549820 | 0.439038 | 0.537918 | 0.025486 |
| Ca8  | 0.436116 | 0.530296 | 0.555904 | 0.025486 |
| S5   | 0.545146 | 0.437132 | 0.474957 | 0.025486 |
| O25  | 0.498238 | 0.431521 | 0.482083 | 0.025486 |
| O26  | 0.561588 | 0.476990 | 0.493633 | 0.025486 |
| O27  | 0.568908 | 0.396744 | 0.486690 | 0.025486 |
| O28  | 0.551849 | 0.443273 | 0.437421 | 0.025486 |
| S6   | 0.420822 | 0.529869 | 0.454568 | 0.025486 |
| O29  | 0.391868 | 0.493973 | 0.441624 | 0.025486 |
| Atom  | x    | y    | z    | Uiso  | Symmetry |
|-------|------|------|------|-------|----------|
| S10   | 0.420822 | 0.529869 | 0.623681 | 0.025486 | S        |
| O53   | 0.391686 | 0.493973 | 0.610738 | 0.025486 | O        |
| O54   | 0.406220 | 0.544215 | 0.658367 | 0.025486 | O        |
| O55   | 0.465839 | 0.512693 | 0.625831 | 0.025486 | O        |
| S11   | 0.419360 | 0.568595 | 0.599788 | 0.025486 | S        |
| O56   | 0.441400 | 0.438788 | 0.707633 | 0.025486 | O        |
| O57   | 0.405364 | 0.406434 | 0.701698 | 0.025486 | O        |
| O58   | 0.435884 | 0.463102 | 0.740657 | 0.025486 | O        |
| O59   | 0.483247 | 0.414360 | 0.707958 | 0.025486 | O        |
| O60   | 0.44106  | 0.471258 | 0.678724 | 0.025486 | O        |
| S12   | 0.565400 | 0.556813 | 0.701698 | 0.025486 | S        |
| O61   | 0.529093 | 0.524363 | 0.703620 | 0.025486 | O        |
| O62   | 0.567526 | 0.582865 | 0.734181 | 0.025486 | O        |
| O63   | 0.606712 | 0.532291 | 0.696648 | 0.025486 | O        |
| O64   | 0.558269 | 0.587733 | 0.672341 | 0.025486 | O        |
| O65   | 0.437625 | 0.358336 | 0.633623 | 0.025486 | O        |
| H33   | 0.437271 | 0.339620 | 0.653587 | 0.025486 | H        |
| H34   | 0.440347 | 0.339289 | 0.613962 | 0.025486 | H        |
| O66   | 0.345165 | 0.428011 | 0.618907 | 0.025486 | O        |
| H35   | 0.322581 | 0.420535 | 0.634736 | 0.025486 | H        |
| O67   | 0.539159 | 0.612895 | 0.618165 | 0.025486 | O        |
| H37   | 0.553069 | 0.640797 | 0.629770 | 0.025486 | H        |
| H38   | 0.545716 | 0.619423 | 0.594637 | 0.025486 | H        |
| O68   | 0.619903 | 0.516588 | 0.627693 | 0.025486 | O        |
| H39   | 0.643223 | 0.518746 | 0.643804 | 0.025486 | H        |
| H40   | 0.631829 | 0.506844 | 0.606249 | 0.025486 | H        |
| O69   | 0.532124 | 0.357378 | 0.707575 | 0.025486 | O        |
| H41   | 0.530004 | 0.333333 | 0.723730 | 0.025486 | H        |
| H42   | 0.524998 | 0.345656 | 0.685382 | 0.025486 | H        |
| O70   | 0.635953 | 0.438970 | 0.693202 | 0.025486 | O        |
| H43   | 0.659032 | 0.443858 | 0.709178 | 0.025486 | H        |
| H44   | 0.648675 | 0.433963 | 0.671092 | 0.025486 | H        |
| O71   | 0.369710 | 0.524076 | 0.723049 | 0.025486 | O        |
| H45   | 0.347301 | 0.520876 | 0.739860 | 0.025486 | H        |
| H46   | 0.356250 | 0.524128 | 0.700880 | 0.025486 | H        |
| O72   | 0.444060 | 0.613907 | 0.715355 | 0.025486 | O        |
| H47   | 0.441719 | 0.632838 | 0.735113 | 0.025486 | H        |
| H48   | 0.449100 | 0.632715 | 0.695847 | 0.025486 | H        |
#Cluster II
#--------------------------------------------------------------------------------- 

# CRYSTAL DATA
#--------------------------------------------------------------------------------- 

data_VESTA_phase_1

| _chemical_name_common | '3D' |
|-----------------------|------|
| _cell_length_a        | 29.00000 |
| _cell_length_b        | 29.00000 |
| _cell_length_c        | 40.00000 |
| _cell_angle_alpha     | 90 |
| _cell_angle_beta      | 90 |
| _cell_angle_gamma     | 90 |
| _space_group_name_H-M_alt | 'P 1' |
| _space_group_IT_number | 1 |

loop_
_space_group_symop_operation_xyz
'x, y, z'

loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_U_iso_or_equiv
_atom_site_type_symbol

|     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|
| Ca1 | 1.0 | 0.581733 | 0.496622 | 0.285867 | Uiso 0.032480 | Ca |
| Ca2 | 1.0 | 0.436309 | 0.587421 | 0.284737 | Uiso 0.032480 | Ca |
| Ca3 | 1.0 | 0.442772 | 0.426736 | 0.291355 | Uiso 0.032480 | Ca |
| S1  | 1.0 | 0.533848 | 0.571579 | 0.280684 | Uiso 0.032480 | S  |
| O1  | 1.0 | 0.534473 | 0.542454 | 0.250000 | Uiso 0.032480 | O  |
| O2  | 1.0 | 0.580953 | 0.590162 | 0.286991 | Uiso 0.032480 | O  |
| O3  | 1.0 | 0.500998 | 0.610545 | 0.275965 | Uiso 0.032480 | O  |
| O4  | 1.0 | 0.405810 | 0.492996 | 0.284182 | Uiso 0.032480 | S  |
| S2  | 1.0 | 0.378141 | 0.449703 | 0.284077 | Uiso 0.032480 | O  |
| O5  | 1.0 | 0.421885 | 0.502887 | 0.318828 | Uiso 0.032480 | O  |
| O6  | 1.0 | 0.446453 | 0.487450 | 0.261752 | Uiso 0.032480 | O  |
| O7  | 1.0 | 0.376760 | 0.531944 | 0.272073 | Uiso 0.032480 | O  |
| O8  | 1.0 | 0.376760 | 0.531944 | 0.272073 | Uiso 0.032480 | O  |
| Atom | 1.0 | x   | y   | z   | Uiso | S     |
|------|-----|-----|-----|-----|------|-------|
| S3   | 0.529766 | 0.383472 | 0.285014 | 0.032480 | S     |
| O9   | 0.507094 | 0.344828 | 0.266782 | 0.032480 | O     |
| O10  | 0.512380 | 0.384995 | 0.285246 | 0.032480 | O     |
| O12  | 0.518964 | 0.427869 | 0.267980 | 0.032480 | O     |
| Ca4  | 0.516146 | 0.583942 | 0.370392 | 0.032480 | Ca    |
| Ca5  | 0.381956 | 0.477238 | 0.369263 | 0.032480 | Ca    |
| S4   | 0.429493 | 0.563870 | 0.365209 | 0.032480 | S     |
| O13  | 0.457151 | 0.554723 | 0.334525 | 0.032480 | O     |
| S5   | 0.535557 | 0.429613 | 0.375881 | 0.032480 | S     |
| O14  | 0.492305 | 0.376378 | 0.368602 | 0.032480 | O     |
| S6   | 0.460753 | 0.416928 | 0.368707 | 0.032480 | S     |
| O17  | 0.492305 | 0.376378 | 0.368602 | 0.032480 | O     |
| O18  | 0.381956 | 0.563870 | 0.365209 | 0.032480 | O     |
| S7   | 0.402403 | 0.463779 | 0.449734 | 0.032480 | S     |
| O19  | 0.459959 | 0.501801 | 0.352506 | 0.032480 | O     |
| Ca7  | 0.412453 | 0.552157 | 0.454917 | 0.032480 | Ca    |
| Ca8  | 0.468159 | 0.390016 | 0.453788 | 0.032480 | Ca    |
| Ca9  | 0.564392 | 0.518859 | 0.460406 | 0.032480 | Ca    |
| O22  | 0.598166 | 0.481263 | 0.404575 | 0.032480 | O     |
| O23  | 0.629274 | 0.542641 | 0.369771 | 0.032480 | O     |
| O24  | 0.605414 | 0.497139 | 0.369540 | 0.032480 | O     |
| Ca10 | 0.551341 | 0.444118 | 0.453232 | 0.032480 | Ca    |
| S8   | 0.552403 | 0.463779 | 0.449734 | 0.032480 | S     |
| O25  | 0.420269 | 0.486788 | 0.419050 | 0.032480 | O     |
| O26  | 0.431867 | 0.476474 | 0.478829 | 0.032480 | O     |
| O27  | 0.354117 | 0.479032 | 0.456041 | 0.032480 | O     |
| O28  | 0.420269 | 0.486788 | 0.419050 | 0.032480 | O     |
| O29  | 0.459959 | 0.501801 | 0.352506 | 0.032480 | O     |
| S9   | 0.504515 | 0.565990 | 0.437031 | 0.032480 | S     |
| Ca10 | 0.523276 | 0.474035 | 0.430802 | 0.032480 | Ca    |
| Ca11 | 0.549356 | 0.395570 | 0.441123 | 0.032480 | Ca    |
| Ca12 | 0.524104 | 0.607271 | 0.454065 | 0.032480 | Ca    |
| S10  | 0.390016 | 0.453788 | 0.369540 | 0.032480 | S     |
| O37  | 0.489196 | 0.644970 | 0.454296 | 0.032480 | O     |
| Atom | U | X  | Y  | Z  | Uiso | Elements |
|------|---|----|----|----|------|----------|
| 38   | 1.0 | 0.486093 | 0.437638 | 0.563354 | 0.032480 | O        |
| 39   | 1.0 | 0.457691 | 0.365217 | 0.540566 | 0.032480 | O        |
| 40   | 1.0 | 0.536552 | 0.389491 | 0.529540 | 0.032480 | O        |
| S11  | 1.0 | 0.556527 | 0.539422 | 0.537758 | 0.032480 | S        |
| 41   | 1.0 | 0.557578 | 0.590791 | 0.537652 | 0.032480 | O        |
| O42  | 1.0 | 0.547962 | 0.522603 | 0.572403 | 0.032480 | O        |
| O43  | 1.0 | 0.518950 | 0.522973 | 0.573625 | 0.032480 | O        |
| S12  | 1.0 | 0.556527 | 0.539422 | 0.537758 | 0.032480 | S        |
| O44  | 1.0 | 0.557578 | 0.590791 | 0.537652 | 0.032480 | O        |
| Ca13 | 1.0 | 0.508736 | 0.405600 | 0.623967 | 0.032480 | Ca       |
| Ca14 | 1.0 | 0.567651 | 0.566036 | 0.622838 | 0.032480 | Ca       |
| Ca15 | 1.0 | 0.411739 | 0.527197 | 0.629456 | 0.032480 | Ca       |
| S13  | 1.0 | 0.572230 | 0.467892 | 0.618784 | 0.032480 | S        |
| O49  | 1.0 | 0.543858 | 0.461284 | 0.588100 | 0.032480 | O        |
| O50  | 1.0 | 0.541352 | 0.476600 | 0.647880 | 0.032480 | O        |
| O51  | 1.0 | 0.600112 | 0.425622 | 0.625091 | 0.032480 | O        |
| O52  | 1.0 | 0.603597 | 0.508061 | 0.614066 | 0.032480 | O        |
| S14  | 1.0 | 0.548969 | 0.577008 | 0.622838 | 0.032480 | S        |
| O53  | 1.0 | 0.420908 | 0.595171 | 0.622177 | 0.032480 | O        |
| O54  | 1.0 | 0.419195 | 0.563313 | 0.656928 | 0.032480 | O        |
| O55  | 1.0 | 0.471910 | 0.536094 | 0.599852 | 0.032480 | O        |
| O56  | 1.0 | 0.501102 | 0.613455 | 0.610173 | 0.032480 | O        |
| S15  | 1.0 | 0.387312 | 0.433159 | 0.623115 | 0.032480 | S        |
| O57  | 1.0 | 0.344828 | 0.447389 | 0.604882 | 0.032480 | O        |
| O58  | 1.0 | 0.385223 | 0.450486 | 0.658150 | 0.032480 | O        |
| O59  | 1.0 | 0.390662 | 0.381890 | 0.623346 | 0.032480 | O        |
| O60  | 1.0 | 0.428534 | 0.452870 | 0.606081 | 0.032480 | O        |
| Ca16 | 1.0 | 0.579645 | 0.488069 | 0.708492 | 0.032480 | Ca       |
| Ca17 | 1.0 | 0.447601 | 0.597416 | 0.707363 | 0.032480 | Ca       |
| Ca18 | 1.0 | 0.432619 | 0.437301 | 0.713981 | 0.032480 | Ca       |
| S16  | 1.0 | 0.542163 | 0.568733 | 0.703309 | 0.032480 | S        |
| O61  | 1.0 | 0.538907 | 0.539784 | 0.672625 | 0.032480 | O        |
| O62  | 1.0 | 0.523633 | 0.542543 | 0.732405 | 0.032480 | O        |
| O63  | 1.0 | 0.591322 | 0.580881 | 0.709616 | 0.032480 | O        |
| O64  | 1.0 | 0.514791 | 0.611724 | 0.698591 | 0.032480 | O        |
| S17  | 1.0 | 0.404805 | 0.507891 | 0.706808 | 0.032480 | S        |
| O65  | 1.0 | 0.371620 | 0.468666 | 0.706702 | 0.032480 | O        |
| O66  | 1.0 | 0.422054 | 0.515554 | 0.741453 | 0.032480 | O        |
| O67  | 1.0 | 0.444348 | 0.496985 | 0.684377 | 0.032480 | O        |
| O68  | 1.0 | 0.381197 | 0.550359 | 0.694698 | 0.032480 | O        |
| S18  | 1.0 | 0.513081 | 0.382843 | 0.707640 | 0.032480 | S        |
| O69  | 1.0 | 0.485467 | 0.347560 | 0.689408 | 0.032480 | O        |
| 070 | 1.0  | 0.496052 | 0.386666 | 0.742675 | Uiso | 0.032480 | O    |
|-----|------|----------|----------|----------|------|----------|------|
| 071 | 1.0  | 0.562520 | 0.368861 | 0.707871 | Uiso | 0.032480 | O    |
| 072 | 1.0  | 0.508284 | 0.428283 | 0.690606 | Uiso | 0.032480 | O    |
#Cluster III

# CRYSTAL DATA

data_VESTA_phase_1

_chemical_name_common                  '3D'
_cell_length_a                         32.00000
_cell_length_b                         32.00000
_cell_length_c                         40.00000
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
'x, y, z'

loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_U_iso_or_equiv
_atom_site_type_symbol
Ca1  1.0 0.572097 0.507783 0.282770 Uiso 0.023903 Ca
Ca2  1.0 0.448458 0.587081 0.286631 Uiso 0.023903 Ca
Ca3  1.0 0.445966 0.433083 0.285596 Uiso 0.023903 Ca
S1   1.0 0.539617 0.572835 0.297714 Uiso 0.023903 S
O1   1.0 0.540862 0.547982 0.266229 Uiso 0.023903 O
O2   1.0 0.521667 0.546842 0.325081 Uiso 0.023903 O
O3   1.0 0.582808 0.585911 0.306892 Uiso 0.023903 O
O4   1.0 0.513130 0.610604 0.292653 Uiso 0.023903 O
S2   1.0 0.415216 0.511457 0.288464 Uiso 0.023903 S
O5   1.0 0.397464 0.469147 0.294803 Uiso 0.023903 O
O6   1.0 0.439695 0.525223 0.318175 Uiso 0.023903 O
O7   1.0 0.443107 0.509860 0.258663 Uiso 0.023903 O
O8   1.0 0.380596 0.541599 0.282213 Uiso 0.023903 O
| Atom | Ux   | Uy   | Uz   | Uiso |
|------|------|------|------|------|
| S3   | 0.530596 | 0.399285 | 0.287877 | 0.023903 |
| O9   | 0.492932 | 0.377089 | 0.275055 | 0.023903 |
| O10  | 0.519892 | 0.421478 | 0.319484 | 0.023903 |
| O11  | 0.564474 | 0.368420 | 0.294456 | 0.023903 |
| O12  | 0.545083 | 0.430154 | 0.262512 | 0.023903 |
| O13  | 0.628864 | 0.473827 | 0.271681 | 0.023903 |
| H1   | 0.637963 | 0.464733 | 0.250000 | 0.023903 |
| H2   | 0.653192 | 0.476032 | 0.285613 | 0.023903 |
| O14  | 0.635739 | 0.550436 | 0.264857 | 0.023903 |
| H3   | 0.628864 | 0.473827 | 0.271681 | 0.023903 |
| H4   | 0.649576 | 0.556969 | 0.303303 | 0.023903 |
| O15  | 0.459663 | 0.652973 | 0.278622 | 0.023903 |
| H5   | 0.463423 | 0.666520 | 0.257420 | 0.023903 |
| H6   | 0.449032 | 0.673453 | 0.293959 | 0.023903 |
| O16  | 0.385784 | 0.630883 | 0.288609 | 0.023903 |
| H7   | 0.373354 | 0.648360 | 0.271607 | 0.023903 |
| H8   | 0.375788 | 0.640303 | 0.311800 | 0.023903 |
| O17  | 0.383325 | 0.410490 | 0.276360 | 0.023903 |
| H9   | 0.370124 | 0.407958 | 0.254904 | 0.023903 |
| H10  | 0.369813 | 0.391182 | 0.291211 | 0.023903 |
| O18  | 0.438509 | 0.356926 | 0.288609 | 0.023903 |
| H11  | 0.430112 | 0.337490 | 0.271607 | 0.023903 |
| H12  | 0.435115 | 0.343318 | 0.309825 | 0.023903 |
| Ca4  | 0.510804 | 0.579543 | 0.366130 | 0.023903 |
| Ca5  | 0.395137 | 0.489013 | 0.369991 | 0.023903 |
| Ca6  | 0.539679 | 0.435824 | 0.368956 | 0.023903 |
| S4   | 0.438678 | 0.570359 | 0.381074 | 0.023903 |
| O19  | 0.462548 | 0.563330 | 0.349589 | 0.023903 |
| O20  | 0.457288 | 0.544834 | 0.408441 | 0.023903 |
| O21  | 0.440593 | 0.615445 | 0.390252 | 0.023903 |
| O22  | 0.394282 | 0.557825 | 0.376013 | 0.023903 |
| S5   | 0.455547 | 0.432670 | 0.371824 | 0.023903 |
| O23  | 0.489625 | 0.401946 | 0.378163 | 0.023903 |
| O24  | 0.450633 | 0.460321 | 0.401535 | 0.023903 |
| O25  | 0.466262 | 0.458470 | 0.342023 | 0.023903 |
| O26  | 0.415666 | 0.409942 | 0.365573 | 0.023903 |
| S6   | 0.599520 | 0.504551 | 0.371237 | 0.023903 |
| O27  | 0.608038 | 0.461672 | 0.358415 | 0.023903 |
| O28  | 0.575038 | 0.501774 | 0.402844 | 0.023903 |
| O29  | 0.639839 | 0.526341 | 0.377816 | 0.023903 |
| O30  | 0.575164 | 0.528417 | 0.345872 | 0.023903 |
| O31  | 0.561597 | 0.621918 | 0.355041 | 0.023903 |
| H13  | 0.573185 | 0.627505 | 0.333360 | 0.023903 |
| H14  | 0.567547 | 0.645611 | 0.368973 | 0.023903 |
| O32  | 0.491552 | 0.653698 | 0.366019 | 0.023903 |
| H15  | 0.492801 | 0.673778 | 0.348217 | 0.023903 |
| Atom  | Fraction | x     | y     | z     | Uiso  |      |
|-------|----------|-------|-------|-------|-------|------|
| H16   | 1.0      | 0.489954 | 0.668916 | 0.386663 | Uiso 0.023903 | H   |
| O33   | 1.0      | 0.336637 | 0.521343 | 0.361982 | Uiso 0.023903 | O   |
| H17   | 1.0      | 0.325091 | 0.529364 | 0.386663 | Uiso 0.023903 | H   |
| H18   | 1.0      | 0.313796 | 0.518069 | 0.377319 | Uiso 0.023903 | H   |
| O34   | 1.0      | 0.333100 | 0.444313 | 0.338232 | Uiso 0.023903 | O   |
| H19   | 1.0      | 0.312500 | 0.438349 | 0.357040 | Uiso 0.023903 | H   |
| H20   | 1.0      | 0.320909 | 0.437988 | 0.395160 | Uiso 0.023903 | H   |
| O35   | 1.0      | 0.540326 | 0.369236 | 0.359720 | Uiso 0.023903 | O   |
| H21   | 1.0      | 0.336409 | 0.524301 | 0.340780 | Uiso 0.023903 | H   |
| H22   | 1.0      | 0.313796 | 0.518069 | 0.377319 | Uiso 0.023903 | H   |
| O36   | 1.0      | 0.333100 | 0.444313 | 0.338232 | Uiso 0.023903 | O   |
| H23   | 1.0      | 0.312500 | 0.438349 | 0.357040 | Uiso 0.023903 | H   |
| H24   | 1.0      | 0.320909 | 0.437988 | 0.395160 | Uiso 0.023903 | H   |
| Ca7   | 1.0      | 0.423238 | 0.546298 | 0.449490 | Uiso 0.023903 | Ca  |
| Ca8   | 1.0      | 0.470509 | 0.407229 | 0.453351 | Uiso 0.023903 | Ca  |
| Ca9   | 1.0      | 0.568433 | 0.526110 | 0.452316 | Uiso 0.023903 | Ca  |
| O37   | 1.0      | 0.408097 | 0.475183 | 0.464434 | Uiso 0.023903 | O   |
| O38   | 1.0      | 0.438334 | 0.484324 | 0.491801 | Uiso 0.023903 | O   |
| O39   | 1.0      | 0.366171 | 0.491875 | 0.473612 | Uiso 0.023903 | O   |
| O40   | 1.0      | 0.405272 | 0.429139 | 0.459373 | Uiso 0.023903 | O   |
| S8    | 1.0      | 0.543636 | 0.445652 | 0.455184 | Uiso 0.023903 | S   |
| O41   | 1.0      | 0.515913 | 0.450143 | 0.484895 | Uiso 0.023903 | O   |
| O42   | 1.0      | 0.522819 | 0.464284 | 0.425383 | Uiso 0.023903 | O   |
| O44   | 1.0      | 0.551924 | 0.400505 | 0.448933 | Uiso 0.023903 | O   |
| S9    | 1.0      | 0.523313 | 0.605284 | 0.454597 | Uiso 0.023903 | O   |
| O45   | 1.0      | 0.566600 | 0.599169 | 0.441775 | Uiso 0.023903 | O   |
| O46   | 1.0      | 0.517852 | 0.581257 | 0.486204 | Uiso 0.023903 | O   |
| O47   | 1.0      | 0.516054 | 0.650536 | 0.461176 | Uiso 0.023903 | O   |
| O48   | 1.0      | 0.492744 | 0.590172 | 0.429232 | Uiso 0.023903 | O   |
| O49   | 1.0      | 0.400006 | 0.608232 | 0.438401 | Uiso 0.023903 | O   |
| H25   | 1.0      | 0.398558 | 0.621015 | 0.416720 | Uiso 0.023903 | O   |
| H26   | 1.0      | 0.398558 | 0.621015 | 0.416720 | Uiso 0.023903 | O   |
| O50   | 1.0      | 0.346885 | 0.552606 | 0.449379 | Uiso 0.023903 | O   |
| H27   | 1.0      | 0.328342 | 0.560413 | 0.431577 | Uiso 0.023903 | H   |
| H28   | 1.0      | 0.331992 | 0.556121 | 0.470023 | Uiso 0.023903 | H   |
| O51   | 1.0      | 0.420679 | 0.362682 | 0.445342 | Uiso 0.023903 | O   |
| H29   | 1.0      | 0.409296 | 0.354431 | 0.424140 | Uiso 0.023903 | H   |
| H30   | 1.0      | 0.416230 | 0.340041 | 0.460679 | Uiso 0.023903 | O   |
| O52   | 1.0      | 0.492223 | 0.333914 | 0.457183 | Uiso 0.023903 | O   |
| H31   | 1.0      | 0.491052 | 0.312500 | 0.440400 | Uiso 0.023903 | H   |
| H32   | 1.0      | 0.494169 | 0.320318 | 0.478520 | Uiso 0.023903 | H   |
| O53   | 1.0      | 0.631501 | 0.504738 | 0.443080 | Uiso 0.023903 | O   |
| H33   | 1.0      | 0.643402 | 0.498491 | 0.421624 | Uiso 0.023903 | H   |
| H34   | 1.0      | 0.654101 | 0.511417 | 0.457931 | Uiso 0.023903 | H   |
| Atom  | Scale Factor | x | y | z | Uiso |
|-------|-------------|---|---|---|------|
| O54   | 1.0         | 0.621727 | 0.581020 | 0.455329 | 0.023903 |
| H35   | 1.0         | 0.640407 | 0.590986 | 0.438326 | 0.023903 |
| H36   | 1.0         | 0.632863 | 0.589546 | 0.476545 | 0.023903 |
| Ca10  | 1.0         | 0.426116 | 0.453588 | 0.532850 | 0.023903 |
| Ca11  | 1.0         | 0.572993 | 0.452299 | 0.536711 | 0.023903 |
| Ca12  | 1.0         | 0.493104 | 0.583978 | 0.535676 | 0.023903 |
| S10   | 1.0         | 0.488246 | 0.415819 | 0.547794 | 0.023903 |
| O55   | 1.0         | 0.473959 | 0.436192 | 0.516309 | 0.023903 |
| O56   | 1.0         | 0.489600 | 0.447378 | 0.575161 | 0.023903 |
| O57   | 1.0         | 0.458649 | 0.381753 | 0.556972 | 0.023903 |
| O58   | 1.0         | 0.530776 | 0.397952 | 0.542733 | 0.023903 |
| S11   | 1.0         | 0.560865 | 0.534011 | 0.538543 | 0.023903 |
| O59   | 1.0         | 0.553362 | 0.579276 | 0.544883 | 0.023903 |
| O60   | 1.0         | 0.547474 | 0.509324 | 0.568255 | 0.023903 |
| O61   | 1.0         | 0.536406 | 0.520512 | 0.508743 | 0.023903 |
| O62   | 1.0         | 0.606218 | 0.526930 | 0.532293 | 0.023903 |
| S12   | 1.0         | 0.403474 | 0.567524 | 0.537956 | 0.023903 |
| O63   | 1.0         | 0.423536 | 0.606367 | 0.525135 | 0.023903 |
| O64   | 1.0         | 0.424351 | 0.554438 | 0.569564 | 0.023903 |
| O65   | 1.0         | 0.358363 | 0.575612 | 0.544536 | 0.023903 |
| O66   | 1.0         | 0.407647 | 0.533681 | 0.512591 | 0.023903 |
| O67   | 1.0         | 0.359985 | 0.452104 | 0.521761 | 0.023903 |
| H37   | 1.0         | 0.347441 | 0.454957 | 0.500080 | 0.023903 |
| H38   | 1.0         | 0.340566 | 0.437284 | 0.535693 | 0.023903 |
| O68   | 1.0         | 0.394956 | 0.383597 | 0.532739 | 0.023903 |
| H39   | 1.0         | 0.381465 | 0.368672 | 0.514936 | 0.023903 |
| H40   | 1.0         | 0.386722 | 0.370700 | 0.553382 | 0.023903 |
| O69   | 1.0         | 0.598594 | 0.390557 | 0.528702 | 0.023903 |
| H41   | 1.0         | 0.602624 | 0.377089 | 0.507500 | 0.023903 |
| H42   | 1.0         | 0.618497 | 0.378883 | 0.544039 | 0.023903 |
| O70   | 1.0         | 0.649367 | 0.448593 | 0.540543 | 0.023903 |
| O43   | 1.0         | 0.669194 | 0.440419 | 0.523760 | 0.023903 |
| H44   | 1.0         | 0.662843 | 0.445942 | 0.561880 | 0.023903 |
| H45   | 1.0         | 0.534098 | 0.636456 | 0.526440 | 0.023903 |
| H46   | 1.0         | 0.543924 | 0.645627 | 0.504984 | 0.023903 |
| O72   | 1.0         | 0.458866 | 0.652412 | 0.538689 | 0.023903 |
| H47   | 1.0         | 0.455625 | 0.673335 | 0.521686 | 0.023903 |
| H48   | 1.0         | 0.454494 | 0.665738 | 0.559905 | 0.023903 |
| Ca13  | 1.0         | 0.514983 | 0.426621 | 0.616210 | 0.023903 |
| Ca14  | 1.0         | 0.564687 | 0.564838 | 0.620071 | 0.023903 |
| Ca15  | 1.0         | 0.414017 | 0.532898 | 0.619036 | 0.023903 |
| S13   | 1.0         | 0.571145 | 0.472800 | 0.631154 | 0.023903 |
| O73   | 1.0         | 0.547197 | 0.466039 | 0.599669 | 0.023903 |
| O74   | 1.0         | 0.541801 | 0.484496 | 0.658521 | 0.023903 |
| O75   | 1.0         | 0.593530 | 0.433616 | 0.640332 | 0.023903 |
|   |   |   |   |   |
|---|---|---|---|---|
| O76 | 1.0 | 0.602050 | 0.507047 | 0.626093 | Uiso | 0.023903 | O |
| S14 | 1.0 | 0.483552 | 0.580365 | 0.621903 | Uiso | 0.023903 | S |
| O77 | 1.0 | 0.438347 | 0.588226 | 0.628243 | Uiso | 0.023903 | O |
| O78 | 1.0 | 0.502434 | 0.559575 | 0.651615 | Uiso | 0.023903 | O |
| O79 | 1.0 | 0.488220 | 0.552820 | 0.592103 | Uiso | 0.023903 | O |
| O80 | 1.0 | 0.505208 | 0.620838 | 0.615653 | Uiso | 0.023903 | O |
| S15 | 1.0 | 0.399959 | 0.442861 | 0.621316 | Uiso | 0.023903 | S |
| O81 | 1.0 | 0.369917 | 0.474621 | 0.608495 | Uiso | 0.023903 | O |
| O82 | 1.0 | 0.419204 | 0.458247 | 0.652924 | Uiso | 0.023903 | O |
| O83 | 1.0 | 0.377433 | 0.402948 | 0.627895 | Uiso | 0.023903 | O |
| O84 | 1.0 | 0.433283 | 0.435628 | 0.595951 | Uiso | 0.023903 | O |
| O85 | 1.0 | 0.494552 | 0.363707 | 0.605121 | Uiso | 0.023903 | O |
| H49 | 1.0 | 0.487719 | 0.352808 | 0.583440 | Uiso | 0.023903 | H |
| H50 | 1.0 | 0.502131 | 0.340484 | 0.619053 | Uiso | 0.023903 | H |
| H51 | 1.0 | 0.580398 | 0.356441 | 0.598296 | Uiso | 0.023903 | H |
| H52 | 1.0 | 0.580219 | 0.362072 | 0.636742 | Uiso | 0.023903 | H |
| O87 | 1.0 | 0.631418 | 0.568621 | 0.612062 | Uiso | 0.023903 | O |
| H53 | 1.0 | 0.645462 | 0.567980 | 0.590860 | Uiso | 0.023903 | H |
| H54 | 1.0 | 0.649009 | 0.583555 | 0.627399 | Uiso | 0.023903 | H |
| O88 | 1.0 | 0.593397 | 0.635707 | 0.623903 | Uiso | 0.023903 | O |
| H55 | 1.0 | 0.607659 | 0.651724 | 0.607120 | Uiso | 0.023903 | H |
| H56 | 1.0 | 0.600349 | 0.647553 | 0.645240 | Uiso | 0.023903 | H |
| O89 | 1.0 | 0.378014 | 0.588917 | 0.609800 | Uiso | 0.023903 | O |
| H57 | 1.0 | 0.372600 | 0.601220 | 0.588344 | Uiso | 0.023903 | H |
| H58 | 1.0 | 0.356177 | 0.597780 | 0.624651 | Uiso | 0.023903 | H |
| O90 | 1.0 | 0.338117 | 0.523171 | 0.622049 | Uiso | 0.023903 | O |
| H59 | 1.0 | 0.317297 | 0.527018 | 0.605046 | Uiso | 0.023903 | H |
| H60 | 1.0 | 0.324094 | 0.523443 | 0.643265 | Uiso | 0.023903 | H |
| Ca16 | 1.0 | 0.570179 | 0.502525 | 0.699570 | Uiso | 0.023903 | Ca |
| Ca17 | 1.0 | 0.456118 | 0.595071 | 0.703431 | Uiso | 0.023903 | Ca |
| Ca18 | 1.0 | 0.436529 | 0.442304 | 0.702395 | Uiso | 0.023903 | Ca |
| S16 | 1.0 | 0.545129 | 0.570783 | 0.714513 | Uiso | 0.023903 | S |
| O91 | 1.0 | 0.543605 | 0.545946 | 0.683029 | Uiso | 0.023903 | O |
| O92 | 1.0 | 0.524402 | 0.546946 | 0.741881 | Uiso | 0.023903 | O |
| O93 | 1.0 | 0.589506 | 0.578978 | 0.723692 | Uiso | 0.023903 | O |
| O94 | 1.0 | 0.523004 | 0.611262 | 0.709453 | Uiso | 0.023903 | O |
| S17 | 1.0 | 0.414678 | 0.523611 | 0.705263 | Uiso | 0.023903 | S |
| O95 | 1.0 | 0.392335 | 0.483535 | 0.711603 | Uiso | 0.023903 | O |
| O96 | 1.0 | 0.440536 | 0.534571 | 0.734975 | Uiso | 0.023903 | O |
| O97 | 1.0 | 0.442219 | 0.518923 | 0.675463 | Uiso | 0.023903 | O |
| O98 | 1.0 | 0.383623 | 0.557413 | 0.699013 | Uiso | 0.023903 | O |
| S18 | 1.0 | 0.516878 | 0.399311 | 0.704676 | Uiso | 0.023903 | S |
| O99 | 1.0 | 0.476981 | 0.381438 | 0.691855 | Uiso | 0.023903 | O |
| O100 | 1.0 | 0.508707 | 0.422556 | 0.736284 | Uiso | 0.023903 | O |
| O101 | 1.0 | 0.547117 | 0.364872 | 0.711255 | Uiso | 0.023903 | O |
| Atom | X   | Y   | Z   | Uiso | Symmetry |
|------|-----|-----|-----|------|----------|
| O102 | 1.0 | 0.534707 | 0.428379 | 0.679311 | O        |
| O103 | 1.0 | 0.622821 | 0.462471 | 0.688481 | O        |
| H61  | 1.0 | 0.630853 | 0.452422 | 0.666800 | H        |
| H62  | 1.0 | 0.647244 | 0.461959 | 0.702413 | H        |
| O104 | 1.0 | 0.638167 | 0.537841 | 0.699459 | O        |
| H63  | 1.0 | 0.658020 | 0.541105 | 0.681656 | H        |
| H64  | 1.0 | 0.652645 | 0.542796 | 0.720102 | H        |
| O105 | 1.0 | 0.474577 | 0.659310 | 0.695421 | O        |
| H65  | 1.0 | 0.479819 | 0.672355 | 0.674220 | H        |
| H66  | 1.0 | 0.466288 | 0.680845 | 0.710759 | H        |
| O106 | 1.0 | 0.398700 | 0.645567 | 0.707262 | O        |
| H67  | 1.0 | 0.388290 | 0.664317 | 0.690480 | H        |
| H68  | 1.0 | 0.389814 | 0.656040 | 0.728599 | H        |
| O107 | 1.0 | 0.371765 | 0.426812 | 0.693160 | O        |
| H69  | 1.0 | 0.358364 | 0.425764 | 0.671704 | H        |
| H70  | 1.0 | 0.356191 | 0.409125 | 0.708011 | H        |
| O108 | 1.0 | 0.420655 | 0.367448 | 0.705409 | O        |
| H71  | 1.0 | 0.410150 | 0.349065 | 0.688406 | H        |
| H72  | 1.0 | 0.415769 | 0.354301 | 0.726625 | H        |
#Cluster IV

# CRYSTAL DATA

data_VESTA_phase_1

_chemical_name_common                  '3D'
_cell_length_a                         89.00000
_cell_length_b                         58.00000
_cell_length_c                         60.00000
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
'x, y, z'

loop_
_atom_site_label
_atom_site_occupancy
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_adp_type
_atom_site_U_iso_or_equiv
_atom_site_type_symbol
Ca1 1.0 0.358073 0.517624 0.529736 Uiso 0.030393 Ca
Ca2 1.0 0.415064 0.521528 0.526043 Uiso 0.030393 Ca
Ca3 1.0 0.304649 0.481850 0.470403 Uiso 0.030393 Ca
Ca4 1.0 0.375574 0.471178 0.467241 Uiso 0.030393 Ca
S1 1.0 0.344904 0.512688 0.482751 Uiso 0.030393 S
O1 1.0 0.353279 0.518268 0.462093 Uiso 0.030393 O
O2 1.0 0.345132 0.531816 0.469125 Uiso 0.030393 O
O3 1.0 0.351586 0.492556 0.494516 Uiso 0.030393 O
O4 1.0 0.329325 0.507260 0.475416 Uiso 0.030393 O
S2 1.0 0.407104 0.523032 0.478102 Uiso 0.030393 S
O5 1.0 0.411722 0.541275 0.462221 Uiso 0.030393 O
O6 1.0 0.400881 0.532545 0.499088 Uiso 0.030393 O
O7 1.0 0.395787 0.508887 0.465995 Uiso 0.030393 O
O8 1.0 0.420079 0.508466 0.484930 Uiso 0.030393 O
S3 1.0 0.324184 0.488731 0.521494 Uiso 0.030393 S
O9 1.0 0.332289 0.473795 0.505457 Uiso 0.030393 O
O10 1.0 0.321045 0.476917 0.542896 Uiso 0.030393 O
O11 1.0 0.333163 0.509486 0.527441 Uiso 0.030393 O
O12 1.0 0.310067 0.495644 0.542896 Uiso 0.030393 O
S4 1.0 0.379982 0.487995 0.531403 Uiso 0.030393 S
O13 1.0 0.380839 0.462793 0.527529 Uiso 0.030393 O
O14 1.0 0.368817 0.494202 0.548720 Uiso 0.030393 O
O15 1.0 0.394562 0.497383 0.539482 Uiso 0.030393 O
O16 1.0 0.376065 0.498256 0.509421 Uiso 0.030393 O
O17 1.0 0.340638 0.545386 0.537422 Uiso 0.030393 O
H1 1.0 0.334656 0.532957 0.541265 Uiso 0.030393 H
H2 1.0 0.336374 0.556586 0.528380 Uiso 0.030393 H
O18 1.0 0.407645 0.547231 0.541373 Uiso 0.030393 O
H3 1.0 0.406389 0.531498 0.463451 Uiso 0.030393 H
H4 1.0 0.414063 0.554600 0.551417 Uiso 0.030393 H
O19 1.0 0.316853 0.448137 0.460313 Uiso 0.030393 O
H5 1.0 0.310478 0.456763 0.458398 Uiso 0.030393 H
H6 1.0 0.312663 0.435300 0.470262 Uiso 0.030393 H
O20 1.0 0.391737 0.444571 0.463455 Uiso 0.030393 O
H7 1.0 0.385962 0.456763 0.458398 Uiso 0.030393 H
H8 1.0 0.386737 0.431034 0.467022 Uiso 0.030393 H
O21 1.0 0.369524 0.539638 0.497053 Uiso 0.030393 O
H9 1.0 0.379837 0.541558 0.496419 Uiso 0.030393 H
H10 1.0 0.363711 0.552879 0.497935 Uiso 0.030393 H
O22 1.0 0.350597 0.458934 0.487248 Uiso 0.030393 O
H11 1.0 0.347467 0.470808 0.478052 Uiso 0.030393 H
H12 1.0 0.348006 0.459913 0.502192 Uiso 0.030393 H
O23 1.0 0.428569 0.548735 0.497171 Uiso 0.030393 O
H13 1.0 0.430703 0.540167 0.493651 Uiso 0.030393 H
H14 1.0 0.425546 0.559794 0.486945 Uiso 0.030393 H
O24 1.0 0.349976 0.514653 0.560384 Uiso 0.030393 O
H15 1.0 0.350992 0.513269 0.575719 Uiso 0.030393 H
H16 1.0 0.353372 0.501019 0.554049 Uiso 0.030393 H
O25 1.0 0.376332 0.537495 0.560029 Uiso 0.030393 O
H17 1.0 0.368654 0.546590 0.565704 Uiso 0.030393 H
H18 1.0 0.382540 0.533487 0.571837 Uiso 0.030393 H
O26 1.0 0.415100 0.505019 0.555056 Uiso 0.030393 O
H19 1.0 0.411123 0.518291 0.548747 Uiso 0.030393 H
H20 1.0 0.410153 0.502547 0.568460 Uiso 0.030393 H
O27 1.0 0.433077 0.539137 0.559479 Uiso 0.030393 O
H21 1.0 0.423760 0.533250 0.555499 Uiso 0.030393 H
H22 1.0 0.432479 0.543748 0.574263 Uiso 0.030393 H
O28 1.0 0.282705 0.471841 0.438876 Uiso 0.030393 O
H23 1.0 0.282943 0.485401 0.430675 Uiso 0.030393 H
| Atom | U (Å²) | x  | y  | z  | Uiso  |Atom |
|------|--------|----|----|----|-------|------|
| H24  | 0.280899 | 0.459845 | 0.428998 | 0.030393 | H |
| O29  | 0.286913 | 0.461295 | 0.495858 | 0.030393 | O |
| H25  | 0.291820 | 0.457976 | 0.509122 | 0.030393 | H |
| H26  | 0.292981 | 0.471319 | 0.487839 | 0.030393 | H |
| O30  | 0.303337 | 0.502383 | 0.443047 | 0.030393 | O |
| H27  | 0.301543 | 0.457976 | 0.509122 | 0.030393 | H |
| H28  | 0.306931 | 0.471319 | 0.487839 | 0.030393 | H |
| O30  | 0.357674 | 0.502383 | 0.443047 | 0.030393 | O |
| H27  | 0.350890 | 0.457976 | 0.509122 | 0.030393 | H |
| H28  | 0.350890 | 0.457976 | 0.509122 | 0.030393 | H |
| O31  | 0.374913 | 0.498301 | 0.431764 | 0.030393 | O |
| O32  | 0.374913 | 0.502383 | 0.443047 | 0.030393 | O |
| H30  | 0.350890 | 0.502383 | 0.443047 | 0.030393 | H |
| O33  | 0.374913 | 0.498301 | 0.431764 | 0.030393 | O |
| O34  | 0.374913 | 0.502383 | 0.443047 | 0.030393 | O |
| O35  | 0.374913 | 0.498301 | 0.431764 | 0.030393 | O |
| O36  | 0.374913 | 0.502383 | 0.443047 | 0.030393 | O |
| O37  | 0.374913 | 0.498301 | 0.431764 | 0.030393 | O |
| O38  | 0.374913 | 0.498301 | 0.431764 | 0.030393 | O |
| O39  | 0.374913 | 0.498301 | 0.431764 | 0.030393 | O |
| S5   | 0.374913 | 0.498301 | 0.431764 | 0.030393 | S |
| O41  | 0.498226 | 0.457976 | 0.509122 | 0.030393 | O |
| H42  | 0.469478 | 0.507260 | 0.475416 | 0.030393 | H |
| O43  | 0.541034 | 0.532545 | 0.499088 | 0.030393 | O |
| O44  | 0.541034 | 0.532545 | 0.499088 | 0.030393 | O |
| S7   | 0.464336 | 0.488731 | 0.521494 | 0.030393 | S |
| O45  | 0.472442 | 0.473976 | 0.505457 | 0.030393 | O |
| O46  | 0.461197 | 0.476917 | 0.542896 | 0.030393 | O |
| O47  | 0.473316 | 0.509486 | 0.527441 | 0.030393 | O |
| O48  | 0.450220 | 0.495644 | 0.509995 | 0.030393 | O |
| S8   | 0.520135 | 0.487995 | 0.531080 | 0.030393 | S |
| O49  | 0.520991 | 0.462793 | 0.527529 | 0.030393 | O |
| O50  | 0.520991 | 0.462793 | 0.527529 | 0.030393 | O |
| O51  | 0.546541 | 0.531498 | 0.543295 | 0.030393 | O |
| O52  | 0.547798 | 0.542731 | 0.541537 | 0.030393 | O |
| H36  | 0.554216 | 0.554600 | 0.551417 | 0.030393 | H |
| H37  | 0.450631 | 0.460313 | 0.460305 | 0.030393 | H |
| H38  | 0.452816 | 0.435300 | 0.470262 | 0.030393 | H |
| Atom | U (ppm) | X | Y | Z | Uiso |
|------|--------|---|---|---|------|
| O52  | 0.526115 | 0.531890 | 0.444571 | 0.463455 | 0.030393 |
| H39  | 0.526890 | 0.539638 | 0.497053 | 0.496419 | 0.030393 |
| H40  | 0.509677 | 0.51558 | 0.497935 | 0.030393 |
| O53  | 0.490750 | 0.458934 | 0.487248 | 0.030393 |
| H41  | 0.487620 | 0.541558 | 0.497171 | 0.030393 |
| H42  | 0.488159 | 0.552879 | 0.493651 | 0.030393 |
| O54  | 0.490129 | 0.514653 | 0.560384 | 0.030393 |
| H43  | 0.491145 | 0.546590 | 0.565704 | 0.030393 |
| H44  | 0.493525 | 0.53487 | 0.571837 | 0.030393 |
| O55  | 0.526890 | 0.539638 | 0.497053 | 0.496419 | 0.030393 |
| H46  | 0.565699 | 0.559794 | 0.486945 | 0.030393 |
| O56  | 0.490129 | 0.514653 | 0.560384 | 0.030393 |
| H47  | 0.491145 | 0.53269 | 0.575719 | 0.030393 |
| H48  | 0.493525 | 0.501019 | 0.554049 | 0.030393 |
| O57  | 0.516485 | 0.537495 | 0.560029 | 0.030393 |
| H49  | 0.508807 | 0.546590 | 0.565704 | 0.030393 |
| H50  | 0.522693 | 0.53487 | 0.571837 | 0.030393 |
| O58  | 0.555253 | 0.505019 | 0.555056 | 0.030393 |
| H51  | 0.51276 | 0.518291 | 0.548747 | 0.030393 |
| H52  | 0.550306 | 0.502547 | 0.568460 | 0.030393 |
| O59  | 0.573230 | 0.539137 | 0.559497 | 0.030393 |
| H53  | 0.563913 | 0.53250 | 0.555499 | 0.030393 |
| H54  | 0.572631 | 0.543748 | 0.574263 | 0.030393 |
| O60  | 0.422858 | 0.471841 | 0.438876 | 0.030393 |
| H55  | 0.423096 | 0.485401 | 0.430675 | 0.030393 |
| H56  | 0.421052 | 0.459845 | 0.428998 | 0.030393 |
| O61  | 0.427066 | 0.461295 | 0.495858 | 0.030393 |
| H57  | 0.431973 | 0.457976 | 0.509122 | 0.030393 |
| H58  | 0.433134 | 0.471319 | 0.487839 | 0.030393 |
| O62  | 0.443490 | 0.502383 | 0.443047 | 0.030393 |
| H59  | 0.441696 | 0.511451 | 0.455509 | 0.030393 |
| H60  | 0.447084 | 0.488268 | 0.448011 | 0.030393 |
| O63  | 0.497827 | 0.457393 | 0.438798 | 0.030393 |
| H61  | 0.506832 | 0.44961 | 0.435770 | 0.030393 |
| H62  | 0.491043 | 0.453201 | 0.427773 | 0.030393 |
| O64  | 0.515066 | 0.498301 | 0.431764 | 0.030393 |
| H63  | 0.514401 | 0.501622 | 0.416667 | 0.030393 |
| H64  | 0.524173 | 0.504066 | 0.436831 | 0.030393 |
| Ca9  | 0.638379 | 0.517624 | 0.529736 | 0.030393 |
| Ca10 | 0.695370 | 0.521528 | 0.526043 | 0.030393 |
| Ca11 | 0.584955 | 0.481850 | 0.470403 | 0.030393 |
| Ca12 | 0.655880 | 0.471178 | 0.467241 | 0.030393 |
| S9   | 0.625210 | 0.512688 | 0.482751 | 0.030393 |
| O65  | 0.633585 | 0.518268 | 0.462093 | 0.030393 |
| O66  | 0.625437 | 0.531816 | 0.499125 | 0.030393 |
|     |     | x    | y    | z    |     |     |
|-----|-----|------|------|------|-----|-----|
| O67 | 1.0 | 0.631892 | 0.492556 | 0.494516 | Uiso 0.030393 | O |
| O68 | 1.0 | 0.609631 | 0.507260 | 0.475416 | Uiso 0.030393 | O |
| S10 | 1.0 | 0.687409 | 0.523032 | 0.478102 | Uiso 0.030393 | S |
| O69 | 1.0 | 0.692027 | 0.541275 | 0.462221 | Uiso 0.030393 | O |
| O70 | 1.0 | 0.681187 | 0.532545 | 0.499088 | Uiso 0.030393 | O |
| O71 | 1.0 | 0.676093 | 0.508887 | 0.465995 | Uiso 0.030393 | O |
| O72 | 1.0 | 0.700385 | 0.508466 | 0.484930 | Uiso 0.030393 | O |
| S11 | 1.0 | 0.604489 | 0.488731 | 0.521494 | Uiso 0.030393 | S |
| O73 | 1.0 | 0.612594 | 0.473795 | 0.505457 | Uiso 0.030393 | O |
| O74 | 1.0 | 0.613135 | 0.479117 | 0.542896 | Uiso 0.030393 | O |
| O75 | 1.0 | 0.613469 | 0.509486 | 0.527441 | Uiso 0.030393 | O |
| O76 | 1.0 | 0.590373 | 0.495644 | 0.509995 | Uiso 0.030393 | O |
| S12 | 1.0 | 0.660288 | 0.487995 | 0.531403 | Uiso 0.030393 | S |
| O77 | 1.0 | 0.661144 | 0.462793 | 0.527529 | Uiso 0.030393 | O |
| O78 | 1.0 | 0.649122 | 0.494202 | 0.548720 | Uiso 0.030393 | O |
| O79 | 1.0 | 0.674686 | 0.497383 | 0.539482 | Uiso 0.030393 | O |
| O80 | 1.0 | 0.656371 | 0.498256 | 0.509421 | Uiso 0.030393 | O |
| O81 | 1.0 | 0.620944 | 0.545386 | 0.537422 | Uiso 0.030393 | O |
| H65 | 1.0 | 0.614962 | 0.532957 | 0.541265 | Uiso 0.030393 | H |
| H66 | 1.0 | 0.616680 | 0.556586 | 0.528380 | Uiso 0.030393 | H |
| O82 | 1.0 | 0.687951 | 0.547231 | 0.541537 | Uiso 0.030393 | O |
| H67 | 1.0 | 0.686694 | 0.531498 | 0.543295 | Uiso 0.030393 | H |
| H68 | 1.0 | 0.694369 | 0.554600 | 0.551417 | Uiso 0.030393 | H |
| O83 | 1.0 | 0.597159 | 0.448137 | 0.463451 | Uiso 0.030393 | O |
| H69 | 1.0 | 0.590784 | 0.460313 | 0.460305 | Uiso 0.030393 | H |
| H70 | 1.0 | 0.592969 | 0.435300 | 0.470262 | Uiso 0.030393 | H |
| O84 | 1.0 | 0.672043 | 0.444571 | 0.463455 | Uiso 0.030393 | O |
| H71 | 1.0 | 0.666268 | 0.456763 | 0.458398 | Uiso 0.030393 | H |
| H72 | 1.0 | 0.667043 | 0.431034 | 0.467022 | Uiso 0.030393 | H |
| O85 | 1.0 | 0.649830 | 0.539638 | 0.497053 | Uiso 0.030393 | O |
| H73 | 1.0 | 0.600143 | 0.541558 | 0.496419 | Uiso 0.030393 | H |
| H74 | 1.0 | 0.644016 | 0.552879 | 0.497935 | Uiso 0.030393 | H |
| O86 | 1.0 | 0.630903 | 0.458934 | 0.487248 | Uiso 0.030393 | O |
| H75 | 1.0 | 0.627773 | 0.470808 | 0.478052 | Uiso 0.030393 | H |
| H76 | 1.0 | 0.628312 | 0.459913 | 0.502192 | Uiso 0.030393 | H |
| O87 | 1.0 | 0.708875 | 0.548735 | 0.497171 | Uiso 0.030393 | O |
| H77 | 1.0 | 0.710219 | 0.540167 | 0.493651 | Uiso 0.030393 | H |
| H78 | 1.0 | 0.705851 | 0.559794 | 0.486945 | Uiso 0.030393 | H |
| O88 | 1.0 | 0.630282 | 0.514653 | 0.560384 | Uiso 0.030393 | O |
| H79 | 1.0 | 0.631298 | 0.513269 | 0.575719 | Uiso 0.030393 | H |
| H80 | 1.0 | 0.633677 | 0.501019 | 0.554049 | Uiso 0.030393 | H |
| O89 | 1.0 | 0.655638 | 0.537495 | 0.560299 | Uiso 0.030393 | O |
| H81 | 1.0 | 0.649860 | 0.546590 | 0.565704 | Uiso 0.030393 | H |
| H82 | 1.0 | 0.662846 | 0.533487 | 0.571837 | Uiso 0.030393 | H |
| O90 | 1.0 | 0.695406 | 0.505019 | 0.555056 | Uiso 0.030393 | O |
| H83 | 1.0 | 0.691429 | 0.518291 | 0.548747 | Uiso 0.030393 | H |
| Atom | Occupation | x     | y     | z     | Uiso  | H/O  |
|------|------------|-------|-------|-------|-------|------|
| H84  | 1.0        | 0.690459 | 0.502547 | 0.568460 | Uiso 0.030393 | H    |
| O91  | 1.0        | 0.713383 | 0.539137 | 0.559479 | Uiso 0.030393 | O    |
| H85  | 1.0        | 0.704066 | 0.533250 | 0.555499 | Uiso 0.030393 | H    |
| H86  | 1.0        | 0.712784 | 0.543748 | 0.574263 | Uiso 0.030393 | H    |
| O92  | 1.0        | 0.563011 | 0.471841 | 0.438876 | Uiso 0.030393 | O    |
| H87  | 1.0        | 0.563249 | 0.485401 | 0.430675 | Uiso 0.030393 | H    |
| H88  | 1.0        | 0.561205 | 0.459845 | 0.428998 | Uiso 0.030393 | H    |
| O93  | 1.0        | 0.567219 | 0.461295 | 0.495858 | Uiso 0.030393 | O    |
| H89  | 1.0        | 0.572126 | 0.457976 | 0.509122 | Uiso 0.030393 | H    |
| H90  | 1.0        | 0.573287 | 0.471319 | 0.487839 | Uiso 0.030393 | H    |
| O94  | 1.0        | 0.583643 | 0.502383 | 0.443047 | Uiso 0.030393 | O    |
| H91  | 1.0        | 0.581849 | 0.511451 | 0.455509 | Uiso 0.030393 | H    |
| H92  | 1.0        | 0.587237 | 0.488268 | 0.448011 | Uiso 0.030393 | H    |
| O95  | 1.0        | 0.637980 | 0.457393 | 0.438798 | Uiso 0.030393 | O    |
| H93  | 1.0        | 0.646985 | 0.449661 | 0.435770 | Uiso 0.030393 | H    |
| H94  | 1.0        | 0.631196 | 0.453201 | 0.427773 | Uiso 0.030393 | H    |
| O96  | 1.0        | 0.655219 | 0.498301 | 0.431764 | Uiso 0.030393 | O    |
| H95  | 1.0        | 0.654554 | 0.501622 | 0.416667 | Uiso 0.030393 | H    |
| H96  | 1.0        | 0.664326 | 0.504066 | 0.436831 | Uiso 0.030393 | H    |
#cluster_I_classical_tr.xyz

24

generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.280001 | 32.360001 | 33.850002 |
| Ca      | 22.490002 | 35.000004 | 35.880001 |
| Ca      | 23.630001 | 30.440002 | 32.910000 |
| Ca      | 22.490002 | 34.810001 | 30.610001 |
| Ca      | 24.810001 | 30.820004 | 27.870003 |
| Ca      | 27.540001 | 32.840000 | 31.370001 |
| Ca      | 29.050003 | 28.200001 | 29.640003 |
| Ca      | 30.670002 | 32.580002 | 26.790001 |
| Ca      | 30.750000 | 28.530003 | 25.020000 |
| Ca      | 34.660000 | 29.340002 | 28.290003 |
| Ca      | 34.230000 | 24.720001 | 26.870001 |
| Ca      | 35.220001 | 28.450001 | 23.230001 |
| S       | 21.340000 | 31.540001 | 35.600002 |
| S       | 20.080002 | 35.490002 | 33.310001 |
| S       | 21.860001 | 31.460001 | 29.710003 |
| S       | 24.680002 | 33.750004 | 33.279999 |
| S       | 26.030003 | 29.640003 | 30.720001 |
| S       | 25.700001 | 34.310001 | 28.680000 |
| S       | 28.290003 | 29.970001 | 26.650002 |
| S       | 30.760002 | 31.160002 | 30.160000 |
| S       | 32.099998 | 27.060001 | 28.180000 |
| S       | 33.180000 | 30.590002 | 25.340002 |
| S       | 33.200001 | 25.880001 | 23.510000 |
| S       | 36.680000 | 27.360001 | 26.470001 |

24

generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.382639 | 32.214893 | 33.783566 |
| Ca      | 22.686935 | 34.711781 | 35.642159 |
| Ca      | 23.456514 | 30.415857 | 32.725616 |
| Ca      | 22.899820 | 34.730812 | 30.487177 |
| Ca      | 25.025219 | 30.925987 | 27.720154 |
| Ca      | 27.686941 | 32.906437 | 31.200424 |
| Ca      | 29.031277 | 28.168602 | 29.698757 |
| Ca      | 30.674175 | 32.451134 | 27.082785 |
| Ca      | 30.706640 | 28.275665 | 25.182442 |
| Ca      | 34.658447 | 29.302114 | 28.425108 |
| Ca      | 34.186771 | 25.062569 | 27.095236 |
| Ca      | 34.752010 | 28.666683 | 23.191090 |
| S       | 21.242472 | 31.449915 | 35.661209 |
| S       | 20.347790 | 35.305504 | 33.035152 |
| S       | 22.067047 | 31.569632 | 29.751125 |
| S       | 24.813843 | 33.424515 | 33.363289 |
| S       | 26.221830 | 29.820816 | 30.530195 |
| S   | 25.985210 | 34.501858 | 28.547548 |
|-----|-----------|-----------|-----------|
| S   | 28.118048 | 30.045206 | 26.654863 |
| S   | 30.725121 | 31.253075 | 30.167288 |
| S   | 31.920599 | 27.058992 | 28.515039 |
| S   | 32.862221 | 30.371290 | 25.550562 |
| S   | 32.829571 | 25.744476 | 23.682564 |
| S   | 36.438889 | 27.922258 | 26.246685 |

24

generated by VMD

| Ca  | 18.429865 | 32.270645 | 33.654480 |
|-----|-----------|-----------|-----------|
| Ca  | 22.833435 | 34.923706 | 35.617962 |
| Ca  | 23.376627 | 30.473579 | 33.091106 |
| Ca  | 22.707108 | 34.858803 | 30.344297 |
| Ca  | 24.772865 | 30.640770 | 27.732357 |
| Ca  | 27.843327 | 32.843971 | 31.320816 |
| Ca  | 28.946514 | 28.168209 | 29.866476 |
| Ca  | 30.768986 | 32.556675 | 27.180307 |
| Ca  | 30.779099 | 28.415518 | 25.023266 |
| Ca  | 34.417469 | 29.223236 | 28.324837 |
| Ca  | 34.264023 | 24.960201 | 26.906704 |
| Ca  | 35.028667 | 28.662251 | 23.176725 |
| S   | 21.210321 | 31.560156 | 35.650394 |
| S   | 20.341568 | 35.275887 | 33.018368 |
| S   | 21.949886 | 31.291821 | 29.611059 |
| S   | 24.967619 | 33.769768 | 33.120567 |
| S   | 26.108456 | 29.628431 | 30.835943 |
| S   | 25.846622 | 34.061630 | 28.755163 |
| S   | 28.209414 | 30.163002 | 26.966621 |
| S   | 30.958586 | 31.091221 | 30.375555 |
| S   | 31.769882 | 27.028126 | 28.195726 |
| S   | 32.923527 | 30.794268 | 25.420717 |
| S   | 32.913948 | 25.880198 | 23.596565 |
| S   | 36.352192 | 27.758053 | 26.424046 |

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generated by VMD

| Ca  | 18.595472 | 32.656624 | 33.799919 |
|-----|-----------|-----------|-----------|
| Ca  | 22.745743 | 35.006470 | 35.740524 |
| Ca  | 23.667160 | 30.389656 | 33.038185 |
| Ca  | 22.530376 | 34.640579 | 30.566446 |
| Ca  | 24.645618 | 30.565010 | 27.662985 |
| Ca  | 27.389917 | 32.755775 | 31.167921 |
| Ca  | 28.910131 | 28.187410 | 29.764660 |
| Ca  | 30.654331 | 32.353077 | 27.253290 |
| Ca  | 30.801340 | 28.438780 | 24.841911 |
| Ca  | 34.665237 | 28.895496 | 28.310833 |
| Ca  | 34.368237 | 24.903757 | 26.745840 |
Ca  35.226604  29.007463  23.361568
S   21.325720  31.640350  35.594646
S   20.267235  35.724754  33.220585
S   21.868933  31.253887  29.903336
S   24.727612  33.795227  33.156654
S   26.054995  29.658415  30.723011
S   25.516031  34.194416  28.400389
S   28.271950  30.102772  26.679031
S   30.571220  31.142994  28.107719
S   32.056824  35.724754  33.220585
S   35.107574  31.142994  28.107719
S   32.056824  35.724754  33.220585
S   36.636971  27.717731  26.346056

24 generated by VMD
Ca  18.081457  32.375511  33.884655
Ca  22.727499  34.722603  35.628407
Ca  23.528744  30.316301  33.091679
Ca  22.681110  34.798973  30.616730
Ca  24.715811  30.787775  27.722948
Ca  27.578049  33.056896  31.423988
Ca  29.136772  28.523119  29.508291
Ca  30.952341  32.486893  26.889149
Ca  30.852247  28.300770  25.139505
Ca  34.819435  29.075800  28.384819
Ca  34.240608  24.787531  26.778980
Ca  35.107574  28.551048  23.069588
S   21.162870  31.420994  35.554829
S   20.136169  35.395218  33.083626
S   21.851284  31.194923  29.956800
S   24.672688  33.763718  33.380127
S   26.139660  29.972391  30.654396
S   25.687973  34.443336  28.724323
S   28.302387  30.301222  26.508919
S   30.627464  31.356575  30.203459
S   31.947792  26.999929  28.359833
S   33.219913  30.455488  25.443222
S   33.039249  25.510918  23.676332
S   36.510918  27.600594  26.255470

24 generated by VMD
Ca  18.462570  32.710739  33.608303
Ca  22.729494  34.905823  35.613323
Ca  23.380104  30.250551  32.942406
Ca  22.712505  34.520294  30.716785
Ca  24.937666  30.357952  27.968227
|   |   |   |   |
|---|---|---|---|
| Ca | 27.556597 | 32.747799 | 31.386963 |
| Ca | 29.055672 | 28.222891 | 29.765818 |
| Ca | 30.748501 | 32.400703 | 26.951443 |
| Ca | 30.612686 | 28.328493 | 24.771725 |
| Ca | 34.422672 | 29.188517 | 28.446674 |
| Ca | 34.136669 | 24.995047 | 26.693851 |
| Ca | 35.144585 | 28.795887 | 23.460215 |
| S  | 21.155996 | 31.647854 | 35.237602 |
| S  | 20.377766 | 35.944336 | 33.042725 |
| S  | 22.077044 | 30.943478 | 30.012684 |
| S  | 24.846289 | 33.690365 | 33.395050 |
| S  | 26.226875 | 29.734119 | 30.892092 |
| S  | 25.798248 | 34.049934 | 28.695934 |
| S  | 28.198889 | 30.018642 | 26.633839 |
| S  | 30.722540 | 31.282507 | 30.227211 |
| S  | 31.866163 | 27.127943 | 28.130354 |
| S  | 32.959206 | 30.565018 | 25.389286 |
| S  | 33.102989 | 26.087254 | 23.449474 |
| S  | 36.488316 | 27.783905 | 26.508043 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 18.256681 | 32.425552 | 33.695518 |
| Ca | 22.256475 | 35.081913 | 35.557808 |
| Ca | 23.577120 | 30.324749 | 32.989853 |
| Ca | 23.213615 | 34.599720 | 31.173038 |
| Ca | 24.827467 | 30.669657 | 27.801580 |
| Ca | 27.535398 | 32.963326 | 31.087292 |
| Ca | 29.054977 | 28.322496 | 29.572287 |
| Ca | 30.736053 | 32.429680 | 26.662518 |
| Ca | 30.789331 | 28.335754 | 24.942442 |
| Ca | 34.355110 | 29.144266 | 28.543571 |
| Ca | 34.378746 | 24.920378 | 26.647909 |
| Ca | 35.188667 | 28.710960 | 23.224281 |
| S  | 21.093065 | 31.528160 | 35.411129 |
| S  | 20.170689 | 35.614693 | 32.985832 |
| S  | 22.095821 | 31.175308 | 30.243492 |
| S  | 24.938814 | 33.810612 | 33.685226 |
| S  | 26.139500 | 29.750439 | 30.697388 |
| S  | 25.868814 | 34.055386 | 28.478226 |
| S  | 28.180988 | 30.041494 | 26.531662 |
| S  | 30.744614 | 31.363113 | 30.263918 |
| S  | 31.862251 | 26.904009 | 28.181091 |
| S  | 33.025146 | 30.478163 | 25.483389 |
| S  | 33.106087 | 25.910135 | 23.459738 |
| S  | 36.324623 | 27.740047 | 26.620916 |
| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| Ca      | 18.292059 | 32.497963 | 33.395390 |
| Ca      | 22.209974 | 34.551353 | 35.938152 |
| Ca      | 23.381695 | 30.368313 | 33.166245 |
| Ca      | 23.240170 | 34.729698 | 30.734381 |
| Ca      | 25.057541 | 30.729780 | 27.930849 |
| Ca      | 27.560991 | 33.261528 | 31.176935 |
| Ca      | 29.285433 | 28.648319 | 29.814875 |
| Ca      | 30.629431 | 32.155201 | 26.502586 |
| Ca      | 30.658972 | 28.162891 | 24.596279 |
| Ca      | 34.314133 | 29.271879 | 28.410442 |
| Ca      | 34.146034 | 25.044252 | 26.972067 |
| Ca      | 35.225395 | 28.549604 | 23.279034 |
| S       | 20.732344 | 31.229654 | 35.561813 |
| S       | 20.323265 | 35.434422 | 33.116409 |
| S       | 22.295311 | 31.431889 | 30.167034 |
| S       | 24.857172 | 33.678234 | 33.743469 |
| S       | 26.254406 | 30.026585 | 30.870737 |
| S       | 26.061781 | 34.180862 | 28.299250 |
| S       | 28.253674 | 29.748037 | 26.691929 |
| S       | 30.852171 | 31.572517 | 30.214657 |
| S       | 31.684336 | 26.893888 | 27.986994 |
| S       | 32.949738 | 30.463892 | 25.275904 |
| S       | 33.044529 | 25.916586 | 23.470663 |
| S       | 36.409504 | 27.752724 | 26.623968 |

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| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| Ca      | 18.199703 | 32.357624 | 33.169029 |
| Ca      | 22.110096 | 34.540543 | 36.071564 |
| Ca      | 23.513496 | 30.459755 | 33.041790 |
| Ca      | 23.278318 | 34.520790 | 31.077793 |
| Ca      | 25.085367 | 30.601187 | 27.845798 |
| Ca      | 27.878538 | 33.357937 | 31.058561 |
| Ca      | 28.956553 | 28.504770 | 29.490891 |
| Ca      | 30.639212 | 32.426159 | 26.354460 |
| Ca      | 30.620630 | 28.083981 | 24.880392 |
| Ca      | 34.244991 | 29.343468 | 28.402578 |
| Ca      | 34.175392 | 25.057590 | 27.055508 |
| Ca      | 35.200825 | 28.461807 | 23.363029 |
| S       | 20.679178 | 31.349493 | 35.484470 |
| S       | 20.280891 | 35.419857 | 33.109856 |
| S       | 22.382401 | 31.435576 | 30.123430 |
| S       | 25.115519 | 33.672421 | 33.887257 |
| S       | 26.309717 | 29.906130 | 31.029312 |
| S       | 26.136608 | 34.122398 | 28.624577 |
| S       | 28.042198 | 30.134203 | 26.338192 |
|    | 30.847246 | 31.653551 | 29.797949 |
|----|-----------|-----------|-----------|
| S  | 31.828798 | 26.968975 | 28.090017 |
| S  | 32.946392 | 30.492279 | 25.301487 |
| S  | 32.991653 | 25.690458 | 23.655237 |
| S  | 36.256329 | 27.761145 | 26.707977 |

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generated by VMD

| Ca | 18.024675 | 32.659847 | 33.120697 |
|----|-----------|-----------|-----------|
| Ca | 22.441912 | 35.124359 | 35.544373 |
| Ca | 23.237465 | 30.179737 | 33.038483 |
| Ca | 23.295544 | 34.579655 | 31.247730 |
| Ca | 24.957380 | 30.522108 | 27.892639 |
| Ca | 27.601736 | 33.079330 | 31.273600 |
| Ca | 29.055737 | 28.429804 | 30.009546 |
| Ca | 30.546532 | 32.061756 | 26.813820 |
| Ca | 30.805321 | 28.140146 | 24.743052 |
| Ca | 34.624451 | 29.630720 | 28.336302 |
| Ca | 34.088524 | 25.118814 | 26.697367 |
| Ca | 35.246391 | 28.387356 | 23.189251 |
| S  | 20.691422 | 31.741385 | 35.455715 |
| S  | 20.118021 | 35.465229 | 33.175610 |
| S  | 22.200533 | 31.355494 | 30.213968 |
| S  | 24.954676 | 33.376133 | 33.795483 |
| S  | 26.225441 | 29.822456 | 30.923069 |
| S  | 25.924562 | 34.007790 | 28.547766 |
| S  | 28.136499 | 29.784145 | 26.675470 |
| S  | 30.835684 | 31.410860 | 30.591352 |
| S  | 31.916021 | 27.186758 | 27.969074 |
| S  | 33.352264 | 30.600992 | 25.053391 |
| S  | 33.078613 | 25.860783 | 23.224478 |
| S  | 36.360626 | 27.774460 | 26.407858 |

24

generated by VMD

| Ca | 18.127764 | 32.443821 | 32.927471 |
|----|-----------|-----------|-----------|
| Ca | 22.171104 | 35.022785 | 35.676369 |
| Ca | 23.387514 | 30.209963 | 33.082115 |
| Ca | 23.298756 | 34.411076 | 31.495028 |
| Ca | 24.969027 | 30.638554 | 27.940371 |
| Ca | 27.685776 | 33.343685 | 31.262627 |
| Ca | 29.187904 | 28.570665 | 29.792999 |
| Ca | 30.661367 | 32.443634 | 26.764811 |
| Ca | 30.792944 | 28.218189 | 24.901806 |
| Ca | 34.575157 | 29.175354 | 28.222244 |
| Ca | 34.095043 | 25.093647 | 26.810099 |
| Ca | 34.969631 | 28.357515 | 23.229685 |
| S  | 20.723124 | 31.527830 | 35.289436 |
S 20.031694 35.585964 33.041405
S 22.306391 31.206762 30.177696
S 25.026236 33.452446 33.768845
S 26.332594 29.839947 30.960756
S 26.034216 34.103725 28.831974
S 28.082626 30.193634 26.523987
S 30.772104 31.495205 30.024492
S 31.995529 27.194397 28.191216
S 33.033665 30.284391 25.099499
S 32.937737 25.703110 23.454487
S 36.522133 27.783739 26.470646

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generated by VMD
Ca 17.876720 32.651703 33.426105
Ca 22.155241 34.905857 35.649780
Ca 23.371407 30.197397 33.127918
Ca 23.169989 34.651730 31.116800
Ca 24.993736 30.893209 27.916298
Ca 27.591066 32.862659 31.417801
Ca 29.205732 28.473919 29.756681
Ca 30.584438 32.398067 26.552322
Ca 30.841295 28.227913 24.865065
Ca 34.549068 29.392859 28.105978
Ca 34.381100 24.980549 26.766695
Ca 35.111000 28.360155 23.203983
S 20.555006 31.637581 35.420582
S 20.166407 35.611614 33.064240
S 22.133459 31.308617 30.315289
S 24.952272 33.364914 33.815132
S 26.162947 29.756992 30.792576
S 25.959545 34.148918 28.745375
S 28.317127 30.079966 26.612226
S 30.857582 31.503937 30.190016
S 31.972385 27.167721 28.138538
S 33.120865 30.406301 24.974066
S 33.102146 25.610147 23.464516
S 36.589558 27.707340 26.502073

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generated by VMD
Ca 18.054768 32.655880 33.261280
Ca 22.376472 34.639698 35.674934
Ca 23.217817 30.392721 33.098095
Ca 23.119411 34.566689 31.238707
Ca 24.948368 30.790560 27.966223
Ca 27.477377 32.992897 31.315554
Ca 29.134075 28.398561 29.636015
| Element | Value1  | Value2  | Value3  |
|--------|--------|--------|--------|
| Ca     | 30.589668 | 32.205925 | 26.665186 |
| Ca     | 30.789715 | 28.063528 | 24.637894 |
| Ca     | 34.547783 | 29.76492 | 28.302572 |
| Ca     | 34.399185 | 24.994074 | 26.977161 |
| Ca     | 35.182259 | 28.731234 | 23.255468 |
| S      | 20.727797 | 31.762470 | 35.386002 |
| S      | 20.234921 | 35.737247 | 33.243031 |
| S      | 22.166565 | 31.455435 | 30.277046 |
| S      | 25.022816 | 33.631725 | 33.740986 |
| S      | 26.205805 | 29.708900 | 30.887909 |
| S      | 25.805477 | 34.132439 | 28.693480 |
| S      | 28.129934 | 29.815807 | 26.472200 |
| S      | 30.656607 | 31.304413 | 30.180819 |
| S      | 31.923862 | 27.045216 | 27.872770 |
| S      | 32.978851 | 30.427322 | 25.179573 |
| S      | 33.432831 | 25.654861 | 23.631283 |
| S      | 36.597679 | 27.815948 | 26.345863 |

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generated by VMD

| Element | Value1  | Value2  | Value3  |
|--------|--------|--------|--------|
| Ca     | 17.966665 | 32.859127 | 33.481827 |

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generated by VMD
Ca    22.722673  34.993454  35.563927
Ca    23.171532  30.322950  32.985569
Ca    23.235355  34.699123  31.145117
Ca    24.826473  30.375494  28.058500
Ca    27.388634  32.697739  31.259804
Ca    29.036448  28.176105  29.573826
Ca    30.655755  32.347691  26.791307
Ca    30.727823  28.212240  24.605480
Ca    34.565815  29.366501  28.318909
Ca    34.411633  25.125296  26.723881
Ca    35.275845  28.640974  23.366215
Ca    20.982677  31.819374  35.512711
S     20.280186  35.689758  33.158207
S     22.142883  31.390112  30.197567
S     24.928143  33.604662  33.587772
S     26.100388  29.416409  30.993361
S     25.718294  33.810673  28.589851
S     28.039280  29.905155  26.468163
S     30.627825  31.277903  30.174307
S     31.827927  27.184715  27.898678
S     33.141872  30.828833  25.356880
S     33.402065  25.786964  23.423416
S     36.544060  27.768951  26.704792

24
generated by VMD
Ca    18.047045  32.730194  33.338497
Ca    22.727829  34.932625  35.426331
Ca    23.488604  30.274759  33.212078
Ca    23.300272  34.501347  30.908535
Ca    24.960285  30.276167  28.078194
Ca    27.671362  32.726196  30.933790
Ca    29.073557  28.169827  29.910114
Ca    30.639219  32.502010  27.197220
Ca    30.765242  28.420282  24.698963
Ca    33.713374  29.710621  28.613350
Ca    34.160439  24.979767  26.579256
Ca    35.158974  28.738348  23.586653
S     21.149665  31.684555  35.307987
S     20.348293  35.575943  32.834141
S     22.285017  31.248177  30.339373
S     25.232460  33.593803  33.352863
S     26.263800  29.417648  30.914654
S     25.826795  33.892769  28.390111
S     28.165436  30.177622  26.802147
S     30.980873  31.176704  30.152052
S     31.554647  27.005697  27.939251
| Element | X-Position | Y-Position | Z-Position |
|---------|------------|------------|------------|
| S       | 32.991623  | 30.808823  | 25.427471  |
| S       | 33.079823  | 25.822216  | 23.404188  |
| S       | 36.130310  | 27.935787  | 26.586887  |

24 generated by VMD

| Element | X-Position | Y-Position | Z-Position |
|---------|------------|------------|------------|
| Ca      | 18.245543  | 32.526985  | 33.431843  |
| Ca      | 22.867100  | 35.011982  | 35.384296  |
| Ca      | 23.378754  | 30.145927  | 33.280697  |
| Ca      | 23.684738  | 34.532146  | 30.946928  |
| Ca      | 24.679142  | 30.501667  | 27.893303  |
| Ca      | 27.624138  | 32.560219  | 30.755308  |
| Ca      | 28.983681  | 28.117123  | 29.848030  |
| Ca      | 30.569378  | 32.304565  | 27.283318  |
| Ca      | 30.674618  | 28.476887  | 24.816519  |
| Ca      | 33.912338  | 29.827520  | 28.462282  |
| Ca      | 34.244057  | 25.104805  | 26.819208  |
| Ca      | 35.179821  | 28.795109  | 23.636974  |
| S       | 21.095608  | 31.754440  | 35.539314  |
| S       | 20.609194  | 35.402382  | 32.739223  |
| S       | 22.102688  | 31.310951  | 30.252420  |
| S       | 25.282211  | 33.443550  | 33.356937  |
| S       | 25.984419  | 29.621243  | 30.676123  |
| S       | 25.912426  | 34.088314  | 28.379707  |
| S       | 28.050327  | 30.010429  | 26.714163  |
| S       | 30.845720  | 31.107216  | 30.154724  |
| S       | 31.549658  | 26.945669  | 27.877659  |
| S       | 32.881851  | 30.835238  | 25.314648  |
| S       | 33.074394  | 25.929197  | 23.618446  |
| S       | 36.288269  | 27.946487  | 26.757946  |

24 generated by VMD

| Element | X-Position | Y-Position | Z-Position |
|---------|------------|------------|------------|
| Ca      | 18.480247  | 32.494328  | 33.554707  |
| Ca      | 22.792774  | 34.790180  | 35.238800  |
| Ca      | 23.600361  | 30.163464  | 33.019737  |
| Ca      | 23.221664  | 34.784222  | 30.796387  |
| Ca      | 24.697859  | 30.661095  | 27.932375  |
| Ca      | 27.698807  | 32.914116  | 30.793285  |
| Ca      | 29.218683  | 28.094753  | 29.899645  |
| Ca      | 30.600147  | 32.581074  | 27.417919  |
| Ca      | 30.712589  | 28.604053  | 24.993723  |
| Ca      | 33.869556  | 29.796970  | 28.448889  |
| Ca      | 34.070824  | 24.663271  | 26.652954  |
| Ca      | 34.890297  | 28.419292  | 23.541843  |
| S       | 21.213896  | 31.497267  | 35.376144  |
| S       | 20.321079  | 35.453285  | 32.813080  |
| S       | 22.082729  | 31.172829  | 30.222313  |
59

S        25.165146       33.453716       33.323406
S        26.276306       29.610664       30.656895
S        25.807354       34.201160       28.439770
S        28.120146       30.042500       26.993168
S        30.909090       31.231796       30.251749
S        31.708248       27.042706       27.853210
S        32.923588       30.887882       25.227844
S        33.086796       25.930563       23.592972
S        36.251873       27.808880       26.899254

24 generated by VMD
Ca       18.368120       32.646713       33.840199
Ca       22.667145       34.898331       35.364895
Ca       23.548370       30.079052       33.215271
Ca       22.971928       34.880836       30.759531
Ca       24.725073       30.480185       27.889967
Ca       27.709478       32.713730       30.801291
Ca       29.130081       28.157654       29.718809
Ca       30.616108       32.374321       27.117311
Ca       30.692921       28.451820       24.713121
Ca       33.956886       29.821571       28.561684
Ca       34.384686       24.627640       26.740295
Ca       35.090233       28.666348       23.442467
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       35.090233       28.666348       23.442467
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       21.187515       31.559763       35.730457
S        20.153349       35.661091       32.939377
Ca       21.187515       31.559763       35.730457
|   | Ca     | S         | S         |
|---|--------|-----------|-----------|
| 1 | 33.691498 | 29.697748 | 28.362623 |
| 2 | 34.335430 | 24.696514 | 26.803738 |
| 3 | 34.942654 | 35.458305 | 32.935333 |
| 4 | 34.942654 | 28.507868 | 23.536301 |
| 5 | 21.247850 | 31.537123 | 35.556351 |
| 6 | 20.267282 | 31.576782 | 30.175957 |
| 7 | 25.083115 | 33.507301 | 33.244267 |
| 8 | 25.827351 | 31.99076  | 30.046345 |
| 9 | 26.221117 | 29.641920 | 30.798397 |
| 10| 28.122849 | 29.947824 | 26.954865 |
| 11| 30.691217 | 31.199076 | 30.046345 |
| 12| 32.962570 | 31.017736 | 25.302773 |
| 13| 33.294102 | 34.169807 | 28.516453 |
| 14| 36.401505 | 32.401890 | 27.519314 |

24 generated by VMD

|   | Ca     | S         | S         |
|---|--------|-----------|-----------|
| 1 | 18.482790 | 32.745300 | 33.846642 |
| 2 | 22.926758 | 34.784828 | 35.390820 |
| 3 | 23.415867 | 30.272726 | 32.965878 |
| 4 | 23.369123 | 34.793568 | 30.751335 |
| 5 | 24.684759 | 30.612532 | 27.867531 |
| 6 | 27.542032 | 32.554306 | 30.807327 |
| 7 | 28.917566 | 28.096743 | 29.837093 |
| 8 | 30.640137 | 32.401890 | 27.267704 |
| 9 | 30.816797 | 28.323681 | 24.919683 |
|10 | 33.863781 | 29.663832 | 28.401751 |
|11 | 34.513988 | 24.837572 | 26.999233 |
|12 | 35.015427 | 28.850784 | 23.496777 |
|13 | 21.385057 | 31.452900 | 35.551823 |
|14 | 20.336443 | 35.605766 | 33.098434 |
|15 | 21.770115 | 31.501625 | 30.127728 |
|16 | 25.117479 | 33.543449 | 33.089661 |
|17 | 25.789204 | 29.462761 | 30.530676 |
|18 | 25.931564 | 34.088772 | 28.351904 |
|19 | 28.119173 | 29.814123 | 26.836533 |
|20 | 30.682024 | 31.144632 | 30.298023 |
|21 | 31.726124 | 26.941599 | 27.689878 |
|22 | 32.892994 | 30.897321 | 25.328194 |
|23 | 33.323700 | 25.994856 | 23.727919 |
|24 | 36.458157 | 27.922112 | 26.757483 |

24 generated by VMD

|   | Ca     | S         | S         |
|---|--------|-----------|-----------|
| 1 | 18.430260 | 32.760666 | 33.970901 |
| 2 | 22.989344 | 34.903492 | 35.617439 |
| 3 | 23.302315 | 30.179684 | 32.863663 |
|  | Ca     | S      | Ca     |
|---|--------|--------|--------|
| 1 | 23.211855 | 34.675430 | 30.928230 |
| 2 | 24.623615 | 30.430847 | 27.497173 |
| 3 | 27.434303 | 32.426136 | 27.179241 |
| 4 | 29.133963 | 28.078438 | 29.955519 |
| 5 | 30.655693 | 32.604809 | 30.564114 |
| 6 | 30.724270 | 28.322371 | 25.069221 |
| 7 | 33.586880 | 29.751659 | 28.384560 |
| 8 | 34.443462 | 24.792757 | 26.796024 |
| 9 | 35.282963 | 28.917250 | 23.806108 |
| 10 | 21.283371 | 31.743259 | 35.569504 |
| 11 | 20.459942 | 35.789299 | 33.425461 |
| 12 | 21.918785 | 31.355453 | 29.919155 |
| 13 | 25.17969 | 33.407463 | 33.201424 |
| 14 | 25.80295 | 29.348223 | 30.353455 |
| 15 | 25.58573 | 33.986572 | 28.241373 |
| 16 | 28.309656 | 29.896103 | 26.963745 |
| 17 | 31.019894 | 31.314505 | 30.024981 |
| 18 | 31.742144 | 27.013376 | 27.749250 |
| 19 | 32.989414 | 30.893835 | 25.359818 |
| 20 | 33.264626 | 26.34966 | 23.559996 |
| 21 | 36.412941 | 27.673470 | 26.935783 |

24 generated by VMD

|  | Ca     | S      | Ca     |
|---|--------|--------|--------|
| 1 | 18.387947 | 33.038876 | 34.015934 |
| 2 | 22.615084 | 34.980621 | 35.422710 |
| 3 | 23.400076 | 30.183069 | 33.049553 |
| 4 | 23.192366 | 34.654442 | 30.790298 |
| 5 | 24.765045 | 30.384016 | 27.925013 |
| 6 | 27.550375 | 32.518536 | 30.897499 |
| 7 | 29.217869 | 27.993725 | 29.754538 |
| 8 | 30.568254 | 32.626614 | 27.058056 |
| 9 | 30.78943 | 28.464066 | 24.871628 |
| 10 | 33.794327 | 29.807369 | 28.557156 |
| 11 | 34.551079 | 24.810303 | 26.537540 |
| 12 | 35.175980 | 28.656879 | 23.717834 |
| 13 | 21.48162 | 31.761663 | 35.574368 |
| 14 | 20.234190 | 35.571857 | 33.078293 |
| 15 | 21.856186 | 31.452499 | 29.920357 |
| 16 | 25.092260 | 33.417755 | 33.165382 |
| 17 | 26.104324 | 29.348614 | 30.647800 |
| 18 | 25.771576 | 33.915417 | 28.494646 |
| 19 | 28.112682 | 29.904486 | 26.829395 |
| 20 | 30.875471 | 31.193642 | 30.105940 |
| 21 | 31.762581 | 27.025795 | 27.633554 |
| 22 | 32.982376 | 30.857889 | 25.358349 |
| 23 | 33.200249 | 26.060715 | 23.323086 |
|    |    |    |    |
|----|----|----|----|
| S  | 36.277702 | 27.671206 | 27.211136 |
| 24 | generated by VMD |
| Ca | 18.662090 | 32.577595 | 34.248974 |
| Ca | 23.148621 | 35.013859 | 35.609035 |
| Ca | 23.509880 | 30.161762 | 32.967575 |
| Ca | 22.738665 | 34.851738 | 30.555372 |
| Ca | 24.851349 | 30.685318 | 27.635771 |
| Ca | 27.620707 | 32.705750 | 30.758804 |
| Ca | 29.000309 | 27.971115 | 29.679838 |
| Ca | 30.343077 | 32.427483 | 27.121311 |
| Ca | 30.859137 | 28.308968 | 24.902704 |
| Ca | 33.791191 | 29.750166 | 28.537327 |
| Ca | 34.238338 | 24.745445 | 26.729195 |
| Ca | 35.140617 | 28.932852 | 23.879770 |
| S  | 21.557301 | 31.590567 | 35.721115 |
| S  | 20.442495 | 35.545567 | 33.290115 |
| S  | 21.950605 | 31.424856 | 29.690952 |
| S  | 24.824036 | 33.390320 | 33.076759 |
| S  | 26.001041 | 29.597279 | 30.336027 |
| S  | 25.768038 | 34.234467 | 28.369402 |
| S  | 28.157410 | 29.812773 | 26.548382 |
| S  | 30.676857 | 31.029707 | 30.017900 |
| S  | 31.703697 | 26.808739 | 27.847279 |
| S  | 33.005999 | 30.887148 | 25.472179 |
| S  | 33.337162 | 26.132296 | 23.826322 |
| S  | 36.396843 | 27.714312 | 27.117908 |

24

|    |    |    |    |
|----|----|----|----|
| generated by VMD |
| Ca | 18.401825 | 32.522850 | 33.934898 |
| Ca | 22.863724 | 35.120369 | 35.441196 |
| Ca | 23.501022 | 30.474098 | 33.046204 |
| Ca | 22.930998 | 34.751488 | 30.420805 |
| Ca | 24.813345 | 30.468079 | 27.997969 |
| Ca | 27.787582 | 32.574871 | 31.199617 |
| Ca | 29.038618 | 27.911716 | 29.918106 |
| Ca | 30.414835 | 32.453686 | 27.425076 |
| Ca | 30.692245 | 28.514738 | 24.699068 |
| Ca | 33.913513 | 29.850897 | 28.365360 |
| Ca | 34.078430 | 24.581596 | 26.623274 |
| Ca | 35.465714 | 28.981215 | 23.660549 |
| S  | 21.397427 | 31.880161 | 35.686558 |
| S  | 20.337833 | 35.612473 | 32.902077 |
| S  | 21.895266 | 31.350853 | 29.932291 |
| S  | 24.884510 | 33.373966 | 33.030636 |
| S  | 26.182726 | 29.433727 | 30.788940 |
S     25.896975    33.909122    28.540085
S     27.990078    29.692173    26.792946
S     30.905424    31.033022    30.154457
S     31.679077    26.972588    27.804199
S     33.055004    30.979635    25.233345
S     33.391412    26.238625    23.418705
S     36.199810    27.618111    26.923689

24
generated by VMD
Ca     18.780043    32.044250    34.229012
Ca     22.971174    34.887093    35.856781
Ca     23.564007    30.744846    32.895695
Ca     22.691904    39.21185    30.728270
Ca     24.741007    30.753979    27.510355
Ca     27.567858    33.134083    30.798733
Ca     29.108988    28.012218    29.728909
Ca     30.551929    32.377480    26.999277
Ca     30.810415    28.243210    24.587601
Ca     33.647865    29.732071    28.650364
Ca     34.261250    24.486351    26.738907
Ca     35.589657    28.764681    23.994343
S     21.724169    31.536724    35.775600
S     20.296682    35.299789    33.450195
S     21.649080    31.682272    29.597187
S     24.767769    33.504448    33.11492
S     25.954222    29.974110    30.452536
S     25.593153    34.272438    28.396299
S     28.122429    29.707785    26.594849
S     30.780540    31.180183    30.019596
S     31.798340    26.824045    27.762892
S     32.922295    30.665470    25.286123
S     33.541065    26.018532    23.403469
S     36.284248    27.532837    27.371548

24
generated by VMD
Ca     19.037201    32.326298    34.431778
Ca     23.275848    35.168407    35.562344
Ca     23.418959    30.620296    32.794743
Ca     22.643738    34.528206    30.424911
Ca     24.530046    30.487190    27.397680
Ca     27.458397    32.659298    30.894424
Ca     29.112555    28.086853    29.795425
Ca     30.456230    32.242256    27.255198
Ca     30.918993    28.671577    24.574028
Ca     34.045414    29.630049    28.827946
Ca     34.126011    24.550335    26.607050
|   | 35.452988 | 29.046577 | 24.157087 |
|---|-----------|----------|----------|
| S | 21.872585 | 31.754816 | 35.793507 |
| S | 20.442776 | 35.416981 | 33.137115 |
| S | 21.703569 | 31.510050 | 29.668468 |
| S | 24.899216 | 33.657902 | 33.114578 |
| S | 25.858576 | 29.528629 | 30.635777 |
| S | 25.360226 | 33.899410 | 28.275421 |
| S | 28.061842 | 29.950294 | 26.539789 |
| S | 30.793467 | 31.087212 | 30.208815 |
| S | 31.718267 | 26.929905 | 27.703190 |
| S | 32.924721 | 30.922424 | 25.510006 |
| S | 33.404652 | 26.304432 | 23.343294 |
| S | 36.202888 | 27.320694 | 27.287468 |

24 generated by VMD

|   | 18.981276 | 32.271927 | 34.633785 |
|---|-----------|----------|----------|
| Ca| 23.034901 | 35.283115 | 35.518246 |
| Ca| 23.581747 | 30.547260 | 32.858807 |
| Ca| 22.678043 | 34.841873 | 30.549746 |
| Ca| 24.511776 | 30.486038 | 27.539843 |
| Ca| 27.581181 | 32.751064 | 29.026142 |
| Ca| 29.022099 | 27.756056 | 29.640003 |
| Ca| 30.221518 | 32.174892 | 27.151125 |
| Ca| 30.613865 | 28.452961 | 24.517893 |
| Ca| 33.555370 | 29.652784 | 28.673788 |
| Ca| 34.214722 | 24.528175 | 26.481581 |
| Ca| 35.830307 | 29.213064 | 24.093317 |
| S | 21.867889 | 31.886963 | 35.748177 |
| S | 20.424646 | 35.524357 | 33.141846 |
| S | 21.813459 | 31.483276 | 29.751453 |
| S | 24.879999 | 33.606243 | 33.019386 |
| S | 25.922451 | 29.674124 | 30.567747 |
| S | 25.662201 | 33.852066 | 28.251312 |
| S | 28.072945 | 29.552099 | 26.565359 |
| S | 30.647762 | 30.936987 | 30.214020 |
| S | 31.608587 | 26.749771 | 27.550102 |
| S | 33.064419 | 31.047253 | 25.502270 |
| S | 33.633900 | 26.596670 | 23.531452 |
| S | 36.295006 | 27.431040 | 27.512648 |

24 generated by VMD

|   | 19.004923 | 32.204529 | 34.414680 |
|---|-----------|----------|----------|
| Ca| 23.073322 | 35.285168 | 35.387737 |
| Ca| 23.403641 | 30.676613 | 32.952290 |
| Ca| 22.606506 | 34.461422 | 30.300369 |
| Ca| 24.848549 | 30.286032 | 27.665539 |
Ca    27.968632  32.85194  31.029015
Ca    28.960785  28.00116  29.847473
Ca    30.436214  32.43229  27.309929
Ca    30.929993  28.72767  25.005157
Ca    33.519272  29.45288  28.671585
Ca    33.995060  24.48170  26.305033
Ca    35.401627  29.04947  23.852354
S     21.813538  31.96897  35.747158
S     20.444424  35.32924  32.978580
S     21.612110  31.11244  29.542162
S     24.855761  33.72966  33.001980
S     26.082169  29.70712  30.853256
S     25.659637  33.82937  28.241463
S     28.118752  29.89353  26.786503
S     30.928577  31.05607  30.306276
S     31.404285  26.70789  27.262173
S     33.054714  31.17075  25.794849
S     33.612659  26.45639  23.459864
S     35.401627  29.04947  23.852354

24

generated by VMD
Ca    19.163038  31.81806  34.26080
Ca    23.185377  35.33367  35.33514
Ca    23.705368  30.66878  33.01288
Ca    22.620266  34.67091  30.28832
Ca    24.756393  30.48414  27.52535
Ca    27.714193  32.70243  31.03123
Ca    28.849319  27.97292  29.66502
Ca    30.269234  32.33695  27.53963
Ca    30.807440  28.55451  24.96023
Ca    33.393219  29.29020  28.71531
Ca    33.892262  24.60827  26.52933
Ca    35.534584  29.08464  24.02060
S     21.976299  32.12276  35.75316
S     20.364740  35.00302  33.03517
S     22.044674  31.39610  29.63909
S     25.056074  33.97958  32.85109
S     26.126930  29.46989  30.78742
S     25.582001  33.82182  28.07020
S     28.118645  29.86746  26.60493
S     30.744736  30.84475  30.43145
S     31.361277  27.06220  27.44836
S     33.064110  31.16848  25.90358
S     33.351448  26.53682  23.40526
S     36.038387  27.50207  27.12617
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| Ca      | 19.194775 | 31.941866 | 34.275883 |
| Ca      | 22.978041 | 35.445347 | 35.424423 |
| Ca      | 23.828381 | 30.714394 | 33.079216 |
| Ca      | 22.666681 | 34.717854 | 30.366938 |
| Ca      | 24.753935 | 30.362818 | 27.528149 |
| Ca      | 27.361088 | 32.647118 | 30.985567 |
| Ca      | 28.783979 | 27.790972 | 29.558626 |
| Ca      | 30.391428 | 32.052876 | 27.428713 |
| Ca      | 30.879976 | 28.571194 | 24.678764 |
| Ca      | 33.662220 | 29.392632 | 28.780140 |
| Ca      | 33.937550 | 24.669790 | 26.452400 |
| Ca      | 35.624035 | 29.210823 | 24.035194 |
| S       | 22.092457 | 32.114323 | 35.946545 |
| S       | 20.232330 | 35.416916 | 32.958801 |
| S       | 21.856401 | 31.502384 | 29.873396 |
| S       | 24.976164 | 34.074501 | 32.908096 |
| S       | 25.908667 | 29.248175 | 30.598303 |
| S       | 25.487982 | 33.842751 | 28.326237 |
| S       | 28.097784 | 29.724525 | 26.640987 |
| S       | 30.673813 | 30.819489 | 30.347824 |
| S       | 31.492226 | 26.796377 | 27.458435 |
| S       | 32.984467 | 31.122643 | 25.811520 |
| S       | 33.739067 | 26.639469 | 23.296791 |
| S       | 36.116676 | 27.480797 | 27.179129 |
| Ca      | 20.885714 | 32.612823 | 34.318336 |
| Ca      | 23.609958 | 35.530037 | 35.339836 |
| Ca      | 23.597298 | 30.519030 | 32.978577 |
| Ca      | 22.499542 | 34.840717 | 30.332382 |
| Ca      | 24.673409 | 30.440870 | 27.542660 |
| Ca      | 27.416947 | 32.669334 | 31.150408 |
| Ca      | 28.569809 | 27.805553 | 29.649946 |
| Ca      | 30.491255 | 32.214764 | 27.643507 |
| Ca      | 30.625740 | 28.187454 | 24.332783 |
| Ca      | 33.523140 | 29.423569 | 28.530464 |
| Ca      | 34.192070 | 24.831827 | 26.442558 |
| Ca      | 35.688789 | 29.412003 | 24.378666 |
| S       | 22.140079 | 32.090801 | 35.948563 |
| S       | 20.464214 | 35.387917 | 33.010235 |
| S       | 21.833616 | 31.355795 | 29.805618 |
| S       | 24.914797 | 33.769657 | 32.949974 |
| S       | 26.012993 | 29.447090 | 30.853329 |
| S       | 25.423433 | 33.872009 | 28.245619 |
| S       | 28.281519 | 29.715897 | 26.545179 |
|   | 30.486677 | 30.778921 | 30.474274 |
|---|-----------|-----------|-----------|
| S | 31.387800 | 26.926008 | 26.655949 |
| S | 32.967579 | 30.845877 | 27.416138 |
| S | 33.773773 | 30.845877 | 25.483004 |
| S | 36.347466 | 27.416138 | 27.343281 |

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generated by VMD

| Ca  | 19.222746 | 32.115772 | 34.181622 |
|-----|-----------|-----------|-----------|
| Ca  | 23.101946 | 35.496811 | 35.416332 |
| Ca  | 23.405985 | 30.746729 | 32.948109 |
| Ca  | 22.483665 | 34.658241 | 30.354292 |
| Ca  | 24.874315 | 30.350792 | 27.534163 |
| Ca  | 27.590258 | 32.620651 | 31.318977 |
| Ca  | 28.643183 | 27.708334 | 29.915012 |
| Ca  | 30.427450 | 32.434242 | 27.641611 |
| Ca  | 30.585627 | 28.238464 | 24.469202 |
| Ca  | 33.424644 | 29.615145 | 28.313889 |
| Ca  | 34.160126 | 24.864346 | 26.419476 |
| Ca  | 36.066231 | 29.220997 | 24.099142 |
| S   | 22.009665 | 32.016853 | 35.832413 |
| S   | 20.339262 | 35.402317 | 33.061836 |
| S   | 21.885750 | 31.387405 | 29.666981 |
| S   | 24.950981 | 34.017307 | 33.025803 |
| S   | 25.857119 | 29.441824 | 30.832159 |
| S   | 25.674246 | 33.912971 | 28.377716 |
| S   | 28.144249 | 29.637510 | 26.852066 |
| S   | 30.469860 | 30.766207 | 30.509632 |
| S   | 31.389559 | 26.657642 | 27.507158 |
| S   | 33.094559 | 30.786968 | 25.253742 |
| S   | 33.588318 | 26.507195 | 23.161581 |
| S   | 36.330299 | 27.695309 | 27.247164 |

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generated by VMD

| Ca  | 18.734833 | 32.240097 | 34.102898 |
|-----|-----------|-----------|-----------|
| Ca  | 22.646570 | 35.394337 | 35.775375 |
| Ca  | 23.656893 | 30.691200 | 33.016960 |
| Ca  | 22.412346 | 34.425831 | 30.400984 |
| Ca  | 24.979324 | 30.756697 | 27.500195 |
| Ca  | 27.808243 | 32.951252 | 31.311628 |
| Ca  | 28.767384 | 27.835531 | 29.586529 |
| Ca  | 30.712105 | 32.312141 | 27.562687 |
| Ca  | 30.553183 | 28.279423 | 24.446064 |
| Ca  | 33.677311 | 29.440571 | 28.419733 |
| Ca  | 34.156517 | 24.760643 | 26.438412 |
| Ca  | 35.907116 | 28.796808 | 23.863186 |
| S   | 21.666664 | 32.022179 | 35.863289 |
|   | S   |       |       |       |
|---|-----|-------|-------|-------|
|   | S   | 20.053478 | 35.442265 | 33.114010 |
|   | S   | 21.822618 | 31.119602 | 29.774181 |
|   | S   | 24.905077 | 34.015881 | 33.181385 |
|   | S   | 26.261427 | 29.663944 | 30.920883 |
|   | S   | 25.498236 | 33.975014 | 28.448486 |
|   | S   | 28.215742 | 29.686712 | 26.655437 |
|   | S   | 30.790962 | 30.819603 | 30.37566 |
|   | S   | 31.491625 | 26.879116 | 27.534637 |
|   | S   | 33.059166 | 30.789061 | 25.250368 |
|   | S   | 33.513092 | 26.509567 | 23.383549 |
|   | S   | 36.430130 | 27.492611 | 27.015617 |
|24| S   |       |       |       |
|   | S   |       |       |       |
|   |   | 20.053478 | 35.442265 | 33.114010 |
|   |   | 21.822618 | 31.119602 | 29.774181 |
|   |   | 24.905077 | 34.015881 | 33.181385 |
|   |   | 26.261427 | 29.663944 | 30.920883 |
|   |   | 25.498236 | 33.975014 | 28.448486 |
|   |   | 28.215742 | 29.686712 | 26.655437 |
|   |   | 30.790962 | 30.819603 | 30.37566 |
|   |   | 31.491625 | 26.879116 | 27.534637 |
|   |   | 33.059166 | 30.789061 | 25.250368 |
|   |   | 33.513092 | 26.509567 | 23.383549 |
|   |   | 36.430130 | 27.492611 | 27.015617 |

Generated by VMD

|   | Ca  |       |       |       |
|---|-----|-------|-------|-------|
|   | Ca  | 18.881992 | 32.279621 | 34.172424 |
|   | Ca  | 23.101284 | 35.526505 | 35.67066 |
|   | Ca  | 23.748243 | 30.743345 | 33.022442 |
|   | Ca  | 22.316093 | 34.272655 | 30.484512 |
|   | Ca  | 24.997738 | 30.477497 | 27.373316 |
|   | Ca  | 27.664822 | 32.963417 | 31.029303 |
|   | Ca  | 28.610987 | 27.719852 | 29.363651 |
|   | Ca  | 30.549479 | 32.282555 | 27.587490 |
|   | Ca  | 30.750931 | 28.323435 | 24.194935 |
|   | Ca  | 33.422554 | 29.599705 | 28.406012 |
|   | Ca  | 34.005650 | 24.708607 | 26.409075 |
|   | Ca  | 35.850201 | 29.218431 | 24.480991 |
|   | S   | 21.927879 | 32.055656 | 36.026104 |
|   | S   | 20.390297 | 35.368046 | 33.425468 |
|   | S   | 22.143692 | 31.034966 | 29.889315 |
|   | S   | 24.872889 | 34.082806 | 32.980244 |
|   | S   | 26.027409 | 29.601801 | 30.728167 |
|   | S   | 25.363052 | 33.985661 | 28.225079 |
|   | S   | 28.247868 | 29.643436 | 26.477999 |
|   | S   | 30.477097 | 30.755033 | 30.275475 |
|   | S   | 31.419228 | 26.791916 | 27.440659 |
|   | S   | 33.140530 | 30.828264 | 25.539635 |
|   | S   | 33.640270 | 26.571341 | 23.268883 |
|   | S   | 36.169815 | 27.465530 | 27.571768 |

Generated by VMD

|   | Ca  |       |       |       |
|---|-----|-------|-------|-------|
|   | Ca  | 18.699566 | 32.123409 | 34.137375 |
|   | Ca  | 22.908831 | 35.160572 | 35.532185 |
|   | Ca  | 23.481735 | 30.647697 | 32.895184 |
|   | Ca  | 22.545195 | 34.504799 | 30.457346 |
|   | Ca  | 24.975445 | 30.682940 | 27.585896 |
|   | Ca  | 27.729107 | 33.034153 | 31.227507 |
|   | Ca  | 29.001919 | 28.128765 | 29.779854 |
|   | Ca  | Ca  | Ca  |
|---|-----|-----|-----|
|   | 30.847349 | 32.396935 | 27.741833 |
|   | 30.638727 | 28.296663 | 24.222124 |
|   | 33.423161 | 29.612535 | 28.467743 |
|   | 34.022301 | 24.687639 | 26.458233 |
|   | 35.598927 | 28.782703 | 23.95641   |
|   | 21.553579 | 31.762325 | 35.683445 |
|   | 20.288185 | 35.212429 | 33.06704   |
|   | 22.065577 | 30.709944 | 29.752060 |
|   | 24.726395 | 34.141579 | 32.807350 |
|   | 26.372740 | 29.984970 | 31.157969 |
|   | 25.693876 | 34.209347 | 28.513218 |
|   | 28.390923 | 29.784788 | 26.824844 |
|   | 30.889391 | 31.162254 | 30.594097 |
|   | 31.352415 | 26.885162 | 27.643353 |
|   | 33.174995 | 30.780281 | 25.368034 |
|   | 33.192791 | 26.102224 | 23.103153 |
|   | 36.146847 | 27.505976 | 27.024881 |

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generated by VMD

|   | Ca  | Ca  | Ca  |
|---|-----|-----|-----|
|   | 18.532528 | 32.078827 | 34.312099 |
|   | 22.913588 | 35.137222 | 35.493057 |
|   | 23.960144 | 30.506687 | 33.148392 |
|   | 22.416042 | 34.830196 | 30.326048 |
|   | 24.924356 | 30.713747 | 27.683737 |
|   | 27.614832 | 33.054882 | 31.095745 |
|   | 29.100510 | 27.802492 | 29.322887 |
|   | 30.677696 | 32.524635 | 27.799715 |
|   | 30.707737 | 28.270060 | 24.380507 |
|   | 33.481243 | 29.488232 | 28.542614 |
|   | 34.264755 | 24.414810 | 26.506432 |
|   | 35.578175 | 28.865396 | 24.127293 |
|   | 21.667934 | 31.750298 | 35.846497 |
|   | 20.038866 | 35.462250 | 33.152534 |
|   | 22.038863 | 31.329662 | 30.009483 |
|   | 24.981052 | 33.930500 | 32.959045 |
|   | 26.248760 | 29.566765 | 30.578176 |
|   | 25.297977 | 34.264503 | 28.155235 |
|   | 28.403082 | 30.039402 | 26.578960 |
|   | 30.732908 | 31.032127 | 30.45670   |
|   | 31.485676 | 26.721966 | 27.516159 |
|   | 33.017334 | 30.806385 | 25.40781   |
|   | 33.312374 | 26.032652 | 23.448906 |
|   | 36.328568 | 27.676390 | 27.092087 |

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generated by VMD

|   | Ca  | Ca  | Ca  |
|---|-----|-----|-----|
|   | 18.625141 | 32.706001 | 34.186325 |
| Element | Value1  | Value2  | Value3  |
|---------|---------|---------|---------|
| Ca      | 22.788021 | 35.211014 | 35.213326 |
| Ca      | 23.718168 | 30.345387 | 33.144665 |
| Ca      | 22.838271 | 34.338638 | 30.353298 |
| Ca      | 25.167931 | 30.600357 | 27.748360 |
| Ca      | 27.826661 | 32.959866 | 31.407574 |
| Ca      | 29.08177 | 34.73261 | 29.779484 |
| Ca      | 30.64823 | 32.55023 | 27.883572 |
| Ca      | 30.555794 | 28.278730 | 24.189529 |
| Ca      | 33.36021 | 29.725782 | 28.407551 |
| Ca      | 34.069408 | 24.789188 | 26.302210 |
| Ca      | 35.366421 | 29.070219 | 24.134468 |
| S       | 21.40430 | 31.875729 | 35.544556 |
| S       | 20.311483 | 35.552074 | 32.624397 |
| S       | 22.09121 | 30.894695 | 30.040722 |
| S       | 24.826422 | 33.622368 | 33.102680 |
| S       | 26.468781 | 29.613716 | 30.998783 |
| S       | 25.923529 | 33.832268 | 28.575001 |
| S       | 28.38172 | 29.702181 | 26.558262 |
| S       | 30.792692 | 31.068111 | 30.451719 |
| S       | 31.40325 | 26.844137 | 27.427744 |
| S       | 32.595314 | 30.85047 | 25.252171 |
| S       | 33.270763 | 26.286591 | 23.530970 |
| S       | 36.189522 | 27.640635 | 27.082634 |

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Generated by VMD

| Element | Value1  | Value2  | Value3  |
|---------|---------|---------|---------|
| Ca      | 18.516993 | 32.293106 | 33.658813 |
| Ca      | 22.839884 | 35.351521 | 35.426308 |
| Ca      | 23.656729 | 30.391773 | 33.103256 |
| Ca      | 22.797358 | 34.673363 | 30.441679 |
| Ca      | 24.969505 | 30.526760 | 27.856068 |
| Ca      | 27.953922 | 32.835209 | 31.390850 |
| Ca      | 29.095921 | 27.805176 | 29.510456 |
| Ca      | 30.526947 | 32.499500 | 27.752274 |
| Ca      | 30.569012 | 28.072704 | 24.469500 |
| Ca      | 33.496906 | 29.886850 | 28.523968 |
| Ca      | 34.277515 | 24.668228 | 26.381393 |
| Ca      | 35.343052 | 28.985519 | 23.808434 |
| S       | 21.396084 | 31.972195 | 35.546337 |
| S       | 20.235270 | 35.486626 | 32.943939 |
| S       | 22.195505 | 31.195351 | 29.806274 |
| S       | 24.976709 | 33.747078 | 33.202605 |
| S       | 26.398348 | 29.545345 | 31.070431 |
| S       | 25.835371 | 33.914894 | 28.487043 |
| S       | 28.300295 | 29.853729 | 26.627989 |
| S       | 30.816416 | 30.937649 | 30.482666 |
| S       | 31.661724 | 26.670303 | 27.817610 |
|  | 32.630611 | 31.085367 | 25.311741 |
|  | 33.205887 | 26.133583 | 23.441437 |
|  | 36.024075 | 27.768227 | 26.879511 |

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generated by VMD

| Ca  | 18.534550 | 32.700840 | 33.778664 |
| Ca  | 22.624672 | 35.270157 | 35.312023 |
| Ca  | 23.348961 | 30.156525 | 32.940571 |
| Ca  | 22.910997 | 34.762783 | 30.468025 |
| Ca  | 25.051294 | 30.371166 | 27.909973 |
| Ca  | 27.803789 | 32.832596 | 31.477718 |
| Ca  | 29.142384 | 28.098356 | 29.906826 |
| Ca  | 30.799646 | 32.590786 | 27.884813 |
| Ca  | 30.416473 | 27.880953 | 24.730808 |
| Ca  | 33.626389 | 29.759186 | 28.044689 |
| Ca  | 34.329178 | 24.863651 | 26.305748 |
| Ca  | 35.312904 | 29.035015 | 23.800655 |
| S   | 21.249039 | 31.969868 | 35.430126 |
| S   | 20.245701 | 35.598648 | 32.798264 |
| S   | 21.920130 | 31.092251 | 29.865387 |
| S   | 24.899090 | 33.531513 | 33.313461 |
| S   | 26.319710 | 29.562859 | 31.179401 |
| S   | 25.843863 | 33.860603 | 28.553616 |
| S   | 28.356318 | 29.840435 | 26.885012 |
| S   | 31.080248 | 30.974911 | 30.494949 |
| S   | 31.694891 | 26.793262 | 27.641422 |
| S   | 32.705738 | 30.768085 | 25.214031 |
| S   | 33.114643 | 26.164230 | 23.310299 |
| S   | 36.389500 | 27.821411 | 26.693598 |

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generated by VMD

| Ca  | 18.051876 | 32.811329 | 33.452080 |
| Ca  | 22.794418 | 34.866463 | 35.601410 |
| Ca  | 23.241268 | 30.533623 | 33.105125 |
| Ca  | 22.898895 | 34.831379 | 30.503788 |
| Ca  | 24.942093 | 30.377411 | 28.055517 |
| Ca  | 27.981199 | 32.916756 | 31.184307 |
| Ca  | 29.286568 | 27.881371 | 30.098307 |
| Ca  | 30.658550 | 32.384602 | 27.567410 |
| Ca  | 30.280212 | 27.895123 | 24.667231 |
| Ca  | 33.759727 | 29.711525 | 28.150146 |
| Ca  | 34.268463 | 24.831264 | 26.553535 |
| Ca  | 35.380333 | 29.103920 | 23.572664 |
| S   | 20.865339 | 31.723503 | 35.532486 |
| S   | 20.276903 | 35.587940 | 32.991852 |
| S   | 21.976608 | 31.422729 | 29.795898 |
S  24.977339  33.572620  33.224449
S  26.358795  29.591270  28.621986
S  25.898512  33.961945  28.621986
S  28.310476  29.654388  26.947584
S  31.123857  31.084314  30.427570
S  31.867512  26.739355  27.888159
S  32.670616  30.739750  24.941048
S  33.318371  26.176765  23.303064
S  36.532074  27.900661  26.517673

24
generated by VMD
Ca  18.144243  32.758789  33.602173
Ca  22.768444  34.914148  35.381485
Ca  23.558952  30.432291  33.076302
Ca  22.905447  34.647373  30.571280
Ca  24.916370  30.548079  27.886713
Ca  28.051037  32.722340  31.494608
Ca  29.204773  27.838621  29.897839
Ca  30.706566  32.296181  27.674404
Ca  30.357878  27.992685  24.879692
Ca  33.844337  29.917715  28.231611
Ca  34.334373  24.986935  26.424852
Ca  35.384895  28.967419  23.555468
S  21.136921  31.956734  35.401901
S  20.205568  35.692165  32.714844
S  21.955345  31.214415  29.724220
S  25.147312  33.527687  33.390366
S  26.229378  29.613670  31.118958
S  25.923382  33.926937  28.727932
S  28.134781  29.618334  26.819569
S  30.77363  31.089947  30.445866
S  31.920658  26.850527  27.967182
S  32.613876  30.696091  25.194412
S  33.115108  26.185827  23.179939
S  36.383080  27.877838  26.578405

24
generated by VMD
Ca  18.373226  33.105026  33.337849
Ca  22.873627  35.067570  35.485176
Ca  23.275188  30.259398  33.227856
Ca  22.983955  34.379524  30.438168
Ca  25.027559  30.274500  28.018129
Ca  27.900005  32.677872  31.511396
Ca  29.168474  27.915138  30.102436
Ca  30.724483  32.496841  27.554916
Ca  30.310423  27.991917  24.533985
| Element | X1     | Y1     | Z1     |
|---------|--------|--------|--------|
| Ca      | 33.686291 | 30.015862 | 27.958685 |
| Ca      | 34.165836 | 24.859076 | 26.502718 |
| Ca      | 35.428356 | 29.193968 | 23.607572 |
| S       | 20.893456 | 32.064293 | 35.578053 |
| S       | 20.648758 | 35.709679 | 32.596619 |
| S       | 21.936825 | 31.109539 | 29.785915 |
| S       | 24.907618 | 33.470173 | 33.380192 |
| S       | 26.259504 | 29.294632 | 31.246420 |
| S       | 25.959307 | 33.640343 | 28.735172 |
| S       | 28.289591 | 29.844776 | 27.005878 |
| S       | 31.025620 | 30.974663 | 30.489777 |
| S       | 31.676353 | 26.975691 | 27.815437 |
| S       | 32.648537 | 30.742739 | 25.046122 |
| S       | 33.286575 | 26.321003 | 23.239392 |
| S       | 36.270447 | 27.917999 | 26.752733 |

24 generated by VMD

| Element | X2     | Y2     | Z2     |
|---------|--------|--------|--------|
| Ca      | 18.067719 | 32.684555 | 33.354286 |
| Ca      | 22.269299 | 35.103600 | 35.338882 |
| Ca      | 23.555534 | 30.593346 | 33.155460 |
| Ca      | 22.788387 | 34.775631 | 30.764542 |
| Ca      | 25.232475 | 30.461550 | 28.013172 |
| Ca      | 27.852661 | 33.012703 | 31.851151 |
| Ca      | 29.145687 | 27.952959 | 29.972452 |
| Ca      | 30.696383 | 32.388336 | 27.309036 |
| Ca      | 30.444817 | 27.793312 | 24.664066 |
| Ca      | 34.071754 | 29.758911 | 27.636314 |
| Ca      | 34.250084 | 24.770262 | 26.466282 |
| Ca      | 35.639751 | 28.818707 | 23.404800 |
| S       | 20.977310 | 31.783577 | 35.653900 |
| S       | 20.113079 | 35.470085 | 32.718758 |
| S       | 22.018051 | 31.315159 | 29.781317 |
| S       | 24.795738 | 33.634094 | 33.558723 |
| S       | 26.326971 | 29.726562 | 31.332630 |
| S       | 25.930843 | 34.168159 | 29.008083 |
| S       | 28.232800 | 29.713379 | 26.710480 |
| S       | 30.776590 | 31.105677 | 30.440689 |
| S       | 31.885641 | 26.875618 | 27.795258 |
| S       | 32.812031 | 30.643450 | 24.898781 |
| S       | 33.279903 | 26.139471 | 23.287205 |
| S       | 36.556519 | 27.610928 | 26.628441 |

24 generated by VMD

| Element | X3     | Y3     | Z3     |
|---------|--------|--------|--------|
| Ca      | 18.301632 | 33.190460 | 33.563210 |
| Ca      | 22.754707 | 34.982704 | 35.705490 |
| Ca      | 23.444561 | 30.619801 | 32.959183 |
| Element | X-position | Y-position | Z-position |
|---------|------------|------------|------------|
| Ca      | 22.805185  | 34.298752  | 30.713543  |
| Ca      | 24.922045  | 30.440491  | 27.939081  |
| Ca      | 27.844868  | 32.830750  | 31.456688  |
| Ca      | 29.166985  | 27.926477  | 29.965836  |
| Ca      | 30.570110  | 32.466827  | 27.438091  |
| Ca      | 30.425320  | 27.785254  | 24.480305  |
| Ca      | 33.606934  | 29.859768  | 27.786633  |
| Ca      | 34.292114  | 24.887592  | 26.502674  |
| Ca      | 35.754780  | 29.195877  | 23.887733  |
| S       | 21.116726  | 32.062881  | 35.496365  |
| S       | 20.708729  | 35.495564  | 32.859943  |
| S       | 21.827341  | 31.158640  | 29.657125  |
| S       | 24.953087  | 33.71887   | 33.374954  |
| S       | 26.161324  | 29.569832  | 31.359280  |
| S       | 25.781637  | 33.769440  | 28.737894  |
| S       | 28.285900  | 29.714798  | 26.817104  |
| S       | 30.864841  | 31.096640  | 30.156294  |
| S       | 31.647520  | 26.747055  | 27.725744  |
| S       | 32.643044  | 30.715361  | 25.015463  |
| S       | 33.543339  | 26.381903  | 23.323025  |
| S       | 36.297348  | 27.731258  | 27.018438  |

24 generated by VMD

| Element | X-position | Y-position | Z-position |
|---------|------------|------------|------------|
| Ca      | 18.288824  | 32.949417  | 34.073486  |
| Ca      | 22.810532  | 35.113995  | 35.448898  |
| Ca      | 23.375223  | 30.617958  | 33.076775  |
| Ca      | 22.947254  | 34.472195  | 30.539314  |
| Ca      | 24.823547  | 30.592262  | 27.791256  |
| Ca      | 27.946623  | 32.797901  | 31.477844  |
| Ca      | 28.951992  | 27.796856  | 29.763426  |
| Ca      | 30.442684  | 32.341766  | 27.377686  |
| Ca      | 30.397814  | 27.841665  | 24.595905  |
| Ca      | 33.398285  | 29.761932  | 27.983446  |
| Ca      | 34.448204  | 24.920170  | 26.670580  |
| Ca      | 35.657398  | 29.214970  | 23.893551  |
| S       | 21.366745  | 31.728470  | 35.692833  |
| S       | 20.486160  | 35.473228  | 32.678978  |
| S       | 21.845722  | 31.341869  | 29.787142  |
| S       | 25.026514  | 33.529133  | 33.367283  |
| S       | 26.214977  | 29.659142  | 30.962286  |
| S       | 25.815172  | 33.975430  | 28.672239  |
| S       | 28.406357  | 29.647184  | 26.564838  |
| S       | 30.897079  | 30.777605  | 30.300804  |
| S       | 31.624681  | 26.703789  | 27.495098  |
| S       | 32.599022  | 30.737020  | 25.038881  |
| S       | 33.595306  | 26.502110  | 23.502958  |
|    |    |    |    |
|----|----|----|----|
| S  | 36.353897 | 27.803963 | 27.184544 |

24 generated by VMD

| Ca | 18.251503  | 33.094200  | 34.083355  |
|----|------------|------------|------------|
| Ca | 22.897924  | 34.806362  | 35.621502  |
| Ca | 23.407429  | 30.698170  | 33.288048  |
| Ca | 22.938698  | 34.492855  | 30.511778  |
| Ca | 24.902670  | 30.317789  | 27.748615  |
| Ca | 27.939281  | 32.869442  | 31.360565  |
| Ca | 29.092581  | 28.041613  | 29.775076  |
| Ca | 30.354952  | 32.256462  | 27.357227  |

| S  | 21.133953  | 31.712173  | 35.425037  |
|----|------------|------------|------------|
| S  | 20.495409  | 35.523525  | 32.851212  |
| S  | 22.008657  | 31.211720  | 29.749886  |
| S  | 24.977514  | 33.806698  | 33.350338  |
| S  | 26.108273  | 29.653471  | 31.013184  |

24 generated by VMD

| Ca | 18.704340  | 33.599838  | 34.020367  |
|----|------------|------------|------------|
| Ca | 22.730705  | 35.085793  | 35.711552  |
| Ca | 23.407578  | 30.065990  | 33.208961  |
| Ca | 22.768339  | 34.503502  | 30.723185  |
| Ca | 24.807152  | 30.336594  | 27.738535  |
| Ca | 27.592766  | 32.679703  | 31.179350  |
| Ca | 29.086607  | 27.863827  | 29.549673  |
| Ca | 30.216784  | 32.277672  | 27.030628  |
| Ca | 30.458391  | 27.877424  | 24.338051  |
| Ca | 33.516544  | 29.867914  | 28.073105  |
| Ca | 34.556084  | 24.931469  | 26.776848  |
| Ca | 35.886452  | 29.198761  | 24.059193  |
| S | 20.971415  | 31.636307  | 35.308899  |
| S | 20.982727  | 36.180588  | 33.077827  |
| S | 21.990854  | 31.180832  | 30.011707  |
| S | 24.694510  | 33.279613  | 33.580921  |
| S | 26.087770  | 29.453133  | 30.848396  |
S  25.828016  33.735985  28.597929
S  28.185942  29.601879  26.640316
S  30.730810  30.993069  30.278059
S  31.687317  26.911795  27.483633
S  32.725449  30.753757  24.921196
S  33.647308  26.362518  23.432308
S  36.456211  27.922050  27.349419

24
generated by VMD
Ca  18.140339  33.485443  34.513161
Ca  22.533497  34.824852  35.602894
Ca  23.286074  30.623997  32.804207
Ca  22.709829  34.348286  30.552269
Ca  24.953382  30.621847  27.858072
Ca  28.018967  32.949692  31.328609
Ca  29.201702  28.053093  29.988655
Ca  30.387669  32.539406  27.342091
Ca  30.420589  27.755653  24.477608
Ca  33.746590  29.738848  28.001070
Ca  34.456161  24.762287  26.596130
Ca  35.670238  29.101236  23.932415
S  20.879734  31.511694  35.274025
S  20.528513  35.688869  32.974583
S  21.847054  31.110992  29.818211
S  24.800797  33.281391  33.350430
S  26.229164  29.696926  31.074215
S  25.883438  33.951534  28.654879
S  28.210651  29.753204  26.712357
S  31.236813  31.317150  30.186516
S  31.804741  26.831032  27.612175
S  32.657375  30.564980  25.029934
S  33.447044  26.213478  23.248320
S  36.669659  27.574112  27.007206

24
generated by VMD
Ca  18.259811  33.485246  33.816856
Ca  22.500431  34.973042  35.771633
Ca  23.460415  30.499390  32.886311
Ca  22.997433  34.440792  30.672270
Ca  24.877117  30.327703  27.694502
Ca  27.813862  32.729923  31.386097
Ca  29.033936  28.120817  29.869904
Ca  30.459709  32.418850  27.195820
Ca  30.378279  27.740892  24.896271
Ca  33.779236  29.972563  27.878698
Ca  34.467766  24.848114  26.755417
Ca  35.526600  29.327572  23.565834  
S   20.877232  31.607664  35.348827  
S   20.888620  35.802124  32.947876  
S   21.891294  31.297535  29.669973  
S   24.835522  33.207523  33.551968  
S   26.109531  29.515358  31.038620  
S   26.047741  33.660248  28.782885  
S   28.063147  29.760794  26.865753  
S   30.921629  31.139820  30.238209  
S   31.883297  26.904282  27.965260  
S   32.582550  30.477520  24.982727  
S   33.519676  26.275700  23.367245  
S   36.545223  27.782579  26.791096  

24 generated by VMD  
Ca  17.987940  33.594795  34.120026  
Ca  22.357664  34.887844  35.673492  
Ca  23.385941  30.403698  32.930935  
Ca  22.567060  34.206161  30.662277  
Ca  25.093273  30.571133  27.852760  
Ca  27.829268  33.022427  31.572399  
Ca  29.398499  28.167736  30.161713  
Ca  30.595722  32.377327  27.297079  
Ca  30.491566  27.753593  24.686871  
Ca  34.052502  29.836855  27.782553  
Ca  34.371868  24.751522  26.524626  
Ca  35.555626  29.036108  23.481121  
S   20.678572  31.590305  35.121582  
S   20.718990  35.936848  33.095787  
S   22.076847  31.019878  29.671374  
S   24.580936  33.290001  33.389885  
S   26.248995  29.786707  31.144642  
S   25.715443  34.071938  28.722618  
S   28.333647  29.619942  26.903154  
S   30.794649  31.225330  30.567772  
S   32.070942  26.861895  27.835922  
S   32.889420  30.607931  25.045258  
S   33.293663  26.125599  23.232635  
S   36.631004  27.554489  26.463226  

24 generated by VMD  
Ca  18.185802  33.678551  33.645367  
Ca  22.937399  34.397034  35.838772  
Ca  23.503092  30.429668  32.766544  
Ca  22.880327  34.681839  30.758639  
Ca  24.907503  30.421837  27.934849
|   |   |   |   |
|---|---|---|---|
| Ca | 28.015856 | 32.875877 | 31.236462 |
| Ca | 29.170916 | 27.927082 | 29.696243 |
| Ca | 30.255329 | 27.653109 | 24.653191 |
| Ca | 33.556282 | 30.087780 | 27.896242 |
| Ca | 34.646973 | 25.000744 | 27.038700 |
| Ca | 35.411911 | 29.048126 | 23.912983 |
| S  | 20.932903 | 31.468498 | 34.936188 |
| S  | 20.806221 | 35.870735 | 33.401943 |
| S  | 21.858812 | 31.229874 | 29.706787 |
| S  | 25.027012 | 33.171028 | 33.374828 |
| S  | 26.474670 | 29.610229 | 30.958223 |
| S  | 25.733318 | 33.934277 | 28.681641 |
| S  | 28.138462 | 29.727283 | 26.584814 |
| S  | 30.850458 | 31.129337 | 30.237045 |
| S  | 31.739576 | 26.895269 | 27.843693 |
| S  | 32.525837 | 30.537600 | 24.928879 |
| S  | 33.440674 | 26.040335 | 23.583122 |
| S  | 36.430836 | 28.084534 | 27.046509 |
| Ca | 18.034317 | 33.963760 | 33.895737 |
| Ca | 22.613430 | 34.564911 | 35.818867 |
| Ca | 23.460159 | 30.535620 | 32.918114 |
| Ca | 22.799006 | 34.418186 | 30.731094 |
| Ca | 25.009726 | 30.451736 | 28.008301 |
| Ca | 27.741819 | 32.794876 | 31.543917 |
| Ca | 29.163181 | 27.891163 | 29.932541 |
| Ca | 30.498409 | 32.559315 | 27.014885 |
| Ca | 30.489697 | 27.666132 | 24.732853 |
| Ca | 33.655529 | 29.938690 | 27.694809 |
| Ca | 34.766254 | 24.925097 | 26.869648 |
| Ca | 35.448242 | 29.080891 | 23.398045 |
| S  | 20.772509 | 31.725239 | 34.937584 |
| S  | 20.591757 | 35.983154 | 33.055405 |
| S  | 21.922474 | 31.349533 | 29.612490 |
| S  | 24.826740 | 33.013622 | 33.704021 |
| S  | 26.306767 | 29.379940 | 31.055107 |
| S  | 25.921137 | 33.724308 | 28.837593 |
| S  | 28.330832 | 29.721498 | 26.876698 |
| S  | 30.945543 | 31.120945 | 30.260120 |
| S  | 31.909821 | 26.722536 | 27.806396 |
| S  | 32.485840 | 30.601952 | 24.868645 |
| S  | 33.593258 | 26.159678 | 23.525995 |
| S  | 36.433617 | 28.007256 | 26.841160 |
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 17.999954     | 34.309616     | 33.882259     |
| Ca      | 22.603111     | 34.715668     | 36.035900     |
| Ca      | 23.416252     | 30.275751     | 32.914158     |
| Ca      | 22.792728     | 34.140244     | 30.860619     |
| Ca      | 25.136797     | 30.419176     | 27.941952     |
| Ca      | 27.845875     | 32.707359     | 31.525219     |
| Ca      | 29.367542     | 28.117371     | 30.045210     |
| Ca      | 30.295464     | 32.459347     | 27.163465     |
| Ca      | 30.369154     | 27.424301     | 24.676731     |
| Ca      | 33.568062     | 29.922958     | 27.636162     |
| Ca      | 34.688393     | 24.883350     | 26.663471     |
| Ca      | 35.576401     | 29.241997     | 23.589304     |
| S       | 20.613464     | 31.817261     | 34.750145     |
| S       | 20.774521     | 36.077656     | 32.977654     |
| S       | 22.029585     | 31.080009     | 29.585464     |
| S       | 24.756905     | 32.899212     | 33.737518     |
| S       | 26.283272     | 29.573391     | 31.079903     |
| S       | 25.934282     | 33.827240     | 28.874275     |
| S       | 28.169563     | 29.590813     | 26.797729     |
| S       | 30.923218     | 31.264088     | 30.344957     |
| S       | 31.815517     | 26.796356     | 27.837353     |
| S       | 32.387615     | 30.457794     | 24.794796     |
| S       | 33.739754     | 26.239609     | 23.484554     |
| S       | 36.632591     | 28.059532     | 26.741230     |

24

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.266438     | 33.966164     | 34.101307     |
| Ca      | 22.724808     | 34.538750     | 35.792248     |
| Ca      | 23.406818     | 30.435608     | 32.653843     |
| Ca      | 22.638742     | 34.382881     | 30.719379     |
| Ca      | 25.073280     | 30.535519     | 27.742916     |
| Ca      | 27.924257     | 32.569298     | 31.748013     |
| Ca      | 29.344761     | 27.786041     | 30.010910     |
| Ca      | 30.274815     | 32.428566     | 27.278339     |
| Ca      | 30.612085     | 27.550945     | 24.699158     |
| Ca      | 33.572151     | 30.079006     | 27.812523     |
| Ca      | 34.546860     | 24.903412     | 26.903637     |
| Ca      | 35.453098     | 29.280140     | 23.700659     |
| S       | 20.778749     | 31.724899     | 34.831730     |
| S       | 20.817623     | 36.240028     | 33.306374     |
| S       | 21.897352     | 31.288784     | 29.551167     |
| S       | 24.850531     | 33.021706     | 33.444725     |
| S       | 26.356789     | 29.475225     | 30.975761     |
| S       | 25.721798     | 33.792816     | 28.750700     |
| S       | 28.237766     | 29.381968     | 26.801289     |
|     |        |        |        |
|-----|--------|--------|--------|
| S   | 30.781494 | 31.118904 | 30.204819 |
| S   | 31.833273  | 26.858463  | 27.879753  |
| S   | 32.671272  | 30.723621  | 24.670818  |
| S   | 33.631233  | 26.096415  | 23.571014  |
| S   | 36.304153  | 28.120876  | 26.788960  |

24 generated by VMD

|     |        |        |        |
|-----|--------|--------|--------|
| Ca  | 17.883110 | 33.893101 | 34.047741 |
| Ca  | 22.567156  | 34.461128  | 36.059200  |
| Ca  | 23.301701  | 30.672953  | 32.380604  |
| Ca  | 22.712200  | 34.368076  | 30.947418  |
| Ca  | 25.107260  | 30.600191  | 27.665272  |
| Ca  | 27.888149  | 32.872860  | 31.866520  |
| Ca  | 29.227283  | 28.253819  | 29.933506  |
| Ca  | 30.657486  | 32.368645  | 26.821978  |
| Ca  | 30.543804  | 27.438490  | 24.652451  |
| Ca  | 33.926842  | 30.047224  | 27.611177  |
| Ca  | 34.536102  | 24.837780  | 27.041103  |
| Ca  | 35.466702  | 28.988447  | 23.354942  |
| S   | 20.490200  | 31.736973  | 34.810837  |
| S   | 20.542767  | 35.740093  | 33.495895  |
| S   | 21.988205  | 31.197203  | 29.650736  |
| S   | 24.816154  | 33.106243  | 33.734268  |
| S   | 26.238979  | 29.685759  | 31.069023  |
| S   | 25.839008  | 33.881298  | 28.942249  |
| S   | 28.380615  | 29.633291  | 26.594398  |
| S   | 30.760174  | 31.430374  | 30.250723  |
| S   | 31.983118  | 26.957619  | 27.958681  |
| S   | 32.626499  | 30.399666  | 24.838795  |
| S   | 33.641212  | 25.856007  | 23.580441  |
| S   | 36.595337  | 27.872885  | 26.632059  |

24 generated by VMD

|     |        |        |        |
|-----|--------|--------|--------|
| Ca  | 18.159420 | 34.302376 | 34.460976 |
| Ca  | 23.078186  | 34.503654  | 35.771099  |
| Ca  | 23.141113  | 30.368256  | 32.432095  |
| Ca  | 22.556332  | 34.308022  | 30.789024  |
| Ca  | 24.639887  | 30.604227  | 27.552401  |
| Ca  | 27.945255  | 32.533924  | 31.313761  |
| Ca  | 29.171768  | 27.726269  | 29.785341  |
| Ca  | 30.330967  | 32.332706  | 27.300671  |
| Ca  | 30.552904  | 27.767481  | 24.617153  |
| Ca  | 33.847374  | 30.243887  | 27.991346  |
| Ca  | 34.650726  | 24.909779  | 26.750664  |
| Ca  | 35.820282  | 29.074188  | 23.866234  |
| S   | 20.754730  | 31.796543  | 34.988300  |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| S       | 20.744345    | 36.050697    | 33.524788    |
| S       | 21.749868    | 30.961243    | 29.814976    |
| S       | 24.914181    | 33.215790    | 33.442623    |
| S       | 26.059917    | 29.575333    | 30.845135    |
| S       | 25.619341    | 33.781105    | 28.769577    |
| S       | 28.115250    | 29.376045    | 26.662504    |
| S       | 30.938076    | 31.205069    | 30.113188    |
| S       | 31.736792    | 27.090652    | 27.765377    |
| S       | 32.848667    | 30.588697    | 24.986902    |
| S       | 33.709621    | 25.942610    | 23.417709    |
| S       | 36.635086    | 28.041466    | 26.978178    |
| Ca      | 18.292915    | 33.610489    | 34.572914    |
| Ca      | 22.845634    | 34.302078    | 35.701874    |
| Ca      | 23.137259    | 30.195684    | 32.350403    |
| Ca      | 22.670181    | 34.797562    | 30.648556    |
| Ca      | 24.570415    | 30.875992    | 27.721493    |
| Ca      | 27.911394    | 32.822426    | 31.455048    |
| Ca      | 29.048298    | 28.012426    | 29.801767    |
| Ca      | 30.702126    | 32.404785    | 27.307087    |
| Ca      | 30.560623    | 27.712269    | 24.912411    |
| Ca      | 33.928093    | 30.095697    | 27.813305    |
| Ca      | 34.652477    | 25.014063    | 27.053019    |
| Ca      | 35.545013    | 28.644428    | 23.446535    |
| S       | 20.946278    | 31.313618    | 34.819561    |
| S       | 20.744164    | 35.929489    | 33.461952    |
| S       | 21.719519    | 31.152864    | 29.602749    |
| S       | 24.787226    | 33.330776    | 33.230759    |
| S       | 26.076162    | 29.589907    | 30.992290    |
| S       | 25.807667    | 34.046314    | 28.751919    |
| S       | 28.149475    | 29.785110    | 26.680515    |
| S       | 30.899326    | 31.211697    | 30.257790    |
| S       | 31.832779    | 27.036751    | 28.021832    |
| S       | 32.822098    | 30.652756    | 24.802168    |
| S       | 33.310047    | 25.791183    | 23.752447    |
| S       | 36.760864    | 27.971638    | 26.781616    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.074772    | 33.581532    | 34.609158    |
| Ca      | 22.871628    | 34.454983    | 35.646576    |
| Ca      | 23.261742    | 30.219212    | 32.716820    |
| Ca      | 22.600128    | 34.645344    | 30.611366    |
| Ca      | 24.895142    | 30.749680    | 27.630722    |
| Ca      | 27.985861    | 32.690655    | 31.312265    |
| Ca      | 29.222977    | 28.113253    | 29.935951    |
|     | 30.432510 | 32.480583 | 27.357903 |
|-----|-----------|-----------|-----------|
| Ca  | 30.703373 | 27.692890 | 24.695843 |
| Ca  | 33.765579 | 30.094929 | 27.925274 |
| Ca  | 34.385429 | 24.778648 | 26.955345 |
| Ca  | 35.493660 | 28.873466 | 23.529373 |
| S   | 20.915552 | 31.369507 | 34.832577 |
| S   | 20.651260 | 35.921230 | 33.512711 |
| S   | 21.875694 | 31.310226 | 29.694246 |
| S   | 24.756565 | 33.526840 | 33.173347 |
| S   | 26.332314 | 29.525873 | 30.856155 |
| S   | 25.710289 | 33.848061 | 28.586906 |
| S   | 28.280972 | 29.692686 | 26.704651 |
| S   | 30.946266 | 31.312103 | 30.400730 |
| S   | 31.760174 | 26.969564 | 27.757162 |
| S   | 32.764816 | 30.854803 | 25.042347 |
| S   | 33.567089 | 25.822508 | 23.565100 |
| S   | 36.466259 | 27.771484 | 26.887558 |

24

generated by VMD

|     | 18.210203 | 33.156151 | 34.418678 |
| Ca  | 22.628452 | 34.364830 | 35.731529 |
| Ca  | 23.367519 | 30.200897 | 32.379570 |
| Ca  | 22.673544 | 34.383492 | 30.460701 |
| Ca  | 24.991976 | 30.785568 | 27.804911 |
| Ca  | 28.042042 | 33.027523 | 31.201756 |
| Ca  | 29.207119 | 28.288418 | 29.853523 |
| Ca  | 30.484694 | 32.635235 | 27.412605 |
| Ca  | 30.397949 | 28.019653 | 24.872650 |
| Ca  | 33.997765 | 29.903339 | 27.925510 |
| Ca  | 34.284668 | 24.817469 | 26.858282 |
| Ca  | 35.248516 | 28.737345 | 23.79791 |
| S   | 21.045851 | 31.185406 | 35.051346 |
| S   | 20.661808 | 35.793774 | 33.452110 |
| S   | 21.866264 | 31.100864 | 29.585758 |
| S   | 24.856403 | 33.678898 | 33.010071 |
| S   | 26.320824 | 29.916056 | 30.982193 |
| S   | 25.768698 | 34.072056 | 28.515079 |
| S   | 28.328552 | 30.119967 | 26.842184 |
| S   | 31.220848 | 31.127659 | 30.212139 |
| S   | 31.767544 | 26.938444 | 27.936684 |
| S   | 32.717999 | 30.615381 | 25.005510 |
| S   | 33.076538 | 25.790472 | 23.741138 |
| S   | 36.554291 | 27.641136 | 26.906290 |

24

generated by VMD

|     | 17.933998 | 33.449692 | 34.303596 |
|          |                  |                  |                  |
|----------|------------------|------------------|------------------|
| Ca       | 22.652386        | 34.275539        | 35.880108        |
| Ca       | 23.249653        | 30.292870        | 32.901741        |
| Ca       | 22.989727        | 34.675755        | 30.655731        |
| Ca       | 25.015793        | 30.713490        | 27.885490        |
| Ca       | 27.847483        | 32.972588        | 31.264030        |
| Ca       | 29.154922        | 28.077602        | 29.928507        |
| Ca       | 30.510376        | 32.265087        | 27.038330        |
| Ca       | 30.535616        | 27.684811        | 24.611103        |
| Ca       | 33.971798        | 30.022362        | 28.067966        |
| Ca       | 34.301220        | 24.950848        | 26.481606        |
| Ca       | 35.526829        | 28.770260        | 23.873146        |
| S        | 20.679653        | 31.333683        | 35.318329        |
| S        | 20.378941        | 35.662888        | 33.259552        |
| S        | 21.976761        | 31.376406        | 29.760418        |
| S        | 24.714035        | 33.770599        | 33.212669        |
| S        | 26.429134        | 30.016026        | 31.093327        |
| S        | 25.949228        | 34.070320        | 28.398613        |
| S        | 28.315117        | 29.360868        | 26.640762        |
| S        | 30.827375        | 31.313580        | 30.322268        |
| S        | 31.947498        | 27.083624        | 28.029953        |
| S        | 32.800560        | 30.438231        | 25.150459        |
| S        | 33.478447        | 25.905367        | 23.123610        |
| S        | 36.533432        | 27.817642        | 26.738697        |

24 generated by VMD

|          |                  |                  |                  |
|----------|------------------|------------------|------------------|
| Ca       | 18.043915        | 32.973587        | 33.983196        |
| Ca       | 22.882568        | 34.294342        | 35.743156        |
| Ca       | 23.374285        | 30.404848        | 32.902298        |
| Ca       | 22.811726        | 34.967991        | 30.627729        |
| Ca       | 25.014584        | 30.972492        | 28.042328        |
| Ca       | 28.031488        | 32.867550        | 31.450899        |
| Ca       | 29.158207        | 27.826340        | 29.820177        |
| Ca       | 30.472301        | 32.234417        | 27.129650        |
| Ca       | 30.374504        | 27.834276        | 24.436810        |
| Ca       | 33.762253        | 29.971481        | 27.935040        |
| Ca       | 34.491879        | 25.004423        | 26.960154        |
| Ca       | 35.422775        | 28.609415        | 23.999414        |
| S        | 20.902210        | 31.275515        | 35.105293        |
| S        | 20.478376        | 35.668549        | 33.248356        |
| S        | 21.834341        | 31.525013        | 29.751883        |
| S        | 24.887173        | 33.659084        | 33.229591        |
| S        | 26.575317        | 29.874586        | 31.157070        |
| S        | 25.750977        | 34.365665        | 28.556040        |
| S        | 28.124729        | 29.527359        | 26.643299        |
| S        | 30.804020        | 31.074551        | 30.235191        |
| S        | 31.847340        | 26.978523        | 27.662617        |
| S     | 32.610584 | 30.499699 | 24.902296 |
|-------|-----------|-----------|-----------|
| S     | 33.527672 | 25.832157 | 23.497473 |
| S     | 36.536739 | 28.058182 | 26.920139 |

24

generated by VMD

| Ca    | 18.149097 | 33.089897 | 34.167347 |
|-------|-----------|-----------|-----------|
| Ca    | 22.762367 | 34.522972 | 35.769634 |
| Ca    | 23.273035 | 30.145622 | 32.897888 |
| Ca    | 22.714012 | 34.690567 | 30.721104 |
| Ca    | 24.986805 | 31.045704 | 27.813492 |
| Ca    | 27.803719 | 32.945301 | 31.362694 |
| Ca    | 29.031643 | 38.078911 | 29.837231 |
| Ca    | 30.495323 | 32.361752 | 27.096098 |
| Ca    | 30.427872 | 27.646437 | 24.537491 |
| Ca    | 33.863373 | 29.978191 | 27.887962 |
| Ca    | 34.402618 | 24.781578 | 26.905897 |
| Ca    | 35.776600 | 28.852016 | 23.923851 |
| S     | 21.076855 | 31.313486 | 35.279377 |
| S     | 20.467012 | 35.711849 | 33.166073 |
| S     | 21.913546 | 31.315557 | 29.868771 |
| S     | 24.853016 | 33.519947 | 33.153427 |
| S     | 26.384901 | 29.896946 | 31.136654 |
| S     | 25.852745 | 34.254425 | 28.386253 |
| S     | 28.055702 | 29.672045 | 26.731356 |
| S     | 30.879551 | 31.248148 | 30.207041 |
| S     | 31.787577 | 26.995838 | 27.742071 |
| S     | 32.739632 | 30.548367 | 24.937065 |
| S     | 33.442860 | 26.152590 | 23.501698 |
| S     | 36.580231 | 27.531960 | 26.909571 |

24

generated by VMD

| Ca    | 18.281446 | 32.808147 | 33.564621 |
|-------|-----------|-----------|-----------|
| Ca    | 22.694166 | 34.551147 | 35.565510 |
| Ca    | 23.601660 | 30.175831 | 32.797604 |
| Ca    | 22.591827 | 34.711426 | 30.688591 |
| Ca    | 24.960155 | 30.981369 | 28.024118 |
| Ca    | 27.710247 | 33.059063 | 31.731121 |
| Ca    | 29.300728 | 28.329826 | 29.677128 |
| Ca    | 30.544765 | 32.258110 | 27.052214 |
| Ca    | 30.312426 | 27.919662 | 24.631613 |
| Ca    | 34.068317 | 29.791595 | 27.694315 |
| Ca    | 34.386566 | 24.718765 | 26.822977 |
| Ca    | 35.398914 | 28.748650 | 23.791986 |
| S     | 21.123440 | 31.325195 | 35.271141 |
| S     | 20.296457 | 35.868458 | 33.071545 |
| S     | 21.912228 | 31.307964 | 30.025331 |
S  24.656628  33.601070  33.219147
S  26.583656  29.785225  30.902950
S  25.725473  34.333031  28.759966
S  28.190166  29.612854  26.849728
S  31.051943  31.411715  30.539976
S  31.879835  26.889200  27.823019
S  32.713501  30.556934  25.091734
S  33.084286  26.065062  23.568678
S  36.651211  27.489721  26.775047

24 generated by VMD
Ca  18.310888  32.860218  33.963291
Ca  22.632168  34.366611  35.778732
Ca  23.488035  30.193123  32.672421
Ca  22.839542  34.702492  30.382687
Ca  25.260872  31.058580  28.095329
Ca  27.804733  32.898689  31.562447
Ca  29.197306  28.127640  29.773502
Ca  30.624290  32.446075  27.012981
Ca  30.230000  27.712877  24.403870
Ca  33.698853  29.963840  27.976698
Ca  34.587540  25.043266  26.783020
Ca  35.242119  28.554529  23.942202
S  20.966702  31.250633  35.326294
S  20.608204  35.677643  33.170807
S  22.061405  31.449085  29.813766
S  24.783756  33.568485  33.164967
S  26.553457  29.927967  31.041842
S  25.850998  34.308365  28.560135
S  28.285606  29.717113  26.777327
S  30.822601  31.454891  30.204691
S  31.782152  26.867365  27.849524
S  32.457100  30.379629  25.055435
S  33.224251  26.018671  23.410587
S  36.407494  27.752295  27.217474

24 generated by VMD
Ca  18.236416  32.759220  33.843052
Ca  22.754532  34.639908  35.892300
Ca  23.393253  30.250715  32.772621
Ca  22.833019  34.857433  30.740543
Ca  25.064266  31.033615  27.815315
Ca  27.917076  32.868256  31.506519
Ca  28.930273  28.002964  29.597466
Ca  30.504475  32.247643  27.138283
Ca  30.478933  27.788877  24.491692
Ca  33.755775  30.067863  27.817183
Ca  34.375114  24.935623  27.095860
Ca  35.613586  28.577728  23.869089
S   21.101017  31.364861  35.276726
S   20.331535  35.629475  33.354988
S   21.98602   31.486031  29.740156
S   24.845989  33.710518  33.445232
S   26.401066  29.867201  30.880173
S   25.937954  34.226688  28.663582
S   27.999241  29.622108  26.629496
S   30.844845  31.093616  30.219770
S   31.827160  26.943092  27.725857
S   32.615707  30.515781  24.760139
S   33.570335  25.759861  23.631924
S   36.399872  28.050930  27.032055

24
generated by VMD
Ca  18.505180  32.752110  33.855988
Ca  22.804609  34.492596  35.967815
Ca  23.496815  30.442549  32.910210
Ca  22.880779  35.057072  30.608128
Ca  24.978691  30.845911  27.73391
Ca  27.657824  32.935303  31.411716
Ca  29.025648  27.867008  29.540369
Ca  30.201954  32.423168  26.91781
Ca  30.386265  27.615288  24.556076
Ca  33.511093  29.869854  27.845589
Ca  34.775028  24.839272  26.988684
Ca  35.712105  29.001772  24.029087
S   21.108486  31.175571  35.365398
S   20.637821  35.805275  33.423645
S   22.092953  31.512838  29.819231
S   24.869287  33.745155  33.365177
S   26.361446  29.825220  30.935699
S   25.793190  34.238285  28.493500
S   28.089762  29.591999  26.385635
S   30.503185  31.188793  30.099226
S   31.716393  26.751469  27.729717
S   32.631706  30.440598  24.898754
S   33.579136  26.103617  23.754557
S   36.400627  27.779388  27.304623

24
generated by VMD
Ca  18.647041  32.869766  33.668423
Ca  22.728739  34.511345  35.809105
Ca  23.570217  30.122459  33.171299
| Ca  | 22.812834 | 34.643490 | 30.683014 |
|-----|-----------|-----------|-----------|
| Ca  | 25.020678 | 30.738586 | 27.787333 |
| Ca  | 27.897007 | 32.827133 | 31.449139 |
| Ca  | 28.747250 | 32.827133 | 31.449139 |
| Ca  | 30.481205 | 32.687969 | 26.876268 |
| Ca  | 30.522831 | 27.802837 | 24.262638 |
| Ca  | 33.375500 | 30.126589 | 27.816658 |
| Ca  | 34.259399 | 24.763533 | 27.052637 |
| Ca  | 35.735420 | 28.803787 | 24.233786 |
| S   | 21.223713 | 31.521332 | 35.364120 |
| S   | 20.544012 | 35.772953 | 33.241325 |
| S   | 21.981815 | 31.182806 | 29.929499 |
| S   | 24.963062 | 33.437332 | 33.474930 |
| S   | 26.374287 | 29.893244 | 31.078556 |
| S   | 25.815620 | 34.146683 | 28.575966 |
| S   | 28.214396 | 29.932753 | 26.290733 |
| S   | 30.784901 | 31.289869 | 30.151995 |
| S   | 31.486414 | 26.965458 | 27.495424 |
| S   | 32.557388 | 30.523582 | 24.874039 |
| S   | 33.581635 | 25.852606 | 23.613297 |
| S   | 36.394684 | 27.715729 | 27.516102 |

24 generated by VMD

| Ca  | 18.222858 | 33.221195 | 33.409859 |
|-----|-----------|-----------|-----------|
| Ca  | 22.542053 | 34.588947 | 35.981804 |
| Ca  | 23.282187 | 30.277550 | 33.017998 |
| Ca  | 22.926382 | 34.685776 | 30.633245 |
| Ca  | 25.157969 | 30.507641 | 27.888321 |
| Ca  | 27.962715 | 32.899696 | 31.830978 |
| Ca  | 28.962738 | 28.099964 | 29.867966 |
| Ca  | 30.543983 | 32.376305 | 26.749760 |
| Ca  | 30.462292 | 27.635033 | 24.522434 |
| Ca  | 33.749268 | 29.902126 | 27.642393 |
| Ca  | 34.429897 | 25.052814 | 26.947971 |
| Ca  | 35.577652 | 28.969763 | 23.646667 |
| S   | 20.630821 | 31.559582 | 35.310715 |
| S   | 20.560488 | 35.784519 | 33.443851 |
| S   | 22.018017 | 31.322186 | 29.806423 |
| S   | 24.861134 | 33.697258 | 33.541382 |
| S   | 26.285307 | 29.635012 | 31.271915 |
| S   | 25.845833 | 33.958752 | 28.638844 |
| S   | 28.272007 | 29.577732 | 26.493397 |
| S   | 30.839754 | 31.281761 | 30.272979 |
| S   | 31.657455 | 26.925217 | 27.879730 |
| S   | 32.789375 | 30.529060 | 24.831245 |
| S   | 33.466728 | 26.033886 | 23.442360 |
|   | 36.673149 | 27.778311 | 26.867977 |
|---|-----------|-----------|-----------|

generated by VMD

| Ca | 18.472786 | 33.244171 | 33.642635 |
|----|-----------|-----------|-----------|
| Ca | 22.775867 | 34.653576 | 35.861046 |
| Ca | 23.344379 | 30.253387 | 33.054626 |
| Ca | 22.664640 | 34.785461 | 30.693455 |
| Ca | 24.887077 | 30.522898 | 27.786575 |
| Ca | 28.002104 | 32.876648 | 31.557060 |
| Ca | 29.022707 | 28.046616 | 29.642239 |
| Ca | 30.423771 | 32.243572 | 27.200129 |
| Ca | 30.412109 | 27.742352 | 24.434834 |
| Ca | 33.652935 | 29.998665 | 27.950993 |
| Ca | 34.568962 | 24.863613 | 26.576286 |
| Ca | 35.757339 | 29.136097 | 24.011049 |
| S  | 21.092476 | 31.519003 | 35.376053 |
| S  | 20.648775 | 35.901878 | 33.383823 |
| S  | 21.833597 | 31.282063 | 29.767139 |
| S  | 24.851574 | 33.682758 | 33.195606 |
| S  | 26.363338 | 29.697342 | 31.061739 |
| S  | 25.593895 | 33.860023 | 28.421820 |
| S  | 28.088696 | 29.588955 | 26.535259 |
| S  | 30.897253 | 31.030422 | 30.328304 |
| S  | 31.783985 | 26.905020 | 27.832733 |
| S  | 32.623314 | 30.600466 | 24.970688 |
| S  | 33.420021 | 26.101000 | 23.483763 |
| S  | 36.538502 | 27.764059 | 27.172203 |

generated by VMD

| Ca | 18.285761 | 33.163536 | 33.291275 |
|----|-----------|-----------|-----------|
| Ca | 22.724615 | 34.577930 | 35.858231 |
| Ca | 23.364576 | 30.180984 | 33.070072 |
| Ca | 22.838362 | 34.922749 | 30.505432 |
| Ca | 24.924854 | 30.594259 | 28.200035 |
| Ca | 27.775532 | 32.791737 | 31.536196 |
| Ca | 29.126755 | 27.898537 | 29.697369 |
| Ca | 30.527874 | 32.194424 | 27.087105 |
| Ca | 30.277359 | 27.931047 | 24.494183 |
| Ca | 33.942673 | 29.826538 | 27.703533 |
| Ca | 34.627144 | 25.013218 | 26.774904 |
| Ca | 35.603531 | 28.937857 | 23.648230 |
| S  | 20.732189 | 31.589373 | 35.372478 |
| S  | 20.625002 | 35.916229 | 33.250629 |
| S  | 21.955248 | 31.367086 | 29.999508 |
| S  | 24.689457 | 33.573547 | 33.281311 |
| S  | 26.432728 | 29.696102 | 31.232155 |
|  | 25.852022 | 33.900024 | 28.601517 |
|  | 28.154245 | 29.502213 | 26.852680 |
|  | 31.682667 | 27.007637 | 27.771336 |
|  | 32.808510 | 30.616848 | 24.975073 |
|  | 33.385292 | 26.042473 | 23.562389 |
|  | 36.517090 | 27.911123 | 26.815819 |

24

generated by VMD

|  | 18.212637 | 33.278610 | 32.908787 |
|  | 22.568260 | 34.820126 | 35.746815 |
|  | 23.721165 | 30.270166 | 33.04195 |
|  | 22.853237 | 34.661999 | 30.620647 |
|  | 25.035351 | 30.049351 | 28.092548 |
|  | 28.005783 | 32.953457 | 31.760456 |
|  | 29.002165 | 27.969007 | 29.802622 |
|  | 30.437046 | 32.534054 | 27.144875 |
|  | 30.358265 | 27.725746 | 24.511988 |
|  | 33.801865 | 29.755461 | 27.708450 |
|  | 34.292191 | 25.037096 | 26.610815 |
|  | 35.543285 | 29.040131 | 23.745213 |
|  | 20.849918 | 31.676275 | 35.101723 |
|  | 20.634720 | 35.943588 | 33.102528 |
|  | 22.082338 | 31.001553 | 30.157988 |
|  | 25.050617 | 33.595245 | 33.450871 |
|  | 26.462353 | 29.558605 | 31.421309 |
|  | 25.820934 | 33.841465 | 28.771193 |
|  | 28.064831 | 29.719641 | 26.712431 |
|  | 30.730705 | 31.125874 | 30.193695 |
|  | 31.664112 | 26.992508 | 27.554176 |
|  | 32.633945 | 30.632448 | 24.972057 |
|  | 33.484528 | 26.381773 | 23.372721 |
|  | 36.409054 | 27.735857 | 27.171917 |

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generated by VMD

|  | 18.213923 | 33.619057 | 32.893147 |
|  | 22.741533 | 34.750912 | 35.961540 |
|  | 23.79478 | 30.219332 | 33.417156 |
|  | 22.929726 | 34.379108 | 30.767841 |
|  | 25.135900 | 30.147591 | 27.972198 |
|  | 28.026766 | 32.894184 | 31.529055 |
|  | 28.864243 | 27.985001 | 29.789032 |
|  | 30.364182 | 32.406975 | 27.168549 |
|  | 30.703552 | 27.926661 | 24.849598 |
|  | 33.291111 | 29.964611 | 27.714766 |
|  | 34.208961 | 24.927485 | 26.385321 |
|     | Ca   | S     | S     | S     | S     | S     | S     | S     |
|-----|------|-------|-------|-------|-------|-------|-------|-------|
|     | 35.755177 | 29.314068 | 23.943735 |       |       |       |       |       |
|     | 20.591076  | 31.949186  | 35.123413  |       |       |       |       |       |
|     | 20.673233  | 36.123024  | 33.190037  |       |       |       |       |       |
|     | 22.095179  | 30.812754  | 30.274845  |       |       |       |       |       |
|     | 25.124901  | 33.339531  | 33.381145  |       |       |       |       |       |
|     | 26.443802  | 29.499184  | 31.329498  |       |       |       |       |       |
|     | 25.840076  | 33.658463  | 28.608120  |       |       |       |       |       |
|     | 28.085791  | 29.470037  | 26.669903  |       |       |       |       |       |
|     | 30.923445  | 31.039471  | 30.066900  |       |       |       |       |       |
|     | 31.818314  | 27.204256  | 27.904043  |       |       |       |       |       |
|     | 32.636993  | 30.618586  | 24.629925  |       |       |       |       |       |
|     | 33.642639  | 26.287241  | 23.348076  |       |       |       |       |       |
|     | 36.230087  | 27.763407  | 27.022198  |       |       |       |       |       |

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generated by VMD

|     | Ca   | S     | S     | S     | S     | S     | S     | S     |
|-----|------|-------|-------|-------|-------|-------|-------|-------|
|     | 18.407654  | 33.617973  | 33.528416  |       |       |       |       |       |
|     | 22.882671  | 34.753662  | 35.748375  |       |       |       |       |       |
|     | 23.282166  | 30.342857  | 33.079700  |       |       |       |       |       |
|     | 22.683491  | 34.425720  | 30.509262  |       |       |       |       |       |
|     | 25.023262  | 30.195791  | 28.106499  |       |       |       |       |       |
|     | 27.874569  | 32.705933  | 31.248003  |       |       |       |       |       |
|     | 28.801928  | 27.920238  | 29.515766  |       |       |       |       |       |
|     | 30.340233  | 32.491894  | 27.428017  |       |       |       |       |       |
|     | 30.745987  | 28.028715  | 24.821136  |       |       |       |       |       |
|     | 33.506935  | 29.832729  | 27.973722  |       |       |       |       |       |
|     | 34.185635  | 24.804543  | 26.502956  |       |       |       |       |       |
|     | 35.653198  | 29.253633  | 23.771488  |       |       |       |       |       |
|     | 20.945501  | 31.811396  | 35.481869  |       |       |       |       |       |
|     | 20.668470  | 35.947510  | 33.134384  |       |       |       |       |       |
|     | 21.924423  | 30.913801  | 30.216774  |       |       |       |       |       |
|     | 24.907223  | 33.706787  | 33.115364  |       |       |       |       |       |
|     | 26.318943  | 29.364582  | 31.159710  |       |       |       |       |       |
|     | 25.740929  | 33.663975  | 28.631527  |       |       |       |       |       |
|     | 28.096767  | 29.752560  | 26.586102  |       |       |       |       |       |
|     | 30.839233  | 30.846531  | 30.158325  |       |       |       |       |       |
|     | 31.901867  | 27.155010  | 27.897804  |       |       |       |       |       |
|     | 32.893299  | 30.900480  | 24.988802  |       |       |       |       |       |
|     | 33.756119  | 26.211193  | 23.404690  |       |       |       |       |       |
|     | 36.339581  | 27.652502  | 26.931366  |       |       |       |       |       |

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generated by VMD

|     | Ca   | S     | S     | S     | S     | S     | S     | S     |
|-----|------|-------|-------|-------|-------|-------|-------|-------|
|     | 18.569016  | 33.445980  | 33.406799  |       |       |       |       |       |
|     | 23.041359  | 34.788559  | 35.805992  |       |       |       |       |       |
|     | 23.469999  | 30.250147  | 33.265705  |       |       |       |       |       |
|     | 22.716106  | 34.400364  | 30.619881  |       |       |       |       |       |
|     | 24.854939  | 30.282402  | 27.867828  |       |       |       |       |       |
|   | Ca    | S     |
|---|-------|-------|
|   | 27.795002 | 32.876656 | 31.434208 |
|   | 28.850178 | 27.828239 | 29.555325 |
|   | 30.455982 | 32.397129 | 27.245586 |
|   | 30.662228 | 27.970625 | 24.615211 |
|   | 33.453892 | 29.758747 | 27.969393 |
|   | 34.199734 | 24.820721 | 26.612743 |
|   | 35.851891 | 29.265816 | 24.283231 |
| S | 20.905233 | 31.775719 | 35.397186 |
| S | 20.884449 | 35.958252 | 33.219555 |
| S | 21.998501 | 30.730368 | 30.182041 |
| S | 24.920200 | 33.733376 | 33.184879 |
| S | 26.360405 | 29.589169 | 31.050339 |
| S | 25.581785 | 33.788162 | 28.458450 |
| S | 28.051624 | 29.792179 | 26.608147 |
| S | 30.695583 | 30.889441 | 30.033699 |
| S | 31.755234 | 27.100796 | 27.823971 |
| S | 32.564663 | 30.760916 | 24.860449 |
| S | 33.764229 | 26.443779 | 23.328234 |
| S | 36.317795 | 27.652533 | 27.112114 |

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generated by VMD

|   | Ca    | S     |
|---|-------|-------|
|   | 18.625076 | 33.679779 | 33.437222 |
|   | 23.066713 | 34.704609 | 35.766457 |
|   | 23.443642 | 30.161308 | 33.223045 |
|   | 22.791773 | 34.180153 | 30.562269 |
|   | 24.992672 | 30.186131 | 27.982357 |
|   | 27.893595 | 32.776070 | 31.324669 |
|   | 28.621262 | 28.041882 | 29.651810 |
|   | 30.275805 | 32.552559 | 27.313759 |
|   | 30.728739 | 28.088039 | 24.534729 |
|   | 33.296616 | 29.800388 | 28.030039 |
|   | 34.213516 | 24.738459 | 26.448689 |
|   | 35.727127 | 29.161236 | 24.506886 |
| S | 20.991373 | 31.831347 | 35.517784 |
| S | 21.028811 | 35.967743 | 32.921310 |
| S | 22.006725 | 30.558720 | 30.250463 |
| S | 24.991381 | 33.542805 | 33.165886 |
| S | 26.296047 | 29.379265 | 31.086899 |
| S | 25.878403 | 33.704876 | 28.489655 |
| S | 28.205101 | 29.912146 | 26.348665 |
| S | 30.541100 | 31.082306 | 30.020798 |
| S | 31.800854 | 27.117008 | 27.872654 |
| S | 32.595959 | 30.970325 | 24.935734 |
| S | 33.601719 | 26.370756 | 23.410313 |
| S | 36.106010 | 27.792107 | 27.137955 |
| Element | X (Å)   | Y (Å)   | Z (Å)   |
|---------|---------|---------|---------|
| Ca      | 18.30184| 33.62595| 33.63267|
| Ca      | 22.84705| 34.70335| 35.69237|
| Ca      | 23.43013| 30.17933| 33.10010|
| Ca      | 22.65505| 34.45142| 30.54278|
| Ca      | 24.98488| 30.09541| 28.00620|
| Ca      | 28.05680| 32.82658| 31.25270|
| Ca      | 28.84226| 27.86477| 29.64937|
| Ca      | 30.43613| 32.43185| 27.47394|
| Ca      | 30.69262| 27.98837| 24.76398|
| Ca      | 33.51128| 29.76693| 27.96756|
| Ca      | 34.31786| 24.84873| 26.62395|
| Ca      | 35.52719| 29.30782| 23.89129|
| S       | 20.73282| 31.70428| 35.14110|
| S       | 20.92336| 36.05846| 33.22401|
| S       | 22.03364| 31.03699| 29.94738|
| S       | 24.84296| 33.59454| 33.14139|
| S       | 26.53275| 29.46384| 31.37943|
| S       | 25.68865| 33.59137| 28.53239|
| S       | 28.25342| 29.74153| 26.68694|
| S       | 30.82222| 30.91819| 30.08605|
| S       | 31.83757| 27.15829| 27.98358|
| S       | 32.64796| 30.98736| 25.04631|
| S       | 33.40131| 26.22916| 23.42358|
| S       | 36.40051| 27.72539| 26.75093|

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| Element | X (Å)   | Y (Å)   | Z (Å)   |
|---------|---------|---------|---------|
| Ca      | 18.05436| 33.52679| 33.64204|
| Ca      | 23.00851| 34.96489| 35.58847|
| Ca      | 23.59969| 30.42921| 33.27153|
| Ca      | 22.89100| 34.58276| 30.54851|
| Ca      | 24.93887| 29.96527| 27.98367|
| Ca      | 27.97549| 32.72622| 31.34004|
| Ca      | 28.80688| 27.75348| 29.53445|
| Ca      | 30.42906| 32.46897| 27.33496|
| Ca      | 30.50960| 28.16213| 24.73539|
| Ca      | 33.49408| 29.74660| 28.10023|
| Ca      | 34.09201| 24.79971| 26.38143|
| Ca      | 35.90328| 29.29531| 24.20183|
| S       | 20.96131| 31.87651| 35.06172|
| S       | 20.63221| 35.94717| 33.26818|
| S       | 22.10063| 30.73784| 30.10204|
| S       | 24.97242| 33.65677| 33.25255|
| S       | 26.44727| 29.34154| 31.28134|
| S       | 25.71292| 33.54716| 28.60862|
| S       | 28.10207| 29.58980| 26.64747|
|  |  |  |  |
|---|---|---|---|
| S  | 30.744198 | 30.989235 | 30.160748 |
| S  | 31.670670 | 27.037731 | 27.755966 |
| S  | 32.621811 | 30.965889 | 24.780836 |
| S  | 33.764019 | 26.407650 | 23.360708 |
| S  | 36.287621 | 27.781349 | 26.996954 |

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generated by VMD

| Ca  | 18.304840 | 33.441948 | 33.478413 |
| Ca  | 22.982878 | 35.029247 | 35.586102 |
| Ca  | 23.563206 | 30.175980 | 33.260094 |
| Ca  | 22.694090 | 34.440155 | 30.478523 |
| Ca  | 25.120760 | 29.882544 | 27.952503 |
| Ca  | 27.765413 | 32.720123 | 31.470779 |
| Ca  | 29.055653 | 27.963181 | 29.917843 |
| Ca  | 30.455334 | 32.374794 | 27.407074 |
| Ca  | 30.735847 | 28.193813 | 24.753132 |
| Ca  | 33.602570 | 29.822071 | 28.049747 |
| Ca  | 33.726334 | 24.729202 | 26.415649 |
| Ca  | 35.659096 | 29.291943 | 23.950546 |
| S  | 21.071112 | 31.828766 | 35.215996 |
| S  | 20.680838 | 36.055050 | 33.000885 |
| S  | 22.025871 | 30.875404 | 30.036987 |
| S  | 24.811253 | 33.527924 | 33.297874 |
| S  | 26.371922 | 29.458807 | 31.370285 |
| S  | 25.697224 | 33.438656 | 28.414181 |
| S  | 28.164133 | 29.902401 | 26.757481 |
| S  | 30.965797 | 30.854897 | 30.242535 |
| S  | 31.807789 | 27.171833 | 27.942034 |
| S  | 32.627884 | 31.154133 | 24.841038 |
| S  | 33.642433 | 26.473671 | 23.172134 |
| S  | 36.187744 | 27.493559 | 26.928188 |

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generated by VMD

| Ca  | 18.238230 | 33.405708 | 33.896904 |
| Ca  | 23.028635 | 34.945198 | 35.642559 |
| Ca  | 23.258934 | 30.335024 | 33.207024 |
| Ca  | 22.833128 | 34.638584 | 30.353016 |
| Ca  | 24.805180 | 30.163542 | 28.020638 |
| Ca  | 27.948477 | 32.775925 | 31.127041 |
| Ca  | 28.926392 | 27.751316 | 29.751467 |
| Ca  | 30.429529 | 32.384911 | 27.515564 |
| Ca  | 30.732559 | 28.060249 | 24.779877 |
| Ca  | 33.467327 | 29.648449 | 28.039093 |
| Ca  | 34.283539 | 24.788403 | 26.340761 |
| Ca  | 35.802231 | 29.569464 | 24.074650 |
| S  | 21.029686 | 31.901449 | 35.522205 |
S        20.746326       35.970879       33.032051
S        21.825897       30.964773       30.007896
S        24.874233       33.557037       33.069824
S        26.282131       29.441462       31.298166
S        25.626476       33.521137       28.305428
S        28.202850       29.682610       26.739956
S        30.768047       30.811047       30.236382
S        31.817570       26.987278       27.890518
S        32.674858       30.833527       24.997370
S        33.704483       26.582952       23.199539
S        36.413300       27.579090       26.892101

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generated by VMD

Ca       18.412838       33.567661       34.126869
Ca       23.238281       34.726059       35.732822
Ca       23.418919       34.480134       32.925220
Ca       22.576672       34.349070       30.527046
Ca       24.875107       30.160217       27.849556
Ca       27.862684       32.826115       31.073711
Ca       28.879230       27.905565       29.608883
Ca       30.331724       32.391502       27.515968
Ca       30.652769       28.036427       24.715466
Ca       33.576637       29.630075       28.185030
Ca       34.229691       24.687485       26.486345
Ca       35.741886       29.465406       24.169636
S        21.239086       31.699541       35.218803
S        21.051830       36.002251       33.410572
S        21.759705       30.866817       29.859131
S        24.847479       33.751358       32.699551
S        26.379303       29.588810       31.156441
S        25.371582       33.497002       28.264742
S        28.112988       29.666571       26.545498
S        30.663500       30.849100       30.233450
S        31.817688       27.011190       27.723129
S        32.735569       30.928692       25.316578
S        33.676537       26.616375       23.453079
S        36.268314       27.628923       27.142511

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generated by VMD

Ca       18.436382       33.433998       34.172215
Ca       23.267687       34.716690       35.828777
Ca       23.442207       30.434719       32.728386
Ca       22.442852       34.430218       30.601799
Ca       24.827297       30.333174       27.769058
Ca       27.658831       32.914349       30.932858
Ca       28.845356       27.908194       29.598482
|   |   |   |
|---|---|---|
| Ca | 30.199018 | 32.382675 | 27.491440 |
| Ca | 30.701740 | 27.962431 | 24.527300 |
| Ca | 33.415043 | 29.599491 | 28.234665 |
| Ca | 34.243969 | 24.588333 | 26.686510 |
| Ca | 35.808029 | 29.299797 | 24.335190 |
| S  | 21.246891 | 31.601786 | 35.216942 |
| S  | 20.889784 | 35.809734 | 33.66192 |
| S  | 21.963223 | 30.990377 | 29.843609 |
| S  | 24.926090 | 33.762104 | 32.833790 |
| S  | 26.530750 | 29.815332 | 31.058662 |
| S  | 25.353025 | 33.698730 | 28.307804 |
| S  | 28.085335 | 29.639660 | 26.53243 |
| S  | 30.754160 | 31.037533 | 30.226109 |
| S  | 31.681923 | 27.057489 | 27.682997 |
| S  | 32.764725 | 30.796003 | 25.036797 |
| S  | 33.869202 | 26.520264 | 23.415607 |
| S  | 36.366524 | 27.566956 | 27.213648 |

24 generated by VMD

| Ca | 18.493105 | 33.437153 | 33.907879 |
| Ca | 23.056570 | 34.699387 | 35.934509 |
| Ca | 23.618427 | 30.216917 | 33.081310 |
| Ca | 22.581448 | 34.691223 | 30.467226 |
| Ca | 24.785515 | 30.393070 | 27.862545 |
| Ca | 27.670708 | 32.774311 | 31.136663 |
| Ca | 28.840828 | 27.893751 | 29.491333 |
| Ca | 30.600515 | 32.387386 | 27.249878 |
| Ca | 30.637285 | 28.113510 | 24.528091 |
| Ca | 33.576344 | 29.855526 | 28.345701 |
| Ca | 34.083790 | 24.812557 | 26.752214 |
| Ca | 35.758076 | 29.018219 | 24.079510 |
| S  | 21.050425 | 31.497692 | 35.358120 |
| S  | 20.819750 | 35.877029 | 33.444069 |
| S  | 21.872700 | 30.867432 | 29.979992 |
| S  | 24.924669 | 33.752193 | 33.036041 |
| S  | 26.518238 | 29.509182 | 31.133177 |
| S  | 25.410801 | 33.818657 | 28.197895 |
| S  | 28.273214 | 29.747684 | 26.516243 |
| S  | 30.624334 | 30.960424 | 30.081860 |
| S  | 31.701183 | 27.204527 | 27.77719 |
| S  | 32.866425 | 30.868217 | 24.955561 |
| S  | 33.685986 | 26.333660 | 23.414104 |
| S  | 36.269745 | 27.570381 | 27.208416 |

24 generated by VMD

| Ca | 18.306362 | 33.032669 | 33.800282 |
|   | Ca       | 22.930542   | 34.406441   | 36.073296   |
|---|----------|-------------|-------------|-------------|
|   | Ca       | 23.329773   | 30.366825   | 32.772881   |
|   | Ca       | 22.839794   | 34.772343   | 30.632454   |
|   | Ca       | 24.966042   | 30.458519   | 28.017769   |
|   | Ca       | 27.950119   | 32.936932   | 31.060469   |
|   | Ca       | 28.900721   | 31.13798    | 29.635015   |
|   | Ca       | 30.584614   | 32.703808   | 26.923927   |
|   | Ca       | 30.646431   | 30.016891   | 24.854347   |
|   | Ca       | 33.594418   | 29.746208   | 27.800385   |
|   | Ca       | 33.934013   | 24.608486   | 26.561234   |
|   | Ca       | 35.871120   | 28.912693   | 24.335941   |
|   | S        | 20.945818   | 31.422142   | 35.338493   |
|   | S        | 20.549809   | 35.764000   | 33.569435   |
|   | S        | 21.825787   | 31.215042   | 30.062191   |
|   | S        | 24.864601   | 33.668312   | 33.117966   |
|   | S        | 26.509602   | 29.806568   | 31.108606   |
|   | S        | 25.383022   | 33.936863   | 28.320036   |
|   | S        | 28.171272   | 29.746105   | 26.505161   |
|   | S        | 30.850990   | 31.205320   | 29.794828   |
|   | S        | 31.876020   | 27.169512   | 28.027210   |
|   | S        | 32.667011   | 30.753540   | 24.725504   |
|   | S        | 33.727497   | 26.162037   | 23.775099   |
|   | S        | 36.494678   | 27.375057   | 27.127529   |

24 generated by VMD

|   | Ca       | 18.111874   | 33.240791   | 33.547047   |
|---|----------|-------------|-------------|-------------|
|   | Ca       | 22.756502   | 34.517540   | 36.005676   |
|   | Ca       | 23.645302   | 30.417950   | 33.010799   |
|   | Ca       | 22.612156   | 34.381065   | 30.724792   |
|   | Ca       | 24.979111   | 30.412865   | 27.821585   |
|   | Ca       | 27.862839   | 33.232075   | 31.571941   |
|   | Ca       | 29.108145   | 28.197021   | 29.816706   |
|   | Ca       | 30.745472   | 32.432980   | 27.138887   |
|   | Ca       | 30.739473   | 27.813772   | 24.682003   |
|   | Ca       | 33.403542   | 29.748060   | 27.755630   |
|   | Ca       | 34.027081   | 24.477039   | 26.654556   |
|   | Ca       | 35.713432   | 29.037451   | 23.971443   |
|   | S        | 20.793293   | 31.554932   | 35.201397   |
|   | S        | 20.503225   | 35.936024   | 33.489178   |
|   | S        | 21.834890   | 30.945850   | 29.976093   |
|   | S        | 24.713974   | 33.789528   | 33.105179   |
|   | S        | 26.523594   | 29.877621   | 31.192781   |
|   | S        | 25.659008   | 33.802250   | 28.543451   |
|   | S        | 28.495457   | 29.732424   | 26.573704   |
|   | S        | 30.937317   | 31.194393   | 30.395756   |
|   | S        | 31.929634   | 27.104549   | 27.917974   |
S  32.749470  30.732254  24.612915
S  33.638542  26.201836  23.456133
S  36.236683  27.519783  26.774460

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| Ca   | 18.416044 | 33.234596 | 33.707279 |
| Ca   | 22.786999 | 34.822586 | 35.776669 |
| Ca   | 23.447346 | 30.186720 | 33.085693 |
| Ca   | 22.871021 | 34.876987 | 30.448397 |
| Ca   | 24.969162 | 30.435234 | 27.669828 |
| Ca   | 27.717010 | 32.797836 | 31.399879 |
| Ca   | 29.001356 | 27.835632 | 29.804138 |
| Ca   | 30.306143 | 32.366051 | 27.368000 |
| Ca   | 30.658424 | 27.760403 | 24.930765 |
| Ca   | 33.523674 | 29.699827 | 27.967388 |
| Ca   | 34.352268 | 24.648609 | 26.595839 |
| Ca   | 35.440315 | 29.468136 | 23.883408 |
| S    | 20.886551 | 31.657135 | 35.539330 |
| S    | 20.623993 | 36.080906 | 33.289108 |
| S    | 22.147324 | 31.252554 | 29.890600 |
| S    | 24.807898 | 33.579845 | 33.258385 |
| S    | 26.278145 | 29.482496 | 30.905300 |
| S    | 25.788265 | 33.814190 | 28.433390 |
| S    | 28.028023 | 29.548992 | 26.654659 |
| S    | 30.796837 | 30.863802 | 30.216503 |
| S    | 32.038853 | 26.991915 | 28.114775 |
| S    | 32.536343 | 30.795370 | 24.842573 |
| S    | 33.856750 | 26.266050 | 23.455433 |
| S    | 36.441307 | 27.834202 | 26.702694 |

24

| Ca   | 18.322126 | 33.404163 | 33.563999 |
| Ca   | 22.812487 | 34.772354 | 35.878162 |
| Ca   | 23.253654 | 30.291035 | 32.923779 |
| Ca   | 22.812742 | 34.328918 | 30.809164 |
| Ca   | 25.039974 | 30.417709 | 27.888672 |
| Ca   | 27.845154 | 32.895504 | 31.352196 |
| Ca   | 28.988235 | 27.709339 | 29.831526 |
| Ca   | 30.292835 | 32.255264 | 27.273090 |
| Ca   | 30.705704 | 27.725533 | 24.978222 |
| Ca   | 33.615395 | 29.788235 | 28.057470 |
| Ca   | 34.437305 | 24.856630 | 26.359747 |
| Ca   | 35.579765 | 29.139885 | 23.775793 |
| S    | 20.694637 | 31.791006 | 28.114775 |
| S    | 20.563594 | 36.022541 | 33.245478 |
| S    | 21.890682 | 31.023281 | 29.792179 |
| El | x1     | y1     | z1     |
|----|--------|--------|--------|
| S  | 24.707170 | 33.738537 | 33.129269 |
| S  | 26.420761 | 29.716143 | 31.194174 |
| S  | 25.772346 | 34.079521 | 28.632233 |
| S  | 28.289085 | 29.516350 | 26.857487 |
| S  | 30.868891 | 30.929909 | 30.098274 |
| S  | 32.122787 | 27.068874 | 28.028839 |
| S  | 32.619621 | 30.823915 | 24.945702 |
| S  | 33.484798 | 26.183533 | 23.230120 |
| S  | 36.460278 | 27.822384 | 26.735659 |

24 generated by VMD

| El | x2     | y2     | z2     |
|----|--------|--------|--------|
| Ca | 18.185184 | 33.222260 | 33.674740 |
| Ca | 22.754028 | 34.630020 | 35.780655 |
| Ca | 23.335258 | 30.276060 | 32.931278 |
| Ca | 22.750977 | 34.624947 | 30.742216 |
| Ca | 25.192682 | 30.487608 | 28.021673 |
| Ca | 27.853624 | 32.903774 | 31.445320 |
| Ca | 29.177761 | 27.856722 | 30.110910 |
| Ca | 30.384069 | 32.325859 | 27.241898 |
| Ca | 30.562073 | 27.889305 | 24.594978 |
| Ca | 33.633076 | 29.883625 | 27.838345 |
| Ca | 34.480396 | 24.639883 | 26.582424 |
| Ca | 35.583157 | 29.033146 | 23.981033 |
| S  | 20.751827 | 31.572979 | 35.175846 |
| S  | 20.578045 | 35.951214 | 33.288818 |
| S  | 21.863108 | 31.162764 | 29.736637 |
| S  | 24.753830 | 33.855656 | 33.228996 |
| S  | 26.495001 | 29.862154 | 31.213835 |
| S  | 25.789608 | 34.022488 | 28.867661 |
| S  | 28.037626 | 29.487350 | 26.618540 |
| S  | 30.897667 | 31.041407 | 30.067247 |
| S  | 31.990913 | 26.989441 | 27.796783 |
| S  | 32.594669 | 30.813829 | 24.805174 |
| S  | 33.553562 | 26.110895 | 23.402346 |
| S  | 36.521912 | 27.656715 | 26.792719 |

24 generated by VMD

| El | x3     | y3     | z3     |
|----|--------|--------|--------|
| Ca | 18.386524 | 33.260567 | 33.424191 |
| Ca | 23.016151 | 34.341618 | 36.063602 |
| Ca | 23.589573 | 30.490137 | 32.915894 |
| Ca | 22.719542 | 34.577873 | 30.769274 |
| Ca | 25.000881 | 30.719973 | 27.791237 |
| Ca | 27.776077 | 32.919029 | 31.120686 |
| Ca | 29.094357 | 27.880241 | 29.564484 |
| Ca | 30.371101 | 32.543751 | 27.110096 |
| Ca | 30.414452 | 27.863255 | 24.661995 |
| Element | X    | Y    | Z    |
|---------|------|------|------|
| Ca      | 33.612404 | 29.907749 | 28.146324 |
| Ca      | 34.340122  | 24.691923  | 26.758633  |
| Ca      | 35.687172  | 29.022640  | 24.037209  |
| S       | 20.955528  | 31.446583  | 35.320889  |
| S       | 20.805294  | 35.688919  | 33.596519  |
| S       | 21.982765  | 31.010750  | 30.068258  |
| S       | 24.684380  | 33.829281  | 32.998405  |
| S       | 26.403233  | 29.937513  | 31.000860  |
| S       | 25.595198  | 34.043438  | 28.416492  |
| S       | 28.076542  | 29.569864  | 26.585682  |
| S       | 30.742107  | 31.234943  | 30.084381  |
| S       | 31.810743  | 26.957581  | 27.914982  |
| S       | 32.768230  | 30.522800  | 24.940269  |
| S       | 33.427921  | 26.089563  | 23.490711  |
| S       | 36.459721  | 27.750046  | 27.158966  |

24

generated by VMD

| Element | X    | Y    | Z    |
|---------|------|------|------|
| Ca      | 18.368095 | 33.374260 | 33.479034 |
| Ca      | 23.060528  | 34.713776  | 35.908211  |
| Ca      | 24.428978  | 30.404524  | 32.946911  |
| Ca      | 22.773087  | 34.503067  | 30.683979  |
| Ca      | 25.087193  | 30.686977  | 27.958088  |
| Ca      | 27.811960  | 32.778824  | 31.454643  |
| Ca      | 28.947868  | 27.808338  | 29.667862  |
| Ca      | 30.163233  | 32.159813  | 27.436979  |
| Ca      | 30.531025  | 27.700464  | 24.97349  |
| Ca      | 33.571594  | 30.097786  | 28.112022  |
| Ca      | 34.444225  | 24.857922  | 26.537178  |
| Ca      | 35.678062  | 29.109104  | 24.041342  |
| S       | 21.007526  | 31.708488  | 35.375645  |
| S       | 20.587120  | 35.965031  | 33.268227  |
| S       | 21.988331  | 30.967030  | 29.974602  |
| S       | 24.799961  | 33.730355  | 33.016697  |
| S       | 26.393887  | 29.703213  | 31.174122  |
| S       | 25.788761  | 33.894291  | 28.561531  |
| S       | 28.324503  | 29.242046  | 26.608059  |
| S       | 30.648653  | 31.056311  | 30.181763  |
| S       | 31.844767  | 26.894056  | 27.802238  |
| S       | 32.509789  | 30.748796  | 25.002785  |
| S       | 33.667416  | 26.433092  | 23.229702  |
| S       | 36.293415  | 27.759808  | 27.021080  |

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generated by VMD

| Element | X    | Y    | Z    |
|---------|------|------|------|
| Ca      | 18.204367 | 32.720531 | 33.388065 |
| Ca      | 22.799046  | 34.630451  | 36.021473  |
| Ca      | 23.474510  | 30.631039  | 32.916870  |
|   |   |   |
|---|---|---|
| Ca | 22.827686 | 34.721546 | 30.799847 |
| Ca | 25.063519 | 30.679882 | 27.813375 |
| Ca | 27.912216 | 32.256310 | 26.831352 |
| Ca | 29.018063 | 28.153566 | 29.712173 |
| Ca | 30.319588 | 32.256310 | 26.831352 |
| Ca | 30.657682 | 27.714470 | 24.451355 |
| Ca | 33.580765 | 29.940617 | 28.003872 |
| Ca | 34.190346 | 24.836714 | 26.617947 |
| Ca | 35.723969 | 28.947224 | 24.152542 |
| S  | 20.908232 | 31.498207 | 35.547676 |
| S  | 20.413792 | 35.644615 | 33.365417 |
| S  | 22.075609 | 31.172226 | 30.122267 |
| S  | 24.877319 | 33.916004 | 33.287582 |
| S  | 26.569347 | 29.96184 | 31.020908 |
| S  | 25.723566 | 34.152363 | 28.702202 |
| S  | 28.165911 | 29.384995 | 26.574163 |
| S  | 30.781216 | 31.173885 | 30.017221 |
| S  | 31.799232 | 26.897011 | 27.796911 |
| S  | 32.778030 | 30.549488 | 24.944492 |
| S  | 33.559311 | 26.149534 | 23.23795 |
| S  | 36.296738 | 27.572605 | 27.278652 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.486629 | 32.273941 | 33.734264 |
| Ca | 22.808626 | 34.737820 | 35.909611 |
| Ca | 23.627207 | 30.547218 | 32.982323 |
| Ca | 22.672386 | 34.824112 | 30.32510 |
| Ca | 25.110886 | 30.859404 | 27.809158 |
| Ca | 27.613197 | 33.084721 | 31.446880 |
| Ca | 29.206810 | 28.027866 | 29.678073 |
| Ca | 30.586107 | 32.534504 | 27.27986 |
| Ca | 30.316337 | 27.905060 | 24.389904 |
| Ca | 33.631893 | 29.911192 | 27.914989 |
| Ca | 34.129364 | 24.547203 | 26.779524 |
| Ca | 35.539738 | 28.807398 | 24.210674 |
| S  | 21.310593 | 31.587540 | 35.603325 |
| S  | 20.412842 | 35.147152 | 33.249538 |
| S  | 22.121456 | 31.166981 | 29.722122 |
| S  | 24.842045 | 33.936195 | 32.967636 |
| S  | 26.226078 | 29.742895 | 31.019306 |
| S  | 25.838463 | 34.453442 | 28.734219 |
| S  | 28.321632 | 29.902554 | 26.705112 |
| S  | 30.786659 | 31.460609 | 30.287352 |
| S  | 31.782597 | 27.016722 | 27.514954 |
| S  | 32.642345 | 30.588989 | 25.089516 |
| S  | 33.493279 | 25.935888 | 23.449064 |
S     36.212349  27.300617  27.143488

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generated by VMD

Ca  18.673199  32.309517  33.725525
Ca  22.886452  34.610794  35.974251
Ca  23.658556  30.981775  32.865349
Ca  22.808281  34.651897  30.779520
Ca  24.915056  30.598660  27.671841
Ca  27.892302  33.068123  31.157578
Ca  29.036381  28.197472  29.783085
Ca  30.380474  32.379665  27.352104
Ca  30.535173  27.946077  24.424519
Ca  33.461582  29.851749  27.977016
Ca  34.010784  24.578747  26.831945
Ca  35.750286  28.983463  24.201134
S   21.302977  31.562124  35.330444
S   20.414398  35.249577  33.391396
S   22.034578  31.243193  29.643772
S   24.787497  33.954853  33.001381
S   26.288301  29.854544  30.872616
S   25.863693  34.188107  28.557325
S   28.149391  29.635950  26.803921
S   30.964449  31.208214  30.171654
S   31.577682  27.004498  27.838886
S   32.498962  30.693499  24.906815
S   33.571335  26.163963  23.466032
S   36.258236  27.383591  27.206364

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generated by VMD

Ca  18.342361  32.478115  33.755638
Ca  22.857399  34.506512  35.689720
Ca  23.750875  30.753590  32.873520
Ca  22.907845  34.727676  30.775574
Ca  24.859673  30.827494  27.815449
Ca  27.930080  33.015133  31.247765
Ca  29.173584  28.113239  29.668633
Ca  30.363632  32.373150  27.281763
Ca  30.313923  27.839764  24.574047
Ca  33.619659  29.857319  28.020275
Ca  34.327538  24.678356  26.615049
Ca  35.619900  28.859755  24.211758
S   21.255009  31.518610  35.357773
S   20.273478  35.394371  33.092346
S   21.948936  31.336258  29.993723
S   25.043343  34.022594  33.158226
S   26.340496  29.835762  30.924484
| S   | 25.700577  | 34.086185  | 28.539339 |
|-----|------------|------------|------------|
| S   | 27.959850  | 29.563158  | 26.629803 |
| S   | 30.897778  | 31.274776  | 30.264240 |
| S   | 31.808128  | 26.871571  | 27.629539 |
| S   | 32.692932  | 30.648781  | 25.137209 |
| S   | 33.422424  | 26.289753  | 23.399359 |
| S   | 36.310669  | 27.428122  | 27.284828 |

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generated by VMD

| Ca  | 18.213411  | 32.790192  | 33.911816 |
|-----|------------|------------|------------|
| Ca  | 22.935349  | 34.336998  | 35.930622 |
| Ca  | 23.510782  | 30.856705  | 32.893291 |
| Ca  | 22.850021  | 34.480457  | 30.565731 |
| Ca  | 25.059250  | 30.691452  | 27.868408 |
| Ca  | 28.016388  | 33.129089  | 31.267254 |
| Ca  | 28.860540  | 27.918472  | 29.651714 |
| Ca  | 30.452799  | 32.274132  | 27.050495 |
| Ca  | 30.587090  | 27.845634  | 24.538250 |
| Ca  | 33.697224  | 29.890392  | 27.993984 |
| Ca  | 33.979530  | 24.849483  | 26.614714 |
| Ca  | 35.742355  | 28.870066  | 24.204365 |
| S   | 21.188179  | 31.541416  | 35.429520 |
| S   | 20.571648  | 35.335644  | 33.168915 |
| S   | 21.847633  | 31.106997  | 29.822231 |
| S   | 24.952122  | 34.041695  | 33.102280 |
| S   | 26.505089  | 29.977858  | 31.045408 |
| S   | 25.641479  | 34.210365  | 28.557949 |
| S   | 28.041071  | 29.558807  | 26.658592 |
| S   | 30.704544  | 31.182125  | 30.147182 |
| S   | 31.621014  | 26.826950  | 27.841141 |
| S   | 32.722488  | 30.575779  | 24.979382 |
| S   | 33.511864  | 26.469488  | 23.434984 |
| S   | 36.508118  | 27.539858  | 27.261806 |

24

generated by VMD

| Ca  | 18.204239  | 33.400223  | 34.059586 |
|-----|------------|------------|------------|
| Ca  | 23.001850  | 34.628693  | 35.780392 |
| Ca  | 23.412663  | 30.352564  | 33.054672 |
| Ca  | 22.747261  | 34.540524  | 30.354759 |
| Ca  | 25.015512  | 30.669422  | 27.834377 |
| Ca  | 27.891542  | 32.879570  | 31.284119 |
| Ca  | 29.031120  | 27.874302  | 29.772421 |
| Ca  | 30.380310  | 32.228294  | 27.333372 |
| Ca  | 30.384689  | 27.966976  | 24.256664 |
| Ca  | 33.506630  | 29.967289  | 28.279202 |
| Ca  | 34.410896  | 24.966539  | 26.534464 |
Ca   35.625023  29.115931  24.045456
S    21.034113  31.385862  35.411236
S    20.602558  35.821392  33.260983
S    21.878601  31.025822  29.989225
S    24.911930  33.727150  32.901741
S    26.393211  29.867990  31.096855
S    25.948437  33.836235  28.390030
S    28.198841  29.338892  26.659079
S    30.798264  31.160025  30.259996
S    31.662766  26.828913  27.675850
S    32.720524  30.604542  25.088596
S    33.445732  26.410934  23.380690
S    36.513340  27.701988  27.236217

24
generated by VMD
Ca   18.094885  33.345577  33.650097
Ca   22.670017  34.695869  35.788898
Ca   23.529392  30.322044  33.294319
Ca   22.929548  34.619534  30.483721
Ca   25.178013  30.357288  27.940357
Ca   27.893274  32.914539  31.353056
Ca   29.074692  28.006489  29.960018
Ca   30.576015  32.231979  27.314976
Ca   30.485140  27.912621  24.547703
Ca   33.499577  29.855091  28.017344
Ca   34.204765  24.985388  26.426720
Ca   35.705452  29.020086  23.987099
S    20.995062  31.536320  35.358128
S    20.536919  35.741940  33.104736
S    22.044930  30.966040  29.949095
S    24.877602  33.823124  33.233669
S    26.403019  29.812618  31.27497
S    25.809404  33.828686  28.485668
S    28.256092  29.371666  26.852947
S    30.890388  31.222542  30.075191
S    31.534725  26.860167  27.555531
S    32.667606  30.743732  24.895046
S    33.555847  26.538017  23.254284
S    36.307690  27.588692  27.136658

24
generated by VMD
Ca   18.295460  33.453506  33.398235
Ca   22.962950  34.610615  35.753426
Ca   23.218592  30.429417  33.164417
Ca   22.499855  34.434986  30.897606
Ca   25.132122  30.481316  28.052296
|   | 27.730576 | 32.983356 | 31.150688 |
|---|-----------|-----------|-----------|
| Ca| 29.060038 | 28.039816 | 30.062727 |
| Ca| 30.547222 | 32.149685 | 27.300289 |
| Ca| 30.438789 | 27.914385 | 24.399635 |
| Ca| 33.853069 | 29.904221 | 28.076540 |
| Ca| 34.303352 | 24.717018 | 26.403210 |
| Ca| 35.868313 | 28.954052 | 23.895872 |
| S | 20.825111 | 31.539064 | 35.350773 |
| S | 20.470438 | 35.794697 | 33.378281 |
| S | 21.970955 | 30.936607 | 30.070175 |
| S | 24.647745 | 33.874454 | 33.128139 |
| S | 26.565449 | 30.037125 | 31.235701 |
| S | 25.443508 | 33.980865 | 28.587175 |
| S | 28.347836 | 29.416267 | 26.710602 |
| S | 31.069008 | 31.186237 | 30.169437 |
| S | 31.677109 | 26.995062 | 27.611618 |
| S | 32.843124 | 30.509064 | 25.001484 |
| S | 33.524826 | 26.361115 | 23.094288 |
| S | 36.424606 | 27.597122 | 27.047472 |

24

generated by VMD

|   | 18.307280 | 33.087406 | 33.501488 |
|---|-----------|-----------|-----------|
| Ca| 23.196201 | 34.506001 | 35.760399 |
| Ca| 23.410713 | 30.314070 | 33.024689 |
| Ca| 22.687492 | 34.589764 | 30.503746 |
| Ca| 24.807335 | 30.768782 | 27.895441 |
| Ca| 27.836796 | 32.775566 | 31.182474 |
| Ca| 29.179001 | 28.074095 | 30.060482 |
| Ca| 30.438864 | 32.225288 | 27.408134 |
| Ca| 30.392925 | 27.852299 | 24.730587 |
| Ca| 33.965023 | 29.958899 | 28.041744 |
| Ca| 34.219627 | 24.841743 | 26.449825 |
| Ca| 35.704727 | 28.978722 | 23.847153 |
| S | 21.059469 | 31.494884 | 35.222191 |
| S | 20.542191 | 35.703869 | 33.443363 |
| S | 21.672476 | 31.154949 | 29.907761 |
| S | 24.937355 | 33.768524 | 32.933098 |
| S | 26.471750 | 29.910349 | 31.191090 |
| S | 25.584677 | 33.983376 | 28.282101 |
| S | 28.143326 | 29.533157 | 26.821667 |
| S | 30.893650 | 31.278114 | 30.278782 |
| S | 31.842167 | 26.903145 | 27.915016 |
| S | 32.747810 | 30.627178 | 25.132038 |
| S | 33.250930 | 26.477142 | 23.358385 |
| S | 36.428211 | 27.492727 | 27.048370 |
Ca   18.465233   33.607479   34.001568
Ca   23.092617   34.399109   36.094238
Ca   23.315014   30.464809   32.899132
Ca   22.792486   34.388126   30.683109
Ca   24.708317   30.712803   27.811283
Ca   27.640118   32.789383   30.890968
Ca   28.874245   27.877661   29.756723
Ca   30.579157   32.349911   27.046141
Ca   30.360985   28.074894   24.604898
Ca   33.781765   29.862274   28.213982
Ca   34.361576   25.004593   26.711161
Ca   35.941734   28.901291   23.976490
S    21.134773   31.582706   35.422577
S    20.932961   35.670509   33.622593
S    21.715164   30.816216   29.907076
S    24.703964   33.658630   32.804688
S    26.318365   29.925573   30.926443
S    25.427050   34.020733   28.12950
S    28.129105   29.606665   26.640137
S    30.741940   30.978504   30.014782
S    31.734159   26.734861   27.795527
S    32.954510   30.778095   25.133423
S    33.473145   26.356110   23.430029
S    36.541706   27.739126   27.423866
Ca   18.444630   33.592079   34.252556
Ca   23.400341   34.424843   35.755306
Ca   23.366055   30.694933   32.800610
Ca   22.608681   34.261284   30.595518
Ca   24.742031   30.612362   27.660187
Ca   27.768831   32.851097   30.928391
Ca   28.676088   27.703396   29.723709
Ca   30.548950   32.163948   27.465996
Ca   30.550497   28.127525   24.673977
Ca   33.750847   29.899155   28.356541
Ca   34.418598   24.936205   26.687206
Ca   35.775356   29.087162   23.923546
S    21.261051   31.719418   35.543819
S    20.828135   35.699123   33.525444
S    21.638275   30.968262   29.777948
S    24.849014   33.695889   32.678932
S    26.171339   29.835102   30.837334
S    25.651917   33.915794   28.206406
S    28.089262   29.597624   26.698906
|  |  |  |  |
|----|----|----|----|
| S  | 30.579191 | 30.871826 | 30.125038 |
| S  | 31.674654 | 26.865767 | 27.907234 |
| S  | 32.954910 | 30.779110 | 25.178053 |
| S  | 33.448174 | 26.448458 | 23.375095 |
| S  | 36.523170 | 27.782597 | 27.262318 |

24 generated by VMD

| Ca  | 18.422684 | 33.141167 | 33.800571 |
| Ca  | 22.860104 | 34.807064 | 35.769958 |
| Ca  | 23.589035 | 30.279823 | 33.144348 |
| Ca  | 22.715477 | 34.546501 | 30.578716 |
| Ca  | 24.903915 | 30.735970 | 27.726929 |
| Ca  | 27.773716 | 32.768845 | 31.198940 |
| Ca  | 29.090340 | 27.745949 | 29.561987 |
| Ca  | 30.339725 | 32.814800 | 27.145699 |
| Ca  | 30.370232 | 27.970198 | 24.481613 |
| Ca  | 33.578148 | 29.872683 | 28.087711 |
| Ca  | 34.627861 | 24.853752 | 26.384830 |
| Ca  | 35.696968 | 29.111256 | 24.378304 |
| S   | 21.192581 | 31.665054 | 35.585220 |
| S   | 20.427042 | 35.804970 | 33.160175 |
| S   | 21.997066 | 31.084026 | 30.078566 |
| S   | 24.866934 | 33.819862 | 33.237614 |
| S   | 26.521580 | 29.793449 | 31.056541 |
| S   | 25.660694 | 34.145714 | 28.384071 |
| S   | 28.061947 | 29.428104 | 26.633615 |
| S   | 30.748447 | 31.023016 | 29.968924 |
| S   | 31.734079 | 26.777958 | 27.519308 |
| S   | 32.765835 | 30.607351 | 25.183197 |
| S   | 33.482521 | 26.621181 | 23.392025 |
| S   | 36.293125 | 27.514658 | 27.481182 |

24 generated by VMD

| Ca  | 18.180622 | 33.179867 | 34.007591 |
| Ca  | 22.931376 | 34.446354 | 35.912861 |
| Ca  | 23.569714 | 30.520761 | 32.934341 |
| Ca  | 22.636082 | 34.838825 | 30.741734 |
| Ca  | 24.798468 | 30.819307 | 27.865978 |
| Ca  | 27.791653 | 32.636578 | 31.051331 |
| Ca  | 28.875900 | 27.833227 | 29.625652 |
| Ca  | 30.427891 | 32.240162 | 27.038446 |
| Ca  | 30.412659 | 27.806488 | 24.488539 |
| Ca  | 33.693806 | 29.886986 | 27.917797 |
| Ca  | 34.708252 | 24.891207 | 26.618610 |
| Ca  | 35.794220 | 28.839664 | 24.253941 |
| S   | 21.102875 | 31.513809 | 35.491234 |
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| S | 20.538284 | 35.80162 | 33.52321 |
| S | 21.833868 | 31.32661 | 29.97231 |
| S | 24.832323 | 33.783813 | 32.964657 |
| S | 26.270472 | 29.886742 | 31.005299 |
| S | 25.503895 | 34.144341 | 28.442097 |
| S | 28.075420 | 29.378828 | 26.587029 |
| S | 30.746937 | 30.900293 | 29.922815 |
| S | 31.838669 | 26.770763 | 27.713541 |
| S | 32.851112 | 30.645716 | 24.922150 |
| S | 33.761688 | 26.530453 | 23.550125 |
| S | 36.543892 | 27.651047 | 27.384653 |

24 generated by VMD

| Ca  |  |  |  |
|-----|--------|--------|--------|
| Ca  | 18.506821 | 32.930656 | 33.819176 |
| Ca  | 22.753510 | 34.854221 | 35.887615 |
| Ca  | 23.474129 | 30.357254 | 32.996437 |
| Ca  | 22.464806 | 34.748672 | 30.492846 |
| Ca  | 24.927141 | 30.722200 | 27.753834 |
| Ca  | 27.693756 | 32.938759 | 31.394390 |
| Ca  | 29.119423 | 27.924248 | 29.646742 |
| Ca  | 30.583138 | 32.330585 | 27.219677 |
| Ca  | 30.556587 | 28.064295 | 24.374651 |
| Ca  | 33.939121 | 29.778673 | 28.102692 |
| Ca  | 34.389702 | 24.837273 | 26.497772 |
| Ca  | 35.681984 | 28.805428 | 23.910065 |
| S   | 21.205631 | 31.554333 | 35.672916 |
| S   | 20.410706 | 35.743504 | 33.148571 |
| S   | 21.807964 | 31.132669 | 30.050060 |
| S   | 24.744253 | 33.801262 | 33.129387 |
| S   | 26.433556 | 29.789307 | 31.037527 |
| S   | 25.572449 | 33.937874 | 28.485416 |
| S   | 28.219772 | 29.585493 | 26.660774 |
| S   | 30.712296 | 31.154106 | 30.367966 |
| S   | 31.797436 | 27.028839 | 27.620174 |
| S   | 32.906338 | 30.561243 | 25.134401 |
| S   | 33.399532 | 26.337463 | 23.293249 |
| S   | 36.419991 | 27.381664 | 27.243702 |

24 generated by VMD
Ca 30.372892 32.206345 27.227570
Ca 30.473722 27.834093 24.498287
Ca 34.596203 24.896751 26.662146
Ca 35.721054 28.861530 23.890028
S 21.118069 31.547525 35.337738
S 20.545044 35.742302 33.238834
S 21.829388 31.334944 29.791103
S 24.925320 33.856735 33.291031
S 26.314260 29.917070 30.942991
S 25.679535 33.880844 28.583647
S 28.059856 29.378502 26.868023
S 30.710852 31.136868 30.091135
S 31.875904 26.948322 27.737747
S 32.897194 30.581055 24.933743
S 33.492466 26.303345 23.320833
S 36.473572 27.593609 27.235321

24 generated by VMD
Ca 18.403435 32.731186 34.148266
Ca 22.696373 34.827179 35.770233
Ca 23.867493 30.446217 32.851196
Ca 22.816772 34.775661 30.510759
Ca 25.001308 30.706219 27.656912
Ca 27.721577 32.865040 31.465603
Ca 29.035378 28.012775 29.642296
Ca 30.599781 32.202190 27.130352
Ca 30.385109 27.975153 24.434250
Ca 33.815090 29.998112 28.002203
Ca 34.161259 24.865498 26.490662
Ca 35.749073 28.694542 24.142693
S 21.452265 31.639030 35.772171
S 20.234974 35.397499 33.080315
S 21.985008 31.194452 29.814331
S 24.759216 33.791752 33.195206
S 26.279419 29.842934 31.012333
S 25.755432 34.206741 28.584126
S 28.184128 29.542139 26.615242
S 30.739685 31.263752 30.259869
S 31.747805 26.951698 27.743935
S 32.969521 30.609064 24.992229
S 33.524769 26.401970 23.282700
S 36.315910 27.359232 27.341652

24 generated by VMD
Ca 18.550474 32.865452 34.272781
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 23.106991    | 34.613190    | 35.800194    |
| Ca      | 23.567787    | 30.417549    | 32.892593    |
| Ca      | 22.642225    | 34.982552    | 30.384716    |
| Ca      | 24.788589    | 30.797514    | 27.612236    |
| Ca      | 27.484516    | 32.687679    | 31.069366    |
| Ca      | 28.913052    | 27.643867    | 29.591700    |
| Ca      | 30.357876    | 32.339237    | 27.290873    |
| Ca      | 31.517864    | 28.195595    | 24.516361    |
| Ca      | 33.849922    | 29.892365    | 28.218515    |
| Ca      | 34.379494    | 24.889658    | 26.579659    |
| Ca      | 35.504547    | 28.895277    | 24.095272    |
| S       | 21.674345    | 31.520802    | 35.432930    |
| S       | 30.474380    | 35.640453    | 33.378998    |
| S       | 22.072077    | 31.385977    | 29.813520    |
| S       | 24.924866    | 33.923847    | 32.889771    |
| S       | 26.120190    | 29.610471    | 30.972836    |
| S       | 25.318184    | 33.995789    | 28.317993    |
| S       | 28.126553    | 29.521635    | 26.646091    |
| S       | 30.608747    | 30.844818    | 30.044502    |
| S       | 31.900835    | 26.963802    | 27.764343    |
| S       | 32.995300    | 30.824905    | 25.271027    |
| S       | 33.376713    | 26.277241    | 23.405052    |
| S       | 36.464558    | 27.579365    | 27.678699    |

24

generated by VMD

| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.280701    | 32.411522    | 34.028732    |
| Ca      | 22.805880    | 34.671097    | 36.001663    |
| Ca      | 23.353928    | 30.401308    | 32.880775    |
| Ca      | 22.909996    | 34.835041    | 30.531448    |
| Ca      | 24.878048    | 30.657055    | 27.659065    |
| Ca      | 27.583590    | 33.076145    | 31.303396    |
| Ca      | 29.169590    | 28.532013    | 29.655626    |
| Ca      | 30.693439    | 32.467846    | 27.147137    |
| Ca      | 30.405102    | 28.235382    | 24.595427    |
| Ca      | 34.386360    | 29.796700    | 27.624151    |
| Ca      | 34.090263    | 24.707451    | 26.591797    |
| Ca      | 35.633453    | 28.177803    | 24.014351    |
| S       | 21.044071    | 31.298553    | 35.690922    |
| S       | 20.520905    | 35.342495    | 33.240181    |
| S       | 21.981464    | 31.267845    | 29.645321    |
| S       | 24.883274    | 33.811810    | 33.280518    |
| S       | 26.111065    | 29.787773    | 30.969656    |
| S       | 25.639030    | 34.121704    | 28.392845    |
| S       | 28.214546    | 29.785343    | 26.685970    |
| S       | 30.728436    | 31.651669    | 30.227238    |
| S       | 31.894154    | 27.239422    | 27.701817    |
|   |   |   |   |
|---|---|---|---|
| S  | 32.970341 | 30.698015 | 25.011827 |
| S  | 33.170578 | 26.151720 | 23.565651 |
| S  | 36.371792 | 27.174320 | 27.494606 |

24 generated by VMD

| Ca | 18.587070 | 32.105881 | 34.066277 |
| Ca | 22.941959 | 34.699142 | 35.987648 |
| Ca | 23.195021 | 30.722765 | 32.824234 |
| Ca | 22.708803 | 34.999020 | 30.401581 |
| Ca | 25.036655 | 30.436451 | 27.731554 |
| Ca | 27.680523 | 33.105518 | 31.316429 |
| Ca | 29.048517 | 28.320625 | 29.744694 |
| Ca | 30.813463 | 32.223145 | 27.235550 |
| Ca | 30.348026 | 28.189129 | 24.533150 |
| Ca | 34.209396 | 29.516979 | 27.659626 |
| Ca | 34.026588 | 24.828434 | 26.482023 |
| Ca | 35.743950 | 28.371582 | 24.024708 |
| S  | 21.306202 | 31.507711 | 35.830284 |
| S  | 20.388155 | 35.195095 | 33.307831 |
| S  | 21.941294 | 31.347736 | 29.585518 |
| S  | 24.650803 | 34.160309 | 32.975471 |
| S  | 26.121645 | 29.872105 | 31.164310 |
| S  | 25.622673 | 33.960304 | 28.319315 |
| S  | 28.170595 | 29.743080 | 26.675350 |
| S  | 30.741879 | 31.476330 | 30.430740 |
| S  | 31.601711 | 27.073347 | 27.561844 |
| S  | 32.997528 | 30.802771 | 25.188284 |
| S  | 33.472721 | 26.419086 | 23.440941 |
| S  | 36.364841 | 27.223549 | 27.452698 |

24 generated by VMD

| Ca | 18.195568 | 32.406700 | 34.366940 |
| Ca | 22.599930 | 34.573856 | 35.818115 |
| Ca | 23.357090 | 30.455688 | 32.686737 |
| Ca | 22.517593 | 34.939007 | 30.402443 |
| Ca | 25.018171 | 30.793003 | 27.670441 |
| Ca | 27.685467 | 33.351307 | 31.525467 |
| Ca | 29.185255 | 28.332733 | 29.977840 |
| Ca | 30.925972 | 32.298725 | 27.091080 |
| Ca | 30.330835 | 27.931206 | 24.831264 |
| Ca | 34.344200 | 29.523922 | 27.564171 |
| Ca | 34.134323 | 24.680290 | 26.472343 |
| Ca | 35.728477 | 28.550510 | 23.761497 |
| S  | 21.463867 | 31.369011 | 35.663170 |
| S  | 20.163090 | 35.330345 | 33.134434 |
| S  | 21.841413 | 31.394260 | 29.659988 |
|   | 24.443827 | 33.947140 | 33.046440 |
|---|-----------|-----------|-----------|
| S | 26.283579 | 30.105915 | 30.966675 |
| S | 25.619740 | 34.136059 | 28.578581 |
| S | 28.355204 | 29.710854 | 26.821400 |
| S | 30.881239 | 31.528229 | 30.619198 |
| S | 31.821995 | 27.032005 | 27.786259 |
| S | 33.003739 | 30.452223 | 25.072815 |
| S | 33.166260 | 26.387825 | 23.304096 |
| S | 36.653172 | 27.066238 | 27.118622 |

24
generated by VMD

| Ca | 18.208221 | 32.641289 | 33.994392 |
|----|-----------|-----------|-----------|
| Ca | 22.662706 | 34.738712 | 35.936832 |
| Ca | 23.109421 | 30.585089 | 32.885475 |
| Ca | 22.655354 | 34.802368 | 30.441696 |
| Ca | 25.136332 | 30.644157 | 27.728321 |
| Ca | 27.659155 | 33.197765 | 31.403465 |
| Ca | 29.312998 | 28.130417 | 29.809830 |
| Ca | 30.644871 | 32.177963 | 27.194855 |
| Ca | 30.497719 | 28.004448 | 24.584328 |
| Ca | 34.544910 | 29.692341 | 27.675240 |
| Ca | 33.972977 | 24.852629 | 26.403759 |
| Ca | 35.742424 | 28.585520 | 23.809208 |
| S  | 21.044683 | 31.533993 | 35.693596 |
| S  | 20.108850 | 35.493542 | 33.191681 |
| S  | 22.124875 | 31.103119 | 29.852428 |
| S  | 24.732838 | 33.970432 | 33.215580 |
| S  | 26.352062 | 29.908661 | 31.198965 |
| S  | 25.573069 | 34.132713 | 28.481548 |
| S  | 28.235886 | 29.617016 | 26.852440 |
| S  | 30.624748 | 31.375694 | 30.575989 |
| S  | 31.983925 | 27.098667 | 27.676228 |
| S  | 33.020557 | 30.533766 | 25.079830 |
| S  | 33.261517 | 26.342857 | 23.100708 |
| S  | 36.506325 | 27.136902 | 27.153706 |

24
generated by VMD

| Ca | 18.490128 | 32.300869 | 33.870209 |
|----|-----------|-----------|-----------|
| Ca | 22.721905 | 34.685150 | 35.634453 |
| Ca | 23.370594 | 30.454380 | 33.003262 |
| Ca | 22.689720 | 34.954559 | 30.438370 |
| Ca | 25.055500 | 30.680634 | 27.985928 |
| Ca | 27.902008 | 33.025162 | 31.204185 |
| Ca | 29.210892 | 28.163210 | 30.025013 |
| Ca | 30.668415 | 32.341221 | 27.131678 |
| Ca | 30.355711 | 28.116325 | 24.315584 |
|   | Ca     | S       |   |
|---|--------|---------|---|
| Ca| 33.703869| 29.771139 | 27.891674 |
| Ca| 33.864632| 24.723455 | 26.516739 |
| Ca| 35.670067| 28.593563 | 24.142115 |
| S | 21.330664| 31.553768 | 35.808708 |
| S | 20.22517 | 35.283325 | 32.989883 |
| S | 21.974043| 31.305473 | 29.769892 |
| S | 24.765306| 33.859238 | 33.110077 |
| S | 26.594992| 29.634792 | 31.186283 |
| S | 25.833172| 33.975010 | 28.552261 |
| S | 28.201485| 29.703991 | 26.686493 |
| S | 30.961811| 31.376972 | 30.343960 |
| S | 31.401375| 26.987782 | 27.529003 |
| S | 33.002708| 30.720646 | 25.053837 |
| S | 33.390102| 26.485737 | 23.462023 |
| S | 36.338417| 27.303665 | 27.288422 |

24 generated by VMD

| Ca | 18.229868 | 32.784561 | 33.820648 |
| Ca | 22.538731 | 34.984787 | 35.567085 |
| Ca | 23.421387 | 30.531841 | 32.952106 |
| Ca | 22.760811 | 34.765289 | 30.593933 |
| Ca | 25.129416 | 30.422684 | 27.764786 |
| Ca | 29.148556 | 28.022589 | 29.792652 |
| Ca | 30.675941 | 32.424530 | 27.221096 |
| Ca | 30.442219 | 27.935684 | 24.476093 |
| Ca | 33.870281 | 29.872175 | 27.948109 |
| Ca | 34.108608 | 24.983973 | 26.517826 |
| Ca | 35.605057 | 28.750332 | 24.046656 |
| S  | 21.142536 | 31.713230 | 35.694229 |
| S  | 20.270144 | 35.366520 | 33.001465 |
| S  | 21.999243 | 31.168379 | 29.970425 |
| S  | 24.727962 | 34.006454 | 33.336849 |
| S  | 26.514814 | 29.662580 | 31.105326 |
| S  | 25.758366 | 33.862770 | 28.663464 |
| S  | 28.469669 | 29.774778 | 26.615555 |
| S  | 30.877573 | 31.245010 | 30.314667 |
| S  | 31.819281 | 26.920507 | 27.669434 |
| S  | 32.900501 | 30.733171 | 25.073601 |
| S  | 33.273548 | 26.280947 | 23.103056 |
| S  | 36.302818 | 27.279266 | 26.973324 |

24 generated by VMD

| Ca | 18.384302 | 32.362000 | 33.731892 |
| Ca | 22.491129 | 34.751747 | 35.587883 |
| Ca | 23.535515 | 30.466526 | 33.066463 |
|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 22.924683 | 34.824337 | 30.333742 |
| Ca  | 24.765924 | 30.477373 | 27.966640 |
| Ca  | 27.942589 | 33.073208 | 31.403301 |
| Ca  | 29.259155 | 28.364157 | 30.005848 |
| Ca  | 30.880594 | 32.365536 | 27.038555 |
| Ca  | 30.302912 | 28.157372 | 24.443964 |
| Ca  | 33.009298 | 24.829908 | 26.447001 |
| Ca  | 35.634327 | 28.481146 | 23.976974 |
| S   | 21.213104 | 31.307194 | 35.705364 |
| S   | 20.259350 | 35.244770 | 32.834049 |
| S   | 21.910440 | 31.518166 | 29.882570 |
| S   | 24.853222 | 33.935768 | 33.278854 |
| S   | 26.396765 | 29.815281 | 31.279839 |
| S   | 25.813938 | 34.016441 | 28.737061 |
| S   | 28.085651 | 29.732635 | 26.728153 |
| S   | 31.190905 | 31.315888 | 30.324390 |
| S   | 31.585461 | 27.183599 | 27.584112 |
| S   | 32.856293 | 30.661251 | 24.873110 |
| S   | 33.303761 | 26.479495 | 23.473167 |
| S   | 36.318207 | 27.155056 | 27.209139 |

24 generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 18.230297 | 32.834949 | 33.977726 |
| Ca  | 22.676924 | 34.527649 | 35.721348 |
| Ca  | 23.457840 | 30.166300 | 33.058151 |
| Ca  | 22.817028 | 34.769184 | 30.629795 |
| Ca  | 25.097248 | 30.739956 | 27.860832 |
| Ca  | 27.716454 | 32.790386 | 31.265257 |
| Ca  | 29.254910 | 28.234854 | 30.030533 |
| Ca  | 30.848057 | 32.551449 | 26.760708 |
| Ca  | 30.187609 | 28.094364 | 24.619049 |
| Ca  | 33.749855 | 29.679722 | 27.716572 |
| Ca  | 34.218464 | 24.927616 | 26.852367 |
| Ca  | 35.732075 | 28.541737 | 23.853287 |
| S   | 21.115341 | 31.504555 | 35.626572 |
| S   | 20.336029 | 35.391335 | 32.995937 |
| S   | 22.156307 | 31.368759 | 29.869755 |
| S   | 24.927837 | 33.344864 | 33.282700 |
| S   | 26.135471 | 29.794441 | 30.815250 |
| S   | 25.915215 | 34.375900 | 28.521336 |
| S   | 28.386549 | 29.835430 | 26.795691 |
| S   | 30.928341 | 31.498123 | 30.126856 |
| S   | 31.469107 | 26.854977 | 27.749702 |
| S   | 32.788025 | 30.560268 | 24.801434 |
| S   | 33.221703 | 26.207647 | 23.586535 |
|   | 36.353374 | 27.705635 | 27.422686 |
|---|-----------|-----------|-----------|
| S |           |           |           |
| Ca| 18.328384 | 32.766052 | 33.904213 |
| Ca| 22.598209 | 34.833092 | 35.611855 |
| Ca| 23.470026 | 30.362131 | 32.963036 |
| Ca| 22.888153 | 34.743870 | 30.763836 |
| Ca| 25.135445 | 30.570242 | 27.903938 |
| Ca| 27.795517 | 33.098419 | 31.420076 |
| Ca| 29.077549 | 28.008993 | 29.934071 |
| Ca| 30.604725 | 32.555939 | 27.376093 |
| Ca| 30.347538 | 27.976721 | 24.545807 |
| Ca| 33.695518 | 29.971115 | 28.114475 |
| Ca| 34.340527 | 24.985313 | 26.423367 |
| Ca| 35.760464 | 28.472666 | 23.904921 |
| S | 21.206606 | 31.651897 | 35.591465 |
| S | 20.359364 | 35.392532 | 32.884747 |
| S | 21.973232 | 31.445316 | 29.687792 |
| S | 24.949093 | 33.239830 | 33.339989 |
| S | 26.275747 | 29.806087 | 30.972227 |
| S | 25.780224 | 34.139980 | 28.673250 |
| S | 28.276859 | 29.774712 | 26.713413 |
| S | 30.755781 | 31.305859 | 30.129002 |
| S | 31.784725 | 27.005026 | 27.710976 |
| S | 32.813229 | 30.534634 | 24.810444 |
| S | 33.134926 | 25.966587 | 23.328737 |
| S | 36.368217 | 27.693089 | 27.232336 |

24 generated by VMD

|   | 36.353374 | 27.705635 | 27.422686 |
|---|-----------|-----------|-----------|
| S |           |           |           |
| Ca| 18.195801 | 32.966591 | 33.982338 |
| Ca| 22.867327 | 35.191803 | 35.567566 |
| Ca| 23.523224 | 30.282913 | 33.135551 |
| Ca| 22.935238 | 34.751415 | 30.642166 |
| Ca| 24.731594 | 30.451679 | 27.786160 |
| Ca| 27.905008 | 32.900593 | 31.272888 |
| Ca| 28.992649 | 27.885941 | 29.767704 |
| Ca| 30.414314 | 32.229660 | 27.376976 |
| Ca| 30.411423 | 28.023609 | 24.571171 |
| Ca| 33.564480 | 29.792332 | 28.157539 |
| Ca| 34.526665 | 24.955360 | 26.583149 |
| Ca| 35.866425 | 29.014160 | 23.830463 |
| S | 20.995068 | 31.783564 | 35.749660 |
| S | 20.500710 | 35.497799 | 32.846390 |
| S | 22.033585 | 31.479813 | 29.821592 |
| S | 24.920731 | 33.409813 | 33.416874 |
| S | 26.192261 | 29.593380 | 30.818316 |
S  25.840435  33.919209  28.437954
S  28.102425  29.522472  26.822426
S  30.955917  30.900898  30.306679
S  31.640408  26.791954  27.761223
S  32.725857  30.629406  24.972057
S  33.549026  26.443356  23.224236
S  36.329422  27.882351  27.088997

24
generated by VMD
Ca  18.424282  32.998184  34.034489
Ca  22.831470  34.748566  35.752701
Ca  23.496716  30.357340  33.220757
Ca  22.970736  34.613937  30.233292
Ca  25.102772  30.590683  27.782118
Ca  27.874737  32.886440  31.283590
Ca  29.049469  27.856039  30.040245
Ca  30.668684  32.338043  27.445398
Ca  30.363039  27.734573  24.775854
Ca  33.639938  29.763855  28.182281
Ca  34.388695  25.038746  26.629185
Ca  35.575302  29.057329  23.703440
S  21.197931  31.509077  35.67654
S  20.473778  35.601280  32.833054
S  21.781984  31.294594  29.461781
S  24.780735  33.509132  33.139526
S  26.120848  29.706306  30.991295
S  26.045290  34.067883  28.491585
S  28.282274  29.765482  26.867130
S  30.858383  31.067013  30.376368
S  31.594151  26.798260  27.829411
S  32.529961  30.638550  25.008598
S  33.334354  26.349424  23.270510
S  36.334511  27.927418  26.910715

24
generated by VMD
Ca  18.256638  33.231590  34.231644
Ca  22.568554  34.871834  35.761074
Ca  23.348309  30.262691  32.927868
Ca  22.663166  34.581226  30.555897
Ca  24.964985  30.683352  27.807566
Ca  27.931435  32.879780  31.604946
Ca  29.173576  28.004179  29.829046
Ca  30.674707  32.474770  27.335550
Ca  30.323961  27.505743  24.764742
Ca  33.568947  29.739971  27.853611
Ca  34.670410  24.982731  26.536409
|   |   |   |   |
|---|---|---|---|
| Ca | 35.687538 | 29.072681 | 23.781660 |
| S  | 21.182686 | 31.736488 | 35.514584 |
| S  | 20.467466 | 35.765007 | 32.869865 |
| S  | 21.824211 | 31.397408 | 29.532145 |
| S  | 24.790245 | 33.434853 | 33.416855 |
| S  | 26.090282 | 29.579102 | 30.936214 |
| S  | 25.927753 | 34.014896 | 28.656546 |
| S  | 28.279282 | 29.547333 | 26.686337 |
| S  | 30.972820 | 31.222414 | 30.315441 |
| S  | 31.815868 | 26.659996 | 27.740515 |
| S  | 32.477585 | 30.462662 | 24.936291 |
| S  | 33.553581 | 26.358700 | 23.309286 |
| S  | 36.506020 | 27.830692 | 27.035971 |

24 generated by VMD

| Ca | 18.308540 | 33.013870 | 33.942562 |
| Ca | 22.553329 | 34.931747 | 35.736900 |
| Ca | 23.527775 | 30.395000 | 33.044205 |
| Ca | 22.944458 | 34.09904  | 30.476330 |
| Ca | 25.047482 | 30.532448 | 27.937723 |
| Ca | 27.924683 | 32.966934 | 31.326866 |
| Ca | 29.062916 | 28.090405 | 30.007900 |
| Ca | 30.572472 | 32.564548 | 27.509142 |
| Ca | 30.484108 | 27.916328 | 24.621510 |
| Ca | 33.628056 | 29.933783 | 28.005419 |
| Ca | 34.223076 | 24.891449 | 26.675264 |
| Ca | 35.590794 | 28.913727 | 23.700068 |
| S  | 21.124454 | 31.608149 | 35.563080 |
| S  | 20.398245 | 35.41605  | 32.718697 |
| S  | 22.009815 | 31.152842 | 29.765476 |
| S  | 24.941984 | 33.387154 | 33.354134 |
| S  | 26.281780 | 29.748894 | 30.997650 |
| S  | 25.992123 | 33.998283 | 28.438782 |
| S  | 28.404676 | 29.847466 | 26.810707 |
| S  | 30.950981 | 31.225468 | 30.299593 |
| S  | 31.457153 | 26.865494 | 27.791481 |
| S  | 32.804951 | 30.623638 | 25.014366 |
| S  | 33.223465 | 26.259384 | 23.232819 |
| S  | 36.262749 | 27.581528 | 26.969412 |

24 generated by VMD

| Ca | 18.448549 | 32.965771 | 34.075424 |
| Ca | 22.739649 | 34.763702 | 35.605820 |
| Ca | 23.190119 | 30.339817 | 33.053619 |
| Ca | 22.889690 | 34.737705 | 30.474785 |
| Ca | 24.970848 | 30.674095 | 27.749233 |
| Ca  | 27.866238 | 32.950844 | 31.380110 |
|-----|-----------|-----------|-----------|
| Ca  | 28.774099 | 28.019321 | 29.782480 |
| Ca  | 30.591391 | 32.460060 | 27.436544 |
| Ca  | 30.698460 | 27.535992 | 24.782379 |
| Ca  | 33.431534 | 29.746346 | 27.994989 |
| Ca  | 34.623466 | 25.120480 | 26.949158 |
| Ca  | 35.524593 | 29.056564 | 23.496302 |
| S   | 21.187479 | 31.450157 | 35.656620 |
| S   | 20.632339 | 35.672077 | 32.980537 |
| S   | 22.005409 | 31.496399 | 29.796129 |
| S   | 24.860489 | 33.755553 | 33.253525 |
| S   | 26.000072 | 29.712193 | 30.789190 |
| S   | 25.863712 | 34.012424 | 28.656610 |
| S   | 28.312363 | 30.010870 | 26.689741 |
| S   | 30.828354 | 30.879168 | 30.295746 |
| S   | 31.594725 | 26.793760 | 27.731955 |
| S   | 32.649429 | 30.590916 | 24.769926 |
| S   | 33.602127 | 25.937860 | 23.561848 |
| S   | 36.434914 | 27.997993 | 26.977413 |

24
generated by VMD

| Ca  | 18.571369 | 32.354168 | 33.918549 |
|-----|-----------|-----------|-----------|
| Ca  | 22.672634 | 34.964546 | 35.654793 |
| Ca  | 23.493572 | 30.541805 | 32.784550 |
| Ca  | 22.661795 | 34.940536 | 30.657314 |
| Ca  | 25.012434 | 30.921185 | 27.934752 |
| Ca  | 27.745396 | 32.834343 | 31.047171 |
| Ca  | 29.063313 | 27.863024 | 30.001581 |
| Ca  | 30.663727 | 32.330788 | 27.487326 |
| Ca  | 30.425640 | 27.700344 | 24.899260 |
| Ca  | 33.599957 | 29.724398 | 27.877842 |
| Ca  | 34.482536 | 24.883850 | 26.804356 |
| Ca  | 35.619144 | 29.110977 | 23.635675 |
| S   | 21.531265 | 31.544697 | 35.588360 |
| S   | 20.263809 | 35.542297 | 33.146034 |
| S   | 21.926147 | 31.599327 | 29.779333 |
| S   | 24.834290 | 33.489124 | 33.030914 |
| S   | 26.121792 | 29.728046 | 30.673920 |
| S   | 25.699478 | 34.345852 | 28.485514 |
| S   | 28.310745 | 29.765759 | 26.946056 |
| S   | 30.903191 | 31.017929 | 30.281765 |
| S   | 31.567711 | 26.601940 | 27.833759 |
| S   | 32.723576 | 30.695942 | 25.056112 |
| S   | 33.498245 | 26.109236 | 23.458296 |
| S   | 36.328274 | 27.689972 | 26.956816 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 18.468559 | 32.513245 | 34.075668 |
| Ca      | 22.902193  | 34.905346  | 35.748646  |
| Ca      | 23.304569  | 30.758642  | 32.859089  |
| Ca      | 22.898872  | 34.455650  | 30.484280  |
| Ca      | 25.086514  | 30.990860  | 27.652395  |
| Ca      | 27.920868  | 32.912769  | 31.349884  |
| Ca      | 28.894396  | 27.914845  | 29.870049  |
| Ca      | 30.488945  | 32.333031  | 27.546478  |
| Ca      | 30.406849  | 27.627590  | 24.612162  |
| Ca      | 33.307892  | 29.821735  | 27.862497  |
| Ca      | 34.579792  | 24.853891  | 26.884029  |
| Ca      | 35.608059  | 29.227581  | 23.785378  |
| S       | 21.483311  | 31.749012  | 35.559662  |
| S       | 20.220783  | 35.332500  | 32.893200  |
| S       | 22.050842  | 31.356976  | 29.659767  |
| S       | 24.996071  | 33.466682  | 33.325207  |
| S       | 26.275034  | 29.859715  | 31.021019  |
| S       | 26.092222  | 34.096550  | 28.592358  |
| S       | 28.271852  | 29.626673  | 26.526062  |
| S    | 30.790539 | 31.058132 | 30.319439 |
| S    | 31.632164 | 26.897038 | 27.879389 |
| S    | 32.523834 | 30.684898 | 25.057148 |
| S    | 33.334572 | 25.967295 | 23.413305 |
| S    | 36.162460 | 27.671286 | 27.071688 |

24 generated by VMD

| Ca   | 18.447498 | 32.356789 | 33.694069 |
| Ca   | 22.745249 | 34.623421 | 35.696091 |
| Ca   | 23.405113 | 30.489662 | 32.918182 |
| Ca   | 23.052908 | 34.783096 | 30.534620 |
| Ca   | 25.251865 | 30.737446 | 27.689507 |
| Ca   | 28.097996 | 33.109688 | 31.472603 |
| Ca   | 28.730209 | 28.159443 | 29.728905 |
| Ca   | 30.744980 | 32.788391 | 27.274834 |
| Ca   | 30.419460 | 27.576496 | 24.796167 |
| Ca   | 33.395699 | 30.074928 | 28.104240 |
| Ca   | 34.215195 | 24.832165 | 27.113045 |
| Ca   | 35.355610 | 28.817131 | 23.722336 |
| S    | 21.207493 | 31.398546 | 35.685951 |
| S    | 20.361496 | 35.152763 | 33.088100 |
| S    | 22.081686 | 31.511391 | 29.562220 |
| S    | 25.014729 | 33.452374 | 33.423813 |
| S    | 26.394855 | 29.878094 | 30.860878 |
| S    | 26.082611 | 34.244244 | 28.590517 |
| S    | 28.562471 | 29.985489 | 26.482748 |
| S    | 30.749203 | 31.213753 | 30.135429 |
| S    | 31.556295 | 26.904232 | 28.118073 |
| S    | 32.628212 | 30.544119 | 24.732929 |
| S    | 33.331043 | 25.831894 | 23.702717 |
| S    | 35.888161 | 27.834497 | 26.812065 |

24 generated by VMD

| Ca   | 18.485416 | 32.612484 | 33.519363 |
| Ca   | 22.550753 | 34.669464 | 35.883522 |
| Ca   | 23.446562 | 30.441086 | 33.108055 |
| Ca   | 23.019745 | 34.676132 | 30.736698 |
| Ca   | 24.974018 | 30.997433 | 27.759972 |
| Ca   | 27.768015 | 33.029144 | 31.361570 |
| Ca   | 29.042944 | 28.154240 | 29.737392 |
| Ca   | 30.610065 | 32.524769 | 26.964966 |
| Ca   | 30.461697 | 27.803139 | 24.635923 |
| Ca   | 33.445095 | 29.778309 | 28.093893 |
| Ca   | 34.331512 | 24.685074 | 26.936609 |
| Ca   | 35.547291 | 28.790760 | 23.688873 |
| S    | 21.128864 | 31.474098 | 35.714825 |
S      20.388569       35.405205       32.913296
S      21.999931       31.423309       29.852995
S      25.072302       33.324043       33.517464
S      26.202137       29.892757       30.733322
S      25.965380       34.281513       28.661388
S      28.416435       29.922497       26.559521
S      30.800697       31.181812       30.165783
S      31.759375       26.967430       27.963417
S      32.508888       30.496441       24.786673
S      33.436039       25.815434       23.735252
S      36.358330       27.953495       26.909260

24
generated by VMD

Ca     18.291168       32.532745       34.093410
Ca     22.615723       35.117970       35.581314
Ca     23.471926       30.369951       33.039009
Ca     22.587290       34.966705       30.469366
Ca     25.071093       30.760395       27.841785
Ca     27.560280       32.696877       31.507710
Ca     29.179964       28.135614       29.667982
Ca     30.665348       32.563976       27.615692
Ca     30.544573       27.668354       24.626713
Ca     33.721355       29.820812       27.746496
Ca     34.419430       24.790051       26.686066
Ca     35.713276       28.751904       23.739582
S      21.252846       31.670107       35.897221
S      20.165297       35.553089       32.921669
S      22.001345       31.549995       29.775713
S      24.687279       33.647346       33.203289
S      26.090073       29.510836       30.617409
S      25.870564       34.145180       28.766928
S      28.586498       30.048994       26.552971
S      30.775379       30.859579       30.702187
S      31.982897       26.780991       28.021900
S      32.648121       30.769489       24.758675
S      33.281021       25.930017       23.410215
S      36.537354       27.659073       26.696728

24
generated by VMD

Ca     18.327408       32.493362       33.378502
Ca     22.473526       34.835670       35.502136
Ca     23.654308       30.328171       33.271080
Ca     22.855667       34.957359       30.350895
Ca     25.211836       30.829258       27.939190
Ca     27.670158       32.960121       31.616545
Ca     29.136494       28.139698       29.931328
| Element | X Coord | Y Coord | Z Coord |
|---------|---------|---------|---------|
| Ca      | 30.590021 | 32.411407 | 27.452539 |
| Ca      | 30.290247 | 27.812893 | 24.692551 |
| Ca      | 33.685795 | 34.563732 | 26.644459 |
| Ca      | 35.358505 | 28.859768 | 23.792589 |
| S       | 21.216579 | 31.425728 | 27.452539 |
| S       | 20.241243 | 35.409565 | 32.948280 |
| S       | 22.163549 | 31.334108 | 30.051201 |
| S       | 24.811230 | 33.745922 | 33.288765 |
| S       | 26.408922 | 29.726164 | 30.893705 |
| S       | 26.172966 | 34.263519 | 28.690563 |
| S       | 28.368620 | 30.052505 | 26.497400 |
| S       | 30.939522 | 31.108665 | 30.488493 |
| S       | 31.633450 | 26.815521 | 27.807301 |
| S       | 32.490883 | 30.530363 | 24.986938 |
| S       | 33.128078 | 25.895752 | 23.475224 |
| S       | 36.327297 | 27.701569 | 26.790058 |
| Ca      | 18.433516 | 32.869873 | 33.967503 |
| Ca      | 22.871204 | 34.941757 | 35.318981 |
| Ca      | 33.724548 | 30.026051 | 27.929533 |
| Ca      | 27.726631 | 32.472977 | 31.196861 |
| Ca      | 28.972363 | 27.895071 | 29.800100 |
| Ca      | 30.565649 | 32.518131 | 27.608093 |
| Ca      | 30.431208 | 27.917885 | 24.596394 |
| Ca      | 33.724548 | 30.026051 | 27.929533 |
| Ca      | 34.525772 | 24.785885 | 26.710251 |
| Ca      | 35.695251 | 29.020576 | 23.943302 |
| S       | 21.139694 | 31.606997 | 35.521320 |
| S       | 20.389023 | 35.718258 | 32.855789 |
| S       | 21.872055 | 31.337217 | 30.121639 |
| S       | 25.021523 | 33.583076 | 33.222145 |
| S       | 26.080023 | 29.608734 | 30.695274 |
| S       | 25.989162 | 34.213657 | 28.660492 |
| S       | 28.255285 | 29.782396 | 26.800381 |
| S       | 30.861855 | 30.860630 | 30.178225 |
| S       | 31.715363 | 26.766968 | 27.781132 |
| S       | 32.575996 | 30.760765 | 24.961380 |
| S       | 33.463943 | 26.155846 | 23.623451 |
| S       | 36.516048 | 27.753342 | 26.821651 |

24

generated by VMD

| Element | X Coord | Y Coord | Z Coord |
|---------|---------|---------|---------|
| Ca      | 18.433907 | 33.127625 | 34.090012 |

24

generated by VMD
|  | Ca   | S    | 24 |
|---|------|------|----|
| Ca| 23.087688 | 34.938858 | 35.478416 |
| Ca| 23.053391 | 30.311996 | 33.031376 |
| Ca| 22.731857 | 34.775032 | 30.355404 |
| Ca| 24.882532 | 30.445780 | 27.818821 |
| Ca| 27.586842 | 32.537006 | 31.359030 |
| Ca| 28.908089 | 27.839848 | 29.866856 |
| Ca| 30.561705 | 32.357681 | 27.561253 |
| Ca| 30.406773 | 27.953251 | 24.542572 |
| Ca| 33.849831 | 29.862858 | 27.906242 |
| Ca| 34.571430 | 24.886765 | 26.605957 |
| Ca| 35.704266 | 29.115404 | 23.743530 |
| S | 21.210754 | 31.795223 | 35.632324 |
| S | 20.742878 | 35.800156 | 33.163052 |
| S | 21.828951 | 31.229290 | 29.930374 |
| S | 24.715935 | 33.570454 | 33.151428 |
| S | 26.026472 | 29.381413 | 30.773922 |
| S | 25.901421 | 33.918793 | 28.378607 |
| S | 28.236774 | 29.748634 | 26.746281 |
| S | 30.764599 | 30.875000 | 30.369537 |
| S | 31.796286 | 26.843822 | 27.822269 |
| S | 32.662056 | 30.759272 | 25.108982 |
| S | 33.516659 | 26.374029 | 23.498856 |
| S | 36.538960 | 27.853199 | 27.004948 |

24 generated by VMD
S 32.857624 30.661964 25.071451
S 33.271141 26.163721 23.302624
S 36.456894 27.72844 26.611977

24
generated by VMD

Ca 18.455803 32.710506 34.180542
Ca 22.940443 34.875038 35.569500
Ca 23.592773 30.393520 32.934223
Ca 22.914494 34.861610 30.435179
Ca 24.771847 30.588507 27.669165
Ca 27.707771 32.698441 31.109442
Ca 28.855865 27.832186 29.587982
Ca 30.427979 32.537125 27.340021
Ca 30.467728 28.026318 24.758459
Ca 33.614822 29.923416 28.201088
Ca 34.266647 24.778240 26.864334
Ca 35.562023 29.099234 23.944874
S 21.340927 31.524513 35.504951
S 20.738115 35.525635 33.165115
S 22.020554 31.170307 29.805447
S 25.100563 33.657349 33.091354
S 26.061312 29.592201 30.622253
S 25.772224 34.058464 28.431473
S 28.155457 29.904255 26.622910
S 30.765568 30.940109 30.231695
S 31.662678 26.835825 28.063622
S 32.691746 30.892201 25.109333
S 33.358128 26.252430 23.685175
S 36.474567 27.622150 27.011892

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Ca 18.398464 32.850044 33.943909
Ca 23.094090 35.236244 35.437946
Ca 23.715967 30.344303 33.040062
Ca 22.814152 34.743698 30.566332
Ca 24.745880 30.393400 27.749025
Ca 27.733215 32.650917 31.111113
Ca 28.841745 27.819006 29.573845
Ca 30.398006 32.417717 27.626947
Ca 30.613937 28.147001 24.685106
Ca 33.527489 29.722027 28.244585
Ca 34.442234 24.739422 26.489746
Ca 35.755142 29.194136 24.032022
S 21.415234 31.860500 35.533787
S 20.374821 35.767883 33.145561
S 21.932034 31.152340 29.966747
|   | X    | Y    | Z    |
|---|------|------|------|
| S | 24.879150 | 33.687675 | 33.154770 |
| S | 26.137020 | 29.340908 | 30.884077 |
| S | 25.749475 | 33.726997 | 30.925089 |
| S | 28.067078 | 29.752495 | 26.676188 |
| S | 30.624519 | 26.932201 | 27.820225 |
| S | 31.896545 | 26.490065 | 23.391462 |
| S | 36.300339 | 27.535126 | 26.994513 |

generated by VMD

| Ca | X    | Y    | Z    |
|----|------|------|------|
| Ca | 18.191254 | 32.541901 | 33.847240 |
| Ca | 22.779415 | 32.541901 | 35.613876 |
| Ca | 23.499268 | 30.423992 | 33.072781 |
| Ca | 22.986534 | 34.927849 | 30.629238 |
| Ca | 24.726517 | 30.725657 | 27.826674 |
| Ca | 27.944502 | 32.842163 | 31.133772 |
| Ca | 29.189327 | 27.852938 | 29.53178 |
| Ca | 30.594318 | 32.404594 | 27.518085 |
| Ca | 30.429928 | 27.963642 | 24.752581 |
| Ca | 33.837284 | 29.907549 | 27.916149 |
| Ca | 34.341022 | 24.758831 | 26.815842 |
| Ca | 35.510380 | 28.825867 | 24.034126 |
| S | 21.217749 | 31.621798 | 35.533524 |
| S | 20.243187 | 35.422180 | 33.117348 |
| S | 21.903709 | 31.374741 | 29.979773 |
| S | 25.006886 | 33.870121 | 33.127514 |
| S | 26.322723 | 29.681576 | 30.901741 |
| S | 25.694473 | 34.062057 | 28.350803 |
| S | 28.183220 | 29.985123 | 26.768555 |
| S | 30.779787 | 30.906570 | 30.150291 |
| S | 31.782217 | 26.951603 | 27.788450 |
| S | 32.816650 | 30.748405 | 24.969734 |
| S | 33.200970 | 26.301853 | 23.54149 |
| S | 36.538727 | 27.463947 | 26.955355 |

generated by VMD

| Ca | X    | Y    | Z    |
|----|------|------|------|
| Ca | 18.359919 | 32.821114 | 33.651852 |
| Ca | 22.945000 | 34.768429 | 35.634529 |
| Ca | 23.680557 | 30.517437 | 33.281357 |
| Ca | 23.003859 | 34.665009 | 30.380268 |
| Ca | 24.667572 | 30.483185 | 27.757576 |
| Ca | 27.984802 | 32.972942 | 31.304352 |
| Ca | 28.844631 | 27.947540 | 29.851589 |
| Ca | 30.446178 | 32.339779 | 27.501085 |
| Ca | 30.264812 | 27.854939 | 24.501488 |
| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 33.742886 | 29.838902 | 28.047171 |
| Ca      | 34.299789  | 24.923672 | 26.548615 |
| Ca      | 35.660221  | 29.085550 | 23.90525  |
| S       | 21.108744  | 31.580986 | 35.479046 |
| S       | 20.568287  | 35.530403 | 32.890167 |
| S       | 22.147564  | 31.204838 | 23.950525 |
| S       | 24.940392  | 33.763477 | 33.20515  |
| S       | 26.242634  | 29.664227 | 31.125647 |
| S       | 25.809517  | 33.935600 | 28.465895 |
| S       | 28.063448  | 29.782215 | 26.807068 |
| S       | 30.717222  | 31.042778 | 30.265488 |
| S       | 31.551947  | 26.884995 | 27.642172 |
| S       | 32.722683  | 30.556870 | 25.163698 |
| S       | 33.479645  | 26.438435 | 23.359047 |
| S       | 36.467751  | 27.696724 | 27.115988 |

24 generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 18.284046 | 32.938713 | 34.097878 |
| Ca      | 22.956127 | 34.723555 | 35.950584 |
| Ca      | 23.456520 | 30.530750 | 32.885998 |
| Ca      | 22.807796 | 34.639832 | 30.470303 |
| Ca      | 24.851093 | 30.535694 | 27.598011 |
| Ca      | 27.833694 | 32.808754 | 31.288675 |
| Ca      | 28.819027 | 27.937183 | 29.661276 |
| Ca      | 30.432510 | 32.353401 | 27.349064 |
| Ca      | 30.414864 | 27.883934 | 24.334461 |
| Ca      | 33.751106 | 29.954613 | 28.003298 |
| Ca      | 34.225109 | 24.766582 | 26.775267 |
| Ca      | 35.752708 | 28.941437 | 24.191637 |
| S       | 21.337654 | 31.710499 | 35.543968 |
| S       | 20.494793 | 35.515160 | 33.286507 |
| S       | 21.955969 | 31.140411 | 29.919443 |
| S       | 24.987862 | 33.818661 | 33.116657 |
| S       | 26.266567 | 29.672661 | 30.825268 |
| S       | 25.686625 | 33.894917 | 28.429123 |
| S       | 28.124580 | 29.874207 | 26.527063 |
| S       | 30.835785 | 31.116852 | 30.234356 |
| S       | 31.596464 | 26.856070 | 27.536554 |
| S       | 32.840084 | 30.712971 | 25.013460 |
| S       | 33.624554 | 26.266216 | 23.495550 |
| S       | 36.382500 | 27.707012 | 27.405693 |

24 generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 18.238352 | 32.934555 | 33.961136 |
| Ca      | 22.855330 | 34.771030 | 35.791836 |
| Ca      | 23.347878 | 30.357468 | 33.035519 |
|   |                  |                  |                  |
|---|----------------|----------------|----------------|
| Ca | 22.906282       | 34.350170       | 30.395454       |
| Ca | 24.979122       | 30.667513       | 27.731575       |
| Ca | 27.903828       | 32.936962       | 31.319555       |
| Ca | 29.095165       | 28.103788       | 29.769438       |
| Ca | 30.496014       | 32.444057       | 27.461042       |
| Ca | 30.441965       | 27.886387       | 24.491734       |
| Ca | 33.743454       | 29.859684       | 28.131975       |
| Ca | 34.079720       | 24.619299       | 26.619699       |
| Ca | 35.615147       | 29.069597       | 24.075544       |
| S  | 21.169708       | 31.708654       | 35.692184       |
| S  | 20.506567       | 35.560703       | 32.922371       |
| S  | 21.905642       | 30.977221       | 29.969257       |
| S  | 24.938889       | 33.787376       | 33.102535       |
| S  | 26.266657       | 29.650171       | 30.97240       |
| S  | 25.874578       | 34.021343       | 28.302595       |
| S  | 28.224312       | 30.005936       | 26.475374       |
| S  | 30.884102       | 31.136703       | 30.549280       |
| S  | 31.767275       | 26.962494       | 27.863819       |
| S  | 32.571800       | 30.725563       | 25.187000       |
| S  | 33.430428       | 26.183884       | 23.309416       |
| S  | 36.477821       | 27.579466       | 26.809008       |
|   | generated by VMD |                  |                  |
| Ca | 18.302076       | 33.055489       | 33.423000       |
| Ca | 22.825233       | 34.866646       | 35.685310       |
| Ca | 23.478432       | 30.194901       | 33.110134       |
| Ca | 23.151369       | 34.621494       | 30.389685       |
| Ca | 24.865791       | 30.347939       | 27.704285       |
| Ca | 27.861778       | 32.517689       | 31.242311       |
| Ca | 29.143360       | 28.272488       | 30.060261       |
| Ca | 30.305000       | 32.636856       | 27.562180       |
| Ca | 30.400290       | 27.936691       | 24.763103       |
| Ca | 33.905754       | 30.023842       | 27.880880       |
| Ca | 34.055305       | 24.661791       | 26.669716       |
| Ca | 35.409252       | 29.144184       | 24.116602       |
| S  | 21.024654       | 31.685333       | 35.459557       |
| S  | 20.618561       | 35.800674       | 32.925060       |
| S  | 21.976597       | 31.221260       | 29.867718       |
| S  | 24.974987       | 33.460461       | 33.165390       |
| S  | 26.257298       | 29.322495       | 31.169693       |
| S  | 26.031038       | 33.654877       | 28.483362       |
| S  | 28.139938       | 29.869408       | 26.982634       |
| S  | 30.913544       | 31.161484       | 30.448330       |
| S  | 31.898928       | 27.167185       | 27.868349       |
| S  | 32.398746       | 30.987129       | 25.065777       |
| S  | 33.265629       | 26.208893       | 23.414719       |
|    |      |      |      |
|----|------|------|------|
| S  | 36.516483 | 27.480820 | 26.481634 |
| Ca | 18.272072 | 33.039078 | 33.510403 |
| Ca | 23.012886 | 34.839966 | 35.637951 |
| Ca | 23.139427 | 30.341000 | 33.139824 |
| Ca | 23.165375 | 34.783039 | 30.535645 |
| Ca | 24.784557 | 30.540798 | 27.690659 |
| Ca | 28.036697 | 32.409538 | 31.393047 |
| Ca | 29.013494 | 27.911596 | 30.154476 |
| Ca | 30.724869 | 32.389153 | 27.620808 |
| Ca | 30.433186 | 27.722187 | 24.647015 |
| Ca | 33.695457 | 29.935785 | 27.937614 |
| Ca | 34.295788 | 25.035175 | 26.750332 |
| Ca | 35.274410 | 29.163006 | 23.685705 |
| S  | 20.973419 | 31.752411 | 35.539520 |
| S  | 20.584345 | 35.727451 | 32.964836 |
| S  | 21.815067 | 31.273514 | 29.798466 |
| S  | 25.002090 | 33.531609 | 33.155075 |
| S  | 26.097984 | 29.444824 | 31.007580 |
| S  | 26.001270 | 33.835033 | 28.469131 |
| S  | 28.107525 | 29.601982 | 26.845894 |
| S  | 30.958237 | 31.025293 | 30.412100 |
| S  | 31.837040 | 26.932999 | 27.924826 |
| S  | 32.410782 | 30.656780 | 25.026470 |
| S  | 33.535244 | 26.308496 | 23.488733 |
| S  | 36.546989 | 28.099335 | 26.602959 |

generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 18.620100 | 32.371346 | 33.307610 |
| Ca | 22.814507 | 34.841980 | 35.578369 |
| Ca | 23.776508 | 30.539728 | 33.222000 |
| Ca | 22.801893 | 34.839256 | 30.267773 |
| Ca | 24.869949 | 30.509972 | 27.838421 |
| Ca | 27.860567 | 32.944157 | 31.488195 |
| Ca | 29.041210 | 28.039845 | 29.886818 |
| Ca | 30.488991 | 32.233009 | 27.486944 |
| Ca | 30.423046 | 27.812965 | 24.688366 |
| Ca | 33.710594 | 29.979359 | 28.237543 |
| Ca | 33.979538 | 24.903940 | 26.450363 |
| Ca | 35.582771 | 29.045378 | 23.835875 |
| S  | 21.207695 | 31.689098 | 35.592384 |
| S  | 20.461884 | 35.434841 | 32.938766 |
| S  | 21.981382 | 31.564217 | 29.959589 |
| S  | 24.957535 | 33.961449 | 33.062614 |
| S  | 26.149834 | 29.619919 | 31.170494 |
|   | 2010.001637 | 33.749054 | 28.562395 |
|---|-------------|------------|------------|
| S | 28.154968   | 29.619081  | 26.792587  |
| S | 30.742632   | 31.007450  | 30.533958  |
| S | 31.903595   | 28.50395   | 27.919065  |
| S | 32.603256   | 30.533096  | 25.182810  |
| S | 33.170055   | 26.496344  | 23.074469  |
| S | 36.415920   | 27.714184  | 26.862619  |

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generated by VMD

| Ca | 18.391222 | 32.673855 | 33.736202 |
|----|-----------|-----------|-----------|
| Ca | 22.934402 | 35.241043 | 35.468689 |
| Ca | 23.372822 | 30.492676 | 33.081886 |
| Ca | 22.751173 | 34.745514 | 30.349880 |
| Ca | 24.908268 | 30.355946 | 27.733492 |
| Ca | 27.819139 | 32.594894 | 31.700056 |
| Ca | 28.951420 | 27.944254 | 29.855474 |
| Ca | 30.684582 | 32.318333 | 27.562843 |
| Ca | 30.523670 | 27.961685 | 24.769152 |
| Ca | 34.007717 | 29.713774 | 28.102526 |
| Ca | 34.169930 | 24.929146 | 26.223064 |
| Ca | 35.655064 | 29.112356 | 23.706259 |
| S  | 21.118969 | 31.946609 | 35.904850 |
| S  | 20.235754 | 35.628662 | 32.737541 |
| S  | 21.824951 | 31.205399 | 29.952473 |
| S  | 24.829008 | 33.956951 | 33.148407 |
| S  | 26.041588 | 29.506126 | 31.092585 |
| S  | 25.864147 | 33.833225 | 28.665478 |
| S  | 28.131248 | 29.722317 | 26.715679 |
| S  | 30.782854 | 30.734032 | 30.634703 |
| S  | 32.019756 | 26.955973 | 27.772160 |
| S  | 32.660793 | 30.651207 | 25.215656 |
| S  | 33.354527 | 26.328684 | 23.123527 |
| S  | 36.687042 | 27.747423 | 26.687754 |

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generated by VMD

| Ca | 18.440998 | 32.525726 | 33.720917 |
|----|-----------|-----------|-----------|
| Ca | 22.878448 | 35.129990 | 35.390587 |
| Ca | 23.370602 | 30.423775 | 33.208450 |
| Ca | 22.963402 | 34.850739 | 30.246750 |
| Ca | 25.046200 | 30.468004 | 27.970783 |
| Ca | 27.722691 | 32.474312 | 31.340563 |
| Ca | 28.949274 | 27.980207 | 29.800463 |
| Ca | 30.549717 | 32.545998 | 27.673874 |
| Ca | 30.417900 | 27.811337 | 24.599569 |
| Ca | 33.669006 | 29.894289 | 27.992754 |
| Ca | 34.189308 | 24.765356 | 26.478155 |
|   | Ca     | S       | S       |
|---|--------|---------|---------|
| S | 35.564785     | 29.132744     | 23.871843     |
| S | 21.238213     | 31.909592     | 35.908813     |
| S | 20.246822     | 35.359383     | 32.698395     |
| S | 21.951077     | 31.240936     | 30.019125     |
| S | 25.026512     | 33.688843     | 33.146141     |
| S | 26.001663     | 29.493607     | 30.878469     |
| S | 25.991127     | 34.053345     | 28.612844     |
| S | 28.313770     | 30.060951     | 26.924942     |
| S | 30.876846     | 30.971060     | 30.439589     |
| S | 31.925541     | 26.998550     | 27.918573     |
| S | 32.712463     | 30.634121     | 25.046677     |
| S | 33.336861     | 26.297596     | 23.162426     |
| S | 36.336861     | 27.589569     | 26.889381     |

24 generated by VMD

|   | Ca     | S       | S       |
|---|--------|---------|---------|
| Ca | 18.587006     | 32.383659     | 33.523167     |
| Ca | 22.705912     | 35.225449     | 34.882477     |
| Ca | 23.643951     | 30.348492     | 33.383625     |
| Ca | 22.982285     | 34.734798     | 30.423300     |
| Ca | 25.009438     | 30.449617     | 28.136889     |
| Ca | 27.809135     | 32.771698     | 31.550394     |
| Ca | 28.946022     | 27.931763     | 29.870182     |
| Ca | 30.606794     | 32.462780     | 27.692055     |
| Ca | 30.563368     | 28.190483     | 24.663786     |
| Ca | 33.480576     | 29.649982     | 27.909838     |
| Ca | 34.134342     | 24.687546     | 26.172277     |
| Ca | 35.504959     | 29.103661     | 23.939293     |
| S | 21.256870     | 31.994625     | 35.959118     |
| S | 20.015390     | 35.352318     | 32.156971     |
| S | 22.065647     | 31.155676     | 30.138937     |
| S | 24.829515     | 33.964424     | 33.156494     |
| S | 26.370287     | 29.352955     | 31.165670     |
| S | 26.048569     | 33.966911     | 28.956486     |
| S | 28.332304     | 29.926453     | 27.002453     |
| S | 30.834202     | 30.916508     | 30.493542     |
| S | 31.902538     | 26.959290     | 27.815575     |
| S | 32.794743     | 30.934910     | 25.087233     |
| S | 33.086327     | 26.423958     | 23.091057     |
| S | 36.209831     | 27.412060     | 26.769232     |

24 generated by VMD

|   | Ca     | S       | S       |
|---|--------|---------|---------|
| Ca | 18.432766     | 32.757675     | 33.598198     |
| Ca | 22.768280     | 35.457279     | 34.998219     |
| Ca | 23.497368     | 30.314304     | 33.573040     |
| Ca | 22.865141     | 34.632229     | 30.524975     |
| Ca | 24.912678     | 30.392300     | 28.107376     |
| Ca   | 27.824282 | 32.603313 | 31.306356 |
| Ca   | 29.001377 | 27.591011 | 29.884884 |
| Ca   | 30.631447 | 32.343048 | 27.470354 |
| Ca   | 30.365795 | 28.272486 | 24.349060 |
| Ca   | 33.796211 | 29.672430 | 28.209850 |
| Ca   | 33.979233 | 24.811539 | 26.186310 |
| Ca   | 35.550446 | 29.542694 | 23.986950 |
| S    | 21.420494 | 32.267010 | 35.889423 |
| S    | 20.227869 | 35.533463 | 32.210995 |
| S    | 21.999454 | 30.905033 | 30.169588 |
| S    | 24.945839 | 33.786190 | 33.219566 |
| S    | 26.192131 | 29.224522 | 31.181295 |
| S    | 26.001408 | 33.820953 | 28.810364 |
| S    | 28.375059 | 29.678589 | 26.837202 |
| S    | 30.797716 | 30.738701 | 30.479979 |
| S    | 31.630753 | 26.816067 | 27.695881 |
| S    | 32.770870 | 30.723206 | 25.229406 |
| S    | 33.417511 | 26.759163 | 23.098103 |
| S    | 36.315945 | 27.656830 | 26.922649 |

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generated by VMD

| Ca   | 18.874081 | 32.470638 | 33.632633 |
| Ca   | 22.992754 | 35.349106 | 35.124763 |
| Ca   | 23.486252 | 30.433342 | 33.149128 |
| Ca   | 22.982489 | 34.845284 | 30.605661 |
| Ca   | 25.037529 | 30.333197 | 27.928648 |
| Ca   | 27.795006 | 32.660469 | 31.515394 |
| Ca   | 28.794617 | 27.669544 | 29.700697 |
| Ca   | 30.289448 | 32.131706 | 27.398689 |
| Ca   | 30.399273 | 27.826138 | 24.491898 |
| Ca   | 33.356544 | 29.961967 | 28.308491 |
| Ca   | 34.116707 | 25.094334 | 26.393492 |
| Ca   | 35.784012 | 29.427195 | 24.039215 |
| S    | 21.464336 | 32.074249 | 35.695236 |
| S    | 20.356514 | 35.497681 | 32.700806 |
| S    | 22.035400 | 31.401451 | 29.896608 |
| S    | 25.035355 | 33.777988 | 33.270103 |
| S    | 26.145489 | 29.438999 | 31.106594 |
| S    | 25.913929 | 33.811146 | 28.698853 |
| S    | 28.093714 | 29.476688 | 26.743979 |
| S    | 30.669954 | 30.747072 | 30.426331 |
| S    | 31.637012 | 26.747526 | 27.662737 |
| S    | 32.591927 | 30.627949 | 25.178990 |
| S    | 33.652264 | 26.705688 | 23.098173 |
| S    | 36.215462 | 27.790707 | 27.173044 |
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.694668     | 32.173584     | 33.947884     |
| Ca      | 22.659008     | 35.538582     | 35.180809     |
| Ca      | 23.614742     | 30.480465     | 33.355141     |
| Ca      | 22.786678     | 34.703224     | 30.244049     |
| Ca      | 24.920647     | 30.443087     | 28.034979     |
| Ca      | 27.927280     | 32.769684     | 31.421211     |
| Ca      | 28.832081     | 27.742752     | 29.646862     |
| Ca      | 30.632099     | 32.505886     | 27.607492     |
| Ca      | 30.498310     | 28.360420     | 24.49944      |
| Ca      | 33.543266     | 29.611195     | 28.054436     |
| Ca      | 33.935417     | 24.622097     | 26.188700     |
| Ca      | 35.756798     | 29.148682     | 24.329861     |
| S       | 21.575893     | 32.233284     | 35.901970     |
| S       | 20.106249     | 35.227108     | 32.566761     |
| S       | 22.090923     | 31.181057     | 29.984894     |
| S       | 24.848076     | 33.808510     | 33.045944     |
| S       | 26.378738     | 29.412596     | 31.162430     |
| S       | 25.896482     | 33.893307     | 28.643097     |
| S       | 28.148914     | 29.928478     | 26.639109     |
| S       | 30.697319     | 30.909636     | 30.374504     |
| S       | 31.715725     | 26.826675     | 27.659935     |
| S       | 32.656406     | 30.820570     | 25.211761     |
| S       | 33.562019     | 26.621857     | 23.100586     |
| S       | 36.242283     | 27.337296     | 27.134151     |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.602600     | 32.638126     | 33.968010     |
| Ca      | 23.024368     | 35.323395     | 34.932907     |
| Ca      | 23.698647     | 30.191273     | 33.320843     |
| Ca      | 22.631859     | 34.397224     | 30.313974     |
| Ca      | 25.092884     | 30.723433     | 28.016775     |
| Ca      | 27.612549     | 32.741470     | 31.356674     |
| Ca      | 28.737055     | 27.702894     | 29.628222     |
| Ca      | 30.659054     | 32.319374     | 27.254068     |
| Ca      | 30.415548     | 28.197754     | 24.380789     |
| Ca      | 33.529430     | 29.838993     | 28.365845     |
| Ca      | 33.951248     | 24.892654     | 26.186810     |
| Ca      | 35.868656     | 29.188511     | 24.307915     |
| S       | 21.705772     | 32.133125     | 35.908089     |
| S       | 20.350159     | 35.552425     | 32.566761     |
| S       | 22.059437     | 30.947384     | 30.180443     |
| S       | 24.899940     | 33.682098     | 33.112995     |
| S       | 26.228123     | 29.300789     | 31.079390     |
| S       | 26.020226     | 33.890480     | 28.795956     |
| S       | 28.194296     | 29.844540     | 26.535627     |
|  |  |  |  |  |  |  |
|---|---|---|---|---|---|---|
| S | 30.589903 | 30.868835 | 30.352270 |
| S | 31.438972 | 26.831196 | 27.589529 |
| S | 32.826195 | 30.823627 | 25.207212 |
| S | 33.495960 | 26.623325 | 23.228554 |
| S | 36.087158 | 27.647148 | 27.350391 |

24
generated by VMD

| Ca | 18.426083 | 32.357883 | 33.936909 |
| Ca | 22.739326 | 35.291149 | 34.924908 |
| Ca | 23.499645 | 30.300665 | 33.293022 |
| Ca | 22.999537 | 34.777855 | 30.530579 |
| Ca | 24.908855 | 30.484875 | 28.108318 |
| Ca | 27.895679 | 32.837204 | 31.633787 |
| Ca | 28.960217 | 27.861164 | 29.690017 |
| Ca | 30.468563 | 32.207527 | 27.106085 |
| Ca | 30.615143 | 28.371264 | 24.464155 |
| Ca | 33.467846 | 29.926353 | 28.293289 |
| Ca | 33.940884 | 24.865913 | 26.157242 |
| Ca | 35.851173 | 28.833450 | 24.088221 |
| S  | 21.316589 | 32.119328 | 35.804379 |
| S  | 20.242437 | 35.213013 | 32.382401 |
| S  | 22.149017 | 31.168531 | 30.015287 |
| S  | 25.018448 | 33.741062 | 33.347809 |
| S  | 26.337685 | 29.589977 | 31.188938 |
| S  | 26.106024 | 33.835648 | 28.870155 |
| S  | 28.108509 | 29.576260 | 26.692829 |
| S  | 30.860798 | 30.912584 | 30.363979 |
| S  | 31.570194 | 27.056841 | 27.627390 |
| S  | 32.988464 | 30.879654 | 25.087229 |
| S  | 33.394722 | 26.487612 | 23.069456 |
| S  | 35.854156 | 27.604183 | 27.255730 |

24
generated by VMD

| Ca | 18.361696 | 32.500416 | 33.887909 |
| Ca | 22.595909 | 35.269684 | 35.048889 |
| Ca | 23.883415 | 30.371988 | 33.431179 |
| Ca | 22.801769 | 34.671997 | 30.426970 |
| Ca | 25.065596 | 30.493607 | 28.036539 |
| Ca | 28.046322 | 32.964428 | 31.690691 |
| Ca | 29.018303 | 27.853317 | 29.836975 |
| Ca | 30.559921 | 32.336494 | 27.549723 |
| Ca | 30.487349 | 28.025764 | 24.179794 |
| Ca | 33.548279 | 29.667850 | 28.260876 |
| Ca | 33.958843 | 24.874657 | 26.076195 |
| Ca | 35.675224 | 29.027311 | 23.944859 |
| S  | 21.331451 | 31.884979 | 35.723961 |
S  19.951164  35.540916  32.399769
S  22.190331  31.203011  30.148426
S  24.701862  33.893600  33.348087
S  26.544176  29.665434  31.192488
S  25.994282  33.929420  28.663294
S  28.125679  29.648966  26.674416
S  30.845636  30.923000  30.485741
S  31.568283  26.830318  27.543571
S  32.593639  30.568764  25.268318
S  33.598568  26.507383  22.929752
S  36.272301  27.646698  27.191645
24
generated by VMD
Ca  18.667807  32.345104  34.113365
Ca  22.952225  35.108318  35.292008
Ca  23.411331  30.381371  33.184437
Ca  22.870159  34.716305  30.330160
Ca  24.631718  30.510450  27.775045
Ca  27.876186  32.973881  31.273474
Ca  28.652966  27.739710  29.805868
Ca  30.481245  32.349361  27.495762
Ca  30.674574  28.051548  24.283157
Ca  33.616219  29.837872  28.359795
Ca  34.009926  24.886913  26.228001
Ca  35.819767  29.018967  24.136204
S  21.586193  31.887524  35.975179
S  20.227833  35.416550  32.785843
S  21.965687  31.312904  30.014412
S  24.921850  33.828297  33.140450
S  26.204609  29.722801  31.032856
S  25.791302  34.020985  28.425966
S  28.118748  29.651966  26.670189
S  30.701071  30.962265  30.276518
S  31.443310  26.792490  27.763702
S  33.117962  30.769682  25.205814
S  33.561031  26.448771  23.071356
S  36.416298  27.566042  27.290011
24
generated by VMD
Ca  18.523350  32.525620  33.962051
Ca  22.782211  35.094067  35.632771
Ca  23.636742  30.690441  33.156422
Ca  22.842752  34.706390  30.455999
Ca  24.932123  30.520599  27.808409
Ca  27.759758  32.979836  31.455702
Ca  28.909782  27.944952  29.618021
| Element | Ca 0.462364 | Ca 0.513201 | Ca 0.420540 | Ca 0.179718 | Ca 0.898304 | S 1.494400 | S 2.763900 | S 1.924278 | S 0.83565  | S 0.381901 | S 0.789471 | S 0.054344 | S 0.615238 | S 0.479975 | S 0.792870 | S 0.567551 | S 0.399162 | 24 generated by VMD | Ca 0.874313 | Ca 0.71883 | Ca 0.781418 | Ca 0.722446 | Ca 0.777000 | Ca 0.016594 | Ca 0.851170 | Ca 0.400534 | Ca 0.519001 | Ca 0.556103 | Ca 0.322222 | Ca 0.746731 | S 1.826843 | S 0.254196 | S 0.938639 | S 0.020512 | S 0.268475 | S 0.654379 | S 1.20865 | S 0.806379 | S 1.483141 | S 0.710838 | S 0.477028 | S 0.209389 | 24 generated by VMD | Ca 0.442795 | 32.312134 | 33.893143 |
|   |     |     |     |
|---|-----|-----|-----|
| Ca| 22.727516 | 35.085808 | 35.509430 |
| Ca| 23.593533 | 30.538784 | 33.112038 |
| Ca| 22.552599 | 34.750381 | 30.322380 |
| Ca| 25.129467 | 30.731798 | 28.120529 |
| Ca| 27.881931 | 32.943222 | 31.358374 |
| Ca| 28.836468 | 27.965336 | 29.774323 |
| Ca| 30.344641 | 32.523045 | 27.349558 |
| Ca| 30.481182 | 27.958269 | 24.576336 |
| Ca| 33.368504 | 29.635759 | 27.948826 |
| Ca| 33.879093 | 24.575590 | 26.168972 |
| Ca| 36.176868 | 29.143518 | 24.562449 |
| S | 21.570917 | 31.778648 | 35.836788 |
| S | 20.249952 | 35.405697 | 32.773476 |
| S | 22.034382 | 31.240143 | 30.141577 |
| S | 24.941853 | 33.957260 | 32.986549 |
| S | 26.544819 | 29.773708 | 31.368134 |
| S | 25.741898 | 33.887199 | 28.476873 |
| S | 28.163465 | 29.664330 | 26.680296 |
| S | 30.767626 | 30.966042 | 30.067245 |
| S | 31.451368 | 26.95917 | 27.354412 |
| S | 32.76682 | 30.936405 | 25.039061 |
| S | 33.780190 | 26.571215 | 23.353907 |
| S | 36.292274 | 27.259827 | 27.165382 |

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generated by VMD

|   |     |     |     |
|---|-----|-----|-----|
| Ca| 18.466259 | 32.084137 | 34.026665 |
| Ca| 22.827765 | 35.002232 | 35.534271 |
| Ca| 23.512939 | 30.668221 | 33.012962 |
| Ca| 22.515524 | 34.809933 | 30.204880 |
| Ca| 25.198170 | 30.589806 | 28.095085 |
| Ca| 27.910244 | 33.078178 | 31.220222 |
| Ca| 29.242714 | 27.919600 | 29.729885 |
| Ca| 30.687571 | 32.581589 | 27.379068 |
| Ca| 30.546755 | 28.011173 | 24.269508 |
| Ca| 33.488178 | 29.579620 | 28.129589 |
| Ca| 33.654190 | 24.754505 | 26.314316 |
| Ca| 35.798424 | 29.078186 | 24.418072 |
| S | 21.494505 | 31.689642 | 35.930843 |
| S | 20.243391 | 35.137291 | 33.042068 |
| S | 21.802910 | 31.253450 | 29.925051 |
| S | 24.898027 | 34.062801 | 32.940414 |
| S | 26.620113 | 29.886513 | 31.249075 |
| S | 25.710480 | 34.099838 | 28.337229 |
| S | 28.363041 | 29.692841 | 26.662834 |
| S | 30.827728 | 31.285110 | 30.286369 |
| S | 31.273458 | 26.689686 | 27.534349 |
S        32.860229       30.548086       25.151848  
S        33.587391       26.489109       23.143074  
S        36.190086       27.308519       27.402411  

24  generated by VMD
Ca       18.641895       32.084427       33.964661  
Ca       23.040422       34.919037       35.662476  
Ca       23.512375       30.637363       33.040192  
Ca       22.666946       34.875786       30.169203  
Ca       24.823738       30.748955       27.913429  
Ca       27.694017       32.874252       31.224522  
Ca       28.829819       27.953938       29.527458  
Ca       30.457108       32.591110       27.490587  
Ca       30.474180       28.101315       24.563894  
Ca       33.532234       29.819954       28.030766  
Ca       34.178360       24.710213       26.525114  
Ca       35.866459       28.854992       24.329973  
S        21.564255       31.700977       35.88638  
S        20.508066       35.181984       33.047565  
S        21.964352       31.314743       29.979149  
S        24.959389       33.934097       33.059708  
S        26.290298       29.789242       30.967308  
S        25.538532       34.263546       28.343678  
S        28.072674       29.831923       26.661766  
S        30.724091       31.084831       30.103348  
S        31.503208       26.714577       27.479141  
S        32.922729       30.618050       25.117750  
S        33.569878       26.340305       23.307499  
S        36.384972       27.354420       27.542236  

24  generated by VMD
Ca       19.035250       31.678324       33.905724  
Ca       22.845438       35.138245       35.573296  
Ca       23.512634       30.621880       32.939560  
Ca       22.718473       35.092743       30.374065  
Ca       24.964994       30.924259       27.719967  
Ca       27.892437       33.033516       31.288275  
Ca       28.927921       27.962204       29.715479  
Ca       30.513466       32.501553       27.343945  
Ca       30.365938       27.900959       24.611536  
Ca       33.536133       29.722136       28.129061  
Ca       34.274765       24.831169       26.453535  
Ca       35.632732       28.855045       24.492727  
S        21.569031       31.776794       35.930408  
S        20.263529       34.945057       33.034691  
S        21.955406       31.461140       29.711914  

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|  |  |  |
|---|---|---|
| S | 24.869991 | 33.983631 | 33.174 |
| S | 26.325848 | 29.832014 | 30.817852 |
| S | 25.707363 | 34.163040 | 28.394777 |
| S | 28.254368 | 29.778687 | 26.603821 |
| S | 30.744232 | 30.970655 | 30.172796 |
| S | 31.550499 | 26.634525 | 27.663855 |
| S | 32.731182 | 30.650394 | 25.227854 |
| S | 33.329689 | 26.456814 | 23.390413 |
| S | 36.198761 | 27.385262 | 27.269964 |

24

generated by VMD

| Ca | 19.045858 | 31.795700 | 33.845467 |
| Ca | 22.617702 | 35.098572 | 35.692726 |
| Ca | 23.565763 | 30.591316 | 33.132153 |
| Ca | 22.823139 | 34.979843 | 30.275808 |
| Ca | 24.966469 | 30.533108 | 27.814085 |
| Ca | 27.653166 | 33.102474 | 31.345505 |
| Ca | 29.075033 | 28.044434 | 29.781445 |
| Ca | 30.747883 | 32.587612 | 27.138556 |
| Ca | 30.439363 | 28.121769 | 24.409479 |
| Ca | 33.369011 | 29.714485 | 28.192934 |
| Ca | 34.106407 | 24.703075 | 26.419538 |
| Ca | 35.800003 | 28.674677 | 24.150906 |
| S | 21.373451 | 31.579857 | 35.902725 |
| S | 20.296314 | 35.213943 | 32.925919 |
| S | 22.027746 | 31.383846 | 29.851257 |
| S | 24.793606 | 34.012802 | 33.206375 |
| S | 26.270790 | 29.845345 | 31.152521 |
| S | 25.683304 | 34.026272 | 28.430090 |
| S | 28.416838 | 29.831421 | 26.756407 |
| S | 30.815302 | 31.297430 | 30.318079 |
| S | 31.341679 | 26.833893 | 27.595421 |
| S | 32.955715 | 30.633434 | 25.096210 |
| S | 33.451225 | 26.483019 | 23.176233 |
| S | 36.084328 | 27.211727 | 27.330299 |

24

generated by VMD

| Ca | 18.558281 | 32.293262 | 33.930840 |
| Ca | 22.493027 | 35.191193 | 35.697670 |
| Ca | 23.548059 | 30.687828 | 33.054939 |
| Ca | 22.691715 | 34.719189 | 30.222347 |
| Ca | 25.123138 | 30.353214 | 28.085165 |
| Ca | 27.522617 | 33.097790 | 31.610273 |
| Ca | 29.199249 | 28.108532 | 29.829187 |
| Ca | 30.599792 | 32.350487 | 27.419912 |
| Ca | 30.521564 | 28.059753 | 24.304424 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 34.125710    | 29.346270    | 27.682045    |
| Ca      | 33.994350    | 24.557167    | 26.236824    |
| Ca      | 35.804779    | 29.039436    | 24.069511    |
| S       | 21.363358    | 31.920780    | 35.937580    |
| S       | 20.273872    | 35.267570    | 32.799854    |
| S       | 21.994946    | 31.242479    | 29.774696    |
| S       | 24.763515    | 34.051647    | 33.203896    |
| S       | 26.500854    | 29.727638    | 31.337049    |
| S       | 25.769056    | 33.817871    | 28.489584    |
| S       | 28.153967    | 29.692963    | 26.594316    |
| S       | 30.450508    | 31.434484    | 30.665949    |
| S       | 31.675781    | 26.882801    | 27.267454    |
| S       | 32.812763    | 30.767143    | 25.323421    |
| S       | 33.549038    | 26.572081    | 23.006638    |
| S       | 36.230076    | 27.118492    | 27.396498    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.456656    | 32.137928    | 33.994118    |
| Ca      | 22.675600    | 35.086113    | 35.612831    |
| Ca      | 23.732700    | 30.548803    | 33.115875    |
| Ca      | 22.776388    | 35.011589    | 30.172400    |
| Ca      | 24.915913    | 30.247173    | 28.043247    |
| Ca      | 27.676327    | 33.109669    | 31.210588    |
| Ca      | 29.146358    | 27.977158    | 29.765968    |
| Ca      | 30.792109    | 32.362385    | 27.671993    |
| Ca      | 30.423185    | 28.230177    | 24.275011    |
| Ca      | 33.810375    | 29.577217    | 28.072542    |
| Ca      | 33.946934    | 24.794249    | 26.348343    |
| Ca      | 35.742172    | 28.963114    | 24.118568    |
| S       | 21.529331    | 31.691576    | 35.765144    |
| S       | 20.160416    | 35.319122    | 32.869026    |
| S       | 22.072224    | 31.267887    | 29.942055    |
| S       | 24.837397    | 34.130997    | 33.022346    |
| S       | 26.484993    | 29.864742    | 31.186869    |
| S       | 25.522493    | 33.967064    | 28.270382    |
| S       | 28.167297    | 29.800474    | 26.719931    |
| S       | 30.811764    | 31.052872    | 30.620911    |
| S       | 31.588295    | 26.717464    | 27.491955    |
| S       | 32.766960    | 30.781605    | 25.374760    |
| S       | 33.468742    | 26.498016    | 23.105991    |
| S       | 36.215416    | 27.162689    | 27.169256    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.564054    | 32.090927    | 34.156143    |
| Ca      | 22.788078    | 35.192715    | 35.789032    |
| Ca      | 23.794338    | 30.687281    | 32.948929    |
| Element | X Value | Y Value | Z Value |
|---------|---------|---------|---------|
| Ca      | 22.918079 | 34.432312 | 30.449953 |
| Ca      | 25.085493 | 30.356565 | 27.718895 |
| Ca      | 27.839138 | 33.180851 | 31.121466 |
| Ca      | 28.511791 | 28.108763 | 29.567482 |
| Ca      | 30.592827 | 32.513382 | 27.601368 |
| Ca      | 30.662241 | 28.315430 | 24.212009 |
| Ca      | 33.334694 | 29.677856 | 28.166740 |
| Ca      | 33.733635 | 24.771587 | 26.498810 |
| Ca      | 35.740849 | 28.751492 | 24.485117 |
| S       | 21.722025 | 31.693905 | 35.948933 |
| S       | 20.311192 | 35.073490 | 32.974480 |
| S       | 22.174917 | 30.880203 | 29.916378 |
| S       | 24.887474 | 34.261276 | 32.912376 |
| S       | 26.516293 | 30.044010 | 31.050623 |
| S       | 25.665016 | 33.843060 | 28.375418 |
| S       | 28.304661 | 30.108706 | 26.313574 |
| S       | 30.722969 | 31.029930 | 30.252525 |
| S       | 31.164019 | 26.842569 | 27.438295 |
| S       | 32.971886 | 30.791241 | 25.218245 |
| S       | 33.822666 | 26.386120 | 23.205637 |
| S       | 35.891708 | 27.266314 | 27.617594 |

24 generated by VMD
|   |    |    |    |
|---|---|---|---|
| S | 36.064327 | 27.146233 | 27.519180 |
| 24 generated by VMD | Ca | 18.512707 | 32.249985 | 33.910492 |
| Ca | 22.643871 | 35.081596 | 35.730042 |
| Ca | 23.506714 | 30.609961 | 33.043758 |
| Ca | 22.768749 | 34.837021 | 30.447607 |
| Ca | 24.986034 | 30.605833 | 27.812880 |
| Ca | 27.568317 | 32.814419 | 31.193615 |
| Ca | 29.043858 | 28.038258 | 29.869997 |
| Ca | 30.778725 | 32.491234 | 27.321619 |
| Ca | 30.414644 | 28.196793 | 24.573099 |
| Ca | 33.787094 | 29.764391 | 28.091185 |
| Ca | 34.158997 | 24.727907 | 26.366947 |
| Ca | 35.834137 | 28.724289 | 24.015451 |
| S | 21.441088 | 31.726772 | 35.983372 |
| S | 20.231766 | 35.294113 | 33.103146 |
| S | 22.066879 | 31.243843 | 29.796022 |
| S | 24.790844 | 33.976013 | 33.058487 |
| S | 26.217815 | 29.734169 | 31.131844 |
| S | 25.531918 | 34.026436 | 28.186642 |
| S | 28.317062 | 29.911415 | 26.819172 |
| S | 30.740046 | 31.089840 | 30.466726 |
| S | 31.522903 | 26.878134 | 27.589024 |
| S | 33.094368 | 30.622837 | 25.130342 |
| S | 33.372952 | 26.430067 | 23.244986 |
| S | 36.388702 | 27.224728 | 27.053656 |
| 24 generated by VMD | Ca | 18.841064 | 32.166695 | 34.565086 |
| Ca | 22.965508 | 34.913887 | 35.606766 |
| Ca | 23.332253 | 30.519623 | 32.862801 |
| Ca | 22.650150 | 34.933754 | 30.155647 |
| Ca | 25.002073 | 30.648581 | 27.771635 |
| Ca | 27.568031 | 32.695969 | 30.952539 |
| Ca | 28.959917 | 27.950863 | 29.693195 |
| Ca | 30.853399 | 32.605778 | 27.372032 |
| Ca | 30.556532 | 28.062572 | 24.578724 |
| Ca | 33.310062 | 29.693239 | 28.375553 |
| Ca | 34.125206 | 24.671371 | 26.699833 |
| Ca | 35.933445 | 28.873924 | 24.032972 |
| S | 21.849512 | 31.620705 | 36.074341 |
| S | 20.401073 | 35.164017 | 33.076324 |
| S | 21.776217 | 31.464235 | 29.701700 |
| S | 24.890823 | 33.888626 | 32.806778 |
| S | 26.123928 | 29.732307 | 31.048412 |
|    | 25.518875 | 34.044456 | 28.166157 |
|----|-----------|-----------|-----------|
| S  | 28.260071 | 30.268152 | 26.637022 |
| S  | 30.636814 | 30.972511 | 30.243345 |
| S  | 31.382160 | 26.946926 | 27.607712 |
| S  | 33.026756 | 30.704708 | 25.174726 |
| S  | 33.504364 | 26.383507 | 23.311314 |
| S  | 36.251781 | 27.373627 | 27.425421 |
| 24 | generated by VMD |
| Ca | 18.526426 | 32.001442 | 34.364758 |
| Ca | 22.810055 | 35.196022 | 35.633102 |
| Ca | 23.392326 | 30.639416 | 32.863266 |
| Ca | 22.763208 | 34.625023 | 30.511511 |
| Ca | 24.974209 | 30.512045 | 27.753527 |
| Ca | 27.871153 | 33.011162 | 31.161783 |
| Ca | 28.933865 | 28.145012 | 29.828426 |
| Ca | 30.792034 | 32.621029 | 27.411175 |
| Ca | 30.497536 | 28.163839 | 24.372284 |
| Ca | 33.549030 | 29.629162 | 28.194643 |
| Ca | 33.944389 | 24.706158 | 26.359377 |
| Ca | 35.944427 | 28.675129 | 24.302654 |
| S  | 21.635498 | 31.842136 | 36.031044 |
| S  | 20.255581 | 34.922653 | 33.010254 |
| S  | 21.968697 | 31.042345 | 29.652626 |
| S  | 24.895617 | 34.093491 | 32.975025 |
| S  | 26.181498 | 29.849892 | 30.986515 |
| S  | 25.641945 | 34.029926 | 28.378685 |
| S  | 28.391804 | 30.064922 | 26.615850 |
| S  | 30.890305 | 31.208426 | 30.180470 |
| S  | 31.355814 | 27.055153 | 27.472973 |
| S  | 33.051674 | 30.787571 | 25.101746 |
| S  | 33.473640 | 26.394279 | 23.171097 |
| S  | 35.979294 | 27.083836 | 27.607254 |
| 24 | generated by VMD |
| Ca | 18.257683 | 32.210705 | 33.884556 |
| Ca | 22.654251 | 35.072372 | 35.541641 |
| Ca | 23.791546 | 30.500496 | 33.189384 |
| Ca | 22.837414 | 34.654839 | 30.299532 |
| Ca | 25.256844 | 30.432158 | 27.919165 |
| Ca | 27.859468 | 33.129700 | 31.529543 |
| Ca | 28.877914 | 28.074793 | 29.737427 |
| Ca | 30.949905 | 32.515522 | 27.214239 |
| Ca | 30.390053 | 28.252031 | 24.289730 |
| Ca | 33.485268 | 29.733898 | 28.193842 |
| Ca | 33.825485 | 24.501270 | 26.567307 |
|  | Ca     |  |  |  |
|---|--------|---|---|---|
|  | 35.904488 | 28.791382 | 24.132812 |
| S | 21.400944 | 31.763845 | 35.863930 |
| S | 20.167305 | 35.106007 | 32.761398 |
| S | 22.303082 | 31.005005 | 29.965174 |
| S | 24.904690 | 33.874390 | 33.273285 |
| S | 26.629139 | 29.922672 | 31.236546 |
| S | 25.768955 | 33.999722 | 28.576691 |
| S | 28.302071 | 30.022947 | 26.642092 |
| S | 30.688091 | 31.265177 | 30.220148 |
| S | 31.211048 | 26.856094 | 27.290928 |
| S | 32.969101 | 30.906618 | 24.847023 |
| S | 33.354877 | 26.334587 | 23.401695 |
| S | 35.930443 | 27.373825 | 27.361938 |

24

*generated by VMD*

|  | Ca     |  |  |  |
|---|--------|---|---|---|
|  | 18.981155 | 32.069466 | 33.853500 |
| Ca | 22.895443 | 35.227165 | 35.332520 |
| Ca | 23.629246 | 30.706623 | 33.108543 |
| Ca | 22.891289 | 34.667751 | 30.522928 |
| Ca | 24.957294 | 30.389128 | 27.830767 |
| Ca | 27.675339 | 32.903603 | 31.117512 |
| Ca | 28.478737 | 27.904087 | 29.398352 |
| Ca | 30.774487 | 32.495274 | 27.587757 |
| Ca | 30.511837 | 28.080484 | 24.492977 |
| Ca | 33.354584 | 29.842499 | 28.350647 |
| Ca | 33.908482 | 24.742756 | 26.483826 |
| Ca | 35.936958 | 29.028675 | 24.135382 |
| S  | 21.743330 | 31.942589 | 35.878765 |
| S  | 20.545338 | 35.131935 | 33.135582 |
| S  | 22.139816 | 31.160164 | 29.879234 |
| S  | 25.050491 | 33.978958 | 32.901436 |
| S  | 26.160145 | 29.693081 | 31.200304 |
| S  | 25.449924 | 33.807930 | 28.365290 |
| S  | 28.239700 | 30.022305 | 26.445219 |
| S  | 30.466276 | 30.823200 | 30.319584 |
| S  | 31.295883 | 26.861183 | 27.667040 |
| S  | 32.957199 | 30.775337 | 25.243895 |
| S  | 33.600121 | 26.466600 | 23.251831 |
| S  | 36.076950 | 27.579208 | 27.437178 |

24

*generated by VMD*

|  | Ca     |  |  |  |
|---|--------|---|---|---|
| Ca | 18.820866 | 32.448586 | 34.224163 |
| Ca | 23.108124 | 35.497677 | 35.099026 |
| Ca | 23.434017 | 30.542801 | 33.093979 |
| Ca | 22.724979 | 34.624168 | 30.178072 |
| Ca | 25.030724 | 30.365337 | 27.696131 |
|  | Ca   | S    |
|---|------|------|
|   | 27.681728 | 32.206581 | 31.359598 |
|   | 28.673859 | 27.670357 | 29.685101 |
|   | 30.592960 | 32.376583 | 27.483295 |
|   | 30.433607 | 28.248711 | 24.500694 |
|   | 33.558388 | 29.677711 | 28.437475 |
|   | 33.962650 | 24.987986 | 26.298058 |
|   | 35.796989 | 29.302017 | 24.301555 |
|   | 21.856907 | 32.290134 | 35.983696 |
|   | 20.314365 | 35.450249 | 32.889259 |
|   | 22.089939 | 31.084053 | 29.828186 |
|   | 25.085182 | 33.853790 | 32.890072 |
|   | 26.166603 | 29.264164 | 31.173443 |
|   | 25.610756 | 33.743900 | 28.297960 |
|   | 28.246300 | 29.675125 | 26.651308 |
|   | 30.482632 | 30.676403 | 30.427069 |
|   | 31.434692 | 26.784500 | 27.616158 |
|   | 32.943432 | 30.954529 | 25.487787 |
|   | 33.468414 | 26.977905 | 23.153656 |
|   | 36.201927 | 27.596766 | 27.183708 |

24 generated by VMD

|  | Ca   | S    |
|---|------|------|
|   | 18.637014 | 32.509308 | 34.029106 |
|   | 23.133560 | 35.035789 | 35.346291 |
|   | 23.628241 | 30.651276 | 33.208649 |
|   | 22.653370 | 34.584908 | 30.467943 |
|   | 24.774567 | 30.260599 | 27.904243 |
|   | 27.899265 | 32.751251 | 31.174690 |
|   | 28.729301 | 27.887949 | 29.619198 |
|   | 30.464619 | 32.474197 | 27.567474 |
|   | 30.626377 | 28.332581 | 24.490116 |
|   | 33.428558 | 29.614990 | 25.362766 |
|   | 34.013512 | 24.860081 | 26.145399 |
|   | 36.026222 | 29.180801 | 24.343163 |
|   | 21.705421 | 32.121490 | 35.671474 |
|   | 20.355953 | 35.435928 | 32.765633 |
|   | 21.989548 | 31.119076 | 30.025320 |
|   | 25.028294 | 33.884800 | 32.832367 |
|   | 26.370956 | 29.589920 | 31.230909 |
|   | 25.576374 | 33.595322 | 28.382959 |
|   | 28.070501 | 29.806702 | 26.567942 |
|   | 30.641787 | 30.927048 | 30.330030 |
|   | 31.402142 | 26.753237 | 27.477949 |
|   | 32.861351 | 30.940378 | 25.417477 |
|   | 33.499912 | 26.605181 | 23.301414 |
|   | 36.203209 | 27.413029 | 27.277555 |

24
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 18.591341 | 32.397266 | 33.830582 |
| Ca      | 22.895733 | 34.965935 | 35.535023 |
| Ca      | 23.561296 | 30.442516 | 33.119591 |
| Ca      | 22.711340 | 34.857876 | 30.586002 |
| Ca      | 25.068401 | 30.505432 | 27.833235 |
| Ca      | 27.653246 | 32.948730 | 31.217449 |
| Ca      | 28.826275 | 27.927254 | 29.694387 |
| Ca      | 30.596603 | 32.514729 | 27.245081 |
| Ca      | 30.756664 | 28.044510 | 24.293234 |
| Ca      | 33.430305 | 29.746782 | 28.068737 |
| Ca      | 34.049149 | 24.682598 | 26.717304 |
| Ca      | 35.773827 | 29.099968 | 24.027002 |
| S       | 21.500469 | 31.802292 | 35.803288 |
| S       | 20.238285 | 35.301693 | 33.142841 |
| S       | 22.052349 | 31.279587 | 29.897095 |
| S       | 24.914520 | 33.805031 | 33.155441 |
| S       | 26.379395 | 29.889696 | 31.240736 |
| S       | 25.660107 | 33.989964 | 28.396912 |
| S       | 28.180824 | 29.877045 | 26.635384 |
| S       | 30.570259 | 31.083971 | 30.294020 |
| S       | 31.289314 | 26.792511 | 27.466969 |
| S       | 33.057606 | 30.663008 | 25.140303 |
| S       | 33.749977 | 26.220715 | 23.370010 |
| S       | 36.212746 | 27.460938 | 27.229427 |

24

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 18.418768 | 32.103191 | 33.719177 |
| Ca      | 22.693863 | 35.135841 | 35.422173 |
| Ca      | 23.576187 | 30.652010 | 33.391659 |
| Ca      | 22.659184 | 34.785503 | 30.636553 |
| Ca      | 25.241173 | 30.857780 | 28.078320 |
| Ca      | 27.551647 | 32.944889 | 31.203428 |
| Ca      | 29.037960 | 27.979877 | 29.605885 |
| Ca      | 30.803339 | 32.559326 | 27.131521 |
| Ca      | 30.391823 | 28.056648 | 24.522896 |
| Ca      | 33.666523 | 29.576685 | 27.962013 |
| Ca      | 34.049221 | 24.536125 | 26.291531 |
| Ca      | 35.916241 | 29.040155 | 24.172668 |
| S       | 21.337839 | 31.956284 | 35.890293 |
| S       | 19.984547 | 35.171989 | 32.812042 |
| S       | 22.017368 | 31.292675 | 30.232052 |
| S       | 24.919659 | 33.703125 | 33.239685 |
| S       | 26.599308 | 29.890898 | 31.220469 |
| S       | 25.529079 | 34.091957 | 28.419979 |
| S       | 28.450939 | 29.797525 | 26.579041 |
|   | S        | 30.596741 | 31.142410 | 30.223860 |
|   | S        | 31.499947 | 26.760220 | 27.635105 |
|   | S        | 33.120625 | 30.606922 | 25.142296 |
|   | S        | 33.390018 | 26.388783 | 23.188110 |
|   | S        | 36.268055 | 27.269281 | 27.219297 |

24 generated by VMD

|   | Ca       | 18.881327 | 32.369644 | 34.249641 |
|   | Ca       | 23.069172 | 35.497711 | 35.358105 |
|   | Ca       | 23.722179 | 30.623289 | 33.007710 |
|   | Ca       | 22.575552 | 34.566521 | 30.346924 |
|   | Ca       | 24.920544 | 30.473328 | 27.453789 |
|   | Ca       | 27.674372 | 32.745800 | 31.107389 |
|   | Ca       | 28.673719 | 27.746758 | 29.563175 |
|   | Ca       | 30.352022 | 32.218487 | 27.710745 |
|   | Ca       | 30.502136 | 28.189060 | 24.437695 |
|   | Ca       | 33.694500 | 29.741772 | 28.340771 |
|   | Ca       | 33.956432 | 24.933498 | 26.133509 |
|   | Ca       | 35.969780 | 29.226860 | 24.309893 |
|   | S        | 21.842615 | 32.070820 | 35.965214 |
|   | S        | 20.303135 | 35.497402 | 33.102074 |
|   | S        | 22.067451 | 31.185188 | 29.708702 |
|   | S        | 24.980545 | 33.624054 | 33.074997 |
|   | S        | 26.102533 | 29.583715 | 30.920488 |
|   | S        | 25.546120 | 33.777534 | 28.271875 |
|   | S        | 28.130207 | 29.626564 | 26.533817 |
|   | S        | 30.674030 | 30.854076 | 30.467514 |
|   | S        | 31.463402 | 26.769999 | 27.661966 |
|   | S        | 32.850433 | 30.632313 | 25.434347 |
|   | S        | 33.446156 | 26.738316 | 23.200958 |
|   | S        | 36.321754 | 27.607357 | 27.578751 |

24 generated by VMD

|   | Ca       | 18.573219 | 32.447350 | 34.344776 |
|   | Ca       | 22.894016 | 35.439522 | 35.166618 |
|   | Ca       | 23.678894 | 30.416029 | 33.221909 |
|   | Ca       | 22.478149 | 34.520683 | 30.400753 |
|   | Ca       | 24.797277 | 30.671364 | 27.633121 |
|   | Ca       | 27.732891 | 33.010571 | 31.423771 |
|   | Ca       | 28.704174 | 27.775539 | 29.568516 |
|   | Ca       | 30.518280 | 32.205833 | 27.495052 |
|   | Ca       | 30.558704 | 28.310333 | 24.420065 |
|   | Ca       | 33.834885 | 29.730747 | 28.285093 |
|   | Ca       | 33.928757 | 24.818083 | 26.220263 |
|   | Ca       | 35.913372 | 29.106724 | 24.317276 |
|   | S        | 21.750513 | 32.194477 | 35.901134 |
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| S       | 20.22462      | 35.345337     | 32.842415     |
| S       | 21.771038     | 31.114281     | 30.034397     |
| S       | 25.066259     | 33.684818     | 33.203537     |
| S       | 26.046310     | 29.541443     | 30.915602     |
| S       | 25.629333     | 33.952660     | 28.320784     |
| S       | 28.153990     | 29.684664     | 26.487907     |
| S       | 30.735998     | 30.663059     | 30.346207     |
| S       | 31.629925     | 26.817238     | 27.532873     |
| S       | 33.097790     | 26.682758     | 23.282307     |
| S       | 33.645920     | 25.337004     |                |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.836725     | 32.152241     | 34.125839     |
| Ca      | 22.896332     | 35.105881     | 35.530869     |
| Ca      | 23.696600     | 30.702724     | 32.895950     |
| Ca      | 22.686359     | 34.573853     | 30.275131     |
| Ca      | 24.922602     | 30.496433     | 27.583055     |
| Ca      | 27.640663     | 32.977848     | 31.247431     |
| Ca      | 29.093510     | 27.970108     | 29.717333     |
| Ca      | 30.597729     | 32.414871     | 27.694191     |
| Ca      | 30.477299     | 28.322824     | 24.377638     |
| Ca      | 33.547604     | 29.641426     | 28.663944     |
| Ca      | 34.006439     | 24.605167     | 26.432758     |
| Ca      | 35.572788     | 28.937496     | 24.154085     |
| S       | 21.788340     | 31.693230     | 35.765503     |
| S       | 20.394073     | 35.113800     | 33.004578     |
| S       | 21.967663     | 31.382559     | 29.583080     |
| S       | 25.056414     | 34.094086     | 32.942444     |
| S       | 26.334980     | 29.775658     | 31.025200     |
| S       | 25.624222     | 33.857754     | 28.403940     |
| S       | 28.092665     | 29.852764     | 26.656870     |
| S       | 30.598190     | 31.139299     | 30.475199     |
| S       | 31.564438     | 26.925617     | 27.571861     |
| S       | 32.829994     | 30.763622     | 25.356932     |
| S       | 33.335529     | 26.326962     | 23.317848     |
| S       | 36.158840     | 27.473816     | 27.138323     |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.661751     | 32.598595     | 33.996941     |
| Ca      | 22.988728     | 34.876629     | 35.664970     |
| Ca      | 23.332012     | 30.507345     | 33.058678     |
| Ca      | 22.745535     | 34.758755     | 30.493128     |
| Ca      | 24.836273     | 30.612385     | 27.675138     |
| Ca      | 27.832565     | 32.775063     | 31.156528     |
| Ca      | 28.854145     | 27.904434     | 29.714354     |
|    | Ca     | S       | Ca     |
|----|--------|---------|--------|
|    | 30.391417 | 32.289139 | 27.286068 |
|    | 30.799690 | 28.108356 | 24.597071 |
|    | 33.108189 | 29.102325 | 23.957014 |
|    | 34.473961 | 29.089636 | 24.063818 |
|    | 35.918701 | 29.721361 | 28.195509 |
|    | 35.918701 | 30.799690 | 24.597071 |
|    | 30.391417 | 32.289139 | 27.286068 |
|    | 30.799690 | 28.108356 | 24.597071 |
|    | 33.108189 | 29.102325 | 23.957014 |
|    | 34.473961 | 29.089636 | 24.063818 |
|    | 35.918701 | 29.721361 | 28.195509 |
|    | 35.918701 | 30.799690 | 24.597071 |
|    | 30.391417 | 32.289139 | 27.286068 |
|    | 30.799690 | 28.108356 | 24.597071 |
|    | 33.108189 | 29.102325 | 23.957014 |
|    | 34.473961 | 29.089636 | 24.063818 |
|    | 35.918701 | 29.721361 | 28.195509 |
|    | 35.918701 | 30.799690 | 24.597071 |
|    | 30.391417 | 32.289139 | 27.286068 |
|    | 30.799690 | 28.108356 | 24.597071 |
|    | 33.108189 | 29.102325 | 23.957014 |
|    | 34.473961 | 29.089636 | 24.063818 |
|    | 35.918701 | 29.721361 | 28.195509 |
|    | 35.918701 | 30.799690 | 24.597071 |
|    | 30.391417 | 32.289139 | 27.286068 |
|    | 30.799690 | 28.108356 | 24.597071 |
|    | 33.108189 | 29.102325 | 23.957014 |
|    | 34.473961 | 29.089636 | 24.063818 |
|    | 35.918701 | 29.721361 | 28.195509 |
|    | 35.918701 | 30.799690 | 24.597071 |
|    | 30.391417 | 32.289139 | 27.286068 |
|    | 30.799690 | 28.108356 | 24.597071 |
|    | 33.108189 | 29.102325 | 23.957014 |
|    | 34.473961 | 29.089636 | 24.063818 |
|    | 35.918701 | 29.721361 | 28.195509 |
|    | 35.918701 | 30.799690 | 24.597071 |
|    | 30.391417 | 32.289139 | 27.286068 |
|    | 30.799690 | 28.108356 | 24.597071 |
|    | 33.108189 | 29.102325 | 23.957014 |
|    | 34.473961 | 29.089636 | 24.063818 |
|    | 35.918701 | 29.721361 | 28.195509 |
|    | 35.918701 | 30.799690 | 24.597071 |
|    | 30.391417 | 32.289139 | 27.286068 |
|    | 30.799690 | 28.108356 | 24.597071 |
|    | 33.108189 | 29.102325 | 23.957014 |
|    | 34.473961 | 29.089636 | 24.063818 |
|    | 35.918701 | 29.721361 | 28.195509 |
|    | 35.918701 | 30.799690 | 24.597071 |

generated by VMD

|    | Ca     | S�       |
|----|--------|---------|
|    | 19.094421 | 32.064194 |
|    | 22.914595 | 34.972290 |
|    | 23.599640 | 30.560596 |
|    | 22.945251 | 34.809143 |
|    | 24.665825 | 30.749245 |
|    | 27.763819 | 33.005394 |
|    | 28.679531 | 27.929035 |
|    | 30.566917 | 32.370262 |
|    | 30.416088 | 28.070536 |
|    | 33.688087 | 29.768623 |
|    | 34.172054 | 24.753899 |
|    | 35.568848 | 29.089636 |
|    | 34.172054 | 24.753899 |
|    | 35.568848 | 29.089636 |
|    | 30.042980 | 29.683691 |
|    | 25.844482 | 34.072124 |
|    | 27.952211 | 29.778994 |
|    | 30.622559 | 30.852222 |
|    | 31.725796 | 26.897118 |
|    | 32.751663 | 30.733295 |
|    | 33.716640 | 26.284607 |
|    | 36.328354 | 27.705198 |

24

24

generated by VMD

|    | Ca     | S�       |
|----|--------|---------|
|    | 18.704840 | 32.675392 |
|    | 25.844482 | 34.072124 |
|    | 27.952211 | 29.778994 |
|    | 30.622559 | 30.852222 |
|    | 31.725796 | 26.897118 |
|    | 32.751663 | 30.733295 |
|    | 33.716640 | 26.284607 |
|    | 36.328354 | 27.705198 |

|    | Ca     | S�       |
|----|--------|---------|
|    | 31.472886 | 26.273281 |
|    | 35.918701 | 29.721361 |
|    | 36.273804 | 27.616013 |

24

generated by VMD
| Ca     | 22.937382 | 35.196548 | 35.591812 |
|--------|-----------|-----------|-----------|
| Ca     | 23.596773 | 30.732601 | 32.832211 |
| Ca     | 22.801128 | 34.513252 | 30.479164 |
| Ca     | 24.639700 | 30.469028 | 27.477762 |
| Ca     | 27.657978 | 32.543922 | 31.176098 |
| Ca     | 29.010103 | 27.670465 | 29.830336 |
| Ca     | 30.504360 | 32.173763 | 27.572882 |
| Ca     | 30.274616 | 28.011482 | 24.627451 |
| Ca     | 33.589432 | 29.847221 | 28.232670 |
| Ca     | 34.514839 | 25.061493 | 26.380920 |
| Ca     | 35.756882 | 29.090164 | 24.048527 |
| S      | 21.591776 | 31.959936 | 35.739502 |
| S      | 20.451456 | 35.775959 | 32.973358 |
| S      | 21.915867 | 31.388466 | 29.650293 |
| S      | 25.068363 | 33.398922 | 33.319733 |
| S      | 25.927408 | 29.536493 | 30.675510 |
| S      | 25.655224 | 33.969353 | 28.472174 |
| S      | 28.122150 | 29.594393 | 26.731796 |
| S      | 30.792183 | 30.765987 | 30.408302 |
| S      | 31.794733 | 26.833258 | 27.857159 |
| S      | 32.580109 | 30.692169 | 25.125092 |
| S      | 33.464508 | 26.675037 | 23.338032 |
| S      | 36.368156 | 27.724768 | 27.295021 |

24

generated by VMD

| Ca     | 18.491070 | 32.856087 | 33.755035 |
|--------|-----------|-----------|-----------|
| Ca     | 22.834105 | 35.097919 | 35.528828 |
| Ca     | 23.399143 | 30.330406 | 33.098709 |
| Ca     | 23.153723 | 34.701115 | 30.300051 |
| Ca     | 25.094213 | 30.422377 | 28.014265 |
| Ca     | 27.801853 | 32.836796 | 31.472065 |
| Ca     | 28.935261 | 27.872120 | 29.809662 |
| Ca     | 30.272255 | 32.375816 | 27.364815 |
| Ca     | 30.650730 | 27.917282 | 24.412176 |
| Ca     | 33.290329 | 29.760616 | 28.251858 |
| Ca     | 34.407463 | 24.772778 | 26.451622 |
| Ca     | 35.786667 | 29.235071 | 24.053728 |
| S      | 21.329697 | 31.830837 | 35.627960 |
| S      | 20.572136 | 35.535057 | 32.832008 |
| S      | 21.982548 | 31.291838 | 30.027519 |
| S      | 24.985100 | 33.650909 | 33.320503 |
| S      | 26.330971 | 29.470842 | 31.119537 |
| S      | 26.061527 | 33.856365 | 28.530167 |
| S      | 28.068086 | 29.429947 | 26.621376 |
| S      | 30.431816 | 31.058737 | 30.208887 |
| S      | 31.559933 | 26.755009 | 27.845469 |
|     |     |     |     |
|-----|-----|-----|-----|
| S   | 32.609547 | 30.808987 | 24.953669 |
| S   | 33.582909 | 26.586403 | 23.228975 |
| S   | 36.096184 | 27.846699 | 27.111181 |

24 generated by VMD

|     |     |     |     |
|-----|-----|-----|-----|
| Ca  | 18.426182 | 32.900116 | 33.963112 |
| Ca  | 23.234097 | 34.777359 | 35.400902 |
| Ca  | 23.334980 | 30.128304 | 32.862129 |
| Ca  | 22.881931 | 34.848385 | 30.419405 |
| Ca  | 24.587568 | 30.600725 | 27.790890 |
| Ca  | 27.797714 | 32.546776 | 31.205631 |
| Ca  | 28.813931 | 27.980232 | 29.660912 |
| Ca  | 30.648283 | 32.422577 | 27.537079 |
| Ca  | 30.326878 | 27.998615 | 24.883377 |
| Ca  | 33.818523 | 30.089088 | 28.085274 |
| Ca  | 34.304790 | 25.009243 | 26.664530 |
| Ca  | 35.698307 | 28.985825 | 24.064003 |
| S   | 21.486721 | 31.684917 | 35.655029 |
| S   | 20.619650 | 35.588760 | 32.980057 |
| S   | 21.784698 | 31.374014 | 29.922495 |
| S   | 25.141649 | 33.545471 | 32.979130 |
| S   | 26.103436 | 29.458424 | 30.822838 |
| S   | 25.650579 | 33.785622 | 28.395657 |
| S   | 28.134083 | 29.882231 | 26.733061 |
| S   | 30.802856 | 30.870304 | 30.278166 |
| S   | 31.757225 | 27.090450 | 28.108627 |
| S   | 32.724236 | 30.717415 | 25.142786 |
| S   | 33.258278 | 26.320772 | 23.368832 |
| S   | 36.383461 | 27.694382 | 27.016167 |

24 generated by VMD

|     |     |     |     |
|-----|-----|-----|-----|
| Ca  | 18.421265 | 33.049519 | 33.821125 |
| Ca  | 22.665565 | 34.965679 | 35.707920 |
| Ca  | 23.419855 | 30.055529 | 33.144657 |
| Ca  | 22.806181 | 34.625965 | 30.437428 |
| Ca  | 25.014790 | 30.629295 | 27.736235 |
| Ca  | 27.470102 | 32.719788 | 31.335493 |
| Ca  | 29.142220 | 27.962654 | 29.924259 |
| Ca  | 30.643253 | 32.445362 | 27.494875 |
| Ca  | 30.386280 | 27.776451 | 24.575331 |
| Ca  | 33.789627 | 30.040077 | 28.104254 |
| Ca  | 34.226238 | 24.848120 | 26.560921 |
| Ca  | 35.723564 | 29.100105 | 23.742493 |
| S   | 21.161728 | 31.742910 | 35.809578 |
| S   | 20.550842 | 35.817333 | 32.986759 |
| S   | 22.029549 | 31.283787 | 29.878616 |
|  |     |     |     |
|---|-----|-----|-----|
| S | 24.800329 | 33.458225 | 33.277538 |
| S | 26.141205 | 29.569382 | 31.013168 |
| S | 25.790764 | 34.021133 | 28.310329 |
| S | 28.279369 | 29.696758 | 26.725391 |
| S | 30.880062 | 31.071213 | 30.243084 |
| S | 31.806414 | 26.915318 | 27.709732 |
| S | 32.709846 | 30.630325 | 25.118776 |
| S | 33.388500 | 26.297554 | 23.385151 |
| S | 36.472450 | 27.577520 | 26.896952 |

24

generated by VMD

| Ca  |     |     |     |
|-----|-----|-----|-----|
| Ca  | 18.577724 | 33.029499 | 33.601074 |
| Ca  | 22.630802 | 35.030533 | 35.536453 |
| Ca  | 23.307453 | 30.251438 | 33.115612 |
| Ca  | 23.040049 | 34.885162 | 30.287947 |
| Ca  | 24.958723 | 30.296951 | 28.063911 |
| Ca  | 27.646427 | 32.818817 | 31.532820 |
| Ca  | 29.254950 | 27.982204 | 29.801834 |
| Ca  | 30.345650 | 32.374481 | 27.664646 |
| Ca  | 30.712193 | 27.966644 | 24.537470 |
| Ca  | 33.432873 | 29.696535 | 28.135565 |
| Ca  | 34.492584 | 25.029945 | 26.387182 |
| Ca  | 35.549809 | 29.178011 | 23.689510 |
| S   | 21.126392 | 31.743851 | 35.720955 |
| S   | 20.576973 | 35.757854 | 32.767113 |
| S   | 22.003420 | 31.359184 | 29.839733 |
| S   | 24.737820 | 33.586716 | 33.247120 |
| S   | 26.416412 | 29.438902 | 31.393101 |
| S   | 25.797691 | 33.663676 | 28.595892 |
| S   | 28.368790 | 29.719271 | 26.748304 |
| S   | 30.734264 | 31.094414 | 30.428158 |
| S   | 31.687622 | 26.727264 | 27.891403 |
| S   | 32.601738 | 30.687820 | 25.047581 |
| S   | 33.383888 | 26.256092 | 23.141712 |
| S   | 36.335815 | 27.722178 | 26.764936 |

24

generated by VMD

| Ca  |     |     |     |
|-----|-----|-----|-----|
| Ca  | 18.492338 | 32.527870 | 33.745678 |
| Ca  | 22.908031 | 35.443329 | 35.161922 |
| Ca  | 23.650593 | 30.477283 | 33.196846 |
| Ca  | 22.598469 | 34.644344 | 30.404655 |
| Ca  | 25.061653 | 30.562590 | 27.782022 |
| Ca  | 27.690563 | 32.690239 | 31.535950 |
| Ca  | 28.867695 | 27.797525 | 29.890360 |
| Ca  | 30.477293 | 32.346367 | 27.842791 |
| Ca  | 30.648685 | 27.975191 | 24.515804 |
| Element | x1       | y1       | z1       |
|---------|----------|----------|----------|
| Ca      | 33.611740| 29.654333| 28.386736|
| Ca      | 34.330391| 24.804256| 26.343054|
| Ca      | 35.673279| 29.260723| 23.587719|
| S       | 21.506718| 31.995094| 35.734535|
| S       | 20.188334| 35.650608| 32.913616|
| S       | 22.028828| 31.265549| 29.833200|
| S       | 24.961126| 33.728783| 33.268631|
| S       | 26.049980| 29.400734| 31.064508|
| S       | 25.769157| 33.905060| 28.568354|
| S       | 28.173000| 29.756516| 26.755733|
| S       | 30.678749| 30.831669| 30.481503|
| S       | 31.758633| 26.680624| 27.812309|
| S       | 32.783714| 30.790422| 25.145969|
| S       | 33.350407| 26.347549| 23.132261|
| S       | 36.460667| 27.763390| 26.835844|

24 generated by VMD

| Element | x2       | y2       | z2       |
|---------|----------|----------|----------|
| Ca      | 18.544823| 32.570213| 33.879303|
| Ca      | 22.811317| 35.354462| 35.657139|
| Ca      | 23.544901| 30.618507| 32.964275|
| Ca      | 23.097137| 34.528694| 30.526125|
| Ca      | 24.803288| 30.576283| 27.556173|
| Ca      | 27.781746| 32.585373| 31.549681|
| Ca      | 28.791458| 27.852905| 29.709541|
| S       | 20.484009| 32.462662| 27.297148|
| S       | 30.559517| 27.945299| 24.529060|
| S       | 33.622417| 29.896343| 28.083134|
| S       | 34.391056| 24.812901| 26.623529|
| S       | 35.667595| 29.179754| 23.963476|
| S       | 21.334023| 32.157173| 35.824314|
| S       | 20.385468| 35.567425| 33.028282|
| S       | 21.848907| 31.389734| 29.746975|
| S       | 24.984135| 33.429085| 33.371559|
| S       | 25.952875| 29.483814| 30.808764|
| S       | 25.828213| 33.702652| 28.597189|
| S       | 28.232727| 29.521450| 26.669611|
| S       | 30.657146| 30.956779| 30.290649|
| S       | 31.635162| 26.800209| 27.625561|
| S       | 32.687225| 30.826004| 25.180435|
| S       | 33.570641| 26.374542| 23.407253|
| S       | 36.504234| 27.707716| 27.050877|

24 generated by VMD

| Element | x3       | y3       | z3       |
|---------|----------|----------|----------|
| Ca      | 18.498663| 32.505108| 33.712730|
| Ca      | 23.019154| 35.101158| 35.356468|
| Ca      | 23.396122| 30.291651| 33.050900|
| Ca    | 23.008102 | 34.694008 | 30.668537 |
|-------|-----------|-----------|-----------|
| Ca    | 25.010170 | 30.587393 | 27.810152 |
| Ca    | 27.827656 | 32.554283 | 27.589266 |
| Ca    | 30.618374 | 27.770521 | 24.551405 |
| Ca    | 33.473087 | 29.942158 | 28.210537 |
| Ca    | 34.082726 | 24.784719 | 26.738636 |
| Ca    | 35.681797 | 29.152678 | 23.902845 |
| S     | 21.324471 | 32.004063 | 35.684700 |
| S     | 20.527859 | 35.381577 | 32.867752 |
| S     | 22.104298 | 31.135605 | 29.956284 |
| S     | 24.981133 | 33.658665 | 33.183556 |
| S     | 26.330193 | 29.567638 | 31.113808 |
| S     | 25.772907 | 33.891582 | 28.552008 |
| S     | 28.227448 | 29.990459 | 26.554052 |
| S     | 30.644287 | 30.924820 | 30.353823 |
| S     | 31.516037 | 26.912220 | 27.821236 |
| S     | 32.734287 | 30.788921 | 24.992020 |
| S     | 33.579048 | 26.164417 | 23.329056 |
| S     | 36.142166 | 27.792257 | 26.974268 |

24 generated by VMD

| Ca    | 18.538319 | 33.121822 | 33.861824 |
|-------|-----------|-----------|-----------|
| Ca    | 23.090649 | 35.255348 | 35.133541 |
| Ca    | 23.649498 | 30.276649 | 33.231003 |
| Ca    | 22.605371 | 34.635952 | 30.247259 |
| Ca    | 24.908840 | 30.257618 | 28.083055 |
| Ca    | 27.642963 | 32.376263 | 31.342735 |
| Ca    | 29.120825 | 27.781570 | 29.629276 |
| Ca    | 30.589186 | 32.630306 | 27.768591 |
| Ca    | 30.587582 | 28.055843 | 24.594246 |
| Ca    | 33.449547 | 29.601307 | 28.334782 |
| Ca    | 34.358597 | 24.789534 | 26.188738 |
| Ca    | 35.436867 | 29.400375 | 23.994089 |
| S     | 21.464886 | 32.088058 | 35.585060 |
| S     | 20.470547 | 35.828064 | 32.755547 |
| S     | 21.892937 | 31.099653 | 30.028357 |
| S     | 24.795164 | 33.482948 | 32.864838 |
| S     | 26.325378 | 29.390095 | 31.372330 |
| S     | 25.542923 | 33.595779 | 28.322023 |
| S     | 28.316677 | 30.022926 | 26.862745 |
| S     | 30.764008 | 30.679760 | 30.681709 |
| S     | 31.821983 | 26.762024 | 27.732204 |
| S     | 32.612045 | 30.871147 | 25.353659 |
| S     | 33.378677 | 26.577154 | 23.049746 |
|   | X-coordinate | Y-coordinate | Z-coordinate |
|---|--------------|--------------|--------------|
| S | 36.356220    | 27.719872    | 26.922705    |

24 generated by VMD

| Ca | 18.324301    | 33.280933    | 33.864727    |
|    | 22.687531    | 35.012482    | 35.470963    |
|    | 23.567883    | 30.365093    | 32.963722    |
|    | 22.901121    | 34.797607    | 30.541498    |
|    | 24.793053    | 30.256285    | 27.948462    |
|    | 27.651308    | 32.748112    | 31.473768    |
|    | 29.031357    | 27.659157    | 29.854012    |
|    | 30.412594    | 32.126122    | 27.679611    |
|    | 30.498005    | 27.947464    | 24.484362    |
|    | 33.684013    | 29.920193    | 28.335880    |
|    | 34.537590    | 24.866470    | 26.571253    |
|    | 35.551117    | 29.313446    | 23.631220    |
| S | 21.091099    | 31.896999    | 35.382668    |
|    | 20.524708    | 35.866714    | 32.860718    |
|    | 22.046886    | 31.289494    | 29.983963    |
|    | 24.970339    | 33.570435    | 33.247971    |
|    | 26.375866    | 29.542767    | 31.093777    |
|    | 25.777416    | 33.757725    | 28.636847    |
|    | 28.102818    | 29.531559    | 26.771332    |
|    | 30.720402    | 30.694557    | 30.442215    |
|    | 31.848526    | 26.861687    | 27.696489    |
|    | 32.519753    | 30.807621    | 25.131681    |
|    | 33.604614    | 26.273294    | 23.107761    |
|    | 36.497787    | 27.913860    | 26.765081    |

24 generated by VMD

| Ca | 18.365433    | 33.242905    | 33.862782    |
|    | 23.163754    | 34.968201    | 35.683247    |
|    | 23.614100    | 30.303530    | 33.050568    |
|    | 22.959274    | 34.903172    | 30.458616    |
|    | 24.612560    | 30.349030    | 27.755093    |
|    | 27.602463    | 32.497826    | 31.170315    |
|    | 28.873652    | 27.584736    | 29.638142    |
|    | 30.334295    | 32.136940    | 27.508287    |
|    | 30.658337    | 28.196569    | 24.377575    |
|    | 33.553398    | 29.768612    | 28.445843    |
|    | 34.408085    | 24.898022    | 26.687355    |
|    | 35.708603    | 29.415638    | 24.067131    |
| S | 21.457642    | 32.056107    | 35.471371    |
|    | 20.583591    | 35.841442    | 33.209499    |
|    | 21.866148    | 31.225325    | 30.144424    |
|    | 25.055286    | 33.613964    | 33.018841    |
|    | 26.176136    | 29.347332    | 30.899395    |
| S | 25.479614 | 33.670364 | 28.408672 |
| S | 28.009094 | 29.411833 | 26.561592 |
| S | 30.616901 | 30.736347 | 30.269840 |
| S | 31.654869 | 26.804943 | 27.706600 |
| S | 32.753136 | 30.850288 | 25.120264 |
| S | 33.752594 | 26.436964 | 23.336296 |
| S | 36.461090 | 28.039951 | 27.088282 |

24 generated by VMD

| Ca | 18.316921 | 32.997578 | 33.667252 |
| Ca | 22.953480 | 34.815323 | 35.543583 |
| Ca | 23.345428 | 30.508808 | 32.901390 |
| Ca | 22.987850 | 34.772301 | 30.485611 |
| Ca | 25.143251 | 30.403112 | 28.006786 |
| Ca | 27.822521 | 32.650269 | 31.502258 |
| Ca | 28.867218 | 27.877399 | 29.765228 |
| Ca | 30.205065 | 32.304749 | 27.468573 |
| Ca | 30.614607 | 27.728394 | 24.595343 |
| Ca | 33.519539 | 29.895172 | 28.087177 |
| Ca | 34.273018 | 25.069912 | 26.622444 |
| Ca | 35.650333 | 29.237492 | 23.882097 |
| S | 21.274029 | 31.847250 | 35.589191 |
| S | 20.576099 | 35.644287 | 33.114452 |
| S | 22.164871 | 31.362408 | 29.813553 |
| S | 24.928881 | 33.773922 | 33.147758 |
| S | 26.450815 | 29.392105 | 31.318438 |
| S | 25.847054 | 33.675087 | 28.483715 |
| S | 28.092749 | 29.593451 | 26.517792 |
| S | 30.616146 | 30.859402 | 30.231068 |
| S | 31.592243 | 26.790890 | 27.669624 |
| S | 32.559193 | 30.772625 | 24.993019 |
| S | 33.482269 | 26.487240 | 23.357782 |
| S | 36.436501 | 27.840830 | 27.175949 |

24 generated by VMD

| Ca | 18.409496 | 33.313591 | 34.131390 |
| Ca | 23.045403 | 35.069527 | 35.578163 |
| Ca | 23.380669 | 30.156923 | 32.914841 |
| Ca | 22.701839 | 34.757973 | 30.367342 |
| Ca | 25.076359 | 30.593685 | 27.983959 |
| Ca | 27.783848 | 32.374126 | 31.470741 |
| Ca | 28.773045 | 27.509830 | 29.666565 |
| Ca | 30.277128 | 32.297981 | 27.430521 |
| Ca | 30.441799 | 27.876518 | 24.352976 |
| Ca | 33.586311 | 30.054346 | 28.183836 |
| Ca | 34.593033 | 25.192204 | 26.604580 |
|   | 155   | 29.194231 | 24.108025 |
|---|-------|-----------|-----------|
| S | 21.180887 | 31.915249 | 35.654358 |
| S | 20.576565 | 36.030750 | 33.097240 |
| S | 22.020578 | 31.344828 | 29.835423 |
| S | 24.891071 | 33.351784 | 32.995667 |
| S | 26.330219 | 29.395515 | 31.060192 |
| S | 25.829929 | 33.89046 | 28.430456 |
| S | 28.184090 | 29.296982 | 26.565813 |
| S | 30.534729 | 30.61865 | 30.277727 |
| S | 31.808405 | 26.831425 | 27.727970 |
| S | 32.607018 | 30.773485 | 25.092117 |
| S | 33.558521 | 26.449712 | 23.248388 |
| S | 36.466965 | 28.013477 | 27.161728 |

24
generated by VMD

|   | 18.778351 | 33.064453 | 34.027622 |
|---|-----------|-----------|-----------|
| Ca | 22.932606 | 35.072067 | 35.336872 |
| Ca | 23.376091 | 30.330990 | 32.842400 |
| Ca | 22.925884 | 34.872742 | 30.461708 |
| Ca | 24.671915 | 30.228695 | 27.79182 |
| Ca | 27.704411 | 32.566525 | 31.385651 |
| Ca | 28.818199 | 27.678164 | 29.715982 |
| Ca | 30.333649 | 32.323154 | 27.583981 |
| Ca | 30.641003 | 27.992102 | 24.709703 |
| Ca | 33.439541 | 29.785952 | 28.144260 |
| Ca | 34.574493 | 24.911203 | 26.563850 |
| Ca | 35.624687 | 29.282267 | 23.945330 |
| S | 21.317074 | 31.851101 | 35.649803 |
| S | 20.733133 | 36.017403 | 32.974907 |
| S | 21.800205 | 31.383169 | 29.800938 |
| S | 24.982624 | 33.390697 | 33.111893 |
| S | 26.102005 | 29.204582 | 30.905830 |
| S | 25.894585 | 33.574883 | 28.620321 |
| S | 28.095728 | 29.669985 | 26.600012 |
| S | 30.643772 | 30.674959 | 30.358791 |
| S | 31.969631 | 27.080868 | 28.001163 |
| S | 32.591640 | 30.966888 | 25.033802 |
| S | 33.551777 | 26.430529 | 23.447718 |
| S | 36.217098 | 27.946684 | 26.938282 |

24
generated by VMD

|   | 18.223377 | 33.159966 | 33.975891 |
|---|-----------|-----------|-----------|
| Ca | 23.055853 | 34.876011 | 35.712173 |
| Ca | 23.405449 | 30.378277 | 32.876060 |
| Ca | 22.896944 | 34.698086 | 30.625359 |
| Ca | 24.616383 | 30.417429 | 27.895596 |
|   | Ca   | S    | Ca   |
|---|------|------|------|
|   | 27.767578 | 32.552597 | 31.153301 |
| Ca | 28.868372  | 27.819340  | 29.765236  |
| Ca | 30.475401  | 32.364788  | 27.395790  |
| Ca | 30.596424  | 27.898306  | 24.783678  |
| Ca | 33.808346  | 29.965139  | 28.025833  |
| Ca | 34.526489  | 25.028067  | 26.643597  |
| Ca | 35.779858  | 28.914406  | 23.886066  |
| S  | 21.094608  | 31.743023  | 35.397205  |
| S  | 20.654118  | 35.763355  | 33.281357  |
| S  | 21.718884  | 31.566982  | 29.740114  |
| S  | 24.966866  | 33.283447  | 33.254562  |
| S  | 26.063631  | 29.438307  | 31.021490  |
| S  | 25.848436  | 33.948318  | 28.360069  |
| S  | 28.066278  | 29.643858  | 26.806925  |
| S  | 30.566132  | 30.857796  | 30.064711  |
| S  | 32.004395  | 27.149738  | 27.971245  |
| S  | 32.711830  | 30.737522  | 24.843830  |
| S  | 33.419250  | 26.322445  | 23.408617  |
| S  | 36.585117  | 27.772850  | 27.051395  |

generated by VMD

|   | Ca   | S    | Ca   |
|---|------|------|------|
| Ca | 18.390156 | 33.506012 | 33.991760 |
| Ca | 22.769089 | 35.051079 | 35.466415 |
| Ca | 23.215416 | 30.217896 | 33.059311 |
| Ca | 23.043362 | 34.651310 | 30.316359 |
| Ca | 24.862041 | 30.449137 | 27.854794 |
| Ca | 27.769554 | 32.373863 | 31.635048 |
| Ca | 29.040367 | 27.812939 | 29.925507 |
| Ca | 30.539345 | 32.412663 | 27.619471 |
| Ca | 30.349693 | 27.687380 | 24.556629 |
| Ca | 33.748341 | 30.129448 | 27.879025 |
| Ca | 34.588161 | 25.176731 | 26.668818 |
| Ca | 35.633450 | 29.054071 | 23.675152 |
| S  | 20.791910 | 31.613537 | 35.480690 |
| S  | 20.921024 | 36.038193 | 32.937550 |
| S  | 21.855171 | 31.351223 | 29.838596 |
| S  | 24.818897 | 33.266258 | 33.195354 |
| S  | 26.037861 | 29.116547 | 31.095016 |
| S  | 25.942755 | 33.771683 | 28.550606 |
| S  | 28.149660 | 29.611555 | 26.831007 |
| S  | 30.959564 | 30.896709 | 30.511631 |
| S  | 31.787392 | 27.033113 | 27.738651 |
| S  | 32.497238 | 30.715733 | 24.849186 |
| S  | 33.483063 | 26.396210 | 23.485199 |
| S  | 36.526524 | 27.966742 | 26.778254 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.382750 | 33.337135 | 33.911602 |
| Ca      | 22.823757 | 34.644382 | 35.758072 |
| Ca      | 23.155607 | 30.095383 | 32.924553 |
| Ca      | 22.974470 | 34.700264 | 30.664467 |
| Ca      | 24.744965 | 30.423878 | 27.806641 |
| Ca      | 27.517845 | 32.903164 | 31.239763 |
| Ca      | 29.103893 | 28.080017 | 29.964851 |
| Ca      | 30.315584 | 32.606674 | 27.477177 |
| Ca      | 30.546379 | 27.780930 | 24.683613 |
| Ca      | 33.878857 | 30.051800 | 28.081804 |
| Ca      | 34.376804 | 25.091047 | 26.687380 |
| Ca      | 35.696373 | 28.607775 | 23.593987 |
| S       | 20.960440 | 31.415691 | 35.526711 |
| S       | 20.642426 | 35.878754 | 33.074394 |
| S       | 21.827232 | 31.485210 | 29.840872 |
| S       | 24.906811 | 33.279366 | 33.448715 |
| S       | 26.122089 | 29.623253 | 30.835011 |
| S       | 25.792587 | 33.973198 | 28.536228 |
| S       | 28.066292 | 29.766125 | 26.605371 |
| S       | 30.934540 | 31.351484 | 30.194670 |
| S       | 32.025433 | 26.972676 | 27.989199 |
| S       | 32.757378 | 30.491245 | 24.761648 |
| S       | 33.564049 | 26.175549 | 23.338531 |
| S       | 36.603451 | 27.562092 | 26.994778 |

24 generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.329575 | 33.197392 | 33.969284 |
| Ca      | 22.904285 | 34.851006 | 35.784016 |
| Ca      | 23.285892 | 30.235954 | 32.958431 |
| Ca      | 22.806496 | 34.739494 | 30.558401 |
| Ca      | 25.030756 | 30.441353 | 27.845551 |
| Ca      | 27.711664 | 32.680283 | 31.130287 |
| Ca      | 29.123016 | 27.915291 | 29.959713 |
| Ca      | 30.545471 | 32.536079 | 27.288185 |
| Ca      | 30.563847 | 27.644281 | 24.781300 |
| Ca      | 33.615005 | 29.937506 | 28.031889 |
| Ca      | 34.166042 | 25.052395 | 26.537682 |
| Ca      | 35.848732 | 28.937222 | 23.860035 |
| S       | 21.007748 | 31.644323 | 35.628555 |
| S       | 20.530472 | 35.871544 | 33.181145 |
| S       | 21.911970 | 31.208210 | 29.839813 |
| S       | 24.896729 | 33.416977 | 33.102982 |
| S       | 26.128750 | 29.498898 | 30.860357 |
| S       | 25.716259 | 33.996735 | 28.298183 |
| S       | 28.324221 | 29.753059 | 26.903666 |
|   | X     | Y     | Z     |
|---|-------|-------|-------|
| S | 30.982956 | 31.054920 | 30.314585 |
| S | 31.873577 | 26.869823 | 27.887442 |
| S | 32.519001 | 30.764948 | 24.978773 |
| S | 33.545216 | 26.384323 | 23.218853 |
| S | 36.352356 | 27.668015 | 27.020983 |

generated by VMD

| Ca | X     | Y     | Z     |
|----|-------|-------|-------|
| Ca | 18.524212 | 33.510342 | 33.761440 |
| Ca | 23.225801 | 34.773148 | 35.739418 |
| Ca | 23.511576 | 30.208153 | 33.144390 |
| Ca | 22.904379 | 34.616684 | 30.712645 |
| Ca | 24.385836 | 30.439285 | 27.612930 |
| Ca | 27.495800 | 32.602928 | 31.036114 |
| Ca | 28.860111 | 27.775610 | 29.491066 |
| Ca | 30.431168 | 32.061371 | 27.301674 |
| Ca | 30.549263 | 27.905647 | 24.623709 |
| Ca | 33.913876 | 30.041756 | 28.318548 |
| Ca | 34.770809 | 24.989532 | 26.743713 |
| Ca | 35.729668 | 29.151338 | 23.833839 |
| S  | 21.109268 | 31.813202 | 35.504086 |
| S  | 20.924530 | 36.025845 | 33.280792 |
| S  | 21.807322 | 31.451168 | 30.103807 |
| S  | 24.909302 | 33.393932 | 33.440678 |
| S  | 25.785965 | 29.211109 | 30.440937 |
| S  | 25.480518 | 33.841431 | 28.580376 |
| S  | 27.938288 | 29.538357 | 26.521778 |
| S  | 30.623581 | 30.864288 | 30.142181 |
| S  | 31.852417 | 27.064037 | 27.873335 |
| S  | 32.826633 | 30.874693 | 24.904295 |
| S  | 33.697746 | 26.212952 | 23.567413 |
| S  | 36.462013 | 27.933498 | 27.260899 |

generated by VMD

| Ca | X     | Y     | Z     |
|----|-------|-------|-------|
| Ca | 18.202583 | 33.268139 | 33.946136 |
| Ca | 23.181133 | 34.790367 | 35.768559 |
| Ca | 23.477276 | 30.535736 | 33.037018 |
| Ca | 22.991753 | 34.687119 | 30.712557 |
| Ca | 24.534042 | 30.473640 | 27.738461 |
| Ca | 27.687351 | 32.638950 | 31.085306 |
| Ca | 28.805927 | 27.610806 | 29.613039 |
| Ca | 30.414970 | 32.001831 | 27.419235 |
| Ca | 30.649572 | 27.868839 | 24.591684 |
| Ca | 33.672951 | 30.086500 | 28.207930 |
| Ca | 34.541965 | 25.158869 | 26.824055 |
| Ca | 35.739021 | 28.997757 | 23.765656 |
| S  | 21.137823 | 31.837666 | 35.472702 |
| S     | 20.755859 | 35.892864 | 33.137070 |
|------|-----------|-----------|-----------|
| S     | 21.800365 | 31.434570 | 29.858376 |
| S     | 25.062216 | 33.276405 | 33.424732 |
| S     | 25.917255 | 29.503407 | 30.760754 |
| S     | 25.634977 | 33.840294 | 28.499380 |
| S     | 27.983757 | 29.612759 | 26.623724 |
| S     | 30.636681 | 30.762306 | 30.183491 |
| S     | 31.918463 | 27.067652 | 27.748333 |
| S     | 32.685692 | 30.645456 | 25.021118 |
| S     | 33.857330 | 26.240473 | 23.303383 |
| S     | 36.431118 | 28.067604 | 27.197392 |

24
generated by VMD

| Ca    | 18.234650 | 33.219479 | 33.962574 |
|-------|-----------|-----------|-----------|
| Ca    | 23.238935 | 35.059471 | 35.614735 |
| Ca    | 23.406116 | 30.371845 | 33.234436 |
| Ca    | 22.903862 | 34.510948 | 30.720394 |
| Ca    | 24.806538 | 30.299423 | 27.713690 |
| Ca    | 27.682810 | 32.628902 | 31.129040 |
| Ca    | 28.972759 | 27.945236 | 29.625252 |
| Ca    | 30.258801 | 32.296074 | 27.420862 |
| Ca    | 30.555393 | 27.925518 | 24.431952 |
| Ca    | 33.625549 | 29.847675 | 28.135399 |
| Ca    | 34.361378 | 25.000858 | 26.529509 |
| Ca    | 35.979790 | 29.278008 | 24.111105 |
| S     | 21.237980 | 31.975586 | 35.720760 |
| S     | 20.682062 | 35.701797 | 33.051998 |
| S     | 21.849192 | 31.348824 | 29.874516 |
| S     | 25.025909 | 33.281670 | 33.294006 |
| S     | 25.931023 | 29.454336 | 30.648647 |
| S     | 25.739456 | 33.895416 | 28.478094 |
| S     | 27.953560 | 29.552849 | 26.546858 |
| S     | 30.622377 | 30.923843 | 30.147619 |
| S     | 31.665714 | 26.899660 | 27.839371 |
| S     | 32.809479 | 30.574032 | 25.018007 |
| S     | 33.642323 | 26.446011 | 23.447058 |
| S     | 36.534389 | 27.862606 | 27.244242 |

24
generated by VMD

| Ca    | 18.441212 | 33.204571 | 33.937393 |
|-------|-----------|-----------|-----------|
| Ca    | 22.964077 | 35.093632 | 35.388275 |
| Ca    | 23.589474 | 30.076832 | 33.371597 |
| Ca    | 22.850109 | 34.725525 | 30.701773 |
| Ca    | 24.603367 | 30.502155 | 27.695295 |
| Ca    | 27.691008 | 32.421181 | 31.244425 |
| Ca    | 28.892994 | 27.758644 | 29.469095 |
|    | Ca      |    |      |     |      |
|----|---------|----|------|-----|------|
|    | 30.453106 |   | 32.179146 |    | 27.349928 |
|    | 30.618290 |   | 28.169804 |    | 24.567320 |
|    | 33.593399 |   | 29.996923 |    | 28.018015 |
|    | 34.290558 |   | 24.874683 |    | 26.560200 |
|    | 36.010696 |   | 28.958179 |    | 23.912428 |
|    | 21.368549 |   | 31.873688 |    | 35.577888 |
|    | 20.313774 |   | 36.036232 |    | 32.875267 |
|    | 21.855503 |   | 31.237894 |    | 30.385284 |
|    | 24.987694 |   | 33.500137 |    | 33.363968 |
|    | 25.927784 |   | 29.366444 |    | 30.646645 |
|    | 25.671692 |   | 33.906281 |    | 28.677963 |
|    | 28.041348 |   | 29.548447 |    | 26.545021 |
|    | 30.639679 |   | 30.634892 |    | 30.234119 |
|    | 31.817177 |   | 27.259892 |    | 27.802853 |
|    | 32.866386 |   | 30.759687 |    | 24.971663 |
|    | 33.788002 |   | 26.402405 |    | 23.349686 |
|    | 36.444180 |   | 27.812798 |    | 27.293953 |

24

generated by VMD

|    | Ca      |    |      |     |      |
|----|---------|----|------|-----|------|
|    | 18.532120 |   | 32.963795 |    | 34.229061 |
|    | 23.293045 |   | 35.175797 |    | 35.457405 |
|    | 23.590652 |   | 30.319878 |    | 33.044514 |
|    | 22.782646 |   | 34.485756 |    | 33.067755 |
|    | 24.625847 |   | 30.623854 |    | 27.349728 |
|    | 27.694748 |   | 32.493187 |    | 30.921371 |
|    | 28.665442 |   | 27.910351 |    | 29.600212 |
|    | 30.553772 |   | 32.627651 |    | 27.494535 |
|    | 30.634417 |   | 28.185429 |    | 24.653297 |
|    | 33.683598 |   | 29.812622 |    | 28.322306 |
|    | 34.275280 |   | 24.764149 |    | 26.735937 |
|    | 35.489609 |   | 29.112700 |    | 24.038879 |
|    | 21.627968 |   | 31.774540 |    | 35.563087 |
|    | 20.473679 |   | 35.687557 |    | 33.295635 |
|    | 21.878819 |   | 31.292839 |    | 29.762402 |
|    | 24.993572 |   | 33.450783 |    | 33.297974 |
|    | 25.878700 |   | 29.299789 |    | 30.552073 |
|    | 25.479721 |   | 33.711788 |    | 28.369022 |
|    | 28.247280 |   | 29.969568 |    | 26.579338 |
|    | 30.611202 |   | 30.975403 |    | 30.194237 |
|    | 31.784369 |   | 26.997417 |    | 27.784931 |
|    | 32.866665 |   | 30.843828 |    | 25.213263 |
|    | 33.615784 |   | 26.062496 |    | 23.549751 |
|    | 36.441086 |   | 27.758894 |    | 27.263359 |

24

generated by VMD

|    | Ca      |    |      |     |      |
|----|---------|----|------|-----|------|
|    | 18.136829 |   | 33.158260 |    | 34.349541 |
|   | Ca     | S      |
|---|--------|--------|
|   | 23.013851 | 35.108624 | 35.327255 |
|   | 23.565451 | 30.405050 | 33.077030 |
|   | 22.657888 | 34.987545 | 30.625263 |
|   | 24.767557 | 30.305042 | 27.680935 |
|   | 27.852753 | 32.522114 | 31.194778 |
|   | 28.739336 | 27.617912 | 29.570677 |
|   | 30.690187 | 32.054279 | 27.511106 |
|   | 30.438856 | 27.976318 | 24.391220 |
|   | 33.729221 | 29.557829 | 28.246624 |
|   | 34.599396 | 25.253853 | 26.702888 |
|   | 35.769928 | 29.249424 | 23.780645 |
|   | 21.213619 | 31.903316 | 35.600658 |
|   | 20.253048 | 35.866886 | 33.144234 |
|   | 21.957420 | 31.391550 | 29.912468 |
|   | 24.924049 | 33.721619 | 33.222652 |
|   | 26.061062 | 29.234848 | 30.882504 |
|   | 25.770370 | 33.869526 | 28.560148 |
|   | 28.137154 | 29.664127 | 26.599468 |
|   | 30.671322 | 30.542284 | 30.444159 |
|   | 31.676922 | 26.644720 | 27.705906 |
|   | 32.705181 | 30.569632 | 25.035984 |
|   | 33.718098 | 26.424561 | 23.424631 |
|   | 36.665760 | 28.270729 | 26.949266 |

24 generated by VMD

|   | Ca     | S      |
|---|--------|--------|
|   | 18.392202 | 33.178005 | 34.186821 |
|   | 22.980183 | 35.058884 | 35.612740 |
|   | 23.118317 | 30.352043 | 33.064854 |
|   | 23.102501 | 34.657547 | 30.598473 |
|   | 24.774515 | 30.641308 | 27.568834 |
|   | 27.789173 | 32.601337 | 31.337803 |
|   | 28.647936 | 27.818832 | 29.812841 |
|   | 30.688843 | 32.007996 | 27.550550 |
|   | 30.577179 | 27.844006 | 24.385405 |
|   | 33.614998 | 29.831480 | 28.285942 |
|   | 34.726982 | 25.330730 | 26.837767 |
|   | 35.636734 | 28.903555 | 23.550274 |
|   | 21.252335 | 31.934351 | 35.788132 |
|   | 20.649342 | 35.635117 | 32.937138 |
|   | 21.671621 | 31.306465 | 29.742750 |
|   | 24.988607 | 33.179264 | 33.268436 |
|   | 25.853827 | 29.570179 | 30.796024 |
|   | 25.807587 | 34.049530 | 28.366379 |
|   | 28.210285 | 29.560120 | 26.820086 |
|   | 30.730309 | 30.724789 | 30.434656 |
|   | 31.591234 | 26.909599 | 27.646490 |
S  32.696178  30.644699  25.053892
S  33.726376  26.255642  23.289745
S  36.492821  28.304577  27.004065

24
generated by VMD

Ca  18.322975  32.935966  34.332500
Ca  22.784945  35.084396  35.550720
Ca  23.358009  30.297165  32.966911
Ca  22.828133  34.583351  30.502592
Ca  25.035576  30.504999  27.685371
Ca  27.677958  32.748100  31.349918
Ca  28.981287  27.974293  29.761114
Ca  31.100571  32.422844  27.384367
Ca  30.408623  28.136757  24.559114
Ca  33.793900  29.809708  28.410040
Ca  34.439709  25.105007  26.852728
Ca  35.633957  28.599243  23.466776
S  21.170906  31.818382  35.773900
S  20.443485  35.576904  32.985279
S  21.894171  31.187363  29.568571
S  24.765549  33.331142  33.180260
S  26.159744  29.578028  30.820139
S  25.794273  34.001846  28.622147
S  28.390953  30.024963  26.672445
S  30.831079  30.852230  30.465847
S  31.714951  26.876892  27.731314
S  32.816509  30.638710  24.950678
S  33.136261  26.185825  23.412691
S  36.236496  28.025902  26.931168

24
generated by VMD

Ca  18.521111  32.935893  34.051125
Ca  22.980562  35.171719  35.380167
Ca  23.592499  30.213917  32.883312
Ca  22.843288  34.609314  30.591228
Ca  24.629425  30.716492  27.597143
Ca  27.735226  32.352531  31.420195
Ca  28.973644  27.882185  29.652029
Ca  30.538708  32.494518  27.690836
Ca  30.301834  28.065460  24.976933
Ca  33.829208  29.700031  28.313698
Ca  35.459444  24.922588  26.911745
Ca  35.419407  29.021877  23.305307
S  21.351212  31.816177  35.573502
S  20.436493  35.695663  32.869644
S  21.888790  31.245960  29.687571
S   24.978502  33.406185  33.138100
S   25.912737  29.338562  30.575079
S   26.017029  34.112659  28.689856
S   28.068630  29.919193  26.812298
S   30.744446  30.932207  30.332130
S   31.879230  26.791349  27.966640
S   32.721474  30.747858  25.126226
S   33.296211  26.179390  23.694801
S   36.521019  28.060343  26.708687
24
generated by VMD
Ca   18.443630  32.930286  33.538227
Ca   23.110281  35.208477  35.174461
Ca   23.570423  30.075003  33.045906
Ca   22.889931  34.776100  30.608061
Ca   24.633244  30.589409  27.955109
Ca   27.862423  32.345234  31.357144
Ca   29.141079  27.708229  29.878057
Ca   30.490627  32.246761  27.583752
Ca   30.336744  28.173054  25.07126
Ca   33.991367  29.999115  28.145014
Ca   34.226929  24.923534  26.409538
Ca   35.458046  29.093412  23.578045
S   21.267736  31.908895  35.297348
S   20.390373  35.918530  32.610474
S   21.841465  31.237398  30.048332
S   25.060234  33.276360  33.141724
S   26.032028  29.159748  30.940268
S   25.897602  33.887886  28.734110
S   28.029346  29.759649  27.009600
S   30.878395  30.821655  30.455652
S   31.914375  27.118919  28.036060
S   32.619301  30.763210  25.156872
S   33.149483  26.413387  23.465805
S   36.485088  27.965839  26.700142
24
generated by VMD
Ca   18.256765  33.019016  33.861427
Ca   23.000563  35.188534  35.188725
Ca   23.414759  30.169657  33.068733
Ca   22.778900  34.521191  30.600769
Ca   24.931297  30.531410  27.940290
Ca   27.795345  32.717758  31.517290
Ca   29.119740  27.966230  29.812351
Ca   30.834530  32.253693  27.628870
Ca   30.235807  28.059448  24.661251
|   | Ca       | 33.859669 | 29.864992 | 28.254951 |
|---|----------|-----------|-----------|-----------|
|   | Ca       | 34.402561 | 25.053654 | 26.515556 |
|   | Ca       | 35.384583 | 28.941883 | 23.549303 |
|   | S        | 21.304180 | 31.862558 | 35.338440 |
|   | S        | 20.350658 | 35.869976 | 32.752262 |
|   | S        | 22.025175 | 28.941883 | 23.549303 |
|   | S        | 24.879292 | 33.384712 | 33.273628 |
|   | S        | 26.042318 | 29.306534 | 30.827227 |
|   | S        | 25.984419 | 34.009697 | 28.722197 |
|   | S        | 28.286868 | 29.726986 | 26.845001 |
|   | S        | 30.980286 | 30.889553 | 30.611013 |
|   | S        | 31.809677 | 26.807888 | 27.791416 |
|   | S        | 32.478943 | 30.710571 | 25.061752 |
|   | S        | 33.102924 | 26.367592 | 23.395811 |
|   | S        | 36.460945 | 28.047600 | 26.886969 |

24 generated by VMD

|   | Ca       | 18.215326 | 32.922630 | 33.703712 |
|---|----------|-----------|-----------|-----------|
|   | Ca       | 23.101011 | 35.152615 | 35.051285 |
|   | Ca       | 23.552162 | 30.329496 | 33.201805 |
|   | Ca       | 22.898838 | 34.585312 | 30.628990 |
|   | Ca       | 24.737751 | 30.609375 | 27.997910 |
|   | Ca       | 28.010952 | 32.562599 | 31.514606 |
|   | Ca       | 28.790840 | 27.735390 | 29.634863 |
|   | Ca       | 30.435820 | 32.310738 | 27.601576 |
|   | Ca       | 30.282957 | 28.102427 | 24.629566 |
|   | Ca       | 33.917671 | 29.793678 | 28.054214 |
|   | Ca       | 34.299519 | 24.937441 | 26.576490 |
|   | Ca       | 35.607777 | 29.305002 | 23.771944 |
|   | S        | 21.160543 | 32.179459 | 35.323929 |
|   | S        | 20.320465 | 35.595741 | 32.679703 |
|   | S        | 21.994619 | 31.043114 | 29.913008 |
|   | S        | 25.073549 | 33.489906 | 33.436913 |
|   | S        | 26.276451 | 29.412350 | 31.193602 |
|   | S        | 25.758480 | 33.940418 | 28.749084 |
|   | S        | 27.915047 | 29.779020 | 26.817867 |
|   | S        | 30.863354 | 30.802332 | 30.314627 |
|   | S        | 31.714367 | 26.892166 | 27.768570 |
|   | S        | 32.650536 | 30.742123 | 25.281092 |
|   | S        | 33.459274 | 26.277367 | 23.374990 |
|   | S        | 36.682686 | 27.799379 | 26.719719 |

24 generated by VMD

|   | Ca       | 18.364174 | 33.042389 | 33.710869 |
|---|----------|-----------|-----------|-----------|
|   | Ca       | 22.885702 | 34.979286 | 35.462280 |
|   | Ca       | 23.649088 | 30.410332 | 33.036644 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 22.798180 | 34.638527 | 30.522337 |
| Ca      | 24.800518 | 30.412285 | 27.930786 |
| Ca      | 27.955154 | 32.736534 | 31.524246 |
| Ca      | 28.897013 | 27.818218 | 29.524048 |
| Ca      | 30.547289 | 32.324856 | 27.729910 |
| Ca      | 30.461063 | 27.971127 | 24.457672 |
| Ca      | 33.560532 | 29.881794 | 28.040920 |
| Ca      | 34.276779 | 24.920551 | 26.579391 |
| Ca      | 35.621250 | 29.132406 | 23.804596 |
| S       | 21.209137 | 31.813231 | 35.523457 |
| S       | 20.391623 | 35.723091 | 32.854076 |
| S       | 22.075417 | 31.198160 | 29.969414 |
| S       | 24.830601 | 33.699860 | 33.234474 |
| S       | 26.317947 | 29.528006 | 31.222589 |
| S       | 25.763279 | 33.817139 | 28.664377 |
| S       | 28.115475 | 29.663960 | 26.678518 |
| S       | 30.890404 | 30.798504 | 30.418018 |
| S       | 31.571644 | 26.925396 | 27.702477 |
| S       | 32.749687 | 30.771679 | 24.964554 |
| S       | 33.655380 | 26.196918 | 23.454624 |
| S       | 36.332775 | 27.895750 | 26.929800 |

24 generated by VMD

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 18.189240 | 32.970474 | 33.567390 |
| Ca      | 22.680939 | 34.701900 | 35.567390 |
| Ca      | 23.515810 | 30.518953 | 32.968132 |
| Ca      | 22.905392 | 34.873009 | 30.730570 |
| Ca      | 25.029385 | 30.588579 | 27.980093 |
| Ca      | 27.766048 | 32.731335 | 31.476645 |
| Ca      | 29.079197 | 27.914099 | 29.938955 |
| Ca      | 30.649933 | 32.335236 | 27.478281 |
| Ca      | 30.533638 | 27.731541 | 24.557840 |
| Ca      | 33.781288 | 29.810440 | 27.960480 |
| Ca      | 34.430458 | 24.811548 | 26.732847 |
| Ca      | 35.393066 | 29.259361 | 23.664740 |
| S       | 21.035915 | 31.574535 | 35.457863 |
| S       | 20.426132 | 35.712570 | 33.023499 |
| S       | 22.017452 | 31.230488 | 29.860231 |
| S       | 24.899586 | 33.847168 | 33.253189 |
| S       | 26.335430 | 29.589954 | 31.129141 |
| S       | 25.884102 | 33.997154 | 28.615772 |
| S       | 28.124718 | 29.648956 | 26.813681 |
| S       | 30.810150 | 30.962006 | 30.199486 |
| S       | 31.843910 | 26.902020 | 27.778893 |
| S       | 32.548386 | 30.708771 | 24.917692 |
| S       | 33.403358 | 26.053349 | 23.419916 |
|   | 36.436550 | 27.826641 | 26.847363 |
|---|------------|------------|------------|

24 generated by VMD

|   | 18.304893  | 33.019505  | 33.511497  |
|---|------------|------------|------------|
| Ca| 22.850212  | 34.869446  | 35.628757  |
| Ca| 23.683790  | 30.144161  | 33.032356  |
| Ca| 22.787430  | 34.594673  | 30.587145  |
| Ca| 25.060738  | 30.565104  | 27.907305  |
| Ca| 27.907219  | 33.092064  | 31.450228  |
| Ca| 29.095278  | 27.908073  | 29.641565  |
| Ca| 30.596625  | 32.492233  | 27.660721  |
| Ca| 30.393366  | 27.783619  | 24.569677  |
| Ca| 33.628807  | 30.041811  | 28.268410  |
| Ca| 34.264633  | 24.815479  | 26.536215  |
| Ca| 35.291283  | 28.951231  | 23.776114  |
| S | 21.105789  | 31.592844  | 35.265785  |
| S | 20.369976  | 35.556404  | 32.780617  |
| S | 22.149025  | 31.081585  | 30.019743  |
| S | 24.949074  | 33.609612  | 33.403156  |
| S | 26.576290  | 29.855145  | 31.116362  |
| S | 25.782978  | 34.041908  | 28.618074  |
| S | 28.238846  | 29.778603  | 26.642109  |
| S | 30.942120  | 31.076923  | 30.390284  |
| S | 31.718510  | 26.960814  | 27.775732  |
| S | 32.558891  | 30.747303  | 25.042440  |
| S | 33.144009  | 25.879082  | 23.191986  |
| S | 36.317337  | 27.842411  | 27.123745  |

24 generated by VMD

|   | 18.324860  | 32.891556  | 33.866657  |
|---|------------|------------|------------|
| Ca| 22.830544  | 34.952286  | 35.700485  |
| Ca| 23.487982  | 30.330292  | 32.937233  |
| Ca| 22.734150  | 34.960075  | 30.504759  |
| Ca| 25.053417  | 30.491814  | 27.878237  |
| Ca| 27.664185  | 32.635712  | 31.221920  |
| Ca| 29.016920  | 27.773083  | 29.610729  |
| Ca| 30.421780  | 32.579468  | 27.639656  |
| Ca| 30.559322  | 27.956881  | 24.481924  |
| Ca| 33.671684  | 29.930611  | 27.936707  |
| Ca| 34.352322  | 24.646755  | 26.646376  |
| Ca| 35.755577  | 28.951303  | 23.949871  |
| S | 21.383228  | 31.597754  | 35.616196  |
| S | 20.326378  | 35.759613  | 33.188835  |
| S | 21.907097  | 31.312939  | 29.996380  |
| S | 24.806128  | 33.758472  | 33.123459  |
| S | 26.470348  | 29.723778  | 31.041943  |
| S    | 25.568050 | 33.858917 | 28.483437 |
|------|-----------|-----------|-----------|
| S    | 28.326374 | 29.687748 | 26.729359 |
| S    | 30.605824 | 31.077404 | 30.322739 |
| S    | 31.621712 | 26.919132 | 27.599203 |
| S    | 32.843788 | 30.662460 | 25.038380 |
| S    | 33.528915 | 26.185705 | 23.360918 |
| S    | 36.459496 | 27.656271 | 27.064651 |

24 generated by VMD

| Ca   | 18.320694 | 32.990952 | 33.375118 |
|------|-----------|-----------|-----------|
| Ca   | 22.852310 | 35.046028 | 35.668503 |
| Ca   | 23.546280 | 30.208235 | 33.215515 |
| Ca   | 22.789364 | 34.702118 | 30.486046 |
| Ca   | 25.047440 | 30.565508 | 28.130018 |
| Ca   | 27.695770 | 32.793602 | 31.402641 |
| Ca   | 29.042665 | 27.897137 | 29.794189 |
| Ca   | 30.575853 | 32.269913 | 27.526180 |
| Ca   | 30.426762 | 28.043568 | 24.557564 |
| Ca   | 33.790306 | 29.937122 | 27.725031 |
| Ca   | 34.452942 | 24.601978 | 26.412989 |
| Ca   | 35.553139 | 29.106913 | 23.914879 |
| S    | 21.045351 | 31.792873 | 35.496758 |
| S    | 20.431087 | 35.786240 | 33.027542 |
| S    | 21.905815 | 31.146130 | 29.938129 |
| S    | 24.796551 | 33.597237 | 33.331188 |
| S    | 26.429985 | 29.678396 | 31.351727 |
| S    | 25.680679 | 33.907478 | 28.372414 |
| S    | 28.198956 | 29.667747 | 26.744781 |
| S    | 30.769497 | 30.957920 | 30.409527 |
| S    | 31.716465 | 26.878359 | 27.732975 |
| S    | 32.649281 | 30.916050 | 25.135015 |
| S    | 33.494286 | 26.210636 | 23.279575 |
| S    | 36.508568 | 27.597940 | 26.911722 |

24 generated by VMD

| Ca   | 18.418352 | 32.788006 | 33.777206 |
|------|-----------|-----------|-----------|
| Ca   | 22.801125 | 34.886921 | 35.606647 |
| Ca   | 23.541864 | 30.210560 | 33.134026 |
| Ca   | 22.853649 | 34.884804 | 30.546270 |
| Ca   | 25.179779 | 30.650040 | 27.940842 |
| Ca   | 27.787836 | 32.816051 | 31.083549 |
| Ca   | 29.185204 | 27.711082 | 29.724855 |
| Ca   | 30.462578 | 32.320442 | 27.783665 |
| Ca   | 30.461330 | 27.895863 | 24.513260 |
| Ca   | 33.513451 | 29.776268 | 28.133289 |
| Ca   | 34.522957 | 24.820698 | 26.610142 |
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 35.302795  | 29.156071  | 23.886021  |
| S       | 21.103134  | 31.643166  | 35.568268  |
| S       | 20.426367  | 35.674641  | 32.984360  |
| S       | 22.092836  | 31.375015  | 29.823547  |
| S       | 25.008955  | 33.570446  | 33.273396  |
| S       | 26.570164  | 29.790356  | 31.060852  |
| S       | 25.623960  | 34.117813  | 28.226547  |
| S       | 28.294735  | 29.829525  | 26.726177  |
| S       | 30.666996  | 30.862549  | 30.296940  |
| S       | 31.631115  | 26.786156  | 27.638199  |

24 generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 18.114536  | 32.965370  | 33.480736  |
| Ca      | 22.478952  | 34.705559  | 35.736183  |
| Ca      | 23.694391  | 30.307049  | 33.084534  |
| Ca      | 22.828278  | 35.015064  | 30.442917  |
| Ca      | 25.054058  | 30.506361  | 28.058992  |
| Ca      | 27.780396  | 32.975662  | 31.260389  |
| Ca      | 29.179070  | 27.986507  | 29.628773  |
| Ca      | 30.563961  | 32.366787  | 27.647198  |
| Ca      | 30.337917  | 27.992794  | 24.508808  |
| Ca      | 33.962234  | 29.735678  | 28.190882  |
| Ca      | 34.525723  | 25.033333  | 26.446558  |
| Ca      | 35.454281  | 28.714882  | 23.749142  |
| S       | 20.934338  | 31.636726  | 35.491909  |
| S       | 20.290285  | 35.686626  | 33.087929  |
| S       | 22.053730  | 31.474112  | 30.174175  |
| S       | 24.785057  | 33.722382  | 33.265022  |
| S       | 26.579092  | 29.760567  | 31.192883  |
| S       | 25.740982  | 33.742577  | 28.495241  |
| S       | 28.139288  | 29.783388  | 26.626945  |
| S       | 30.870975  | 30.997562  | 30.433012  |
| S       | 31.823059  | 26.758224  | 27.734375  |
| S       | 32.747005  | 30.539295  | 25.276484  |
| S       | 33.156109  | 25.871288  | 23.368803  |
| S       | 36.626308  | 28.022278  | 26.558134  |

24 generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 18.187241  | 33.078346  | 33.769238  |
| Ca      | 22.771614  | 34.629158  | 35.433777  |
| Ca      | 23.367931  | 30.260071  | 32.830544  |
| Ca      | 22.808285  | 34.725403  | 30.648645  |
| Ca      | 24.922483  | 30.570301  | 27.942310  |
|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 27.961151 | 32.742989 | 31.299025 |
| Ca  | 29.025711 | 27.829809 | 29.816193 |
| Ca  | 30.757027 | 32.459641 | 27.584110 |
| Ca  | 30.423874 | 27.858418 | 24.772306 |
| Ca  | 33.819660 | 29.862516 | 27.962164 |
| Ca  | 34.416626 | 25.040659 | 26.711960 |
| Ca  | 35.142612 | 29.029247 | 23.494474 |
| S   | 20.981955 | 31.775959 | 35.332397 |
| S   | 20.390160 | 35.788166 | 32.933624 |
| S   | 22.110203 | 31.372068 | 29.985376 |
| S   | 24.832201 | 33.552368 | 33.266155 |
| S   | 26.367004 | 29.618504 | 31.245344 |
| S   | 25.788788 | 33.937706 | 28.513903 |
| S   | 28.368439 | 29.814384 | 26.906496 |
| S   | 30.907314 | 30.871098 | 30.451124 |
| S   | 31.754833 | 26.779945 | 27.822441 |
| S   | 32.730663 | 30.688026 | 25.095772 |
| S   | 33.301979 | 25.946304 | 23.469374 |
| S   | 36.582359 | 28.068918 | 26.653275 |

24

generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 18.048405 | 32.805496 | 33.671421 |
| Ca  | 22.738697 | 34.702347 | 35.876431 |
| Ca  | 23.471092 | 30.230801 | 32.814751 |
| Ca  | 22.802643 | 34.677338 | 30.447275 |
| Ca  | 24.992113 | 30.694477 | 27.782631 |
| Ca  | 28.019314 | 32.886974 | 31.382631 |
| Ca  | 29.106453 | 28.023346 | 29.867470 |
| Ca  | 30.638542 | 32.594604 | 27.513634 |
| Ca  | 30.196400 | 27.853952 | 24.722200 |
| Ca  | 34.004383 | 29.900412 | 27.858036 |
| Ca  | 34.398911 | 24.896423 | 26.690409 |
| Ca  | 35.372318 | 28.751488 | 23.597153 |
| S   | 21.009727 | 31.711540 | 35.399082 |
| S   | 20.419781 | 35.497520 | 33.137955 |
| S   | 22.055773 | 31.232887 | 29.878271 |
| S   | 24.979275 | 33.655697 | 33.218452 |
| S   | 26.287220 | 29.682697 | 30.868956 |
| S   | 25.952858 | 34.192982 | 28.522032 |
| S   | 28.241339 | 29.862858 | 26.843290 |
| S   | 30.961424 | 31.055786 | 30.361834 |
| S   | 31.813480 | 27.016579 | 27.906591 |
| S   | 32.654354 | 30.636765 | 25.117580 |
| S   | 33.041981 | 25.848446 | 23.514595 |
| S   | 36.513519 | 27.888647 | 26.947355 |

24
generated by VMD

| Element | X1     | Y1     | Z1     |
|---------|--------|--------|--------|
| Ca      | 18.124619 | 32.533558 | 33.445724 |
| Ca      | 22.744267 | 34.630135 | 35.727604 |
| Ca      | 23.566990 | 30.421360 | 32.886276 |
| Ca      | 22.816374 | 34.927341 | 30.677023 |
| Ca      | 24.880243 | 30.652775 | 27.817331 |
| Ca      | 27.873158 | 33.112820 | 31.426590 |
| Ca      | 29.315458 | 28.035378 | 29.855757 |
| Ca      | 30.699980 | 32.496086 | 27.531422 |
| Ca      | 30.194124 | 27.557018 | 24.939981 |
| Ca      | 33.769363 | 29.592886 | 27.855282 |
| Ca      | 34.545372 | 24.764210 | 26.554749 |
| Ca      | 35.265274 | 28.991238 | 23.631105 |
| S       | 21.157520 | 31.745285 | 35.244118 |
| S       | 20.290474 | 35.412262 | 33.061634 |
| S       | 22.015371 | 31.500381 | 29.702587 |
| S       | 24.996304 | 33.711185 | 33.427330 |
| S       | 26.344402 | 29.786522 | 31.129015 |
| S       | 25.818573 | 34.070374 | 28.479271 |
| S       | 28.408037 | 29.986755 | 26.870775 |
| S       | 30.827038 | 31.270981 | 30.553303 |
| S       | 31.815899 | 26.721909 | 27.836468 |
| S       | 32.489937 | 30.502708 | 25.072443 |
| S       | 33.212055 | 25.931395 | 23.54231 |
| S       | 36.549213 | 27.945515 | 26.671846 |

24 generated by VMD

| Element | X1     | Y1     | Z1     |
|---------|--------|--------|--------|
| Ca      | 18.569984 | 32.270775 | 33.429039 |
| Ca      | 22.992535 | 34.412029 | 35.720215 |
| Ca      | 23.347513 | 30.424131 | 32.836624 |
| Ca      | 23.028635 | 34.805298 | 30.631107 |
| Ca      | 24.874853 | 30.705723 | 27.766012 |
| Ca      | 28.007849 | 32.861969 | 31.316887 |
| Ca      | 28.938396 | 27.992054 | 29.719513 |
| Ca      | 30.655483 | 32.457699 | 27.456367 |
| Ca      | 30.349590 | 28.104252 | 25.096912 |
| Ca      | 33.823486 | 30.081882 | 28.133606 |
| Ca      | 34.277664 | 24.802111 | 26.801725 |
| Ca      | 35.113293 | 28.695261 | 23.636700 |
| S       | 21.253483 | 31.619015 | 35.477364 |
| S       | 20.495491 | 35.501854 | 33.113564 |
| S       | 22.034355 | 31.493038 | 29.549326 |
| S       | 24.969341 | 33.704285 | 32.966537 |
| S       | 26.174198 | 29.751503 | 31.031935 |
| S       | 25.899734 | 34.097046 | 28.517775 |
| S       | 28.116404 | 29.918631 | 26.721109 |
|    | 30.867359  | 31.083014  | 30.334068  |
|----|------------|------------|------------|
| 30.867359 | 31.905373  | 27.142162  | 28.168983  |
| 32.625538 | 30.605202  | 25.114740  |
| 32.980087 | 25.860859  | 23.651007  |
| 36.419441 | 27.910275  | 26.748962  |

24 generated by VMD

| Ca  | 18.351458 | 32.365086 | 33.293396 |
|-----|-----------|-----------|-----------|
| Ca  | 22.469231 | 34.538048 | 35.715851 |
| Ca  | 23.392719 | 30.536699 | 33.021370 |
| Ca  | 23.123421 | 35.113453 | 30.583172 |
| Ca  | 24.844845 | 30.579733 | 27.988602 |
| Ca  | 27.846987 | 33.191376 | 31.509558 |
| Ca  | 29.247124 | 28.057199 | 29.968943 |
| Ca  | 30.579924 | 32.268509 | 27.664711 |
| Ca  | 30.374916 | 27.884087 | 24.962469 |
| Ca  | 34.147877 | 29.989429 | 27.774696 |
| Ca  | 34.316944 | 24.709114 | 26.623598 |
| Ca  | 35.087307 | 28.819824 | 23.411819 |
| S   | 20.874657 | 31.482063 | 35.346939 |
| S   | 20.395149 | 35.380028 | 32.863365 |
| S   | 21.968674 | 31.613468 | 29.692516 |
| S   | 24.863457 | 33.844650 | 33.264671 |
| S   | 26.363579 | 29.713005 | 31.276033 |
| S   | 26.014305 | 33.947906 | 28.543829 |
| S   | 28.253410 | 29.846630 | 26.906595 |
| S   | 30.828762 | 31.227808 | 30.580532 |
| S   | 32.148335 | 27.026772 | 28.068655 |
| S   | 32.756599 | 30.773209 | 25.058205 |
| S   | 32.914242 | 25.852524 | 23.512466 |
| S   | 36.556137 | 27.539476 | 26.308062 |

24 generated by VMD

| Ca  | 18.304569 | 32.678017 | 33.554893 |
|-----|-----------|-----------|-----------|
| Ca  | 22.681877 | 34.816223 | 35.302505 |
| Ca  | 23.249149 | 30.288506 | 32.830082 |
| Ca  | 22.921604 | 34.676731 | 30.295792 |
| Ca  | 25.329964 | 30.505051 | 28.117554 |
| Ca  | 28.074028 | 32.946663 | 31.725636 |
| Ca  | 28.868801 | 28.040827 | 29.864992 |
| Ca  | 30.622215 | 32.672195 | 27.967394 |
| Ca  | 30.316191 | 27.896576 | 24.798054 |
| Ca  | 33.844185 | 29.975922 | 27.867334 |
| Ca  | 34.357319 | 24.746891 | 26.749062 |
| Ca  | 34.999851 | 28.869400 | 23.399332 |
| S   | 21.072496 | 31.646772 | 35.293858 |
|   | 20.421291 | 35.565063 | 32.749016 |
|---|-----------|-----------|-----------|
|  S | 22.092924 | 31.230774 | 29.676693 |
|  S | 24.869854 | 33.647694 | 33.281647 |
|  S | 26.505306 | 29.659899 | 31.344452 |
|  S | 26.127823 | 33.779037 | 28.811338 |
|  S | 28.359648 | 30.005844 | 26.810999 |
|  S | 30.977358 | 31.045589 | 30.568111 |
|  S | 31.963488 | 27.066376 | 27.847082 |
|  S | 32.586849 | 30.771032 | 25.100620 |
|  S | 32.821510 | 25.904278 | 23.535351 |
|  S | 36.351757 | 27.864717 | 26.448246 |

24

generated by VMD

|   | 18.270643 | 32.748993 | 33.327675 |
|---|-----------|-----------|-----------|
|  Ca | 22.698742 | 34.714264 | 35.589142 |
|  Ca | 23.498398 | 30.317425 | 33.121071 |
|  Ca | 22.910954 | 35.013031 | 30.582020 |
|  Ca | 24.775515 | 30.480888 | 27.975859 |
|  Ca | 27.843349 | 32.990059 | 31.321787 |
|  Ca | 29.091055 | 28.003635 | 29.790808 |
|  Ca | 30.563519 | 32.513336 | 27.662769 |
|  Ca | 30.353226 | 28.013184 | 24.776699 |
|  Ca | 33.767254 | 29.879105 | 28.041559 |
|  Ca | 34.594353 | 24.651962 | 26.639200 |
|  Ca | 35.301094 | 28.889111 | 23.575266 |
|  S  | 20.958923 | 31.668280 | 35.378433 |
|  S  | 20.457502 | 35.543686 | 32.758896 |
|  S  | 22.121651 | 31.473665 | 30.026340 |
|  S  | 25.062969 | 33.553642 | 33.443596 |
|  S  | 26.288593 | 29.672382 | 31.237316 |
|  S  | 25.767265 | 33.987267 | 28.588358 |
|  S  | 28.267414 | 29.747593 | 26.861794 |
|  S  | 30.853310 | 31.006062 | 30.396107 |
|  S  | 31.905537 | 26.863209 | 27.846172 |
|  S  | 32.642067 | 30.843481 | 24.949358 |
|  S  | 33.292488 | 25.945492 | 23.505182 |
|  S  | 36.434265 | 27.780342 | 26.544640 |

24

generated by VMD

|   | 18.129631 | 32.950790 | 33.686214 |
|---|-----------|-----------|-----------|
|  Ca | 22.934132 | 34.471859 | 35.670792 |
|  Ca | 23.445427 | 30.367813 | 32.982315 |
|  Ca | 22.861008 | 34.848042 | 30.586290 |
|  Ca | 24.936180 | 30.617878 | 27.938879 |
|  Ca | 27.797379 | 32.895149 | 31.173761 |
|  Ca | 29.092838 | 27.754879 | 29.931213 |
Ca | 30.664944 | 32.207588 | 27.527807
---|---|---|---
Ca | 30.405066 | 27.917194 | 24.700890
Ca | 33.803619 | 30.188353 | 28.054585
Ca | 34.424187 | 24.993761 | 26.687647
Ca | 35.411701 | 28.880236 | 23.661158
S  | 20.978043 | 31.690571 | 35.261814
S  | 20.425591 | 35.732613 | 33.042057
S  | 21.996094 | 31.514622 | 29.816925
S  | 24.881533 | 33.551510 | 33.265656
S  | 26.291218 | 29.551638 | 31.014719
S  | 25.931414 | 34.097557 | 28.697012
S  | 28.284151 | 29.689693 | 26.885052
S  | 30.934601 | 30.863888 | 30.236141
S  | 31.938322 | 26.874401 | 27.950766
S  | 32.525879 | 30.590677 | 24.851707
S  | 33.164734 | 25.985283 | 23.516516
S  | 36.462337 | 28.064104 | 26.800117

24 generated by VMD
Ca | 18.662580 | 32.08124 | 33.619564
Ca | 22.782028 | 35.103474 | 35.810356
Ca | 23.172886 | 30.455870 | 32.875206
Ca | 23.116821 | 34.729473 | 30.534740
Ca | 24.912018 | 30.286053 | 27.681059
Ca | 27.680519 | 32.697075 | 31.375591
Ca | 29.031185 | 27.855940 | 29.844828
Ca | 30.595219 | 32.454166 | 27.719786
Ca | 30.446507 | 27.833317 | 24.672600
Ca | 33.764706 | 29.965641 | 28.098875
Ca | 34.419273 | 24.901335 | 26.643257
Ca | 35.257389 | 29.835086 | 23.264340
S  | 21.119053 | 31.945629 | 35.510445
S  | 20.618301 | 35.675224 | 33.000252
S  | 21.938568 | 31.585400 | 29.647757
S  | 24.812433 | 33.366146 | 33.396614
S  | 26.246433 | 29.401821 | 31.036600
S  | 25.791504 | 33.792595 | 28.399361
S  | 28.303329 | 29.807850 | 26.738178
S  | 30.851105 | 31.000305 | 30.446047
S  | 31.799652 | 26.970182 | 27.971540
S  | 32.764263 | 30.687923 | 25.093807
S  | 33.164803 | 26.188463 | 23.588015
S  | 36.469494 | 27.952988 | 26.611254

24 generated by VMD
Ca | 18.640339 | 32.526016 | 33.875984
|   | Ca     |      |      |
|---|--------|------|------|
|   | 23.051901 | 34.923347 | 35.699806 |
|   | 23.403679 | 30.483690 | 33.072491 |
|   | 22.692719 | 34.808388 | 30.324709 |
|   | 24.971432 | 27.803213 |
|   | 30.283066 | 32.486145 | 27.617989 |
|   | 30.527905 | 28.319794 | 24.327372 |
|   | 33.624779 | 29.854549 | 28.256941 |
|   | 34.382900 | 26.404087 |
|   | 35.692940 | 24.024893 |
|   | 21.304443 | 31.657265 | 35.689598 |
|   | 20.462421 | 35.674618 | 33.055210 |
|   | 21.881170 | 31.489521 | 29.819233 |
|   | 24.845324 | 33.724762 | 33.101494 |
|   | 26.282642 | 29.496458 | 31.243483 |
|   | 25.684071 | 33.826042 | 28.452759 |
|   | 28.185503 | 29.717579 | 26.585037 |
|   | 30.620693 | 30.995323 | 30.297535 |
|   | 31.639599 | 26.885643 | 27.716572 |
|   | 32.917400 | 25.162882 |
|   | 33.463043 | 23.416960 |
|   | 36.487858 | 27.051970 |

24 generated by VMD

|   | Ca     |      |      |
|---|--------|------|------|
|   | 18.575026 | 32.962147 | 34.191013 |
|   | 23.057625 | 34.761040 | 35.963139 |
|   | 23.342644 | 30.336948 | 32.958885 |
|   | 22.883781 | 34.660984 | 30.460670 |
|   | 24.821796 | 30.507240 | 27.621122 |
|   | 27.692505 | 32.726688 | 31.202841 |
|   | 28.936184 | 27.949266 | 29.589930 |
|   | 30.451454 | 32.627754 | 27.440525 |
|   | 30.518181 | 27.974335 | 24.583426 |
|   | 33.497372 | 30.081284 | 28.290741 |
|   | 34.441437 | 24.784100 | 26.773621 |
|   | 35.573463 | 28.808414 | 24.198914 |
|   | 21.471428 | 31.650163 | 35.600609 |
|   | 20.769554 | 35.652294 | 33.097549 |
|   | 21.892256 | 31.374115 | 29.600752 |
|   | 25.034250 | 33.412148 | 33.147919 |
|   | 25.947254 | 29.459330 | 30.666683 |
|   | 25.724220 | 33.856617 | 28.350452 |
|   | 28.206501 | 29.941633 | 26.394800 |
|   | 30.620468 | 31.058977 | 30.226238 |
|   | 31.801956 | 26.838894 | 27.838205 |
|  |  |  |
|---|---|---|
| S  | 32.857868 | 30.860033 | 24.899639 |
| S  | 33.322601 | 26.028736 | 23.586445 |
| S  | 36.280209 | 27.981081 | 27.255924 |
| 24 | generated by VMD |
| Ca | 18.360426 | 32.532776 | 34.051437 |
| Ca | 22.637783 | 35.160465 | 35.714764 |
| Ca | 23.336704 | 30.564697 | 32.964577 |
| Ca | 22.717562 | 34.785484 | 30.621178 |
| Ca | 24.923122 | 30.911938 | 27.859558 |
| Ca | 27.836830 | 32.855366 | 31.201115 |
| Ca | 28.869596 | 27.793745 | 29.635382 |
| Ca | 30.452227 | 32.403942 | 27.547251 |
| Ca | 30.648727 | 27.884403 | 24.490038 |
| Ca | 33.887238 | 29.771259 | 28.278141 |
| Ca | 34.402031 | 24.839970 | 26.837387 |
| Ca | 35.856716 | 28.686832 | 23.474760 |
| S  | 21.124790 | 31.782646 | 35.683060 |
| S  | 20.200253 | 35.489491 | 33.426819 |
| S  | 21.786926 | 31.639801 | 29.762867 |
| S  | 24.750465 | 33.543198 | 33.180672 |
| S  | 26.390934 | 29.627420 | 30.918341 |
| S  | 25.745394 | 34.128941 | 28.599253 |
| S  | 28.166826 | 29.659645 | 26.456572 |
| S  | 30.675228 | 30.877941 | 30.327574 |
| S  | 31.862036 | 26.853527 | 27.823399 |
| S  | 33.303869 | 30.712006 | 24.950222 |
| S  | 33.568539 | 25.905573 | 23.392059 |
| S  | 36.481010 | 27.888977 | 26.743614 |
| 24 | generated by VMD |
| Ca | 18.494038 | 32.576530 | 33.864281 |
| Ca | 23.213356 | 34.696201 | 35.769119 |
| Ca | 23.179024 | 30.474682 | 32.946449 |
| Ca | 22.913532 | 34.697826 | 30.554573 |
| Ca | 24.903566 | 30.719223 | 27.533331 |
| Ca | 27.739273 | 32.900940 | 31.091726 |
| Ca | 29.000153 | 27.974951 | 29.743320 |
| Ca | 30.489336 | 32.496971 | 27.667788 |
| Ca | 30.360325 | 27.899391 | 24.632477 |
| Ca | 33.640259 | 29.887383 | 28.330978 |
| Ca | 34.560738 | 24.887577 | 27.069054 |
| Ca | 35.532345 | 28.824615 | 23.640961 |
| S  | 21.249695 | 31.745636 | 35.465828 |
| S  | 20.560429 | 35.534821 | 33.373604 |
| S  | 21.872919 | 31.383755 | 29.584908 |
S  25.032188  33.392502  33.094440
S  26.036522  29.578058  30.708998
S  25.826855  34.094883  28.410580
S  28.203838  30.854298  24.920816
S  30.932932  29.048998  26.831482
S  31.694340  30.708998  27.779764
S  32.553673  31.123537  30.385487
S  33.327892  34.094883  28.410580
S  36.402817  28.410580  26.914644

24 generated by VMD
Ca  18.480560  32.416386  33.439274
Ca  22.765625  34.846046  35.990971
Ca  23.409992  30.517611  32.952080
Ca  22.844059  34.846046  30.790272
Ca  24.943760  30.561911  27.797066
Ca  27.853542  32.870296  31.169178
Ca  29.001656  28.035614  29.784325
Ca  30.623241  32.498154  27.223852
Ca  30.452496  27.842529  24.605370
Ca  33.867317  29.882336  27.750774
Ca  34.608063  24.678749  27.036562
Ca  35.387642  28.866745  23.828506
S  21.221035  31.566154  35.409279
S  20.319450  35.464706  33.422081
S  21.932577  31.747343  29.556330
S  24.993961  33.535168  33.425468
S  26.061499  29.637196  30.884598
S  25.723297  34.272797  28.551477
S  28.261738  29.753386  26.672159
S  30.882902  31.265896  30.218018
S  31.640537  26.975765  27.693521
S  32.663139  30.655476  25.082949
S  33.318764  25.843435  23.713488
S  36.463200  27.721987  26.942490

24 generated by VMD
Ca  18.419666  32.635826  33.693298
Ca  22.963051  34.858189  35.813347
Ca  23.506052  30.627554  32.996719
Ca  22.686066  34.542877  30.688589
Ca  24.752747  30.651657  27.641087
Ca  27.845669  32.986881  31.203362
Ca  28.962631  28.049435  29.939661
Ca  30.567532  32.389290  27.409096
Ca  30.616899  27.787155  24.354109
|   |   |   |   |
|---|---|---|---|
| Ca | 33.756073 | 29.771624 | 28.043388 |
| Ca | 34.284958 | 24.913385 | 27.009459 |
| Ca | 35.557068 | 28.976076 | 23.757490 |
| S  | 21.148869 | 31.595798 | 35.392189 |
| S  | 20.450344 | 35.378956 | 33.461388 |
| S  | 21.791542 | 31.483707 | 29.638674 |
| S  | 25.009872 | 33.586067 | 33.248363 |
| S  | 26.130239 | 29.807825 | 30.854336 |
| S  | 25.725937 | 34.118778 | 28.581974 |
| S  | 28.271149 | 29.934399 | 26.612650 |
| S  | 30.857157 | 31.115829 | 30.381590 |
| S  | 31.662184 | 26.905796 | 27.814596 |
| S  | 32.715855 | 30.649231 | 25.004515 |
| S  | 33.500778 | 25.881500 | 23.550165 |
| S  | 36.537735 | 27.652178 | 26.850025 |

24
generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 18.549879 | 32.404015 | 33.656902 |
| Ca | 22.722887 | 34.953724 | 35.978607 |
| Ca | 23.551548 | 30.582129 | 32.748032 |
| Ca | 22.842745 | 34.684921 | 30.703300 |
| Ca | 24.850700 | 30.789436 | 27.576599 |
| Ca | 27.765297 | 32.643051 | 31.573881 |
| Ca | 28.993666 | 27.973679 | 29.624775 |
| Ca | 30.495472 | 32.465172 | 27.179300 |
| Ca | 30.293604 | 27.717888 | 24.602144 |
| Ca | 33.534882 | 29.915564 | 27.903725 |
| Ca | 34.678307 | 24.972340 | 27.024799 |
| Ca | 35.611458 | 28.709839 | 23.895710 |
| S  | 21.242605 | 31.855551 | 35.439072 |
| S  | 20.377419 | 35.511612 | 33.332825 |
| S  | 22.018976 | 31.593914 | 29.614727 |
| S  | 24.930452 | 33.621639 | 33.446255 |
| S  | 26.030088 | 29.608991 | 30.798098 |
| S  | 25.969692 | 34.057865 | 28.726530 |
| S  | 28.182924 | 29.842827 | 26.683502 |
| S  | 30.887701 | 31.036667 | 30.305981 |
| S  | 31.678539 | 26.835381 | 27.658043 |
| S  | 32.567341 | 30.692480 | 24.761612 |
| S  | 33.451450 | 25.993341 | 23.639009 |
| S  | 36.492447 | 27.838158 | 27.066595 |

24
generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 18.453547 | 32.666687 | 33.824623 |
| Ca | 23.074368 | 34.627251 | 35.772316 |
| Ca | 23.426437 | 30.363979 | 32.800270 |
|   | Ca     | S     |
|---|--------|-------|
|   | 23.112602 | 34.726089 | 30.507183 |
|   | 24.850645 | 30.755997 | 27.682230 |
|   | 27.761049 | 32.817589 | 31.516235 |
|   | 28.906179 | 28.072483 | 29.800526 |
|   | 30.472969 | 32.611568 | 27.281952 |
|   | 30.324297 | 27.911245 | 24.544744 |
|   | 33.462746 | 29.886379 | 27.795374 |
|   | 34.319405 | 24.887585 | 27.082376 |
|   | 35.609154 | 28.937603 | 23.995056 |
|   | 21.439087 | 31.613386 | 35.531940 |
|   | 20.679718 | 35.361015 | 33.128334 |
|   | 21.990604 | 31.511463 | 29.659483 |
|   | 25.012236 | 33.331375 | 33.136528 |
|   | 26.097088 | 29.464748 | 30.902794 |
|   | 25.948288 | 34.150734 | 28.578562 |
|   | 28.245319 | 29.839558 | 26.677835 |
|   | 30.649080 | 31.279072 | 30.139776 |
|   | 31.415421 | 27.100222 | 27.78097 |
|   | 32.603424 | 30.582100 | 24.716524 |
|   | 33.550468 | 25.927639 | 23.783144 |
|   | 36.315952 | 27.874269 | 27.304131 |

generated by VMD

|   | Ca     | S     |
|---|--------|-------|
|   | 18.224354 | 32.924667 | 33.704842 |
|   | 23.079544 | 34.437859 | 35.934006 |
|   | 23.468155 | 30.304785 | 32.788010 |
|   | 22.934155 | 34.917297 | 30.492693 |
|   | 24.742762 | 30.544216 | 27.754257 |
|   | 27.945488 | 32.808922 | 31.124998 |
|   | 29.114662 | 28.070951 | 29.663465 |
|   | 30.434093 | 32.764877 | 27.204908 |
|   | 30.345522 | 27.742052 | 24.834627 |
|   | 33.747017 | 30.056919 | 27.992113 |
|   | 34.284348 | 24.899940 | 27.018234 |
|   | 35.576950 | 28.791351 | 23.885403 |
|   | 21.047272 | 31.405697 | 35.396370 |
|   | 20.586582 | 35.657616 | 33.450333 |
|   | 21.856735 | 31.623875 | 29.763210 |
|   | 24.961847 | 33.346268 | 33.083275 |
|   | 26.250864 | 29.437794 | 30.837353 |
|   | 25.973053 | 34.021877 | 28.595480 |
|   | 28.134499 | 29.958410 | 26.704718 |
|   | 30.952690 | 31.171032 | 29.972723 |
|   | 31.746811 | 26.913885 | 28.04458 |
|   | 32.612122 | 30.540539 | 24.893740 |
|   | 33.228863 | 25.873873 | 23.721403 |
|   | 36.471653 | 28.085346 | 27.079453 |
|---|-----------|-----------|-----------|
| 24| generated by VMD |
| Ca| 18.284702 | 32.423603 | 33.462261 |
| Ca| 22.797844 | 34.622536 | 35.686302 |
| Ca| 23.381886 | 30.242563 | 32.890938 |
| Ca| 22.830072 | 35.107174 | 30.567404 |
| Ca| 25.085562 | 30.794487 | 27.882687 |
| Ca| 27.861940 | 32.760773 | 31.419529 |
| Ca| 29.374702 | 28.135487 | 29.815426 |
| Ca| 30.604870 | 32.734539 | 27.237707 |
| Ca| 30.262136 | 27.632721 | 24.919847 |
| Ca| 33.655332 | 30.028446 | 27.937227 |
| Ca| 34.520988 | 24.749573 | 26.890560 |
| Ca| 35.139072 | 28.699631 | 23.501638 |
| S | 20.964733 | 31.415680 | 35.393608 |
| S | 20.432076 | 35.594830 | 33.165905 |
| S | 22.020344 | 31.719431 | 29.631451 |
| S | 24.837923 | 33.544094 | 33.370586 |
| S | 26.216099 | 29.655006 | 30.822187 |
| S | 25.871838 | 34.247227 | 28.707525 |
| S | 28.425087 | 30.020336 | 26.908852 |
| S | 31.076811 | 31.118801 | 30.406387 |
| S | 31.899261 | 26.750757 | 28.090107 |
| S | 32.521107 | 30.586742 | 24.839289 |
| S | 33.123512 | 25.776518 | 23.834972 |
| S | 36.531017 | 27.939053 | 26.552933 |

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|   | generated by VMD |
|---|-----------|-----------|-----------|
| Ca| 18.227245 | 32.800636 | 33.605080 |
| Ca| 23.171574 | 34.125282 | 35.704849 |
| Ca| 23.267578 | 30.379601 | 32.841507 |
| Ca| 23.061207 | 34.741180 | 30.682032 |
| Ca| 24.925657 | 30.988972 | 27.622843 |
| Ca| 27.917850 | 32.899586 | 31.124897 |
| Ca| 29.019135 | 28.219919 | 29.809616 |
| Ca| 30.524576 | 32.480934 | 27.384657 |
| Ca| 30.087166 | 27.619406 | 24.801962 |
| Ca| 33.697094 | 29.945881 | 27.975288 |
| Ca| 34.582710 | 25.121893 | 27.028864 |
| Ca| 35.270645 | 28.746918 | 23.669138 |
| S | 20.986931 | 31.246502 | 35.243073 |
| S | 20.618610 | 35.535454 | 33.353592 |
| S | 21.866465 | 31.593018 | 29.628201 |
| S | 25.236927 | 33.314686 | 33.487068 |
| S | 26.274448 | 30.021191 | 30.799721 |
| \(\text{S} \) | 25.798660 | 34.256958 | 28.233688 |
| \(\text{S} \) | 28.163731 | 30.023903 | 26.709156 |
| \(\text{S} \) | 30.965736 | 31.171120 | 30.245125 |
| \(\text{S} \) | 31.798058 | 26.885380 | 28.238913 |
| \(\text{S} \) | 32.379162 | 30.361794 | 25.018843 |
| \(\text{S} \) | 33.193005 | 25.712049 | 23.988827 |
| \(\text{S} \) | 36.685814 | 28.107777 | 26.743120 |

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Generated by VMD

| \(\text{Ca} \) | 18.150717 | 32.924217 | 34.170288 |
| \(\text{Ca} \) | 23.146591 | 34.598869 | 35.849644 |
| \(\text{Ca} \) | 23.190971 | 30.365257 | 32.705082 |
| \(\text{Ca} \) | 22.643635 | 34.822891 | 30.745543 |
| \(\text{Ca} \) | 24.618944 | 30.930105 | 27.619963 |
| \(\text{Ca} \) | 27.664494 | 32.719925 | 31.300081 |
| \(\text{Ca} \) | 28.823689 | 28.196411 | 29.761021 |
| \(\text{Ca} \) | 30.752987 | 32.458862 | 26.991850 |
| \(\text{Ca} \) | 30.622700 | 27.760910 | 24.565323 |
| \(\text{Ca} \) | 33.872383 | 30.078686 | 27.770685 |
| \(\text{Ca} \) | 34.443256 | 24.759806 | 27.195250 |
| \(\text{Ca} \) | 35.850121 | 28.714558 | 23.717710 |
| \(\text{S} \) | 21.170429 | 31.403267 | 35.515076 |
| \(\text{S} \) | 20.585526 | 35.618362 | 33.571709 |
| \(\text{S} \) | 21.620646 | 31.480349 | 29.667213 |
| \(\text{S} \) | 24.844168 | 33.280624 | 33.299202 |
| \(\text{S} \) | 26.014206 | 29.681011 | 30.721062 |
| \(\text{S} \) | 25.633097 | 34.267483 | 28.631247 |
| \(\text{S} \) | 28.183294 | 29.857332 | 26.625637 |
| \(\text{S} \) | 30.970051 | 31.240921 | 29.919233 |
| \(\text{S} \) | 31.677948 | 27.057640 | 28.025679 |
| \(\text{S} \) | 33.046753 | 30.503042 | 24.778822 |
| \(\text{S} \) | 33.621620 | 25.863316 | 23.719505 |
| \(\text{S} \) | 36.571823 | 27.716228 | 27.073240 |

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Generated by VMD

| \(\text{Ca} \) | 18.390923 | 33.099564 | 33.650497 |
| \(\text{Ca} \) | 23.054802 | 34.960358 | 35.826771 |
| \(\text{Ca} \) | 23.395275 | 30.264845 | 32.880379 |
| \(\text{Ca} \) | 22.970192 | 34.676155 | 30.667744 |
| \(\text{Ca} \) | 24.735741 | 30.659355 | 27.688112 |
| \(\text{Ca} \) | 27.863781 | 32.495991 | 31.414387 |
| \(\text{Ca} \) | 29.082970 | 27.881601 | 29.620070 |
| \(\text{Ca} \) | 30.443531 | 32.418156 | 27.527367 |
| \(\text{Ca} \) | 30.486204 | 27.988525 | 24.820808 |
| \(\text{Ca} \) | 33.839878 | 30.115076 | 27.957558 |
| \(\text{Ca} \) | 34.520378 | 24.902149 | 26.695763 |
|   |   |   |
|---|---|---|
| Ca | 35.163315 | 28.979458 | 23.818769 |
| S  | 21.181240 | 31.815298 | 35.289181 |
| S  | 20.524998 | 35.883270 | 33.062981 |
| S  | 21.827333 | 31.306137 | 29.682415 |
| S  | 24.89902  | 33.121670 | 33.296585 |
| S  | 26.142727 | 29.425632 | 30.913715 |
| S  | 25.871040 | 33.915810 | 28.587729 |
| S  | 28.097996 | 29.778713 | 26.621668 |
| S  | 30.795795 | 30.864048 | 30.289276 |
| S  | 32.050323 | 26.980675 | 27.863958 |
| S  | 32.661182 | 30.717899 | 25.051878 |
| S  | 33.212437 | 25.903778 | 23.852938 |
| S  | 36.518082 | 28.145863 | 26.859512 |

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generated by VMD

| Ca | 18.126781 | 33.529671 | 33.802612 |
| Ca | 22.726192 | 34.148567 | 36.004082 |
| Ca | 23.11534  | 30.183350 | 32.789871 |
| Ca | 22.977482 | 34.663174 | 30.894459 |
| Ca | 24.992865 | 30.843571 | 27.667280 |
| Ca | 27.808517 | 32.757664 | 31.550375 |
| Ca | 29.032127 | 28.148563 | 29.682020 |
| Ca | 30.524225 | 32.438332 | 26.753935 |
| Ca | 30.538897 | 27.653538 | 24.561541 |
| Ca | 33.848278 | 30.236908 | 27.785543 |
| Ca | 34.652790 | 25.053139 | 27.025478 |
| Ca | 35.424698 | 28.514874 | 23.749407 |
| Ca | 20.773602 | 31.487366 | 23.749407 |
| Ca | 20.724396 | 35.938778 | 33.511261 |
| Ca | 21.937897 | 31.506903 | 29.678268 |
| Ca | 24.775768 | 33.231266 | 33.483208 |
| Ca | 26.224155 | 29.612194 | 31.010355 |
| Ca | 25.867634 | 33.948090 | 28.683332 |
| Ca | 28.146862 | 29.747753 | 26.492508 |
| Ca | 30.832287 | 31.342306 | 30.221214 |
| Ca | 31.902065 | 27.138214 | 27.814711 |
| Ca | 32.815975 | 30.381094 | 24.754595 |
| Ca | 33.424541 | 25.587753 | 23.829092 |
| Ca | 36.530441 | 28.206968 | 26.955574 |

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generated by VMD

| Ca | 18.718882 | 32.850426 | 33.642780 |
| Ca | 22.726368 | 34.522781 | 35.841827 |
| Ca | 23.320564 | 30.351963 | 32.831806 |
| Ca | 22.995655 | 34.917297 | 30.578527 |
| Ca | 24.958527 | 30.784033 | 27.642105 |
| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 27.76473  | 32.784763 | 31.453804 |
| Ca      | 29.067825 | 28.042374 | 29.808664 |
| Ca      | 30.242723 | 32.510788 | 27.022663 |
| Ca      | 30.460037 | 27.780262 | 24.741539 |
| Ca      | 33.710892 | 30.223310 | 27.814789 |
| Ca      | 34.682785 | 24.756927 | 26.937876 |
| Ca      | 35.415993 | 28.66447  | 23.812504 |
| S       | 20.797901 | 31.344444 | 35.665207 |
| S       | 20.805973 | 35.645844 | 33.384308 |
| S       | 21.841396 | 31.711697 | 29.655743 |
| S       | 24.893871 | 33.404999 | 33.421539 |
| S       | 26.006165 | 29.694607 | 30.787930 |
| S       | 25.903311 | 34.113831 | 28.603531 |
| S       | 28.164045 | 29.610744 | 26.658981 |
| S       | 30.703968 | 31.213036 | 30.133228 |
| S       | 31.883024 | 27.093723 | 27.954397 |
| S       | 32.732037 | 30.541344 | 24.860857 |
| S       | 33.401314 | 25.904484 | 23.610826 |
| S       | 36.522335 | 27.829906 | 27.074598 |

24 generated by VMD

| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 18.273510 | 32.923588 | 33.407085 |
| Ca      | 22.627647 | 34.920547 | 35.643925 |
| Ca      | 23.422548 | 30.386963 | 33.002914 |
| Ca      | 23.075344 | 34.618298 | 30.735857 |
| Ca      | 24.867674 | 30.658894 | 27.729940 |
| Ca      | 27.694012 | 32.600380 | 31.534496 |
| Ca      | 29.177597 | 27.907864 | 30.132584 |
| Ca      | 30.649693 | 32.312195 | 27.157000 |
| Ca      | 30.318447 | 27.828873 | 24.620703 |
| Ca      | 33.789726 | 30.084587 | 27.871454 |
| Ca      | 34.342243 | 25.014158 | 26.509367 |
| Ca      | 35.385414 | 28.715197 | 23.685770 |
| S       | 20.981075 | 31.663380 | 35.302391 |
| S       | 20.459698 | 35.713383 | 33.221298 |
| S       | 22.017914 | 31.537991 | 29.808628 |
| S       | 25.070889 | 33.488075 | 33.424088 |
| S       | 26.120789 | 29.430706 | 31.076498 |
| S       | 25.929501 | 34.014969 | 28.687672 |
| S       | 28.289722 | 29.557255 | 26.947840 |
| S       | 30.741238 | 31.052092 | 30.205667 |
| S       | 31.883728 | 27.040771 | 27.795574 |
| S       | 32.708252 | 30.826740 | 24.894642 |
| S       | 33.263626 | 26.030203 | 23.576990 |
| S       | 36.629700 | 27.972954 | 26.967693 |

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| Element | X Coordinate 1 | Y Coordinate 1 | Z Coordinate 1 | X Coordinate 2 | Y Coordinate 2 | Z Coordinate 2 |
|---------|----------------|----------------|----------------|----------------|----------------|----------------|
| Ca      | 18.295952      | 33.040230      | 33.835155      | 24.742670      | 30.991125      | 27.795593      |
| Ca      | 23.053711      | 34.571106      | 35.911270      | 27.93276       | 32.555573      | 31.125221      |
| Ca      | 22.903847      | 29.946823      | 32.927635      | 30.730740      | 27.889643      | 24.682169      |
| Ca      | 22.880104      | 34.786980      | 30.680677      | 30.367926      | 30.048357      | 27.899569      |
| Ca      | 24.742670      | 30.991125      | 27.795593      | 30.367926      | 30.048357      | 27.899569      |
| Ca      | 27.93276       | 32.555573      | 31.125221      | 35.694160      | 28.680016      | 23.745741      |
| Ca      | 22.758213      | 34.571106      | 35.911270      | 20.967197      | 31.687996      | 35.572517      |
| Ca      | 20.613987      | 35.863964      | 33.383034      | 20.613987      | 35.863964      | 33.383034      |
| Ca      | 21.692780      | 31.525383      | 29.887177      | 21.692780      | 31.525383      | 29.887177      |
| Ca      | 24.916592      | 33.061928      | 33.212196      | 24.916592      | 33.061928      | 33.212196      |
| Ca      | 26.102562      | 29.681362      | 30.983353      | 26.102562      | 29.681362      | 30.983353      |
| Ca      | 25.764185      | 34.122169      | 28.442245      | 25.764185      | 34.122169      | 28.442245      |
| Ca      | 28.061760      | 29.861916      | 26.621538      | 28.061760      | 29.861916      | 26.621538      |
| Ca      | 30.858047      | 31.202719      | 29.948881      | 30.858047      | 31.202719      | 29.948881      |
| Ca      | 31.917923      | 27.075806      | 28.019979      | 31.917923      | 27.075806      | 28.019979      |
| Ca      | 32.914421      | 30.357279      | 24.904284      | 32.914421      | 30.357279      | 24.904284      |
| Ca      | 33.408108      | 25.716946      | 23.552212      | 33.408108      | 25.716946      | 23.552212      |
| Ca      | 36.686924      | 28.202753      | 27.103662      | 36.686924      | 28.202753      | 27.103662      |

| 24      | generated by VMD |
|---------|----------------|
| Ca      | 18.312145      | 32.837570      | 33.630196      |
| Ca      | 22.758213      | 34.763664      | 35.858070      |
| Ca      | 23.175318      | 30.197115      | 32.934181      |
| Ca      | 22.916601      | 34.892502      | 30.693800      |
| Ca      | 24.897308      | 30.756771      | 27.850220      |
| Ca      | 27.719906      | 32.679451      | 31.384556      |
| Ca      | 29.260624      | 28.186859      | 29.979195      |
| Ca      | 30.693642      | 32.141762      | 26.841312      |
| Ca      | 30.328859      | 27.970444      | 24.587151      |
| Ca      | 34.015327      | 30.129972      | 28.003433      |
| Ca      | 34.281723      | 24.867262      | 26.808603      |
| Ca      | 35.591053      | 28.723736      | 23.674440      |
| S       | 20.869251      | 31.618296      | 35.715759      |
| S       | 20.478130      | 35.627953      | 33.214523      |
| S       | 21.965014      | 31.616261      | 29.734665      |
| S       | 24.784124      | 33.376564      | 33.372543      |
| S       | 26.066620      | 29.433784      | 30.752964      |
| S       | 25.948265      | 34.159222      | 28.705446      |
| S       | 28.113979      | 29.652658      | 26.824081      |
|      | X    | Y    | Z    |
|------|------|------|------|
| S    | 30.975855 | 31.291214 | 30.195223 |
| S    | 31.931803 | 27.133747 | 27.731117 |
| S    | 32.706181 | 30.542051 | 24.924923 |
| S    | 33.399055 | 25.847767 | 23.541660 |
| S    | 36.531113 | 27.853495 | 26.981991 |

24 generated by VMD

|      | X    | Y    | Z    |
|------|------|------|------|
| Ca   | 18.404079 | 32.936634 | 33.788124 |
| Ca   | 22.863241 | 34.538486 | 35.650757 |
| Ca   | 23.214729 | 30.111202 | 32.880081 |
| Ca   | 22.905291 | 34.950050 | 30.713367 |
| Ca   | 25.095461 | 30.772442 | 27.881031 |
| Ca   | 27.691982 | 32.807175 | 31.298422 |
| Ca   | 29.212902 | 28.086267 | 29.888632 |
| Ca   | 30.509876 | 32.575447 | 27.055094 |
| Ca   | 30.345110 | 27.629112 | 24.592102 |
| Ca   | 33.518166 | 29.989466 | 28.067532 |
| Ca   | 34.624962 | 24.817123 | 26.982708 |
| Ca   | 35.612732 | 28.884447 | 23.703608 |
| S    | 20.961189 | 31.230953 | 35.475559 |
| S    | 20.471916 | 35.839302 | 33.242283 |
| S    | 21.896076 | 31.526413 | 29.934214 |
| S    | 24.749054 | 33.592381 | 33.235626 |
| S    | 26.264368 | 29.722902 | 30.883102 |
| S    | 25.996521 | 34.201546 | 28.861361 |
| S    | 28.363678 | 29.661102 | 26.697701 |
| S    | 30.783463 | 31.421570 | 30.103083 |
| S    | 31.703573 | 26.759937 | 27.729956 |
| S    | 32.660252 | 30.593697 | 24.738222 |
| S    | 33.516464 | 25.771713 | 23.503210 |
| S    | 36.354988 | 27.880693 | 27.034271 |

24 generated by VMD

|      | X    | Y    | Z    |
|------|------|------|------|
| Ca   | 18.364628 | 33.268375 | 34.140083 |
| Ca   | 22.920412 | 34.964252 | 35.758522 |
| Ca   | 23.291628 | 30.236364 | 32.865379 |
| Ca   | 22.793930 | 34.524788 | 30.496830 |
| Ca   | 25.012932 | 30.647346 | 27.806997 |
| Ca   | 27.619427 | 32.665855 | 31.270292 |
| Ca   | 29.058144 | 27.972645 | 29.821257 |
| Ca   | 30.442089 | 32.298656 | 27.170212 |
| Ca   | 30.450336 | 27.922319 | 24.558962 |
| Ca   | 33.736526 | 30.079067 | 27.894934 |
| Ca   | 34.455723 | 24.829887 | 26.838573 |
| Ca   | 35.523216 | 28.987551 | 23.851650 |
| S    | 21.058765 | 31.448669 | 35.444920 |
|   | S          |   | S          |   | S          |   | S          |   |
|---|-----------|---|-----------|---|-----------|---|-----------|---|
|   | 20.828583 |   | 35.688740 |   | 33.157608 |   |           |   |
| S | 21.704262 |   | 31.474163 |   | 29.558683 |   |           |   |
| S | 24.828384 |   | 33.168892 |   | 33.351570 |   |           |   |
| S | 26.051508 |   | 29.622387 |   | 30.788679 |   |           |   |
| S | 25.946716 |   | 34.236179 |   | 28.756525 |   |           |   |
| S | 28.215595 |   | 29.476385 |   | 26.714123 |   |           |   |
| S | 30.780560 |   | 31.229874 |   | 30.156456 |   |           |   |
| S | 31.927401 |   | 26.946980 |   | 27.905014 |   |           |   |
| S | 32.785759 |   | 30.766476 |   | 25.085445 |   |           |   |
| S | 33.455780 |   | 25.995543 |   | 23.575800 |   |           |   |
| S | 36.467842 |   | 27.848663 |   | 26.971508 |   |           |   |

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generated by VMD

|   | Ca       |   | Ca       |   | Ca       |   | Ca       |   | Ca       |   |
|---|----------|---|----------|---|----------|---|----------|---|----------|---|
|   | 18.295502|   | 33.111652|   | 33.879951|   |           |   |           |   |
| Ca| 22.653225|   | 34.581200|   | 35.744888|   |           |   |           |   |
| Ca| 23.273430|   | 30.342916|   | 32.876892|   |           |   |           |   |
| Ca| 22.873890|   | 34.818130|   | 30.686333|   |           |   |           |   |
| Ca| 24.748922|   | 30.778919|   | 27.623949|   |           |   |           |   |
| Ca| 27.869484|   | 32.727062|   | 31.196070|   |           |   |           |   |
| Ca| 29.111546|   | 28.097017|   | 29.980051|   |           |   |           |   |
| Ca| 30.752081|   | 32.237663|   | 27.356981|   |           |   |           |   |
| Ca| 30.416306|   | 27.895195|   | 24.659124|   |           |   |           |   |
| Ca| 33.787689|   | 29.974632|   | 28.108158|   |           |   |           |   |
| Ca| 34.573059|   | 25.109598|   | 26.831202|   |           |   |           |   |
| Ca| 35.595802|   | 28.568630|   | 23.486301|   |           |   |           |   |
| S | 21.031706|   | 31.288101|   | 35.531357|   |           |   |           |   |
| S | 20.550316|   | 35.675217|   | 33.125534|   |           |   |           |   |
| S | 21.822788|   | 31.564507|   | 29.821678|   |           |   |           |   |
| S | 25.038719|   | 33.519295|   | 33.250759|   |           |   |           |   |
| S | 26.072216|   | 29.545948|   | 30.760120|   |           |   |           |   |
| S | 25.749046|   | 34.040909|   | 28.552881|   |           |   |           |   |
| S | 28.356277|   | 29.846272|   | 26.866293|   |           |   |           |   |
| S | 30.947695|   | 31.107903|   | 30.344534|   |           |   |           |   |
| S | 31.788414|   | 26.961681|   | 27.869724|   |           |   |           |   |
| S | 32.705818|   | 30.593288|   | 25.044268|   |           |   |           |   |
| S | 33.221382|   | 25.781662|   | 23.686380|   |           |   |           |   |
| S | 36.484741|   | 28.132633|   | 26.656567|   |           |   |           |   |

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generated by VMD

|   | Ca       |   | Ca       |   | Ca       |   | Ca       |   |
|---|----------|---|----------|---|----------|---|----------|---|
|   | 18.334446|   | 32.807575|   | 33.935783|   |           |   |
| Ca| 22.861353|   | 35.018150|   | 35.589375|   |           |   |
| Ca| 23.556314|   | 30.227556|   | 32.884079|   |           |   |
| Ca| 22.735819|   | 34.711132|   | 30.727041|   |           |   |
| Ca| 25.021183|   | 30.598291|   | 27.895815|   |           |   |
| Ca| 27.682140|   | 32.754559|   | 31.054760|   |           |   |
| Ca| 28.988529|   | 28.017498|   | 29.846256|   |           |   |
|   | Ca       | 30.674942 | 32.427311 | 27.30466   |
|---|----------|-----------|-----------|------------|
| Ca| 30.323046| 28.034229 | 24.308182 |
| Ca| 33.698505| 29.875519 | 28.103174 |
| Ca| 34.309410| 24.948576 | 26.908747 |
| Ca| 35.610996| 28.870665 | 23.904600 |
| S | 21.304121| 31.646795 | 35.468727 |
| S | 20.295891| 35.475555 | 33.172150 |
| S | 21.968052| 31.322330 | 29.838974 |
| S | 24.964226| 33.372913 | 33.378262 |
| S | 26.158321| 29.663952 | 30.77067  |
| S | 25.737995| 34.273849 | 28.561674 |
| S | 28.239037| 29.876677 | 26.729416 |
| S | 30.850863| 31.830440 | 30.264992 |
| S | 31.503521| 26.950562 | 27.639791 |
| S | 33.025265| 30.590849 | 25.095011 |
| S | 33.305649| 25.986294 | 23.651031 |
| S | 36.570427| 27.663120 | 26.900217 |

24 generated by VMD

|   | Ca       | 18.177944 | 33.271950 | 33.547089 |
|---|----------|-----------|-----------|-----------|
| Ca| 22.962172| 34.823315 | 35.541283 |
| Ca| 23.361248| 30.187160 | 33.075371 |
| Ca| 23.016634| 34.674896 | 30.624660 |
| Ca| 24.842770| 30.425114 | 27.901405 |
| Ca| 27.692869| 32.538559 | 31.234150 |
| Ca| 29.216801| 29.939507 | 29.969660 |
| Ca| 30.733479| 32.426498 | 27.543371 |
| Ca| 30.408146| 27.876852 | 24.688292 |
| Ca| 33.712978| 29.884359 | 28.190435 |
| Ca| 34.563148| 25.101664 | 26.914873 |
| Ca| 35.363289| 28.939344 | 23.424509 |
| S | 20.788338| 31.706575 | 35.423908 |
| S | 20.593632| 35.906567 | 32.967575 |
| S | 21.931421| 31.316641 | 29.900343 |
| S | 24.987137| 33.197205 | 33.434563 |
| S | 26.017967| 29.484585 | 30.837975 |
| S | 25.931185| 33.915634 | 28.594162 |
| S | 28.359257| 29.776760 | 26.907099 |
| S | 30.989805| 31.064400 | 30.454418 |
| S | 31.740799| 26.849903 | 27.975769 |
| S | 32.600494| 30.797657 | 24.797552 |
| S | 33.229889| 26.038092 | 23.495090 |
| S | 36.498680| 28.156843 | 26.496511 |

24 generated by VMD

|   | Ca       | 18.228683 | 33.262932 | 33.944214 |
| Element | X  | Y  | Z   |
|---------|----|----|-----|
| Ca      | 22.774250 | 35.062935 | 35.412556 |
| Ca      | 23.488663 | 30.186050 | 33.048927 |
| Ca      | 22.766541 | 34.633869 | 30.599606 |
| Ca      | 24.782274 | 30.515038 | 27.929352 |
| Ca      | 27.883728 | 32.615524 | 31.259960 |
| Ca      | 29.030445 | 28.037155 | 29.809681 |
| Ca      | 30.642630 | 32.285034 | 27.606981 |
| Ca      | 30.383812 | 28.022594 | 24.613924 |
| Ca      | 33.808712 | 29.659521 | 28.351231 |
| Ca      | 34.591522 | 24.969810 | 26.651594 |
| Ca      | 35.537079 | 28.987886 | 23.422552 |
| S       | 21.029970 | 31.795784 | 35.430687 |
| S       | 20.493744 | 35.773972 | 32.827129 |
| S       | 21.895304 | 31.218353 | 29.862240 |
| S       | 25.020470 | 33.417797 | 33.456940 |
| S       | 26.104450 | 29.376593 | 30.751900 |
| S       | 25.756172 | 33.918362 | 28.807472 |
| S       | 28.162819 | 29.818966 | 26.763161 |
| S       | 30.972866 | 30.955170 | 30.340042 |
| S       | 31.658772 | 26.823013 | 27.794569 |
| S       | 32.793839 | 30.734482 | 25.043982 |
| S       | 33.356716 | 26.032625 | 23.536394 |
| S       | 36.556599 | 28.196600 | 26.674961 |

24 generated by VMD

| Element | X  | Y  | Z   |
|---------|----|----|-----|
| Ca      | 18.297054 | 33.042297 | 33.899757 |
| Ca      | 22.828304 | 34.868061 | 35.517671 |
| Ca      | 23.325666 | 30.395233 | 32.773216 |
| Ca      | 22.806862 | 34.790565 | 30.411850 |
| Ca      | 24.997795 | 30.417122 | 28.233025 |
| Ca      | 27.834366 | 32.736687 | 31.263464 |
| Ca      | 29.130306 | 27.693087 | 30.069309 |
| Ca      | 30.666286 | 32.432255 | 27.597401 |
| Ca      | 30.418877 | 28.034500 | 24.658329 |
| Ca      | 33.665836 | 29.855976 | 27.976473 |
| Ca      | 34.470055 | 24.870537 | 26.688368 |
| Ca      | 35.498329 | 28.974255 | 23.612860 |
| S       | 21.173279 | 31.531904 | 35.528824 |
| S       | 20.425442 | 35.901978 | 32.990242 |
| S       | 21.764503 | 31.422970 | 29.801777 |
| S       | 24.851322 | 33.372536 | 33.143295 |
| S       | 26.313255 | 29.567535 | 30.884947 |
| S       | 25.716677 | 33.992928 | 28.544756 |
| S       | 28.161060 | 29.777203 | 26.827330 |
| S       | 31.035877 | 30.970375 | 30.388674 |
| S       | 31.731617 | 26.781034 | 27.840782 |
|      | 18.192493 | 32.805809 | 33.858181 |
|------|------------|------------|------------|
| Ca   | 22.923645  | 34.453842  | 35.703362  |
| Ca   | 23.118650  | 30.268368  | 32.549149  |
| Ca   | 22.886753  | 35.112564  | 30.693848  |
| Ca   | 25.181751  | 30.638851  | 28.190428  |
| Ca   | 27.817289  | 32.809502  | 31.126925  |
| Ca   | 29.230457  | 28.147289  | 29.914724  |
| Ca   | 30.481050  | 32.661400  | 27.266283  |
| Ca   | 30.543257  | 27.770870  | 24.720488  |
| Ca   | 33.668224  | 29.963676  | 28.062162  |
| Ca   | 34.234127  | 24.716824  | 26.910252  |
| Ca   | 35.285065  | 28.872622  | 23.682201  |
| S    | 21.147110  | 31.343487  | 35.284775  |
| S    | 20.491859  | 35.836494  | 33.269997  |
| S    | 22.006550  | 31.502571  | 29.806271  |
| S    | 24.915829  | 33.369522  | 33.133835  |
| S    | 26.350355  | 29.395004  | 30.809551  |
| S    | 25.740297  | 34.025948  | 28.433758  |
| S    | 28.331493  | 29.837067  | 26.887014  |
| S    | 30.971542  | 31.367641  | 30.298050  |
| S    | 31.937943  | 27.125746  | 27.916607  |
| S    | 32.657753  | 30.639946  | 24.843496  |
| S    | 33.316261  | 25.868631  | 23.717846  |
| S    | 36.290298  | 27.766386  | 26.860859  |

---

|      | 20.785808  | 30.747139  | 24.978756  |
|------|------------|------------|------------|
| S    | 33.401772  | 26.201113  | 23.496120  |
| S    | 36.467739  | 27.922750  | 26.758818  |

---

24 generated by VMD
S  24.875370  33.409222  33.372078
S  26.367208  29.484663  30.866869
S  30.417896  27.915926  24.711853
S  25.673641  33.964073  28.387186
S  28.434097  29.883614  26.918472
S  30.874739  31.086212  28.017523
S  31.917076  27.019728  28.017523
S  32.800011  30.816601  25.041372
S  33.129150  25.909170  23.355061
S  36.345303  27.750816  26.365486

24 generated by VMD
Ca  18.123669  32.912834  33.798080
Ca  22.862938  34.851383  35.256271
Ca  23.418304  30.197449  33.124359
Ca  22.627617  34.828274  30.297848
Ca  25.108410  30.588951  28.445282
Ca  27.745312  32.663071  31.123257
Ca  29.618380  27.941650  30.056154
Ca  30.870068  32.488331  27.584900
Ca  30.422749  28.299107  24.846306
Ca  33.750629  29.652540  28.116278
Ca  34.237717  24.717587  26.203375
Ca  35.338760  28.760424  23.679726
S  21.089588  31.592510  35.430305
S  20.116928  35.904217  33.080917
S  21.815523  31.297844  30.035017
S  24.797218  33.450802  32.940819
S  26.333981  29.343716  30.891476
S  25.766975  34.011768  28.292957
S  28.465475  29.930058  27.161615
S  31.106453  31.148979  30.482254
S  31.917912  26.992594  27.881451
S  32.747150  30.859737  25.187351
S  33.043465  26.120281  23.439335
S  36.394882  27.745987  26.584740

24 generated by VMD
Ca  18.543724  32.655243  33.646488
Ca  23.014435  34.606632  35.662880
Ca  23.204618  30.182686  32.991714
Ca  22.891560  34.820297  30.451637
Ca  25.131378  30.690321  28.065403
Ca  27.713881  32.793182  31.117477
Ca  29.328056  28.160370  29.916281
Ca  30.673565  32.556198  27.193764
Ca  30.417896  27.915926  24.711853
| Element | Ca 1 | Ca 2 | Ca 3 |
|---------|------|------|------|
| Ca      | 33.797058 | 34.266102 | 35.331409 |
| Ca      | 29.994905 | 24.617014 | 28.034052 |
| Ca      | 28.034052 | 26.538858 | 23.866676 |

| Element | Ca 1 | Ca 2 | Ca 3 |
|---------|------|------|------|
| S       | 21.001865 | 21.937437 | 25.161514 |
| S       | 31.336708 | 31.336309 | 30.756363 |
| S       | 35.720016 | 29.794930 | 27.613780 |
| S       | 33.124046 | 29.165289 | 25.078318 |

24

generated by VMD

| Element | Ca 1 | Ca 2 | Ca 3 |
|---------|------|------|------|
| Ca      | 18.516033 | 22.667980 | 23.518898 |
| Ca      | 32.843056 | 34.856659 | 30.558170 |
| Ca      | 33.145531 | 35.882034 | 33.169266 |

| Element | Ca 1 | Ca 2 | Ca 3 |
|---------|------|------|------|
| S       | 21.000622 | 21.987381 | 24.914490 |
| S       | 31.681789 | 31.313732 | 33.44347 |
| S       | 35.622360 | 29.812632 | 33.406563 |
| S       | 33.542290 | 29.002029 | 26.305365 |

24

generated by VMD

| Element | Ca 1 | Ca 2 | Ca 3 |
|---------|------|------|------|
| Ca      | 18.371704 | 22.831495 | 23.476349 |
| Ca      | 32.755421 | 35.060387 | 30.222713 |
| Ca      | 33.542290 | 35.458302 | 32.907158 |
|   |      |      |      |
|---|------|------|------|
| Ca| 22.803616 | 34.662659 | 30.507906 |
| Ca| 25.267147 | 30.694221 | 28.310944 |
| Ca| 27.809381 | 32.831070 | 31.263548 |
| Ca| 29.341169 | 27.923615 | 30.074963 |
| Ca| 30.743839 | 32.569733 | 27.528072 |
| Ca| 30.252337 | 27.946053 | 24.515745 |
| Ca| 33.670563 | 29.689896 | 28.103786 |
| Ca| 34.314671 | 24.837805 | 26.512268 |
| Ca| 35.413780 | 28.971079 | 23.830311 |
| S | 21.193653 | 31.634174 | 35.526329 |
| S | 20.334419 | 35.685474 | 32.926643 |
| S | 22.213755 | 31.138542 | 29.852501 |
| S | 24.780430 | 33.484871 | 33.216339 |
| S | 26.423260 | 29.454453 | 30.917356 |
| S | 25.690798 | 34.091034 | 28.501734 |
| S | 28.365644 | 29.841021 | 26.977432 |
| S | 30.832237 | 31.308311 | 30.379673 |
| S | 31.558771 | 26.800926 | 27.71652 |
| S | 32.630238 | 30.813499 | 25.054094 |
| S | 33.088394 | 26.173393 | 23.419140 |
| S | 36.312431 | 27.709721 | 26.841875 |

24 generated by VMD

|   |      |      |      |
|---|------|------|------|
| Ca| 18.312174 | 32.850719 | 33.880352 |
| Ca| 22.678711 | 34.662838 | 35.715263 |
| Ca| 23.428755 | 30.371807 | 32.982689 |
| Ca| 23.016254 | 34.725098 | 30.756546 |
| Ca| 25.279240 | 30.690680 | 28.093657 |
| Ca| 27.705563 | 32.862083 | 31.277863 |
| Ca| 29.147854 | 28.086636 | 29.873796 |
| Ca| 30.872667 | 32.357597 | 26.885458 |
| Ca| 30.502995 | 27.814537 | 24.462090 |
| Ca| 33.609390 | 30.004524 | 28.150335 |
| Ca| 34.181946 | 24.898939 | 26.837761 |
| Ca| 35.603146 | 28.687281 | 23.769142 |
| S | 21.017778 | 31.334461 | 35.490097 |
| S | 20.330296 | 35.577847 | 33.141045 |
| S | 22.013016 | 31.556187 | 29.877382 |
| S | 24.929386 | 33.378567 | 33.383287 |
| S | 26.243015 | 29.681435 | 30.826597 |
| S | 25.923225 | 34.328754 | 28.440916 |
| S | 28.282444 | 29.605442 | 26.684814 |
| S | 30.707092 | 31.349655 | 30.009043 |
| S | 31.555414 | 26.874313 | 27.773027 |
| S | 32.887634 | 30.823215 | 24.997496 |
| S | 33.405228 | 25.938789 | 23.671957 |
| Element | X1    | Y1    | Z1    |
|---------|-------|-------|-------|
| S       | 36.286896 | 27.838699 | 26.958889 |
| Ca      | 18.429047  | 32.697136  | 33.687099 |
| Ca      | 22.856512  | 34.858440  | 35.708286 |
| Ca      | 23.244102  | 30.538687  | 32.943848 |
| Ca      | 22.918829  | 34.698692  | 30.457098 |
| Ca      | 25.141788  | 30.944351  | 28.061460 |
| Ca      | 27.653009  | 32.464165  | 31.219391 |
| Ca      | 29.173306  | 28.116360  | 30.185469 |
| Ca      | 30.716719  | 32.476978  | 27.156246 |
| Ca      | 30.345737  | 27.838453  | 24.792257 |
| Ca      | 33.633976  | 29.945625  | 28.164085 |
| Ca      | 34.530334  | 24.943682  | 26.551020 |
| Ca      | 35.574150  | 28.770582  | 23.653111 |
| S       | 20.925545  | 31.616373  | 35.638470 |
| S       | 20.616215  | 35.516136  | 33.140816 |
| S       | 21.846041  | 31.490688  | 29.783575 |
| S       | 24.889191  | 33.187550  | 33.308941 |
| S       | 25.983650  | 29.711979  | 30.680130 |
| S       | 25.876249  | 34.095898  | 28.450462 |
| S       | 28.394609  | 29.729515  | 26.898058 |
| S       | 30.886215  | 31.194374  | 30.284233 |
| S       | 31.832825  | 26.931686  | 27.874250 |
| S       | 32.821678  | 30.653442  | 24.947620 |
| S       | 33.089489  | 25.882385  | 23.563059 |
| S       | 36.340824  | 27.996782  | 26.791061 |

*24 generated by VMD*
| S   | 25.550220 | 34.133240 | 28.420723 |
| S   | 28.251184 | 29.645821 | 26.654558 |
| S   | 30.634378 | 31.245415 | 30.164742 |
| S   | 31.705406 | 27.026722 | 28.114857 |
| S   | 32.791840 | 30.688370 | 24.859797 |
| S   | 33.359661 | 25.896997 | 23.752373 |
| S   | 36.416084 | 28.031996 | 27.276865 |

24 generated by VMD

| Ca  | 18.802559 | 32.106659 | 33.686501 |
| Ca  | 23.158278 | 34.412224 | 35.874516 |
| Ca  | 23.472435 | 30.389391 | 32.618130 |
| Ca  | 22.918739 | 34.748211 | 30.522446 |
| Ca  | 25.068748 | 30.996883 | 27.718666 |
| Ca  | 27.584341 | 33.112488 | 30.983692 |
| Ca  | 29.326923 | 28.532967 | 30.018011 |
| Ca  | 30.781704 | 32.603291 | 27.257660 |
| Ca  | 30.085966 | 27.781332 | 24.908197 |
| Ca  | 33.674313 | 30.029892 | 28.237518 |
| Ca  | 33.962051 | 24.881916 | 26.689428 |
| Ca  | 35.398544 | 28.497417 | 24.033030 |
| S   | 21.357971 | 31.091177 | 35.485992 |
| S   | 20.614111 | 35.121067 | 33.200981 |
| S   | 22.009188 | 31.470604 | 29.512897 |
| S   | 24.910469 | 33.399853 | 33.377186 |
| S   | 26.206652 | 30.060413 | 30.420664 |
| S   | 25.910543 | 34.415478 | 28.257650 |
| S   | 28.337385 | 30.014587 | 26.758606 |
| S   | 30.930069 | 31.703991 | 30.184900 |
| S   | 31.606615 | 27.014721 | 28.210989 |
| S   | 32.773555 | 30.418957 | 25.079897 |
| S   | 32.656330 | 25.631340 | 23.749414 |
| S   | 36.168770 | 27.865192 | 27.153053 |

24 generated by VMD

| Ca  | 18.655951 | 32.351948 | 33.859837 |
| Ca  | 23.203449 | 34.551514 | 35.874573 |
| Ca  | 23.182331 | 30.519258 | 32.856239 |
| Ca  | 22.956982 | 34.869473 | 30.758181 |
| Ca  | 25.258533 | 30.851141 | 27.890261 |
| Ca  | 27.585005 | 32.800976 | 30.791771 |
| Ca  | 28.977711 | 28.150719 | 29.895388 |
| Ca  | 30.673843 | 32.286030 | 26.874765 |
| Ca  | 30.426006 | 28.047283 | 24.634739 |
| Ca  | 33.489708 | 29.947975 | 28.466728 |
| Ca  | 34.249763 | 24.815262 | 26.776119 |
|    |      |      |      |
|----|------|------|------|
| Ca | 35.907673 | 35.907673 | 28.506021 | 35.907673 |
| S  | 21.339718 | 31.532812 | 35.726093 | 21.339718 |
| S  | 20.578255 | 35.363239 | 33.466179 | 20.578255 |
| S  | 21.832005 | 31.637863 | 29.694162 | 21.832005 |
| S  | 24.864933 | 33.388569 | 33.185474 | 24.864933 |
| S  | 25.923624 | 30.899940 | 30.613710 | 25.923624 |
| S  | 25.663038 | 34.245823 | 28.206667 | 25.663038 |
| S  | 28.256115 | 29.696436 | 26.742098 | 28.256115 |
| S  | 30.618309 | 31.430595 | 30.082594 | 30.618309 |
| S  | 31.581450 | 27.083872 | 27.938356 | 31.581450 |
| S  | 32.926384 | 30.518658 | 24.850433 | 32.926384 |
| S  | 33.313992 | 26.038561 | 23.470917 | 33.313992 |
| S  | 36.255314 | 27.966084 | 27.232870 | 36.255314 |

24

generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 18.670650 | 32.556713 | 33.908070 | 18.670650 |
| Ca | 23.140610 | 34.500965 | 35.690094 | 23.140610 |
| Ca | 23.182199 | 34.343433 | 33.030029 | 23.182199 |
| Ca | 22.975502 | 34.962509 | 30.512369 | 22.975502 |
| Ca | 24.979492 | 30.731115 | 27.914906 | 24.979492 |
| Ca | 27.573713 | 32.903042 | 30.942669 | 27.573713 |
| Ca | 29.055059 | 28.206158 | 29.895639 | 29.055059 |
| Ca | 30.630249 | 32.423477 | 27.054567 | 30.630249 |
| Ca | 30.385538 | 27.961155 | 24.629534 | 30.385538 |
| Ca | 33.579247 | 29.916115 | 28.349564 | 33.579247 |
| Ca | 34.165504 | 24.764397 | 26.742226 | 34.165504 |
| Ca | 35.709084 | 28.785091 | 23.922085 | 35.709084 |
| S  | 21.321077 | 31.344933 | 35.743454 | 21.321077 |
| S  | 20.585117 | 35.377983 | 33.103500 | 20.585117 |
| S  | 22.018799 | 31.490807 | 29.806274 | 22.018799 |
| S  | 25.052494 | 33.472996 | 33.325420 | 25.052494 |
| S  | 25.942350 | 29.736988 | 30.718340 | 25.942350 |
| S  | 25.642223 | 34.265335 | 28.057205 | 25.642223 |
| S  | 28.212523 | 29.742146 | 26.794037 | 28.212523 |
| S  | 30.739302 | 31.432905 | 30.115952 | 30.739302 |
| S  | 31.592598 | 26.889181 | 27.982557 | 31.592598 |
| S  | 32.809074 | 30.587601 | 25.061684 | 32.809074 |
| S  | 33.389427 | 26.192913 | 23.395397 | 33.389427 |
| S  | 36.368252 | 27.712044 | 27.244951 | 36.368252 |

24

generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 18.447941 | 32.739317 | 34.124619 | 18.447941 |
| Ca | 23.111256 | 34.822880 | 35.651756 | 23.111256 |
| Ca | 23.385670 | 30.346272 | 32.889305 | 23.385670 |
| Ca | 22.829420 | 34.928078 | 30.579975 | 22.829420 |
| Ca | 24.998610 | 30.630362 | 27.884197 | 24.998610 |
|    |      |      |      |
|----|------|------|------|
| Ca | 27.637981 | 32.719746 | 30.967308 |
| Ca | 29.092232 | 27.931419 | 29.908072 |
| Ca | 30.375526 | 32.389343 | 27.005342 |
| Ca | 30.582083 | 28.030813 | 24.447725 |
| Ca | 33.586903 | 29.878490 | 28.346819 |
| Ca | 34.217590 | 24.766094 | 26.617641 |
| Ca | 35.869015 | 28.980772 | 24.173840 |
| S  | 21.436907 | 31.625286 | 35.731426 |
| S  | 20.520695 | 35.712143 | 33.312309 |
| S  | 21.900944 | 31.535027 | 29.786688 |
| S  | 24.886627 | 33.360069 | 33.198418 |
| S  | 26.032238 | 29.466068 | 30.609436 |
| S  | 25.600578 | 34.098648 | 28.299421 |
| S  | 28.200882 | 29.426905 | 26.658745 |
| S  | 30.576504 | 31.320347 | 30.169224 |
| S  | 31.679888 | 26.907181 | 27.844030 |
| S  | 32.830799 | 30.778927 | 25.154293 |
| S  | 33.557499 | 26.254379 | 23.435902 |
| S  | 36.362247 | 27.656834 | 27.143568 |

24 generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 18.616768 | 32.685600 | 33.898651 |
| Ca | 23.196365 | 34.675270 | 35.710171 |
| Ca | 23.103495 | 30.347664 | 32.921852 |
| Ca | 22.760769 | 34.512093 | 30.698374 |
| Ca | 25.012321 | 31.054617 | 27.875952 |
| Ca | 27.680351 | 32.814301 | 30.950176 |
| Ca | 29.103199 | 28.179657 | 30.130161 |
| Ca | 30.496431 | 32.343750 | 27.174471 |
| Ca | 30.589993 | 28.003605 | 24.786631 |
| Ca | 33.696285 | 29.972244 | 27.992981 |
| Ca | 34.227608 | 24.604553 | 26.757496 |
| Ca | 35.687523 | 28.731121 | 24.106180 |
| S  | 21.228680 | 31.443609 | 35.671211 |
| S  | 20.567333 | 35.584217 | 33.335869 |
| S  | 21.840309 | 31.596191 | 29.650194 |
| S  | 24.851400 | 33.153450 | 33.253784 |
| S  | 25.832800 | 29.789440 | 30.444521 |
| S  | 25.729935 | 34.271645 | 28.377525 |
| S  | 28.067358 | 29.587801 | 26.831333 |
| S  | 30.920622 | 31.311432 | 29.970263 |
| S  | 31.863686 | 27.152306 | 27.999165 |
| S  | 32.863358 | 30.704624 | 24.685646 |
| S  | 33.406578 | 26.057146 | 23.511381 |
| S  | 36.376896 | 27.723694 | 27.206045 |
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 18.34687   | 32.717682  | 34.236145  |
| Ca      | 23.32234   | 34.540947  | 35.844238  |
| Ca      | 23.195854  | 30.458023  | 32.833221  |
| Ca      | 22.802917  | 34.714264  | 30.543196  |
| Ca      | 25.135082  | 30.950005  | 27.820999  |
| Ca      | 27.76560   | 32.866989  | 30.764175  |
| Ca      | 29.017498  | 28.029741  | 29.628981  |
| Ca      | 30.567301  | 32.475792  | 27.025339  |
| Ca      | 30.475079  | 27.922947  | 24.560392  |
| Ca      | 33.420074  | 29.984430  | 28.342215  |
| Ca      | 34.280712  | 24.768135  | 27.069578  |
| Ca      | 35.914959  | 28.845015  | 23.940411  |
| S       | 21.286020  | 31.409483  | 35.805973  |
| S       | 20.582859  | 35.577110  | 33.597229  |
| S       | 22.077854  | 31.581921  | 29.643810  |
| S       | 24.833214  | 33.267105  | 33.107296  |
| S       | 26.033558  | 29.647152  | 30.611055  |
| S       | 25.576891  | 34.203148  | 28.067490  |
| S       | 28.311646  | 29.691681  | 26.729134  |
| S       | 30.721607  | 31.281708  | 30.083323  |
| S       | 31.454395  | 26.755096  | 27.792645  |
| S       | 32.792187  | 30.633417  | 24.886620  |
| S       | 33.519028  | 26.079140  | 23.666315  |
| S       | 36.285881  | 27.899094  | 27.340288  |

24

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 18.202038  | 33.030067  | 33.646446  |
| Ca      | 22.901035  | 35.155907  | 35.591164  |
| Ca      | 23.329853  | 30.279915  | 33.178089  |
| Ca      | 22.950718  | 34.445206  | 30.788147  |
| Ca      | 25.225925  | 30.798592  | 28.009075  |
| Ca      | 27.753830  | 32.785824  | 31.199440  |
| Ca      | 28.918806  | 28.053061  | 29.976051  |
| Ca      | 30.647717  | 32.344063  | 27.390877  |
| Ca      | 30.344946  | 27.762768  | 24.554804  |
| Ca      | 33.726799  | 29.830502  | 27.867567  |
| Ca      | 34.408787  | 24.868198  | 26.698347  |
| Ca      | 35.727104  | 29.094145  | 23.783653  |
| S       | 20.967272  | 31.862347  | 35.643272  |
| S       | 20.443493  | 35.663860  | 32.991898  |
| S       | 22.018421  | 31.172674  | 29.799431  |
| S       | 24.880783  | 33.192337  | 33.331093  |
| S       | 26.095470  | 29.521692  | 30.804237  |
| S       | 25.880213  | 34.050098  | 28.628510  |
| S       | 28.321201  | 29.687124  | 26.753012  |
|   | 30.743397  | 30.980087  | 30.240387  |
|---|------------|------------|------------|
| S | 31.717365  | 26.847157  | 27.907801  |
| S | 32.630630  | 30.703857  | 24.900959  |
| S | 33.377708  | 26.249702  | 23.437712  |
| S | 36.506565  | 27.920803  | 26.818106  |

24 generated by VMD

| Ca | 18.298790 | 32.883907 | 33.942909 |
|    | 22.844370 | 34.928337 | 35.594269 |
| Ca | 23.328373 | 30.269526 | 33.042229 |
| Ca | 22.704613 | 34.825665 | 30.739904 |
| Ca | 25.155294 | 30.923010 | 26.053410 |
| Ca | 27.702410 | 32.609749 | 31.181658 |
| Ca | 29.184700 | 27.929707 | 29.588772 |
| Ca | 30.726490 | 32.465244 | 27.410433 |
| Ca | 30.403109 | 27.876066 | 24.747540 |
| Ca | 33.758484 | 29.943501 | 28.224333 |
| Ca | 34.827965 | 25.103863 | 26.592466 |
| Ca | 35.509567 | 28.517712 | 23.796078 |
| S  | 21.312050 | 31.803873 | 35.514786 |
| S  | 20.250328 | 36.005985 | 33.119980 |
| S  | 21.892166 | 31.387835 | 29.963659 |
| S  | 24.852882 | 33.284233 | 33.197163 |
| S  | 25.885658 | 29.035570 | 30.565561 |
| S  | 25.537430 | 33.995800 | 28.596039 |
| S  | 28.276361 | 29.963036 | 26.616922 |
| S  | 30.763187 | 31.134609 | 30.273809 |
| S  | 31.997074 | 26.953785 | 27.759148 |
| S  | 32.925682 | 30.609901 | 25.087620 |
| S  | 33.154102 | 25.989647 | 23.360437 |
| S  | 36.428879 | 27.859478 | 26.970850 |

24 generated by VMD

| Ca  | 18.449123 | 33.084721 | 33.923134 |
| Ca  | 22.925652 | 34.570950 | 35.630974 |
| Ca  | 23.294674 | 30.260948 | 33.043159 |
| Ca  | 22.968073 | 34.798019 | 30.497143 |
| Ca  | 25.051416 | 30.971495 | 27.751024 |
| Ca  | 27.779753 | 32.466576 | 31.043310 |
| Ca  | 29.077925 | 27.900730 | 29.727545 |
| Ca  | 30.587318 | 32.250542 | 27.380167 |
| Ca  | 30.412140 | 27.751221 | 24.833630 |
| Ca  | 33.742500 | 29.916494 | 28.348848 |
| Ca  | 34.638447 | 25.231813 | 26.994511 |
| Ca  | 35.306633 | 28.852926 | 23.466505 |
| S   | 21.289200 | 31.449722 | 35.515785 |
|    |   X      |   Y      |   Z      |
|----|----------|----------|----------|
| S  | 20.467537| 35.851837| 33.217766|
| S  | 21.988043| 31.526321| 29.823324|
| S  | 24.913006| 33.279236| 33.208107|
| S  | 25.853384| 29.466093| 30.455397|
| S  | 25.901197| 34.236221| 28.349250|
| S  | 28.110531| 29.676598| 26.794620|
| S  | 30.794632| 30.961548| 30.337818|
| S  | 31.820791| 26.936779| 28.131540|
| S  | 32.669899| 30.586550| 25.106980|
| S  | 33.179512| 25.979029| 23.583841|
| S  | 36.498692| 28.293663| 26.778954|

24 generated by VMD

|    |   X      |   Y      |   Z      |
|----|----------|----------|----------|
| Ca | 18.433750| 33.451756| 33.839020|
| Ca | 23.144453| 34.684147| 35.854328|
| Ca | 23.194483| 30.010054| 33.002640|
| Ca | 22.812782| 34.631512| 30.692873|
| Ca | 25.098675| 30.834366| 27.988327|
| Ca | 27.626181| 32.616924| 31.073942|
| Ca | 29.061287| 27.900978| 29.800608|
| Ca | 30.381746| 32.355862| 27.427492|
| Ca | 30.357983| 27.702389| 24.437855|
| Ca | 33.625099| 29.942139| 28.037807|
| Ca | 34.608517| 25.300827| 27.069441|
| Ca | 35.644375| 28.892927| 23.819962|
| S  | 21.031153| 31.608238| 35.286064|
| S  | 20.757488| 35.935825| 33.313148|
| S  | 21.947412| 31.388119| 29.885822|
| S  | 24.945126| 33.136856| 33.201996|
| S  | 25.991674| 29.416546| 30.431753|
| S  | 25.755243| 34.207031| 28.482025|
| S  | 28.154358| 29.548496| 26.753077|
| S  | 30.767017| 31.026262| 30.149902|
| S  | 31.893383| 26.888908| 27.768322|
| S  | 32.539196| 30.656212| 24.880493|
| S  | 33.441059| 25.990635| 23.652018|
| S  | 36.507641| 28.173054| 27.092600|

24 generated by VMD

|    |   X      |   Y      |   Z      |
|----|----------|----------|----------|
| Ca | 18.204926| 33.135864| 33.718037|
| Ca | 23.258335| 34.710758| 35.536301|
| Ca | 23.367449| 30.124491| 33.159737|
| Ca | 23.067343| 34.601360| 30.632357|
| Ca | 25.112860| 30.813309| 27.981390|
| Ca | 27.576109| 32.530563| 30.964520|
| Ca | 29.337730| 28.025906| 29.981031|
|   |         |         |         |
|---|---------|---------|---------|
| Ca | 30.549940 | 32.736671 | 27.223869 |
| Ca | 30.331448 | 27.991657 | 24.685530 |
| Ca | 33.520336 | 29.923161 | 28.075157 |
| Ca | 34.429615 | 24.943628 | 26.696178 |
| Ca | 35.631657 | 28.851597 | 23.982752 |
| S  | 21.113050 | 31.606056 | 35.457031 |
| S  | 20.586851 | 35.876053 | 33.323460 |
| S  | 21.999928 | 31.257515 | 29.857382 |
| S  | 24.893822 | 33.151112 | 33.287548 |
| S  | 25.868149 | 29.414196 | 30.546412 |
| S  | 25.759598 | 33.976925 | 28.368364 |
| S  | 28.417671 | 29.817829 | 26.880239 |
| S  | 30.669106 | 31.288036 | 30.133553 |
| S  | 31.621775 | 26.908600 | 27.800947 |
| S  | 32.686291 | 30.581873 | 24.915749 |
| S  | 33.238930 | 26.020741 | 23.760027 |
| S  | 36.477139 | 28.012096 | 26.972502 |

24

generated by VMD

|   |         |         |         |
|---|---------|---------|---------|
| Ca | 18.414532 | 33.150978 | 34.009514 |
| Ca | 23.076185 | 34.659870 | 35.709175 |
| Ca | 23.338619 | 30.296886 | 32.912598 |
| Ca | 23.038387 | 34.341869 | 30.620770 |
| Ca | 24.967651 | 31.045162 | 27.904404 |
| Ca | 27.702265 | 32.685741 | 31.028275 |
| Ca | 29.070137 | 27.808083 | 29.675589 |
| Ca | 30.557501 | 32.331505 | 27.303122 |
| Ca | 30.313797 | 27.845467 | 24.715548 |
| Ca | 33.690399 | 30.000870 | 28.213060 |
| Ca | 34.650822 | 25.085255 | 27.020203 |
| Ca | 35.729164 | 28.96201 | 23.68950 |
| S  | 21.120892 | 31.630276 | 35.548553 |
| S  | 20.804159 | 35.870506 | 33.299202 |
| S  | 21.668457 | 31.509109 | 29.876883 |
| S  | 24.935623 | 33.088364 | 33.296440 |
| S  | 25.717052 | 29.604170 | 30.280375 |
| S  | 25.823214 | 34.058361 | 28.395964 |
| S  | 27.923983 | 29.616447 | 26.655087 |
| S  | 30.703514 | 31.138680 | 30.154430 |
| S  | 31.771738 | 26.896589 | 27.988564 |
| S  | 32.716236 | 30.468754 | 24.942293 |
| S  | 33.437656 | 26.094997 | 23.684883 |
| S  | 36.548004 | 28.110098 | 27.015287 |

24

generated by VMD

|   |         |         |         |
|---|---------|---------|---------|
| Ca | 18.729944 | 33.002163 | 34.132309 |
|   |    |    |    |
|---|---|---|---|
| Ca | 23.023247 | 34.487370 | 35.915699 |
| Ca | 23.106878 | 30.358362 | 32.685329 |
| Ca | 22.908125 | 34.869164 | 30.519926 |
| Ca | 25.076475 | 31.076099 | 27.676090 |
| Ca | 27.666952 | 32.490585 | 31.069326 |
| Ca | 29.098289 | 27.979994 | 29.699835 |
| Ca | 30.592329 | 32.336071 | 27.058416 |
| Ca | 30.311741 | 27.676361 | 24.799173 |
| Ca | 33.624474 | 30.079336 | 28.098345 |
| Ca | 34.465851 | 25.194420 | 27.471241 |
| Ca | 35.544930 | 28.555382 | 23.729424 |
| S  | 21.187725 | 31.192032 | 35.672192 |
| S  | 20.966955 | 35.544853 | 33.429600 |
| S  | 21.899075 | 31.713112 | 29.523720 |
| S  | 24.872477 | 33.146683 | 33.283020 |
| S  | 25.877256 | 29.570101 | 30.290382 |
| S  | 25.764166 | 34.332066 | 28.551693 |
| S  | 28.232567 | 29.804966 | 26.506649 |
| S  | 30.604977 | 31.181776 | 30.083252 |
| S  | 31.726400 | 27.059233 | 27.949350 |
| S  | 32.544395 | 30.626747 | 24.894384 |
| S  | 33.413467 | 25.728750 | 23.740723 |
| S  | 36.486797 | 28.294399 | 27.160004 |

24

generated by VMD

|   |    |    |    |
|---|---|---|---|
| Ca | 18.688656 | 32.197388 | 33.654037 |
| Ca | 22.568130 | 34.523678 | 35.936764 |
| Ca | 23.380405 | 30.422527 | 32.901741 |
| Ca | 22.906219 | 35.079067 | 30.494333 |
| Ca | 25.275579 | 31.263765 | 28.038864 |
| Ca | 27.646761 | 33.026035 | 31.453777 |
| Ca | 28.973257 | 28.201303 | 29.801111 |
| Ca | 30.570059 | 32.420902 | 26.962336 |
| Ca | 30.339834 | 27.784628 | 24.735907 |
| Ca | 33.735687 | 29.840683 | 27.855288 |
| Ca | 34.454002 | 24.994846 | 27.018812 |
| Ca | 35.661457 | 28.599834 | 23.602396 |
| S  | 21.153364 | 31.187788 | 35.719833 |
| S  | 20.301104 | 35.271317 | 33.211800 |
| S  | 21.998703 | 31.791958 | 29.963058 |
| S  | 24.814837 | 33.851917 | 33.316334 |
| S  | 26.019289 | 29.861494 | 30.512691 |
| S  | 26.145493 | 34.288986 | 28.523220 |
| S  | 28.170937 | 29.644888 | 26.711035 |
| S  | 30.735626 | 31.269279 | 30.182032 |
| S  | 31.546679 | 26.908894 | 27.829794 |
|   |         |         |         |
|---|---------|---------|---------|
| S | 32.617092 | 30.475023 | 24.755005 |
| S | 33.591873 | 25.750149 | 23.751818 |
| S | 36.425018 | 27.643669 | 27.008097 |

24

generated by VMD

| Ca  |         |         |         |
|-----|---------|---------|---------|
| Ca  | 18.618113 | 32.332153 | 33.544220 |
| Ca  | 22.806950 | 34.330170 | 35.863304 |
| Ca  | 23.280405 | 30.314930 | 32.874413 |
| Ca  | 22.949997 | 35.040337 | 30.511879 |
| Ca  | 25.228672 | 31.121441 | 27.971319 |
| Ca  | 27.845615 | 32.903835 | 31.045160 |
| Ca  | 29.101358 | 28.041874 | 29.836576 |
| Ca  | 30.497025 | 32.499809 | 27.067057 |
| Ca  | 30.281330 | 27.722736 | 25.043192 |
| Ca  | 33.393017 | 29.814548 | 27.804485 |
| Ca  | 34.504143 | 24.893227 | 27.229980 |
| Ca  | 35.449295 | 28.791077 | 23.690372 |
| S   | 21.044458 | 31.237309 | 35.592674 |
| S   | 20.575367 | 35.471100 | 33.310028 |
| S   | 22.142258 | 31.675354 | 29.908667 |
| S   | 25.036285 | 33.539822 | 33.213776 |
| S   | 26.133072 | 29.656033 | 30.583740 |
| S   | 25.872726 | 34.562019 | 28.496490 |
| S   | 28.139404 | 29.800665 | 26.710333 |
| S   | 30.778175 | 31.343674 | 30.061335 |
| S   | 31.434263 | 27.084492 | 27.904873 |
| S   | 32.700584 | 30.586079 | 24.883837 |
| S   | 33.433819 | 25.753887 | 23.886425 |
| S   | 36.473675 | 27.783438 | 26.905912 |

24

generated by VMD

| Ca  |         |         |         |
|-----|---------|---------|---------|
| Ca  | 18.200428 | 32.606060 | 33.552998 |
| Ca  | 22.950081 | 34.431557 | 35.779751 |
| Ca  | 23.375053 | 30.310223 | 32.818771 |
| Ca  | 22.931126 | 35.170017 | 30.686775 |
| Ca  | 25.115311 | 31.075788 | 28.221609 |
| Ca  | 27.750631 | 32.770836 | 31.268835 |
| Ca  | 29.260826 | 28.091118 | 30.019175 |
| Ca  | 30.579735 | 32.387154 | 26.891989 |
| Ca  | 30.367496 | 27.435783 | 24.711723 |
| Ca  | 33.414288 | 29.988041 | 27.867064 |
| Ca  | 34.473984 | 24.825134 | 27.155340 |
| Ca  | 35.613823 | 29.003124 | 23.899321 |
| S   | 21.019806 | 31.274353 | 35.341587 |
| S   | 20.425203 | 35.527252 | 33.315315 |
| S   | 22.070299 | 31.691326 | 29.954796 |
S 24.913059 33.477295 33.369316
S 26.171486 29.742533 30.699556
S 26.009619 34.362873 28.661922
S 28.247114 29.775103 26.629971
S 30.831408 31.223984 30.052832
S 31.635403 26.855022 27.798622
S 32.442341 30.594948 24.505531
S 33.570873 25.754772 23.791306
S 36.350658 27.925838 26.945946

24 generated by VMD
Ca 18.622398 32.584301 33.550354
Ca 22.658079 34.624638 35.646332
Ca 23.525127 30.247871 33.109818
Ca 22.981741 34.838779 30.613102
Ca 25.121944 30.966743 27.867493
Ca 27.570189 32.838383 31.337433
Ca 29.227003 28.102604 29.873108
Ca 30.481209 32.437981 27.539684
Ca 30.336618 27.612930 24.902554
Ca 33.609463 29.931835 27.737371
Ca 34.368416 24.828728 26.948700
Ca 35.387203 29.063160 23.841141
Ca 21.113945 31.486294 35.292278
S 20.611597 35.658195 33.271744
S 22.144285 31.503635 29.896450
S 24.932362 33.470516 33.291969
S 26.119747 29.812077 30.532082
S 25.876930 34.222179 28.385033
S 28.262764 29.653969 26.652100
S 30.887638 31.127813 30.278437
S 31.689922 26.951067 27.891586
S 32.364597 30.604877 24.942028
S 33.369560 25.928869 23.713741
S 36.457340 27.802635 26.825512

24 generated by VMD
Ca 18.691256 32.603722 34.156525
Ca 23.254992 34.238369 35.976616
Ca 23.291967 30.569628 32.689381
Ca 22.914717 34.997841 30.529118
Ca 24.902840 31.068241 27.741959
Ca 27.517088 32.810482 30.717089
Ca 28.874022 27.747305 29.688366
Ca 30.616840 32.405205 27.291615
Ca 30.336763 27.675247 24.936626

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| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 33.860134  | 30.008524  | 28.115416  |
| Ca      | 34.729488  | 24.836227  | 27.381588  |
| Ca      | 35.511318  | 35.441952  | 33.518837  |
| S       | 21.343340  | 31.204082  | 35.504700  |
| S       | 20.767963  | 29.024429  | 23.838633  |
| S       | 25.045017  | 33.497414  | 33.162468  |
| S       | 25.719988  | 29.763460  | 30.255903  |
| S       | 25.583851  | 34.477470  | 28.078840  |
| S       | 30.004192  | 29.671295  | 26.654512  |
| S       | 30.638212  | 30.954678  | 30.113440  |
| S       | 31.639809  | 26.876743  | 28.120485  |
| S       | 32.486046  | 30.519369  | 24.929096  |
| S       | 33.550468  | 25.972446  | 23.889565  |
| S       | 36.655312  | 27.956802  | 26.947161  |

24

generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 18.802773  | 33.028557  | 33.888927  |
| Ca      | 23.002449  | 34.162647  | 36.012592  |
| Ca      | 23.289452  | 30.264107  | 32.725258  |
| Ca      | 23.292074  | 34.908161  | 30.540541  |
| Ca      | 25.017296  | 30.907757  | 27.647228  |
| Ca      | 27.633747  | 32.612991  | 31.031725  |
| Ca      | 28.903538  | 27.833706  | 29.754250  |
| Ca      | 30.233023  | 32.504398  | 27.294168  |
| Ca      | 30.313818  | 27.640564  | 25.148491  |
| Ca      | 33.597832  | 30.209625  | 27.966009  |
| Ca      | 34.502338  | 25.134705  | 27.136824  |
| Ca      | 35.374691  | 28.940552  | 23.804867  |
| S       | 21.280594  | 31.511824  | 35.468681  |
| S       | 20.983709  | 35.702286  | 33.376991  |
| S       | 21.906475  | 31.739996  | 29.554258  |
| S       | 25.028976  | 33.179260  | 33.235703  |
| S       | 25.856667  | 29.450977  | 30.287729  |
| S       | 25.772343  | 34.114246  | 27.933985  |
| S       | 28.130903  | 29.563290  | 26.644251  |
| S       | 30.717236  | 31.027729  | 30.259430  |
| S       | 31.861750  | 27.069683  | 28.493711  |
| S       | 32.336803  | 30.771175  | 25.015251  |
| S       | 33.412941  | 26.063271  | 23.840754  |
| S       | 36.468567  | 27.958546  | 26.878395  |

24

generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 18.350876  | 32.737305  | 34.486000  |
| Ca      | 23.072329  | 34.217323  | 35.725182  |
| Ca      | 23.335140  | 30.469297  | 32.680408  |
| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 22.899162 | 35.211754 | 30.526014 |
| Ca      | 24.95629 | 31.073814 | 27.760305 |
| Ca      | 27.804474 | 32.744648 | 30.803696 |
| Ca      | 28.921518 | 27.928844 | 29.586454 |
| Ca      | 30.431108 | 32.416550 | 27.087885 |
| Ca      | 30.323332 | 27.787594 | 25.048960 |
| Ca      | 33.982719 | 30.062492 | 28.002367 |
| Ca      | 34.514603 | 24.837418 | 27.139481 |
| Ca      | 35.556286 | 28.824215 | 23.932854 |
| S       | 21.387386 | 31.176018 | 35.670090 |
| S       | 20.550070 | 35.261189 | 33.436 |
| S       | 21.814934 | 31.955463 | 29.724516 |
| S       | 25.046818 | 33.622715 | 32.960255 |
| S       | 25.814724 | 29.444904 | 30.134275 |
| S       | 27.878372 | 34.348492 | 28.208445 |
| S       | 30.760229 | 31.085911 | 30.038507 |
| S       | 31.802814 | 27.043257 | 28.227856 |
| S       | 32.745647 | 30.553268 | 25.152016 |
| S       | 33.368107 | 26.096149 | 23.882393 |
| S       | 36.692513 | 27.697138 | 27.078775 |
| 24      | 24.1832032 | 32.907799 | 30.631721 |
| Ca      | 23.026003 | 34.862999 | 35.534126 |
| Ca      | 23.215391 | 30.292370 | 32.950485 |
| Ca      | 23.004623 | 35.134766 | 30.498430 |
| Ca      | 25.077312 | 30.852722 | 28.249460 |
| Ca      | 27.581028 | 32.352061 | 31.049566 |
| Ca      | 29.077600 | 27.600128 | 30.009460 |
| Ca      | 30.607361 | 32.220783 | 27.557890 |
| Ca      | 30.391273 | 27.724302 | 24.933109 |
| Ca      | 33.707775 | 29.909498 | 28.250202 |
| Ca      | 34.567612 | 25.145233 | 26.551098 |
| Ca      | 35.436390 | 29.243528 | 23.527824 |
| S       | 21.298874 | 31.730366 | 35.466702 |
| S       | 20.515869 | 35.777328 | 33.044983 |
| S       | 21.938797 | 31.685570 | 30.002911 |
| S       | 24.826920 | 33.457806 | 33.180885 |
| S       | 25.892883 | 29.295336 | 30.593212 |
| S       | 25.741077 | 34.018597 | 28.278749 |
| S       | 28.223946 | 29.501762 | 27.076687 |
| S       | 30.901314 | 30.784134 | 30.457190 |
| S       | 32.026047 | 26.897125 | 28.078482 |
| S       | 32.471703 | 30.533367 | 25.03396 |
| S       | 33.411182 | 26.070034 | 23.368866 |
|     |      |      |      |
|-----|------|------|------|
| S   | 36.451008 | 28.299435 | 26.614578 |

24

generated by VMD

Ca  | 18.618114 | 32.912933 | 34.229424 |
Ca  | 23.103291 | 34.806244 | 35.561485 |
Ca  | 23.378977 | 30.341484 | 32.714951 |
Ca  | 22.767551 | 34.831684 | 30.257795 |
Ca  | 24.972115 | 30.773014 | 27.961014 |
Ca  | 27.690084 | 32.355003 | 30.835846 |
Ca  | 29.114941 | 27.968468 | 29.825991 |
Ca  | 30.493660 | 32.334362 | 27.463142 |
Ca  | 30.214163 | 28.085789 | 24.709538 |
Ca  | 33.883556 | 29.908852 | 28.383854 |
Ca  | 34.248604 | 25.014900 | 26.781183 |
Ca  | 35.587711 | 29.039246 | 23.930300 |
S   | 21.652077 | 31.507065 | 35.836258 |
S   | 20.658464 | 35.615036 | 32.979301 |
S   | 21.777122 | 31.378056 | 29.859047 |
S   | 24.817329 | 33.604218 | 33.042099 |
S   | 25.940348 | 29.341576 | 30.330404 |
S   | 25.581181 | 33.986610 | 28.268963 |
S   | 28.190289 | 29.890259 | 26.757057 |
S   | 30.799374 | 30.843880 | 30.494793 |
S   | 31.717091 | 26.988571 | 27.894588 |
S   | 32.915939 | 30.660269 | 25.290815 |
S   | 33.105728 | 26.240049 | 23.529837 |
S   | 36.492397 | 27.872503 | 27.002329 |

24

generated by VMD

Ca  | 18.441156 | 32.755474 | 34.018688 |
Ca  | 23.026575 | 34.702473 | 35.561226 |
Ca  | 23.303650 | 30.510494 | 32.487770 |
Ca  | 22.710505 | 35.136082 | 30.452307 |
Ca  | 25.058338 | 31.082420 | 27.967674 |
Ca  | 27.823404 | 32.364861 | 30.966568 |
Ca  | 29.108311 | 27.723955 | 29.748199 |
Ca  | 30.514786 | 32.221333 | 27.500437 |
Ca  | 30.236210 | 27.554031 | 25.019791 |
Ca  | 33.854992 | 29.853123 | 28.286058 |
Ca  | 34.872169 | 25.118801 | 26.519512 |
Ca  | 35.292553 | 29.156553 | 23.787125 |
S   | 21.512180 | 31.463879 | 35.598938 |
S   | 20.588446 | 35.641453 | 33.343941 |
S   | 21.805086 | 31.818268 | 29.839424 |
S   | 24.992170 | 33.671249 | 32.940697 |
S   | 26.037003 | 29.343002 | 30.426323 |
|    |        |        |        |
|----|--------|--------|--------|
| S  | 25.532169 | 34.176556 | 28.253914 |
| S  | 28.034468 | 29.660881 | 26.919107 |
| S  | 30.730455 | 30.867975 | 30.452744 |
| S  | 31.925964 | 26.787718 | 27.893671 |
| S  | 32.507549 | 30.401608 | 25.357635 |
| S  | 33.266693 | 26.007978 | 23.606884 |
| S  | 36.545219 | 28.279877 | 26.991426 |
| 24 | generated by VMD |
| Ca | 18.574379 | 33.128555 | 33.955727 |
| Ca | 23.265408 | 34.541035 | 35.620914 |
| Ca | 23.194487 | 30.137669 | 32.706680 |
| Ca | 22.730156 | 34.807129 | 30.509356 |
| Ca | 25.003883 | 30.557693 | 28.080336 |
| Ca | 27.757246 | 32.553249 | 30.932224 |
| Ca | 29.214754 | 28.064682 | 29.890968 |
| Ca | 30.486614 | 32.544281 | 27.481516 |
| Ca | 30.338717 | 27.991070 | 24.836952 |
| Ca | 33.728935 | 29.954903 | 28.061403 |
| Ca | 34.376858 | 24.995049 | 26.837196 |
| Ca | 35.433941 | 29.011778 | 23.939770 |
| S  | 21.409643 | 31.616550 | 35.574068 |
| S  | 20.678349 | 35.751747 | 33.216766 |
| S  | 21.887619 | 31.327963 | 29.813358 |
| S  | 24.922483 | 33.339733 | 32.757942 |
| S  | 26.037205 | 29.326744 | 30.444679 |
| S  | 25.556871 | 34.052921 | 28.385817 |
| S  | 28.348427 | 29.903431 | 26.836634 |
| S  | 30.845947 | 31.127409 | 30.221727 |
| S  | 31.691837 | 26.916914 | 27.923340 |
| S  | 32.682854 | 30.773861 | 25.226423 |
| S  | 33.170746 | 26.108692 | 23.536970 |
| S  | 36.382675 | 27.766964 | 27.145926 |
| 24 | generated by VMD |
| Ca | 18.519243 | 32.629581 | 33.866898 |
| Ca | 22.994753 | 34.492340 | 35.884674 |
| Ca | 22.963566 | 30.569691 | 32.798370 |
| Ca | 23.058508 | 35.031712 | 30.437366 |
| Ca | 25.174816 | 30.737064 | 28.028101 |
| Ca | 27.677055 | 32.829903 | 31.087879 |
| Ca | 28.903450 | 28.088253 | 30.081030 |
| Ca | 30.559544 | 32.334885 | 27.350658 |
| Ca | 30.397066 | 27.790007 | 24.725868 |
| Ca | 33.941929 | 29.984777 | 28.036144 |
| Ca | 34.394051 | 24.907078 | 26.733200 |
Ca       35.444778       28.886295       23.977762
S        21.158104       31.416151       29.604361
S        20.727386       35.466187       33.018749
S        21.848473       31.566614       29.604361
S        24.940947       33.668083       33.018749
S        25.971581       29.567879       30.766056
S        25.745358       34.032513       28.106812
S        28.176979       29.649096       26.824848
S        30.818630       31.130762       30.345100
S        31.768124       26.906818       27.965107
S        32.703220       30.692642       25.074654
S        33.394661       26.020290       23.449804
S        36.437813       27.901382       26.779915

24

generated by VMD

Ca       18.687185       32.557484       33.826576
Ca       22.882114       34.730034       35.445114
Ca       23.527010       30.317514       32.947281
Ca       22.802256       35.056915       30.331463
Ca       25.190905       30.774277       28.189948
Ca       27.843470       32.730392       31.263945
Ca       29.028564       27.866131       29.776167
Ca       30.473848       32.484047       27.391590
Ca       30.381838       27.950867       24.530281
Ca       33.588799       29.808674       28.265646
Ca       34.310760       25.084709       26.592588
Ca       35.519669       28.841318       24.105154
S        21.382202       31.418697       35.725304
S        20.557707       35.527126       33.055374
S        22.112057       31.540684       29.970726
S        24.949942       33.593594       32.981789
S        26.104027       29.408911       30.653111
S        25.683626       34.199825       28.296736
S        28.154856       29.755259       26.774033
S        30.758322       31.115488       30.188757
S        31.647079       26.882561       27.886047
S        32.651901       30.677765       25.064161
S        33.201668       26.071808       23.441330
S        36.280220       27.905989       27.237968

24

generated by VMD

Ca       18.337124       32.618462       33.538113
Ca       22.779598       34.524231       35.745159
Ca       23.458603       30.300177       33.049313
Ca       22.825779       34.933697       30.447439
Ca       25.395136       31.008867       28.298437
Ca       27.832258       33.044178       31.055649
Ca       29.083773       27.957897       29.901295
Ca       30.712320       32.467125       27.612869
Ca       30.282324       27.836510       24.637339
Ca       33.741634       30.015953       27.906174
Ca       34.273663       32.467125       27.612869
Ca       30.282324       27.836510       24.637339
Ca       33.741634       30.015953       27.906174
S        21.065041       31.347471       35.609264
S        20.282343       35.517082       33.159782
S        22.268391       31.548744       30.027084
S        24.903709       33.770718       33.050713
S        26.244654       29.665718       30.876163
S        25.515194       34.130562       28.094265
S        28.404531       29.721931       26.837812
S        30.863375       31.047729       30.321466
S        31.711920       26.952351       27.842871
S        32.748789       30.705067       25.085463
S        33.241695       25.928776       23.529148
S        36.355885       27.775078       26.820454
S        21.186859       31.372730       35.338516
S        20.491787       35.659142       32.994698
S        22.090555       31.416832       29.922897
S        24.889378       33.838413       33.194527
S        26.278460       29.775232       30.823757
S        25.704348       34.076611       28.439047
S        28.332458       29.619347       27.010548
S        31.046730       30.903393       30.502760
S        31.643614       26.765667       27.871859
S        32.525894       30.579868       25.245232
S        33.170933       26.034195       23.391865
S        36.264828       28.022003       26.804108

24

generated by VMD

Ca       18.399605       32.757133       33.475037
Ca       22.977106       34.527435       35.496124
Ca       23.642122       30.484262       33.056580
Ca       22.744940       34.950485       30.407938
Ca       25.048756       30.588654       28.115643
Ca       27.823935       32.826939       31.081255
Ca       29.295000       27.826546       30.010258
Ca       30.662540       32.351051       27.621307
Ca       30.266758       27.870600       24.647249
Ca       33.560562       30.021648       28.314232
Ca       34.346180       24.955780       26.609303
Ca       35.326721       29.076038       23.564978
S        21.186859       31.372730       35.338516
S        20.491787       35.659142       32.994698
S        22.090555       31.416832       29.922897
S        24.889378       33.838413       33.194527
S        26.278460       29.775232       30.823757
S        25.704348       34.076611       28.439047
S        28.332458       29.619347       27.010548
S        31.046730       30.903393       30.502760
S        31.643614       26.765667       27.871859
S        32.525894       30.579868       25.245232
S        33.170933       26.034195       23.391865
S        36.264828       28.022003       26.804108

24
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 18.528381 | 32.431961 | 33.602901 |
| Ca      | 22.446396  | 34.542881 | 35.663216 |
| Ca      | 23.747427  | 30.464081 | 33.021843 |
| Ca      | 22.829021  | 34.905571 | 30.435343 |
| Ca      | 25.339666  | 30.758141 | 27.925606 |
| Ca      | 27.652496  | 33.259380 | 31.370411 |
| Ca      | 29.189365  | 28.105480 | 30.077839 |
| Ca      | 30.686321  | 32.447071 | 27.525488 |
| Ca      | 30.258127  | 27.805359 | 24.759953 |
| Ca      | 33.694107  | 29.966223 | 27.981882 |
| Ca      | 34.186398  | 24.568409 | 26.740927 |
| Ca      | 35.109409  | 28.976341 | 23.755573 |
| S       | 21.293621  | 31.231194 | 35.345055 |
| S       | 20.345863  | 35.437485 | 32.893532 |
| S       | 22.288540  | 31.379322 | 29.600883 |
| S       | 24.971352  | 33.805290 | 33.301716 |
| S       | 26.406324  | 29.771679 | 31.160868 |
| S       | 25.826227  | 34.228428 | 28.363377 |
| S       | 28.355080  | 29.742802 | 26.935205 |
| S       | 31.003094  | 31.304237 | 30.304438 |
| S       | 31.688353  | 26.893707 | 27.788279 |
| S       | 32.702995  | 30.630224 | 25.189461 |
| S       | 32.940392  | 26.029396 | 23.277056 |
| S       | 36.231064  | 27.615385 | 26.919231 |

24

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 18.208252 | 32.943066 | 33.736588 |
| Ca      | 22.924433  | 34.774353 | 35.581612 |
| Ca      | 23.419064  | 30.239920 | 33.019745 |
| Ca      | 22.696831  | 34.921627 | 30.302502 |
| Ca      | 25.139385  | 30.497906 | 28.299866 |
| Ca      | 27.689804  | 32.651192 | 31.117266 |
| Ca      | 29.216221  | 27.958891 | 30.158207 |
| Ca      | 30.570024  | 32.514359 | 27.307417 |
| Ca      | 30.385246  | 27.945896 | 24.766657 |
| Ca      | 33.674034  | 29.860544 | 27.978607 |
| Ca      | 34.229408  | 24.882286 | 26.580669 |
| Ca      | 35.466351  | 29.224295 | 23.774353 |
| S       | 21.102852  | 31.654377 | 35.449677 |
| S       | 20.486086  | 35.801426 | 33.123611 |
| S       | 21.976068  | 31.334332 | 29.943169 |
| S       | 24.873291  | 33.667305 | 33.032295 |
| S       | 26.180683  | 29.467094 | 30.904966 |
| S       | 25.743126  | 33.848595 | 28.452745 |
| S       | 28.270927  | 29.674168 | 27.056730 |
| Element | X1  | Y1  | Z1  |
|---------|-----|-----|-----|
| S       | 31.103821 | 30.966839 | 30.254202 |
| S       | 31.692947 | 26.833174 | 27.827074 |
| S       | 32.782673 | 30.694572 | 25.182741 |
| S       | 33.459457 | 26.342131 | 23.253563 |
| S       | 36.429008 | 27.601730 | 26.835783 |

24 generated by VMD

| Ca      | 18.500526 | 32.904015 | 33.549026 |
|---------|-----------|-----------|-----------|
| Ca      | 22.875183 | 34.729095 | 35.524994 |
| Ca      | 23.507837 | 30.169786 | 33.030811 |
| Ca      | 22.625637 | 35.009003 | 30.719469 |
| Ca      | 25.236076 | 30.718494 | 28.240162 |
| Ca      | 27.696304 | 32.850117 | 30.970650 |
| Ca      | 29.331882 | 27.855907 | 30.058203 |
| Ca      | 30.513012 | 32.513557 | 27.383257 |
| Ca      | 30.250122 | 27.874695 | 24.685411 |
| Ca      | 33.738235 | 29.988049 | 28.113840 |
| Ca      | 34.545406 | 24.803204 | 26.451799 |
| Ca      | 35.401840 | 28.889282 | 23.973009 |
| S       | 21.113077 | 31.424362 | 35.402428 |
| S       | 20.44317 | 35.798576 | 33.095268 |
| S       | 22.093012 | 31.454226 | 30.97248 |
| S       | 24.836458 | 33.526554 | 33.110001 |
| S       | 26.268372 | 29.485573 | 30.791079 |
| S       | 25.483883 | 34.142700 | 28.257711 |
| S       | 28.262363 | 29.762001 | 26.973948 |
| S       | 30.924955 | 31.121557 | 30.181673 |
| S       | 31.819014 | 26.680527 | 27.808220 |
| S       | 32.600170 | 30.604877 | 25.057810 |
| S       | 33.230106 | 26.411480 | 23.384724 |
| S       | 36.422268 | 27.582357 | 27.079330 |

24 generated by VMD

| Ca      | 18.293715 | 33.104435 | 33.690155 |
|---------|-----------|-----------|-----------|
| Ca      | 22.914190 | 35.061356 | 35.359970 |
| Ca      | 23.714834 | 30.332394 | 33.541042 |
| Ca      | 22.533697 | 34.676952 | 30.400015 |
| Ca      | 25.140022 | 30.621168 | 28.166765 |
| Ca      | 27.662449 | 32.619640 | 31.057299 |
| Ca      | 29.222534 | 27.765715 | 30.079460 |
| Ca      | 30.660282 | 32.427513 | 27.806183 |
| Ca      | 30.342031 | 27.912376 | 24.549423 |
| Ca      | 33.560047 | 29.793072 | 28.136581 |
| Ca      | 34.281395 | 24.918991 | 25.984859 |
| Ca      | 35.569180 | 29.141521 | 24.007977 |
| S       | 21.072985 | 31.873732 | 35.630398 |
|   | X    | Y    | Z    |
|---|------|------|------|
| S | 20.307297 | 35.720123 | 32.755142 |
| S | 22.172960 | 31.060307 | 30.211470 |
| S | 24.853859 | 33.703049 | 33.136665 |
| S | 26.028528 | 29.383137 | 30.749155 |
| S | 25.664665 | 33.918945 | 28.183964 |
| S | 28.374577 | 29.717323 | 27.183756 |
| S | 31.011478 | 30.940556 | 30.406702 |
| S | 31.789940 | 26.681322 | 27.545969 |
| S | 32.757038 | 30.706549 | 25.330687 |
| S | 33.323997 | 26.429296 | 23.102436 |
| S | 36.468418 | 27.790545 | 26.924026 |

24

generated by VMD

| Ca | X    | Y    | Z    |
|----|------|------|------|
| Ca | 18.173294 | 32.739193 | 33.546028 |
| Ca | 22.491909 | 35.071762 | 35.630634 |
| Ca | 23.586876 | 30.377974 | 33.089558 |
| Ca | 22.916342 | 34.896130 | 30.485355 |
| Ca | 25.088816 | 30.693859 | 28.033619 |
| Ca | 27.850372 | 32.693352 | 31.463114 |
| Ca | 29.126812 | 27.752426 | 29.812260 |
| Ca | 30.680387 | 32.359413 | 27.437933 |
| Ca | 30.273092 | 27.542774 | 24.528475 |
| Ca | 33.549896 | 29.613590 | 27.973160 |
| Ca | 34.747082 | 25.061317 | 26.672253 |
| Ca | 35.398502 | 29.298262 | 23.523022 |
| S  | 20.907413 | 31.821863 | 35.591507 |
| S  | 20.120144 | 35.757835 | 32.926208 |
| S  | 22.198845 | 31.530762 | 30.019289 |
| S  | 24.858421 | 33.678383 | 33.566078 |
| S  | 26.130295 | 29.543724 | 30.891298 |
| S  | 26.049704 | 34.055466 | 28.595848 |
| S  | 28.297600 | 29.663927 | 26.843222 |
| S  | 30.947922 | 30.880892 | 30.427032 |
| S  | 31.833595 | 26.583878 | 27.803093 |
| S  | 32.471661 | 30.515942 | 25.103163 |
| S  | 33.427963 | 26.064369 | 23.428980 |
| S  | 36.593071 | 28.102983 | 26.547802 |

24

generated by VMD

| Ca | X    | Y    | Z    |
|----|------|------|------|
| Ca | 18.293491 | 33.383289 | 33.444595 |
| Ca | 23.019014 | 34.907055 | 35.638512 |
| Ca | 23.397518 | 30.287434 | 33.212181 |
| Ca | 22.883411 | 35.064568 | 30.504452 |
| Ca | 25.026058 | 30.263639 | 28.072588 |
| Ca | 27.504406 | 32.486023 | 31.171570 |
| Ca | 29.182384 | 27.786108 | 29.960888 |
Ca  30.250631  32.291309  27.597118
Ca  30.362160  27.765175  24.693621
Ca  33.581818  29.884172  27.923632
Ca  34.748112  24.952578  26.444799
Ca  35.615295  29.320513  23.878468
S   21.104404  31.708054  35.466614
S   20.596798  35.911354  33.121063
S   22.133110  31.352825  29.837788
S   24.936096  33.545158  33.327034
S   26.107426  29.369724  30.905230
S   25.724722  33.752777  28.389420
S   28.195129  29.624289  27.006601
S   30.772949  30.818623  30.390039
S   31.625507  26.892588  27.647627
S   32.512238  30.712391  25.164783
S   33.586071  26.201204  23.390636
S   36.561333  28.019159  26.750801
24
generated by VMD
Ca  18.482994  33.186882  33.475098
Ca  22.798225  34.997665  35.491478
Ca  23.452091  30.205862  33.012074
Ca  22.907753  34.629665  30.820127
Ca  24.964832  30.475510  28.053671
Ca  27.723986  32.678768  31.420113
Ca  29.101959  27.924015  29.791065
Ca  30.411562  32.392509  27.562767
Ca  30.506502  27.658381  24.664230
Ca  33.700657  30.017433  28.157961
Ca  34.488758  24.896061  26.513287
Ca  35.337357  29.173363  23.723454
S   21.087011  31.730469  35.434013
S   20.531662  35.961727  32.927734
S   22.052200  31.374935  29.719740
S   24.827278  33.324207  33.465179
S   26.243580  29.546429  30.909281
S   25.803576  33.893734  28.679094
S   28.059509  29.464088  26.846855
S   30.832977  31.176334  30.301058
S   31.871864  26.968744  27.802794
S   32.628952  30.570894  25.083614
S   33.491783  26.122444  23.279894
S   36.413010  27.929955  26.805454
24
generated by VMD
Ca  18.120621  33.142006  33.708725
|   | Ca   | S      | S      |
|---|------|--------|--------|
| Ca| 22.909565 | 34.864491 | 35.713509 |
| Ca| 23.524376 | 30.272644 | 32.884476 |
| Ca| 22.922392 | 34.487267 | 30.616882 |
| Ca| 25.082787 | 30.547081 | 28.082998 |
| Ca| 27.598686 | 32.808697 | 31.181231 |
| Ca| 29.348223 | 28.125589 | 29.859066 |
| Ca| 30.506124 | 32.370239 | 27.611418 |
| Ca| 33.598668 | 32.808697 | 31.181231 |
| Ca| 29.348223 | 28.125589 | 29.859066 |
| Ca| 30.506124 | 32.370239 | 27.611418 |
| Ca| 33.598668 | 32.808697 | 31.181231 |
| Ca| 29.348223 | 28.125589 | 29.859066 |
| Ca| 30.506124 | 32.370239 | 27.611418 |
| Ca| 33.598668 | 32.808697 | 31.181231 |
| S | 21.243307 | 31.705652 | 35.331108 |
| S | 20.513264 | 35.805405 | 33.184372 |
| S | 21.970760 | 31.499962 | 29.717478 |
| S | 24.952747 | 33.308842 | 33.378998 |
| S | 26.116987 | 29.480938 | 30.712196 |
| S | 25.832378 | 33.873741 | 28.439709 |
| S | 28.469456 | 29.896877 | 26.652370 |
| S | 30.743370 | 31.098984 | 30.346403 |
| S | 31.781164 | 26.786018 | 27.994762 |
| S | 32.575180 | 30.617542 | 25.195644 |
| S | 33.440037 | 25.933935 | 23.389917 |
| S | 36.373131 | 28.009432 | 26.742521 |

Generated by VMD
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| S       | 32.630642    | 30.733799    | 25.077158    |
| S       | 33.378017    | 26.256447    | 23.558064    |
| S       | 36.497631    | 27.957760    | 26.943613    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.377153    | 33.261158    | 33.514351    |
| Ca      | 22.809242    | 34.889111    | 35.879120    |
| Ca      | 23.369507    | 30.395336    | 33.080208    |
| Ca      | 22.921082    | 34.521000    | 30.523207    |
| Ca      | 25.252163    | 30.446115    | 27.968687    |
| Ca      | 27.663456    | 32.671890    | 31.307100    |
| Ca      | 29.247608    | 27.938217    | 29.981518    |
| Ca      | 30.514622    | 32.258755    | 27.444292    |
| Ca      | 30.508730    | 27.803953    | 24.676214    |
| Ca      | 33.393597    | 29.939526    | 28.181036    |
| Ca      | 34.534380    | 25.003529    | 26.415026    |
| Ca      | 35.122742    | 29.106464    | 23.806717    |
| S       | 21.031435    | 31.782040    | 35.420418    |
| S       | 20.725857    | 35.960468    | 33.175362    |
| S       | 22.146769    | 31.345528    | 29.558523    |
| S       | 24.840775    | 33.279697    | 33.329071    |
| S       | 26.132748    | 29.268997    | 30.952942    |
| S       | 25.962173    | 33.742168    | 28.316992    |
| S       | 28.200928    | 29.579929    | 26.840225    |
| S       | 30.752235    | 31.111731    | 30.474258    |
| S       | 31.767546    | 27.004770    | 27.660875    |
| S       | 32.689735    | 30.782217    | 25.076256    |
| S       | 33.353714    | 26.093517    | 23.610815    |
| S       | 36.392677    | 28.113909    | 26.746872    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.463299    | 33.483498    | 33.825237    |
| Ca      | 23.279177    | 34.570213    | 35.908806    |
| Ca      | 23.099407    | 30.095314    | 32.912209    |
| Ca      | 23.005070    | 34.475365    | 30.670698    |
| Ca      | 25.014313    | 30.626026    | 27.881001    |
| Ca      | 27.644051    | 32.558865    | 31.022562    |
| Ca      | 29.135843    | 28.001068    | 29.971836    |
| Ca      | 30.577837    | 32.370621    | 27.067772    |
| Ca      | 30.479530    | 27.849403    | 24.626350    |
| Ca      | 33.562363    | 30.036522    | 28.168093    |
| Ca      | 34.470005    | 25.017269    | 26.737322    |
| Ca      | 35.514534    | 28.965485    | 23.923794    |
| S       | 21.025320    | 31.812126    | 35.443619    |
| S       | 20.918989    | 35.988384    | 33.445877    |
| S       | 21.718142    | 31.300146    | 29.713619    |
generated by VMD

Calculated coordinates for S and Ca from VMD output:

S (x, y, z) = (24.826124, 32.903469, 33.227997)
S (x, y, z) = (25.900745, 29.477066, 30.624048)
S (x, y, z) = (25.552683, 33.940720, 28.222122)
S (x, y, z) = (28.352688, 29.748747, 26.840117)
S (x, y, z) = (30.671457, 31.218719, 30.168089)
S (x, y, z) = (31.693626, 26.912785, 27.887522)
S (x, y, z) = (32.900200, 30.804504, 24.911663)
S (x, y, z) = (33.493382, 25.996876, 23.745708)
S (x, y, z) = (36.421177, 28.146873, 26.994047)

Ca (x, y, z) = (18.383759, 33.415657, 33.927555)
Ca (x, y, z) = (23.182083, 34.542625, 36.016956)
Ca (x, y, z) = (23.208408, 30.274132, 32.516121)
Ca (x, y, z) = (22.876034, 34.622139, 30.688980)
Ca (x, y, z) = (25.025486, 30.521103, 27.919371)
Ca (x, y, z) = (27.603083, 32.575394, 30.890043)
Ca (x, y, z) = (29.191486, 27.924255, 30.090969)
Ca (x, y, z) = (30.428968, 32.295059, 27.292269)
Ca (x, y, z) = (30.407866, 27.657623, 24.753222)
Ca (x, y, z) = (33.723660, 30.032402, 28.217094)
Ca (x, y, z) = (34.436016, 25.105690, 26.790726)
Ca (x, y, z) = (35.491222, 29.156406, 23.695604)
Ca (x, y, z) = (21.171480, 31.692501, 35.387943)
S (x, y, z) = (20.884743, 36.074535, 33.520061)
S (x, y, z) = (21.838928, 31.505888, 29.522739)
S (x, y, z) = (24.799757, 33.082123, 33.052677)
S (x, y, z) = (25.963028, 29.334820, 30.556234)
S (x, y, z) = (25.672228, 33.974712, 28.364955)
S (x, y, z) = (28.203014, 29.478239, 26.879387)
S (x, y, z) = (30.785004, 31.168417, 30.221012)
S (x, y, z) = (31.835670, 26.914982, 27.966125)
S (x, y, z) = (32.645119, 30.704481, 25.010046)
S (x, y, z) = (33.409546, 26.097797, 23.634356)
S (x, y, z) = (36.550583, 28.124361, 27.024038)
Ca  33.708843  30.114944  28.019279
Ca  34.319096  24.968563  26.604691
Ca  35.587746  35.748466  33.276131
S   20.873861  31.730133  35.299011
S   20.706581  31.459351  29.607334
S   24.864983  33.207298  33.225288
S   26.042746  29.635080  30.680407
S   25.834446  34.135391  28.548386
S   28.289608  29.373602  26.959690
S   30.797911  31.288593  30.268379
S   31.914795  26.979851  27.897659
S   32.639278  30.616253  25.006571
S   33.426006  36.423782  27.912697  26.954657

generated by VMD

Ca  18.174324  33.617744  33.658607
Ca  23.138887  34.725605  35.886665
Ca  23.441475  30.364841  32.889618
Ca  22.831888  34.347408  30.823420
Ca  25.012423  30.752974  27.798872
Ca  27.798403  32.445786  31.066835
Ca  29.172354  27.816898  29.854750
Ca  30.316319  32.311920  27.380819
Ca  30.506710  27.610186  24.707579
Ca  33.642754  30.165577  28.143517
Ca  34.592422  33.617744  33.658607
Ca  35.470085  29.029049  23.709940
S   20.824497  31.806364  35.290478
S   20.764835  35.857292  33.425049
S   21.810764  31.417650  29.533951
S   25.037725  33.161873  33.326317
S   26.074406  29.584293  30.618973
S   25.692072  33.982800  28.611521
S   28.130650  29.439285  26.887878
S   30.707806  31.041021  30.222904
S   31.937569  26.922552  27.918995
S   32.562012  30.637138  25.066763
S   33.533272  26.013142  23.731728
S   36.546341  28.225122  26.741819

generated by VMD

Ca  18.065599  33.350548  33.725441
Ca  23.072763  34.535404  35.696770
Ca  23.498367  30.444092  33.067757
|   |     |     |     |
|---|-----|-----|-----|
| Ca | 22.875893 | 34.717537 | 30.716553 |
| Ca | 25.089188 | 30.629990 | 28.018595 |
| Ca | 27.764132 | 32.510296 | 31.140615 |
| Ca | 29.337624 | 27.901047 | 29.776785 |
| Ca | 30.457550 | 32.499554 | 27.271669 |
| Ca | 30.330669 | 27.790199 | 24.982199 |
| Ca | 33.740707 | 29.947468 | 28.025293 |
| Ca | 34.674038 | 24.933828 | 26.586924 |
| Ca | 35.119892 | 28.985777 | 23.801991 |
| S  | 20.840611 | 31.578697 | 35.113369 |
| S  | 20.603806 | 35.819336 | 33.271660 |
| S  | 21.997803 | 31.557829 | 29.738298 |
| S  | 25.017815 | 33.402729 | 33.232178 |
| S  | 26.115623 | 31.281654 | 30.553654 |
| S  | 25.799536 | 34.059185 | 28.524681 |
| S  | 28.340353 | 31.490204 | 26.830444 |
| S  | 30.659367 | 31.190083 | 30.128426 |
| S  | 32.117401 | 26.899750 | 28.059570 |
| S  | 32.468254 | 30.607845 | 25.290251 |
| S  | 33.199051 | 26.008245 | 23.571789 |
| S  | 36.533978 | 28.158722 | 26.815166 |

24 generated by VMD

|   |     |     |     |
|---|-----|-----|-----|
| Ca | 18.564636 | 33.261635 | 33.468224 |
| Ca | 23.040586 | 34.373451 | 35.989159 |
| Ca | 23.287592 | 30.236286 | 32.896690 |
| Ca | 23.134377 | 34.582302 | 30.773876 |
| Ca | 25.113075 | 30.870075 | 27.712576 |
| Ca | 27.887909 | 32.798145 | 31.184746 |
| Ca | 29.045582 | 27.795189 | 29.671133 |
| Ca | 30.142763 | 32.512711 | 27.061604 |
| Ca | 30.305891 | 27.615749 | 24.851898 |
| Ca | 33.553146 | 30.293489 | 28.059473 |
| Ca | 34.682461 | 24.992201 | 27.016600 |
| Ca | 35.207699 | 28.948406 | 23.953012 |
| S  | 20.904821 | 31.459717 | 35.249435 |
| S  | 21.104134 | 35.833984 | 33.525406 |
| S  | 22.182150 | 31.540409 | 29.624634 |
| S  | 24.905699 | 33.061737 | 33.307114 |
| S  | 25.941343 | 29.560474 | 30.314003 |
| S  | 25.981430 | 34.145008 | 28.627815 |
| S  | 27.993267 | 29.583370 | 26.514675 |
| S  | 30.599066 | 31.211384 | 30.128937 |
| S  | 31.993206 | 27.148251 | 28.180235 |
| S  | 32.355171 | 30.516056 | 24.929773 |
| S  | 33.341393 | 25.639153 | 23.904850 |
|   |       |       |       |
|---|-------|-------|-------|
| S | 36.452660 | 28.320816 | 26.994137 |

24

generated by VMD

| Ca |       |       |       |
|----|-------|-------|-------|
| 18.452492 | 33.140156 | 33.652206 |
| 23.017258 | 34.464584 | 36.054581 |
| 23.153978 | 30.381649 | 32.571098 |
| 23.027212 | 34.467621 | 30.814152 |
| 25.170818 | 30.882732 | 27.722654 |
| 27.714245 | 32.834042 | 30.975508 |
| 29.055126 | 27.912888 | 29.836098 |
| 30.294991 | 32.335552 | 27.287653 |
| 30.452377 | 27.624157 | 24.870571 |
| 33.628933 | 30.228416 | 27.871611 |
| 34.683624 | 24.883844 | 26.968241 |
| 35.335991 | 28.877312 | 23.909870 |
| S | 21.074715 | 31.526623 | 35.236469 |
| 20.871006 | 35.842033 | 33.851597 |
| 21.994207 | 31.607315 | 29.424023 |
| 24.886637 | 33.021202 | 33.299751 |
| 25.960211 | 29.650169 | 30.414669 |
| S | 25.810936 | 34.407127 | 28.581722 |
| 28.202919 | 29.343504 | 26.666559 |
| S | 30.704296 | 31.283903 | 30.027637 |
| 32.022186 | 26.996887 | 28.113478 |
| S | 32.484753 | 30.665245 | 24.885756 |
| 33.320267 | 25.736557 | 23.983509 |
| S | 36.400848 | 28.186535 | 26.920614 |

24

generated by VMD

| Ca |       |       |       |
|----|-------|-------|-------|
| 18.128639 | 33.454224 | 33.397202 |
| 22.831942 | 34.072701 | 36.042530 |
| 23.303699 | 30.366903 | 32.533409 |
| 22.861603 | 34.467995 | 31.201429 |
| 24.992741 | 30.943546 | 27.705845 |
| 27.778170 | 32.789246 | 31.527481 |
| 29.158981 | 28.219469 | 30.014900 |
| 30.434605 | 32.262123 | 26.765804 |
| 30.405041 | 27.492115 | 24.917597 |
| 33.874218 | 30.140299 | 27.599495 |
| 34.835434 | 25.075151 | 27.424652 |
| 35.275501 | 28.595318 | 23.145142 |
| S | 20.714029 | 31.461021 | 34.862923 |
| 20.582195 | 35.709949 | 33.704376 |
| S | 21.935358 | 31.818710 | 29.526722 |
| S | 24.846289 | 33.090408 | 33.491447 |
| S | 26.115141 | 29.753670 | 30.787405 |
Ca       35.181583       28.827526       23.321371
S        20.649319       31.485802       35.097015
S        20.781057       35.706028       33.580956
S        21.989347       31.590157       29.619358
S        24.925505       33.205170       33.367706
S        26.214420       29.752190       30.830954
S        25.903877       34.168144       28.590893
S        28.281141       29.445282       26.970974
S        30.839836       31.433809       30.231134
S        31.876472       27.009985       28.078018
S        32.504887       30.439981       24.879032
S        33.194363       25.765697       23.582844
S        36.532406       28.180292       26.568979

24
generated by VMD
Ca       18.325130       33.487129       33.496964
Ca       23.057327       34.194187       36.011806
Ca       23.325850       30.075832       32.849873
Ca       22.892694       34.713692       31.049309
Ca       24.767920       30.767881       27.652151
Ca       27.731640       32.588791       31.125488
Ca       29.204321       28.039936       29.971653
Ca       30.327419       32.397175       26.777639
Ca       30.436239       27.523254       24.662083
Ca       33.676765       30.235912       28.111702
Ca       34.620033       25.262173       27.133350
Ca       35.654827       28.760994       23.756521
S        20.846889       31.482759       35.059692
S        20.996216       36.101757       33.748985
S        21.890724       31.673832       29.753199
S        24.990549       33.000801       33.580925
S        25.999071       29.524208       30.475065
S        25.708269       34.225140       28.718740
S        28.203257       29.540918       26.421240
S        30.606745       31.318933       29.922981
S        31.779829       27.106712       27.987402
S        32.620365       30.433346       24.782673
S        33.582432       25.515697       23.914776
S        36.475510       28.329014       26.975882

24
generated by VMD
Ca       18.503227       33.325184       33.584183
Ca       23.165504       34.302414       36.014877
Ca       23.407799       30.400791       32.777184
Ca       22.838964       34.450508       31.192635
Ca       24.901646       30.704945       27.599379
Ca   27.627102  33.274593  30.925066
Ca   29.058203  28.277725  29.580355
Ca   30.44185  32.257755  27.072901
Ca   30.60397  27.662367  24.437191
Ca   33.675442  30.178604  28.271526
Ca   34.519062  24.808472  27.079262
Ca   35.621140  28.691628  23.87231
S    20.772184  31.278164  35.389305
S    20.653097  35.767128  33.834717
S    21.924103  31.584435  29.622530
S    24.890366  33.294106  33.440006
S    26.246294  29.817074  30.681309
S    25.421982  34.161556  28.600428
S    28.159073  29.540257  26.477291
S    30.781668  31.427841  29.894720
S    31.946404  26.950771  27.848394
S    32.684898  30.519009  24.846390
S    33.540188  25.713528  23.561768
S    36.333519  27.911219  27.336390

24
generated by VMD
Ca   18.553411  33.220665  33.775742
Ca   23.072771  34.420082  36.028385
Ca   23.442469  30.391096  32.792027
Ca   22.941628  34.471745  30.882217
Ca   24.846046  30.750645  27.507162
Ca   27.802258  32.929688  31.230007
Ca   28.877254  27.939831  29.620974
Ca   30.265648  32.196831  27.115932
Ca   30.478926  27.756519  24.365520
Ca   33.530014  29.984285  28.083387
Ca   34.668938  25.028852  27.406673
Ca   35.517986  28.989719  23.877720
S    21.121677  31.443640  35.461086
S    20.937830  35.748962  33.455173
S    21.839767  31.664616  29.535986
S    24.915182  33.161079  33.450584
S    26.188986  29.796314  30.543341
S    25.725382  34.294594  28.509048
S    28.020214  29.280092  26.505051
S    30.644588  31.164677  30.101492
S    31.492359  27.035067  27.860285
S    32.611816  30.743023  24.900457
S    33.756092  25.878819  23.892767
S    36.468807  28.009239  27.039032
|   | 0.260501  | 0.326001  | 0.270501  |
|---|-----------|-----------|-----------|
| Ca | 18.494431 | 33.091816 | 33.631126 |
| Ca | 23.158674 | 34.350201 | 36.223465 |
| Ca | 23.365429 | 30.198540 | 32.755371 |
| Ca | 22.891556 | 34.720009 | 30.962427 |
| Ca | 24.887436 | 31.054039 | 27.473278 |
| Ca | 27.650692 | 32.765011 | 31.158928 |
| Ca | 28.988794 | 28.121655 | 29.785118 |
| Ca | 30.527815 | 32.347931 | 26.934996 |
| Ca | 30.461632 | 27.703133 | 24.514580 |
| Ca | 33.598125 | 30.241043 | 28.105604 |
| Ca | 34.527527 | 24.921732 | 27.391079 |
| Ca | 35.422752 | 28.818939 | 23.745003 |
| S  | 21.066055 | 31.413921 | 35.341072 |
| S  | 20.784243 | 35.758690 | 33.576271 |
| S  | 21.821911 | 31.469019 | 29.608242 |
| S  | 24.975004 | 33.140282 | 33.482704 |
| S  | 25.935410 | 29.843655 | 30.421097 |
| S  | 25.720039 | 34.336044 | 28.607353 |
| S  | 28.206047 | 29.487991 | 26.631796 |
| S  | 30.806938 | 31.289761 | 30.023520 |
| S  | 31.723072 | 27.040882 | 27.873087 |
| S  | 32.540661 | 30.612953 | 24.577385 |
| S  | 33.808151 | 25.548162 | 23.896252 |
| S  | 36.357651 | 28.024677 | 27.220322 |

---

|   | 0.173001  | 0.236001  | 0.176001  |
|---|-----------|-----------|-----------|
| Ca | 18.272413 | 33.043289 | 33.949837 |
| Ca | 22.918072 | 34.728157 | 36.063412 |
| Ca | 23.279049 | 30.164112 | 32.537552 |
| Ca | 22.945961 | 34.579586 | 30.927345 |
| Ca | 24.952177 | 31.189398 | 27.678173 |
| Ca | 27.702898 | 32.648659 | 31.315306 |
| Ca | 29.125408 | 28.180840 | 29.744970 |
| Ca | 30.508514 | 32.163673 | 26.912148 |
| Ca | 30.419243 | 27.391733 | 24.717054 |
| Ca | 33.684711 | 30.025177 | 27.860090 |
| Ca | 34.634026 | 25.115374 | 27.400585 |
| Ca | 35.653381 | 28.919903 | 23.642017 |
| S  | 21.075312 | 31.484665 | 35.367565 |
| S  | 20.577368 | 35.665585 | 33.529533 |
| S  | 21.823162 | 31.922815 | 29.477831 |
| S  | 24.761169 | 32.965157 | 33.472313 |
| S  | 25.942562 | 29.773296 | 30.433205 |
| S  | 25.932816 | 34.357468 | 28.726114 |
| S  | 28.177204 | 29.355408 | 26.714293 |
|   |        |        |        |
|---|--------|--------|--------|
| S | 30.911915 | 31.389389 | 30.060139 |
| S | 31.798073 | 26.922421 | 27.869701 |
| S | 32.541664 | 30.380180 | 24.808140 |
| S | 33.539406 | 25.828476 | 23.886986 |
| S | 36.543568 | 28.105309 | 26.845766 |

24

generated by VMD

| Ca | 18.387257 | 33.362068 | 33.958717 |
| Ca | 23.170538 | 34.349487 | 35.983002 |
| Ca | 23.028231 | 30.168011 | 32.748814 |
| Ca | 23.020042 | 34.976837 | 30.736607 |
| Ca | 24.870920 | 30.704382 | 27.428608 |
| Ca | 27.449196 | 32.602562 | 31.068747 |
| Ca | 29.072353 | 28.021561 | 29.895771 |
| Ca | 30.445902 | 32.450397 | 27.230789 |
| Ca | 30.456469 | 27.585873 | 24.974091 |
| Ca | 33.739971 | 30.180843 | 28.001251 |
| Ca | 34.683037 | 24.841118 | 26.933678 |
| Ca | 35.589287 | 28.916332 | 23.722088 |
| Ca | 36.543568 | 28.105309 | 26.845766 |

S

| 21.085598 | 31.419315 | 35.575523 |
| 20.782591 | 35.699852 | 33.475670 |
| 21.915859 | 31.621002 | 29.591339 |
| 24.932974 | 33.349197 | 33.279667 |
| 25.692345 | 29.492180 | 30.397486 |
| 25.773420 | 34.111633 | 28.413000 |
| 28.216339 | 29.661293 | 26.809772 |
| 30.902563 | 31.212894 | 30.043428 |
| 31.927826 | 26.976421 | 28.358875 |
| 32.629299 | 30.551498 | 24.745621 |
| 33.470398 | 25.887886 | 23.665169 |
| 36.477608 | 28.157372 | 26.902378 |

24

generated by VMD

| Ca | 18.092075 | 33.378933 | 33.815140 |
| Ca | 22.778751 | 34.625423 | 35.947067 |
| Ca | 23.229336 | 30.188438 | 33.034927 |
| Ca | 22.842768 | 34.594448 | 30.540686 |
| Ca | 25.091829 | 30.784874 | 27.795700 |
| Ca | 27.895983 | 32.845928 | 31.736799 |
| Ca | 29.123726 | 27.984329 | 29.760944 |
| Ca | 30.595818 | 32.302246 | 26.857019 |
| Ca | 30.470486 | 27.730907 | 24.447750 |
| Ca | 33.620674 | 30.067200 | 28.025654 |
| Ca | 34.587173 | 24.985989 | 26.902399 |
| Ca | 35.389362 | 28.778555 | 23.685696 |
| S | 20.769920 | 31.555397 | 35.422333 |
S   20.617249  35.744892  33.314503
S   22.002785  31.164650  29.786701
S   24.811163  33.431515  33.407604
S   26.217955  29.637512  31.039095
S   26.026480  34.218300  28.626661
S   28.327396  29.529306  26.564785
S   30.748341  31.228386  30.182285
S   31.777321  27.054621  27.697433
S   32.792988  30.537348  24.747238
S   33.549889  25.990755  23.407063
S   36.360634  27.940096  27.194616

24 generated by VMD
Ca  18.219645  33.345818  33.575588
Ca  23.058826  34.265228  36.011978
Ca  23.176926  30.248598  32.783882
Ca  23.142735  34.841713  30.481918
Ca  25.086182  30.755013  27.701591
Ca  27.685831  32.679489  31.392109
Ca  29.126558  28.086460  29.852751
Ca  30.520458  32.372131  27.155020
Ca  30.486118  27.497265  24.868299
Ca  33.622631  30.287811  27.984268
Ca  34.574505  24.919827  26.971565
Ca  35.101768  29.065853  23.435951
S   20.754822  31.478693  35.208107
S   20.869375  35.788738  33.504341
S   22.007616  31.262230  29.792183
S   24.873262  33.410740  33.192085
S   26.147339  29.532200  30.777836
S   26.011364  34.083885  28.418217
S   28.349369  29.573517  26.770424
S   30.902273  31.225300  30.373451
S   31.940777  26.981062  28.200788
S   32.354778  30.560799  24.944262
S   33.349594  25.960461  23.708241
S   36.357246  28.077230  26.835146

24 generated by VMD
Ca  17.974388  33.221371  33.445923
Ca  22.816277  34.586155  35.816734
Ca  23.331282  29.926956  33.074368
Ca  22.990408  34.812813  30.456583
Ca  25.083141  30.655506  27.882126
Ca  27.949783  32.656334  31.458776
Ca  29.307859  28.116783  30.126844
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 30.526661 | 32.495136 | 27.312962 |
| Ca      | 30.525064 | 27.867954 | 25.025    |
| Ca      | 33.675522 | 30.107067 | 27.900169 |
| Ca      | 34.474449 | 24.905783 | 26.779079 |
| Ca      | 35.043755 | 28.589869 | 23.237217 |
| S       | 20.632341 | 31.532459 | 35.054115 |
| S       | 20.586149 | 35.794189 | 33.196411 |
| S       | 22.059769 | 31.312286 | 29.693434 |
| S       | 24.905979 | 33.265678 | 33.254845 |
| S       | 26.249134 | 29.498690 | 30.977234 |
| S       | 26.076788 | 34.048855 | 28.743477 |
| S       | 28.296593 | 29.821796 | 26.976721 |
| S       | 31.006207 | 31.284458 | 30.299663 |
| S       | 32.218464 | 27.260101 | 28.294971 |
| S       | 32.728920 | 30.718143 | 24.846592 |
| S       | 32.954617 | 25.886799 | 23.486862 |
| S       | 36.312641 | 27.934837 | 26.599171 |

24 generated by VMD

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 31.819547 | 33.014656 | 33.706322 |
| Ca      | 22.874269 | 34.397247 | 35.693077 |
| Ca      | 23.388250 | 30.277571 | 33.037251 |
| Ca      | 22.796829 | 34.758804 | 30.439606 |
| Ca      | 24.780277 | 30.887981 | 27.906376 |
| Ca      | 27.831678 | 32.698742 | 31.347265 |
| Ca      | 29.114323 | 28.132717 | 29.717896 |
| Ca      | 30.695053 | 32.352837 | 27.305937 |
| Ca      | 30.319683 | 27.648800 | 24.918385 |
| Ca      | 34.024216 | 29.810524 | 27.984114 |
| Ca      | 34.540245 | 25.065983 | 26.875454 |
| Ca      | 35.422234 | 28.679729 | 23.495934 |
| S       | 20.970669 | 31.410757 | 35.523956 |
| S       | 20.760933 | 35.629791 | 33.094154 |
| S       | 21.827473 | 31.269714 | 29.850630 |
| S       | 24.941078 | 33.662373 | 33.005116 |
| S       | 26.066505 | 29.618023 | 30.760818 |
| S       | 25.782055 | 34.324127 | 28.860247 |
| S       | 28.240753 | 29.951000 | 26.737537 |
| S       | 30.686010 | 31.224117 | 30.288557 |
| S       | 31.883495 | 27.033504 | 28.113647 |
| S       | 32.771164 | 30.509802 | 24.951559 |
| S       | 33.214504 | 26.085430 | 23.607512 |
| S       | 36.588795 | 27.855778 | 26.718693 |

24 generated by VMD

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 18.199547 | 33.014656 | 33.706322 |
| Ca      | 22.874269 | 34.397247 | 35.693077 |
| Ca      | 23.388250 | 30.277571 | 33.037251 |
| Ca      | 22.796829 | 34.758804 | 30.439606 |
| Ca      | 24.780277 | 30.887981 | 27.906376 |
| Ca      | 27.831678 | 32.698742 | 31.347265 |
| Ca      | 29.114323 | 28.132717 | 29.717896 |
| Ca      | 30.695053 | 32.352837 | 27.305937 |
| Ca      | 30.319683 | 27.648800 | 24.918385 |
| Ca      | 34.024216 | 29.810524 | 27.984114 |
| Ca      | 34.540245 | 25.065983 | 26.875454 |
| Ca      | 35.422234 | 28.679729 | 23.495934 |
| S       | 20.970669 | 31.410757 | 35.523956 |
| S       | 20.760933 | 35.629791 | 33.094154 |
| S       | 21.827473 | 31.269714 | 29.850630 |
| S       | 24.941078 | 33.662373 | 33.005116 |
| S       | 26.066505 | 29.618023 | 30.760818 |
| S       | 25.782055 | 34.324127 | 28.860247 |
| S       | 28.240753 | 29.951000 | 26.737537 |
| S       | 30.686010 | 31.224117 | 30.288557 |
| S       | 31.883495 | 27.033504 | 28.113647 |
| S       | 32.771164 | 30.509802 | 24.951559 |
| S       | 33.214504 | 26.085430 | 23.607512 |
| S       | 36.588795 | 27.855778 | 26.718693 |

24 generated by VMD

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 18.148018 | 33.327808 | 33.628601 |
|   | Ca   |       |       |   |
|---|------|-------|-------|---|
|   | 22.963053 | 34.617153 | 35.713509 |   |
| Ca | 23.070692 | 30.209267 | 32.932762 |   |
| Ca | 23.021173 | 34.593929 | 30.601009 |   |
| Ca | 24.833303 | 30.633532 | 27.749195 |   |
| Ca | 27.972307 | 32.468834 | 31.190954 |   |
| Ca | 29.246426 | 27.962416 | 30.018007 |   |
| Ca | 30.531599 | 32.595150 | 27.517296 |   |
| Ca | 33.711517 | 30.091660 | 28.026079 |   |
| Ca | 34.668659 | 24.885532 | 26.832167 |   |
| Ca | 35.192120 | 28.708569 | 23.481998 |   |
| S  | 20.904011 | 31.656864 | 35.627270 |   |
| S  | 20.895678 | 35.797550 | 33.131256 |   |
| S  | 21.753292 | 31.358685 | 29.704233 |   |
| S  | 24.798580 | 33.275002 | 33.089836 |   |
| S  | 26.166304 | 29.266140 | 30.580299 |   |
| S  | 25.805199 | 34.088882 | 28.741589 |   |
| S  | 28.341553 | 29.763800 | 26.940020 |   |
| S  | 30.990686 | 31.334175 | 30.188545 |   |
| S  | 31.876648 | 26.899723 | 27.874393 |   |
| S  | 32.643127 | 30.863739 | 24.930992 |   |
| S  | 33.143250 | 25.985378 | 23.676258 |   |
| S  | 36.345623 | 28.061169 | 26.714598 |   |
|   | 18.015652 | 33.172062 | 33.216694 |   |
| Ca | 22.728424 | 34.318844 | 35.752983 |   |
| Ca | 23.514877 | 30.256557 | 33.038460 |   |
| Ca | 23.008863 | 34.820351 | 30.761011 |   |
| Ca | 24.790749 | 30.809118 | 27.928999 |   |
| Ca | 28.137379 | 32.801426 | 31.421602 |   |
| Ca | 29.241413 | 28.047646 | 29.875874 |   |
| Ca | 30.694206 | 32.406693 | 27.212070 |   |
| Ca | 30.397186 | 27.500172 | 24.917740 |   |
| Ca | 33.603088 | 30.145496 | 27.960609 |   |
| Ca | 34.586430 | 25.170198 | 26.851873 |   |
| Ca | 35.222740 | 28.650120 | 23.434553 |   |
| S  | 20.623329 | 31.347649 | 34.970959 |   |
| S  | 20.557247 | 35.729576 | 33.401100 |   |
| S  | 21.887459 | 31.438971 | 29.856945 |   |
| S  | 25.056311 | 33.572479 | 33.208633 |   |
| S  | 26.251881 | 29.610291 | 31.093786 |   |
| S  | 26.077612 | 34.062859 | 28.861885 |   |
| S  | 28.351816 | 29.657116 | 26.796082 |   |
| S  | 31.060169 | 31.221901 | 30.130470 |   |
| S  | 31.861832 | 26.991423 | 28.141539 |   |
|    |     |     |     |
|----|----|----|----|
| S  | 32.535450 | 30.531841 | 24.736359 |
| S  | 33.095722 | 25.858330 | 23.621416 |
| S  | 36.420235 | 28.178932 | 26.748459 |
| Ca | 18.330147 | 33.167320 | 33.625374 |
| Ca | 22.884346 | 34.342625 | 36.006413 |
| Ca | 23.318846 | 30.359146 | 32.859871 |
| Ca | 23.010590 | 34.628639 | 30.768818 |
| Ca | 24.823263 | 30.679445 | 27.478836 |
| Ca | 27.820522 | 33.056164 | 31.164000 |
| Ca | 29.490261 | 28.287716 | 29.817797 |
| Ca | 30.599522 | 32.421291 | 27.216579 |
| Ca | 30.239231 | 27.694405 | 24.887449 |
| Ca | 33.738190 | 30.006338 | 28.082499 |
| Ca | 34.477303 | 24.958055 | 26.876755 |
| Ca | 35.393368 | 28.692833 | 23.793631 |
| S  | 20.808125 | 31.323486 | 35.254265 |
| S  | 20.843153 | 35.504379 | 33.462051 |
| S  | 21.935001 | 31.142036 | 29.820175 |
| S  | 24.930092 | 33.571800 | 33.237793 |
| S  | 26.203999 | 29.893959 | 30.734827 |
| S  | 25.743614 | 34.074883 | 28.498127 |
| S  | 28.268015 | 29.861515 | 26.615145 |
| S  | 31.021515 | 31.372620 | 30.152349 |
| S  | 31.857914 | 26.975483 | 27.958101 |
| S  | 32.526604 | 30.532654 | 24.909050 |
| S  | 33.169178 | 25.991455 | 23.494404 |
| S  | 36.287197 | 27.761806 | 27.225811 |

24 generated by VMD

|    |     |     |     |
|----|----|----|----|
| Ca | 18.166792 | 33.192219 | 33.569103 |
| Ca | 23.005049 | 34.765957 | 35.732487 |
| Ca | 23.254620 | 29.996513 | 33.045013 |
| Ca | 23.190004 | 34.699802 | 30.518541 |
| Ca | 24.741558 | 30.583870 | 27.732252 |
| Ca | 27.690668 | 32.649620 | 31.159622 |
| Ca | 29.143715 | 28.083145 | 29.934973 |
| Ca | 30.588366 | 32.383507 | 27.506809 |
| Ca | 30.429562 | 28.016745 | 24.929222 |
| Ca | 33.854660 | 30.189499 | 27.826889 |
| Ca | 34.342407 | 24.784182 | 26.988811 |
| Ca | 35.470085 | 28.892555 | 23.569302 |
| S  | 20.880611 | 31.416176 | 35.482437 |
| S  | 20.684299 | 35.794975 | 33.074127 |
| S  | 22.078026 | 31.302603 | 30.037884 |
|   | 25.052738 | 33.309376 | 33.457085 |
|---|-----------|-----------|-----------|
| S | 26.014629 | 29.459248 | 30.723228 |
| S | 25.723989 | 34.086727 | 28.390829 |
| S | 28.186352 | 29.750568 | 26.842537 |
| S | 31.011007 | 31.235714 | 30.129505 |
| S | 31.744398 | 27.108265 | 27.873959 |
| S | 32.764359 | 30.726009 | 24.929302 |
| S | 33.358231 | 26.092731 | 23.697655 |
| S | 36.343929 | 27.780075 | 26.788458 |

24

generated by VMD

|   | 18.018167 | 33.296116 | 33.683846 |
| Ca| 22.903601 | 34.569778 | 35.614677 |
| Ca| 23.494411 | 30.162598 | 33.064735 |
| Ca| 22.783384 | 34.695885 | 30.962847 |
| Ca| 24.893993 | 30.738037 | 27.77597 |
| Ca| 27.800037 | 32.688404 | 31.090269 |
| Ca| 29.224993 | 28.177549 | 29.965864 |
| Ca| 30.701185 | 32.355019 | 27.404108 |
| Ca| 30.451553 | 27.517864 | 24.768847 |
| Ca| 33.933708 | 30.063652 | 27.938467 |
| Ca| 34.392090 | 24.975380 | 26.887014 |
| Ca| 35.274307 | 28.911644 | 23.387754 |
| S | 20.846806 | 31.476509 | 35.032715 |
| S | 20.328533 | 35.807705 | 33.147625 |
| S | 21.958122 | 31.168533 | 29.927448 |
| S | 25.071306 | 33.535099 | 33.354435 |
| S | 26.110867 | 29.669149 | 30.575169 |
| S | 25.787876 | 34.151154 | 28.819395 |
| S | 28.385546 | 29.911261 | 26.815935 |
| S | 30.995066 | 31.160027 | 30.347546 |
| S | 32.011036 | 26.891306 | 28.116928 |
| S | 32.606140 | 30.532784 | 25.028486 |
| S | 33.179955 | 25.951813 | 23.497223 |
| S | 36.567356 | 27.892797 | 26.731121 |

24

generated by VMD

|   | 18.318808 | 32.910629 | 33.641121 |
| Ca| 23.095112 | 34.565243 | 35.633804 |
| Ca| 23.172920 | 30.235428 | 32.850277 |
| Ca| 22.854076 | 34.773590 | 30.536402 |
| Ca| 24.791592 | 30.848366 | 27.696285 |
| Ca| 27.754456 | 32.898453 | 31.205914 |
| Ca| 29.005581 | 27.914341 | 29.827168 |
| Ca| 30.655510 | 32.279045 | 27.485977 |
| Ca| 30.412365 | 28.076290 | 24.950327 |
|   | Ca       | 34.214695 | 29.944571 | 27.945707 |
|---|----------|-----------|-----------|-----------|
|   | Ca       | 34.219452 | 29.944571 | 27.945707 |
|   | Ca       | 35.155289 | 29.944571 | 27.945707 |
| S | 21.068876 | 31.439774 | 35.405037 |
| S | 20.593769 | 31.439774 | 35.405037 |
| S | 21.766148 | 31.439774 | 35.405037 |
| S | 24.909298 | 31.439774 | 35.405037 |
| S | 26.310356 | 31.439774 | 35.405037 |
| S | 25.674950 | 31.439774 | 35.405037 |
| S | 28.223206 | 31.439774 | 35.405037 |
| S | 30.916452 | 31.439774 | 35.405037 |
| S | 31.959490 | 31.439774 | 35.405037 |
| S | 32.789330 | 31.439774 | 35.405037 |
| S | 33.117100 | 31.439774 | 35.405037 |
| S | 36.741207 | 31.439774 | 35.405037 |

24

generated by VMD

|   | Ca       | 18.347649 | 32.859642 | 33.772961 |
|---|----------|-----------|-----------|-----------|
|   | Ca       | 22.861704 | 34.958569 | 35.724503 |
|   | Ca       | 23.471333 | 30.339630 | 32.930603 |
|   | Ca       | 22.917595 | 34.639183 | 30.490978 |
|   | Ca       | 24.968122 | 30.554838 | 27.659098 |
|   | Ca       | 27.699823 | 32.876019 | 31.178032 |
|   | Ca       | 29.096418 | 27.719110 | 29.774923 |
|   | Ca       | 30.672203 | 32.495316 | 27.844053 |
|   | Ca       | 30.346760 | 27.884443 | 24.846748 |
|   | Ca       | 33.857712 | 29.956570 | 27.890976 |
|   | Ca       | 34.332050 | 24.917067 | 26.690510 |
|   | Ca       | 35.265381 | 29.082561 | 23.606865 |
| S | 21.145397 | 31.674530 | 35.444695 |
| S | 20.461994 | 35.782154 | 33.062077 |
| S | 21.804695 | 31.311520 | 29.693102 |
| S | 25.060711 | 33.494194 | 33.215546 |
| S | 26.047016 | 29.473614 | 30.787971 |
| S | 25.792179 | 33.997238 | 28.552914 |
| S | 28.332333 | 29.765810 | 26.949944 |
| S | 30.859241 | 31.001801 | 30.489277 |
| S | 31.941557 | 26.903816 | 28.015974 |
| S | 32.698532 | 30.707546 | 25.006008 |
| S | 33.172920 | 26.038652 | 23.550100 |
| S | 36.566650 | 27.866243 | 26.762142 |

24

generated by VMD

|   | Ca       | 18.282911 | 32.688374 | 33.753334 |
|---|----------|-----------|-----------|-----------|
|   | Ca       | 22.835949 | 34.664043 | 35.714691 |
|   | Ca       | 23.427738 | 30.421104 | 32.936050 |
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 22.558641     | 34.671421     | 30.444050     |
| Ca      | 24.891682     | 30.805519     | 27.804033     |
| Ca      | 27.786449     | 33.037853     | 31.229464     |
| Ca      | 29.082438     | 28.190445     | 29.804033     |
| Ca      | 30.77493      | 32.308487     | 27.659781     |
| Ca      | 30.387253     | 27.795666     | 24.776688     |
| Ca      | 34.000187     | 29.841869     | 28.033201     |
| Ca      | 34.392677     | 24.870491     | 26.822309     |
| Ca      | 35.263313     | 28.708708     | 23.403921     |
| S       | 21.205589     | 31.410845     | 35.303936     |
| S       | 20.394600     | 35.644520     | 33.251648     |
| S       | 21.731762     | 31.279846     | 29.876175     |
| S       | 24.847733     | 33.678391     | 33.197365     |
| S       | 26.202566     | 29.765793     | 30.778877     |
| S       | 25.834404     | 34.289875     | 28.558758     |
| S       | 28.293772     | 29.990362     | 26.753128     |
| S       | 31.084229     | 31.052822     | 30.556633     |
| S       | 31.832211     | 26.985031     | 28.000502     |
| S       | 32.739086     | 30.504962     | 25.148840     |
| S       | 33.264481     | 25.938896     | 23.474743     |
| S       | 36.602837     | 27.754627     | 26.657841     |

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generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.290239     | 32.844284     | 33.706459     |
| Ca      | 22.782185     | 34.622524     | 35.827286     |
| Ca      | 23.409407     | 30.365356     | 33.017151     |
| Ca      | 22.610146     | 34.738777     | 30.611971     |
| Ca      | 24.965435     | 30.657282     | 27.819965     |
| Ca      | 27.516842     | 33.000328     | 31.257366     |
| Ca      | 29.259529     | 28.217022     | 29.910625     |
| Ca      | 30.673258     | 32.500576     | 27.218372     |
| Ca      | 30.423927     | 27.971462     | 24.668243     |
| Ca      | 33.878670     | 29.887184     | 28.096849     |
| Ca      | 34.365768     | 24.725513     | 26.745527     |
| Ca      | 35.531342     | 28.699064     | 23.610872     |
| S       | 20.981550     | 31.501289     | 35.508186     |
| S       | 20.380234     | 35.628609     | 33.338707     |
| S       | 21.974251     | 31.368465     | 29.769106     |
| S       | 24.854172     | 33.661926     | 33.268333     |
| S       | 26.277496     | 29.620125     | 30.835873     |
| S       | 25.545773     | 34.195290     | 28.532856     |
| S       | 28.391981     | 29.879047     | 26.750006     |
| S       | 31.172646     | 31.232544     | 30.136047     |
| S       | 31.801598     | 26.833271     | 27.848118     |
| S       | 32.856659     | 30.616501     | 25.122208     |
| S       | 33.161057     | 26.001335     | 23.512335     |
|   | 36.615887 | 27.532280 | 26.827610 |
|---|-----------|-----------|-----------|
| 24 | generated by VMD |
| Ca | 18.348524 | 32.828682 | 33.487564 |
| Ca | 22.919836 | 34.969147 | 35.663849 |
| Ca | 23.467438 | 30.328579 | 33.094204 |
| Ca | 22.882593 | 34.660439 | 30.250362 |
| Ca | 24.841532 | 30.598236 | 27.883249 |
| Ca | 27.870813 | 32.805267 | 31.341959 |
| Ca | 28.995872 | 27.802380 | 30.028204 |
| Ca | 30.684832 | 32.349148 | 27.690485 |
| Ca | 30.289669 | 28.006193 | 24.788673 |
| Ca | 33.619553 | 29.870392 | 28.045620 |
| Ca | 34.383217 | 24.885290 | 26.460609 |
| Ca | 35.413109 | 29.102623 | 23.682423 |
| S  | 21.167240 | 31.770195 | 35.508591 |
| S  | 20.749676 | 35.51605  | 32.903114 |
| S  | 21.912537 | 31.120296 | 29.704058 |
| S  | 24.980835 | 33.693012 | 33.127384 |
| S  | 26.383873 | 29.691437 | 31.146914 |
| S  | 25.729866 | 33.806778 | 28.569412 |
| S  | 28.257967 | 29.633369 | 26.881847 |
| S  | 30.961258 | 30.912123 | 30.490974 |
| S  | 31.632124 | 26.924515 | 27.771158 |
| S  | 32.713337 | 30.780220 | 25.150103 |
| S  | 33.206638 | 26.292980 | 23.415646 |
| S  | 36.307766 | 27.917168 | 26.853605 |
| 24 | generated by VMD |
| Ca | 18.089975 | 33.165016 | 33.534313 |
| Ca | 22.773548 | 34.746342 | 35.897392 |
| Ca | 23.402176 | 30.292471 | 33.072441 |
| Ca | 22.813072 | 34.616920 | 30.426497 |
| Ca | 25.037008 | 30.642138 | 27.760466 |
| Ca | 27.691917 | 32.858734 | 31.480181 |
| Ca | 29.265339 | 27.929907 | 30.123928 |
| Ca | 30.683254 | 32.344635 | 27.554287 |
| Ca | 30.236010 | 28.032570 | 24.623070 |
| Ca | 33.813946 | 30.015705 | 27.858057 |
| Ca | 34.457664 | 24.796501 | 26.532938 |
| Ca | 35.481789 | 28.848532 | 23.584377 |
| S  | 20.863798 | 31.608814 | 35.461994 |
| S  | 20.538704 | 35.643185 | 33.109913 |
| S  | 21.930647 | 30.984310 | 29.787146 |
| S  | 24.787636 | 33.775040 | 33.186958 |
| S  | 26.381510 | 29.539906 | 31.134890 |
|  | X     | Y     | Z     |
|---|-------|-------|-------|
| S | 25.793150 | 34.142578 | 28.511101 |
| S | 28.346092 | 29.773281 | 26.865959 |
| S | 31.128450 | 31.186586 | 30.436737 |
| S | 31.728256 | 27.042919 | 27.783957 |
| S | 32.722015 | 30.593758 | 25.018923 |
| S | 33.176563 | 26.087532 | 23.457401 |
| S | 36.577568 | 27.632748 | 26.736670 |

24 generated by VMD

| Ca | 18.549618 | 33.198486 | 33.863213 |
|----|-----------|-----------|-----------|
| Ca | 22.417824 | 34.925858 | 35.614265 |
| Ca | 23.268784 | 30.299168 | 32.994762 |
| Ca | 22.915451 | 34.880577 | 30.349785 |
| Ca | 24.848606 | 30.316593 | 27.954399 |
| Ca | 27.623283 | 32.785374 | 31.523726 |
| Ca | 29.213116 | 27.742535 | 29.930424 |
| Ca | 30.640272 | 32.295567 | 27.651976 |
| Ca | 30.486591 | 27.696501 | 24.622803 |
| Ca | 33.817917 | 29.764301 | 28.295853 |
| Ca | 34.564404 | 24.918091 | 26.369818 |
| Ca | 35.299332 | 29.296444 | 23.636175 |
| S  | 21.050407 | 31.679600 | 35.441414 |
| S  | 20.339451 | 35.999638 | 32.927170 |
| S  | 21.984585 | 31.243341 | 29.921661 |
| S  | 24.789967 | 33.702499 | 33.243675 |
| S  | 26.184990 | 29.450947 | 31.106943 |
| S  | 25.915529 | 34.053223 | 28.597719 |
| S  | 28.265247 | 29.599724 | 26.821501 |
| S  | 31.092693 | 30.851084 | 30.313345 |
| S  | 32.098614 | 26.694527 | 27.832264 |
| S  | 32.521622 | 30.692017 | 24.980095 |
| S  | 33.373466 | 26.262249 | 23.323458 |
| S  | 36.458252 | 27.951694 | 26.623590 |

24 generated by VMD

| Ca | 18.215916 | 33.316662 | 33.746124 |
|----|-----------|-----------|-----------|
| Ca | 22.822731 | 34.977211 | 35.708755 |
| Ca | 23.551987 | 30.418701 | 32.947765 |
| Ca | 22.623947 | 34.779903 | 30.513435 |
| Ca | 24.648493 | 30.309582 | 27.944616 |
| Ca | 27.803041 | 32.595928 | 31.435184 |
| Ca | 29.391134 | 27.701107 | 29.909538 |
| Ca | 30.474733 | 32.368973 | 27.622423 |
| Ca | 30.615459 | 27.920958 | 24.695814 |
| Ca | 33.751156 | 29.776371 | 27.969488 |
| Ca | 34.609932 | 24.739479 | 26.511021 |
|      |        |        |        |
|------|--------|--------|--------|
| Ca   | 35.454708 | 29.301628 | 23.790794 |
| S    | 21.126467  | 31.736858  | 35.127106  |
| S    | 20.456192  | 35.893738  | 33.050980  |
| S    | 21.847561  | 31.303383  | 29.908426  |
| S    | 24.956499  | 33.956814  | 33.041542  |
| S    | 26.162937  | 29.290390  | 30.980011  |
| S    | 25.615084  | 33.690414  | 28.710768  |
| S    | 28.167826  | 29.610668  | 27.033779  |
| S    | 30.971296  | 30.861919  | 30.327805  |
| S    | 31.924530  | 26.737663  | 27.703030  |
| S    | 32.563595  | 30.836205  | 25.246338  |
| S    | 33.306652  | 26.414669  | 23.386312  |
| S    | 36.658257  | 27.760845  | 26.628990  |

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generated by VMD

|      |        |        |        |
|------|--------|--------|--------|
| Ca   | 18.248646 | 33.330811 | 33.097569 |
| Ca   | 22.803604 | 34.662804 | 35.722061 |
| Ca   | 23.520386 | 30.347698 | 33.370361 |
| Ca   | 22.950132 | 34.799324 | 30.508188 |
| Ca   | 24.900871 | 30.378670 | 28.040295 |
| Ca   | 27.772152 | 32.626122 | 31.243797 |
| Ca   | 29.291929 | 27.849022 | 29.935480 |
| Ca   | 30.661703 | 32.258381 | 27.494852 |
| Ca   | 30.325653 | 27.791176 | 24.779961 |
| Ca   | 33.620811 | 30.006420 | 28.144037 |
| Ca   | 34.662815 | 25.038864 | 26.422131 |
| Ca   | 35.260212 | 29.081810 | 23.546801 |
| S    | 20.811584 | 31.722351 | 35.086063 |
| S    | 20.642059 | 35.870476 | 33.078705 |
| S    | 21.977642 | 31.184546 | 30.232252 |
| S    | 24.883671 | 33.830437 | 33.423935 |
| S    | 26.139061 | 29.416533 | 30.949604 |
| S    | 25.811939 | 33.846081 | 28.582706 |
| S    | 28.386913 | 29.675495 | 26.896097 |
| S    | 30.854506 | 30.894409 | 30.341763 |
| S    | 31.960659 | 26.772251 | 27.982372 |
| S    | 32.505520 | 30.705025 | 25.105310 |
| S    | 33.302849 | 26.148140 | 23.275290 |
| S    | 36.424732 | 28.063229 | 26.680357 |

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generated by VMD

|      |        |        |        |
|------|--------|--------|--------|
| Ca   | 18.450733 | 33.579967 | 33.475826 |
| Ca   | 23.000061 | 34.680794 | 35.546284 |
| Ca   | 23.273411 | 30.179096 | 33.252274 |
| Ca   | 22.767372 | 34.616806 | 30.316343 |
| Ca   | 24.826658 | 30.430107 | 27.907051 |
|  | Ca  |  |  |  |
|---|---|---|---|---|
|  | 27.718754 | 32.396671 | 31.265518 |
| Ca | 29.290527 | 27.950275 | 29.990147 |
| Ca | 30.787113 | 32.450039 | 27.547926 |
| Ca | 30.465002 | 27.933334 | 24.99937 |
| Ca | 33.910786 | 29.842865 | 27.994022 |
| Ca | 34.572086 | 25.014874 | 26.713831 |
| Ca | 35.126133 | 29.139488 | 23.423380 |
| S  | 20.891052 | 31.785942 | 35.267372 |
| S  | 20.802940 | 36.069565 | 33.012024 |
| S  | 21.740005 | 31.127619 | 30.095871 |
| S  | 24.763529 | 33.277531 | 33.220009 |
| S  | 26.149815 | 29.301647 | 30.647259 |
| S  | 25.888588 | 33.785736 | 28.644983 |
| S  | 28.331997 | 29.752975 | 26.925367 |
| S  | 30.890461 | 30.938408 | 30.561357 |
| S  | 31.896198 | 26.912682 | 27.800177 |
| S  | 32.527264 | 30.842440 | 25.139170 |
| S  | 33.173386 | 26.139641 | 23.619818 |
| S  | 36.476204 | 28.151531 | 26.574120 |

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generated by VMD

|  | Ca  |  |  |  |
|---|---|---|---|---|
|  | 18.575794 | 33.700546 | 33.627262 |
| Ca | 23.027208 | 34.677284 | 35.905190 |
| Ca | 23.448071 | 30.049103 | 33.092499 |
| Ca | 22.874973 | 34.668743 | 30.431597 |
| Ca | 24.873955 | 30.241089 | 27.920431 |
| Ca | 27.524513 | 32.521561 | 31.118185 |
| Ca | 29.113350 | 27.960155 | 29.854933 |
| Ca | 30.482773 | 32.529976 | 27.346088 |
| Ca | 30.594246 | 27.969181 | 24.517946 |
| Ca | 33.435066 | 30.010626 | 27.995819 |
| Ca | 34.477989 | 24.928337 | 26.900949 |
| Ca | 35.475094 | 28.982153 | 23.940535 |
| S  | 20.935329 | 31.691422 | 35.355934 |
| S  | 20.930733 | 36.066750 | 33.306679 |
| S  | 21.864918 | 31.120190 | 29.887581 |
| S  | 24.857885 | 33.355289 | 33.189243 |
| S  | 26.156265 | 29.200237 | 30.776812 |
| S  | 25.731783 | 33.670731 | 28.573481 |
| S  | 28.248995 | 29.817892 | 26.922970 |
| S  | 30.695049 | 31.178452 | 30.216873 |
| S  | 31.609936 | 26.989069 | 27.567263 |
| S  | 32.712482 | 30.941620 | 24.979311 |
| S  | 33.659672 | 26.122322 | 23.569845 |
| S  | 36.414009 | 27.907314 | 26.942608 |

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| Element | X1      | Y1      | Z1      |
|---------|---------|---------|---------|
| Ca      | 18.164265 | 33.607903 | 33.657501 |
| Ca      | 22.926743  | 34.540131 | 35.821728  |
| Ca      | 23.638401  | 30.283619 | 33.091797  |
| Ca      | 22.848408  | 34.507973 | 30.679712  |
| Ca      | 24.942165  | 30.352905 | 27.899696  |
| Ca      | 27.584072  | 32.604897 | 31.125010  |
| Ca      | 29.397793  | 28.085869 | 30.194784  |
| Ca      | 30.550720  | 32.441193 | 27.544973  |
| Ca      | 30.552378  | 29.834442 | 28.057352  |
| Ca      | 34.381939  | 24.709301 | 26.733530  |
| Ca      | 35.388744  | 29.254538 | 23.576687  |
| S       | 21.081673  | 31.609367 | 34.951599  |
| S       | 20.770027  | 35.816906 | 33.222527  |
| S       | 22.068535  | 30.997002 | 29.748560  |
| S       | 24.950176  | 33.734825 | 32.942390  |
| S       | 26.133528  | 29.439793 | 30.849812  |
| S       | 25.790699  | 33.841175 | 28.549124  |
| S       | 28.323868  | 29.591373 | 27.005123  |
| S       | 30.828478  | 31.317566 | 30.406181  |
| S       | 31.700684  | 26.950047 | 27.674984  |
| S       | 32.522404  | 30.752954 | 24.981159  |
| S       | 33.419304  | 26.254251 | 23.456354  |
| S       | 36.227745  | 27.794941 | 26.835663  |

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| Element | X1      | Y1      | Z1      |
|---------|---------|---------|---------|
| Ca      | 18.229389 | 33.727135 | 33.878624 |
| Ca      | 22.886200  | 34.562183 | 36.034824  |
| Ca      | 23.556976  | 30.242367 | 33.059483  |
| Ca      | 22.607124  | 34.446579 | 30.665525  |
| Ca      | 24.995190  | 30.457615 | 27.806604  |
| Ca      | 27.586195  | 32.576160 | 31.220720  |
| Ca      | 29.194395  | 28.021286 | 29.949898  |
| Ca      | 30.375103  | 32.603310 | 27.172064  |
| Ca      | 30.766573  | 27.793610 | 24.763903  |
| Ca      | 33.685116  | 29.996735 | 27.799522  |
| Ca      | 34.350418  | 24.903883 | 26.784863  |
| Ca      | 35.796886  | 28.938797 | 23.921349  |
| S       | 21.013670  | 31.606098 | 35.450783  |
| S       | 20.706463  | 35.966919 | 33.303165  |
| S       | 21.896702  | 31.100683 | 29.950882  |
| S       | 24.700573  | 33.629135 | 33.235523  |
| S       | 26.019772  | 29.425713 | 30.641233  |
| S       | 25.699526  | 33.901268 | 28.557379  |
| S       | 28.212408  | 29.744873 | 26.654118  |
|   |             |             |             |
|---|-------------|-------------|-------------|
| 24 | generated by VMD |
| Ca | 18.253408   | 34.008049   | 34.103958   |
| Ca | 22.972195   | 34.632843   | 35.792915   |
| Ca | 23.510477   | 30.312508   | 33.007713   |
| Ca | 22.574142   | 34.684799   | 30.697807   |
| Ca | 24.938023   | 30.185871   | 27.767000   |
| Ca | 27.560736   | 32.288101   | 30.935753   |
| Ca | 29.125706   | 27.771893   | 29.923161   |
| Ca | 30.482971   | 32.474094   | 27.453718   |
| Ca | 30.810677   | 27.891968   | 25.029240   |
| Ca | 33.538754   | 29.835188   | 28.201759   |
| Ca | 34.719250   | 24.934891   | 26.561502   |
| Ca | 35.393673   | 29.252464   | 23.664072   |
| Ca | 20.986588   | 31.861197   | 35.285248   |
| Ca | 20.802412   | 36.093964   | 33.496971   |
| Ca | 22.020378   | 31.056557   | 29.746763   |
| Ca | 24.945358   | 33.526806   | 32.987583   |
| Ca | 26.001244   | 29.113873   | 30.557928   |
| Ca | 25.533905   | 33.809433   | 28.404348   |
| Ca | 28.381845   | 29.660831   | 26.721722   |
| Ca | 30.698013   | 30.937256   | 30.364679   |
| Ca | 31.738602   | 26.833687   | 27.723694   |
| Ca | 32.617931   | 30.907597   | 25.055696   |
| Ca | 33.589520   | 26.189022   | 23.496885   |
| Ca | 36.524281   | 28.037098   | 26.959976   |

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|   |             |             |             |
|---|-------------|-------------|-------------|
| generated by VMD |
| Ca | 18.494339   | 33.816780   | 34.463993   |
| Ca | 23.114246   | 34.444595   | 35.818993   |
| Ca | 23.358030   | 30.240845   | 32.793396   |
| Ca | 22.918264   | 34.914402   | 30.215630   |
| Ca | 24.543970   | 30.241007   | 27.636608   |
| Ca | 27.520905   | 32.323391   | 31.081913   |
| Ca | 29.055489   | 27.861790   | 29.958618   |
| Ca | 30.367804   | 32.453838   | 27.490772   |
| Ca | 30.663092   | 27.720188   | 25.103502   |
| Ca | 33.533554   | 29.717365   | 28.085768   |
| Ca | 34.708748   | 25.236841   | 26.932837   |
| Ca | 35.413147   | 29.382046   | 23.740646   |
| S  | 21.155602   | 31.611465   | 35.364700   |
S  20.879597  35.833260  33.323303
S  21.860018  31.456507  29.667755
S  25.052422  33.446655  32.772522
S  25.970631  29.273661  30.544426
S  25.821896  33.769127  28.283020
S  28.209698  29.710846  26.792780
S  30.769684  30.945198  30.410105
S  31.663090  26.727249  27.829924
S  32.416801  30.776917  25.221031
S  33.602989  26.358532  23.591324
S  36.625996  28.037537  26.816484

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generated by VMD

Ca  18.325251  33.918736  34.040981
Ca  22.719795  34.635773  35.580513
Ca  23.440453  30.111511  33.039604
Ca  22.874828  34.603191  30.428978
Ca  24.876236  30.251350  27.911486
Ca  27.715326  32.707581  31.315895
Ca  29.205889  27.849228  29.968523
Ca  30.476503  32.426102  27.479410
Ca  30.731722  27.999210  24.883858
Ca  33.427063  29.763508  28.071098
Ca  34.466995  24.928497  26.605042
Ca  35.576153  29.095335  23.662495
S  20.881237  31.549347  35.234699
S  20.687653  35.972679  33.123280
S  22.059988  31.152546  29.855478
S  24.987082  33.526070  33.168152
S  26.380262  29.422363  31.052391
S  25.905685  33.699944  28.540104
S  28.273462  29.940022  26.880192
S  30.699629  31.035933  30.209257
S  31.604736  26.846088  27.642979
S  32.472488  30.792583  24.810316
S  33.602367  26.432590  23.523344
S  36.329300  28.039841  26.911926

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generated by VMD

Ca  18.037994  33.262947  34.589481
Ca  22.828548  34.551907  35.706886
Ca  23.320305  30.482698  32.735836
Ca  22.965263  34.793976  30.481485
Ca  24.980339  30.432240  27.861925
Ca  28.007641  32.741444  31.126896
Ca  29.145393  28.168671  29.767996
| Element | Ca   | S    | generated by VMD |
|---------|------|------|------------------|
|         | 30.447884 | 32.611229 | 27.110361 |
|         | 30.715113 | 27.840549 | 25.017965 |
|         | 33.478569 | 29.725632 | 27.776075 |
|         | 34.401112 | 24.765219 | 26.970367 |
|         | 35.670872 | 28.899467 | 24.121742 |
|         | 20.974651 | 31.325588 | 35.328663 |
|         | 20.494781 | 35.439224 | 33.248249 |
|         | 22.017469 | 31.350353 | 29.727020 |
|         | 24.973146 | 33.671787 | 33.026932 |
|         | 26.309687 | 29.545223 | 30.866041 |
|         | 25.884838 | 34.012978 | 28.637051 |
|         | 28.307018 | 29.930363 | 26.717098 |
|         | 30.809290 | 31.250408 | 30.010578 |
|         | 31.518353 | 26.717854 | 27.578503 |
|         | 32.534245 | 30.788271 | 24.858620 |
|         | 33.493752 | 26.248209 | 23.572243 |
|         | 36.403763 | 27.743820 | 27.102001 |

24

generated by VMD

| Element | Ca   | S    | generated by VMD |
|---------|------|------|------------------|
|         | 18.168503 | 33.088768 | 34.426254 |
|         | 22.806084 | 34.804504 | 35.814114 |
|         | 23.556511 | 30.478004 | 32.843788 |
|         | 23.027491 | 34.395065 | 30.480164 |
|         | 24.846302 | 30.417702 | 27.753277 |
|         | 27.703806 | 32.725719 | 31.527002 |
|         | 29.273380 | 28.184368 | 29.920246 |
|         | 30.767517 | 32.659622 | 27.370176 |
|         | 30.707497 | 27.951065 | 24.985435 |
|         | 33.567814 | 29.831753 | 28.091640 |
|         | 34.228172 | 24.818497 | 26.638302 |
|         | 35.570210 | 28.869057 | 23.952593 |
|         | 21.214775 | 31.514891 | 35.332912 |
|         | 20.543297 | 35.439575 | 33.016693 |
|         | 22.041162 | 31.249901 | 29.407921 |
|         | 24.826780 | 33.803215 | 33.014725 |
|         | 26.095856 | 29.505491 | 30.868576 |
|         | 25.803288 | 33.906578 | 28.506937 |
|         | 28.356501 | 29.918865 | 26.818047 |
|         | 30.838905 | 31.357906 | 30.342625 |
|         | 31.594753 | 26.918682 | 27.714735 |
|         | 32.605621 | 30.721609 | 24.860477 |
|         | 33.271969 | 26.116535 | 23.313042 |
|         | 36.303867 | 27.622650 | 26.940355 |

24

generated by VMD

| Element | Ca   | S    | generated by VMD |
|---------|------|------|------------------|
|         | 18.329866 | 32.962727 | 34.398987 |

238
Ca   22.699934 34.754028 35.529858
Ca   23.398285 30.331621 32.931160
Ca   22.970707 34.890274 30.479885
Ca   24.937811 30.377577 27.772957
Ca   27.743912 32.909096 31.402943
Ca   29.200455 28.075062 29.984337
Ca   30.639086 32.547508 27.236874
Ca   30.622629 28.127176 24.798004
Ca   33.572613 29.754152 27.995794
Ca   34.253090 24.783493 26.816465
Ca   35.545769 28.685757 23.635773
S    21.145365 31.339628 35.543991
S    20.467556 35.558372 32.967216
S    22.140263 31.349400 29.564098
S    24.831570 33.490791 33.121841
S    26.209419 29.476566 31.048470
S    25.897715 34.134789 28.604851
S    28.267975 29.882145 26.772242
S    30.695471 31.327848 30.282831
S    31.554089 26.879143 27.546570
S    32.824585 30.819994 24.879316
S    33.396610 26.086559 23.457777
S    36.375206 27.756371 27.167767

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generated by VMD
Ca   18.297756 32.632835 34.330025
Ca   23.134804 34.701714 35.523670
Ca   23.382799 30.315945 32.710999
Ca   22.982208 34.783024 30.521931
Ca   24.836708 30.680653 27.736448
Ca   27.878204 32.843231 31.070618
Ca   29.201784 28.183245 29.908463
Ca   30.609814 32.744980 27.301367
Ca   30.569332 27.965277 24.929255
Ca   33.345097 29.900185 28.157326
Ca   34.265373 24.421051 26.680950
Ca   35.667969 28.831715 24.115667
S    21.263050 31.382885 35.690147
S    20.351469 35.282272 33.225187
S    21.995180 31.278285 29.671661
S    24.968849 33.794392 32.880825
S    26.262331 29.637142 30.809523
S    25.787140 34.127880 28.375763
S    28.373680 30.013348 26.870655
S    30.816624 31.424217 30.183054
S    31.476614 26.892673 27.511847
S        32.700329       30.860260       24.929659
S        33.355839       26.104641       23.600679
S        36.197113       27.497738       27.204306

24 generated by VMD
Ca       18.459969       32.714111       34.150860
Ca       22.944080       34.846283       35.587891
Ca       23.463614       30.234974       32.699162
Ca       22.486622       34.548294       30.369604
Ca       25.077663       30.609554       27.773966
Ca       27.959423       32.945065       31.135712
Ca       29.184698       28.096878       30.007351
Ca       30.651333       32.802277       27.436989
Ca       30.608225       28.092224       24.819901
Ca       33.389702       29.853256       27.774683
Ca       34.063046       24.602924       26.560015
Ca       35.725563       28.732798       24.484741
S        21.627232       31.565960       35.607399
S        20.447363       35.476570       33.246880
S        21.859565       31.077763       29.674927
S        24.783762       33.724682       32.899529
S        26.358980       29.536045       31.005510
S        25.598591       34.107891       28.622545
S        28.283255       30.026678       26.849728
S        31.040276       31.415777       30.103121
S        31.317276       26.877464       27.398643
S        32.820217       30.854382       24.918842
S        33.403786       26.293224       23.448093
S        36.169403       27.265015       27.363894

24 generated by VMD
Ca       18.328825       32.749207       34.159779
Ca       22.999517       34.825066       35.626225
Ca       23.318361       30.411123       32.927643
Ca       22.687300       34.539383       30.506361
Ca       25.067619       30.403217       27.843351
Ca       27.836031       32.667919       31.053974
Ca       29.128571       28.140335       29.851795
Ca       30.771988       32.823112       27.306261
Ca       30.721115       28.164948       24.798899
Ca       33.562717       29.674475       28.147202
Ca       34.111343       24.511086       26.772863
Ca       35.725140       28.664150       23.873177
S        21.158371       31.641794       35.660549
S        20.445835       35.468636       33.297657
S        21.974371       31.108223       29.704876
|   | 1st Coordinate | 2nd Coordinate | 3rd Coordinate |
|---|----------------|----------------|----------------|
| S | 24.697273      | 33.747189      | 33.119354      |
| S | 26.195564      | 29.641672      | 30.908096      |
| S | 25.601889      | 34.115147      | 28.389200      |
| S | 28.417595      | 30.041008      | 26.761749      |
| S | 30.970547      | 31.391628      | 30.241701      |
| S | 31.644356      | 27.076931      | 27.466637      |
| S | 32.788452      | 30.962429      | 24.999945      |
| S | 33.360645      | 26.133106      | 23.454613      |
| S | 36.206593      | 27.398233      | 27.068151      |

24 generated by VMD

| Ca  | 18.457817 | 32.337097 | 33.692085 |
|-----|-----------|-----------|-----------|
| Ca  | 23.074310 | 34.746597 | 35.869972 |
| Ca  | 23.387430 | 30.625416 | 32.939449 |
| Ca  | 22.959427 | 34.903473 | 30.361361 |
| Ca  | 24.847721 | 30.305035 | 27.722794 |
| Ca  | 27.748381 | 32.896919 | 31.267326 |
| Ca  | 29.095531 | 27.975958 | 29.789122 |
| Ca  | 30.569700 | 32.588547 | 27.216160 |
| Ca  | 30.649700 | 28.031403 | 24.983128 |
| Ca  | 33.410431 | 29.708958 | 28.067099 |
| Ca  | 34.096729 | 24.675409 | 26.980820 |
| Ca  | 35.675987 | 28.950590 | 23.819881 |
| S   | 21.316257 | 31.634771 | 35.623394 |
| S   | 20.642900 | 35.202854 | 33.340332 |
| S   | 22.024937 | 31.486393 | 29.657005 |
| S   | 25.053665 | 33.791618 | 33.022587 |
| S   | 26.147587 | 29.689991 | 30.879953 |
| S   | 25.637545 | 34.018314 | 28.348156 |
| S   | 28.307007 | 29.901833 | 26.715374 |
| S   | 30.742798 | 31.197800 | 30.333397 |
| S   | 31.614052 | 26.820072 | 27.726555 |
| S   | 32.748558 | 30.858118 | 24.937874 |
| S   | 33.271214 | 26.329617 | 23.624537 |
| S   | 36.240402 | 27.623276 | 27.021679 |

24 generated by VMD

| Ca  | 18.482668 | 32.697769 | 33.633064 |
|-----|-----------|-----------|-----------|
| Ca  | 22.915310 | 34.767223 | 35.758617 |
| Ca  | 23.525763 | 30.428644 | 32.901928 |
| Ca  | 22.909264 | 34.692513 | 30.373796 |
| Ca  | 25.020639 | 30.314812 | 27.948162 |
| Ca  | 27.787319 | 33.035362 | 31.249783 |
| Ca  | 29.311907 | 28.132788 | 29.877804 |
| Ca  | 30.375198 | 32.607021 | 27.371017 |
| Ca  | 30.592144 | 27.900871 | 25.007631 |
| Element | Ca       | 33.155144 | 29.606544 | 28.010681 |
|---------|----------|-----------|-----------|-----------|
|         | Ca       | 34.273643 | 24.690014 | 26.707973 |
|         | Ca       | 35.629826 | 29.073044 | 23.854200 |
|         | Ca       | 35.629826 | 35.646637 | 33.312225 |
|         | S        | 22.096241 | 31.370584 | 29.638412 |
| S       | 24.964764 | 33.706367 | 33.242981 |
|         | S        | 25.723015 | 29.673641 | 31.531313 |
| S       | 30.857632 | 29.774303 | 31.531313 |
|         | S        | 31.417286 | 26.648365 | 27.557018 |
| S       | 32.497711 | 26.481355 | 24.890869 |
|         | S        | 33.438763 | 26.296717 | 23.533327 |
| S       | 36.224033 | 27.716190 | 27.119116 |
|         | generated by VMD |
| Ca      | 18.344753 | 32.524372 | 33.665901 |
|         | Ca       | 22.813278 | 34.939384 | 35.822075 |
| Ca      | 23.568314 | 30.439425 | 33.054108 |
|         | Ca       | 22.938854 | 34.815434 | 33.588276 |
| Ca      | 25.027958 | 30.387081 | 27.937115 |
|         | Ca       | 27.976370 | 33.024429 | 31.434002 |
| Ca      | 29.050072 | 28.125401 | 29.727215 |
|         | Ca       | 30.515245 | 32.355988 | 27.217163 |
| Ca      | 30.563061 | 27.899696 | 24.776655 |
|         | Ca       | 33.383976 | 29.701260 | 28.069334 |
| Ca      | 34.194176 | 24.885572 | 26.845057 |
|         | Ca       | 35.681911 | 29.012749 | 23.884785 |
| S       | 21.192215 | 31.450239 | 35.415993 |
|         | S       | 20.463957 | 25.359357 | 32.960018 |
|         | S       | 22.135603 | 31.503361 | 29.810671 |
| S       | 24.984926 | 33.646111 | 33.338470 |
|         | S       | 26.388927 | 29.846333 | 31.150063 |
| S       | 25.796516 | 33.910355 | 28.323963 |
|         | S       | 28.176598 | 29.856882 | 26.599674 |
| S       | 30.705414 | 30.893204 | 30.318481 |
|         | S       | 31.480103 | 26.916487 | 27.545471 |
| S       | 32.615677 | 30.726467 | 24.844765 |
|         | S       | 33.401070 | 26.252377 | 23.610519 |
| S       | 36.321014 | 27.713840 | 27.000278 |
|         | generated by VMD |
| Ca      | 18.749065 | 32.514488 | 33.779137 |
|         | Ca       | 22.752476 | 34.705879 | 35.733700 |
| Ca      | 23.443144 | 30.365686 | 32.880703 |
Ca       22.775146       34.984398       30.458767
Ca       24.899195       32.914644       29.872906
Ca       27.817606       33.093788       31.124966
Ca       29.103724       30.510071       27.982903
Ca       30.432417       27.979836       27.593037
Ca       30.622965       24.875931
Ca       33.591370       29.594803       27.71293
Ca       34.334583       24.746897       26.711880
Ca       35.633698       23.935854
S        21.324938       31.589218       35.564430
S        20.513401       35.533459       33.045124
S        21.925776       31.369400       29.777264
S        25.061260       32.742203       32.987095
S        26.330357       31.146173
S        25.682861       28.970169       28.391300
S        28.118326       29.783045       26.773876
S        30.712019       30.439875
S        31.389606       26.764618       27.423872
S        32.680645       29.862610       24.961092
S        33.516911       26.443233       23.581856
S        36.308548       27.685455       27.180984

24

generated by VMD

Ca       18.523815       32.695042       34.050560
Ca       22.886444       34.810196       35.769310
Ca       23.581331       30.443174       32.820419
Ca       22.704123       34.841545       30.738846
Ca       24.814983       30.425503       27.657604
Ca       27.562084       32.913715       31.292206
Ca       29.017681       29.753629       29.792591
Ca       30.601225       32.541290       27.387505
Ca       30.670582       27.780798       24.796379
Ca       33.466572       29.685177       27.898682
Ca       34.227032       24.947720       26.737465
Ca       35.659683       29.003841       23.940973
S        21.526394       31.661093       35.630051
S        20.252264       35.611053       33.267784
S        21.853130       31.586691       29.784306
S        24.783642       33.687065       33.185593
S        26.144135       29.657719       30.820948
S        25.693562       33.989174       28.288919
S        28.316826       29.824711       26.588238
S        30.883009       31.037205       30.131100
S        31.465059       26.717949       27.682297
S        32.820427       30.541483       25.044958
S        33.837791       26.293493       23.526222
|   | 36.428146 | 27.650803 | 27.107096 |
|---|-----------|-----------|-----------|

generated by VMD

|   | 18.468678 | 32.689255 | 33.294540 |
|---|-----------|-----------|-----------|
| Ca | 22.685492 | 35.080696 | 35.608505 |
| Ca | 23.397352 | 30.435081 | 33.251465 |
| Ca | 22.855560 | 34.884270 | 30.628681 |
| Ca | 24.980690 | 30.418781 | 27.691277 |
| Ca | 27.812794 | 32.867889 | 31.501049 |
| Ca | 29.098789 | 28.020782 | 29.771049 |
| Ca | 30.569670 | 32.344830 | 27.468412 |
| Ca | 30.659134 | 27.964794 | 24.936186 |
| Ca | 33.586601 | 29.749559 | 27.869284 |
| Ca | 34.483467 | 24.730574 | 26.642410 |
| Ca | 35.447155 | 28.984623 | 23.668987 |
| S  | 21.282579 | 31.965961 | 35.651680 |
| S  | 20.261337 | 35.578457 | 32.934135 |
| S  | 22.015633 | 31.313908 | 29.848726 |
| S  | 24.932104 | 33.558342 | 33.571941 |
| S  | 26.192217 | 29.521971 | 31.048065 |
| S  | 25.694645 | 33.851738 | 28.625988 |
| S  | 28.275126 | 29.709755 | 26.750328 |
| S  | 30.841473 | 30.981152 | 30.410164 |
| S  | 31.766930 | 26.804893 | 27.520042 |
| S  | 32.677670 | 30.733418 | 24.972446 |
| S  | 33.379753 | 26.392220 | 23.385624 |
| S  | 36.355202 | 27.717144 | 26.889021 |
|   | 18.601318 | 32.304913 | 33.812954 |
| Ca | 22.834536 | 34.987892 | 35.580704 |
| Ca | 23.723633 | 30.484398 | 33.084091 |
| Ca | 22.581717 | 34.821838 | 30.425682 |
| Ca | 24.911770 | 30.506172 | 27.692898 |
| Ca | 27.690174 | 32.904842 | 31.197886 |
| Ca | 29.180395 | 27.997540 | 30.095333 |
| Ca | 30.541561 | 32.491318 | 27.549883 |
| Ca | 30.629129 | 28.232277 | 24.838812 |
| Ca | 33.504829 | 29.476288 | 28.038185 |
| Ca | 34.073803 | 24.649628 | 26.427002 |
| Ca | 35.906536 | 28.909855 | 24.043041 |
| S  | 21.268869 | 31.761173 | 35.817329 |
| S  | 20.349777 | 35.533310 | 32.904400 |
| S  | 21.963448 | 31.403786 | 30.005619 |
| S  | 24.893755 | 33.863224 | 33.096081 |
| S  | 26.309404 | 29.679104 | 31.055155 |
| S   | 25.496117 | 33.913422 | 28.405073 |
|-----|-----------|-----------|-----------|
| S   | 28.321184 | 29.709312 | 26.876251 |
| S   | 30.752211 | 31.144039 | 30.279568 |
| S   | 31.490377 | 26.842138 | 27.337446 |
| S   | 32.896214 | 30.993809 | 25.121044 |
| S   | 35.545727 | 26.321907 | 23.364727 |
| S   | 36.253620 | 27.367847 | 26.890909 |

24 generated by VMD

| Ca  | 18.417044 | 32.647148 | 33.983280 |
|-----|-----------|-----------|-----------|
| Ca  | 23.078217 | 35.146278 | 35.528889 |
| Ca  | 23.566124 | 30.378916 | 32.969284 |
| Ca  | 22.434494 | 34.673729 | 30.438190 |
| Ca  | 25.118029 | 30.711712 | 27.815014 |
| Ca  | 27.649532 | 32.764954 | 31.193813 |
| Ca  | 29.195992 | 27.834740 | 29.938910 |
| Ca  | 30.910332 | 32.346436 | 27.436710 |
| Ca  | 30.470848 | 28.008188 | 24.875481 |
| Ca  | 33.644001 | 29.747772 | 28.287212 |
| Ca  | 34.320095 | 24.931906 | 26.374908 |
| Ca  | 35.659664 | 28.882755 | 23.987204 |
| S   | 21.438589 | 31.833735 | 35.699356 |
| S   | 20.317610 | 35.439972 | 33.252186 |
| S   | 22.042999 | 31.165419 | 29.681704 |
| S   | 24.707357 | 33.728172 | 32.897583 |
| S   | 26.251457 | 29.512981 | 30.921471 |
| S   | 25.601139 | 33.943577 | 28.392378 |
| S   | 28.502001 | 29.940594 | 26.796085 |
| S   | 30.787718 | 31.108894 | 30.351994 |
| S   | 31.624943 | 26.671066 | 27.705313 |
| S   | 32.781525 | 30.778738 | 25.008219 |
| S   | 32.997326 | 26.522362 | 23.140387 |
| S   | 36.202999 | 27.579948 | 27.269030 |

24 generated by VMD

| Ca  | 18.524488 | 32.315272 | 33.942944 |
|-----|-----------|-----------|-----------|
| Ca  | 22.633274 | 35.417545 | 35.302582 |
| Ca  | 23.637739 | 30.459381 | 33.229259 |
| Ca  | 22.947056 | 34.485046 | 30.267506 |
| Ca  | 25.034166 | 30.485460 | 27.871216 |
| Ca  | 27.881250 | 32.898521 | 31.540913 |
| Ca  | 28.947157 | 27.992937 | 29.794945 |
| Ca  | 30.730806 | 32.459152 | 27.422176 |
| Ca  | 30.616142 | 28.107697 | 24.528824 |
| Ca  | 33.251446 | 29.560810 | 28.369858 |
| Ca  | 34.140423 | 24.957596 | 26.186663 |
|   | Ca   | 35.703018 | 29.054878 | 24.053940 |
|---|------|-----------|-----------|-----------|
| S | 21.440062 | 32.080528 | 36.009098 |
| S | 20.160437 | 35.324162 | 32.605331 |
| S | 22.097649 | 31.107536 | 29.856586 |
| S | 24.910660 | 33.711266 | 33.249725 |
| S | 26.416712 | 29.723545 | 31.237667 |
| S | 26.001112 | 33.806427 | 28.509262 |
| S | 28.310070 | 29.802174 | 26.752089 |
| S | 30.816742 | 30.928120 | 30.317596 |
| S | 31.293549 | 26.721947 | 27.583151 |
| S | 32.718781 | 30.748123 | 25.053854 |
| S | 33.444294 | 26.630753 | 22.996510 |
| S | 36.063004 | 27.523857 | 27.258385 |

24

Ca 18.638657 32.120464 33.670395
Ca 22.648182 35.343990 35.152683
Ca 23.801622 30.579929 33.493916
Ca 22.896000 34.597656 30.171543
Ca 25.132414 30.433296 27.928631
Ca 27.881660 33.017643 31.458588
Ca 28.960176 27.994698 29.854271
Ca 30.333845 32.304211 27.826620
Ca 30.644590 28.178646 24.451984
Ca 33.425133 29.452374 28.350035
Ca 33.925121 24.811169 26.100830
Ca 35.569942 29.190706 23.974812
S 21.516548 32.011547 35.911060
S 20.214321 35.120262 32.371197
S 22.150309 31.094471 30.032146
S 25.062559 33.993271 33.165813
S 26.470776 29.793247 31.178478
S 25.835201 33.714630 28.463806
S 28.470449 30.024471 26.831358
S 30.811319 31.005291 30.671177
S 31.281982 26.607592 27.500919
S 32.502205 30.928217 25.083614
S 33.402740 26.727062 23.141678
S 36.144192 27.255199 27.154476

24

generated by VMD

|   | Ca   | 18.592424 | 32.404747 | 33.934746 |
|---|------|-----------|-----------|-----------|
| Ca 22.634287 | 35.669769 | 35.183697 |
| Ca 23.601276 | 30.342236 | 33.336678 |
| Ca 22.761248 | 34.606865 | 30.510040 |
| Ca 24.975550 | 30.416233 | 27.834606 |
| Element | Ca   | S    |
|---------|------|------|
| 27.95   | 21.44 |       |
| 27.95   | 20.60 |       |
| 27.95   | 22.14 |       |
| 27.95   | 24.88 |       |
| 27.95   | 26.31 |       |
| 27.95   | 25.77 |       |
| 27.95   | 28.12 |       |
| 27.95   | 30.82 |       |
| 27.95   | 31.30 |       |
| 27.95   | 32.85 |       |
| 27.95   | 33.55 |       |
| 27.95   | 36.27 |       |

generated by VMD

| Element | Ca   | S    |
|---------|------|------|
| 18.72   | 21.38 |       |
| 22.68   | 20.23 |       |
| 23.64   | 22.12 |       |
| 23.02   | 25.08 |       |
| 28.08   | 28.78 |       |
| 30.39   | 30.60 |       |
| 33.26   | 34.21 |       |
| 35.56   | 21.38 |       |
| 20.23   | 22.12 |       |
| 25.08   | 26.36 |       |
| 26.01   | 28.17 |       |
| 30.53   | 32.72 |       |
| 31.39   | 33.62 |       |
| 36.19   | 24.72 |       |

24

24
| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 18.549435 | 32.007542 | 33.845798 |
| Ca      | 22.577284 | 35.563118 | 34.979706 |
| Ca      | 23.738049 | 30.437618 | 33.415749 |
| Ca      | 22.945333 | 34.567242 | 30.069841 |
| Ca      | 24.992720 | 28.4567242 | 30.069841 |
| Ca      | 27.919813 | 32.710201 | 31.590258 |
| Ca      | 29.138535 | 27.895052 | 29.795597 |
| Ca      | 30.590027 | 32.516357 | 27.774761 |
| Ca      | 30.521839 | 28.416529 | 24.677448 |
| Ca      | 32.80647 | 29.448101 | 28.087986 |
| Ca      | 33.989517 | 24.708584 | 26.154301 |
| Ca      | 35.677898 | 28.943501 | 24.153255 |
| S       | 21.545097 | 32.243298 | 35.812283 |
| S       | 19.983688 | 35.128742 | 32.221142 |
| S       | 22.086420 | 30.822304 | 30.221935 |
| S       | 25.006054 | 33.889275 | 33.204231 |
| S       | 26.567455 | 29.779793 | 31.315792 |
| S       | 25.963680 | 33.988213 | 28.577160 |
| S       | 28.082710 | 30.023916 | 26.802174 |
| S       | 30.763214 | 30.841240 | 30.273270 |
| S       | 31.413397 | 26.905815 | 27.199806 |
| S       | 32.819622 | 31.006149 | 25.312244 |
| S       | 33.447884 | 26.714096 | 22.989733 |
| S       | 36.113804 | 27.102352 | 27.131790 |
| 24      |
| Ca      | 18.881315 | 32.093800 | 34.042114 |
| Ca      | 22.518993 | 35.690125 | 35.137154 |
| Ca      | 23.685215 | 30.744701 | 33.327835 |
| Ca      | 22.665003 | 34.450111 | 30.075375 |
| Ca      | 25.045527 | 30.424175 | 28.095734 |
| Ca      | 27.460051 | 32.746590 | 31.318245 |
| Ca      | 28.963839 | 27.961308 | 29.665455 |
| Ca      | 30.749487 | 32.270294 | 27.693722 |
| Ca      | 30.595171 | 28.315109 | 24.818096 |
| Ca      | 33.494835 | 29.201389 | 28.329491 |
| Ca      | 33.901310 | 24.729084 | 25.901754 |
| Ca      | 35.881283 | 29.235601 | 24.171307 |
| S       | 21.554974 | 32.296001 | 36.033913 |
| S       | 20.150085 | 34.978752 | 32.545868 |
| S       | 22.082375 | 30.994312 | 30.044060 |
| S       | 25.036057 | 33.944527 | 33.063148 |
| S       | 26.270969 | 29.952850 | 31.260708 |
| S       | 25.612968 | 33.933533 | 28.442331 |
| S       | 28.207504 | 29.982414 | 26.773659 |
|     |         |         |         |
|-----|---------|---------|---------|
| S   | 30.841026 | 30.614063 | 30.537508 |
| S   | 31.390842 | 26.840431 | 27.439768 |
| S   | 32.874195 | 30.940033 | 25.273674 |
| S   | 33.592796 | 26.789528 | 23.027384 |
| S   | 36.264179 | 27.171322 | 26.921772 |
| S   | 34.280010 | 28.749847 | 26.068859 |
| S   | 35.760254 | 28.829559 | 24.268547 |
| Ca  | 18.457722 | 32.491642 | 33.821381 |
| Ca  | 22.508476 | 35.197838 | 35.319641 |
| Ca  | 23.727127 | 30.343801 | 33.302666 |
| Ca  | 22.803425 | 34.759930 | 30.379124 |
| Ca  | 25.115194 | 30.473537 | 28.038765 |
| Ca  | 27.795458 | 32.926125 | 31.299763 |
| Ca  | 29.124132 | 29.792147 | 29.874313 |
| Ca  | 30.477251 | 32.578011 | 27.651451 |
| Ca  | 30.604292 | 28.331959 | 24.820141 |
| Ca  | 33.275742 | 29.532421 | 28.051964 |
| Ca  | 34.280010 | 28.749847 | 26.068859 |
| Ca  | 35.760254 | 29.829559 | 24.268547 |
| S   | 21.436361 | 31.939411 | 35.619347 |
| S   | 20.142284 | 35.436134 | 32.765205 |
| S   | 22.180805 | 31.060982 | 30.129288 |
| S   | 24.936563 | 33.786079 | 33.175716 |
| S   | 26.568167 | 29.664646 | 31.314491 |
| S   | 25.691086 | 33.932400 | 28.269245 |
| S   | 28.364347 | 29.813839 | 26.895609 |
| S   | 30.813372 | 31.007885 | 30.258102 |
| S   | 31.473082 | 26.748671 | 27.203209 |
| S   | 32.630749 | 30.865898 | 25.060211 |
| S   | 33.403606 | 26.557915 | 23.065372 |
| S   | 36.150558 | 27.278530 | 27.287628 |

24 generated by VMD

|     |         |         |         |
|-----|---------|---------|---------|
| Ca  | 18.495134 | 32.940269 | 33.838505 |
| Ca  | 22.763252 | 35.289490 | 35.079647 |
| Ca  | 23.704617 | 30.233292 | 33.369678 |
| Ca  | 22.788956 | 34.527706 | 30.509350 |
| Ca  | 25.051489 | 30.249550 | 27.946121 |
| Ca  | 27.761122 | 32.591537 | 31.391684 |
| Ca  | 28.966833 | 27.734335 | 29.771820 |
| Ca  | 30.608620 | 32.516930 | 27.561768 |
| Ca  | 30.739820 | 28.341606 | 24.716145 |
| Ca  | 33.329014 | 29.612705 | 28.289795 |
| Ca  | 34.192078 | 24.704098 | 26.221657 |
| Ca  | 35.868000 | 29.209032 | 24.136253 |
| S   | 21.484861 | 32.145775 | 35.676037 |

24 generated by VMD
| S   | 20.101591 | 35.836895 | 32.459091 |
|-----|-----------|-----------|-----------|
| S   | 22.126202 | 30.941507 | 30.281246 |
| S   | 24.978140 | 33.534809 | 33.158222 |
| S   | 26.536749 | 29.344099 | 31.310635 |
| S   | 25.696970 | 33.737907 | 28.500927 |
| S   | 28.386871 | 29.832371 | 26.817537 |
| S   | 30.708214 | 30.918232 | 30.409702 |
| S   | 31.339830 | 26.721313 | 27.306751 |
| S   | 32.767391 | 31.136421 | 25.007456 |
| S   | 33.396915 | 26.528095 | 23.169945 |
| S   | 35.927406 | 27.672106 | 27.010056 |

24 generated by VMD

| Ca  | 18.542454 | 32.621998 | 34.077293 |
|-----|-----------|-----------|-----------|
| Ca  | 22.990496 | 35.525742 | 35.104763 |
| Ca  | 23.855129 | 30.273891 | 33.228004 |
| Ca  | 22.573235 | 34.514870 | 30.391354 |
| Ca  | 24.828566 | 30.342957 | 27.960506 |
| Ca  | 27.814117 | 32.753876 | 31.227699 |
| Ca  | 28.805573 | 27.731428 | 29.646391 |
| Ca  | 30.463480 | 32.425877 | 27.703072 |
| Ca  | 30.742998 | 28.443913 | 25.061041 |
| Ca  | 33.256882 | 29.493919 | 28.446728 |
| Ca  | 34.063843 | 24.831217 | 26.081112 |
| Ca  | 35.746227 | 29.244022 | 24.113773 |
| S   | 21.720034 | 32.115368 | 35.542252 |
| S   | 20.301554 | 35.512135 | 32.664928 |
| S   | 22.139883 | 31.003548 | 30.063885 |
| S   | 25.063845 | 33.709549 | 33.014008 |
| S   | 26.420050 | 29.597511 | 31.029575 |
| S   | 25.457125 | 33.676758 | 28.349453 |
| S   | 28.206156 | 29.869816 | 26.738575 |
| S   | 30.733408 | 30.697258 | 30.403702 |
| S   | 31.363836 | 26.809513 | 27.405884 |
| S   | 32.891380 | 31.071152 | 25.425396 |
| S   | 33.471161 | 26.621862 | 23.235970 |
| S   | 36.268612 | 27.411831 | 27.024731 |

24 generated by VMD

| Ca  | 18.360973 | 32.617630 | 33.977020 |
|-----|-----------|-----------|-----------|
| Ca  | 22.775465 | 35.401955 | 35.015884 |
| Ca  | 23.687626 | 30.473476 | 33.296150 |
| Ca  | 22.665192 | 34.490753 | 30.549053 |
| Ca  | 25.123064 | 30.345596 | 27.935732 |
| Ca  | 27.836803 | 32.836456 | 31.382156 |
| Ca  | 28.883053 | 27.924204 | 29.835505 |
| Ca       | 30.737368 | 32.607327 | 27.594330 |
| Ca       | 30.732002 | 28.354650 | 24.725231 |
| Ca       | 33.481392 | 29.475424 | 27.992241 |
| Ca       | 33.970932 | 24.529875 | 26.317251 |
| Ca       | 35.736954 | 29.213337 | 24.116131 |
| S        | 21.556681 | 31.976337 | 35.736313 |
| S        | 20.039478 | 35.609592 | 32.583466 |
| S        | 22.033640 | 30.972382 | 30.013235 |
| S        | 24.948044 | 33.637085 | 33.206451 |
| S        | 26.456003 | 29.627960 | 31.209381 |
| S        | 25.687943 | 33.688065 | 28.588221 |
| S        | 28.354744 | 29.846264 | 26.899681 |
| S        | 30.703527 | 30.948496 | 30.389793 |
| S        | 31.353729 | 26.774508 | 27.209986 |
| S        | 32.790844 | 31.015623 | 25.143938 |
| S        | 33.557751 | 26.505356 | 23.257765 |
| S        | 36.246773 | 27.427711 | 26.965101 |

24 generated by VMD

| Ca       | 18.483980 | 32.826290 | 34.050274 |
| Ca       | 22.842701 | 35.265404 | 35.194172 |
| Ca       | 23.488853 | 30.263809 | 33.184513 |
| Ca       | 22.784281 | 34.833084 | 30.233257 |
| Ca       | 25.006735 | 30.576763 | 27.969753 |
| Ca       | 27.790869 | 32.609653 | 31.226509 |
| Ca       | 28.908567 | 27.588020 | 29.722168 |
| Ca       | 30.490200 | 32.248978 | 27.559494 |
| Ca       | 30.742918 | 28.302795 | 24.803703 |
| Ca       | 33.426018 | 29.488161 | 28.244820 |
| Ca       | 34.357597 | 24.944515 | 26.509415 |
| Ca       | 35.659821 | 29.231201 | 23.891491 |
| S        | 21.541922 | 31.949045 | 35.806358 |
| S        | 20.282110 | 35.562424 | 32.751312 |
| S        | 21.999962 | 31.194672 | 30.052662 |
| S        | 24.859711 | 33.524143 | 32.960098 |
| S        | 26.318394 | 29.584681 | 31.249729 |
| S        | 25.849466 | 33.939346 | 28.436373 |
| S        | 28.114769 | 29.696598 | 26.868414 |
| S        | 30.787554 | 30.626198 | 30.443981 |
| S        | 31.467657 | 26.755310 | 27.278103 |
| S        | 32.778484 | 30.906545 | 25.181854 |
| S        | 33.416893 | 26.454494 | 23.299999 |
| S        | 36.320610 | 27.937931 | 27.021620 |

24 generated by VMD

| Ca       | 18.509180 | 33.097031 | 33.804199 |
|  Ca      |  5 Ca  |  10 Ca |
|---------|--------|--------|
| 22.711994 | 35.070908 | 35.586666 |
| 23.545029 | 30.390606 | 33.204594 |
| 22.627899 | 34.457352 | 30.309593 |
| 24.997211 | 30.570517 | 28.040972 |
| 27.861588 | 32.615700 | 31.383888 |
| 28.908333 | 27.855778 | 29.688103 |
| 30.577759 | 32.185829 | 27.678146 |
| 30.593508 | 28.111055 | 24.621098 |
| 33.673763 | 29.647160 | 28.160332 |
| 34.529896 | 24.919800 | 26.467213 |
| 35.602287 | 29.075157 | 23.813183 |
| 21.261349 | 31.898163 | 35.653980 |
| 20.444086 | 35.655521 | 32.837112 |
| 21.852842 | 31.119259 | 29.910709 |
| 24.904636 | 33.720047 | 33.079334 |
| 26.497229 | 29.601334 | 31.184799 |
| 25.735378 | 33.952782 | 28.413628 |
| 28.003971 | 29.784748 | 26.820347 |
| 30.752922 | 30.846531 | 30.414948 |
| 31.501747 | 26.611570 | 27.376232 |
| 32.613373 | 30.778994 | 25.167755 |
| 33.466652 | 26.522522 | 23.371908 |
| 36.477497 | 27.811718 | 26.951324 |

24

generated by VMD

|  Ca      |  5 Ca  |  10 Ca |
|---------|--------|--------|
| 18.081749 | 32.919365 | 33.808277 |
| 22.741125 | 34.972862 | 35.375435 |
| 23.526457 | 30.279795 | 33.167423 |
| 22.782667 | 34.546421 | 30.528637 |
| 24.801754 | 30.854216 | 27.943771 |
| 27.893930 | 32.850128 | 31.343508 |
| 29.069620 | 27.904100 | 29.682705 |
| 30.579338 | 32.413418 | 27.522030 |
| 30.378893 | 28.029491 | 24.672409 |
| 33.846107 | 29.868692 | 27.930073 |
| 34.292130 | 24.706108 | 26.581673 |
| 35.795818 | 28.771553 | 23.800880 |
| 21.102106 | 31.519655 | 35.599045 |
| 20.336800 | 35.446968 | 33.024338 |
| 21.852619 | 31.080513 | 29.888475 |
| 25.016962 | 33.664192 | 33.250587 |
| 26.348083 | 29.937292 | 31.102985 |
| 25.877674 | 34.026287 | 28.682858 |
| 28.025438 | 29.955711 | 26.679775 |
| 31.049845 | 31.050150 | 30.189734 |
| 31.049845 | 26.998346 | 27.650557 |
|   |   |   |   |
|---|---|---|---|
| S | 32.840069 | 30.863667 | 24.934856 |
| S | 33.346931 | 26.117624 | 23.640221 |
| S | 36.410564 | 27.523499 | 26.939777 |

24

generated by VMD

| Ca |   |   |   |
|----|---|---|---|
| 18.337189 | 32.882832 | 33.405052 |
| 22.716370 | 34.671009 | 35.596291 |
| 23.538383 | 30.098301 | 32.975136 |
| 22.863815 | 34.899185 | 30.580482 |
| 24.979494 | 30.765795 | 27.964451 |
| 27.691187 | 32.648026 | 31.220222 |
| 29.329281 | 27.902130 | 29.917107 |
| 30.285784 | 32.718502 | 27.451283 |
| 30.500565 | 27.863121 | 25.130573 |
| 33.530228 | 29.832939 | 28.050299 |
| 34.510159 | 24.943752 | 26.686411 |
| 35.336464 | 28.786648 | 23.497887 |
| S | 21.146866 | 31.475416 | 35.284916 |
| S | 20.351831 | 35.812538 | 33.101479 |
| S | 22.126362 | 31.357250 | 29.968056 |
| S | 24.826868 | 33.476936 | 30.977771 |
| S | 26.624825 | 29.835644 | 31.192581 |
| S | 25.944357 | 34.271778 | 28.479454 |
| S | 28.304394 | 29.752941 | 26.824421 |
| S | 30.993414 | 30.988300 | 30.396324 |
| S | 31.812849 | 26.766350 | 27.918907 |
| S | 32.432961 | 30.559959 | 24.965229 |
| S | 33.221916 | 26.163532 | 23.461281 |
| S | 36.314564 | 27.827183 | 26.774445 |

24

generated by VMD

| Ca |   |   |   |
|----|---|---|---|
| 18.339888 | 33.102341 | 33.580273 |
| 23.008249 | 34.828766 | 35.718788 |
| 23.306496 | 30.316391 | 32.845234 |
| 22.832108 | 34.485874 | 30.430433 |
| 24.735632 | 30.495136 | 27.921806 |
| 27.956272 | 32.655033 | 31.510975 |
| 29.046398 | 27.938423 | 29.738827 |
| 30.651014 | 32.293549 | 27.689278 |
| 30.333830 | 28.022734 | 24.814978 |
| 33.696964 | 29.925106 | 27.997726 |
| 34.556664 | 24.801817 | 26.600296 |
| 35.605278 | 28.989880 | 23.770256 |
| S | 21.142380 | 31.833916 | 35.569077 |
| S | 20.492329 | 35.847942 | 33.094494 |
| S | 21.600079 | 31.257505 | 29.888657 |
| S  | 24.849655 | 33.606884 | 33.020485 |
|----|-----------|-----------|-----------|
| S  | 26.301163 | 29.619053 | 31.168419 |
| S  | 25.758175 | 33.853729 | 28.436062 |
| S  | 28.236973 | 29.680840 | 26.820061 |
| S  | 31.091246 | 30.880440 | 30.420029 |
| S  | 31.729458 | 26.833544 | 27.698961 |
| S  | 32.551235 | 30.844999 | 24.924179 |
| S  | 33.376709 | 26.284983 | 23.422100 |
| S  | 36.521919 | 27.901173 | 26.858635 |

24 generated by VMD

| Ca | 18.117855 | 33.483963 | 33.540642 |
|----|-----------|-----------|-----------|
| Ca | 22.897516 | 34.620522 | 35.758381 |
| Ca | 23.212757 | 30.222740 | 33.121361 |
| Ca | 22.922960 | 34.719894 | 30.512564 |
| Ca | 24.875736 | 30.378576 | 27.941763 |
| Ca | 27.774277 | 32.783623 | 31.246655 |
| Ca | 29.160603 | 27.983116 | 29.974768 |
| Ca | 30.500793 | 32.439651 | 27.561106 |
| Ca | 30.508549 | 27.900158 | 24.987865 |
| Ca | 33.760399 | 29.838165 | 27.863995 |
| Ca | 34.592163 | 24.788275 | 26.611553 |
| Ca | 35.691624 | 28.939030 | 23.392696 |
| S  | 20.692110 | 31.671919 | 35.391586 |
| S  | 20.634598 | 35.894630 | 33.187782 |
| S  | 21.812065 | 31.262596 | 29.966385 |
| S  | 24.928019 | 33.613617 | 33.199097 |
| S  | 26.220575 | 29.554289 | 31.064978 |
| S  | 25.684883 | 33.749130 | 28.530621 |
| S  | 28.262609 | 29.672901 | 26.915108 |
| S  | 30.804289 | 30.988052 | 30.420919 |
| S  | 32.006046 | 26.734106 | 27.783529 |
| S  | 32.828705 | 30.847187 | 24.827284 |
| S  | 33.303631 | 26.196480 | 23.479887 |
| S  | 36.527332 | 28.017426 | 26.659504 |

24 generated by VMD

| Ca | 18.315342 | 33.590176 | 33.112114 |
|----|-----------|-----------|-----------|
| Ca | 22.811218 | 34.693535 | 35.698055 |
| Ca | 23.228979 | 30.278606 | 33.096275 |
| Ca | 23.026756 | 34.316216 | 30.660271 |
| Ca | 25.087837 | 30.343056 | 28.298798 |
| Ca | 27.856764 | 32.626560 | 31.286617 |
| Ca | 29.154612 | 27.896069 | 30.112797 |
| Ca | 30.511433 | 32.404644 | 27.408524 |
| Ca | 30.494989 | 27.835484 | 24.933548 |
| Ca  | 33.818172 | 29.998135 | 27.904192 |
|-----|-----------|-----------|-----------|
| Ca  | 34.368347 | 25.053556 | 26.583208 |
| Ca  | 35.376999 | 29.054050 | 23.606228 |
| S   | 20.618114 | 31.805429 | 35.290447 |
| S   | 20.703087 | 35.982483 | 33.100559 |
| S   | 21.916733 | 31.067451 | 30.089062 |
| S   | 24.860220 | 33.521259 | 33.011131 |
| S   | 26.208059 | 29.352272 | 31.071604 |
| S   | 26.038832 | 33.741024 | 28.516380 |
| S   | 28.277222 | 29.694912 | 26.946194 |
| S   | 31.085226 | 30.957775 | 30.283840 |
| S   | 31.873980 | 26.887131 | 27.939026 |
| S   | 32.464375 | 30.684669 | 25.038776 |
| S   | 33.101154 | 26.350965 | 23.396179 |
| S   | 36.521519 | 27.914627 | 26.556221 |

24 generated by VMD

| Ca  | 18.233149 | 33.389534 | 33.556118 |
|-----|-----------|-----------|-----------|
| Ca  | 22.726698 | 34.594666 | 35.778687 |
| Ca  | 23.311216 | 30.223782 | 32.990334 |
| Ca  | 22.864313 | 34.770462 | 30.443935 |
| Ca  | 24.779472 | 30.496410 | 28.081402 |
| Ca  | 27.899323 | 32.680984 | 31.159389 |
| Ca  | 29.191936 | 28.069845 | 30.152885 |
| Ca  | 30.628979 | 32.428066 | 27.466747 |
| Ca  | 30.372616 | 27.922804 | 25.008638 |
| Ca  | 33.933075 | 29.824909 | 27.952911 |
| Ca  | 34.551117 | 24.908619 | 26.494488 |
| Ca  | 35.478092 | 29.049309 | 23.685001 |
| S   | 20.943621 | 31.447605 | 35.279823 |
| S   | 20.550652 | 35.875160 | 33.139622 |
| S   | 21.778881 | 31.159893 | 29.889812 |
| S   | 24.829313 | 33.606457 | 33.189255 |
| S   | 26.484356 | 29.606220 | 30.926544 |
| S   | 25.700920 | 33.883980 | 28.412186 |
| S   | 28.219261 | 29.748594 | 27.016628 |
| S   | 31.053341 | 31.126396 | 30.327757 |
| S   | 31.882191 | 26.924561 | 27.944775 |
| S   | 32.646431 | 30.614170 | 24.920713 |
| S   | 33.055496 | 26.304808 | 23.483891 |
| S   | 36.605694 | 27.642784 | 26.638527 |

24 generated by VMD

| Ca  | 18.8383615 | 33.348282 | 33.786121 |
|-----|------------|-----------|-----------|
| Ca  | 22.933743 | 34.708794 | 35.725620 |
| Ca  | 23.534922 | 30.242947 | 32.961044 |
| Element | X1  | Y1  | Z1  |
|---------|-----|-----|-----|
| Ca      | 22.833899 | 34.770912 | 30.135202 |
| Ca      | 24.749352 | 30.298847 | 27.913628 |
| Ca      | 27.888500 | 32.622025 | 31.305410 |
| Ca      | 29.187136 | 27.928955 | 30.013294 |
| Ca      | 30.578272 | 32.344852 | 27.776093 |
| Ca      | 30.328863 | 28.093607 | 24.643095 |
| Ca      | 33.678955 | 30.123840 | 27.953728 |
| Ca      | 34.358181 | 24.866993 | 26.516083 |
| Ca      | 35.683449 | 29.055267 | 23.953381 |
| S       | 21.101290 | 31.569492 | 35.448154 |
| S       | 20.811747 | 35.809471 | 32.947193 |
| S       | 21.796787 | 31.218582 | 29.918957 |
| S       | 24.753660 | 33.658440 | 33.055275 |
| S       | 26.163803 | 29.330139 | 31.050480 |
| S       | 25.859541 | 33.680264 | 28.420475 |
| S       | 28.251183 | 29.719578 | 27.025124 |
| S       | 30.931021 | 31.071037 | 30.386927 |
| S       | 31.688799 | 27.004145 | 27.648998 |
| S       | 32.569183 | 30.755932 | 25.079105 |
| S       | 33.193676 | 26.283222 | 23.443653 |
| S       | 36.460560 | 27.794445 | 26.833006 |
|    | 18.215921 | 33.281952 | 33.851540 |
|----|-----------|-----------|-----------|
| Ca | 22.915232 | 34.126991 | 35.909454 |
| Ca | 23.205456 | 30.393749 | 32.757267 |
| Ca | 23.049322 | 34.774708 | 30.447477 |
| Ca | 24.913237 | 30.600027 | 27.498108 |
| Ca | 27.963070 | 32.837685 | 31.322699 |
| Ca | 29.071136 | 27.906303 | 29.842785 |
| Ca | 30.523216 | 32.363701 | 27.430515 |
| Ca | 30.371759 | 27.698568 | 24.872963 |
| Ca | 33.880821 | 30.181761 | 28.000904 |
| Ca | 34.583576 | 24.943218 | 26.911217 |
| Ca | 35.188122 | 28.957844 | 23.661182 |
| S  | 20.869247 | 31.373735 | 35.328384 |
| S  | 20.754330 | 35.769993 | 33.314854 |
| S  | 22.071037 | 31.411560 | 29.721668 |
| S  | 25.009836 | 33.628689 | 33.141846 |
| S  | 26.114439 | 29.696590 | 30.902975 |
| S  | 25.853260 | 33.993927 | 28.433895 |
| S  | 28.195345 | 29.634403 | 26.807434 |
| S  | 30.858809 | 31.084822 | 30.200199 |
| S  | 32.011726 | 26.996384 | 28.171623 |
| S  | 32.487503 | 30.658047 | 24.960772 |
| S  | 33.232857 | 26.031126 | 23.686401 |
| S  | 36.380798 | 27.954277 | 26.763887 |

24 generated by VMD

|    | 18.140266 | 33.400459 | 33.647293 |
|----|-----------|-----------|-----------|
| Ca | 22.771126 | 34.317562 | 36.254414 |
| Ca | 23.234734 | 30.589920 | 32.556435 |
| Ca | 22.881130 | 34.908669 | 30.731060 |
| Ca | 24.813560 | 30.501141 | 27.769577 |
| Ca | 27.787058 | 32.753616 | 31.395536 |
| Ca | 29.014322 | 27.843102 | 29.913624 |
| Ca | 30.441835 | 32.221870 | 27.186354 |
| Ca | 30.411194 | 27.536930 | 24.721136 |
| Ca | 33.747120 | 30.004635 | 27.993229 |
| Ca | 34.841637 | 25.273357 | 26.807381 |
| Ca | 35.692001 | 28.857254 | 23.486496 |
| S  | 20.902735 | 31.555962 | 35.084908 |
| S  | 20.720922 | 35.844112 | 33.520584 |
| S  | 21.912216 | 31.498165 | 29.786880 |
| S  | 24.990211 | 33.834976 | 33.370811 |
| S  | 26.058350 | 29.513367 | 30.945248 |
| S     | 25.692602 | 33.909275 | 28.625914 |
| S     | 28.103380 | 29.465080 | 26.749249 |
| S     | 30.827394 | 31.058327 | 30.116611 |
| S     | 32.056122 | 26.774662 | 28.037994 |
| S     | 32.602730 | 30.458099 | 24.865849 |
| S     | 33.435692 | 26.089304 | 23.488171 |
| S     | 36.641689 | 28.090225 | 26.885300 |

24

generated by VMD

| Ca    | 18.501318 | 33.469601 | 33.807831 |
| Ca    | 23.045809 | 34.320873 | 35.870125 |
| Ca    | 23.340528 | 30.296978 | 32.955883 |
| Ca    | 23.007967 | 34.866043 | 30.427383 |
| Ca    | 24.771864 | 30.397707 | 27.823130 |
| Ca    | 27.634491 | 32.642422 | 30.927567 |
| Ca    | 28.990730 | 28.017900 | 29.958220 |
| Ca    | 30.489880 | 32.255291 | 27.382566 |
| Ca    | 30.258070 | 27.795807 | 24.678873 |
| Ca    | 33.840939 | 30.094259 | 28.095985 |
| Ca    | 34.585182 | 25.148693 | 26.713734 |
| Ca    | 35.567123 | 29.083782 | 23.897572 |
| S     | 20.891743 | 31.448769 | 35.414017 |
| S     | 20.938725 | 35.949577 | 33.204712 |
| S     | 21.847439 | 31.422039 | 29.974636 |
| S     | 24.981312 | 33.523945 | 33.000763 |
| S     | 25.999718 | 29.449978 | 30.845646 |
| S     | 25.725620 | 33.937042 | 28.441872 |
| S     | 28.169001 | 29.239698 | 26.798069 |
| S     | 30.815125 | 31.120380 | 30.351509 |
| S     | 31.863842 | 26.914936 | 27.749405 |
| S     | 32.585262 | 30.613297 | 25.122961 |
| S     | 33.350662 | 26.323883 | 23.430630 |
| S     | 36.517719 | 27.967163 | 27.063271 |

24

generated by VMD

| Ca    | 18.391359 | 33.636215 | 33.907509 |
| Ca    | 23.074327 | 34.516182 | 35.842545 |
| Ca    | 23.107553 | 30.251541 | 32.984375 |
| Ca    | 22.846991 | 34.617371 | 30.598633 |
| Ca    | 24.819719 | 30.392046 | 27.760765 |
| Ca    | 27.721590 | 32.675682 | 31.168045 |
| Ca    | 29.043003 | 27.864115 | 29.861393 |
| Ca    | 30.340132 | 32.384178 | 27.544779 |
| Ca    | 30.428698 | 27.853588 | 24.483862 |
| Ca    | 33.726841 | 30.046131 | 27.827337 |
| Ca    | 34.537560 | 25.063168 | 26.837883 |
| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 35.754597 | 28.884895 | 24.067930 |
| S       | 21.117247  | 31.754328  | 35.280586  |
| S       | 20.924898  | 35.900101  | 33.618393  |
| S       | 21.816893  | 31.130283  | 29.815674  |
| S       | 24.955677  | 33.482491  | 33.026054  |
| S       | 26.028141  | 29.423046  | 30.693470  |
| S       | 25.618952  | 33.939644  | 28.351009  |
| S       | 28.158825  | 29.626867  | 26.707500  |
| S       | 30.717480  | 31.090046  | 30.195164  |
| S       | 31.810755  | 26.843254  | 27.724857  |
| S       | 32.585621  | 30.627655  | 25.017292  |
| S       | 33.670528  | 26.367849  | 23.499382  |
| S       | 36.522671  | 27.929398  | 27.125576  |

24 generated by VMD

| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 18.288252 | 33.611954 | 33.965996 |
| Ca      | 22.950216  | 34.689537  | 35.836933  |
| Ca      | 23.483891  | 30.224922  | 32.811127  |
| Ca      | 22.794518  | 34.560963  | 30.555737  |
| Ca      | 24.694418  | 30.454084  | 27.741699  |
| Ca      | 27.748243  | 32.655209  | 31.200502  |
| Ca      | 29.127213  | 27.798332  | 29.749819  |
| Ca      | 30.467159  | 32.365788  | 27.560074  |
| Ca      | 30.449680  | 27.999737  | 24.626549  |
| Ca      | 33.957943  | 29.963406  | 28.218365  |
| Ca      | 34.655701  | 25.083115  | 26.685877  |
| Ca      | 35.669731  | 28.793205  | 23.883595  |
| S       | 21.022766  | 31.696287  | 35.484787  |
| S       | 20.732800  | 35.969631  | 33.241455  |
| S       | 21.918764  | 31.023289  | 29.773434  |
| S       | 24.747469  | 33.620876  | 33.163422  |
| S       | 26.156342  | 29.345982  | 30.912106  |
| S       | 25.615696  | 33.812572  | 28.406445  |
| S       | 28.253723  | 29.805605  | 26.807972  |
| S       | 30.690285  | 31.123718  | 30.397110  |
| S       | 31.953394  | 26.958057  | 27.769737  |
| S       | 32.786850  | 30.681843  | 24.999146  |
| S       | 33.314137  | 26.235039  | 23.223076  |
| S       | 36.240932  | 27.826889  | 26.925085  |

24 generated by VMD

| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 18.256886  | 32.983692  | 33.665562  |
| Ca      | 22.961716  | 34.733364  | 35.880817  |
| Ca      | 23.483603  | 30.666912  | 32.778702  |
| Ca      | 23.031828  | 34.761902  | 30.895641  |
| Ca      | 24.572275  | 30.550819  | 27.632833  |
| Element | 1st Value     | 2nd Value     | 3rd Value     |
|---------|---------------|---------------|---------------|
| Ca      | 27.792473     | 32.720093     | 31.222275     |
| Ca      | 29.051764     | 27.802235     | 29.792362     |
| Ca      | 30.555634     | 32.239388     | 27.469650     |
| Ca      | 30.386309     | 27.896564     | 24.744827     |
| Ca      | 33.875641     | 29.970219     | 27.935114     |
| Ca      | 34.683048     | 25.193096     | 26.705446     |
| Ca      | 35.515076     | 28.624725     | 23.788551     |
| S       | 20.880877     | 31.656811     | 35.382378     |
| S       | 20.683186     | 35.573044     | 33.327885     |
| S       | 21.809916     | 31.148186     | 29.820051     |
| S       | 25.003548     | 33.895592     | 33.174423     |
| S       | 26.219473     | 29.675285     | 30.639004     |
| S       | 25.660175     | 34.104881     | 28.660658     |
| S       | 28.023396     | 29.610392     | 26.552376     |
| S       | 30.832453     | 30.764364     | 30.352581     |
| S       | 31.938520     | 26.922562     | 27.916481     |
| S       | 32.620041     | 30.646845     | 25.071018     |
| S       | 33.346844     | 26.181953     | 23.474453     |
| S       | 36.535309     | 27.977137     | 27.056953     |

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generated by VMD

| Element | 1st Value     | 2nd Value     | 3rd Value     |
|---------|---------------|---------------|---------------|
| Ca      | 18.183144     | 33.170727     | 33.617264     |
| Ca      | 22.827135     | 34.603676     | 35.742218     |
| Ca      | 23.399073     | 30.675350     | 32.768661     |
| Ca      | 23.179441     | 34.456787     | 30.628558     |
| Ca      | 24.895815     | 30.460903     | 27.862633     |
| Ca      | 27.862963     | 32.713692     | 31.419254     |
| Ca      | 29.050888     | 27.925938     | 29.811178     |
| Ca      | 30.626991     | 32.519619     | 27.633839     |
| Ca      | 30.349857     | 27.955399     | 24.614300     |
| Ca      | 33.885937     | 30.084900     | 27.956406     |
| Ca      | 34.662437     | 25.101955     | 26.714706     |
| Ca      | 35.161682     | 28.853245     | 23.539299     |
| S       | 20.836512     | 31.625614     | 35.451080     |
| S       | 20.678553     | 35.744434     | 33.278324     |
| S       | 21.853588     | 31.110268     | 29.703642     |
| S       | 24.925432     | 33.695148     | 32.984840     |
| S       | 26.185869     | 29.414001     | 31.052280     |
| S       | 25.854109     | 33.910233     | 28.515858     |
| S       | 28.293583     | 29.740944     | 26.811251     |
| S       | 31.011536     | 31.065603     | 30.291222     |
| S       | 31.927095     | 26.926720     | 27.857746     |
| S       | 32.638130     | 30.631182     | 25.192192     |
| S       | 32.962971     | 26.007410     | 23.369892     |
| S       | 36.467270     | 27.906326     | 27.123362     |

24
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.373150 | 33.307903 | 33.672798 |
| Ca      | 23.148121  | 34.456566  | 35.608150  |
| Ca      | 23.503527  | 30.183126  | 32.784477  |
| Ca      | 22.710583  | 34.683624  | 30.670883  |
| Ca      | 24.627222  | 30.661127  | 27.952469  |
| Ca      | 28.014729  | 32.895206  | 31.232037  |
| Ca      | 29.041931  | 28.065102  | 29.657284  |
| Ca      | 30.642895  | 32.343819  | 27.236885  |
| Ca      | 30.183979  | 28.030350  | 24.678135  |
| Ca      | 33.936104  | 29.993721  | 28.108597  |
| Ca      | 34.507504  | 25.149712  | 26.845531  |
| Ca      | 35.349373  | 28.691170  | 23.837223  |
| S       | 20.993973  | 31.498890  | 35.297646  |
| S       | 20.593910  | 35.589577  | 33.281528  |
| S       | 21.593010  | 31.323360  | 29.669563  |
| S       | 24.897585  | 33.399498  | 33.033840  |
| S       | 26.231653  | 29.656193  | 30.966850  |
| S       | 25.851761  | 33.931709  | 28.759073  |
| S       | 28.114498  | 29.700651  | 26.854794  |
| S       | 31.081459  | 31.197018  | 30.235935  |
| S       | 31.856998  | 27.132948  | 27.899963  |
| S       | 32.663246  | 30.551716  | 25.083691  |
| S       | 33.115170  | 26.109316  | 23.554092  |
| S       | 36.687660  | 27.747761  | 27.018585  |

24

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.402937 | 33.867111 | 33.600464 |
| Ca      | 23.248732 | 34.502644 | 35.801121 |
| Ca      | 23.35029  | 30.230988 | 32.944977 |
| Ca      | 22.673330 | 34.330898 | 30.881783 |
| Ca      | 24.688812 | 30.598110 | 27.583672 |
| Ca      | 27.707617 | 32.720722 | 31.006294 |
| Ca      | 28.964243 | 27.876438 | 29.764038 |
| Ca      | 30.554230 | 32.500031 | 27.306931 |
| Ca      | 30.418600 | 27.948074 | 24.802471 |
| Ca      | 33.970310 | 30.023388 | 28.020468 |
| Ca      | 34.704315 | 24.771713 | 26.736961 |
| Ca      | 35.377197 | 29.054457 | 23.968500 |
| S       | 20.819160 | 31.672243 | 35.088783 |
| S       | 21.090919 | 35.864197 | 33.659039 |
| S       | 21.697262 | 30.727192 | 29.781704 |
| S       | 24.833918 | 33.589455 | 32.949322 |
| S       | 26.214735 | 29.524162 | 30.900867 |
| S       | 25.510939 | 33.816029 | 28.495153 |
| S       | 28.152084 | 29.664640 | 26.747311 |
|    | 30.955599 | 31.169453 | 30.232946 |
|----|-----------|-----------|-----------|
| S  | 31.936266 | 27.043858 | 27.794058 |
| S  | 32.749283 | 30.830858 | 25.309679 |
| S  | 33.136654 | 26.171036 | 23.629740 |
| S  | 36.558887 | 27.802349 | 26.933758 |
|    | 33.136654 | 26.171036 | 23.629740 |

24 generated by VMD

|    | 18.163960 | 33.300972 | 33.791325 |
|----|-----------|-----------|-----------|
| Ca | 23.046513 | 34.475914 | 35.900040 |
| Ca | 23.521008 | 30.299973 | 32.626358 |
| Ca | 22.755146 | 34.541534 | 31.016457 |
| Ca | 24.920998 | 30.845863 | 27.536514 |
| Ca | 27.881382 | 32.833790 | 31.216412 |
| Ca | 28.976719 | 27.832731 | 29.700186 |
| Ca | 30.423122 | 32.272915 | 27.313196 |
| Ca | 30.511999 | 28.009329 | 24.486977 |
| Ca | 33.872372 | 30.216888 | 28.060969 |
| Ca | 34.517395 | 24.890558 | 26.961140 |
| Ca | 35.331020 | 28.627510 | 23.750523 |
| S  | 21.017231 | 31.461777 | 35.287018 |
| S  | 20.675999 | 35.667767 | 33.488106 |
| S  | 21.670061 | 31.101503 | 29.699165 |
| S  | 24.750500 | 33.715302 | 33.252682 |
| S  | 26.276932 | 29.839127 | 30.736204 |
| S  | 25.731508 | 34.266060 | 28.700455 |
| S  | 28.268980 | 29.547798 | 26.609188 |
| S  | 30.914265 | 31.189642 | 30.185966 |
| S  | 31.886972 | 27.084553 | 27.878029 |
| S  | 32.710182 | 30.679893 | 24.973766 |
| S  | 33.302761 | 25.725222 | 23.629831 |
| S  | 36.593040 | 27.873436 | 27.139793 |

24 generated by VMD

|    | 18.521154 | 33.046707 | 33.542576 |
|----|-----------|-----------|-----------|
| Ca | 22.989552 | 34.315414 | 36.075249 |
| Ca | 23.424320 | 30.425211 | 32.646732 |
| Ca | 22.557528 | 34.582413 | 30.744038 |
| Ca | 25.006882 | 30.847799 | 27.576574 |
| Ca | 27.767900 | 32.955269 | 31.367437 |
| Ca | 29.149952 | 28.084633 | 29.659184 |
| Ca | 30.506142 | 32.515259 | 27.361423 |
| Ca | 30.383389 | 27.997046 | 24.609789 |
| Ca | 33.708210 | 30.033806 | 28.182194 |
| Ca | 34.445301 | 24.685246 | 26.854633 |
| Ca | 35.411324 | 28.566452 | 23.795033 |
| S  | 21.276932 | 31.408901 | 35.220367 |
S  20.646605  35.506310  33.580177
S  22.040995  30.971363  29.640949
S  24.873817  34.022343  33.081474
S  26.284603  29.843212  30.777252
S  25.527361  34.175720  28.570477
S  28.232376  29.825191  26.661337
S  30.852283  31.247807  30.165043
S  31.948170  27.013321  28.035099
S  32.689476  30.668570  25.094448
S  30.021626  25.797266  23.661339
S  36.545052  27.764740  27.037218

24 generated by VMD
Ca  18.385756  33.217484  33.668968
Ca  22.931089  34.391815  36.172325
Ca  23.538078  30.804928  32.649715
Ca  22.573368  34.688232  30.588612
Ca  24.936075  30.575068  27.884228
Ca  27.879169  32.937622  31.372160
Ca  28.985325  27.898441  29.829927
Ca  30.570269  32.386086  27.231182
Ca  30.660208  27.743443  24.516872
Ca  33.598957  29.987944  28.174931
Ca  34.391335  24.760057  26.678892
Ca  35.637577  28.997545  23.770943
S  21.118732  31.551556  35.357174
S  20.580639  35.616352  33.478165
S  21.754036  30.964056  29.874962
S  24.783636  34.157032  32.959145
S  26.355530  29.786777  30.874941
S  25.561132  33.981846  28.748266
S  28.252424  29.535557  26.679491
S  30.762332  31.007254  30.280354
S  31.674976  26.757328  27.730274
S  32.842545  30.664516  24.943199
S  33.677010  26.021177  23.410662
S  36.269932  27.867931  27.067200

24 generated by VMD
Ca  18.480263  32.989464  33.840019
Ca  23.255613  34.531563  36.000538
Ca  23.584822  30.285954  32.952225
Ca  22.645355  34.748299  30.504066
Ca  24.939419  30.535168  27.554678
Ca  27.551702  32.682587  31.043058
Ca  28.955973  27.978798  29.709442
| Ca   | 30.739578 | 32.767857 | 27.316292 |
| Ca   | 30.445608 | 27.954191 | 24.583359 |
| Ca   | 33.435757 | 30.038887 | 28.097878 |
| Ca   | 34.365509 | 24.698856 | 26.917017 |
| Ca   | 35.641731 | 28.888447 | 23.847778 |
| S    | 21.201872 | 31.564650 | 35.646328 |
| S    | 20.664782 | 35.676300 | 33.403122 |
| S    | 21.925161 | 31.189651 | 29.785847 |
| S    | 24.779627 | 33.855408 | 33.006493 |
| S    | 25.990400 | 29.441578 | 30.812428 |
| S    | 25.658140 | 33.934170 | 28.377842 |
| S    | 28.434607 | 30.012651 | 26.641197 |
| S    | 30.627800 | 31.165377 | 30.185677 |
| S    | 31.791567 | 26.866610 | 27.937290 |
| S    | 32.848698 | 30.819118 | 25.059868 |
| S    | 33.365219 | 26.055361 | 23.656860 |
| S    | 36.390877 | 27.619106 | 27.060715 |

24

generated by VMD

| Ca   | 18.510540 | 33.095566 | 33.651917 |
| Ca   | 23.013145 | 34.771263 | 36.140991 |
| Ca   | 23.292341 | 30.513725 | 32.710972 |
| Ca   | 22.731703 | 34.629055 | 30.784428 |
| Ca   | 24.931215 | 30.381855 | 27.512115 |
| Ca   | 27.837402 | 32.587093 | 31.380692 |
| Ca   | 28.839720 | 27.949413 | 29.625988 |
| Ca   | 30.406033 | 32.382378 | 27.463493 |
| Ca   | 30.444426 | 27.842363 | 24.614527 |
| Ca   | 33.744801 | 30.131874 | 27.947739 |
| Ca   | 34.366959 | 24.859985 | 26.825695 |
| Ca   | 35.680187 | 28.903027 | 23.996330 |
| S    | 21.266382 | 31.850052 | 35.191341 |
| S    | 20.732508 | 35.937519 | 33.612225 |
| S    | 21.817854 | 30.990826 | 29.673397 |
| S    | 24.941326 | 33.660416 | 33.102230 |
| S    | 26.189133 | 29.576143 | 30.812019 |
| S    | 25.566351 | 33.819855 | 28.685837 |
| S    | 28.239798 | 29.588036 | 26.443504 |
| S    | 30.679464 | 31.085884 | 30.299927 |
| S    | 31.841022 | 26.943533 | 27.863468 |
| S    | 32.681385 | 30.776791 | 24.960741 |
| S    | 33.426014 | 26.119160 | 23.595013 |
| S    | 36.540333 | 27.904243 | 27.045441 |

24

generated by VMD

| Ca   | 18.384176 | 32.756275 | 33.867584 |
|  | Ca   |  | S   |  |  |
|---|---|---|---|---|---|
| Ca | 23.055391 | 35.023766 | 35.753700 |  |  |
| Ca | 23.477024 | 30.446405 | 32.778366 |  |  |
| Ca | 22.714769 | 34.663254 | 30.525707 |  |  |
| Ca | 24.830942 | 30.420467 | 27.802513 |  |  |
| Ca | 27.851486 | 32.832275 | 31.215803 |  |  |
| Ca | 29.079765 | 27.780851 | 29.866623 |  |  |
| Ca | 30.497078 | 32.455467 | 27.617760 |  |  |
| Ca | 30.655844 | 28.092941 | 24.401915 |  |  |
| Ca | 33.676594 | 29.832619 | 28.217869 |  |  |
| Ca | 34.347092 | 24.666893 | 26.564199 |  |  |
| Ca | 35.446579 | 29.128452 | 23.858292 |  |  |
| S  | 21.163763 | 31.881454 | 35.541492 |  |  |
| S  | 20.508711 | 35.790131 | 33.265606 |  |  |
| S  | 21.717175 | 31.130140 | 29.886215 |  |  |
| S  | 24.891438 | 33.791824 | 33.001293 |  |  |
| S  | 26.162781 | 29.445507 | 31.011669 |  |  |
| S  | 25.722404 | 33.934570 | 28.527298 |  |  |
| S  | 28.121805 | 29.659077 | 26.662773 |  |  |
| S  | 30.761314 | 31.094971 | 30.429047 |  |  |
| S  | 31.697693 | 26.844698 | 27.491808 |  |  |
| S  | 32.932854 | 30.742498 | 25.275766 |  |  |
| S  | 33.569725 | 26.033085 | 23.358372 |  |  |
| S  | 36.453667 | 27.852440 | 27.018335 |  |  |

24 generated by VMD

|  | Ca   |  | S   |  |  |
|---|---|---|---|---|---|
| Ca | 18.307636 | 32.857224 | 33.908875 |  |  |
| Ca | 23.079369 | 34.698650 | 35.934738 |  |  |
| Ca | 23.07482 | 30.685291 | 33.115910 |  |  |
| Ca | 23.058905 | 34.563469 | 30.600327 |  |  |
| Ca | 24.749914 | 30.441341 | 27.643646 |  |  |
| Ca | 27.803730 | 32.861446 | 31.182264 |  |  |
| Ca | 28.669306 | 28.007975 | 29.783268 |  |  |
| Ca | 30.449364 | 32.380821 | 27.379248 |  |  |
| Ca | 30.589596 | 28.010979 | 24.498812 |  |  |
| Ca | 33.576237 | 29.986147 | 28.112379 |  |  |
| Ca | 34.210136 | 24.837780 | 26.739128 |  |  |
| Ca | 35.812046 | 29.016619 | 23.997719 |  |  |
| S  | 21.166164 | 31.692011 | 35.414665 |  |  |
| S  | 20.596231 | 35.418610 | 33.153553 |  |  |
| S  | 21.979893 | 31.152252 | 29.931107 |  |  |
| S  | 24.903196 | 33.927692 | 33.075256 |  |  |
| S  | 26.157885 | 29.705841 | 30.996740 |  |  |
| S  | 25.811270 | 33.930340 | 28.365192 |  |  |
| S  | 28.147486 | 29.578938 | 26.681675 |  |  |
| S  | 30.773726 | 30.989388 | 30.200878 |  |  |
| S  | 31.682335 | 26.928787 | 27.775482 |  |  |
| Element | X Position     | Y Position     | Z Position     |
|---------|----------------|----------------|----------------|
| S       | 32.838997      | 30.710808      | 25.097227      |
| S       | 33.568642      | 26.349419      | 23.450291      |
| S       | 36.480480      | 27.568222      | 26.901623      |

24 generated by VMD

| Element | X Position     | Y Position     | Z Position     |
|---------|----------------|----------------|----------------|
| Ca      | 18.452087      | 33.234821      | 33.751274      |
| Ca      | 23.139324      | 34.871376      | 35.799057      |
| Ca      | 23.411705      | 30.447201      | 32.890884      |
| Ca      | 22.905649      | 34.631821      | 30.262110      |
| Ca      | 24.678728      | 30.161209      | 27.931484      |
| Ca      | 27.630861      | 32.620651      | 31.147078      |
| Ca      | 29.024639      | 27.728268      | 30.027132      |
| Ca      | 30.403137      | 32.155884      | 27.668203      |
| Ca      | 30.645935      | 28.157969      | 24.542019      |
| Ca      | 33.719116      | 29.932371      | 28.178770      |
| Ca      | 34.243862      | 24.849804      | 26.478294      |
| Ca      | 35.544838      | 29.513298      | 23.790195      |
| S       | 21.209192      | 31.952816      | 35.567574      |
| S       | 20.838703      | 35.561234      | 32.897415      |
| S       | 21.835207      | 31.125805      | 29.775400      |
| S       | 25.019661      | 33.790466      | 32.987343      |
| S       | 26.208506      | 29.433159      | 31.210283      |
| S       | 25.714886      | 33.774609      | 28.328228      |
| S       | 28.117880      | 29.445230      | 26.962101      |
| S       | 30.716497      | 30.916557      | 30.449076      |
| S       | 31.573376      | 26.972118      | 27.770725      |
| S       | 32.815540      | 30.885712      | 25.450443      |
| S       | 33.489719      | 26.504993      | 23.352497      |
| S       | 36.380966      | 27.632713      | 26.722410      |

24 generated by VMD

| Element | X Position     | Y Position     | Z Position     |
|---------|----------------|----------------|----------------|
| Ca      | 18.308809      | 33.086414      | 33.573860      |
| Ca      | 22.746250      | 34.567150      | 35.860680      |
| Ca      | 23.490303      | 30.466764      | 33.046459      |
| Ca      | 23.024195      | 34.618069      | 30.422092      |
| Ca      | 25.104967      | 30.493771      | 27.904884      |
| Ca      | 27.858398      | 32.869854      | 31.346066      |
| Ca      | 29.070095      | 27.923870      | 29.958971      |
| Ca      | 30.561621      | 32.478699      | 27.350256      |
| Ca      | 30.408703      | 27.861074      | 24.533440      |
| Ca      | 33.559174      | 30.013172      | 28.327171      |
| Ca      | 34.284294      | 24.892853      | 26.524082      |
| Ca      | 35.377224      | 28.931610      | 23.593048      |
| S       | 20.961390      | 31.633598      | 35.405128      |
| S       | 20.525953      | 35.598782      | 33.072166      |
| S       | 22.160608      | 31.102560      | 29.872269      |
|   | 24 generated by VMD |
|---|-------------------|
| S | 24.903435         |
| S | 26.269165         |
| S | 25.857012         |
| S | 28.368803         |
| S | 30.795145         |
| S | 31.751043         |
| S | 32.776379         |
| S | 33.157471         |
| S | 36.399612         |
| Ca| 18.467626         |
| Ca| 22.762264         |
| Ca| 23.575130         |
| Ca| 23.009014         |
| Ca| 25.219664         |
| Ca| 27.914434         |
| Ca| 28.996071         |
| Ca| 30.699581         |
| Ca| 30.383360         |
| Ca| 33.495289         |
| Ca| 34.052391         |
| Ca| 35.322132         |
| S | 21.141062         |
| S | 20.538095         |
| S | 22.045614         |
| S | 24.858667         |
| S | 26.567347         |
| S | 25.743839         |
| S | 28.534622         |
| S | 30.930471         |
| S | 31.545547         |
| S | 32.699133         |
| S | 33.108864         |
| S | 36.110695         |
| Ca| 18.168379         |
| Ca| 22.651438         |
| Ca| 23.492792         |
| Ca| 22.820202         |
| Ca| 25.087173         |
| Ca| 27.778368         |
| Ca| 29.051332         |
| Ca| 30.616810         |
| Ca| 30.719152         |
|   |   |   |
|---|---|---|
| Ca | 33.511845 | 29.616478 | 28.309107 |
| Ca | 34.222569 | 24.760841 | 26.189392 |
| Ca | 35.501774 | 29.116062 | 23.651085 |
| S  | 20.953867 | 31.958817 | 35.672958 |
| S  | 20.650690 | 35.781311 | 32.755726 |
| S  | 22.133438 | 30.856119 | 30.043350 |
| S  | 24.901558 | 33.850842 | 32.983562 |
| S  | 26.426435 | 29.483372 | 31.331882 |
| S  | 25.820976 | 33.644279 | 28.508453 |
| S  | 28.220894 | 29.611996 | 26.688107 |
| S  | 30.647886 | 30.960007 | 30.440208 |
| S  | 31.837303 | 26.952394 | 27.676743 |
| S  | 32.762844 | 31.094114 | 25.213547 |
| S  | 33.428802 | 26.488214 | 23.118919 |
| S  | 36.313507 | 27.769333 | 26.838985 |

24

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generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.480185 | 33.155334 | 34.033257 |
| Ca | 22.650560 | 34.799694 | 35.583076 |
| Ca | 23.339134 | 30.482918 | 33.167580 |
| Ca | 22.870010 | 34.431263 | 30.164864 |
| Ca | 24.962355 | 30.495121 | 27.990059 |
| Ca | 27.837967 | 32.650230 | 31.369007 |
| Ca | 28.994209 | 27.976307 | 29.772121 |
| Ca | 30.555813 | 32.457821 | 27.586525 |
| Ca | 30.524506 | 28.172123 | 24.408726 |
| Ca | 33.573936 | 29.589916 | 28.489561 |
| Ca | 34.193760 | 24.873959 | 26.574890 |
| Ca | 35.730232 | 29.167320 | 23.584949 |
| S  | 21.251614 | 31.804594 | 35.776035 |
| S  | 20.501276 | 35.531879 | 32.794533 |
| S  | 22.069124 | 31.009138 | 29.970570 |
| S  | 24.834457 | 33.791302 | 33.085804 |
| S  | 26.332449 | 29.813250 | 31.231297 |
| S  | 25.876743 | 33.805511 | 28.411591 |
| S  | 28.181402 | 29.742567 | 26.607920 |
| S  | 30.723881 | 30.979336 | 30.312553 |
| S  | 31.504190 | 26.740980 | 27.705397 |
| S  | 32.943413 | 30.653366 | 25.254440 |
| S  | 33.441006 | 26.230125 | 23.242420 |
| S  | 36.347809 | 27.945993 | 26.822845 |

24

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generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.429152 | 33.231575 | 34.070068 |
| Ca | 22.837893 | 35.125065 | 35.471073 |
| Ca | 23.404613 | 30.348618 | 32.999317 |
|   |      |      |      |
|---|------|------|------|
| Ca  | 22.644190 | 34.528385 | 30.408215 |
| Ca  | 24.834225 | 30.417126 | 28.026239 |
| Ca  | 27.643463 | 32.547050 | 31.351070 |
| Ca  | 29.028669 | 27.961504 | 29.723019 |
| Ca  | 30.861685 | 32.431664 | 27.541380 |
| Ca  | 30.551645 | 28.507147 | 24.308434 |
| Ca  | 33.613304 | 29.723978 | 28.253866 |
| Ca  | 34.341747 | 24.681625 | 26.528927 |
| Ca  | 35.613251 | 28.991432 | 23.918234 |
| S   | 21.364113 | 31.770752 | 35.603241 |
| S   | 20.343599 | 35.610954 | 32.948949 |
| S   | 21.841692 | 30.961697 | 29.987591 |
| S   | 24.888391 | 33.633915 | 33.048363 |
| S   | 26.389051 | 29.527542 | 31.201307 |
| S   | 25.566525 | 33.838501 | 28.470449 |
| S   | 28.285734 | 29.787729 | 26.747272 |
| S   | 30.886206 | 31.023279 | 30.444043 |
| S   | 31.504898 | 26.997940 | 27.374538 |
| S   | 32.943939 | 30.901451 | 25.070030 |
| S   | 33.385792 | 26.175591 | 23.407501 |
| S   | 36.516350 | 27.575562 | 27.037003 |

generated by VMD

|   |      |      |      |
|---|------|------|------|
| Ca  | 18.400324 | 33.367905 | 33.783863 |
| Ca  | 22.735910 | 35.062885 | 35.935917 |
| Ca  | 23.398088 | 30.347836 | 33.130856 |
| Ca  | 22.851982 | 34.454659 | 30.336845 |
| Ca  | 24.945322 | 30.012165 | 28.096226 |
| Ca  | 27.837706 | 32.565918 | 31.340508 |
| Ca  | 28.996626 | 27.954884 | 29.798349 |
| Ca  | 30.531118 | 32.371468 | 27.371956 |
| Ca  | 30.795843 | 28.593224 | 24.678860 |
| Ca  | 33.726002 | 29.569763 | 28.349598 |
| Ca  | 34.199017 | 24.801407 | 26.398924 |
| Ca  | 35.491192 | 29.020214 | 23.554237 |
| S   | 21.083883 | 31.988777 | 35.419777 |
| S   | 20.406137 | 35.838348 | 32.914024 |
| S   | 21.889915 | 30.878662 | 30.001133 |
| S   | 24.872282 | 33.821545 | 33.099194 |
| S   | 26.484335 | 29.354099 | 31.392555 |
| S   | 25.652546 | 33.521309 | 28.397442 |
| S   | 28.087400 | 29.762383 | 26.692461 |
| S   | 30.753889 | 31.002909 | 30.123850 |
| S   | 31.710823 | 26.920048 | 27.418106 |
| S   | 33.048389 | 31.081985 | 25.447094 |
| S   | 33.448891 | 26.384806 | 23.276705 |
|     | 36.372540 | 27.622875 | 26.981518 |
|-----|-----------|-----------|-----------|
| 24  | generated by VMD |
| Ca  | 18.391972 | 33.069065 | 33.855698 |
| Ca  | 22.878815 | 34.900383 | 35.753670 |
| Ca  | 23.649105 | 30.579212 | 33.063572 |
| Ca  | 22.784725 | 34.491745 | 30.280201 |
| Ca  | 24.652990 | 30.338665 | 27.872959 |
| Ca  | 27.865385 | 32.825005 | 31.079378 |
| Ca  | 28.954426 | 27.673786 | 29.791573 |
| Ca  | 30.318310 | 32.242329 | 27.462719 |
| Ca  | 30.722692 | 28.634562 | 24.606600 |
| Ca  | 33.792076 | 29.600094 | 28.575443 |
| Ca  | 34.081821 | 24.778780 | 26.498722 |
| Ca  | 35.504860 | 29.122253 | 23.720482 |
| S   | 21.296015 | 31.903006 | 35.522442 |
| S   | 20.448242 | 35.772163 | 32.954578 |
| S   | 21.997490 | 30.845184 | 30.201767 |
| S   | 25.097654 | 33.766068 | 33.029140 |
| S   | 26.391302 | 29.572519 | 31.054310 |
| S   | 25.509096 | 33.830540 | 28.250441 |
| S   | 28.084194 | 29.488064 | 26.699999 |
| S   | 30.820690 | 30.711330 | 30.194653 |
| S   | 31.602381 | 26.779640 | 27.717100 |
| S   | 33.207035 | 31.196609 | 25.502520 |
| S   | 33.417168 | 26.452553 | 23.309204 |
| S   | 36.251625 | 27.726465 | 26.942919 |
| 24  | generated by VMD |
| Ca  | 18.470816 | 33.257259 | 33.718361 |
| Ca  | 22.965790 | 35.194695 | 35.579914 |
| Ca  | 23.654892 | 30.470549 | 33.050526 |
| Ca  | 22.710176 | 34.524231 | 30.547646 |
| Ca  | 24.735834 | 30.291315 | 27.983341 |
| Ca  | 27.742922 | 32.627758 | 31.098446 |
| Ca  | 28.692192 | 27.641033 | 29.735874 |
| Ca  | 30.584457 | 31.940662 | 27.633917 |
| Ca  | 30.465294 | 28.256851 | 24.255165 |
| Ca  | 33.647263 | 29.775478 | 28.372965 |
| Ca  | 34.278484 | 24.965252 | 26.486567 |
| Ca  | 35.868374 | 29.289413 | 23.981039 |
| S   | 21.438162 | 31.902147 | 35.575783 |
| S   | 20.601067 | 35.828342 | 33.033333 |
| S   | 21.890053 | 30.976536 | 30.176306 |
| S   | 24.936434 | 33.840324 | 33.041290 |
| S   | 26.223194 | 29.500706 | 31.201788 |
|  | 25.568071 | 33.575012 | 28.237375 |
|---|---|---|---|
| S | 28.142069 | 29.410999 | 26.831207 |
| S | 30.643795 | 30.632553 | 30.384539 |
| S | 31.489769 | 26.932987 | 27.490412 |
| S | 32.909851 | 30.884466 | 25.321890 |
| S | 33.622868 | 26.743095 | 23.145769 |
| S | 36.438179 | 27.838364 | 27.056616 |

24 generated by VMD

| Ca  | 18.518328 | 33.012268 | 33.935707 |
|-----|---|---|---|
| Ca  | 22.974531 | 35.359795 | 35.349915 |
| Ca  | 23.601767 | 30.324596 | 33.163212 |
| Ca  | 22.811699 | 34.389500 | 30.273079 |
| Ca  | 24.901443 | 30.188038 | 27.872501 |
| Ca  | 27.595486 | 32.678280 | 31.152294 |
| Ca  | 28.862366 | 27.696110 | 29.890875 |
| Ca  | 30.843565 | 32.247414 | 27.763090 |
| Ca  | 30.380896 | 28.482084 | 24.561035 |
| Ca  | 33.700443 | 29.542667 | 28.484423 |
| Ca  | 34.174923 | 25.013058 | 26.208023 |
| Ca  | 35.762321 | 29.195948 | 23.932953 |
| S   | 21.587587 | 32.103138 | 35.689308 |
| S   | 20.386923 | 35.774364 | 32.787842 |
| S   | 22.034159 | 30.755745 | 30.060099 |
| S   | 25.007183 | 33.732712 | 33.078606 |
| S   | 26.177391 | 29.249657 | 30.996861 |
| S   | 25.509991 | 33.732956 | 28.276140 |
| S   | 28.257278 | 29.836761 | 26.893326 |
| S   | 30.710428 | 30.679092 | 30.477854 |
| S   | 31.503315 | 26.932322 | 27.370377 |
| S   | 33.011208 | 30.997078 | 25.382059 |
| S   | 33.106873 | 26.551125 | 23.291405 |
| S   | 36.299946 | 27.825348 | 27.049080 |

24 generated by VMD

| Ca  | 18.339302 | 32.901520 | 34.017654 |
|-----|---|---|---|
| Ca  | 22.903400 | 34.860462 | 35.509514 |
| Ca  | 23.643049 | 30.571438 | 33.121025 |
| Ca  | 22.784599 | 34.737000 | 30.514921 |
| Ca  | 24.816936 | 30.507284 | 27.908159 |
| Ca  | 27.915733 | 32.781391 | 31.234917 |
| Ca  | 28.953884 | 27.783487 | 29.777925 |
| Ca  | 30.764214 | 32.320930 | 27.385120 |
| Ca  | 30.412592 | 28.171963 | 24.503368 |
| Ca  | 33.539169 | 29.700157 | 28.356853 |
| Ca  | 34.471855 | 24.944221 | 26.362991 |
|   | Ca     | S       | S       | S       | S       | S       | S     |
|---|--------|---------|---------|---------|---------|---------|-------|
| 1 | 35.535793 | 29.043575 | 23.946196 |        |         |         |       |
| 2 | 21.298021  | 31.807606 | 35.745377 |        |         |         |       |
| 3 | 20.351610  | 35.520348 | 32.915405 |        |         |         |       |
| 4 | 21.742956  | 31.180113 | 30.002346 |        |         |         |       |
| 5 | 24.979748  | 33.892620 | 32.909866 |        |         |         |       |
| 6 | 26.315392  | 29.618591 | 30.97156  |        |         |         |       |
| 7 | 25.702040  | 33.821388 | 26.814149 |        |         |         |       |
| 8 | 30.783337  | 30.803169 | 30.420748 |        |         |         |       |
| 9 | 31.501993  | 26.743717 | 27.552925 |        |         |         |       |
| 10| 32.800289  | 30.696163 | 25.346119 |        |         |         |       |
| 11| 28.196981  | 29.634392 | 26.814149 |        |         |         |       |
| 12| 25.702040  | 33.821388 | 26.814149 |        |         |         |       |
| 13| 28.196981  | 29.634392 | 26.814149 |        |         |         |       |
| 14| 30.783337  | 30.803169 | 30.420748 |        |         |         |       |
| 15| 31.501993  | 26.743717 | 27.552925 |        |         |         |       |
| 16| 32.800289  | 30.696163 | 25.346119 |        |         |         |       |
| 17| 28.196981  | 29.634392 | 26.814149 |        |         |         |       |

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generated by VMD

Ca  18.356903  33.049770  34.005898
Ca  22.998001  35.047161  35.408375
Ca  23.511406  30.319799  33.218044
Ca  22.778761  34.636969  30.358580
Ca  24.873817  30.282379  27.904776
Ca  27.926794  32.633724  30.962782
Ca  28.791582  27.694014  29.961374
Ca  30.761406  32.371773  27.568655
Ca  30.558346  28.149843  24.364365
Ca  33.501377  29.711244  28.348392
Ca  34.271889  25.072317  26.417595
Ca  35.814236  29.175032  23.933281
Ca  21.424557  32.075031  35.930072
Ca  20.281433  35.678032  32.825127
Ca  21.877033  31.161003  30.043503
Ca  24.949013  33.540726  33.113075
Ca  26.074112  29.380762  30.989731
Ca  25.659849  33.853311  28.244802
Ca  28.279160  29.577778  26.872837
Ca  30.705404  30.844584  30.379255
Ca  31.641657  26.739563  27.601223
Ca  32.982914  30.998882  25.253435
Ca  33.335876  26.605614  23.164303
Ca  36.364468  27.669146  27.061562

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generated by VMD

Ca  18.810688  32.841599  34.156784
Ca  23.102097  35.047161  35.408375
Ca  23.650785  30.254551  33.144283
Ca  22.789007  34.764305  30.302954
Ca  24.686094  30.302132  27.830032
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 27.412472     | 32.591610     | 31.145794     |
| Ca      | 28.864174     | 27.829174     | 29.792145     |
| Ca      | 30.478182     | 32.480366     | 27.702070     |
| Ca      | 30.420044     | 28.258005     | 24.386963     |
| Ca      | 33.727077     | 29.600376     | 28.319500     |
| Ca      | 34.177113     | 25.051861     | 26.458109     |
| Ca      | 35.777283     | 29.186926     | 24.253906     |
| S       | 21.686804     | 31.909523     | 35.766064     |
| S       | 20.558426     | 35.651176     | 32.931107     |
| S       | 21.849157     | 31.218983     | 29.951008     |
| S       | 25.000797     | 33.545219     | 33.001640     |
| S       | 25.940075     | 29.272406     | 30.810204     |
| S       | 25.642523     | 33.810154     | 28.161144     |
| S       | 28.170832     | 29.728168     | 26.757576     |
| S       | 30.541952     | 30.971844     | 30.371973     |
| S       | 31.661852     | 26.788280     | 27.679625     |
| S       | 32.957218     | 30.824142     | 25.372196     |
| S       | 33.489849     | 26.616528     | 23.254162     |
| S       | 36.325562     | 27.597599     | 27.113075     |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.818052     | 32.339973     | 34.401394     |
| Ca      | 22.684462     | 35.214306     | 35.520275     |
| Ca      | 23.726158     | 30.561371     | 33.022102     |
| Ca      | 22.536774     | 34.637280     | 30.346704     |
| Ca      | 24.712088     | 30.560457     | 27.669632     |
| Ca      | 27.763332     | 33.137436     | 31.132864     |
| Ca      | 28.757292     | 28.032558     | 29.618542     |
| Ca      | 30.707653     | 32.482903     | 27.550161     |
| Ca      | 30.392189     | 28.194164     | 24.327087     |
| Ca      | 33.453430     | 29.555178     | 28.179329     |
| Ca      | 34.155300     | 24.669609     | 26.399694     |
| Ca      | 36.030388     | 28.935085     | 24.460762     |
| S       | 21.829782     | 31.773817     | 35.936790     |
| S       | 20.377136     | 35.386574     | 33.074898     |
| S       | 21.954670     | 31.183872     | 29.983198     |
| S       | 24.951765     | 33.716560     | 32.968513     |
| S       | 26.277386     | 29.798824     | 30.723652     |
| S       | 25.431932     | 33.928257     | 28.330116     |
| S       | 28.060619     | 29.787380     | 26.424694     |
| S       | 30.793793     | 31.058647     | 30.294804     |
| S       | 31.336130     | 26.713018     | 27.346403     |
| S       | 32.944801     | 30.695955     | 25.365076     |
| S       | 33.705044     | 26.567993     | 23.257530     |
| S       | 36.319870     | 27.368729     | 27.605856     |
| Element | X  | Y  | Z  |
|---------|----|----|----|
| Ca      | 18.569302 | 32.833279 | 34.139099 |
| Ca      | 23.031971  | 35.465492  | 35.278809  |
| Ca      | 23.587555  | 30.411404  | 33.311668  |
| Ca      | 22.545650  | 34.392422  | 30.309572  |
| Ca      | 24.893827  | 30.509634  | 27.778811  |
| Ca      | 27.527658  | 32.620995  | 31.130226  |
| Ca      | 28.791117  | 27.753197  | 29.731251  |
| Ca      | 30.420822  | 32.380009  | 27.546940  |
| Ca      | 30.561535  | 28.382187  | 24.368891  |
| Ca      | 33.851883  | 29.511616  | 28.329983  |
| Ca      | 34.123928  | 24.802212  | 26.172573  |
| Ca      | 35.994709  | 29.178246  | 24.352535  |
| S       | 21.603535  | 32.299500  | 35.930801  |
| S       | 20.347879  | 35.602036  | 32.904781  |
| S       | 21.861149  | 30.946651  | 29.895878  |
| S       | 24.891077  | 33.675087  | 33.057487  |
| S       | 26.108881  | 29.446486  | 31.260460  |
| S       | 25.492287  | 33.736599  | 28.370049  |
| S       | 28.155071  | 29.660543  | 26.766308  |
| S       | 30.786676  | 30.757891  | 30.375347  |
| S       | 31.483463  | 26.802948  | 27.408129  |
| S       | 32.865482  | 30.985725  | 25.408180  |
| S       | 33.732338  | 26.825666  | 23.055779  |
| S       | 36.492287  | 27.320189  | 27.056522  |

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| Element | X  | Y  | Z  |
|---------|----|----|----|
| Ca      | 18.460659 | 32.688320 | 34.135902 |
| Ca      | 23.071707  | 35.672100  | 35.056709  |
| Ca      | 23.626003  | 30.269753  | 33.318806  |
| Ca      | 22.489330  | 34.552338  | 30.404919  |
| Ca      | 24.869438  | 30.483154  | 27.885349  |
| Ca      | 27.717928  | 32.536171  | 31.217228  |
| Ca      | 28.893602  | 27.841854  | 29.597580  |
| Ca      | 30.598890  | 32.420429  | 27.399067  |
| Ca      | 30.533047  | 28.226532  | 24.336292  |
| Ca      | 33.612209  | 29.560471  | 28.219458  |
| Ca      | 34.130554  | 24.635479  | 26.042303  |
| Ca      | 35.833557  | 29.405598  | 24.593063  |
| S       | 21.548197  | 32.329948  | 35.864388  |
| S       | 20.055290  | 35.557529  | 32.658169  |
| S       | 21.945137  | 30.846367  | 30.168823  |
| S       | 25.006529  | 33.653740  | 33.198002  |
| S       | 26.436058  | 29.490482  | 31.227028  |
| S       | 25.480587  | 33.614971  | 28.513062  |
| S       | 28.183838  | 29.961479  | 26.625065  |
S  30.836157  30.808121  30.303179
S  31.515623  26.733759  27.430201
S  33.036823  30.813271  25.429041
S  33.533928  26.939491  23.071045
S  36.304943  27.258701  27.245369

24 generated by VMD

Ca  18.625072  32.351063  33.851967
Ca  22.893185  35.231293  35.578175
Ca  23.561033  30.553379  33.027802
Ca  22.759199  34.711716  30.141035
Ca  24.966169  30.218868  27.976088
Ca  27.716017  32.836346  31.372429
Ca  28.880274  27.939249  29.608269
Ca  30.553663  32.445904  27.625359
Ca  30.617580  28.427979  24.429939
Ca  33.579838  29.744509  28.290293
Ca  34.096592  24.966637  26.364798
Ca  35.771992  28.844284  24.233749
S  21.601744  31.963840  35.979477
S  20.35623  35.231998  32.964676
S  21.947645  31.148695  29.924561
S  25.036303  33.922417  32.983414
S  26.183735  29.642626  31.190067
S  25.775078  33.677246  28.231834
S  28.218189  29.857353  26.760693
S  30.758774  30.948452  30.379004
S  31.384327  26.966049  27.364435
S  33.106273  30.817299  25.227291
S  33.335575  26.456547  23.090179
S  35.996063  27.396313  27.345975

24 generated by VMD

Ca  18.473736  32.428417  34.139397
Ca  22.776516  34.953728  35.400139
Ca  23.497871  30.471016  33.070034
Ca  22.895075  34.837227  30.226509
Ca  24.953913  30.640217  28.069641
Ca  27.771713  32.742168  31.122622
Ca  28.910961  27.865738  29.689865
Ca  30.486887  32.465469  27.297073
Ca  30.535673  28.010620  24.406353
Ca  33.420395  29.652866  28.160332
Ca  34.115814  24.693756  26.372780
Ca  36.019062  29.091206  24.467165
S  21.508806  31.770367  35.805595
| S   | 20.274273 | 35.596870 | 33.014236 |
| S   | 22.113213 | 31.286253 | 30.239515 |
| S   | 24.880207 | 33.813362 | 33.054047 |
| S   | 26.478657 | 29.735357 | 31.207468 |
| S   | 25.623686 | 33.946449 | 28.309687 |
| S   | 28.198750 | 29.697351 | 26.672523 |
| S   | 30.689440 | 30.962244 | 30.131630 |
| S   | 31.407431 | 26.731243 | 27.455063 |
| S   | 32.740826 | 30.888340 | 25.031384 |
| S   | 33.703644 | 26.537889 | 23.206047 |
| S   | 36.243488 | 27.481892 | 27.390968 |

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Generated by VMD

| Ca  | 18.593372 | 32.353020 | 34.063263 |
| Ca  | 22.999895 | 35.238163 | 35.523922 |
| Ca  | 23.793316 | 30.452812 | 33.108696 |
| Ca  | 22.890184 | 34.452374 | 30.403656 |
| Ca  | 25.017391 | 30.310959 | 27.721294 |
| Ca  | 27.806307 | 33.050087 | 31.055277 |
| Ca  | 28.735765 | 28.014992 | 29.664322 |
| Ca  | 30.674297 | 32.549900 | 27.520399 |
| Ca  | 30.400734 | 28.139439 | 24.254591 |
| Ca  | 33.271629 | 29.797701 | 28.072375 |
| Ca  | 33.892792 | 24.509853 | 26.622044 |
| Ca  | 35.940479 | 29.204231 | 24.634499 |
| S   | 21.587461 | 31.981270 | 35.804276 |
| S   | 20.237471 | 35.238583 | 33.015091 |
| S   | 22.065689 | 31.146748 | 29.986973 |
| S   | 25.177074 | 33.613285 | 33.109737 |
| S   | 26.386597 | 29.543934 | 30.906189 |
| S   | 25.663122 | 33.908752 | 28.316528 |
| S   | 28.145334 | 30.138832 | 26.460403 |
| S   | 30.747372 | 31.037258 | 30.265862 |
| S   | 31.164032 | 26.924210 | 27.318703 |
| S   | 32.787556 | 30.873356 | 25.149164 |
| S   | 33.640617 | 26.456694 | 23.547951 |
| S   | 36.101578 | 27.363615 | 27.414448 |

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Generated by VMD

| Ca  | 18.306356 | 32.899071 | 33.881504 |
| Ca  | 23.127554 | 35.269875 | 35.665565 |
| Ca  | 23.374516 | 30.308552 | 33.253510 |
| Ca  | 22.699627 | 34.357178 | 30.592663 |
| Ca  | 24.897980 | 30.319221 | 27.756001 |
| Ca  | 27.821058 | 33.006927 | 31.140724 |
| Ca  | 28.833225 | 28.035959 | 29.670036 |
|  | Ca  |  |  |  |
|---|---|---|---|---|
|  | 30.483345 | 32.421074 | 27.323549 |  |
|  | 30.668291 | 28.264767 | 24.290928 |  |
|  | 33.532986 | 29.624787 | 25.090500 |  |
|  | 34.006268 | 24.657776 | 26.589802 |  |
|  | 36.035900 | 29.283817 | 24.204348 |  |
| S | 21.334263 | 32.031284 | 35.751305 |  |
| S | 20.458315 | 35.647156 | 33.060467 |  |
| S | 21.955353 | 30.793533 | 30.083252 |  |
| S | 25.126904 | 33.588802 | 33.314373 |  |
| S | 26.264441 | 29.688309 | 31.081272 |  |
| S | 25.449272 | 33.679729 | 28.255646 |  |
|  | 28.199522 | 29.752682 | 26.490995 |  |
|  | 30.562069 | 30.980244 | 30.242046 |  |
| S | 31.286303 | 26.953632 | 27.351009 |  |
|  | 33.146248 | 30.868279 | 25.268398 |  |
| S | 33.708290 | 26.543867 | 23.390823 |  |
| S | 36.441952 | 27.318523 | 27.191326 |  |

24  

|  | Ca  |  |  |  |
|---|---|---|---|---|
|  | 18.297966 | 32.962784 | 34.026539 |  |
|  | 23.154358 | 35.439209 | 35.587330 |  |
|  | 23.531393 | 30.556635 | 33.107288 |  |
|  | 22.786619 | 34.426437 | 30.479105 |  |
|  | 24.750338 | 30.269835 | 27.791939 |  |
|  | 27.832813 | 32.858139 | 30.956974 |  |
|  | 28.746181 | 27.671600 | 29.653133 |  |
|  | 30.635712 | 32.105080 | 27.464397 |  |
|  | 30.577816 | 28.350594 | 24.387402 |  |
|  | 33.498714 | 29.527451 | 28.295277 |  |
|  | 34.390202 | 25.059393 | 26.326391 |  |
|  | 35.943325 | 29.326912 | 24.284767 |  |
| S | 21.561649 | 32.088005 | 35.669868 |  |
| S | 20.450371 | 35.563492 | 33.101631 |  |
| S | 21.811197 | 30.947269 | 30.019161 |  |
| S | 25.115280 | 33.556408 | 33.119728 |  |
| S | 26.248861 | 29.711840 | 31.084641 |  |
| S | 25.308115 | 33.742596 | 28.342049 |  |
| S | 28.047068 | 29.592621 | 26.517941 |  |
| S | 30.713394 | 30.729343 | 30.265240 |  |
| S | 31.343616 | 26.596792 | 27.342068 |  |
| S | 32.985847 | 30.775063 | 25.495842 |  |
| S | 33.607662 | 26.742878 | 23.354944 |  |
| S | 36.381554 | 27.704151 | 27.266397 |  |

24  

|  | Ca  |  |  |  |
|---|---|---|---|---|
|  | 18.580929 | 32.668755 | 34.068604 |  |
|   |   |   |
|---|---|---|
| Ca | 22.823265 | 35.484032 | 35.282104 |
| Ca | 23.501551 | 30.570213 | 27.866962 |
| Ca | 22.560738 | 34.575562 | 30.413565 |
| Ca | 24.913059 | 30.570213 | 27.866962 |
| Ca | 27.763271 | 32.977043 | 31.207825 |
| Ca | 28.991076 | 27.811115 | 29.575500 |
| Ca | 30.507174 | 32.325363 | 27.525173 |
| Ca | 30.478680 | 28.252623 | 24.203096 |
| Ca | 33.631214 | 29.603924 | 28.156942 |
| Ca | 34.337090 | 24.627701 | 26.245861 |
| Ca | 35.932610 | 29.192871 | 24.331181 |
| S  | 21.348736 | 31.937311 | 36.032860 |
| S  | 20.228857 | 35.480461 | 32.840584 |
| S  | 21.922489 | 31.126118 | 30.014465 |
| S  | 24.907972 | 33.517368 | 33.347588 |
| S  | 26.361345 | 29.771572 | 31.092743 |
| S  | 25.602823 | 34.133987 | 28.484180 |
| S  | 28.108324 | 29.506618 | 26.637312 |
| S  | 30.715229 | 30.963287 | 30.274639 |
| S  | 31.574976 | 26.786152 | 27.427891 |
| S  | 32.866764 | 30.738289 | 25.224533 |
| S  | 33.585247 | 26.565975 | 23.194435 |
| S  | 36.476585 | 27.320147 | 27.274017 |

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Generated by VMD
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| S | 33.003544 | 30.735180 | 25.234884 |
| S | 33.240871 | 26.196163 | 23.123125 |
| S | 36.503220 | 27.595959 | 26.662529 |

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generated by VMD

| Ca | X       | Y       | Z       |
|----|---------|---------|---------|
| 18.275618 | 32.768238 | 33.512882 |
| 22.610264 | 35.301853 | 35.263348 |
| 23.383497 | 30.346504 | 33.210560 |
| 22.848833 | 34.947369 | 30.520962 |
| 25.091003 | 30.480179 | 28.293743 |
| 27.786024 | 32.709949 | 31.486465 |
| 29.071909 | 27.787264 | 29.803978 |
| 30.576107 | 32.290409 | 27.591747 |
| 30.640877 | 27.939228 | 24.796757 |
| 33.687336 | 29.460781 | 28.052048 |
| 34.334923 | 24.720001 | 26.215302 |
| 35.377300 | 29.370342 | 23.641064 |

| S | X       | Y       | Z       |
|----|---------|---------|---------|
| 21.165449 | 31.887249 | 35.512074 |
| 20.16916 | 35.503468 | 32.646606 |
| 22.088530 | 31.464039 | 29.995529 |
| 24.987093 | 33.623569 | 33.163002 |
| 26.627001 | 29.729059 | 31.430370 |
| 25.569643 | 33.865292 | 28.635809 |
| 28.265411 | 29.515675 | 26.866657 |
| 30.815445 | 30.766766 | 30.528168 |
| 31.965673 | 26.994568 | 27.878273 |
| 32.495171 | 30.700447 | 25.175421 |
| 33.443367 | 26.434841 | 23.129051 |
| 36.444103 | 27.692932 | 26.590240 |

24

generated by VMD

| Ca | X       | Y       | Z       |
|----|---------|---------|---------|
| 18.480595 | 32.724693 | 34.055477 |
| 22.801085 | 35.230030 | 35.629539 |
| 23.416059 | 30.462051 | 32.734169 |
| 22.646252 | 34.818214 | 30.744772 |
| 24.810160 | 30.539886 | 27.856657 |
| 27.710108 | 32.818077 | 31.283762 |
| 28.896341 | 27.779327 | 29.717663 |
| 30.359020 | 31.923563 | 27.591188 |
| 30.672539 | 27.761353 | 24.395374 |
| 33.738434 | 29.849524 | 28.236433 |
| 34.350323 | 24.923056 | 26.483463 |
| 35.874962 | 29.118160 | 23.848194 |
| 21.420677 | 31.895004 | 35.734299 |
| 20.335388 | 35.651005 | 33.142929 |
| 21.830698 | 31.538111 | 29.800381 |
|    |          |          |          |
|----|----------|----------|----------|
| S  | 24.848969| 33.551407| 33.245674|
| S  | 26.276762| 29.769711| 30.965179|
| S  | 25.481588| 34.164429| 28.481848|
| S  | 27.996838| 29.587822| 26.496056|
| S  | 30.704002| 30.726067| 30.321476|
| S  | 31.838501| 26.762989| 27.862709|
| S  | 32.823708| 30.565792| 25.123505|
| S  | 33.646843| 26.354160| 23.132040|
| S  | 36.760155| 27.785629| 27.057274|
| 24 |          |          |          |

generated by VMD

| Ca |          |          |          |
|----|----------|----------|----------|
| Ca | 18.867094| 32.826256| 34.224731|
| Ca | 22.756975| 35.221050| 35.563080|
| Ca | 23.304192| 30.148697| 33.027672|
| Ca | 22.731865| 34.718735| 30.524433|
| Ca | 25.067926| 30.611265| 27.796101|
| Ca | 27.754770| 32.726582| 31.135624|
| Ca | 28.712751| 27.834087| 29.746962|
| Ca | 30.508390| 32.08871 | 27.394258|
| Ca | 30.571852| 27.943457| 24.330303|
| Ca | 33.707081| 29.927334| 28.306200|
| Ca | 34.205582| 25.017113| 26.599007|
| Ca | 35.861446| 29.084976| 23.906414|
| S  | 21.340281| 31.789009| 35.961788|
| S  | 20.374020| 35.774803| 32.999767|
| S  | 21.948582| 31.392513| 29.706554|
| S  | 24.759245| 33.301056| 33.255394|
| S  | 26.275518| 29.657001| 31.013557|
| S  | 25.747190| 34.137531| 28.412586|
| S  | 28.103046| 29.527557| 26.496159|
| S  | 30.585442| 30.854481| 30.257992|
| S  | 31.551119| 27.006634| 27.742090|
| S  | 32.883869| 30.671782| 25.149046|
| S  | 33.636909| 26.272024| 23.175911|
| S  | 36.464886| 27.767258| 27.214417|

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generated by VMD

| Ca |          |          |          |
|----|----------|----------|----------|
| Ca | 18.552168| 33.058022| 33.884701|
| Ca | 23.121714| 35.343140| 35.328026|
| Ca | 23.518147| 30.397818| 33.328499|
| Ca | 22.795624| 34.365170| 30.374165|
| Ca | 24.888298| 30.160315| 27.824301|
| Ca | 27.770767| 32.688770| 31.057255|
| Ca | 28.841064| 27.626774| 29.588757|
| Ca | 30.509460| 32.189224| 27.766140|
| Ca | 30.461733| 28.320660| 24.283707|
| Ca       | 33.603168 | 29.609173 | 28.536991 |
| Ca       | 34.002060 | 25.123659 | 26.395454 |
| Ca       | 35.756554 | 35.781658 | 23.040489 |
| S        | 21.370209 | 32.043373 | 35.781658 |
| S        | 20.584969 | 35.787334 | 32.87925  |
| S        | 21.988461 | 30.026558 | 30.069107 |
| S        | 25.074498 | 33.554436 | 33.165691 |
| S        | 26.282574 | 29.546446 | 31.090076 |
| S        | 25.554113 | 33.624153 | 28.207062 |
| S        | 28.243351 | 29.651775 | 32.617443 |
| S        | 30.569366 | 30.597370 | 30.381443 |
| S        | 31.547327 | 26.694424 | 27.605400 |
| S        | 32.848530 | 30.884235 | 25.362759 |
| S        | 33.504879 | 26.698246 | 23.206835 |
| S        | 36.330608 | 28.042622 | 27.165142 |

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generated by VMD

| Ca       | 18.430454 | 33.029015 | 34.466583 |
| Ca       | 23.086374 | 35.423496 | 35.425354 |
| Ca       | 22.491949 | 30.626236 | 33.019588 |
| Ca       | 22.877726 | 34.283127 | 30.570652 |
| Ca       | 24.608524 | 30.390509 | 27.643923 |
| Ca       | 27.798801 | 32.779777 | 31.122517 |
| Ca       | 28.624178 | 27.601908 | 29.584839 |
| Ca       | 30.697723 | 32.264938 | 27.600613 |
| Ca       | 30.605173 | 28.336399 | 24.244587 |
| Ca       | 33.549858 | 29.830769 | 28.411921 |
| Ca       | 34.228569 | 25.063951 | 26.657440 |
| Ca       | 35.913212 | 28.904900 | 23.921389 |
| S        | 21.527512 | 32.121010 | 35.793869 |
| S        | 20.545795 | 35.460182 | 32.921833 |
| S        | 21.780922 | 30.928246 | 29.846848 |
| S        | 24.964989 | 33.188519 | 33.098770 |
| S        | 26.045130 | 29.533752 | 30.801064 |
| S        | 25.700655 | 33.864845 | 28.394348 |
| S        | 28.059443 | 29.812962 | 26.686783 |
| S        | 30.545979 | 30.736706 | 30.404247 |
| S        | 31.545099 | 26.963743 | 27.420708 |
| S        | 33.018696 | 30.910614 | 25.265381 |
| S        | 33.552494 | 26.562222 | 23.347137 |
| S        | 36.520813 | 27.684031 | 27.289665 |

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generated by VMD

| Ca       | 18.596285 | 32.895420 | 34.058834 |
| Ca       | 22.838409 | 35.353745 | 35.600437 |
| Ca       | 23.289852 | 30.666641 | 33.073860 |
| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 22.890629 | 34.339447 | 30.417477 |
| Ca      | 24.863119 | 30.159790 | 27.708927 |
| Ca      | 27.847599 | 32.811646 | 31.110491 |
| Ca      | 28.738815 | 27.882755 | 29.610538 |
| Ca      | 30.780638 | 32.194386 | 27.490042 |
| Ca      | 30.637947 | 28.233231 | 24.259903 |
| Ca      | 33.667957 | 29.705181 | 28.481438 |
| Ca      | 34.133755 | 24.786713 | 26.540329 |
| Ca      | 35.757473 | 29.269138 | 24.022575 |
| S       | 21.325884 | 32.061222 | 36.162643 |
| S       | 20.629305 | 35.703407 | 33.027458 |
| S       | 21.794355 | 30.899250 | 29.809757 |
| S       | 24.866131 | 33.488457 | 31.124985 |
| S       | 26.274002 | 29.562954 | 31.199259 |
| S       | 25.586451 | 33.611599 | 28.251980 |
| S       | 28.204996 | 29.859793 | 26.533613 |
| S       | 30.622761 | 30.784269 | 30.403673 |
| S       | 31.440706 | 26.756622 | 27.429779 |
| S       | 33.000652 | 30.993076 | 25.244934 |
| S       | 33.618137 | 26.573013 | 23.239155 |
| S       | 36.314194 | 27.708267 | 27.138025 |

24 generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 18.618229 | 32.805794 | 33.681267 |
| Ca      | 23.101152 | 35.067097 | 35.636700 |
| Ca      | 23.526917 | 30.495842 | 33.154079 |
| Ca      | 22.860828 | 34.493431 | 30.467243 |
| Ca      | 24.871305 | 30.043152 | 27.913551 |
| Ca      | 27.892202 | 33.010609 | 31.018866 |
| Ca      | 28.736732 | 27.935398 | 29.582367 |
| Ca      | 30.417486 | 32.331459 | 27.417114 |
| Ca      | 30.580492 | 28.361876 | 24.235100 |
| Ca      | 33.353336 | 29.644661 | 28.224134 |
| Ca      | 34.178745 | 25.110733 | 26.486223 |
| Ca      | 35.889458 | 29.057482 | 24.310089 |
| S       | 21.316990 | 31.882559 | 35.802521 |
| S       | 20.623379 | 35.706532 | 33.040867 |
| S       | 21.792206 | 31.038387 | 30.116808 |
| S       | 25.121126 | 32.331459 | 27.417114 |
| S       | 28.355101 | 29.651340 | 31.066233 |
| S       | 25.535568 | 33.508877 | 28.363888 |
| S       | 28.120523 | 29.732971 | 26.435726 |
| S       | 30.691071 | 31.093418 | 30.364401 |
| S       | 31.306244 | 26.908844 | 27.351875 |
| S       | 32.936520 | 30.831638 | 25.401255 |
| S       | 33.605606 | 26.452679 | 23.230278 |
|  |  |  |  |
|---|---|---|---|
| S  | 36.288815 | 27.503740 | 27.451843 |
| 24 | generated by VMD |
| Ca | 18.214176  | 33.257080  | 34.040516  |
| Ca | 22.793381  | 34.930576  | 35.521591  |
| Ca | 23.315403  | 30.086601  | 33.204231  |
| Ca | 22.860348  | 34.805008  | 30.274578  |
| Ca | 25.092690  | 30.251549  | 28.011108  |
| Ca | 27.813288  | 32.809052  | 31.436972  |
| Ca | 29.118055  | 28.015728  | 29.829077  |
| Ca | 30.719767  | 32.391243  | 27.446644  |
| Ca | 30.557421  | 28.159462  | 24.567711  |
| Ca | 33.648952  | 29.655386  | 27.985840  |
| Ca | 34.434402  | 24.827599  | 26.552649  |
| Ca | 35.563004  | 29.056337  | 24.044003  |
| S  | 21.113760  | 31.717890  | 35.648220  |
| S  | 20.601618  | 35.680305  | 32.688225  |
| S  | 22.029263  | 31.248276  | 30.037176  |
| S  | 24.774002  | 33.462448  | 33.168858  |
| S  | 26.515909  | 29.585966  | 31.360662  |
| S  | 25.700708  | 33.582577  | 28.372601  |
| S  | 28.386341  | 29.877319  | 26.576988  |
| S  | 30.755831  | 31.059589  | 30.322647  |
| S  | 31.545515  | 26.702686  | 27.504368  |
| S  | 32.746098  | 31.005157  | 25.102879  |
| S  | 33.485016  | 26.311947  | 23.277992  |
| S  | 35.935055  | 27.820282  | 26.964504  |

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generated by VMD

| Ca | 18.463873  | 33.096672  | 33.536263  |
| Ca | 22.659201  | 35.269566  | 35.202118  |
| Ca | 23.798538  | 30.253235  | 33.456188  |
| Ca | 22.833399  | 34.378033  | 30.281685  |
| Ca | 25.361174  | 30.343494  | 28.084835  |
| Ca | 27.895285  | 32.810200  | 31.455780  |
| Ca | 28.805084  | 27.714046  | 29.809048  |
| Ca | 30.671732  | 32.296326  | 27.785103  |
| Ca | 30.458181  | 28.273628  | 24.450062  |
| Ca | 33.290333  | 29.787939  | 28.404633  |
| Ca | 34.014427  | 24.886162  | 26.295048  |
| Ca | 35.470615  | 29.280891  | 23.911318  |
| S  | 21.333954  | 31.936882  | 35.524536  |
| S  | 20.503849  | 35.617519  | 32.498661  |
| S  | 22.340305  | 30.732895  | 30.043304  |
| S  | 24.917458  | 33.801674  | 33.150517  |
| S  | 26.718645  | 29.524538  | 31.647795  |
|   | X Value 1 | Y Value 1 | Z Value 1 |
|---|-----------|-----------|-----------|
| S | 25.907064 | 33.610531 | 28.458691 |
| S | 28.252298 | 29.761612 | 26.738834 |
| S | 30.597734 | 30.707130 | 30.537918 |
| S | 31.397030 | 26.740582 | 27.439495 |
| S | 32.724419 | 31.003685 | 25.146797 |
| S | 33.239571 | 26.515369 | 23.090069 |
| S | 36.065983 | 27.957405 | 26.991320 |

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generated by VMD

|   | X Value 2 | Y Value 2 | Z Value 2 |
|---|-----------|-----------|-----------|
| Ca | 18.496183 | 32.895073 | 33.640327 |
| Ca | 22.684753 | 35.158192 | 35.234650 |
| Ca | 23.659790 | 30.231548 | 33.334007 |
| Ca | 22.883764 | 34.655003 | 30.162340 |
| Ca | 25.141277 | 30.275198 | 28.200613 |
| Ca | 27.856083 | 32.933945 | 31.696938 |
| Ca | 28.911436 | 27.943684 | 29.794895 |
| Ca | 30.658039 | 32.297485 | 27.150677 |
| Ca | 30.487305 | 28.031082 | 24.302511 |
| Ca | 33.242001 | 29.539415 | 28.649632 |
| Ca | 34.174469 | 24.807251 | 26.255365 |
| Ca | 35.658303 | 29.369087 | 23.781834 |
| S  | 21.238108 | 31.891396 | 35.549221 |
| S  | 20.328773 | 35.790813 | 32.756920 |
| S  | 22.017572 | 30.946636 | 30.271526 |
| S  | 24.901632 | 33.723022 | 33.060379 |
| S  | 26.636625 | 29.590660 | 31.520964 |
| S  | 25.905449 | 33.681553 | 28.605804 |
| S  | 28.278366 | 29.714973 | 26.558483 |
| S  | 30.818178 | 30.849810 | 30.407482 |
| S  | 31.301714 | 26.511574 | 27.572435 |
| S  | 32.777973 | 30.823280 | 25.260096 |
| S  | 33.420444 | 26.644093 | 23.243610 |
| S  | 36.242069 | 27.995270 | 26.929276 |

24

generated by VMD

|   | X Value 3 | Y Value 3 | Z Value 3 |
|---|-----------|-----------|-----------|
| Ca | 18.531006 | 33.317841 | 33.443558 |
| Ca | 22.706303 | 35.046196 | 35.656265 |
| Ca | 23.529284 | 30.165356 | 33.187538 |
| Ca | 22.825869 | 34.445171 | 30.731422 |
| Ca | 25.180296 | 30.465092 | 28.046551 |
| Ca | 27.645565 | 32.594612 | 31.407772 |
| Ca | 28.954489 | 28.051834 | 29.612225 |
| Ca | 30.819084 | 32.604038 | 26.975788 |
| Ca | 30.576336 | 28.115742 | 24.425034 |
| Ca | 33.462719 | 29.814075 | 28.571964 |
| Ca | 34.494770 | 24.785110 | 26.885317 |
|    | Ca       | S        | S        |
|----|----------|----------|----------|
|    | 35.255230| 29.034313| 23.579193|
|    | 20.937534| 31.812546| 35.235710 |
|    | 20.675226| 35.826931| 33.035656 |
|    | 22.087912| 31.031027| 29.986290 |
|    | 24.980425| 33.416893| 33.557144 |
|    | 26.397484| 29.516066| 31.314823 |
|    | 25.638102| 33.506664| 28.556513 |
|    | 28.341915| 29.874092| 26.416130 |
|    | 30.735252| 31.014399| 30.066969 |
|    | 31.613964| 26.709450| 27.816065 |
|    | 32.909527| 30.957523| 25.091288 |
|    | 33.218452| 26.164129| 23.437851 |
|    | 36.203236| 28.030947| 26.902992 |

24

generated by VMD

|    | Ca       | S        | S        |
|----|----------|----------|----------|
|    | 18.439241| 33.278248| 33.455479|
|    | 22.688473| 35.017227| 35.679585|
|    | 23.509253| 30.205349| 33.489807|
|    | 22.866386| 34.567650| 30.595266|
|    | 25.038607| 30.341236| 28.081711|
|    | 27.730736| 32.524246| 31.414734|
|    | 28.766430| 27.690243| 29.687901|
|    | 30.833212| 32.242416| 26.893713|
|    | 30.552252| 28.174061| 24.546963|
|    | 33.476883| 29.919308| 28.611694|
|    | 34.312843| 25.084408| 26.451463|
|    | 35.755096| 28.887169| 23.589638|
|    | 20.911171| 31.963385| 35.384750|
|    | 20.556395| 35.988476| 33.134178|
|    | 22.107660| 30.988190| 30.162104|
|    | 24.941879| 33.509460| 33.325443|
|    | 26.387997| 29.363808| 31.254784|
|    | 25.708353| 33.575745| 28.422186|
|    | 28.227316| 29.759905| 26.609066|
|    | 30.659365| 30.999697| 30.166571|
|    | 31.552229| 27.011164| 27.606396|
|    | 33.091354| 30.832657| 24.954626|
|    | 33.351295| 26.374376| 23.340195|
|    | 36.255627| 28.001656| 27.079090|

24

generated by VMD

|    | Ca       | S        | S        |
|----|----------|----------|----------|
|    | 18.659708| 33.480293| 33.576046|
|    | 22.875982| 34.854641| 35.637688|
|    | 23.490835| 30.231817| 33.208786|
|    | 22.948786| 34.592007| 30.435524|
|    | 24.869209| 30.065273| 27.834427|
| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 27.751722 | 32.843857 | 31.320034 |
| Ca      | 28.932251 | 27.797216 | 29.748331 |
| Ca      | 30.409687 | 32.189365 | 27.429539 |
| Ca      | 30.362823 | 27.731331 | 24.454857 |
| Ca      | 33.375786 | 29.913816 | 28.490589 |
| Ca      | 34.521194 | 25.285091 | 26.504269 |
| Ca      | 35.570759 | 29.400650 | 23.768551 |
| S       | 21.098272 | 31.627344 | 35.239197 |
| S       | 20.991049 | 35.981964 | 33.112068 |
| S       | 22.056265 | 31.178066 | 29.892101 |
| S       | 25.022572 | 33.762131 | 33.243031 |
| S       | 26.290016 | 29.469898 | 31.203022 |
| S       | 25.698198 | 33.654213 | 28.384041 |
| S       | 28.177826 | 29.464676 | 26.641773 |
| S       | 30.680771 | 30.811543 | 30.569187 |
| S       | 31.576298 | 26.827408 | 27.746588 |
| S       | 32.560459 | 30.558060 | 25.318226 |
| S       | 33.561401 | 26.474003 | 23.187435 |
| S       | 36.238197 | 28.105381 | 26.994738 |

24

generated by VMD

| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 18.621115 | 33.382706 | 33.844711 |
| Ca      | 23.180294 | 34.677887 | 35.856602 |
| Ca      | 23.170246 | 30.326385 | 33.016628 |
| Ca      | 22.791924 | 34.892529 | 30.231125 |
| Ca      | 24.823919 | 30.260368 | 27.708294 |
| Ca      | 27.708302 | 32.784599 | 31.346153 |
| Ca      | 28.864016 | 27.719074 | 29.643042 |
| Ca      | 30.146057 | 32.052994 | 27.378082 |
| Ca      | 30.443748 | 27.787399 | 24.587263 |
| Ca      | 33.670128 | 29.898756 | 28.262161 |
| Ca      | 34.534142 | 25.082302 | 26.515774 |
| Ca      | 35.689693 | 29.241837 | 24.139053 |
| S       | 21.115824 | 31.821167 | 35.488869 |
| S       | 21.068878 | 36.106895 | 33.488827 |
| S       | 21.950228 | 31.338100 | 29.813286 |
| S       | 24.752094 | 33.482063 | 32.992573 |
| S       | 26.129549 | 29.437141 | 31.028873 |
| S       | 25.554192 | 33.736393 | 28.372787 |
| S       | 28.026054 | 29.184818 | 26.607002 |
| S       | 30.614744 | 30.875063 | 30.331083 |
| S       | 31.936176 | 26.770264 | 27.628542 |
| S       | 32.616383 | 30.696669 | 25.152332 |
| S       | 33.614529 | 26.636793 | 23.408623 |
| S       | 36.697853 | 28.107826 | 27.098349 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.393024    | 32.951889    | 33.675339    |
| Ca      | 23.084919    | 34.864643    | 35.565338    |
| Ca      | 23.491362    | 30.440826    | 33.180874    |
| Ca      | 22.805721    | 34.707489    | 30.481613    |
| Ca      | 24.774109    | 30.475758    | 27.739326    |
| Ca      | 27.802124    | 32.879486    | 31.251717    |
| Ca      | 29.020767    | 27.608246    | 29.953899    |
| Ca      | 30.471516    | 32.056190    | 27.485027    |
| Ca      | 30.260149    | 27.926254    | 24.722084    |
| Ca      | 33.567673    | 29.782381    | 28.370518    |
| Ca      | 34.378796    | 25.132236    | 26.221666    |
| Ca      | 35.757790    | 29.036928    | 23.888546    |
| S       | 21.186033    | 31.728580    | 35.408978    |
| S       | 20.570124    | 35.813362    | 33.096447    |
| S       | 21.881397    | 31.257994    | 30.039097    |
| S       | 25.095778    | 33.626083    | 33.167038    |
| S       | 26.304943    | 29.634808    | 31.183878    |
| S       | 25.680258    | 33.871773    | 28.015680    |
| S       | 28.138069    | 29.386396    | 26.892719    |
| S       | 30.836130    | 30.940664    | 30.417290    |
| S       | 31.620646    | 26.773294    | 27.752472    |
| S       | 32.693771    | 30.828001    | 25.050646    |
| S       | 33.468571    | 26.758198    | 23.179977    |
| S       | 36.436253    | 27.818588    | 27.199924    |
| Ca      | 18.462879    | 33.723846    | 33.431396    |
| Ca      | 22.914631    | 35.003311    | 35.663208    |
| Ca      | 23.392332    | 30.217991    | 33.118832    |
| Ca      | 22.886930    | 34.456421    | 30.393106    |
| Ca      | 24.944145    | 30.239155    | 28.152788    |
| Ca      | 27.775488    | 32.685596    | 31.283003    |
| Ca      | 28.904253    | 27.514755    | 29.756313    |
| Ca      | 30.314791    | 32.156620    | 27.649473    |
| Ca      | 30.279160    | 28.073275    | 24.622478    |
| Ca      | 33.603191    | 29.710693    | 28.217594    |
| Ca      | 34.683399    | 25.151173    | 26.276634    |
| Ca      | 35.663059    | 29.051580    | 23.784187    |
| S       | 20.906481    | 31.890825    | 35.344048    |
| S       | 20.844858    | 36.090889    | 33.021675    |
| S       | 22.012608    | 30.923393    | 30.216011    |
| S       | 24.905657    | 33.533348    | 33.087856    |
| S       | 26.367386    | 29.686958    | 31.309649    |
| S       | 25.667358    | 33.617565    | 28.474991    |
| S       | 28.123356    | 29.371471    | 26.819084    |
S  30.700367  30.683224  30.356730
S  31.665506  26.656441  27.588690
S  32.596481  30.781544  25.059620
S  33.567528  26.838970  23.305372
S  36.538177  28.240993  27.007328

24
generated by VMD
Ca  18.185135  33.549889  33.433270
Ca  22.565727  34.676773  35.920578
Ca  23.169615  30.065502  33.165279
Ca  22.869337  34.396988  30.646935
Ca  25.409199  30.825079  28.089403
Ca  27.766209  32.721535  31.380432
Ca  29.206640  27.791801  29.707981
Ca  30.246532  32.369232  27.339531
Ca  30.357756  27.760006  24.665943
Ca  33.613918  30.009315  27.854910
Ca  34.711330  25.139866  26.573879
Ca  35.507370  28.774162  23.770882
S  20.772909  31.680363  35.302254
S  20.628944  36.017357  33.161980
S  21.976913  31.357920  30.120117
S  24.689991  33.398788  33.312347
S  26.631519  29.698997  31.305313
S  25.952494  33.965401  28.400696
S  28.205276  29.590618  26.805134
S  30.684103  31.080671  30.110168
S  31.921711  26.773689  27.659492
S  32.616035  30.549423  24.868708
S  33.412045  26.227407  23.408867
S  36.619308  27.879234  26.935953

24
generated by VMD
Ca  18.286495  33.579189  33.596062
Ca  22.702515  34.487690  35.676521
Ca  23.220253  30.097824  33.122013
Ca  22.824203  34.533722  30.439987
Ca  24.993025  30.522739  28.309933
Ca  27.792173  32.871857  31.339520
Ca  29.268974  27.819195  30.034697
Ca  30.462891  32.443096  27.300125
Ca  30.457987  27.906563  24.485741
Ca  33.645473  29.975765  28.039011
Ca  34.440174  25.060095  26.384796
Ca  35.677567  28.847973  23.578993
S  20.777159  31.659464  35.393570
S        20.559706       35.958542       32.862492
S        21.914436       31.299156       30.120119
S        24.793566       33.515091       33.251041
S        26.438261       29.730989       31.459826
S        25.952667       33.740391       28.495165
S        28.270973       29.536259       26.944633
S        30.804859       31.041288       30.374924
S        31.807274       26.883163       27.629936
S        32.778400       30.763981       24.862358
S        33.471180       30.763981       24.862358
S        36.379807       27.766991       26.954929

generated by VMD

Ca       18.318981       33.139149       35.540006
Ca       22.874096       34.797722       35.900318
Ca       23.450794       30.226223       32.992950
Ca       22.847708       34.563934       30.477114
Ca       24.826296       30.586452       27.812946
Ca       27.792675       32.822929       31.277348
Ca       28.996000       27.694099       29.772137
Ca       30.457483       32.350784       27.284794
Ca       30.421005       27.843121       24.650483
Ca       33.640385       29.906595       28.043209
Ca       34.573978       24.933012       26.767887
Ca       35.314785       29.049007       23.892754
S        21.155617       31.687786       35.496944
S        20.639690       35.774986       33.259941
S        21.894773       31.216221       29.941067
S        25.024017       33.643066       33.076931
S        26.275215       29.596912       30.979418
S        25.840176       33.977829       28.413641
S        28.189276       29.778103       26.828005
S        30.934521       30.872169       30.181919
S        31.613373       26.907967       27.625053
S        32.653645       30.767864       25.101532
S        33.521954       26.329050       23.472431
S        36.463551       27.835083       27.142616

generated by VMD

Ca       18.236977       33.126717       33.612156
Ca       22.744621       34.721054       35.839333
Ca       23.414791       30.345547       33.018288
Ca       22.779629       34.359760       30.637962
Ca       25.009838       30.640512       27.913412
Ca       27.903603       33.137535       31.254791
Ca       29.169249       27.983704       29.678509
|  |  |  |  |
|---|---|---|---|
| Ca | 30.574408 | 32.556232 | 27.289167 |
| Ca | 30.391302 | 27.700109 | 24.636 |
| Ca | 33.641857 | 29.827579 | 28.071276 |
| Ca | 34.228664 | 24.855255 | 26.536531 |
| Ca | 35.629906 | 28.946327 | 23.849384 |
| S  | 20.972357 | 31.578064 | 35.345173 |
| S  | 20.437824 | 35.733364 | 33.352623 |
| S  | 22.025822 | 31.107515 | 29.953804 |
| S  | 24.811901 | 33.830421 | 33.150684 |
| S  | 26.440304 | 29.697090 | 31.240490 |
| S  | 25.806852 | 33.985439 | 28.443815 |
| S  | 28.282845 | 29.710659 | 26.775665 |
| S  | 30.871607 | 31.141872 | 30.121845 |
| S  | 31.77369 | 26.748352 | 27.791895 |
| S  | 32.579380 | 30.584791 | 25.050154 |
| S  | 33.511818 | 26.362259 | 23.340645 |
| S  | 36.477112 | 27.619930 | 27.035978 |

24

generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 18.257973 | 33.205284 | 33.692558 |
| Ca | 22.970896 | 34.520927 | 35.813324 |
| Ca | 23.540813 | 30.353542 | 32.962852 |
| Ca | 22.609797 | 34.661701 | 30.643885 |
| Ca | 25.077736 | 30.679792 | 27.823711 |
| Ca | 27.747511 | 32.985149 | 31.233868 |
| Ca | 29.121655 | 27.860456 | 29.932194 |
| Ca | 30.433752 | 32.187172 | 27.384407 |
| Ca | 30.607700 | 27.498030 | 24.443001 |
| Ca | 33.591953 | 29.782139 | 28.240906 |
| Ca | 34.201138 | 24.899307 | 26.521446 |
| Ca | 35.830566 | 29.262890 | 23.913288 |
| S  | 20.985390 | 31.617716 | 35.344780 |
| S  | 20.549604 | 35.935539 | 33.426750 |
| S  | 21.867586 | 31.118553 | 29.967241 |
| S  | 24.785288 | 33.857563 | 33.027283 |
| S  | 26.530880 | 29.809177 | 31.080492 |
| S  | 25.489964 | 33.977108 | 28.480885 |
| S  | 28.298346 | 29.347382 | 26.683468 |
| S  | 30.909157 | 31.121365 | 30.221157 |
| S  | 31.798622 | 26.937986 | 27.904196 |
| S  | 32.586170 | 30.605026 | 25.015587 |
| S  | 33.527157 | 26.405819 | 23.257908 |
| S  | 36.400436 | 27.670397 | 26.924898 |

24

generated by VMD

|  |  |  |
|---|---|---|
| Ca | 18.423124 | 33.129234 | 33.675739 |
|   | Ca     | 34.220387 | 35.589733 |
|---|--------|-----------|-----------|
| Ca| 22.682060 | 34.220387 | 35.589733 |
| Ca| 23.395679 | 30.335125 | 33.043522 |
| Ca| 22.737137 | 34.770432 | 30.486403 |
| Ca| 25.039942 | 30.887215 | 27.953957 |
| Ca| 27.821636 | 33.072678 | 31.326048 |
| Ca| 29.098249 | 28.115374 | 29.941025 |
| Ca| 30.777677 | 34.770432 | 30.486403 |
| Ca| 30.467112 | 27.719418 | 24.727882 |
| Ca| 33.674786 | 29.899921 | 28.117680 |
| Ca| 34.210220 | 24.788317 | 26.854912 |
| Ca| 35.653698 | 28.805119 | 23.518173 |
| Ca| 22.834530 | 33.021099 | 33.928551 |
| Ca| 22.834530 | 34.354183 | 35.927147 |
| Ca| 23.349752 | 30.319824 | 32.802055 |
| Ca| 22.785997 | 34.670750 | 30.530460 |
| Ca| 25.031637 | 30.912899 | 27.825394 |
| Ca| 27.710947 | 32.900997 | 31.161764 |
| Ca| 29.192278 | 28.160149 | 29.922728 |
| Ca| 30.594080 | 32.398201 | 27.480154 |
| Ca| 30.364574 | 27.622963 | 24.728252 |
| Ca| 33.928860 | 29.824600 | 27.806507 |
| Ca| 34.427216 | 24.783787 | 26.810539 |
| Ca| 35.478096 | 28.754877 | 23.833845 |
| S  | 21.006001 | 31.221657 | 35.377346 |
| S  | 20.516409 | 35.743580 | 33.341885 |
| S  | 21.770317 | 31.253971 | 29.781713 |
| S  | 24.823238 | 33.623234 | 33.200714 |
| S  | 26.411224 | 30.047762 | 30.893681 |
| S  | 25.526178 | 34.185627 | 28.263229 |
| S  | 28.329466 | 29.877945 | 26.692537 |
| S  | 30.841419 | 31.340384 | 30.290195 |
| S  | 31.645084 | 27.063942 | 27.873199 |
S  32.786377  30.729538  25.012260
S  33.348969  25.969282  23.661240
S  36.625771  27.518837  26.794666

24  generated by VMD

Ca  18.383472  33.193741  33.499992
Ca  22.724085  34.351791  36.009518
Ca  23.381853  30.228340  32.840919
Ca  22.980045  34.833057  30.611540
Ca  25.142788  30.896378  27.897465
Ca  27.586113  32.705952  31.318428
Ca  29.122526  27.874224  29.862293
Ca  30.527521  32.301239  27.292351
Ca  30.511896  27.750946  24.774017
Ca  33.701103  30.133091  28.164482
Ca  34.558479  24.849903  27.007664
Ca  35.360310  28.892830  23.398125
S  21.040453  31.352627  35.294388
S  20.668770  35.885220  33.387212
S  22.024229  31.469088  29.918850
S  24.884867  33.576340  33.120174
S  26.346224  29.734289  31.069811
S  25.712288  34.110214  28.291462
S  28.163086  29.455429  26.672581
S  30.773369  31.049625  30.241320
S  31.809416  26.971912  27.900316
S  32.562176  30.785877  24.887486
S  33.445217  25.929516  23.607140
S  36.309654  27.968431  26.871033

24  generated by VMD

Ca  18.374382  33.358967  33.677002
Ca  22.886494  34.449383  35.908859
Ca  23.183002  30.172331  32.804115
Ca  22.999022  34.618187  30.616650
Ca  24.996817  30.647655  27.923719
Ca  27.788109  32.839371  31.307148
Ca  28.907713  27.994987  29.949759
Ca  30.630238  32.390739  27.257097
Ca  30.452658  27.958626  24.621490
Ca  33.869614  29.974403  27.968977
Ca  34.283962  25.092678  26.829126
Ca  35.513474  28.818605  23.638096
S  21.066027  31.623844  35.294724
S  20.692497  35.811749  33.285107
S  21.915281  31.142076  29.724329
S        24.910328       33.462360       33.281979
S        26.316671       29.515514       26.754463
S        25.685259       33.902950       28.396662
S        28.106783       29.515514       26.754463
S        30.738983       31.161448       30.184875
S        31.578693       27.029446       27.799160
S        32.942612       30.819641       25.022259
S        33.386517       25.957289       23.664804
S        36.494972       27.970907       26.883350
24

generated by VMD
Ca       18.228216       33.122173       33.539734
Ca       23.028334       34.167511       35.873093
Ca       23.335064       30.127258       32.666584
Ca       23.016722       35.006638       30.668560
Ca       24.807280       30.751434       27.897194
Ca       27.914200       32.692539       31.460869
Ca       29.154598       27.996334       29.801903
Ca       30.320616       32.482162       27.390608
Ca       30.273338       27.724716       24.890373
Ca       33.817532       29.965023       27.989761
Ca       34.572853       25.185198       27.063671
Ca       35.344986       28.755417       23.384853
S        20.947918       31.378996       35.167580
S        20.739063       35.830463       33.179558
S        21.921675       31.608259       29.716879
S        24.877283       33.502518       33.052937
S        26.414686       29.697704       31.126001
S        25.906176       34.028656       28.622150
S        27.989937       29.661434       26.726728
S        30.884094       31.109085       30.224537
S        31.828396       26.873230       28.066669
S        32.522148       30.661932       24.835205
S        33.378883       25.813320       23.855415
S        36.496147       28.158077       26.739126
24

generated by VMD
Ca       18.204344       33.478027       33.774487
Ca       22.722479       34.468067       36.075287
Ca       23.281321       30.180979       32.840858
Ca       22.890694       34.709595       30.472073
Ca       25.069321       30.743256       27.800510
Ca       27.795837       32.703972       31.484955
Ca       28.943476       27.784784       29.605766
Ca       30.656382       32.235725       27.542641
Ca       30.343790       27.680847       24.696804
|  | Ca     | S       | 24           |
|---|--------|---------|--------------|
|  | 33.810467 | 29.848942 | 28.219193    |
|  | 34.735733 | 31.560822 | 26.980986    |
|  | 35.415428 | 35.854462 | 33.397964    |
|  | 21.860752 | 28.676331 | 23.250675    |
|  | 24.789656 | 33.428009 | 33.105492    |
|  | 26.327900 | 29.709240 | 26.617126    |
|  | 25.880968 | 34.097580 | 28.323051    |
|  | 28.241987 | 32.851374 | 27.889606    |
|  | 30.728012 | 30.958717 | 30.342913    |
|  | 31.759865 | 28.819763 | 23.735531    |
|  | 32.694336 | 30.667208 | 24.894831    |
|  | 33.415966 | 34.097580 | 28.323051    |
|  | 36.546864 | 32.670204 | 26.617126    |
|  | 18.366436 | 33.619240 | 33.480892    |
|  | 23.228226 | 34.22233 | 35.960861    |
|  | 23.212564 | 30.362745 | 32.712826    |
|  | 22.911228 | 34.386330 | 30.821766    |
|  | 24.953094 | 30.774525 | 27.772270    |
|  | 27.668114 | 32.670204 | 30.952757    |
|  | 28.977631 | 27.956997 | 29.739849    |
|  | 30.452789 | 32.620415 | 27.382027    |
|  | 30.346703 | 27.759346 | 24.803509    |
|  | 33.677547 | 29.972973 | 28.155064    |
|  | 34.667828 | 25.107735 | 26.933590    |
|  | 35.350609 | 28.819763 | 23.735531    |
|  | 31.678615 | 31.464455 | 35.192604    |
|  | 24.953094 | 30.774525 | 27.772270    |
|  | 27.668114 | 32.670204 | 30.952757    |
|  | 28.977631 | 27.956997 | 29.739849    |
|  | 30.452789 | 32.620415 | 27.382027    |
|  | 30.346703 | 27.759346 | 24.803509    |
|  | 33.677547 | 29.972973 | 28.155064    |
|  | 34.667828 | 25.107735 | 26.933590    |
|  | 35.350609 | 28.819763 | 23.735531    |
|  | 21.014053 | 31.464455 | 35.192604    |
|  | 21.100697 | 35.731216 | 33.543282    |
|  | 21.918297 | 31.195545 | 29.664181    |
|  | 24.899212 | 33.434155 | 33.094025    |
|  | 26.314285 | 29.602089 | 30.957542    |
|  | 25.746162 | 33.888260 | 28.290230    |
|  | 28.179520 | 29.821247 | 26.737438    |
|  | 30.825655 | 31.056126 | 30.157089    |
|  | 31.756023 | 26.903034 | 28.044004    |
|  | 32.473213 | 30.751060 | 24.979069    |
|  | 33.137016 | 25.923935 | 23.912708    |
|  | 36.543179 | 28.236439 | 26.916918    |

24

generated by VMD

| Ca     | S       | 24           |
|--------|---------|--------------|
| 18.366436 | 33.619240 | 33.480892    |
| 23.228226 | 34.22233 | 35.960861    |
| 23.212564 | 30.362745 | 32.712826    |
| 22.911228 | 34.386330 | 30.821766    |
| 24.953094 | 30.774525 | 27.772270    |
| 27.668114 | 32.670204 | 30.952757    |
| 28.977631 | 27.956997 | 29.739849    |
| 30.452789 | 32.620415 | 27.382027    |
| 30.346703 | 27.759346 | 24.803509    |
| 33.677547 | 29.972973 | 28.155064    |
| 34.667828 | 25.107735 | 26.933590    |
| 35.350609 | 28.819763 | 23.735531    |
| 21.014053 | 31.464455 | 35.192604    |
| 21.100697 | 35.731216 | 33.543282    |
| 21.918297 | 31.195545 | 29.664181    |
| 24.899212 | 33.434155 | 33.094025    |
| 26.314285 | 29.602089 | 30.957542    |
| 25.746162 | 33.888260 | 28.290230    |
| 28.179520 | 29.821247 | 26.737438    |
| 30.825655 | 31.056126 | 30.157089    |
| 31.756023 | 26.903034 | 28.044004    |
| 32.473213 | 30.751060 | 24.979069    |
| 33.137016 | 25.923935 | 23.912708    |
| 36.543179 | 28.236439 | 26.916918    |

24

generated by VMD

| Ca     | S       |
|--------|---------|
| 18.326696 | 33.582771 |
| 22.994495 | 34.309029 |
| 23.379175 | 30.258154 |
| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 22.816177 | 34.660015 | 30.528955 |
| Ca      | 25.036209  | 30.436962  | 27.726353  |
| Ca      | 27.839926  | 32.796593  | 31.099171  |
| Ca      | 29.165955  | 27.837063  | 29.792456  |
| Ca      | 30.460382  | 32.581841  | 27.643845  |
| Ca      | 30.424591  | 27.753265  | 24.733974  |
| Ca      | 33.694031  | 30.862034  | 28.335419  |
| Ca      | 34.543934  | 25.165949  | 26.913361  |
| Ca      | 35.043442  | 29.014927  | 23.347061  |
| S       | 20.889544  | 31.537382  | 35.175873  |
| S       | 21.054255  | 35.905632  | 33.517029  |
| S       | 21.923666  | 31.230801  | 29.601583  |
| S       | 24.820742  | 33.538780  | 33.032845  |
| S       | 26.329876  | 29.652863  | 31.119719  |
| S       | 25.543978  | 33.836030  | 28.357914  |
| S       | 28.363571  | 29.694654  | 26.829948  |
| S       | 30.893911  | 31.090961  | 30.496460  |
| S       | 31.810279  | 26.795357  | 27.831268  |
| S       | 32.587933  | 30.697132  | 25.146046  |
| S       | 33.251431  | 25.709034  | 23.476238  |
| S       | 36.485909  | 28.353825  | 26.912571  |

24 generated by VMD

| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 18.245687 | 33.769554 | 33.723919 |
| Ca      | 22.801508 | 34.300041 | 35.584801 |
| Ca      | 23.180103 | 30.223412 | 32.667038 |
| Ca      | 22.938633 | 34.685833 | 30.779415 |
| Ca      | 25.065020 | 30.603725 | 27.885923 |
| Ca      | 27.933184 | 32.697273 | 31.224572 |
| Ca      | 29.214281 | 27.805958 | 30.051380 |
| Ca      | 30.518606 | 32.275486 | 27.639488 |
| Ca      | 30.362291 | 27.678745 | 24.910007 |
| Ca      | 33.759029 | 29.962452 | 28.053291 |
| Ca      | 34.550529 | 25.154701 | 26.862679 |
| Ca      | 35.268883 | 29.049778 | 23.282677 |
| S       | 20.880692 | 31.403496 | 35.029831 |
| S       | 20.754606 | 35.971432 | 33.200111 |
| S       | 21.828960 | 31.269979 | 29.765018 |
| S       | 24.903923 | 33.371841 | 33.069210 |
| S       | 26.481430 | 29.795187 | 31.106663 |
| S       | 25.794836 | 34.050732 | 28.673079 |
| S       | 28.360180 | 29.483387 | 26.963547 |
| S       | 30.836258 | 30.991505 | 30.341204 |
| S       | 31.834248 | 26.720207 | 28.072321 |
| S       | 32.435600 | 30.628651 | 24.882483 |
| S       | 33.402233 | 25.986317 | 23.651070 |
|   |      |      |      |
|---|------|------|------|
| S | 36.369232 | 28.420330 | 26.515015 |
| 24 generated by VMD  |
| Ca | 18.344296 | 33.181992 | 33.383747 |
| Ca | 22.951441 | 34.338509 | 36.018436 |
| Ca | 23.242973 | 30.459568 | 32.796581 |
| Ca | 22.914007 | 34.830925 | 30.430670 |
| Ca | 24.945988 | 30.707809 | 27.891325 |
| Ca | 27.956753 | 32.743431 | 31.339302 |
| Ca | 29.101612 | 27.752808 | 29.842955 |
| Ca | 30.550936 | 32.133339 | 27.499500 |
| Ca | 30.275980 | 27.830074 | 25.140682 |
| Ca | 33.824184 | 29.904766 | 28.317675 |
| Ca | 34.613613 | 25.180122 | 26.719730 |
| Ca | 35.249989 | 28.931561 | 23.322351 |
| S | 20.935425 | 31.460722 | 35.201698 |
| S | 20.850552 | 35.767395 | 33.278099 |
| S | 22.014233 | 31.433201 | 29.702126 |
| S | 24.849218 | 33.595657 | 32.968124 |
| S | 26.365751 | 29.500927 | 31.117332 |
| S | 25.816164 | 34.094696 | 28.532654 |
| S | 28.126051 | 29.710209 | 26.799446 |
| S | 30.714575 | 30.930367 | 30.236389 |
| S | 31.992170 | 26.999912 | 28.206642 |
| S | 32.492908 | 30.597382 | 24.974194 |
| S | 33.160862 | 25.812050 | 23.673832 |
| S | 36.430313 | 28.402590 | 26.546532 |

24
generated by VMD

| Ca | 18.391069 | 33.266888 | 33.622654 |
| Ca | 22.981653 | 34.414879 | 36.018860 |
| Ca | 23.264772 | 30.457609 | 32.798103 |
| Ca | 23.012283 | 34.872627 | 30.531551 |
| Ca | 24.859371 | 30.586254 | 27.779617 |
| Ca | 27.627432 | 32.531830 | 31.195312 |
| Ca | 29.071577 | 27.733307 | 29.890282 |
| Ca | 30.611530 | 32.417583 | 27.497015 |
| Ca | 30.363728 | 27.799942 | 24.924507 |
| Ca | 33.652149 | 30.007622 | 28.251749 |
| Ca | 34.631134 | 24.973972 | 26.672237 |
| Ca | 35.309509 | 28.996311 | 23.434147 |
| S | 20.906876 | 31.493183 | 35.366253 |
| S | 20.770182 | 35.891472 | 33.258793 |
| S | 21.838516 | 31.315090 | 29.759037 |
| S | 24.911217 | 33.674179 | 32.960026 |
| S | 26.358889 | 29.535238 | 31.043571 |
| S    | 25.816847 | 33.843121 | 28.353607 |
|------|-----------|-----------|-----------|
| S    | 28.239021 | 29.704247 | 26.783205 |
| S    | 30.821112 | 30.961636 | 30.293316 |
| S    | 31.985531 | 26.814445 | 28.176117 |
| S    | 32.632549 | 30.723751 | 24.959019 |
| S    | 33.243073 | 26.028261 | 23.630466 |
| S    | 36.419975 | 28.256634 | 26.740604 |

24 generated by VMD

| Ca   | 18.368200 | 33.410362 | 33.493767 |
|------|-----------|-----------|-----------|
| Ca   | 22.853483 | 34.323128 | 35.771599 |
| Ca   | 23.381372 | 30.313581 | 32.766830 |
| Ca   | 22.831640 | 34.673416 | 30.761768 |
| Ca   | 25.048929 | 30.901695 | 27.833647 |
| Ca   | 27.819639 | 32.777695 | 31.405704 |
| Ca   | 29.182148 | 27.846922 | 29.766823 |
| Ca   | 30.370876 | 32.371246 | 27.383753 |
| Ca   | 30.305204 | 27.700480 | 24.773277 |
| Ca   | 33.717739 | 30.010645 | 28.206223 |
| Ca   | 34.853096 | 25.059607 | 26.929678 |
| Ca   | 35.246563 | 28.743420 | 23.594513 |
| S    | 20.944824 | 31.363668 | 35.084322 |
| S    | 20.645544 | 35.830173 | 33.313141 |
| S    | 21.921783 | 31.379177 | 30.028362 |
| S    | 24.880199 | 33.704281 | 33.310474 |
| S    | 26.328587 | 29.669678 | 30.850733 |
| S    | 25.841082 | 34.042755 | 28.645041 |
| S    | 26.219698 | 29.645161 | 26.619835 |
| S    | 30.753021 | 30.993912 | 30.166203 |
| S    | 31.844387 | 26.835400 | 27.767979 |
| S    | 32.520981 | 30.671955 | 24.925468 |
| S    | 33.225971 | 25.836521 | 23.793224 |
| S    | 36.614975 | 28.195213 | 26.743578 |

24 generated by VMD

| Ca   | 18.392349 | 33.286896 | 33.514137 |
|------|-----------|-----------|-----------|
| Ca   | 22.905378 | 34.402576 | 35.757244 |
| Ca   | 23.431580 | 29.972260 | 32.687016 |
| Ca   | 22.769838 | 34.769932 | 30.512936 |
| Ca   | 25.011490 | 30.734039 | 27.895555 |
| Ca   | 27.849640 | 32.905361 | 31.351852 |
| Ca   | 29.161966 | 27.865894 | 29.868273 |
| Ca   | 30.493227 | 32.453186 | 27.519045 |
| Ca   | 30.386892 | 27.697132 | 24.786148 |
| Ca   | 33.764099 | 30.142368 | 28.243008 |
| Ca   | 34.501392 | 25.155609 | 26.630316 |
Ca  35.179241   28.698700   23.653660
S   20.925287   31.301975   29.893665
S   20.640692   35.864113   33.350666
S   22.077547   31.356161   29.893665
S   24.910437   33.424210   33.214283
S   26.448236   29.805767   31.063423
S   25.817137   34.227806   28.485661
S   28.180662   29.667110   26.675018
S   30.811129   31.262672   27.972227
S   32.680988   30.602451   25.093483
S   33.095573   25.638565   23.657217
S   36.351330   28.179710   26.740643

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generated by VMD
Ca  18.291269   32.818436   33.147594
Ca  22.751986   34.702728   35.654289
Ca  23.513649   30.338419   32.954281
Ca  22.851587   34.774254   30.622345
Ca  25.048864   30.838879   27.955759
Ca  28.075216   32.871582   31.391310
Ca  29.216866   27.945309   29.862032
Ca  30.614450   32.601589   27.460936
Ca  30.569590   27.661415   24.589125
Ca  33.682980   29.924475   28.271172
Ca  34.435150   24.930950   26.571066
Ca  34.985703   28.846199   23.588314
S   21.031490   31.429794   35.389771
S   20.267525   35.660725   33.174149
S   22.062342   31.299366   29.891148
S   24.825727   33.660088   33.261490
S   26.574125   29.856274   31.195984
S   25.950571   33.992867   28.695606
S   28.269148   29.688993   26.780884
S   30.797239   31.096178   30.148117
S   31.875317   26.844536   27.999462
S   32.724781   30.731243   25.076992
S   33.092239   25.774456   23.533566
S   36.212154   28.011288   26.724625

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generated by VMD
Ca  18.384048   33.149429   33.079594
Ca  22.859861   34.699707   35.789753
Ca  23.754341   30.142456   33.340542
Ca  22.759466   34.303974   30.682236
Ca  24.994005   30.673403   28.002983
| Ca    | 27.918491 | 32.786388 | 31.365091 |
|-------|-----------|-----------|-----------|
| Ca    | 29.046997 | 27.960320 | 29.559210 |
| Ca    | 30.462660 | 32.719124 | 27.44088  |
| Ca    | 30.547207 | 27.942478 | 24.522894 |
| Ca    | 33.355289 | 29.887711 | 28.125235 |
| Ca    | 34.418869 | 24.804249 | 26.563553 |
| Ca    | 35.321651 | 28.823267 | 23.891867 |
| S     | 21.076654 | 31.585539 | 35.046803 |
| S     | 20.499071 | 35.833874 | 33.143761 |
| S     | 21.981548 | 30.917459 | 30.201242 |
| S     | 24.963469 | 33.723289 | 33.298656 |
| S     | 26.517971 | 29.964848 | 31.108074 |
| S     | 25.772511 | 33.958893 | 28.537758 |
| S     | 28.343493 | 30.011700 | 26.663776 |
| S     | 30.688160 | 31.126366 | 30.217112 |
| S     | 31.747845 | 26.716682 | 27.773663 |
| S     | 32.762100 | 30.730431 | 24.973734 |
| S     | 33.205502 | 25.859249 | 23.626102 |
| S     | 36.338829 | 27.979227 | 26.982311 |

24 generated by VMD

| Ca    | 18.123032 | 32.632195 | 33.657768 |
|-------|-----------|-----------|-----------|
| Ca    | 22.852310 | 34.578758 | 35.473186 |
| Ca    | 23.482540 | 30.337948 | 33.116470 |
| Ca    | 22.960304 | 34.354038 | 30.601341 |
| Ca    | 25.019869 | 30.873968 | 27.940536 |
| Ca    | 28.203762 | 33.137562 | 31.337049 |
| Ca    | 29.129290 | 31.145470 | 29.689472 |
| Ca    | 30.863272 | 32.667984 | 27.511257 |
| Ca    | 30.405231 | 27.981613 | 24.596291 |
| Ca    | 33.663574 | 29.904819 | 28.020992 |
| Ca    | 34.120045 | 24.783264 | 26.747885 |
| Ca    | 35.122593 | 28.546535 | 23.814781 |
| S     | 21.034464 | 31.405228 | 35.200729 |
| S     | 20.282150 | 35.433105 | 33.244015 |
| S     | 22.123384 | 30.922569 | 29.795637 |
| S     | 24.857803 | 33.857571 | 33.075169 |
| S     | 26.439972 | 30.047592 | 31.143303 |
| S     | 25.925289 | 34.196598 | 28.705486 |
| S     | 28.544214 | 30.051620 | 26.670073 |
| S     | 30.897758 | 31.219250 | 30.228786 |
| S     | 31.484011 | 26.841877 | 27.733448 |
| S     | 32.750530 | 30.750687 | 25.019749 |
| S     | 33.091343 | 25.764191 | 23.777971 |
| S     | 36.343330 | 27.865623 | 26.838678 |
|  |  |  |  |
|---|---|---|---|
| Ca | 18.319164 | 32.909401 | 33.693573 |
| Ca | 22.995945 | 34.782631 | 35.609776 |
| Ca | 23.344261 | 30.237185 | 33.040829 |
| Ca | 22.935369 | 34.577045 | 30.479378 |
| Ca | 27.903271 | 32.641388 | 31.332495 |
| Ca | 28.959064 | 27.903893 | 29.754959 |
| Ca | 30.605280 | 32.443420 | 27.522539 |
| Ca | 30.340334 | 27.995081 | 24.775887 |
| Ca | 33.770813 | 29.953869 | 28.277367 |
| Ca | 34.330086 | 25.021961 | 26.624527 |
| Ca | 35.313980 | 28.709183 | 23.546936 |
| S  | 20.956036 | 31.515518 | 35.461338 |
| S  | 20.615250 | 35.461628 | 33.026466 |
| S  | 22.004059 | 30.972935 | 29.816696 |
| S  | 24.995848 | 33.511356 | 33.091515 |
| S  | 26.435738 | 29.818806 | 30.947451 |
| S  | 26.019958 | 34.316799 | 28.453424 |
| S  | 28.163380 | 29.938457 | 26.628166 |
| S  | 30.742636 | 31.112017 | 30.205414 |
| S  | 31.669281 | 27.068621 | 27.998241 |
| S  | 32.837074 | 30.780706 | 25.139206 |
| S  | 33.039352 | 25.850376 | 23.722057 |
| S  | 36.396896 | 27.979645 | 26.834030 |

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|  |  |  |  |
|---|---|---|---|
| Ca | 18.115385 | 33.177574 | 33.320141 |
| Ca | 22.607067 | 34.469589 | 35.640016 |
| Ca | 23.669708 | 30.260124 | 33.138866 |
| Ca | 22.766739 | 34.620453 | 30.463093 |
| Ca | 25.060686 | 30.863487 | 28.229488 |
| Ca | 27.972574 | 32.686333 | 31.443466 |
| Ca | 29.091639 | 27.787014 | 29.685795 |
| Ca | 30.507263 | 32.437359 | 27.501593 |
| Ca | 30.303904 | 27.866693 | 24.772438 |
| Ca | 33.783180 | 30.061340 | 28.235481 |
| Ca | 34.486858 | 24.976105 | 26.628426 |
| Ca | 35.332626 | 28.726135 | 23.344761 |
| S  | 20.826069 | 31.477121 | 35.217308 |
| S  | 20.487720 | 35.788109 | 33.027302 |
| S  | 21.984922 | 31.221943 | 29.978346 |
| S  | 24.849899 | 33.773811 | 33.068520 |
| S  | 26.600073 | 29.844759 | 31.311146 |
| S  | 26.005585 | 34.126339 | 28.713062 |
| S  | 28.255308 | 29.642435 | 26.902908 |
|    | S    | Ca    |
|----|------|-------|
|    | 30.938389 | 30.933834 | 30.267918 |
|    | 31.946295 | 26.946640 | 28.034241 |
|    | 32.675507 | 30.724371 | 25.032972 |
|    | 33.146591 | 25.867737 | 23.389 |
|    | 36.306049 | 28.020760 | 26.589493 |
|    | 36.306049 | 28.020760 | 26.589493 |

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generated by VMD

|    | S    | Ca    | Ca |
|----|------|-------|----|
|    | 18.254152 | 32.877853 | 33.538113 |
|    | 22.971300 | 34.930351 | 35.597328 |
|    | 23.455587 | 30.552532 | 33.017529 |
|    | 22.800068 | 34.519943 | 30.429939 |
|    | 25.027334 | 30.558105 | 27.926659 |
|    | 27.950237 | 32.789516 | 31.465469 |
|    | 28.923859 | 27.719765 | 29.812536 |
|    | 30.563412 | 32.331650 | 27.768894 |
|    | 30.534775 | 27.900791 | 24.551130 |
|    | 33.700760 | 29.841871 | 28.228216 |
|    | 34.388790 | 24.964287 | 26.526215 |
|    | 35.168743 | 29.105072 | 23.778763 |
|    | 21.044828 | 31.787735 | 35.419434 |
|    | 20.513649 | 35.656940 | 33.054314 |
|    | 21.897717 | 31.121643 | 29.874687 |
|    | 24.873409 | 33.797554 | 32.955864 |
|    | 26.311947 | 29.747007 | 31.186430 |
|    | 26.039032 | 33.734356 | 28.543026 |
|    | 28.228007 | 29.653934 | 26.865540 |
|    | 30.954552 | 30.793734 | 30.415197 |
|    | 31.712009 | 26.836536 | 27.670616 |
|    | 32.766621 | 30.866440 | 25.238073 |
|    | 33.152744 | 26.104752 | 23.507401 |
|    | 36.485744 | 28.107662 | 26.568705 |

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generated by VMD
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|--------------|--------------|--------------|
| S       | 20.706430    | 35.530449    | 33.261799    |
| S       | 21.777592    | 30.928623    | 29.818947    |
| S       | 24.829926    | 33.642776    | 32.825455    |
| S       | 26.471712    | 29.734356    | 30.885696    |
| S       | 25.680508    | 33.935947    | 28.676571    |
| S       | 28.311220    | 29.962667    | 26.650097    |
| S       | 30.789415    | 30.940155    | 30.267303    |
| S       | 31.660906    | 26.783154    | 27.876148    |
| S       | 32.812687    | 30.814386    | 25.122887    |
| S       | 33.311317    | 25.797981    | 23.640575    |
| S       | 36.425488    | 28.009212    | 26.890079    |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|--------------|--------------|--------------|
| Ca      | 18.421558    | 32.691887    | 33.931038    |
| Ca      | 22.823475    | 34.655930    | 35.634117    |
| Ca      | 23.538237    | 30.436348    | 32.816250    |
| Ca      | 22.692461    | 34.719234    | 30.207348    |
| Ca      | 25.174618    | 30.870935    | 27.919727    |
| Ca      | 27.871500    | 32.952255    | 31.333160    |
| Ca      | 28.930288    | 27.711626    | 29.753521    |
| Ca      | 30.588179    | 32.520615    | 27.562920    |
| Ca      | 30.434006    | 27.963570    | 24.588596    |
| Ca      | 33.692307    | 29.665195    | 28.429638    |
| Ca      | 34.512608    | 24.776333    | 26.756811    |
| Ca      | 35.227249    | 28.951630    | 23.403316    |
| S       | 21.191236    | 31.499228    | 35.607628    |
| S       | 20.486704    | 35.531387    | 33.097668    |
| S       | 21.999102    | 31.152016    | 29.708532    |
| S       | 24.740675    | 33.806389    | 32.903297    |
| S       | 26.501719    | 29.916359    | 31.100704    |
| S       | 25.889238    | 34.288841    | 28.532364    |
| S       | 28.340595    | 29.735832    | 26.735547    |
| S       | 30.874966    | 30.880568    | 30.448467    |
| S       | 31.666842    | 26.779110    | 27.971478    |
| S       | 32.721989    | 30.785988    | 25.144379    |
| S       | 33.159283    | 25.997576    | 23.576487    |
| S       | 36.241177    | 28.011154    | 26.779034    |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|--------------|--------------|--------------|
| Ca      | 18.349873    | 33.038113    | 33.673111    |
| Ca      | 22.964434    | 34.556274    | 35.750519    |
| Ca      | 23.220737    | 30.224949    | 32.747219    |
| Ca      | 22.857676    | 34.630169    | 30.505787    |
| Ca      | 25.024004    | 30.980747    | 28.008663    |
| Ca      | 27.905926    | 32.741154    | 31.331657    |
| Ca      | 29.180325    | 28.039312    | 29.843971    |
|   | 30.547369 | 32.486042 | 27.352131 |
|---|-----------|-----------|-----------|
| Ca| 30.357986 | 27.679436 | 24.814407 |
| Ca| 33.664516 | 30.076735 | 28.056969 |
| Ca| 34.595627 | 25.047180 | 26.702545 |
| Ca| 35.055714 | 28.761442 | 23.792839 |
| S | 21.124548 | 31.505047 | 35.353348 |
| S | 20.587982 | 35.672977 | 33.141758 |
| S | 21.792471 | 31.257362 | 29.709805 |
| S | 24.808266 | 33.496143 | 33.044247 |
| S | 26.335941 | 29.735535 | 30.912720 |
| S | 25.984371 | 34.093819 | 28.559200 |
| S | 28.260695 | 29.776661 | 26.743711 |
| S | 31.063295 | 31.053875 | 30.404543 |
| S | 31.972801 | 26.837864 | 27.950720 |
| S | 32.430698 | 30.649445 | 25.061588 |
| S | 33.125156 | 26.133804 | 23.622940 |
| S | 36.509666 | 27.825966 | 26.855637 |

24 generated by VMD

|   | 18.234791 | 32.789288 | 33.541138 |
|---|-----------|-----------|-----------|
| Ca| 22.733335 | 34.885880 | 35.801098 |
| Ca| 23.652411 | 30.506590 | 33.079838 |
| Ca| 22.840294 | 34.891781 | 30.507305 |
| Ca| 24.594463 | 30.373718 | 27.813589 |
| Ca| 27.673529 | 32.915272 | 31.371578 |
| Ca| 29.197792 | 27.799746 | 29.671989 |
| Ca| 30.592001 | 32.252136 | 27.663565 |
| Ca| 30.458708 | 28.001102 | 24.503811 |
| Ca| 34.001556 | 29.815773 | 28.138893 |
| Ca| 34.650597 | 24.784475 | 26.438507 |
| Ca| 35.290562 | 28.971432 | 23.893936 |
| S | 21.143646 | 31.703388 | 35.495903 |
| S | 20.453285 | 35.681877 | 33.147785 |
| S | 21.931908 | 31.340397 | 30.000759 |
| S | 24.893112 | 33.997421 | 33.277191 |
| S | 26.268259 | 29.656652 | 31.038235 |
| S | 25.592342 | 33.954056 | 28.341431 |
| S | 28.145144 | 29.650921 | 26.685837 |
| S | 30.876873 | 30.886787 | 30.383997 |
| S | 31.976387 | 26.832790 | 27.516922 |
| S | 32.612221 | 30.681736 | 25.263262 |
| S | 33.308990 | 26.261803 | 23.348249 |
| S | 36.597412 | 27.665071 | 27.015228 |

24 generated by VMD

|   | 17.795803 | 32.918484 | 33.431454 |
| Element | X1 | Y1 | Z1 |
|---------|-----|-----|-----|
| Ca      | 22.527943 | 34.532539 | 35.848328 |
| Ca      | 23.424902 | 30.476055 | 32.956432 |
| Ca      | 23.053276 | 34.586174 | 35.848328 |
| Ca      | 25.061527 | 30.918396 | 27.796083 |
| Ca      | 28.012810 | 32.929195 | 27.620106 |
| Ca      | 29.370129 | 28.040489 | 29.999857 |
| Ca      | 30.487524 | 32.453129 | 27.620106 |
| Ca      | 30.187500 | 27.859339 | 25.002846 |
| Ca      | 34.092266 | 30.136814 | 27.842842 |
| Ca      | 34.588055 | 24.906113 | 26.542860 |
| Ca      | 34.965534 | 28.549660 | 23.788395 |
| S       | 20.723400 | 31.440050 | 35.219414 |
| S       | 20.461231 | 35.421547 | 32.911087 |
| S       | 22.070854 | 31.190853 | 30.093872 |
| S       | 24.910084 | 33.875885 | 33.328148 |
| S       | 26.468164 | 29.914631 | 31.083366 |
| S       | 26.094030 | 33.999630 | 28.627556 |
| S       | 28.234453 | 29.774866 | 26.809433 |
| S       | 31.193243 | 31.173264 | 30.303905 |
| S       | 31.978874 | 26.990894 | 27.769588 |
| S       | 32.639828 | 30.702509 | 25.095186 |
| S       | 32.884727 | 25.84692 | 23.319798 |
| S       | 36.493862 | 27.664797 | 26.643642 |

24 generated by VMD

| Element | X1 | Y1 | Z1 |
|---------|-----|-----|-----|
| Ca      | 18.078606 | 32.797314 | 33.493359 |
| Ca      | 22.416023 | 34.480118 | 35.869823 |
| Ca      | 23.370163 | 30.443390 | 32.991871 |
| Ca      | 22.668240 | 34.754971 | 30.848215 |
| Ca      | 25.110003 | 31.058823 | 27.736435 |
| Ca      | 27.729780 | 33.227310 | 31.606798 |
| Ca      | 29.374659 | 28.275936 | 29.742214 |
| Ca      | 30.761179 | 32.508709 | 27.254602 |
| Ca      | 30.521152 | 27.758106 | 24.675577 |
| Ca      | 34.407360 | 29.776054 | 27.414797 |
| Ca      | 34.533295 | 24.583277 | 26.787275 |
| Ca      | 35.144897 | 28.578310 | 23.392803 |
| S       | 20.820644 | 31.434155 | 35.545094 |
| S       | 20.186588 | 35.515209 | 33.182236 |
| S       | 21.959133 | 31.184998 | 29.724899 |
| S       | 24.667143 | 33.709415 | 33.441227 |
| S       | 26.442291 | 29.928566 | 31.026909 |
| S       | 25.715765 | 34.326099 | 28.715904 |
| S       | 28.494061 | 29.845303 | 26.750669 |
| S       | 30.866236 | 31.520210 | 30.530624 |
| S       | 31.908129 | 26.954647 | 27.800789 |
|   | X       | Y       | Z       |
|---|---------|---------|---------|
| S | 32.83389| 30.60392| 25.05973|
| S | 33.08317| 25.59339| 23.60649|
| S | 36.62701| 27.44182| 26.74169|

24

generated by VMD

| Ca  | X       | Y       | Z       |
|-----|---------|---------|---------|
|     | 18.34279| 33.27084| 33.54747|
| Ca  | 22.56767| 34.43499| 35.82007|
| Ca  | 23.39599| 30.17338| 32.99323|
| Ca  | 22.46518| 34.87231| 30.54534|
| Ca  | 24.95182| 30.70550| 27.82219|
| Ca  | 27.49697| 32.80079| 31.67006|
| Ca  | 29.34611| 28.06974| 30.12294|
| Ca  | 30.82256| 32.48978| 27.26952|
| Ca  | 30.46506| 27.96207| 24.76800|
| Ca  | 34.46159| 29.78134| 27.42410|
| Ca  | 34.45398| 24.77279| 26.69131|
| Ca  | 35.33470| 28.61267| 23.29523|
| S   | 20.86621| 31.44562| 35.24614|
| S   | 20.45163| 35.83328| 33.24008|
| S   | 21.94493| 31.41853| 29.78520|
| S   | 24.60669| 33.67189| 33.28233|
| S   | 26.30747| 29.53437| 31.12879|
| S   | 25.61473| 34.16640| 28.65011|
| S   | 28.25848| 29.68135| 26.93283|
| S   | 30.65779| 31.37544| 30.49438|
| S   | 32.21315| 27.16718| 28.00970|
| S   | 32.88044| 30.56774| 25.12137|
| S   | 33.15400| 25.96238| 23.54027|
| S   | 36.65977| 27.52926| 26.53887|

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generated by VMD

| Ca  | X       | Y       | Z       |
|-----|---------|---------|---------|
|     | 18.35286| 32.83967| 33.56708|
| Ca  | 22.37041| 34.27870| 36.07804|
| Ca  | 23.50936| 30.26071| 32.82029|
| Ca  | 22.86685| 34.69078| 30.61519|
| Ca  | 25.28637| 31.08241| 27.66472|
| Ca  | 27.79862| 33.16017| 31.83642|
| Ca  | 29.31670| 28.34217| 29.78430|
| Ca  | 30.75571| 32.41939| 26.78900|
| Ca  | 30.30349| 27.74044| 24.87447|
| Ca  | 34.02068| 30.04620| 27.55083|
| Ca  | 34.42139| 24.76440| 26.98821|
| Ca  | 35.28109| 28.48305| 23.56872|
| S   | 20.95178| 31.09283| 35.29921|
| S   | 20.40209| 35.55237| 33.22615|
| S   | 22.13312| 31.25843| 29.62263|
|   |         |         |         |
|---|---------|---------|---------|
| S | 24.530281 | 33.733971 | 33.438000 |
| S | 26.434952 | 29.782013 | 30.953678 |
| S | 26.105036 | 34.506676 | 28.937328 |
| S | 28.215336 | 29.786972 | 26.510235 |
| S | 30.846386 | 31.701099 | 30.232750 |
| S | 31.924953 | 27.089695 | 27.945602 |
| S | 32.582375 | 30.455753 | 24.788223 |
| S | 32.963707 | 25.728500 | 23.824348 |
| S | 36.346249 | 27.502533 | 27.024620 |

24 generated by VMD

|   |         |         |         |
|---|---------|---------|---------|
| Ca | 17.894665 | 32.971111 | 33.348118 |
| Ca | 22.235584 | 34.276573 | 36.071571 |
| Ca | 23.358337 | 30.416142 | 32.801735 |
| Ca | 22.892879 | 34.947105 | 30.841583 |
| Ca | 25.291737 | 31.100018 | 27.908600 |
| Ca | 27.526627 | 32.941498 | 31.811127 |
| Ca | 29.268162 | 28.297810 | 29.878723 |
| Ca | 30.873524 | 32.315254 | 26.732178 |
| Ca | 30.393032 | 27.571505 | 24.744205 |
| Ca | 34.494305 | 29.772369 | 27.233942 |
| Ca | 34.495270 | 24.661385 | 26.979704 |
| Ca | 35.557888 | 28.414410 | 23.376633 |
| S  | 20.807594 | 31.197041 | 35.207256 |
| S  | 20.308222 | 35.541420 | 33.492535 |
| S  | 22.206589 | 31.588043 | 29.853003 |
| S  | 24.691311 | 33.652027 | 33.374115 |
| S  | 26.468136 | 29.869644 | 31.351677 |
| S  | 25.733917 | 34.413658 | 28.975594 |
| S  | 28.395264 | 29.722572 | 26.652672 |
| S  | 30.362972 | 31.662785 | 30.395309 |
| S  | 32.033272 | 27.159054 | 27.814644 |
| S  | 32.568554 | 30.524260 | 24.504333 |
| S  | 33.326721 | 25.571800 | 23.813152 |
| S  | 36.535576 | 27.712566 | 26.777641 |

24 generated by VMD

|   |         |         |         |
|---|---------|---------|---------|
| Ca | 18.045202 | 32.666512 | 33.401356 |
| Ca | 22.230183 | 34.268547 | 35.849289 |
| Ca | 23.624590 | 30.244011 | 32.850967 |
| Ca | 22.825947 | 35.016720 | 30.690435 |
| Ca | 25.300142 | 31.205168 | 27.923605 |
| Ca | 27.713554 | 32.947624 | 31.997583 |
| Ca | 29.495344 | 28.195347 | 29.896889 |
| Ca | 30.903135 | 32.459145 | 26.757540 |
| Ca | 30.335785 | 27.543659 | 24.837616 |
| Ca    | 34.307396 | 29.782616 | 27.313812 |
|-------|-----------|-----------|-----------|
| Ca    | 34.308968 | 24.731550 | 27.168272 |
| S     | 20.869980 | 31.152920 | 34.921936 |
| S     | 20.098886 | 35.619682 | 33.183937 |
| S     | 22.223343 | 31.586182 | 29.806353 |
| S     | 24.843079 | 33.609936 | 33.401268 |
| S     | 26.550264 | 29.742077 | 31.151093 |
| S     | 26.178989 | 34.380802 | 29.037498 |
| S     | 30.737724 | 31.604748 | 30.426226 |
| S     | 32.011700 | 27.195137 | 27.808716 |
| S     | 32.368526 | 30.564201 | 24.564318 |
| S     | 33.091717 | 25.592285 | 23.950268 |
| S     | 36.364418 | 27.776253 | 26.684738 |

24
generated by VMD

| Ca    | 18.063261 | 32.741028 | 33.415482 |
|-------|-----------|-----------|-----------|
| Ca    | 22.397587 | 34.671124 | 36.083149 |
| Ca    | 23.238564 | 30.383602 | 32.881752 |
| Ca    | 22.988348 | 34.908424 | 30.663668 |
| Ca    | 25.108530 | 30.942158 | 27.883867 |
| Ca    | 27.701563 | 32.770458 | 31.843679 |
| Ca    | 29.228571 | 28.243155 | 29.768145 |
| Ca    | 30.646404 | 32.392078 | 27.002594 |
| Ca    | 30.271124 | 27.524445 | 24.778931 |
| Ca    | 34.213757 | 29.919685 | 27.196167 |
| Ca    | 34.656685 | 24.699471 | 26.790611 |
| Ca    | 35.516705 | 28.576202 | 23.424019 |
| S     | 20.754814 | 31.317045 | 35.414356 |
| S     | 20.324862 | 35.689606 | 33.427380 |
| S     | 22.089743 | 31.454550 | 29.896383 |
| S     | 24.639023 | 33.769279 | 33.351330 |
| S     | 26.300829 | 29.771900 | 30.985081 |
| S     | 26.092478 | 34.244003 | 28.745358 |
| S     | 28.358664 | 29.837141 | 26.581963 |
| S     | 30.667061 | 31.421473 | 30.423616 |
| S     | 32.016369 | 27.014439 | 27.849926 |
| S     | 32.550873 | 30.392673 | 24.836823 |
| S     | 33.294735 | 25.798975 | 23.741470 |
| S     | 36.599510 | 27.817211 | 26.952045 |

24
generated by VMD

| Ca    | 17.969685 | 33.112869 | 33.672089 |
|-------|-----------|-----------|-----------|
| Ca    | 22.774086 | 34.408440 | 36.063408 |
| Ca    | 23.048201 | 30.447186 | 32.779667 |
Ca 22.995975 34.901611 30.730291
Ca 25.047714 30.668781 27.929981
Ca 27.856743 32.459175 31.373983
Ca 29.216515 28.098667 30.012907
Ca 30.495886 32.582001 27.180130
Ca 30.427048 28.098667 30.012907
Ca 31.917862 30.041821 27.360201
Ca 34.614792 24.933092 26.981667
Ca 35.546349 28.718983 23.546886
S 20.637344 31.551846 35.407745
S 20.639376 35.674904 33.461090
S 21.835909 31.505327 29.567150
S 24.771959 33.544952 33.162975
S 26.231655 29.723835 31.12789
S 25.930786 33.991039 28.745567
S 28.407543 29.746346 26.783543
S 30.938608 31.306694 30.178408
S 31.857176 27.059536 27.866184
S 32.617332 30.536316 24.760145
S 33.430672 25.797754 23.567226
S 36.510754 27.879177 26.993034

24

generated by VMD

Ca 18.085400 32.841240 33.481560
Ca 22.862125 34.455437 36.139626
Ca 23.461178 30.111572 32.863380
Ca 22.887957 34.866646 30.783098
Ca 25.037270 30.978449 27.547520
Ca 27.791037 32.843582 31.436872
Ca 29.102394 28.116760 29.543619
Ca 30.401554 32.469193 27.121326
Ca 30.291849 27.551966 24.66981
Ca 33.893429 30.142296 27.585407
Ca 34.407772 25.007809 27.284285
Ca 35.597378 28.589924 23.795776
S 20.925791 31.415417 35.383778
S 20.413458 35.617798 33.479618
S 21.951859 31.611919 29.840630
S 24.957815 33.345238 33.535751
S 26.383677 29.845993 30.723295
S 25.848461 34.368023 28.649725
S 28.029280 29.753006 26.489946
S 30.960161 31.364960 30.106106
S 31.757153 27.158257 27.789764
S 32.655968 30.426687 24.725563
S 33.487511 25.668457 23.952309
|   | 36.529610 | 27.749443 | 27.014090 |
|---|-----------|-----------|-----------|
|24 | generated by VMD |
|Ca| 18.535160 | 32.658142 | 33.746052 |
|Ca| 23.044231 | 34.744144 | 36.022858 |
|Ca| 23.347095 | 30.433796 | 32.692654 |
|Ca| 22.842958 | 34.753357 | 30.765945 |
|Ca| 24.798326 | 30.970009 | 27.436054 |
|Ca| 27.777308 | 32.778095 | 31.149410 |
|Ca| 28.963264 | 28.015812 | 29.573771 |
|Ca| 30.362631 | 32.354259 | 27.296642 |
|Ca| 30.371773 | 27.727364 | 24.613678 |
|Ca| 33.588570 | 29.946831 | 27.736179 |
|Ca| 34.580208 | 25.001011 | 27.227098 |
|Ca| 35.657833 | 28.909826 | 23.959618 |
|S | 21.302357 | 31.569546 | 35.586182 |
|S | 20.767769 | 35.456284 | 33.394272 |
|S | 22.040691 | 31.641060 | 29.565430 |
|S | 24.947252 | 33.240261 | 33.439476 |
|S | 26.170837 | 29.687115 | 30.612375 |
|S | 25.685583 | 34.284210 | 28.493000 |
|S | 28.069798 | 29.663055 | 26.609028 |
|S | 30.725674 | 31.084038 | 30.097986 |
|S | 31.619793 | 26.910414 | 28.007263 |
|S | 32.642769 | 30.628544 | 24.772202 |
|S | 33.408054 | 25.968828 | 23.880238 |
|S | 36.470184 | 27.874058 | 27.262611 |

24 generated by VMD

| Ca | 18.585804 | 32.758186 | 33.643715 |
| Ca | 23.017868 | 34.457123 | 36.197346 |
| Ca | 23.258999 | 30.578354 | 32.843201 |
| Ca | 23.004414 | 34.724457 | 30.914381 |
| Ca | 24.924658 | 30.621027 | 27.526661 |
| Ca | 27.533068 | 32.946098 | 31.108509 |
| Ca | 28.924667 | 28.200661 | 29.644836 |
| Ca | 30.392197 | 32.442039 | 27.099792 |
| Ca | 30.415222 | 27.717951 | 24.507782 |
| Ca | 33.583195 | 30.004480 | 27.875843 |
| Ca | 34.748657 | 25.026939 | 27.107290 |
| Ca | 35.553165 | 28.633951 | 24.020794 |
| S  | 21.257145 | 31.544071 | 35.646526 |
| S  | 20.684265 | 35.567444 | 33.328190 |
| S  | 21.937853 | 31.781683 | 29.536903 |
| S  | 24.892340 | 33.289978 | 33.470181 |
| S  | 26.055729 | 29.715254 | 30.737402 |
|   | 25.830248 | 34.078770 | 28.481653 |
|---|-----------|-----------|-----------|
| S | 28.162777 | 29.850250 | 26.552963 |
| S | 30.622805 | 31.081451 | 30.152733 |
| S | 31.780746 | 26.935116 | 27.666374 |
| S | 32.646442 | 30.538811 | 24.716793 |
| S | 33.47655  | 25.861189 | 23.704166 |
| S | 36.460186 | 27.944813 | 27.455978 |

24

generated by VMD

| Ca | 18.122725 | 33.068176 | 33.430332 |
|----|-----------|-----------|-----------|
| Ca | 23.307003 | 34.696922 | 35.746658 |
| Ca | 23.219103 | 30.250370 | 33.008570 |
| Ca | 23.08526  | 34.608795 | 30.945549 |
| Ca | 24.775095 | 30.534966 | 27.591892 |
| Ca | 27.961170 | 32.826515 | 31.194954 |
| Ca | 28.879017 | 28.018181 | 29.879398 |
| Ca | 30.403639 | 32.501297 | 27.277048 |
| Ca | 30.45644  | 27.951342 | 24.661541 |
| Ca | 33.584351 | 29.967829 | 27.720970 |
| Ca | 34.356045 | 25.011343 | 27.070538 |
| Ca | 35.563766 | 28.862411 | 23.845058 |
| S  | 21.016870 | 31.754440 | 35.437302 |
| S  | 20.698059 | 35.519814 | 33.277920 |
| S  | 21.917759 | 31.422157 | 29.629723 |
| S  | 25.10547  | 33.229473 | 33.401638 |
| S  | 26.187811 | 29.593552 | 31.003765 |
| S  | 25.771187 | 33.955399 | 28.489067 |
| S  | 28.157578 | 29.633812 | 26.589493 |
| S  | 30.920681 | 31.080402 | 30.149696 |
| S  | 31.773298 | 26.974115 | 27.970507 |
| S  | 32.606518 | 30.725698 | 24.856171 |
| S  | 33.392193 | 26.131855 | 23.579643 |
| S  | 36.458481 | 27.981190 | 27.183121 |

24

generated by VMD

| Ca | 18.269636 | 32.812973 | 33.465027 |
|----|-----------|-----------|-----------|
| Ca | 23.101540 | 34.802277 | 35.675186 |
| Ca | 23.421478 | 30.667402 | 33.129089 |
| Ca | 22.649975 | 34.522804 | 30.625002 |
| Ca | 24.825804 | 30.724627 | 27.666092 |
| Ca | 27.809141 | 32.779198 | 31.310953 |
| Ca | 28.977385 | 27.940006 | 29.834631 |
| Ca | 30.624125 | 32.304478 | 27.349182 |
| Ca | 30.551140 | 27.889721 | 24.623695 |
| Ca | 33.911407 | 30.200851 | 28.102398 |
| Ca | 34.456245 | 25.113140 | 26.628881 |
|  |  |  |  |
|---|---|---|---|
| Ca | 35.586285 | 28.462090 | 23.685459 |
| S  | 21.092949 | 31.776482 | 35.701809 |
| S  | 20.389683 | 35.554512 | 33.308891 |
| S  | 21.876871 | 31.271841 | 29.884962 |
| S  | 24.981394 | 33.362011 | 33.311996 |
| S  | 26.016544 | 29.719635 | 30.788387 |
| S  | 25.802166 | 34.174438 | 28.810165 |
| S  | 28.155697 | 29.877842 | 26.664400 |
| S  | 30.688231 | 30.927292 | 30.169067 |
| S  | 31.868975 | 27.004128 | 27.852726 |
| S  | 32.920643 | 30.607054 | 24.787842 |
| S  | 33.287033 | 26.049969 | 23.180567 |
| S  | 36.455418 | 27.755310 | 27.383631 |

24

generated by VMD

| Ca | 18.272427 | 32.528591 | 33.548515 |
| Ca | 22.909023 | 34.804623 | 35.899365 |
| Ca | 23.380087 | 30.416073 | 32.861717 |
| Ca | 22.968601 | 34.695705 | 30.910610 |
| Ca | 25.005733 | 30.868490 | 27.684109 |
| Ca | 27.799419 | 32.950493 | 31.382710 |
| Ca | 28.964596 | 28.128265 | 29.737686 |
| Ca | 30.609060 | 32.365776 | 27.105553 |
| Ca | 30.465250 | 27.607998 | 24.90328 |
| Ca | 33.792439 | 30.098186 | 27.942028 |
| Ca | 34.314693 | 25.011032 | 26.833912 |
| Ca | 35.594353 | 28.642624 | 23.838634 |
| S  | 21.149761 | 31.800728 | 35.619209 |
| S  | 20.319435 | 35.446194 | 33.235088 |
| S  | 22.135258 | 31.532324 | 29.682377 |
| S  | 24.984224 | 33.367073 | 33.436737 |
| S  | 26.166269 | 29.612326 | 30.710419 |
| S  | 25.731777 | 34.183697 | 28.737890 |
| S  | 28.254742 | 29.710657 | 26.590269 |
| S  | 30.966629 | 31.101751 | 30.107599 |
| S  | 31.729195 | 26.913122 | 27.828022 |
| S  | 32.605179 | 30.699020 | 24.767656 |
| S  | 33.298508 | 25.932009 | 23.611103 |
| S  | 36.303448 | 27.883261 | 27.379519 |

24

generated by VMD

| Ca | 18.262222 | 32.747055 | 33.838215 |
| Ca | 23.014805 | 34.601753 | 35.851685 |
| Ca | 23.284840 | 30.242270 | 33.004932 |
| Ca | 22.968927 | 34.898430 | 30.691362 |
| Ca | 25.031733 | 30.683750 | 27.661819 |
|   | Ca  | S     |   |
|---|-----|-------|---|
| Ca| 27.806168 | 32.853127 | 31.196178 |
| Ca| 28.923761 | 28.109379 | 29.584824 |
| Ca| 30.583372 | 32.420570 | 27.093483 |
| Ca| 30.384258 | 27.936602 | 24.519676 |
| Ca| 33.620312 | 30.152184 | 27.868359 |
| Ca| 34.629963 | 24.991627 | 27.010542 |
| Ca| 35.628178 | 28.507999 | 23.861397 |
| S | 21.018454 | 31.616966 | 35.729103 |
| S | 20.409523 | 35.533031 | 33.90980 |
| S | 22.119621 | 31.530100 | 29.817320 |
| S | 24.968979 | 33.278637 | 33.270565 |
| S | 25.971968 | 29.687260 | 30.731522 |
| S | 25.966579 | 34.298878 | 28.604210 |
| S | 28.142029 | 29.676826 | 26.449680 |
| S | 30.727484 | 31.037140 | 30.100266 |
| S | 31.645344 | 27.080971 | 27.798452 |
| S | 32.806469 | 30.702320 | 24.717438 |
| S | 33.418213 | 25.911545 | 23.726093 |
| S | 36.386749 | 27.801579 | 27.421976 |

24

generated by VMD

|   | Ca  | S     |   |
|---|-----|-------|---|
| Ca| 18.869572 | 32.456493 | 33.548504 |
| Ca| 22.845207 | 35.075649 | 35.744232 |
| Ca| 23.187042 | 30.366093 | 33.110737 |
| Ca| 22.951595 | 34.549374 | 30.615614 |
| Ca| 25.148731 | 30.493065 | 27.731873 |
| Ca| 27.858034 | 32.717510 | 31.485394 |
| Ca| 28.766676 | 28.049282 | 29.891617 |
| Ca| 30.388958 | 32.549530 | 27.388550 |
| Ca| 30.442883 | 27.572598 | 24.526760 |
| Ca| 33.622761 | 30.160566 | 27.943508 |
| Ca| 34.035736 | 25.092379 | 26.818199 |
| Ca| 35.639595 | 28.919622 | 23.741959 |
| S | 21.310442 | 31.791893 | 35.514580 |
| S | 20.552414 | 35.621162 | 33.041416 |
| S | 22.086403 | 31.518820 | 29.486317 |
| S | 24.813704 | 33.419487 | 33.402748 |
| S | 26.070465 | 29.579906 | 30.938202 |
| S | 26.126789 | 33.938164 | 28.744499 |
| S | 28.239405 | 29.764082 | 26.623047 |
| S | 30.713415 | 31.092716 | 30.281336 |
| S | 31.711248 | 26.972578 | 27.910812 |
| S | 32.701786 | 30.545792 | 24.960306 |
| S | 33.346771 | 26.144205 | 23.394634 |
| S | 36.290367 | 27.909073 | 27.095253 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.126205    | 32.963173    | 33.543663    |
| Ca      | 22.767681    | 34.801643    | 36.242184    |
| Ca      | 23.376055    | 30.605762    | 32.922157    |
| Ca      | 23.036751    | 34.303223    | 30.751564    |
| Ca      | 25.027351    | 30.650040    | 27.651848    |
| Ca      | 27.917349    | 32.902706    | 31.291569    |
| Ca      | 28.965759    | 28.306488    | 29.839079    |
| Ca      | 30.138367    | 32.729851    | 27.449007    |
| Ca      | 30.633024    | 27.646503    | 24.576603    |
| Ca      | 33.613930    | 30.001362    | 27.925306    |
| Ca      | 34.185524    | 24.819218    | 27.055859    |
| Ca      | 35.782379    | 28.682896    | 23.677773    |
| S       | 20.994383    | 31.761652    | 35.638870    |
| S       | 20.702112    | 35.395710    | 33.250412    |
| S       | 22.040621    | 31.319349    | 29.625896    |
| S       | 24.972834    | 33.251808    | 33.446415    |
| S       | 26.001213    | 29.615913    | 30.786167    |
| S       | 25.919502    | 34.012402    | 28.613701    |
| S       | 28.254419    | 29.910843    | 26.615210    |
| S       | 30.831850    | 31.310734    | 30.078093    |
| S       | 31.694094    | 27.124496    | 27.630737    |
| S       | 32.692085    | 30.567095    | 24.726942    |
| S       | 33.575455    | 25.863121    | 23.574036    |
| S       | 36.471016    | 27.754028    | 27.026953    |

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| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.292189    | 32.976246    | 33.804512    |
| Ca      | 23.013178    | 34.641411    | 36.180305    |
| Ca      | 23.423471    | 30.624039    | 33.050484    |
| Ca      | 22.915903    | 34.506145    | 30.777632    |
| Ca      | 24.811340    | 30.639759    | 27.504087    |
| Ca      | 27.743868    | 32.927002    | 31.037741    |
| Ca      | 29.202963    | 28.188404    | 29.843727    |
| Ca      | 30.433931    | 32.461594    | 26.878575    |
| Ca      | 30.470655    | 27.665089    | 24.619049    |
| Ca      | 33.603161    | 29.943195    | 27.868931    |
| Ca      | 34.215336    | 24.865639    | 27.059139    |
| Ca      | 35.768524    | 29.019539    | 24.075584    |
| S       | 21.022961    | 31.592335    | 35.579666    |
| S       | 20.496967    | 35.571789    | 33.481697    |
| S       | 21.843979    | 31.617052    | 29.531670    |
| S       | 24.979164    | 33.207462    | 33.453991    |
| S       | 26.020737    | 29.699139    | 30.705433    |
| S       | 25.805315    | 33.989933    | 28.506895    |
| S       | 28.264915    | 29.614151    | 26.575899    |
|  |  |  |  |
|---|---|---|---|
| S | 30.774633 | 31.273781 | 30.035831 |
| S | 31.740112 | 26.969173 | 27.850607 |
| S | 32.741928 | 30.583681 | 24.817593 |
| S | 33.785858 | 26.143337 | 23.529320 |
| S | 36.348995 | 27.580189 | 27.171501 |

24
generated by VMD

| Ca | 18.451672 | 33.094826 | 33.832222 |
| Ca | 23.068876 | 34.672443 | 35.851887 |
| Ca | 23.396973 | 30.539211 | 32.977226 |
| Ca | 22.779081 | 34.257790 | 30.472977 |
| Ca | 24.804752 | 30.534246 | 27.620657 |
| Ca | 27.860619 | 33.028183 | 31.362494 |
| Ca | 28.905788 | 28.091812 | 29.801600 |
| Ca | 30.528624 | 32.515087 | 27.431768 |
| Ca | 30.571560 | 27.749771 | 24.580727 |
| Ca | 33.682163 | 30.006344 | 28.118200 |
| Ca | 34.190872 | 24.834976 | 26.662609 |
| Ca | 35.623837 | 29.075634 | 24.052773 |
| S | 21.294069 | 31.839859 | 35.715424 |
| S | 20.710941 | 35.565491 | 33.112469 |
| S | 21.736946 | 31.077755 | 29.650822 |
| S | 25.027540 | 33.262367 | 33.278980 |
| S | 26.194445 | 29.834229 | 30.775469 |
| S | 25.802988 | 33.801373 | 28.507528 |
| S | 28.151474 | 29.895079 | 26.427601 |
| S | 30.800299 | 31.171352 | 30.172129 |
| S | 31.658356 | 26.907745 | 27.806139 |
| S | 32.747921 | 30.664902 | 25.076281 |
| S | 33.397224 | 26.121977 | 23.346294 |
| S | 36.333096 | 27.757574 | 27.305737 |

24
generated by VMD

| Ca | 18.306896 | 33.014053 | 33.553780 |
| Ca | 22.780069 | 35.017262 | 35.781757 |
| Ca | 23.314342 | 30.542496 | 33.099678 |
| Ca | 22.774599 | 34.395714 | 30.772902 |
| Ca | 25.177515 | 30.539955 | 27.726013 |
| Ca | 27.739412 | 32.955601 | 31.524416 |
| Ca | 28.910923 | 28.126980 | 29.863514 |
| Ca | 30.548882 | 32.499290 | 27.394421 |
| Ca | 30.581024 | 27.618948 | 24.438890 |
| Ca | 33.645496 | 29.834431 | 27.620073 |
| Ca | 34.277573 | 25.002394 | 26.702473 |
| Ca | 35.658558 | 28.898537 | 23.884329 |
| S | 21.101126 | 31.819473 | 35.635094 |
| S       | 20.451548     | 35.564949     | 33.158554 |
| S       | 22.025509     | 31.344570     | 29.618429 |
| S       | 24.838614     | 33.253574     | 33.487572 |
| S       | 26.306644     | 29.636761     | 31.021873 |
| S       | 25.793230     | 33.849499     | 28.682898 |
| S       | 28.350716     | 29.764126     | 26.637352 |
| S       | 30.826218     | 31.253525     | 30.306095 |
| S       | 31.595350     | 26.994320     | 27.655270 |
| S       | 32.645668     | 30.544451     | 24.918573 |
| S       | 33.603119     | 26.166740     | 23.436161 |
| S       | 36.466991     | 27.662365     | 27.019917 |

24 generated by VMD

| Ca      | 18.370916     | 33.321747     | 33.765411 |
| Ca      | 22.954298     | 34.688667     | 35.784111 |
| Ca      | 23.362192     | 30.481785     | 32.938187 |
| Ca      | 22.914993     | 34.646008     | 30.813803 |
| Ca      | 24.935652     | 30.381243     | 27.736589 |
| Ca      | 27.816299     | 32.787964     | 31.509567 |
| Ca      | 29.001694     | 27.895092     | 29.819206 |
| Ca      | 30.343739     | 32.133587     | 26.978252 |
| Ca      | 30.605991     | 27.519749     | 24.261435 |
| Ca      | 33.428593     | 29.874763     | 27.923944 |
| Ca      | 34.493759     | 25.086746     | 26.770470 |
| Ca      | 35.771412     | 29.315798     | 24.023666 |
| S       | 21.162138     | 31.806561     | 35.530125 |
| S       | 20.712814     | 35.914955     | 33.239506 |
| S       | 21.856750     | 31.428972     | 29.691130 |
| S       | 24.936523     | 33.208271     | 33.431194 |
| S       | 26.031380     | 29.568686     | 30.994125 |
| S       | 25.782190     | 34.058609     | 28.620543 |
| S       | 28.026566     | 29.351526     | 26.592934 |
| S       | 30.644531     | 31.104595     | 30.220554 |
| S       | 31.551256     | 26.932545     | 27.717201 |
| S       | 32.523895     | 30.606537     | 24.937672 |
| S       | 34.047920     | 26.234379     | 23.451469 |
| S       | 36.444923     | 27.952675     | 27.188946 |

24 generated by VMD

| Ca      | 18.409105     | 32.951759     | 33.583714 |
| Ca      | 23.052164     | 34.871128     | 35.942497 |
| Ca      | 23.299904     | 30.336115     | 32.953655 |
| Ca      | 22.757420     | 34.290596     | 30.671490 |
| Ca      | 25.159426     | 30.771160     | 27.555153 |
| Ca      | 27.537493     | 33.075882     | 31.156122 |
| Ca      | 29.040768     | 27.931568     | 29.748167 |
|   | Ca     | 30.504135 | 32.450153 | 27.365738 |
|---|--------|-----------|-----------|-----------|
|   | Ca     | 30.430471 | 28.033051 | 24.367142 |
|   | Ca     | 33.661053 | 29.920376 | 27.904810 |
|   | Ca     | 34.308113 | 24.840652 | 26.907738 |
|   | Ca     | 35.742680 | 28.949158 | 24.043741 |
|   | S      | 21.272755 | 31.798866 | 35.702240 |
|   | S      | 20.545450 | 35.630638 | 33.433662 |
|   | S      | 22.039999 | 31.318726 | 29.591587 |
|   | S      | 24.903627 | 33.209179 | 33.509438 |
|   | S      | 26.303026 | 29.896664 | 31.032919 |
|   | S      | 25.559713 | 34.017323 | 28.263050 |
|   | S      | 28.378548 | 29.667545 | 26.614836 |
|   | S      | 30.574278 | 31.163094 | 30.245853 |
|   | S      | 31.687658 | 26.822838 | 27.763708 |
|   | S      | 32.765984 | 30.594055 | 25.066816 |
|   | S      | 33.379398 | 25.996346 | 23.490404 |
|   | S      | 36.406841 | 27.763123 | 27.025539 |

24 generated by VMD

| Ca | 18.486465 | 32.938332 | 34.213627 |
|----|-----------|-----------|-----------|
| Ca | 23.173328 | 34.918167 | 35.616219 |
| Ca | 23.352549 | 30.580410 | 32.882679 |
| Ca | 22.691444 | 34.417519 | 30.597530 |
| Ca | 24.872801 | 30.598007 | 27.734882 |
| Ca | 27.894321 | 32.762707 | 31.025452 |
| Ca | 28.922466 | 27.951122 | 29.688520 |
| Ca | 30.349087 | 32.408592 | 27.452995 |
| Ca | 30.413567 | 28.088264 | 24.436033 |
| Ca | 33.745911 | 29.838396 | 28.070286 |
| Ca | 34.345650 | 24.807976 | 26.529221 |
| Ca | 35.815067 | 29.091553 | 24.314369 |
| Ca | 31.086658 | 28.257560 | 27.328856 |
| S  | 21.41938  | 31.922346 | 35.683426 |
| S  | 20.481140 | 35.579670 | 32.968025 |
| S  | 21.742620 | 31.256378 | 29.639179 |
| S  | 24.896790 | 33.309978 | 33.181465 |
| S  | 26.163097 | 29.746246 | 31.017584 |
| S  | 25.548336 | 33.877296 | 28.303419 |
| S  | 28.238218 | 29.800751 | 26.758472 |
| S  | 30.863327 | 30.905590 | 30.250198 |
| S  | 31.735001 | 26.699938 | 27.760284 |
| S  | 32.648869 | 30.761570 | 25.288139 |
| S  | 33.410259 | 26.467098 | 23.411457 |
| S  | 36.514793 | 27.572117 | 27.116619 |

24 generated by VMD

| Ca | 18.317545 | 33.267555 | 34.087822 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 22.926205 | 34.820137 | 35.675007 |
| Ca      | 23.352646 | 30.391684 | 33.029518 |
| Ca      | 23.004230 | 34.647003 | 30.703194 |
| Ca      | 24.824192 | 30.493385 | 27.646290 |
| Ca      | 27.799217 | 32.626354 | 30.962433 |
| Ca      | 28.935577 | 27.911123 | 29.722158 |
| Ca      | 30.757957 | 32.335365 | 27.259041 |
| Ca      | 30.446281 | 27.658926 | 24.806210 |
| Ca      | 33.609135 | 29.966148 | 28.312759 |
| Ca      | 34.430386 | 24.942869 | 26.589447 |
| Ca      | 35.711548 | 29.049110 | 23.805130 |
| S       | 21.332052 | 31.790543 | 35.614838 |
| S       | 20.538893 | 35.838993 | 33.200726 |
| S       | 21.784527 | 31.361725 | 29.766602 |
| S       | 24.959772 | 33.174103 | 33.150795 |
| S       | 26.053926 | 29.493256 | 30.859329 |
| S       | 25.453642 | 33.854881 | 28.427357 |
| S       | 28.249565 | 29.840776 | 26.766787 |
| S       | 30.625137 | 30.972546 | 30.218729 |
| S       | 31.787022 | 26.899469 | 27.872776 |
| S       | 32.734207 | 30.757849 | 25.007698 |
| S       | 33.639130 | 26.342127 | 23.318604 |
| S       | 36.444641 | 27.864128 | 27.136827 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 18.409695 | 33.174984 | 34.151115 |
| Ca      | 23.154869 | 34.539036 | 35.940323 |
| Ca      | 23.244020 | 30.256323 | 32.732811 |
| Ca      | 22.632629 | 34.468498 | 30.821476 |
| Ca      | 24.931662 | 30.897125 | 27.501583 |
| Ca      | 27.661190 | 32.849289 | 31.14403 |
| Ca      | 28.862864 | 28.083357 | 29.608084 |
| Ca      | 30.461342 | 32.478348 | 27.384222 |
| Ca      | 30.621910 | 27.978287 | 24.702698 |
| Ca      | 33.928345 | 30.075451 | 27.94201 |
| Ca      | 34.312218 | 24.713003 | 27.073212 |
| Ca      | 35.570969 | 28.605110 | 23.989933 |
| S       | 21.272919 | 31.597710 | 35.541092 |
| S       | 20.544025 | 35.768646 | 33.392921 |
| S       | 21.724644 | 31.330959 | 29.472403 |
| S       | 24.858435 | 33.161957 | 33.291264 |
| S       | 26.180273 | 29.840534 | 30.704874 |
| S       | 25.510684 | 34.002579 | 28.466248 |
| S       | 28.270107 | 29.719315 | 26.542603 |
| S       | 30.797541 | 31.247372 | 30.037802 |
| S       | 31.917393 | 27.164791 | 28.059961 |
|     | 32.819580 | 30.779291 | 24.977312 |
|-----|-----------|-----------|-----------|
| S   | 33.504383 | 25.984390 | 23.539505 |
| S   | 36.528091 | 27.583664 | 27.069950 |

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generated by VMD

|     | 18.403070 | 32.708778 | 33.503288 |
|-----|-----------|-----------|-----------|
| Ca  | 22.678904 | 34.926430 | 35.591011 |
| Ca  | 23.342051 | 30.645004 | 33.096054 |
| Ca  | 23.051804 | 34.437851 | 30.781435 |
| Ca  | 25.018001 | 30.708235 | 27.767452 |
| Ca  | 27.941774 | 32.929283 | 31.518593 |
| Ca  | 28.921179 | 27.775887 | 29.724810 |
| Ca  | 30.421126 | 32.295227 | 27.215031 |
| Ca  | 30.381163 | 27.867161 | 24.570974 |
| Ca  | 33.554688 | 29.918497 | 27.738585 |
| Ca  | 34.431126 | 24.940479 | 26.699944 |
| Ca  | 35.455879 | 29.049591 | 23.919098 |
| S   | 21.010944 | 31.739540 | 35.727112 |
| S   | 20.449867 | 35.419189 | 32.627167 |
| S   | 22.137135 | 31.677055 | 29.778458 |
| S   | 25.076168 | 33.44893  | 33.669075 |
| S   | 26.442480 | 29.852180 | 31.067665 |
| S   | 25.912886 | 33.947983 | 28.730034 |
| S   | 28.051638 | 29.615656 | 26.704208 |
| S   | 30.712060 | 30.981764 | 30.246391 |
| S   | 31.806412 | 26.888641 | 27.831234 |
| S   | 32.518085 | 30.534414 | 24.987913 |
| S   | 33.484283 | 26.218851 | 23.367477 |
| S   | 36.572739 | 27.77412  | 27.077055 |

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generated by VMD

|     | 18.444725 | 32.613323 | 33.934834 |
|-----|-----------|-----------|-----------|
| Ca  | 22.846529 | 34.772655 | 35.509892 |
| Ca  | 23.448187 | 30.532074 | 33.064171 |
| Ca  | 22.834606 | 34.431469 | 30.764618 |
| Ca  | 24.991957 | 30.768715 | 27.716526 |
| Ca  | 27.778450 | 32.878231 | 31.048313 |
| Ca  | 28.827904 | 28.032227 | 29.494741 |
| Ca  | 30.615755 | 32.549156 | 27.181425 |
| Ca  | 30.416712 | 27.953766 | 24.566605 |
| Ca  | 33.559448 | 30.073013 | 28.036217 |
| Ca  | 34.239681 | 24.728266 | 26.885925 |
| Ca  | 35.721859 | 28.710724 | 23.955111 |
| S   | 21.346176 | 31.390430 | 35.624420 |
| S   | 20.418530 | 35.527035 | 32.951782 |
| S   | 21.988501 | 31.603031 | 29.897821 |
|   | 24.943104 | 33.333225 | 33.612686 |
|---|-----------|-----------|-----------|
| S | 26.364861 | 30.023470 | 30.965208 |
| S | 25.837698 | 34.123802 | 28.622566 |
| S | 28.252241 | 29.842514 | 26.378319 |
| S | 30.676908 | 31.073582 | 30.105091 |
| S | 31.653389 | 26.951021 | 27.847466 |
| S | 32.887466 | 30.639868 | 24.922747 |
| S | 33.389847 | 25.951584 | 23.545900 |
| S | 36.235588 | 27.796879 | 27.307657 |

24 generated by VMD

|   | 18.023977 | 33.397854 | 34.123165 |
|---|-----------|-----------|-----------|
| Ca | 22.889944 | 34.789928 | 35.838219 |
| Ca | 23.146851 | 30.493351 | 32.811470 |
| Ca | 22.841387 | 34.556419 | 30.618237 |
| Ca | 25.018814 | 30.933170 | 27.896662 |
| Ca | 27.713602 | 32.397278 | 31.190077 |
| Ca | 29.012789 | 27.636543 | 29.711010 |
| Ca | 30.423534 | 32.228508 | 27.438387 |
| Ca | 30.421444 | 27.726784 | 24.692589 |
| Ca | 33.788494 | 29.971531 | 28.185177 |
| Ca | 34.701069 | 25.159515 | 26.639008 |
| Ca | 35.486549 | 28.983171 | 23.515877 |
| Ca | 34.046515 | 31.776920 | 35.492447 |
| S | 20.481575 | 35.863094 | 33.061226 |
| S | 21.868965 | 31.510904 | 29.541103 |
| S | 24.789408 | 33.288101 | 33.220596 |
| S | 26.473375 | 29.637886 | 31.344936 |
| S | 25.786947 | 33.891579 | 28.411144 |
| S | 28.189217 | 29.549356 | 26.785622 |
| S | 30.881294 | 30.814190 | 30.321484 |
| S | 31.958021 | 26.763355 | 27.864737 |
| S | 32.727081 | 30.528284 | 24.976513 |
| S | 33.416397 | 26.230160 | 23.362709 |
| S | 36.632862 | 28.172207 | 26.897648 |

24 generated by VMD

|   | 18.458057 | 32.998863 | 33.987240 |
|---|-----------|-----------|-----------|
| Ca | 22.901291 | 34.681667 | 35.773079 |
| Ca | 23.338181 | 30.282295 | 32.930328 |
| Ca | 22.862432 | 34.529850 | 30.528912 |
| Ca | 24.867765 | 30.921654 | 27.873039 |
| Ca | 27.952744 | 32.788113 | 31.213615 |
| Ca | 28.852140 | 28.086790 | 29.543131 |
| Ca | 30.475965 | 32.506218 | 27.148979 |
| Ca | 30.535767 | 27.743109 | 24.615097 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 33.729881 | 30.042110 | 28.011314 |
| Ca      | 34.336571 | 24.740849 | 26.888004 |
| Ca      | 35.581776 | 29.093950 | 24.032171 |
| S       | 21.276613 | 31.550488 | 35.496067 |
| S       | 20.598488 | 35.700050 | 33.211014 |
| S       | 21.713833 | 29.093950 | 24.032171 |
| S       | 24.818245 | 33.187073 | 33.212906 |
| S       | 26.297340 | 29.862492 | 31.043385 |
| S       | 25.796597 | 33.951275 | 28.361668 |
| S       | 28.080574 | 29.803322 | 26.549671 |
| S       | 30.789757 | 31.096434 | 30.115097 |
| S       | 31.881218 | 26.981567 | 27.931892 |
| S       | 32.667492 | 30.695202 | 25.014702 |
| S       | 33.584854 | 26.093323 | 23.508190 |
| S       | 36.322445 | 27.557783 | 27.145271 |

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generated by VMD

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 18.169098 | 32.821198 | 34.026703 |
| Ca      | 23.073227 | 34.838070 | 35.554283 |
| Ca      | 23.331123 | 30.402756 | 32.858639 |
| Ca      | 22.761572 | 34.773094 | 30.563017 |
| Ca      | 24.836256 | 30.624294 | 27.809050 |
| Ca      | 27.954918 | 32.796791 | 31.253162 |
| Ca      | 29.031788 | 28.041527 | 29.799259 |
| Ca      | 30.426325 | 32.508278 | 27.283237 |
| Ca      | 30.295019 | 27.619099 | 24.878498 |
| Ca      | 33.910637 | 29.896881 | 27.981956 |
| Ca      | 34.211479 | 24.979111 | 26.544601 |
| Ca      | 35.530666 | 28.863064 | 23.932861 |
| S       | 21.196806 | 31.544390 | 35.476593 |
| S       | 20.382103 | 35.545540 | 33.106117 |
| S       | 21.870466 | 31.387985 | 29.734524 |
| S       | 24.993023 | 33.393707 | 33.101372 |
| S       | 26.242748 | 29.708502 | 30.960445 |
| S       | 25.804333 | 34.029400 | 28.479191 |
| S       | 28.201326 | 29.905556 | 26.726814 |
| S       | 30.864422 | 31.122997 | 30.308178 |
| S       | 31.847973 | 26.958200 | 28.016449 |
| S       | 32.812008 | 30.533047 | 25.233467 |
| S       | 33.192074 | 26.374708 | 23.317987 |
| S       | 36.780659 | 27.631845 | 26.993614 |

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generated by VMD

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 18.454288 | 32.509102 | 33.441017 |
| Ca      | 22.706078 | 34.981766 | 35.665588 |
| Ca      | 23.477777 | 30.490147 | 33.235928 |
| Ca  | 23.065434 | 34.716408 | 30.547047 |
|-----|-----------|-----------|-----------|
| Ca  | 25.047775 | 30.714510 | 27.944408 |
| Ca  | 28.001415 | 32.864288 | 31.413551 |
| Ca  | 28.923140 | 27.802496 | 29.915176 |
| Ca  | 30.440201 | 32.440895 | 27.230099 |
| Ca  | 30.577654 | 27.835754 | 24.673000 |
| Ca  | 33.602913 | 29.923132 | 28.020998 |
| Ca  | 34.179714 | 24.995888 | 26.663784 |
| Ca  | 35.565308 | 28.977880 | 23.765295 |
| S   | 21.184341 | 31.663036 | 35.493156 |
| S   | 20.333202 | 35.583637 | 32.955734 |
| S   | 21.859406 | 31.327038 | 29.844015 |
| S   | 24.953026 | 33.493397 | 33.336193 |
| S   | 26.326550 | 29.723022 | 31.323330 |
| S   | 26.073938 | 33.997452 | 28.488628 |
| S   | 28.115427 | 29.708332 | 26.479961 |
| S   | 30.749468 | 30.853981 | 30.208866 |
| S   | 31.702072 | 26.995724 | 28.021332 |
| S   | 32.698677 | 30.672653 | 24.927860 |
| S   | 33.262737 | 26.382095 | 23.354858 |
| S   | 36.419498 | 27.647396 | 26.990242 |

24 generated by VMD

| Ca  | 18.551783 | 32.958118 | 34.347031 |
|-----|-----------|-----------|-----------|
| Ca  | 23.185200 | 34.723293 | 35.777901 |
| Ca  | 23.205330 | 30.372993 | 32.856834 |
| Ca  | 22.955349 | 34.771202 | 30.366096 |
| Ca  | 24.821842 | 30.543077 | 27.670141 |
| Ca  | 27.743729 | 32.697636 | 31.227703 |
| Ca  | 28.715004 | 27.937489 | 29.460646 |
| Ca  | 30.409828 | 32.292988 | 27.305885 |
| Ca  | 30.461985 | 27.940048 | 24.612381 |
| Ca  | 33.632225 | 29.901062 | 28.062891 |
| Ca  | 34.386219 | 24.954943 | 26.892067 |
| Ca  | 35.679222 | 29.109062 | 24.298126 |
| S   | 21.465984 | 31.473545 | 35.672382 |
| S   | 20.794344 | 35.710346 | 33.279011 |
| S   | 21.816759 | 31.515783 | 29.544106 |
| S   | 24.887117 | 33.339249 | 33.119930 |
| S   | 26.128380 | 29.705982 | 30.904943 |
| S   | 25.675730 | 33.925011 | 28.226917 |
| S   | 28.021051 | 29.644222 | 26.301708 |
| S   | 30.685930 | 30.898159 | 30.142157 |
| S   | 31.755888 | 27.138710 | 27.984884 |
| S   | 32.600334 | 30.749531 | 25.002840 |
| S   | 33.585518 | 26.332592 | 23.672258 |
|   | S         | 24.586041 | 27.664965 | 27.211208 |
|---|-----------|-----------|-----------|-----------|
| Ca| 18.639956 | 32.961300 | 34.152531 |
| Ca| 22.997612 | 34.719242 | 35.577938 |
| Ca| 23.202919 | 30.248859 | 32.910934 |
| Ca| 22.910889 | 34.822388 | 30.400520 |
| Ca| 24.920601 | 30.682892 | 28.036049 |
| Ca| 27.693504 | 32.481979 | 31.039864 |
| Ca| 28.947769 | 27.746704 | 29.530758 |
| Ca| 30.608152 | 32.676773 | 27.266869 |
| Ca| 30.431229 | 28.007483 | 24.687830 |
| Ca| 33.620533 | 30.051533 | 28.075706 |
| Ca| 34.299034 | 24.838455 | 26.831371 |
| Ca| 35.635635 | 28.976936 | 23.979649 |
| S | 21.238909 | 31.416262 | 35.747276 |
| S | 20.758045 | 35.630219 | 32.973141 |
| S | 21.899691 | 31.515179 | 29.807943 |
| S | 24.597158 | 33.277874 | 33.147442 |
| S | 26.404482 | 29.703007 | 31.024498 |
| S | 25.878323 | 34.109818 | 28.397526 |
| S | 28.129694 | 29.763008 | 26.580254 |
| S | 30.542656 | 31.148193 | 30.059174 |
| S | 31.798344 | 27.072159 | 28.091583 |
| S | 32.802063 | 30.656746 | 25.026077 |
| S | 33.417065 | 26.111860 | 23.559280 |
| S | 36.345863 | 27.681183 | 27.035854 |

24 generated by VMD

|   | S         | 24.586041 | 27.664965 | 27.211208 |
|---|-----------|-----------|-----------|-----------|
| Ca| 18.396187 | 32.585007 | 34.043869 |
| Ca| 23.135515 | 34.548561 | 35.614731 |
| Ca| 23.577501 | 30.284515 | 32.864624 |
| Ca| 22.771793 | 35.040989 | 30.667686 |
| Ca| 24.937748 | 30.842686 | 27.739235 |
| Ca| 27.656780 | 32.679470 | 30.850006 |
| Ca| 29.098822 | 28.025738 | 29.713383 |
| Ca| 30.556475 | 32.525627 | 27.218655 |
| Ca| 30.329437 | 27.841377 | 24.733765 |
| Ca| 33.661572 | 29.840551 | 27.954697 |
| Ca| 34.454037 | 24.705341 | 26.858412 |
| Ca| 35.543556 | 29.147871 | 24.191391 |
| S | 21.458052 | 31.466501 | 35.557976 |
| S | 20.344912 | 35.488865 | 33.253002 |
| S | 21.958595 | 31.550232 | 29.838268 |
| S | 24.917713 | 33.536434 | 33.110073 |
| S | 26.328436 | 29.911957 | 30.895601 |
|   | 25.613962 | 34.321270 | 28.339554 |
|---|-----------|-----------|-----------|
| S | 28.170040 | 29.766575 | 26.586555 |
| S | 30.764141 | 31.073326 | 30.008389 |
| S | 31.631195 | 26.709745 | 27.711720 |
| S | 32.698246 | 30.552345 | 24.986553 |
| S | 33.341419 | 26.243561 | 23.757114 |
| S | 36.373917 | 27.611481 | 27.444775 |

24

generated by VMD

|   | 19.051891 | 32.401112 | 34.083969 |
| Ca| 23.380630 | 34.710335 | 35.717979 |
| Ca| 23.083801 | 30.356342 | 33.139324 |
| Ca| 23.090065 | 35.059662 | 30.388641 |
| Ca| 24.807009 | 30.868790 | 27.642319 |
| Ca| 27.235832 | 32.549149 | 30.761538 |
| Ca| 28.635235 | 27.991896 | 29.595671 |
| Ca| 30.459625 | 32.467361 | 27.195171 |
| Ca| 30.559179 | 27.825985 | 24.556644 |
| Ca| 33.659370 | 30.001461 | 27.965385 |
| Ca| 34.089649 | 24.683609 | 26.938786 |
| Ca| 35.645687 | 29.285328 | 24.240044 |
| S | 21.581562 | 31.427654 | 35.899467 |
| S | 20.943161 | 35.257919 | 33.183224 |
| S | 21.754583 | 31.451735 | 29.690411 |
| S | 25.029526 | 33.461765 | 33.067692 |
| S | 26.143723 | 29.845249 | 30.869465 |
| S | 25.696566 | 34.426231 | 28.112518 |
| S | 28.026575 | 29.801062 | 26.332027 |
| S | 30.368406 | 31.013765 | 30.146324 |
| S | 31.616394 | 26.810795 | 27.961018 |
| S | 32.705250 | 30.664355 | 25.150860 |
| S | 33.725887 | 26.204165 | 23.797337 |
| S | 36.430500 | 27.732235 | 27.504223 |

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generated by VMD

|   | 18.932961 | 32.486137 | 34.258377 |
| Ca| 23.097324 | 34.848972 | 35.713432 |
| Ca| 23.433367 | 30.144615 | 32.806404 |
| Ca| 22.919050 | 34.754883 | 30.558109 |
| Ca| 24.819733 | 30.831059 | 27.554794 |
| Ca| 27.624535 | 32.641701 | 30.861244 |
| Ca| 28.533266 | 28.143057 | 29.345116 |
| Ca| 30.557173 | 32.480873 | 27.181538 |
| Ca| 30.409769 | 27.776524 | 24.592117 |
| Ca| 33.623878 | 29.959696 | 28.082375 |
| Ca| 34.276146 | 24.821564 | 27.132088 |
|      |         |         |         |
|------|---------|---------|---------|
| Ca   | 35.824818 | 29.077160 | 24.303383 |
| S    | 21.576550  | 31.529453 | 35.851044 |
| S    | 20.708212  | 35.488667 | 33.397327 |
| S    | 21.855730  | 31.461279 | 29.764879 |
| S    | 25.074738  | 33.316017 | 33.095425 |
| S    | 26.082952  | 29.872025 | 30.661453 |
| S    | 25.676712  | 34.169029 | 28.178452 |
| S    | 28.063564  | 29.905809 | 26.258030 |
| S    | 30.619135  | 31.053528 | 30.052872 |
| S    | 31.370293  | 26.898891 | 27.860184 |
| S    | 32.780472  | 30.742310 | 25.112225 |
| S    | 33.596146  | 26.228798 | 23.841084 |
| S    | 36.263603  | 27.668045 | 27.478149 |
| Ca   | 18.665951  | 32.837635 | 34.301712 |
| Ca   | 23.187504  | 34.824741 | 35.842056 |
| Ca   | 23.330439  | 30.106537 | 32.547470 |
| Ca   | 22.917553  | 34.758270 | 30.574066 |
| Ca   | 24.852646  | 30.839981 | 27.569313 |
| Ca   | 27.547770  | 32.814095 | 30.911545 |
| Ca   | 28.833122  | 27.927191 | 29.643137 |
| Ca   | 30.417389  | 32.269394 | 27.111450 |
| Ca   | 30.513998  | 27.979492 | 24.701912 |
| Ca   | 33.712383  | 29.860537 | 28.535835 |
| Ca   | 34.525574  | 25.026237 | 26.962811 |
| Ca   | 35.452160  | 28.840115 | 23.886316 |
| S    | 21.530165  | 31.413822 | 35.553169 |
| S    | 20.716797  | 35.717686 | 33.376545 |
| S    | 21.774267  | 31.592468 | 29.643330 |
| S    | 24.966473  | 33.308887 | 33.267345 |
| S    | 26.233501  | 29.838940 | 30.551868 |
| S    | 25.584574  | 34.071648 | 28.300449 |
| S    | 28.085306  | 29.635212 | 26.520056 |
| S    | 30.565399  | 31.050533 | 30.179180 |
| S    | 31.576778  | 26.838818 | 27.908150 |
| S    | 32.552578  | 30.795517 | 25.231752 |
| S    | 33.665855  | 26.038147 | 23.558117 |
| S    | 36.511848  | 27.914200 | 27.262459 |

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generated by VMD

|      |         |         |         |
|------|---------|---------|---------|
| Ca   | 18.751097 | 32.736816 | 34.141563 |
| Ca   | 22.960819 | 35.080444 | 35.670433 |
| Ca   | 22.468348 | 30.312874 | 32.948349 |
| Ca   | 22.714525 | 34.815365 | 30.363951 |
| Ca   | 24.954674 | 30.684467 | 27.878651 |
| Element | Value 1     | Value 2     | Value 3     |
|---------|-------------|-------------|-------------|
| Ca      | 27.359194   | 32.561707   | 30.892693   |
| Ca      | 28.839975   | 27.673527   | 29.603207   |
| Ca      | 30.714231   | 32.410828   | 27.398640   |
| Ca      | 30.504000   | 28.063536   | 24.415249   |
| Ca      | 33.552784   | 29.666451   | 28.260771   |
| Ca      | 34.240566   | 24.954184   | 26.634975   |
| Ca      | 35.838055   | 29.018114   | 24.059366   |
| S       | 21.513716   | 31.607479   | 35.805725   |
| S       | 20.645056   | 35.658134   | 33.228710   |
| S       | 21.835234   | 31.163282   | 29.913231   |
| S       | 24.755926   | 33.627598   | 33.027328   |
| S       | 26.376511   | 29.850838   | 31.065695   |
| S       | 25.553453   | 34.209930   | 28.312645   |
| S       | 28.265427   | 29.647449   | 26.556189   |
| S       | 30.447113   | 30.924906   | 30.153324   |
| S       | 31.589191   | 26.775272   | 27.631958   |
| S       | 32.926865   | 30.702703   | 25.257740   |
| S       | 33.505905   | 26.264248   | 23.364914   |
| S       | 36.407501   | 27.889885   | 27.354715   |

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generated by VMD

| Element | Value 1     | Value 2     | Value 3     |
|---------|-------------|-------------|-------------|
| Ca      | 18.537985   | 32.836586   | 34.178699   |
| Ca      | 22.851721   | 34.966164   | 35.688404   |
| Ca      | 23.450825   | 30.386135   | 32.922455   |
| Ca      | 22.763594   | 34.584568   | 30.690994   |
| Ca      | 24.889833   | 30.737404   | 27.839233   |
| Ca      | 27.535591   | 32.614643   | 30.895794   |
| Ca      | 28.901966   | 27.832415   | 29.658089   |
| Ca      | 30.586269   | 32.369438   | 27.220276   |
| Ca      | 30.591703   | 27.965719   | 24.620964   |
| Ca      | 33.413898   | 29.738779   | 27.975880   |
| Ca      | 34.525673   | 24.664001   | 26.904570   |
| Ca      | 35.904007   | 29.248287   | 24.035427   |
| S       | 21.400930   | 31.598715   | 35.559608   |
| S       | 20.468878   | 35.895653   | 33.357498   |
| S       | 21.798855   | 31.375759   | 29.794546   |
| S       | 24.954586   | 33.323418   | 33.267239   |
| S       | 26.320044   | 29.850174   | 30.961094   |
| S       | 25.694809   | 34.210972   | 28.279411   |
| S       | 28.244814   | 29.716335   | 26.556107   |
| S       | 30.644348   | 30.933277   | 30.057629   |
| S       | 31.431776   | 26.734951   | 27.642735   |
| S       | 32.684368   | 30.702225   | 25.039066   |
| S       | 33.767406   | 26.194212   | 23.621574   |
| S       | 36.356255   | 27.820183   | 27.172729   |

24
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.572887    | 33.047298    | 34.147182    |
| Ca      | 22.990328    | 34.902351    | 35.593517    |
| Ca      | 23.383560    | 30.176336    | 33.127457    |
| Ca      | 22.768293    | 34.506359    | 30.534821    |
| Ca      | 24.855623    | 30.910873    | 27.941349    |
| Ca      | 27.539194    | 32.634567    | 30.807915    |
| Ca      | 28.860884    | 27.928646    | 29.435318    |
| Ca      | 30.658218    | 32.576950    | 27.145765    |
| Ca      | 30.594902    | 27.933155    | 24.581688    |
| Ca      | 33.399639    | 29.728897    | 28.213587    |
| Ca      | 34.406754    | 24.663219    | 26.865852    |
| Ca      | 35.905399    | 28.883234    | 23.955450    |
| S       | 21.398132    | 31.526541    | 35.793076    |
| S       | 20.621046    | 35.692978    | 33.298695    |
| S       | 21.710449    | 31.190208    | 29.827789    |
| S       | 24.852186    | 33.211182    | 33.115440    |
| S       | 26.294317    | 29.927685    | 31.003716    |
| S       | 25.703060    | 34.248386    | 28.358774    |
| S       | 28.238363    | 29.928379    | 26.415375    |
| S       | 30.518892    | 31.087257    | 30.159115    |
| S       | 31.490099    | 26.694284    | 27.698246    |
| S       | 32.928555    | 30.785255    | 25.127293    |
| S       | 33.636932    | 26.097992    | 23.613270    |
| S       | 36.392307    | 28.017963    | 27.179352    |

24

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.253071    | 33.178017    | 34.407475    |
| Ca      | 23.161251    | 34.811455    | 35.541771    |
| Ca      | 23.199173    | 30.240746    | 32.993793    |
| Ca      | 22.855392    | 34.482964    | 30.571102    |
| Ca      | 25.148207    | 30.510563    | 27.821918    |
| Ca      | 27.320713    | 32.483730    | 30.903025    |
| Ca      | 28.909933    | 27.995449    | 29.580763    |
| Ca      | 30.612614    | 32.719902    | 27.106827    |
| Ca      | 30.539577    | 27.780666    | 24.539511    |
| Ca      | 33.389141    | 29.841305    | 28.165913    |
| Ca      | 34.433887    | 24.859159    | 26.953003    |
| Ca      | 35.608784    | 29.177612    | 23.997398    |
| S       | 21.239708    | 31.732868    | 35.627697    |
| S       | 20.665678    | 35.705135    | 33.201530    |
| S       | 22.099310    | 31.358349    | 29.702583    |
| S       | 24.838285    | 33.107327    | 33.356182    |
| S       | 26.279293    | 29.673298    | 31.036736    |
| S       | 25.914169    | 34.035831    | 28.336075    |
| S       | 28.364149    | 29.913532    | 26.471554    |
S  30.687742  31.193542  30.136440
S  31.451677  26.822174  27.566845
S  32.794636  30.820480  25.078537
S  33.560951  26.068150  23.627808
S  36.392654  27.787777  27.215536

24
generated by VMD
Ca  18.424410  32.732594  33.936890
Ca  23.177746  34.777603  35.693741
Ca  23.428555  30.206209  32.994919
Ca  22.782450  34.733131  30.493721
Ca  25.160580  30.704910  27.804089
Ca  27.622822  32.619316  30.977009
Ca  28.886869  27.958057  29.423248
Ca  30.754971  32.584785  27.212933
Ca  30.457596  27.987228  24.620907
Ca  33.372841  29.753885  28.268227
Ca  34.401100  24.652048  27.150002
Ca  35.558659  29.143946  23.861609
S  21.406073  31.512630  35.784153
S  20.557838  35.686100  33.227184
S  22.076208  31.285017  29.886181
S  24.900875  33.488148  33.110912
S  26.340467  29.809101  31.041542
S  25.722414  34.139820  28.312275
S  28.256651  30.008366  26.381771
S  30.547379  30.883139  30.061005
S  31.539846  26.821892  27.705971
S  32.647881  30.900837  24.946085
S  33.605000  26.067902  23.749563
S  36.090851  27.843361  27.296162

24
generated by VMD
Ca  18.263790  33.194420  33.912903
Ca  23.084917  34.511185  35.681000
Ca  23.115149  29.995199  32.800514
Ca  22.862764  35.024467  30.679367
Ca  25.033686  30.702789  27.844587
Ca  27.672379  32.504883  30.978523
Ca  28.963785  27.878603  29.727114
Ca  30.454449  32.324306  27.414597
Ca  30.461130  27.812592  24.840103
Ca  33.642471  30.025963  27.843712
Ca  34.692291  24.920994  27.077480
Ca  35.420197  28.960934  23.733770
S  21.016226  31.551334  35.522274
|    |     |     |     |
|----|-----|-----|-----|
| S  | 20.718489 | 35.739204 | 33.221146 |
| S  | 22.126057 | 31.523365 | 29.737213 |
| S  | 24.950241 | 33.375664 | 33.194221 |
| S  | 26.286001 | 29.782242 | 30.987959 |
| S  | 25.753956 | 34.158192 | 28.595577 |
| S  | 28.150862 | 29.696781 | 26.561550 |
| S  | 30.719744 | 31.004095 | 30.141493 |
| S  | 31.711107 | 26.847475 | 27.792406 |
| S  | 32.506554 | 30.799133 | 24.977705 |
| S  | 33.534515 | 25.915115 | 23.761909 |
| S  | 36.579220 | 28.051064 | 26.912960 |

24

generated by VMD

|    |     |     |     |
|----|-----|-----|-----|
| Ca | 18.274523 | 32.631851 | 33.725296 |
| Ca | 23.058342 | 34.541359 | 35.995373 |
| Ca | 23.333084 | 30.420780 | 33.185940 |
| Ca | 23.216736 | 34.867748 | 30.508081 |
| Ca | 24.793535 | 30.861458 | 27.865932 |
| Ca | 27.615665 | 32.814732 | 31.048399 |
| Ca | 28.638847 | 27.775541 | 29.313068 |
| Ca | 30.520138 | 32.277279 | 27.146336 |
| Ca | 30.278288 | 27.650471 | 24.685299 |
| Ca | 33.657833 | 29.789852 | 28.154396 |
| Ca | 34.542721 | 25.031895 | 27.098835 |
| Ca | 35.654675 | 29.008579 | 23.768427 |
| S  | 20.934885 | 31.718006 | 35.787029 |
| S  | 20.683746 | 35.295189 | 32.995117 |
| S  | 21.909515 | 31.521408 | 29.903946 |
| S  | 25.340944 | 33.579559 | 33.376163 |
| S  | 26.267626 | 29.993067 | 30.969002 |
| S  | 25.839478 | 34.264938 | 28.341345 |
| S  | 27.959190 | 29.839111 | 26.357014 |
| S  | 30.659096 | 30.756104 | 30.010429 |
| S  | 31.679333 | 26.779560 | 27.815889 |
| S  | 32.588280 | 30.594057 | 24.985561 |
| S  | 33.655235 | 26.164745 | 23.752958 |
| S  | 36.618328 | 28.122744 | 27.150150 |

24

generated by VMD

|    |     |     |     |
|----|-----|-----|-----|
| Ca | 18.325520 | 32.405304 | 34.110199 |
| Ca | 23.177734 | 34.772907 | 35.287182 |
| Ca | 23.191160 | 30.284868 | 32.842758 |
| Ca | 22.957087 | 35.017021 | 30.658627 |
| Ca | 25.147985 | 30.863602 | 27.869438 |
| Ca | 27.593359 | 32.526478 | 30.852219 |
| Ca | 28.966995 | 27.995726 | 29.544857 |
|   |   |   |   |
|---|---|---|---|
| Ca | 30.792505 | 32.495052 | 27.381210 |
| Ca | 30.423567 | 27.746338 | 24.664120 |
| Ca | 34.316658 | 24.851429 | 27.005634 |
| Ca | 35.376278 | 29.059343 | 23.819542 |
| S  | 21.428333 | 31.567173 | 35.737040 |
| S  | 20.261303 | 35.378036 | 33.091080 |
| S  | 21.893604 | 31.533508 | 29.813263 |
| S  | 24.870689 | 33.480183 | 33.014309 |
| S  | 25.932541 | 34.394833 | 28.684402 |
| S  | 28.339565 | 30.044559 | 26.570297 |
| S  | 30.736687 | 30.970873 | 30.250822 |
| S  | 32.532948 | 30.514000 | 25.115210 |
| S  | 33.291988 | 25.927050 | 23.648119 |
| S  | 36.505478 | 27.890755 | 26.950279 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 18.332489 | 32.700226 | 33.964695 |
| Ca | 22.956268 | 35.071762 | 35.146465 |
| Ca | 23.215645 | 30.386593 | 33.193668 |
| Ca | 22.775517 | 34.721916 | 30.368242 |
| Ca | 25.019958 | 30.66605 | 28.118484 |
| Ca | 27.726950 | 32.532436 | 31.219414 |
| Ca | 28.994720 | 27.830603 | 29.616282 |
| Ca | 30.625137 | 32.537346 | 27.533745 |
| Ca | 30.511410 | 28.060795 | 24.619762 |
| Ca | 33.556870 | 29.721348 | 28.223087 |
| Ca | 34.343494 | 24.784920 | 26.668514 |
| Ca | 35.474636 | 29.019600 | 23.690830 |
| S  | 21.342747 | 31.885080 | 35.894030 |
| S  | 20.334440 | 35.363274 | 32.630013 |
| S  | 21.911228 | 31.356886 | 29.977924 |
| S  | 25.092052 | 33.368660 | 33.202332 |
| S  | 26.432514 | 29.821087 | 31.106239 |
| S  | 25.728590 | 34.161915 | 28.624004 |
| S  | 28.230219 | 29.961596 | 26.667208 |
| S  | 30.846542 | 30.828777 | 30.295189 |
| S  | 31.572630 | 26.752819 | 27.608881 |
| S  | 32.670879 | 30.838316 | 25.256624 |
| S  | 33.594959 | 26.193420 | 23.344402 |
| S  | 36.430229 | 27.755299 | 26.964619 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.579844 | 32.366753 | 34.013432 |
| Element | x1     | y1     | z1     |
|---------|--------|--------|--------|
| Ca      | 23.078609 | 35.026638 | 35.458118 |
| Ca      | 23.229343 | 30.335196  | 33.108662  |
| Ca      | 22.972881 | 34.781387 | 30.278088 |
| Ca      | 24.993204 | 30.684807 | 27.937981 |
| Ca      | 27.640453 | 32.490593 | 31.215202 |
| Ca      | 28.804184 | 27.843994 | 29.512535 |
| Ca      | 30.752310 | 32.480629 | 27.561722 |
| Ca      | 30.349123 | 28.053959 | 24.690380 |
| Ca      | 33.535698 | 29.910549 | 28.177244 |
| Ca      | 34.373421 | 24.847580 | 26.792156 |
| Ca      | 35.663666 | 29.035381 | 23.918884 |
| S       | 21.285557 | 31.890743 | 35.925926 |
| S       | 20.370956 | 35.318184 | 32.823502 |
| S       | 22.127554 | 31.367008 | 29.795277 |
| S       | 24.959389 | 33.537788 | 33.102577 |
| S       | 26.404449 | 29.761686 | 31.119888 |
| S       | 26.023727 | 34.197723 | 28.479038 |
| S       | 28.019165 | 29.939236 | 26.570869 |
| S       | 30.607517 | 30.883677 | 30.189304 |
| S       | 31.594025 | 26.883427 | 27.828053 |
| S       | 32.705574 | 30.706848 | 24.937551 |
| S       | 33.444313 | 26.236900 | 23.413437 |
| S       | 36.205070 | 27.719387 | 27.098091 |

24 generated by VMD

| Element | x1     | y1     | z1     |
|---------|--------|--------|--------|
| Ca      | 18.411837 | 32.214848 | 34.102390 |
| Ca      | 22.722383 | 34.928860 | 35.342407 |
| Ca      | 23.426598 | 30.486622 | 33.024479 |
| Ca      | 23.089668 | 34.828560 | 30.316284 |
| Ca      | 25.036612 | 30.904205 | 28.003706 |
| Ca      | 27.615599 | 32.662338 | 31.408215 |
| Ca      | 28.813923 | 27.897837 | 29.587687 |
| Ca      | 30.669533 | 32.447357 | 27.451378 |
| Ca      | 30.277111 | 28.068760 | 24.567829 |
| Ca      | 33.696129 | 29.849546 | 28.109932 |
| Ca      | 34.206821 | 24.727650 | 26.816509 |
| Ca      | 35.580486 | 29.007278 | 23.878334 |
| S       | 21.338213 | 31.728115 | 35.855934 |
| S       | 20.238922 | 34.992264 | 32.731472 |
| S       | 22.253870 | 31.363405 | 29.625828 |
| S       | 24.956301 | 33.819389 | 33.309387 |
| S       | 26.479637 | 30.038605 | 31.234390 |
| S       | 26.019373 | 34.293518 | 28.552921 |
| S       | 28.130209 | 29.865917 | 26.603916 |
| S       | 30.720766 | 30.960030 | 30.346565 |
| S       | 31.603567 | 26.909557 | 27.651506 |
S       32.766251       30.726980       24.947329
S       33.277893       25.960594       23.468946
S       36.388294       27.617758       27.002703

24
generated by VMD
Ca       18.359638       32.668541       33.870575
Ca       22.767097       35.307217       35.120583
Ca       23.555964       30.497925       33.276932
Ca       23.078711       34.653923       30.213589
Ca       25.220871       30.685993       28.069088
Ca       27.777756       32.467556       31.385918
Ca       28.733913       27.582850       29.726181
Ca       30.455303       32.208519       27.848782
Ca       30.481291       27.741764       24.609711
Ca       33.584259       29.767376       28.435207
Ca       34.347290       25.010235       26.298782
Ca       35.462181       29.533138       23.710260
S       21.324989       32.102043       35.789394
S       20.319485       35.317535       32.246155
S       22.148355       31.100311       29.902145
S       25.043339       33.670700       33.147934
S       26.378416       29.816895       31.374367
S       26.343708       34.028545       28.664793
S       28.015787       29.472620       26.883984
S       30.639252       30.674850       30.560041
S       31.662756       26.653889       27.744795
S       32.419392       30.709051       25.264759
S       33.306004       26.619961       23.085453
S       36.294231       28.008625       26.710613

24
generated by VMD
Ca       18.492693       32.777336       33.886875
Ca       22.875902       35.449234       35.055664
Ca       23.430283       30.314901       33.153378
Ca       22.674274       34.697685       30.484810
Ca       25.124428       30.562809       27.876816
Ca       27.806454       32.659340       31.753504
Ca       28.799555       27.702858       29.657330
Ca       30.585373       32.228233       27.676365
Ca       30.517179       28.034721       24.412397
Ca       33.809788       29.741369       28.181473
Ca       34.310207       24.903839       26.356611
Ca       35.536285       29.342514       23.690243
S       21.312353       32.277798       35.661663
S       20.046150       35.594372       32.600803
S       21.984882       31.098381       29.980953
S       24.927366       33.723145       33.321331
S       26.189806       29.415798       26.750233
S       25.760160       33.811447       28.816971
S       28.277594       29.699219       26.750
S       30.730791       30.593296       30.605534
S       31.810390       26.829723       27.681601
S       32.688816       30.670691       25.237907
S       33.530369       30.670691       25.237907
S       36.498924       27.758492       26.683834

24
generated by VMD
Ca       18.442387       32.290077       33.721455
Ca       22.535236       35.267296       35.264004
Ca       23.614807       30.612255       33.344807
Ca       23.022144       34.540215       30.232498
Ca       25.044765       30.411102       27.920158
Ca       27.896694       32.729153       31.419189
Ca       29.063931       28.052280       30.016071
Ca       30.708605       32.515984       27.722729
Ca       30.372545       28.092533       24.591240
Ca       33.461910       29.707216       28.051579
Ca       33.976082       24.894131       26.435274
Ca       35.484070       29.076809       23.837229
S       21.378363       32.107071       35.742878
S       20.236370       35.097595       32.391060
S       22.210636       31.178074       29.871994
S       24.906990       33.714817       33.209251
S       26.241941       29.636227       31.123989
S       26.228926       33.897926       28.734953
S       28.300007       29.921585       26.974438
S       30.961090       31.036564       30.648968
S       31.499094       26.653156       27.547602
S       32.693306       30.820782       25.174093
S       33.189388       26.467319       23.279186
S       36.250755       27.579914       26.685455

24
generated by VMD
Ca       18.272078       32.380352       33.662395
Ca       22.579428       35.466892       35.137253
Ca       23.387957       30.648657       33.267685
Ca       22.958160       34.677963       30.221067
Ca       25.002228       30.296688       28.240990
Ca       27.984848       32.806316       31.700806
Ca       29.032337       27.976280       29.996655
Ca       30.754059       32.183460       27.616146
Ca       30.362427       28.000149       24.520414
| Element | First Value | Second Value | Third Value |
|---------|-------------|--------------|-------------|
| Ca      | 33.825195   | 29.662037    | 28.090654   |
| Ca      | 34.112667   | 24.722176    | 26.177399   |
| Ca      | 35.603931   | 29.447899    | 23.719437   |
| S       | 21.140352   | 32.116108    | 35.784321   |
| S       | 20.087502   | 35.231247    | 32.365269   |
| S       | 22.015505   | 31.089050    | 29.929703   |
| S       | 24.897516   | 34.033222    | 33.230934   |
| S       | 26.337669   | 29.467073    | 31.412432   |
| S       | 25.978371   | 33.847950    | 28.764217   |
| S       | 28.252699   | 29.848478    | 26.950895   |
| S       | 21.490917   | 29.194014    | 27.692524   |
| S       | 22.005480   | 30.713774    | 25.256119   |
| S       | 33.185562   | 26.592155    | 23.049501   |
| S       | 36.468590   | 27.529697    | 26.426296   |

generated by VMD

| Element | First Value | Second Value | Third Value |
|---------|-------------|--------------|-------------|
| Ca      | 18.487358   | 32.293846    | 33.752846   |
| Ca      | 22.573166   | 35.447556    | 35.169048   |
| Ca      | 23.580809   | 30.782307    | 33.222069   |
| Ca      | 22.530157   | 34.405319    | 30.272495   |
| Ca      | 24.971167   | 30.570669    | 28.062904   |
| Ca      | 27.94697    | 33.010658    | 31.550381   |
| Ca      | 29.023434   | 27.872684    | 29.978447   |
| Ca      | 30.820961   | 32.244709    | 27.798084   |
| Ca      | 30.415028   | 28.031506    | 24.544218   |
| Ca      | 33.944481   | 29.627756    | 28.227331   |
| Ca      | 33.950886   | 24.759937    | 25.977245   |
| Ca      | 23.654091   | 29.232882    | 23.776409   |
| S       | 21.417229   | 32.273224    | 35.866783   |
| S       | 20.005308   | 35.153919    | 32.544048   |
| S       | 22.002502   | 31.010433    | 29.845634   |
| S       | 24.851212   | 33.793671    | 33.074280   |
| S       | 26.440634   | 29.745600    | 31.274376   |
| S       | 25.802498   | 34.218208    | 28.653618   |
| S       | 28.335306   | 29.682365    | 26.892475   |
| S       | 31.043537   | 30.714836    | 30.754574   |
| S       | 31.601244   | 26.613869    | 27.780888   |
| S       | 32.716888   | 30.783600    | 25.322109   |
| S       | 33.276711   | 26.571121    | 22.892994   |
| S       | 36.328861   | 27.459419    | 26.706787   |

generated by VMD

| Element | First Value | Second Value | Third Value |
|---------|-------------|--------------|-------------|
| Ca      | 18.398310   | 32.357468    | 33.969032   |
| Ca      | 22.699886   | 35.110207    | 35.239574   |
| Ca      | 23.722321   | 30.419708    | 33.247700   |
|   | Ca    | S     | Ca    |
|---|-------|-------|-------|
|   | 23.053083 | 34.495850 | 30.169109 |
|   | 24.845856 | 30.644104 | 28.149639 |
|   | 28.038818 | 33.036976 | 31.270033 |
|   | 28.971407 | 27.989887 | 29.687634 |
|   | 30.605995 | 32.598354 | 27.686277 |
|   | 30.455660 | 28.274389 | 24.415306 |
|   | 33.653442 | 29.813560 | 27.940397 |
|   | 33.972656 | 24.499748 | 26.447582 |
|   | 35.683765 | 29.162781 | 24.261919 |
|   | 21.283527 | 31.746429 | 35.863937 |
|   | 20.310057 | 35.135109 | 32.543396 |
|   | 21.948805 | 31.047558 | 30.073292 |
|   | 24.963249 | 33.708229 | 32.979649 |
|   | 26.531424 | 29.782356 | 31.083719 |
|   | 25.673889 | 34.246262 | 28.530085 |
|   | 28.271210 | 30.068497 | 26.725340 |
|   | 31.011620 | 30.952318 | 30.351578 |
|   | 31.371708 | 26.843657 | 27.663380 |
|   | 32.823578 | 30.885059 | 25.180613 |
|   | 33.314583 | 26.274698 | 23.556114 |
|   | 36.115215 | 27.206860 | 26.904800 |

*24 generated by VMD*
|   |   |   |
|---|---|---|
| **S** | 36.476974 | 27.562756 | 27.074734 |
| **24** generated by VMD |
| **Ca** | 18.652988 | 32.345650 | 34.150280 |
| **Ca** | 22.820107 | 35.134239 | 35.248375 |
| **Ca** | 23.634937 | 30.555489 | 33.153625 |
| **Ca** | 22.671223 | 34.688751 | 30.008024 |
| **Ca** | 25.039852 | 30.310455 | 27.818251 |
| **Ca** | 27.831961 | 32.737617 | 31.525948 |
| **Ca** | 28.908167 | 28.112247 | 29.718267 |
| **Ca** | 30.850061 | 32.537312 | 27.645405 |
| **Ca** | 30.433187 | 28.207172 | 24.606731 |
| **Ca** | 33.424622 | 29.670784 | 28.296238 |
| **Ca** | 34.064373 | 24.777544 | 26.417458 |
| **Ca** | 35.610413 | 29.179720 | 23.852379 |
| **S** | 21.552853 | 32.018494 | 35.753361 |
| **S** | 20.129189 | 35.277809 | 32.674553 |
| **S** | 22.154694 | 31.117802 | 30.004974 |
| **S** | 24.966251 | 34.016037 | 32.919754 |
| **S** | 26.167864 | 29.611168 | 31.185238 |
| **S** | 25.802965 | 33.742981 | 28.521111 |
| **S** | 28.279129 | 30.142679 | 26.814724 |
| **S** | 30.927862 | 30.656204 | 30.650112 |
| **S** | 31.310461 | 26.646555 | 27.542742 |
| **S** | 32.845482 | 30.797947 | 25.216591 |
| **S** | 33.360008 | 26.430830 | 23.177778 |
| **S** | 36.281456 | 27.584591 | 27.038139 |
| **24** generated by VMD |
| **Ca** | 18.338253 | 32.324936 | 33.983944 |
| **Ca** | 22.881943 | 34.959862 | 35.496700 |
| **Ca** | 23.384024 | 30.617687 | 32.953411 |
| **Ca** | 22.965351 | 34.875107 | 30.309448 |
| **Ca** | 24.887999 | 30.500580 | 27.857548 |
| **Ca** | 28.089972 | 32.809425 | 31.220131 |
| **Ca** | 28.861156 | 28.059345 | 29.883034 |
| **Ca** | 30.823875 | 32.497864 | 27.640108 |
| **Ca** | 30.403131 | 27.958324 | 24.620148 |
| **Ca** | 33.701714 | 29.746071 | 27.978458 |
| **Ca** | 33.857975 | 24.916496 | 26.716516 |
| **Ca** | 35.708237 | 29.106844 | 24.057854 |
| **S** | 21.557154 | 31.632999 | 35.745308 |
| **S** | 20.285526 | 35.021767 | 32.881073 |
| **S** | 21.783905 | 31.178875 | 29.932423 |
| **S** | 24.930206 | 34.032791 | 32.963646 |
| **S** | 26.249599 | 29.660156 | 31.105106 |
|     | S             | Ca            |     |
|-----|---------------|---------------|-----|
| S   | 25.946409     | 18.506208     | 32.127167 | 33.868336 |
| S   | 28.294626     | 22.885700     | 34.973259 | 35.435043 |
| S   | 30.895613     | 23.661709     | 30.358704 | 33.355759 |
| S   | 31.470623     | 22.848513     | 34.779579 | 30.156408 |
| S   | 32.673729     | 24.976320     | 30.481649 | 27.877640 |
| S   | 36.428394     | 27.895744     | 33.004902 | 31.101963 |
|     | 24 generated by VMD |           |       |           |
| Ca  | 18.281347     | 22.784647     | 35.114429 | 35.356060 |
| Ca  | 23.441879     | 23.441879     | 30.607330 | 33.111115 |
| Ca  | 22.906891     | 22.906891     | 34.738110 | 30.563950 |
| Ca  | 25.088114     | 25.088114     | 30.361675 | 28.121307 |
| Ca  | 27.833521     | 27.833521     | 32.819538 | 31.544922 |
| Ca  | 28.643051     | 28.643051     | 32.018387 | 29.863836 |
| Ca  | 30.602283     | 30.602283     | 32.548050 | 27.660089 |
| Ca  | 30.683805     | 30.683805     | 27.936897 | 24.548756 |
| Ca  | 33.632565     | 33.632565     | 29.732449 | 28.158371 |
| Ca  | 34.282619     | 34.282619     | 24.780130 | 26.510683 |
| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| Ca   | 35.498379 | 29.177357 | 23.621803 |
| S    | 21.137520  | 31.925343  | 35.492050  |
| S    | 20.247536  | 35.500847  | 32.638039  |
| S    | 22.113596  | 31.93811   | 30.016634  |
| S    | 24.940536  | 33.766289  | 33.270504  |
| S    | 26.364334  | 29.542427  | 31.335819  |
| S    | 25.854221  | 33.810486  | 28.702427  |
| S    | 28.387598  | 29.655735  | 26.689957  |
| S    | 30.766453  | 31.026724  | 30.375378  |
| S    | 31.696018  | 26.733574  | 27.785381  |
| S    | 32.839401  | 30.794422  | 25.154202  |
| S    | 33.428730  | 26.219105  | 23.11580   |
| S    | 36.265038  | 27.697151  | 26.606552  |

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*generated by VMD*

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| Ca   | 18.520590  | 33.152035  | 33.911179  |
| Ca   | 23.099533  | 35.191891  | 35.40085   |
| Ca   | 23.413424  | 30.178108  | 33.164642  |
| Ca   | 23.13347   | 34.689045  | 30.28466   |
| Ca   | 24.592777  | 30.208553  | 27.880169  |
| Ca   | 27.686592  | 32.539703  | 31.218306  |
| Ca   | 28.958935  | 27.616657  | 29.579208  |
| Ca   | 30.352186  | 32.302532  | 27.706593  |
| Ca   | 30.590931  | 28.068684  | 24.708609  |
| Ca   | 33.756180  | 29.645794  | 28.544861  |
| Ca   | 34.306854  | 25.136402  | 26.382328  |
| Ca   | 35.475193  | 29.308050  | 23.794250  |
| S    | 21.329567  | 32.056511  | 35.874329  |
| S    | 20.659607  | 35.759411  | 32.724255  |
| S    | 21.908184  | 31.351215  | 29.900736  |
| S    | 25.043564  | 33.539993  | 33.185013  |
| S    | 25.931593  | 29.326370  | 30.950256  |
| S    | 25.738846  | 33.485645  | 28.280266  |
| S    | 28.073582  | 29.766077  | 26.730465  |
| S    | 30.729502  | 30.68419   | 30.342789  |
| S    | 31.700180  | 26.750298  | 27.831867  |
| S    | 32.622231  | 30.905674  | 25.408661  |
| S    | 33.638268  | 26.493813  | 23.223038  |
| S    | 36.458336  | 28.141262  | 26.913326  |

24

*generated by VMD*

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| Ca   | 18.065529  | 33.352646  | 34.074314  |
| Ca   | 22.920052  | 35.002335  | 35.298542  |
| Ca   | 23.283840  | 30.040934  | 33.136894  |
| Ca   | 22.925102  | 34.567398  | 30.468218  |
| Ca   | 24.744610  | 30.282513  | 28.012447  |
|   | Ca   | S    |   |
|---|------|------|---|
|   | 27.917955 | 32.682755 | 31.322678 |
| Ca | 28.998398 | 28.092985 | 29.861305 |
| Ca | 30.579132 | 32.367661 | 27.540421 |
| Ca | 30.463652 | 28.090767 | 24.517227 |
| Ca | 33.689686 | 29.851292 | 28.187578 |
| Ca | 34.102482 | 24.850262 | 26.503469 |
| Ca | 35.784214 | 29.017515 | 23.825344 |
| S  | 21.057444 | 31.811064 | 35.459106 |
| S  | 20.563803 | 35.850708 | 32.743454 |
| S  | 21.931963 | 30.993050 | 30.117931 |
| S  | 24.978832 | 33.397987 | 33.329765 |
| S  | 26.322975 | 29.397474 | 31.141869 |
| S  | 25.756285 | 33.749580 | 28.407982 |
| S  | 28.254335 | 29.912136 | 26.766075 |
| S  | 30.923800 | 31.090290 | 30.408577 |
| S  | 31.788166 | 26.930655 | 27.624447 |
| S  | 32.739334 | 30.923084 | 25.040342 |
| S  | 33.508343 | 26.334337 | 23.253689 |
| S  | 36.418301 | 27.710625 | 26.898355 |

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generated by VMD

|   | Ca   | S    |   |
|---|------|------|---|
| Ca | 18.096613 | 33.301605 | 34.072670 |
| Ca | 22.744169 | 34.737968 | 35.453274 |
| Ca | 23.325178 | 30.173103 | 33.077675 |
| Ca | 23.073359 | 34.583836 | 30.377853 |
| Ca | 24.946840 | 30.176418 | 28.023064 |
| Ca | 27.938532 | 32.983078 | 31.470871 |
| Ca | 29.198914 | 27.970642 | 29.672020 |
| Ca | 30.397341 | 32.479012 | 27.319389 |
| Ca | 30.505087 | 28.082211 | 24.593971 |
| Ca | 33.608768 | 29.962730 | 28.208580 |
| Ca | 34.234955 | 24.788685 | 26.396244 |
| Ca | 35.499428 | 28.906193 | 23.879408 |
| S  | 21.010391 | 31.70092 | 35.364353 |
| S  | 20.653158 | 35.716209 | 32.725906 |
| S  | 22.040649 | 31.161442 | 29.742626 |
| S  | 24.993679 | 33.380486 | 33.381970 |
| S  | 26.418713 | 29.619822 | 31.299784 |
| S  | 25.915760 | 33.717072 | 28.505833 |
| S  | 28.266203 | 29.816525 | 26.744070 |
| S  | 30.856647 | 31.202423 | 30.494097 |
| S  | 31.800573 | 27.028017 | 27.802200 |
| S  | 32.678238 | 30.785145 | 25.089294 |
| S  | 33.249443 | 26.277122 | 23.368584 |
| S  | 36.267483 | 27.750229 | 26.898472 |

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| Element | X1   | Y1   | Z1   | X2   | Y2   | Z2   |
|---------|------|------|------|------|------|------|
| Ca      | 18.497040 | 33.068970 | 34.171730 | 22.880112 | 35.030212 | 35.341415 |
| Ca      | 23.488611 | 30.400253 | 33.044090 | 22.941280 | 34.561752 | 30.323257 |
| Ca      | 24.744940 | 30.440102 | 27.859097 | 27.805328 | 32.712631 | 31.327049 |
| Ca      | 28.853354 | 27.599556 | 29.758162 | 30.396809 | 32.539413 | 27.827629 |
| Ca      | 30.679226 | 28.351458 | 24.660305 | 30.679226 | 28.351458 | 24.660305 |
| Ca      | 34.231049 | 24.746342 | 26.292301 | 35.607666 | 28.931736 | 23.836853 |
| S       | 21.488670 | 31.813385 | 35.542770 | 20.615479 | 35.578590 | 32.615150 |
| S       | 21.866318 | 31.164810 | 29.842995 | 25.102615 | 33.662563 | 33.161160 |
| S       | 26.177835 | 29.459312 | 31.034090 | 26.177835 | 29.459312 | 31.034090 |
| S       | 25.800545 | 33.637997 | 28.446644 | 28.254402 | 29.687351 | 26.816925 |
| S       | 30.671676 | 30.911648 | 30.403091 | 31.853113 | 26.935045 | 27.798752 |
| S       | 32.734879 | 30.99241 | 25.169170 | 33.387802 | 26.235035 | 23.251589 |
| S       | 36.202229 | 28.025757 | 27.001429 | 36.202229 | 28.025757 | 27.001429 |

| Element | X1   | Y1   | Z1   | X2   | Y2   | Z2   |
|---------|------|------|------|------|------|------|
| Ca      | 18.559017 | 32.565407 | 34.367313 | 22.800348 | 35.090767 | 35.229322 |
| Ca      | 23.355450 | 30.484436 | 33.221619 | 22.787790 | 34.762859 | 30.208420 |
| Ca      | 24.672421 | 30.605988 | 27.968216 | 28.056244 | 32.771240 | 31.118496 |
| Ca      | 28.664272 | 27.603448 | 29.629957 | 30.644497 | 32.325081 | 27.627522 |
| Ca      | 30.607084 | 28.225815 | 24.650473 | 33.645950 | 29.503798 | 28.448399 |
| Ca      | 34.253017 | 24.956341 | 26.269705 | 35.685684 | 28.979998 | 23.931705 |
| S       | 21.535694 | 31.780960 | 35.783241 | 20.446056 | 35.452858 | 32.625950 |
| S       | 21.694708 | 30.985218 | 30.091879 | 24.984976 | 33.698936 | 32.890831 |
| S       | 26.101318 | 29.714481 | 30.969559 | 26.009562 | 34.057549 | 28.464237 |
| S       | 28.097513 | 29.926525 | 26.659111 | 36.202229 | 28.025757 | 27.001429 |
|  | S        | 30.848183 | 30.638336 | 30.399654 |
|  | S        | 31.680439 | 26.822828 | 27.781710 |
|  | S        | 32.849724 | 30.881882 | 25.193954 |
|  | S        | 33.481915 | 26.389746 | 23.395798 |
|  | S        | 36.258091 | 27.875586 | 27.012928 |

24 generated by VMD

| Ca       | 18.262798 | 32.991447 | 34.382198 |
| Ca       | 22.977028 | 34.964043 | 35.347137 |
| Ca       | 23.426113 | 30.348740 | 33.222500 |
| Ca       | 22.990227 | 34.565151 | 30.309635 |
| Ca       | 24.863312 | 30.783340 | 27.822899 |
| Ca       | 27.655922 | 32.534843 | 31.088688 |
| Ca       | 28.760130 | 27.528008 | 29.603516 |
| Ca       | 30.636114 | 32.369595 | 27.433491 |
| Ca       | 30.503704 | 28.392982 | 24.593290 |
| Ca       | 33.707550 | 29.746710 | 28.531433 |
| Ca       | 34.164913 | 25.073433 | 26.229115 |
| Ca       | 35.676502 | 28.664333 | 23.935207 |
| S        | 21.245251 | 31.888998 | 35.826355 |
| S        | 20.565008 | 35.316029 | 32.675667 |
| S        | 22.036415 | 31.121670 | 30.066200 |
| S        | 24.906681 | 33.605545 | 33.101135 |
| S        | 26.271542 | 29.629637 | 31.062656 |
| S        | 25.674109 | 34.074902 | 28.403034 |
| S        | 28.178444 | 29.841408 | 26.659266 |
| S        | 30.588558 | 30.768997 | 30.191832 |
| S        | 31.796803 | 27.082047 | 27.724783 |
| S        | 33.067871 | 30.826347 | 25.138901 |
| S        | 33.333870 | 26.201349 | 23.445635 |
| S        | 36.431145 | 27.980358 | 27.145496 |

24 generated by VMD

| Ca       | 18.143679 | 32.917072 | 34.207191 |
| Ca       | 23.055418 | 34.794132 | 35.589909 |
| Ca       | 23.245600 | 30.291462 | 32.999092 |
| Ca       | 22.911537 | 34.872612 | 30.350916 |
| Ca       | 25.020586 | 30.660351 | 27.954304 |
| Ca       | 27.705669 | 32.751839 | 31.195869 |
| Ca       | 28.789742 | 27.854441 | 29.782572 |
| Ca       | 30.620934 | 32.398052 | 27.285625 |
| Ca       | 30.705454 | 28.135359 | 24.412422 |
| Ca       | 33.804272 | 29.941624 | 28.428558 |
| Ca       | 34.172611 | 24.868433 | 26.479988 |
| Ca       | 35.644165 | 28.799828 | 23.747137 |
| S        | 21.160908 | 31.611206 | 35.681793 |
|   |         |         |         |
|---|---------|---------|---------|
| S | 20.425734 | 35.337730 | 32.913536 |
| S | 22.046076 | 31.182400 | 29.914574 |
| S | 24.872488 | 33.639061 | 33.164635 |
| S | 26.432983 | 29.842928 | 31.258553 |
| S | 25.727470 | 34.110069 | 28.41790 |
| S | 28.096014 | 29.718292 | 26.701710 |
| S | 30.794460 | 31.100418 | 30.102123 |
| S | 31.611404 | 26.913668 | 27.846970 |
| S | 32.858040 | 30.658672 | 24.979328 |
| S | 33.494404 | 26.204124 | 23.290462 |
| S | 36.380436 | 27.696251 | 27.210981 |

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generated by VMD

| Ca | 18.539967 | 32.467739 | 34.139046 |
| Ca | 22.914534 | 35.062328 | 35.686264 |
| Ca | 23.423019 | 30.601610 | 32.810791 |
| Ca | 22.966774 | 34.931637 | 30.267937 |
| Ca | 24.808041 | 30.479498 | 27.665094 |
| Ca | 27.780605 | 32.840572 | 31.306202 |
| Ca | 28.771763 | 27.996761 | 29.673414 |
| Ca | 30.495033 | 32.179493 | 27.456455 |
| Ca | 30.439016 | 28.201281 | 24.271099 |
| Ca | 33.682838 | 29.788975 | 28.272068 |
| Ca | 33.982452 | 24.811537 | 26.636055 |
| Ca | 35.935989 | 28.959751 | 24.224707 |
| S  | 21.714056 | 31.598223 | 35.835094 |
| S  | 20.436756 | 35.208542 | 33.065781 |
| S  | 21.908730 | 31.293911 | 29.921822 |
| S  | 24.984039 | 33.917297 | 33.003250 |
| S  | 26.178715 | 29.772879 | 30.908133 |
| S  | 25.617659 | 33.882732 | 28.424244 |
| S  | 27.991428 | 29.615246 | 26.621058 |
| S  | 30.732025 | 30.893875 | 30.466627 |
| S  | 31.473749 | 27.025570 | 27.481369 |
| S  | 32.976227 | 30.860689 | 25.121174 |
| S  | 33.506596 | 26.258648 | 23.53437 |
| S  | 36.460056 | 27.651337 | 27.147896 |

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generated by VMD

| Ca | 18.376129 | 32.703331 | 34.351215 |
| Ca | 22.862198 | 35.031109 | 35.763763 |
| Ca | 23.448103 | 30.224247 | 33.042309 |
| Ca | 22.917465 | 34.723839 | 30.286255 |
| Ca | 25.063766 | 30.738926 | 27.595829 |
| Ca | 27.636768 | 32.819004 | 31.291382 |
| Ca | 28.957174 | 27.929695 | 29.448345 |
| Element | 1st Value       | 2nd Value       | 3rd Value       |
|---------|-----------------|-----------------|-----------------|
| Ca      | 30.487370       | 32.425213       | 27.331146       |
| Ca      | 30.448175       | 28.116871       | 24.387255       |
| Ca      | 33.737473       | 29.669390       | 28.223759       |
| Ca      | 34.211124       | 24.872559       | 26.791761       |
| Ca      | 35.669216       | 28.983639       | 24.190918       |
| S       | 21.536716       | 31.841068       | 36.067783       |
| S       | 20.392973       | 35.337708       | 33.013725       |
| S       | 22.005922       | 31.222300       | 29.769218       |
| S       | 24.779194       | 33.636284       | 33.179642       |
| S       | 26.183416       | 29.668667       | 30.828218       |
| S       | 25.805708       | 34.013321       | 28.346401       |
| S       | 28.045208       | 29.964664       | 26.418705       |
| S       | 30.638784       | 31.031191       | 30.194199       |
| S       | 31.716661       | 26.849968       | 27.540173       |
| S       | 32.957310       | 30.700302       | 25.098164       |
| S       | 33.466251       | 26.144346       | 23.416096       |
| S       | 36.376942       | 27.652370       | 27.413673       |

24 generated by VMD

| Element | 1st Value       | 2nd Value       | 3rd Value       |
|---------|-----------------|-----------------|-----------------|
| Ca      | 18.511600       | 32.298981       | 34.246323       |
| Ca      | 23.008919       | 35.108345       | 35.594727       |
| Ca      | 23.622185       | 30.482634       | 33.074608       |
| Ca      | 22.879448       | 34.890369       | 30.287004       |
| Ca      | 25.017509       | 30.539639       | 27.689400       |
| Ca      | 27.926579       | 32.793961       | 31.141970       |
| Ca      | 28.903297       | 27.873611       | 29.722389       |
| Ca      | 30.651764       | 32.563675       | 27.307739       |
| Ca      | 30.417156       | 28.174515       | 24.671637       |
| Ca      | 33.137344       | 29.544260       | 28.039719       |
| Ca      | 34.226982       | 24.662710       | 26.721354       |
| Ca      | 35.869442       | 29.049181       | 24.334852       |
| S       | 21.709578       | 31.665054       | 35.829002       |
| S       | 20.213081       | 35.194973       | 32.796085       |
| S       | 21.972490       | 31.480015       | 29.849600       |
| S       | 24.875807       | 33.838398       | 33.145203       |
| S       | 26.175468       | 29.507977       | 30.959400       |
| S       | 25.776428       | 33.983093       | 28.398809       |
| S       | 28.249104       | 30.031460       | 26.726271       |
| S       | 30.766239       | 30.934681       | 30.255680       |
| S       | 31.206221       | 26.675554       | 27.274595       |
| S       | 32.887753       | 31.064529       | 24.994711       |
| S       | 33.622833       | 26.160275       | 23.637978       |
| S       | 36.092743       | 27.782135       | 27.240992       |

24 generated by VMD

| Element | 1st Value       | 2nd Value       | 3rd Value       |
|---------|-----------------|-----------------|-----------------|
| Ca      | 18.505363       | 33.009850       | 34.022026       |
| Element | X coordinates | Y coordinates | Z coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 22.764946     | 34.571236     | 35.732765     |
| Ca      | 23.271076     | 30.488964     | 33.031418     |
| Ca      | 22.977654     | 32.818451     | 31.371315     |
| Ca      | 28.776426     | 27.838692     | 29.671227     |
| Ca      | 30.318153     | 30.192253     | 27.554607     |
| Ca      | 34.248489     | 25.079262     | 26.830250     |
| Ca      | 35.775219     | 28.42182      | 23.566566     |
| S       | 21.372936     | 31.648680     | 35.784279     |
| S       | 20.777729     | 35.491287     | 32.841591     |
| S       | 21.950411     | 31.196198     | 29.773062     |
| S       | 25.010942     | 33.684464     | 32.979851     |
| S       | 26.220650     | 29.591919     | 31.062195     |
| S       | 25.944271     | 33.866879     | 28.336582     |
| S       | 27.884726     | 29.682076     | 26.742796     |
| S       | 30.858679     | 30.914490     | 26.209274     |
| S       | 31.389030     | 26.899578     | 27.715477     |
| S       | 33.111515     | 30.779137     | 25.014086     |
| S       | 33.261108     | 26.330456     | 23.600727     |
| S       | 36.380081     | 28.038237     | 26.938389     |

24 generated by VMD

| Element | X coordinates | Y coordinates | Z coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.379812     | 32.759064     | 34.280205     |
| Ca      | 23.004505     | 34.774426     | 35.518860     |
| Ca      | 23.249046     | 30.415051     | 33.000851     |
| Ca      | 22.812071     | 34.850128     | 30.507486     |
| Ca      | 25.149548     | 30.607769     | 27.940075     |
| Ca      | 27.822691     | 32.674191     | 31.172829     |
| Ca      | 28.792402     | 27.739792     | 29.479431     |
| Ca      | 30.107296     | 32.672417     | 27.305130     |
| Ca      | 30.529400     | 28.127495     | 24.564766     |
| Ca      | 33.512772     | 29.730316     | 28.324623     |
| Ca      | 34.352512     | 24.742365     | 26.778999     |
| Ca      | 36.017830     | 28.901398     | 23.871929     |
| S       | 21.310295     | 31.668842     | 35.837318     |
| S       | 20.361561     | 35.522575     | 33.024197     |
| S       | 21.784599     | 31.398382     | 29.871258     |
| S       | 25.003935     | 33.640877     | 33.074383     |
| S       | 26.347736     | 29.806862     | 31.110023     |
| S       | 25.875679     | 34.031158     | 28.550013     |
| S       | 28.097994     | 29.750443     | 26.419594     |
| S       | 30.604698     | 30.982700     | 29.926344     |
| S       | 31.576021     | 26.767521     | 27.572014     |
|     |     |     |     |
|-----|-----|-----|-----|
| S   | 33.053165 | 30.748844 | 24.989918 |
| S   | 33.588764 | 26.156033 | 23.628582 |
| S   | 36.385735 | 27.831373 | 27.191219 |

24 generated by VMD

| Ca  | 18.674603 | 32.776527 | 33.979759 |
| Ca  | 22.937326 | 34.705956 | 35.590530 |
| Ca  | 23.383089 | 30.329525 | 33.229279 |
| Ca  | 22.874887 | 34.816544 | 30.352165 |
| Ca  | 24.999115 | 30.504662 | 27.921701 |
| Ca  | 27.704201 | 32.720749 | 31.076458 |
| Ca  | 28.803923 | 27.902588 | 29.608583 |
| Ca  | 30.525658 | 32.605022 | 27.586388 |
| Ca  | 30.505623 | 28.111378 | 24.507225 |
| Ca  | 33.319775 | 29.670010 | 28.168110 |
| Ca  | 34.175926 | 24.830805 | 26.866444 |
| Ca  | 35.893242 | 28.917542 | 24.005325 |
| S   | 21.486500 | 31.612417 | 35.680634 |
| S   | 20.569336 | 35.591820 | 33.001442 |
| S   | 22.026134 | 31.347717 | 29.902290 |
| S   | 24.858768 | 33.669155 | 33.175499 |
| S   | 26.401138 | 29.664232 | 31.114649 |
| S   | 25.658241 | 33.959644 | 28.201427 |
| S   | 28.164019 | 29.795971 | 26.644894 |
| S   | 30.579306 | 31.076279 | 30.154667 |
| S   | 31.591845 | 26.705505 | 27.430468 |
| S   | 32.832134 | 30.865757 | 25.022717 |
| S   | 33.497971 | 26.206726 | 23.481224 |
| S   | 36.257301 | 27.913574 | 27.238173 |

24 generated by VMD

| Ca  | 18.527416 | 32.883144 | 34.046932 |
| Ca  | 23.035221 | 34.722321 | 35.766556 |
| Ca  | 23.103666 | 30.355738 | 32.877892 |
| Ca  | 22.998331 | 35.071491 | 30.673304 |
| Ca  | 24.802752 | 30.514721 | 27.745754 |
| Ca  | 27.666397 | 32.582901 | 31.150278 |
| Ca  | 28.726749 | 27.783415 | 29.832092 |
| Ca  | 30.393808 | 32.630974 | 27.526201 |
| Ca  | 30.491619 | 27.905025 | 24.774628 |
| Ca  | 33.705124 | 29.821320 | 28.234177 |
| Ca  | 34.537010 | 25.273554 | 27.006214 |
| Ca  | 35.881184 | 28.61155 | 23.472363 |
| S   | 21.273926 | 31.575554 | 35.653412 |
| S   | 20.581238 | 35.695030 | 33.149540 |
| S   | 21.809031 | 31.785383 | 29.646368 |
|   | 24.980844 | 33.443123 | 33.175278 |
|---|-----------|-----------|-----------|
| 2 | 26.043385 | 29.434383 | 30.985415 |
| 3 | 25.641638 | 33.874313 | 28.453930 |
| 4 | 28.204395 | 29.879398 | 26.717113 |
| 5 | 30.382025 | 30.885405 | 30.057735 |
| 6 | 31.745426 | 26.811756 | 27.796667 |
| 7 | 33.082447 | 30.629257 | 24.813314 |
| 8 | 33.619179 | 25.901318 | 23.523502 |
| 9 | 36.487225 | 28.229378 | 26.861383 |

24 generated by VMD

|   | 18.457527 | 32.998432 | 33.877136 |
|---|-----------|-----------|-----------|
| 2 | 22.821285 | 34.955132 | 35.655087 |
| 3 | 23.226912 | 30.363010 | 33.131599 |
| 4 | 22.985310 | 34.702717 | 30.455864 |
| 5 | 25.021284 | 30.274586 | 27.707951 |
| 6 | 27.757204 | 32.583729 | 31.241671 |
| 7 | 28.768785 | 27.848154 | 29.840969 |
| 8 | 30.560005 | 32.223557 | 27.502365 |
| 9 | 30.415092 | 27.810551 | 24.458475 |
| 10 | 33.718983 | 29.756872 | 28.357527 |
| 11 | 34.374443 | 25.387541 | 26.676392 |
| 12 | 35.597221 | 29.125450 | 23.733574 |
| 13 | 21.253016 | 31.779276 | 35.540833 |
| 14 | 20.750759 | 35.932129 | 33.234486 |
| 15 | 21.925217 | 31.374374 | 29.828779 |
| 16 | 24.859695 | 33.438393 | 33.230259 |
| 17 | 26.106899 | 29.669933 | 31.055374 |
| 18 | 25.876545 | 33.792370 | 28.319084 |
| 19 | 28.260744 | 29.567936 | 26.584551 |
| 20 | 30.658257 | 30.853184 | 30.403267 |
| 21 | 31.590818 | 26.769981 | 27.652763 |
| 22 | 32.843307 | 30.535017 | 25.164791 |
| 23 | 33.416698 | 26.165825 | 23.329168 |
| 24 | 36.474079 | 28.391899 | 26.958094 |

24 generated by VMD

|   | 18.501881 | 32.891567 | 33.856823 |
|---|-----------|-----------|-----------|
| 2 | 22.843061 | 34.568802 | 35.902580 |
| 3 | 23.336559 | 30.392284 | 32.904739 |
| 4 | 23.149309 | 34.881760 | 30.440166 |
| 5 | 25.150696 | 30.558783 | 27.912769 |
| 6 | 27.395687 | 32.765560 | 31.133972 |
| 7 | 28.667885 | 28.042858 | 29.688332 |
| 8 | 30.557201 | 32.190422 | 27.348507 |
| 9 | 30.453911 | 27.834080 | 24.472363 |
|  |  |  |  |
|---|---|---|---|
| Ca | 33.635086 | 29.847145 | 28.268494 |
| Ca | 34.401859 | 24.959019 | 27.037529 |
| Ca | 35.672050 | 28.926506 | 23.634661 |
| S  | 21.182453 | 31.649734 | 35.755920 |
| S  | 20.730820 | 35.552338 | 33.213997 |
| S  | 22.056437 | 31.465378 | 29.649185 |
| S  | 24.903408 | 33.508068 | 33.326012 |
| S  | 26.297447 | 29.802237 | 31.157860 |
| S  | 25.767731 | 33.927135 | 28.279644 |
| S  | 28.128489 | 29.763584 | 26.510162 |
| S  | 30.685198 | 30.867687 | 30.140079 |
| S  | 31.618900 | 32.904919 | 27.739180 |
| S  | 32.796799 | 30.729963 | 24.911545 |
| S  | 33.517540 | 26.085907 | 23.518064 |
| S  | 36.269657 | 28.184349 | 27.137501 |

24 generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 18.143541 | 32.977657 | 34.016220 |
| Ca | 22.886463 | 34.752457 | 35.693768 |
| Ca | 23.270779 | 30.354342 | 33.187237 |
| Ca | 22.978418 | 34.708557 | 30.418190 |
| Ca | 24.867067 | 30.532917 | 27.757053 |
| Ca | 27.875170 | 32.825684 | 31.241123 |
| Ca | 28.895317 | 28.051506 | 29.703716 |
| Ca | 30.657242 | 32.297104 | 27.510010 |
| Ca | 30.616938 | 28.179028 | 24.502411 |
| Ca | 33.751556 | 29.901752 | 28.186333 |
| Ca | 34.297367 | 24.768616 | 26.732925 |
| Ca | 35.610313 | 28.829950 | 23.791512 |
| S  | 20.995781 | 31.672680 | 35.792267 |
| S  | 20.436813 | 35.655045 | 33.046516 |
| S  | 21.892187 | 31.257563 | 29.865795 |
| S  | 24.919876 | 33.447014 | 33.165359 |
| S  | 26.350256 | 29.783577 | 31.087439 |
| S  | 25.811903 | 33.852707 | 28.486065 |
| S  | 28.087959 | 29.801571 | 26.498217 |
| S  | 30.871445 | 31.063211 | 30.157543 |
| S  | 31.721472 | 26.952049 | 27.799911 |
| S  | 32.782467 | 30.862930 | 24.982132 |
| S  | 33.608463 | 26.012999 | 23.396082 |
| S  | 36.391293 | 27.759155 | 26.922226 |

24 generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 18.193399 | 33.026714 | 33.990208 |
| Ca | 22.969288 | 34.905453 | 35.684715 |
| Ca | 23.430244 | 30.340076 | 33.047829 |
| Element | Value 1   | Value 2   | Value 3   |
|---------|----------|----------|----------|
| Ca      | 22.803001| 34.742966| 30.595062|
| Ca      | 24.964561| 30.571880| 27.765877|
| Ca      | 27.873863| 32.698978| 31.086023|
| Ca      | 28.924347| 27.672419| 29.799646|
| Ca      | 30.512028| 32.361252| 27.545267|
| Ca      | 30.345371| 28.035000| 24.525471|
| Ca      | 33.674507| 29.784172| 28.410076|
| Ca      | 34.462612| 25.064541| 26.755119|
| Ca      | 35.715866| 28.956512| 23.745579|
| S       | 21.235565| 31.780653| 35.510231|
| S       | 20.447472| 35.727463| 33.034721|
| S       | 21.980192| 31.378433| 29.837034|
| S       | 25.082633| 33.469276| 33.177040|
| S       | 26.357988| 29.520809| 31.047905|
| S       | 25.802704| 33.793346| 28.466566|
| S       | 28.160915| 29.626337| 26.530413|
| S       | 30.542328| 30.865093| 30.258196|
| S       | 31.580217| 26.879238| 27.669331|
| S       | 32.842670| 30.817663| 24.938286|
| S       | 33.64635 | 26.230064| 23.537958|
| S       | 36.439980| 28.051706| 26.981499|

Generated by VMD
| Element | X-Coordinates | Y-Coordinates | Z-Coordinates |
|---------|---------------|---------------|---------------|
| S       | 36.493542     | 28.284855     | 26.857828     |

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generated by VMD

| Element | X-Coordinates | Y-Coordinates | Z-Coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.364868     | 32.999687     | 33.819210     |
| Ca      | 22.945055     | 35.052643     | 35.491768     |
| Ca      | 23.523428     | 30.351303     | 33.354507     |
| Ca      | 22.755428     | 34.552773     | 30.515999     |
| Ca      | 24.875809     | 30.274593     | 27.916851     |
| Ca      | 27.843761     | 32.790512     | 31.137234     |
| Ca      | 28.960466     | 27.875862     | 29.715229     |
| Ca      | 30.635952     | 32.536792     | 27.511711     |
| Ca      | 30.473642     | 28.347099     | 24.317406     |
| Ca      | 33.751976     | 29.747633     | 28.251682     |
| Ca      | 34.200718     | 24.371902     | 26.592537     |
| Ca      | 35.671890     | 29.076054     | 24.112431     |
| S       | 21.249483     | 31.846064     | 35.607826     |
| S       | 20.325686     | 35.734531     | 32.896423     |
| S       | 21.933146     | 31.025433     | 29.968452     |
| S       | 25.046177     | 33.531780     | 33.114948     |
| S       | 26.259624     | 29.512070     | 31.129532     |
| S       | 25.624577     | 33.839699     | 28.366577     |
| S       | 28.293217     | 29.001850     | 26.714912     |
| S       | 30.903254     | 30.753944     | 30.359936     |
| S       | 31.604145     | 26.863594     | 27.550230     |
| S       | 32.836899     | 31.096447     | 25.105354     |
| S       | 33.335255     | 26.325598     | 23.481766     |
| S       | 36.305607     | 27.646717     | 26.903542     |

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generated by VMD

| Element | X-Coordinates | Y-Coordinates | Z-Coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.320297     | 33.299393     | 33.728653     |
| Ca      | 22.929607     | 34.720093     | 35.864288     |
| Ca      | 23.228897     | 30.346189     | 33.259872     |
| Ca      | 22.878054     | 34.641140     | 30.288349     |
| Ca      | 24.639828     | 30.147274     | 27.991871     |
| Ca      | 27.782764     | 32.678379     | 31.348095     |
| Ca      | 28.925678     | 27.923176     | 29.850836     |
| Ca      | 30.708389     | 32.316277     | 27.430679     |
| Ca      | 30.588634     | 28.056789     | 24.307884     |
| Ca      | 33.755585     | 29.858442     | 28.117012     |
| Ca      | 34.443218     | 25.051825     | 26.414169     |
| Ca      | 35.861885     | 28.826216     | 23.892597     |
| S       | 20.964497     | 31.989677     | 35.701965     |
| S       | 20.612785     | 35.955742     | 33.063667     |
| S       | 21.753765     | 31.145174     | 29.971628     |
| S       | 24.946030     | 33.656334     | 33.237473     |
| S       | 26.127501     | 29.548443     | 31.247210     |
|   |        |        |        |
|---|--------|--------|--------|
| S | 25.675274 | 33.454010 | 28.445698 |
| S | 28.269627  | 29.798386 | 26.678619 |
| S | 30.730730  | 30.897701 | 30.359308 |
| S | 31.585045  | 26.936087 | 27.392586 |
| S | 32.961857  | 30.748814 | 24.987965 |
| S | 33.558086  | 26.270744 | 23.249035 |
| S | 36.471939  | 28.033737 | 27.103374 |

24 generated by VMD

| Ca |        |        |        |
|----|--------|--------|--------|
|    | 18.389668 | 32.980804 | 33.753551 |
| Ca | 22.835655  | 34.753036 | 35.952034 |
| Ca | 23.354910  | 30.399101 | 33.073792 |
| Ca | 22.797699  | 34.778030 | 30.383606 |
| Ca | 24.913588  | 30.378763 | 27.892292 |
| Ca | 27.722067  | 32.744606 | 31.224609 |
| Ca | 28.915770  | 27.921726 | 29.793919 |
| Ca | 30.492775  | 32.433922 | 27.488789 |
| Ca | 30.510328  | 28.192135 | 24.409012 |
| Ca | 33.643681  | 29.883488 | 27.996716 |
| Ca | 34.361629  | 24.772686 | 26.736216 |
| Ca | 35.643074  | 28.921368 | 23.942921 |
| S  | 21.318642  | 31.550976 | 35.615620 |
| S  | 20.662151  | 35.791943 | 33.186607 |
| S  | 21.886654  | 31.331060 | 29.895464 |
| S  | 24.675537  | 33.820290 | 33.070328 |
| S  | 26.437521  | 29.699163 | 31.125538 |
| S  | 25.636274  | 33.761951 | 28.247198 |
| S  | 28.314758  | 29.655550 | 26.687668 |
| S  | 30.719652  | 31.000689 | 30.306835 |
| S  | 31.740486  | 26.773951 | 27.670357 |
| S  | 32.742134  | 30.928246 | 25.138569 |
| S  | 33.477932  | 26.188101 | 23.291130 |
| S  | 36.527370  | 27.638414 | 27.057316 |

24 generated by VMD

| Ca |        |        |        |
|----|--------|--------|--------|
|    | 18.509022 | 33.271263 | 34.150505 |
| Ca | 23.087582  | 34.522636 | 35.852196 |
| Ca | 23.166113  | 30.538986 | 32.910404 |
| Ca | 22.828045  | 34.805691 | 30.316536 |
| Ca | 24.976471  | 30.428635 | 27.873806 |
| Ca | 27.677364  | 32.548275 | 31.231720 |
| Ca | 28.810787  | 27.999413 | 29.658154 |
| Ca | 30.418894  | 32.436371 | 27.519932 |
| Ca | 30.579357  | 27.887287 | 24.231621 |
| Ca | 33.457748  | 29.910736 | 28.112835 |
| Ca | 34.468956  | 24.890209 | 26.824043 |
|   | 35.702225 | 29.049749 | 24.096378 |
|---|-----------|-----------|-----------|
| S | 21.175129 | 31.580517 | 35.761513 |
| S | 20.807507 | 35.667496 | 33.212658 |
| S | 21.788000 | 31.222511 | 29.874208 |
| S | 24.865147 | 33.769379 | 32.883400 |
| S | 26.225769 | 29.661102 | 31.227571 |
| S | 25.598339 | 33.826790 | 28.342560 |
| S | 28.288801 | 29.727165 | 26.501352 |
| S | 30.645359 | 30.952423 | 30.238756 |
| S | 31.614429 | 26.867943 | 27.487930 |
| S | 32.766445 | 30.693481 | 24.999504 |
| S | 33.792992 | 26.211266 | 23.381954 |
| S | 36.469582 | 27.830713 | 27.250473 |

Generated by VMD

|   | 18.207041 | 33.139420 | 33.768223 |
|---|-----------|-----------|-----------|
| Ca| 22.969475 | 34.75548 | 35.949432 |
| Ca| 23.219646 | 30.418701 | 33.111305 |
| Ca| 22.865292 | 34.648621 | 30.382370 |
| Ca| 24.878716 | 30.560509 | 27.823620 |
| Ca| 27.801300 | 32.764851 | 31.441532 |
| Ca| 28.927141 | 28.030239 | 29.806873 |
| Ca| 30.336670 | 32.574829 | 27.496008 |
| Ca| 30.585892 | 27.802288 | 24.411587 |
| Ca| 33.437683 | 29.916601 | 28.057486 |
| Ca| 34.493710 | 24.830498 | 26.691299 |
| Ca| 35.829636 | 28.950956 | 23.798206 |
| S | 20.922447 | 31.723045 | 35.591175 |
| S | 20.771486 | 35.676231 | 33.294029 |
| S | 22.054981 | 31.243572 | 29.860130 |
| S | 24.817423 | 33.650410 | 33.270561 |
| S | 26.254139 | 29.644831 | 31.044231 |
| S | 25.668211 | 33.871750 | 28.559557 |
| S | 28.360184 | 29.651520 | 26.491844 |
| S | 30.628866 | 31.053522 | 30.137453 |
| S | 31.676807 | 26.892319 | 27.727722 |
| S | 32.849289 | 30.660984 | 24.811672 |
| S | 33.588692 | 25.920181 | 23.344418 |
| S | 36.575237 | 27.928640 | 27.069283 |

Generated by VMD

|   | 18.003319 | 33.044823 | 33.708447 |
|---|-----------|-----------|-----------|
| Ca| 23.057623 | 34.453506 | 36.054634 |
| Ca| 23.301785 | 30.661694 | 32.901871 |
| Ca| 22.820774 | 34.609306 | 30.678562 |
| Ca| 24.760981 | 30.558113 | 27.669838 |
|    | 27.931389 | 33.055832 | 31.316002 |
|---|-----------|-----------|-----------|
| Ca| 28.854023 | 27.907545 | 29.880283 |
| Ca| 30.456974 | 32.372890 | 27.202923 |
| Ca| 30.716986 | 27.893684 | 24.514748 |
| Ca| 33.679428 | 29.929981 | 27.858526 |
| Ca| 34.394753 | 28.893684 | 24.024975 |
| Ca| 35.300568 | 28.895063 | 24.024975 |
| S | 20.969582 | 31.473833 | 35.443317 |
| S | 20.769257 | 35.516525 | 33.481117 |
| S | 22.021711 | 31.179691 | 29.891785 |
| S | 24.933771 | 34.020042 | 33.254295 |
| S | 26.255188 | 29.950802 | 31.069754 |
| S | 25.692873 | 33.883110 | 28.393288 |
| S | 28.066210 | 29.713306 | 26.531614 |
| S | 30.654350 | 31.035622 | 30.058247 |
| S | 31.615023 | 26.806633 | 27.701523 |
| S | 32.850342 | 30.671146 | 24.921963 |
| S | 33.608704 | 25.975224 | 23.523390 |
| S | 36.504463 | 27.834198 | 27.097630 |

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generated by VMD

|    | 18.362944 | 33.010647 | 33.967117 |
|---|-----------|-----------|-----------|
| Ca| 23.156689 | 34.842167 | 35.818756 |
| Ca| 23.641586 | 30.439384 | 30.058247 |
| Ca| 22.592651 | 34.533318 | 30.440216 |
| Ca| 24.821030 | 30.262737 | 27.657005 |
| Ca| 27.802391 | 32.866497 | 31.049498 |
| Ca| 29.057112 | 27.837990 | 29.629526 |
| Ca| 30.399405 | 32.544182 | 27.552773 |
| Ca| 30.508484 | 28.212101 | 24.456636 |
| Ca| 33.566536 | 29.717915 | 28.392761 |
| Ca| 34.285637 | 24.790335 | 26.284433 |
| Ca| 35.537807 | 29.072258 | 24.342861 |
| S | 21.476988 | 31.447275 | 35.415359 |
| S | 20.663832 | 35.708706 | 33.378822 |
| S | 21.928577 | 31.023079 | 29.860725 |
| S | 24.883644 | 34.147419 | 32.807121 |
| S | 26.474449 | 29.745975 | 31.034538 |
| S | 25.472124 | 33.814552 | 28.157101 |
| S | 28.151764 | 29.811020 | 26.785141 |
| S | 30.753309 | 31.015644 | 30.252779 |
| S | 31.600765 | 26.753502 | 27.699791 |
| S | 32.815060 | 30.844614 | 25.338268 |
| S | 33.397274 | 26.267708 | 23.351551 |
| S | 36.369915 | 27.590992 | 27.320686 |
|   |          |          |          |
|---|----------|----------|----------|
|   | Ca       | Ca       | Ca       |
|   | 18.460306| 33.209545| 33.374908|
|   | 22.793661| 34.840145| 35.664227|
|   | 23.738750| 30.359470| 33.314701|
|   | 22.656015| 34.528679| 30.439425|
|   | 24.891794| 30.374716| 27.988611|
|   | 27.776270| 32.793930| 31.464447|
|   | 29.049036| 27.946360| 29.884668|
|   | 30.442606| 32.386127| 27.660549|
|   | 30.471130| 27.971333| 24.376318|
|   | 33.623386| 29.992859| 28.265720|
|   | 34.463940| 25.017370| 26.087170|
|   | 35.727322| 28.994385| 24.054379|
|   | S        |          |          |
|   | 20.994072| 31.735662| 35.165577|
|   | 20.577677| 36.093483| 33.064003|
|   | 21.938911| 30.870554| 30.157810|
|   | 24.956467| 33.891312| 33.119312|
|   | 26.440853| 29.668961| 31.391497|
|   | 25.591196| 33.649368| 28.527594|
|   | 28.132753| 29.572321| 26.714420|
|   | 30.859743| 30.923256| 30.411568|
|   | 31.584892| 26.777824| 27.644985|
|   | 32.881264| 30.539341| 25.192345|
|   | 33.331753| 26.327663| 23.112476|
|   | 36.336288| 27.835386| 26.863377|
| 24|          |          |          |
|   | Ca       |          |          |
|   | 18.145641| 33.235600| 33.598770|
|   | 22.924309| 34.817562| 35.547470|
|   | 23.554594| 30.253525| 33.447258|
|   | 22.866982| 34.344448| 30.520121|
|   | 24.918634| 30.395771| 27.976784|
|   | 27.873861| 32.812267| 31.243336|
|   | 29.116903| 27.859127| 29.846565|
|   | 30.426498| 32.271492| 27.463440|
|   | 30.422873| 28.180025| 24.451008|
|   | 33.929001| 29.913134| 28.139099|
|   | 34.275753| 24.653116| 26.277468|
|   | 35.500298| 29.079292| 24.090492|
|   | S        |          |          |
|   | 20.822451| 31.831892| 35.292995|
|   | 20.460782| 35.788002| 32.937096|
|   | 22.015970| 31.001347| 30.201473|
|   | 25.024820| 33.632332| 33.243702|
|   | 26.400944| 29.765427| 31.349960|
|   | 25.823793| 33.812626| 28.257637|
|   | 27.990250| 29.770618| 26.643932|
| S   | 30.835625 | 31.105719 | 30.328484 |
|-----|-----------|-----------|-----------|
| S   | 31.651913 | 26.995647 | 27.642246 |
| S   | 32.790924 | 30.905514 | 25.317406 |
| S   | 33.417885 | 26.286282 | 23.263477 |
| S   | 36.529724 | 27.589359 | 26.859844 |

24

| Ca  | 18.180744 | 33.088814 | 33.806145 |
|-----|-----------|-----------|-----------|
| Ca  | 22.850620 | 34.987923 | 35.858360 |
| Ca  | 23.465408 | 30.406630 | 33.027241 |
| Ca  | 22.734413 | 34.549896 | 30.796705 |
| Ca  | 24.976341 | 30.534203 | 27.926483 |
| Ca  | 27.622728 | 32.735283 | 31.318886 |
| Ca  | 29.033945 | 27.931561 | 29.666588 |
| Ca  | 30.512814 | 32.428303 | 27.269123 |
| Ca  | 30.605392 | 27.905128 | 24.472980 |
| Ca  | 33.643188 | 29.792549 | 28.020374 |
| Ca  | 34.331219 | 24.807579 | 26.507502 |
| Ca  | 35.580437 | 29.148178 | 24.077183 |
| S   | 20.987011 | 31.801533 | 35.463360 |
| S   | 20.344566 | 35.641083 | 33.186859 |
| S   | 21.988754 | 31.124416 | 30.021284 |
| S   | 24.842073 | 34.003731 | 33.212006 |
| S   | 26.341862 | 29.528721 | 31.046381 |
| S   | 25.704237 | 33.940804 | 28.605324 |
| S   | 28.327429 | 29.741463 | 26.469137 |
| S   | 30.866150 | 31.001427 | 30.092201 |
| S   | 31.676899 | 26.796654 | 27.565613 |
| S   | 32.859890 | 30.650845 | 25.097588 |
| S   | 33.641602 | 26.058430 | 23.453487 |
| S   | 36.602322 | 27.694870 | 26.979206 |

24

| Ca  | 18.066891 | 32.804329 | 34.105232 |
|-----|-----------|-----------|-----------|
| Ca  | 22.689909 | 35.030617 | 35.349514 |
| Ca  | 23.592426 | 30.347679 | 33.095551 |
| Ca  | 22.838165 | 34.662025 | 30.520569 |
| Ca  | 25.134235 | 30.824165 | 27.781258 |
| Ca  | 27.991636 | 32.805202 | 31.583874 |
| Ca  | 28.993477 | 27.850540 | 29.666351 |
| Ca  | 30.649807 | 32.408772 | 27.549170 |
| Ca  | 30.485613 | 27.891396 | 24.386127 |
| Ca  | 33.379890 | 29.618469 | 27.892193 |
| Ca  | 34.482498 | 24.962080 | 26.803753 |
| Ca  | 35.660557 | 29.091709 | 23.795023 |
| S   | 21.072178 | 31.838034 | 35.635963 |
S  20.317558  35.518906  32.788
S  22.027241  31.157681  29.940140
S  24.943405  33.645840  33.168404
S  26.442499  29.609489  31.161247
S  26.022026  34.112686  28.837307
S  28.257210  29.627068  26.711262
S  30.788971  31.025843  30.254780
S  31.345503  26.662476  27.399837
S  32.533379  30.827984  24.958134
S  33.625710  26.149599  23.617481
S  36.379318  27.827480  26.938099

24 generated by VMD
Ca  18.408396  32.777321  33.798916
Ca  22.978783  35.141628  35.310165
Ca  23.645348  30.148605  33.162502
Ca  22.814957  34.890388  30.643524
Ca  25.097208  30.804682  27.785341
Ca  27.827332  32.651527  31.616604
Ca  28.671217  27.913239  29.555372
Ca  30.504498  32.239086  27.249594
Ca  30.471848  27.914364  24.406025
Ca  33.412048  29.992641  28.081060
Ca  34.424255  24.988853  26.834127
Ca  35.712494  28.960758  23.808796
S  21.323492  31.646351  35.627914
S  20.282234  35.630119  33.005714
S  22.043482  31.337856  30.000603
S  24.927847  33.549591  33.378365
S  26.208515  29.478878  30.856634
S  25.903656  34.194305  28.881737
S  28.164253  29.560083  26.445412
S  30.599730  30.891783  30.208059
S  31.571814  26.872015  27.633608
S  32.712505  30.677685  24.793468
S  33.711998  26.087831  23.546707
S  36.302124  27.950455  27.309757

24 generated by VMD
Ca  18.138311  32.694485  33.838966
Ca  22.795807  35.038715  35.505833
Ca  23.454882  30.403233  33.104424
Ca  22.794304  34.791843  30.647751
Ca  24.988501  30.559895  27.805939
Ca  27.853468  32.883068  31.682915
Ca  28.929586  27.900753  29.673777
| Element | X1   | X2   | X3     |
|---------|------|------|--------|
| Ca      | 30.856148 | 32.238342 | 26.906469 |
| Ca      | 30.504827 | 27.920834 | 24.575073 |
| Ca      | 33.583817 | 29.809416 | 28.254002 |
| Ca      | 34.207115 | 24.793949 | 26.490738 |
| Ca      | 35.858173 | 29.068760 | 23.594759 |
| S       | 21.006721 | 31.861406 | 35.723114 |
| S       | 20.210772 | 35.570900 | 32.984531 |
| S       | 23.583817 | 29.809416 | 28.254002 |
| S       | 24.207115 | 24.793949 | 26.490738 |
| S       | 25.858173 | 29.068760 | 23.594759 |
| S       | 28.322996 | 29.562469 | 26.560425 |
| S       | 30.828362 | 31.121964 | 30.400181 |
| S       | 31.637127 | 26.933754 | 27.767809 |
| S       | 32.967697 | 30.778078 | 25.014206 |
| S       | 33.569069 | 26.114187 | 23.261608 |
| S       | 36.326805 | 27.706860 | 27.004892 |

24 generated by VMD

| Element | X1   | X2   | X3     |
|---------|------|------|--------|
| Ca      | 18.640377 | 32.882477 | 33.454876 |
| Ca      | 22.503830 | 35.131092 | 35.553749 |
| Ca      | 23.719212 | 30.643503 | 33.250595 |
| Ca      | 22.808882 | 34.220856 | 30.611580 |
| Ca      | 25.201653 | 30.659706 | 28.105312 |
| Ca      | 27.767250 | 32.935585 | 31.732346 |
| Ca      | 28.775953 | 27.818325 | 29.528530 |
| Ca      | 30.741478 | 32.312107 | 26.814877 |
| Ca      | 30.669222 | 27.877495 | 24.418720 |
| Ca      | 33.421917 | 29.799761 | 28.419331 |
| Ca      | 34.298798 | 24.966721 | 26.514521 |
| Ca      | 35.595001 | 29.096600 | 23.876236 |
| S       | 21.147104 | 31.841881 | 35.480133 |
| S       | 20.553207 | 35.625351 | 32.831879 |
| S       | 22.076210 | 31.125584 | 30.045275 |
| S       | 24.974150 | 33.643032 | 33.527988 |
| S       | 26.254164 | 29.449684 | 31.116434 |
| S       | 25.960384 | 33.886581 | 28.928135 |
| S       | 28.226952 | 29.606785 | 26.360909 |
| S       | 30.561008 | 30.992971 | 30.243084 |
| S       | 31.537991 | 26.800644 | 27.661024 |
| S       | 32.776920 | 30.795490 | 25.005829 |
| S       | 33.382107 | 26.148169 | 23.372105 |
| S       | 36.128548 | 28.039648 | 27.085705 |

24 generated by VMD

| Element | X1   | X2   | X3     |
|---------|------|------|--------|
| Ca      | 18.219402 | 32.965775 | 34.050262 |
|   |   |   |
|---|---|---|
| Ca | 22.636480 | 34.927231 | 35.527328 |
| Ca | 23.538010 | 30.332394 | 33.084129 |
| Ca | 22.872625 | 34.594193 | 30.456280 |
| Ca | 25.395857 | 30.727406 | 27.979618 |
| Ca | 27.794300 | 32.810989 | 31.592896 |
| Ca | 28.983259 | 28.053505 | 29.783283 |
| Ca | 30.726961 | 32.280655 | 26.608435 |
| Ca | 30.493681 | 32.280655 | 26.608435 |
| Ca | 32.611150 | 29.816938 | 28.463718 |
| Ca | 34.236389 | 24.992903 | 26.512701 |
| Ca | 35.561092 | 29.098827 | 23.808208 |
| S  | 21.054394 | 31.590237 | 35.510239 |
| S  | 20.469101 | 35.517189 | 32.840427 |
| S  | 22.327873 | 31.224880 | 29.779114 |
| S  | 24.942116 | 33.549004 | 33.421898 |
| S  | 26.322975 | 29.702959 | 31.092056 |
| S  | 26.125891 | 34.076157 | 28.991077 |
| S  | 28.399824 | 29.488243 | 26.421553 |
| S  | 30.694645 | 31.226740 | 30.121881 |
| S  | 31.353754 | 26.712881 | 27.801870 |
| S  | 32.697197 | 30.533587 | 24.940218 |
| S  | 33.468464 | 26.266665 | 23.39466 |
| S  | 36.144650 | 28.142622 | 27.073975 |

24

generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.374916 | 33.179070 | 33.445168 |
| Ca | 22.684853 | 35.113380 | 35.638485 |
| Ca | 23.551525 | 30.281517 | 33.295849 |
| Ca | 23.167179 | 34.407654 | 30.588987 |
| Ca | 25.137878 | 30.357939 | 28.115614 |
| Ca | 27.889717 | 32.732563 | 31.755499 |
| Ca | 28.771137 | 27.933319 | 29.764601 |
| Ca | 30.660187 | 32.336998 | 26.573940 |
| Ca | 30.668854 | 27.840931 | 24.407856 |
| Ca | 33.365803 | 29.820772 | 28.529020 |
| Ca | 34.185028 | 24.961609 | 26.714596 |
| Ca | 35.538231 | 29.272924 | 23.744020 |
| S  | 20.980116 | 31.733038 | 35.463585 |
| S  | 20.500422 | 35.816483 | 32.861053 |
| S  | 22.195805 | 31.151215 | 30.184217 |
| S  | 24.945526 | 33.374069 | 33.465824 |
| S  | 26.329308 | 29.533134 | 31.131887 |
| S  | 26.120419 | 33.764660 | 28.739677 |
| S  | 28.160257 | 29.545391 | 26.492071 |
| S  | 30.502203 | 31.121971 | 30.057671 |
| S  | 31.454662 | 26.902096 | 27.739985 |
|    |       |       |       |
|----|-------|-------|-------|
| S  | 32.772186 | 30.727688 | 24.926256 |
| S  | 33.636620  | 26.282400  | 23.181583 |
| S  | 36.127308  | 28.109272  | 27.122585 |

24 generated by VMD

| Ca  |       |       |       |
|-----|-------|-------|-------|
| Ca  | 18.518896 | 32.763180 | 33.709457 |
| Ca  | 22.796797  | 34.958702  | 35.927261 |
| Ca  | 23.308386  | 30.343632  | 33.047760 |
| Ca  | 22.955034  | 34.681488  | 30.440744 |
| Ca  | 25.309952  | 30.603252  | 27.979412 |
| Ca  | 27.746677  | 32.744686  | 31.719631 |
| Ca  | 28.727827  | 28.072731  | 29.660122 |
| Ca  | 30.645960  | 32.451729  | 26.362053 |
| Ca  | 30.565411  | 27.721067  | 24.329971 |
| Ca  | 33.278267  | 29.944609  | 28.354107 |
| Ca  | 34.162556  | 24.859325  | 26.888721 |
| Ca  | 35.656319  | 29.049496  | 23.928370 |

| S  |       |       |       |
|----|-------|-------|-------|
| S  | 21.126600 | 31.609047  | 35.770927 |
| S  | 20.625948  | 35.674583  | 33.092167 |
| S  | 22.183403  | 31.309406  | 29.726227 |
| S  | 24.868490  | 33.563297  | 33.396660 |
| S  | 26.165705  | 29.384665  | 30.944160 |
| S  | 26.041279  | 33.966614  | 28.694084 |
| S  | 28.223833  | 29.645901  | 26.486713 |
| S  | 30.747902  | 31.086161  | 30.247543 |
| S  | 31.456142  | 26.978321  | 27.687342 |
| S  | 32.756195  | 30.735157  | 24.818096 |
| S  | 33.579151  | 26.073210  | 23.492805 |
| S  | 36.273380  | 28.079792  | 27.235725 |

24 generated by VMD

| Ca  |       |       |       |
|-----|-------|-------|-------|
| Ca  | 18.337559 | 32.933678 | 34.267639 |
| Ca  | 22.836689  | 34.780010  | 35.636345 |
| Ca  | 23.365852  | 30.311691  | 33.070450 |
| Ca  | 22.757570  | 34.901657  | 30.529972 |
| Ca  | 25.434126  | 30.815792  | 28.037109 |
| Ca  | 27.520237  | 32.565460  | 31.281364 |
| Ca  | 29.134300  | 27.942093  | 29.687607 |
| Ca  | 30.681152  | 32.435158  | 26.686155 |
| Ca  | 30.463537  | 27.783588  | 24.506699 |
| Ca  | 33.249615  | 29.767490  | 28.668438 |
| Ca  | 34.522316  | 25.006615  | 26.838112 |
| Ca  | 35.438988  | 29.138840  | 23.708736 |
| S  | 21.187891  | 31.516550  | 35.712341 |
| S  | 20.437954  | 35.654411  | 33.082760 |
| S  | 22.251814  | 31.517242  | 29.739178 |
| S    | 24.882639 | 33.407600 | 33.347435 |
| S    | 26.121965 | 29.480419 | 30.664322 |
| S    | 25.905590 | 34.101906 | 28.420517 |
| S    | 28.335840 | 29.741959 | 26.641455 |
| S    | 30.686506 | 31.205015 | 29.859943 |
| S    | 31.502836 | 26.632792 | 27.874252 |
| S    | 32.903309 | 30.589249 | 25.069593 |
| S    | 33.563496 | 26.062946 | 23.539106 |
| S    | 36.198341 | 28.007887 | 27.070522 |

24

generated by VMD

| Ca   | 18.258299 | 32.856590 | 34.490738 |
| Ca   | 23.189493 | 34.950329 | 35.531364 |
| Ca   | 23.383547 | 30.191822 | 32.903458 |
| Ca   | 22.593956 | 34.832390 | 30.437923 |
| Ca   | 25.256794 | 30.784771 | 28.080471 |
| Ca   | 27.522982 | 32.598637 | 31.185753 |
| Ca   | 29.218636 | 28.072418 | 29.536747 |
| Ca   | 30.635376 | 32.789051 | 26.662895 |
| Ca   | 30.450388 | 27.806870 | 24.454988 |
| Ca   | 33.067715 | 29.581886 | 28.787216 |
| Ca   | 34.560493 | 25.000706 | 26.684650 |
| Ca   | 35.554226 | 29.005135 | 24.001652 |
| S    | 21.508797 | 31.673122 | 35.724731 |
| S    | 20.550369 | 35.540802 | 33.253544 |
| S    | 21.936289 | 31.324162 | 29.786755 |
| S    | 24.866171 | 33.441742 | 33.069431 |
| S    | 26.113750 | 29.426157 | 30.516777 |
| S    | 25.875807 | 34.031036 | 28.394619 |
| S    | 28.382223 | 29.925066 | 26.552071 |
| S    | 30.860764 | 31.324890 | 30.038504 |
| S    | 31.407560 | 26.333469 | 27.774916 |
| S    | 32.771423 | 30.597847 | 25.249165 |
| S    | 33.680103 | 26.196301 | 23.320831 |
| S    | 36.074860 | 28.014843 | 27.500847 |

24

generated by VMD

| Ca   | 18.389297 | 33.306107 | 34.193836 |
| Ca   | 22.944780 | 34.858639 | 35.475372 |
| Ca   | 23.198280 | 30.157604 | 32.910786 |
| Ca   | 22.789639 | 34.655418 | 30.604771 |
| Ca   | 25.286398 | 30.547958 | 28.032948 |
| Ca   | 27.610252 | 32.593582 | 31.436483 |
| Ca   | 29.281221 | 27.911839 | 29.894497 |
| Ca   | 30.669149 | 32.493156 | 26.711018 |
| Ca   | 30.392063 | 27.681938 | 24.705029 |
| Element | Value1   | Value2   | Value3   |
|---------|----------|----------|----------|
| Ca      | 33.203091| 29.782379| 28.511242|
| Ca      | 34.662514| 25.003180| 26.622341|
| Ca      | 35.442093| 29.139420| 23.483749|
| S       | 21.156628| 31.693270| 35.436073|
| S       | 20.463686| 35.904335| 33.039227|
| S       | 22.198345| 31.196384| 29.552025|
| S       | 24.762682| 33.480614| 33.258438|
| S       | 26.106544| 29.374016| 30.860758|
| S       | 26.120945| 34.110779| 28.726597|
| S       | 28.449768| 29.583450| 26.837786|
| S       | 30.752235| 30.894552| 30.205019|
| S       | 31.740253| 26.588545| 27.817753|
| S       | 32.642719| 29.374016| 29.843260|
| S       | 33.281097| 26.327620| 23.360905|
| S       | 36.176308| 28.280010| 27.256536|

24 generated by VMD

| Element | Value1   | Value2   | Value3   |
|---------|----------|----------|----------|
| Ca      | 18.220680| 33.51617 | 33.660484|
| Ca      | 22.911175| 34.717522| 35.483505|
| Ca      | 23.513105| 30.120886| 32.989319|
| Ca      | 22.769392| 34.432575| 30.776165|
| Ca      | 25.255926| 30.848648| 28.074612|
| Ca      | 27.599503| 32.822411| 31.486546|
| Ca      | 29.329861| 27.876320| 29.843260|
| Ca      | 30.615837| 32.610016| 26.988426|
| Ca      | 30.581482| 27.725567| 24.683712|
| Ca      | 33.379524| 29.859297| 28.480974|
| Ca      | 34.551949| 25.125710| 26.814243|
| Ca      | 34.929745| 28.893105| 23.530956|
| S       | 21.195507| 31.691479| 35.132004|
| S       | 20.435198| 35.844597| 32.981598|
| S       | 22.137093| 31.140862| 29.657043|
| S       | 24.892778| 33.414345| 33.570812|
| S       | 26.193998| 29.510214| 30.778240|
| S       | 25.924055| 34.043877| 28.784784|
| S       | 28.439838| 29.745510| 26.776197|
| S       | 30.905497| 31.272694| 30.230061|
| S       | 31.804909| 26.636053| 28.043936|
| S       | 32.754517| 30.558254| 25.104702|
| S       | 33.196487| 26.022282| 23.226334|
| S       | 36.181923| 28.136196| 26.841684|

24 generated by VMD

| Element | Value1   | Value2   | Value3   |
|---------|----------|----------|----------|
| Ca      | 18.189568| 32.920670| 33.611584|
| Ca      | 22.894674| 34.820786| 35.538033|
| Ca      | 23.338234| 30.191174| 32.839764|
Ca | 23.002247 | 34.695038 | 30.562351
Ca | 25.267048 | 30.844891 | 28.201748
Ca | 27.767788 | 32.454384 | 31.587658
Ca | 29.390121 | 28.024570 | 29.974926
Ca | 30.547136 | 32.409546 | 26.778322
Ca | 30.320881 | 27.544266 | 24.901033
Ca | 33.560715 | 29.858963 | 28.504532
Ca | 34.680855 | 25.227980 | 26.455292
Ca | 35.176041 | 29.057247 | 23.626001
S  | 20.944359 | 31.721966 | 35.471161
S  | 20.495468 | 35.772186 | 32.926994
S  | 22.081696 | 31.407391 | 29.668121
S  | 24.836163 | 33.388260 | 33.135307
S  | 26.20477  | 29.553215 | 30.858923
S  | 26.111338 | 34.044838 | 28.735712
S  | 28.174101 | 29.634331 | 26.977583
S  | 31.116112 | 31.255611 | 30.403416
S  | 31.890364 | 26.747070 | 28.017126
S  | 32.350880 | 30.485479 | 25.100990
S  | 33.047520 | 26.184536 | 23.180687
S  | 36.287292 | 28.055641 | 26.883301

24 generated by VMD

Ca | 18.328823 | 33.154861 | 33.831360
Ca | 23.035553 | 34.917824 | 35.446800
Ca | 23.366255 | 30.141426 | 32.644173
Ca | 22.822136 | 34.560173 | 30.871603
Ca | 25.135365 | 30.686172 | 28.081964
Ca | 27.692511 | 32.481777 | 31.625216
Ca | 29.223263 | 27.823334 | 29.686394
Ca | 30.542679 | 32.422565 | 26.800245
Ca | 30.332439 | 27.757805 | 24.935652
Ca | 33.544930 | 29.966255 | 28.587440
Ca | 34.571400 | 25.374741 | 26.583633
Ca | 35.315758 | 28.832256 | 23.615601
S  | 21.388950 | 31.674294 | 35.090393
S  | 20.526457 | 35.948997 | 33.024632
S  | 22.003904 | 31.178211 | 29.704851
S  | 24.949818 | 33.582809 | 33.332867
S  | 26.091473 | 29.360685 | 30.683323
S  | 25.918257 | 34.000340 | 28.866808
S  | 28.295284 | 29.679173 | 26.795832
S  | 30.701965 | 31.126688 | 30.248003
S  | 31.863281 | 26.738430 | 28.001083
S  | 32.594902 | 30.621101 | 25.142048
S  | 33.277145 | 26.169540 | 23.357599
|   | 36.197559 | 28.100601 | 26.981964 |
|---|------------|------------|------------|
| 24 generated by VMD | | | |
| Ca | 18.275692 | 33.247383 | 33.780800 |
| Ca | 23.099258 | 34.967667 | 35.552368 |
| Ca | 23.473946 | 30.229771 | 33.114250 |
| Ca | 22.730637 | 34.472622 | 30.504080 |
| Ca | 25.208618 | 30.910007 | 28.090080 |
| Ca | 27.670389 | 32.625107 | 31.098104 |
| Ca | 29.323479 | 27.854515 | 29.749352 |
| Ca | 30.798454 | 32.647285 | 27.234673 |
| Ca | 30.458460 | 27.671667 | 24.778631 |
| Ca | 33.419262 | 29.622345 | 28.620844 |
| Ca | 34.756725 | 25.013107 | 26.514105 |
| Ca | 35.132973 | 29.330429 | 23.444759 |
| S  | 21.107079 | 31.739853 | 35.590439 |
| S  | 20.538637 | 35.916264 | 33.137772 |
| S  | 21.954678 | 31.155245 | 29.933130 |
| S  | 24.803301 | 33.377258 | 33.109619 |
| S  | 26.009388 | 29.383598 | 30.565268 |
| S  | 25.794378 | 33.861305 | 28.279043 |
| S  | 28.433287 | 29.769072 | 26.718159 |
| S  | 30.951256 | 31.033600 | 30.403847 |
| S  | 31.841272 | 26.323114 | 27.887060 |
| S  | 32.488510 | 30.698116 | 25.354502 |
| S  | 33.271061 | 26.226316 | 23.488161 |
| S  | 36.179283 | 28.224371 | 26.990978 |
| 24 generated by VMD | | | |
| Ca | 18.417274 | 33.186920 | 33.355789 |
| Ca | 23.095676 | 34.929882 | 35.303471 |
| Ca | 23.502201 | 30.052052 | 33.193771 |
| Ca | 22.776554 | 34.428150 | 30.625324 |
| Ca | 25.322571 | 30.910913 | 28.271811 |
| Ca | 27.664572 | 32.610001 | 31.541725 |
| Ca | 29.346867 | 27.995815 | 29.839344 |
| Ca | 30.776726 | 32.507317 | 26.933500 |
| Ca | 30.316246 | 27.764233 | 24.610399 |
| Ca | 33.327232 | 29.584991 | 28.635136 |
| Ca | 34.417747 | 25.109915 | 26.339584 |
| Ca | 35.305531 | 29.035963 | 23.730873 |
| S  | 21.280304 | 31.771641 | 35.469776 |
| S  | 20.385479 | 35.743889 | 32.779343 |
| S  | 22.082958 | 31.100887 | 30.095465 |
| S  | 24.910305 | 33.376328 | 33.178692 |
| S  | 26.112825 | 29.297955 | 30.907253 |
|  |  |  |  |
|---|---|---|---|
| S  | 25.901066 | 34.094437 | 28.694483 |
| S  | 28.317713 | 29.857460 | 26.760300 |
| S  | 30.741657 | 31.235844 | 30.326582 |
| S  | 31.664175 | 26.667744 | 27.820261 |
| S  | 32.441975 | 30.741709 | 25.121958 |
| S  | 33.271107 | 26.082241 | 23.441120 |
| S  | 36.341305 | 28.213734 | 26.964119 |

24 generated by VMD

| Ca  | 18.269499 | 32.998722 | 33.763100 |
| Ca  | 22.811251 | 34.976833 | 35.742844 |
| Ca  | 23.386757 | 30.283112 | 32.797615 |
| Ca  | 22.643408 | 34.790035 | 30.699974 |
| Ca  | 25.219360 | 30.693188 | 28.114689 |
| Ca  | 27.603466 | 32.696331 | 31.581059 |
| Ca  | 29.273657 | 28.002951 | 29.783073 |
| Ca  | 30.716288 | 32.456459 | 27.190216 |
| Ca  | 30.449171 | 27.631794 | 24.742220 |
| Ca  | 33.629646 | 29.908104 | 27.988182 |
| Ca  | 34.542843 | 34.941223 | 26.634098 |
| Ca  | 35.530685 | 28.907505 | 23.752823 |
| S  | 21.145567 | 31.667641 | 35.357414 |
| S  | 20.316439 | 35.734314 | 33.196365 |
| S  | 21.956768 | 31.451473 | 29.761717 |
| S  | 24.788933 | 33.413277 | 33.268566 |
| S  | 26.180382 | 29.404655 | 30.670134 |
| S  | 25.873796 | 34.194481 | 28.733128 |
| S  | 28.304724 | 29.771957 | 26.684317 |
| S  | 30.879097 | 31.117550 | 30.342583 |
| S  | 31.842909 | 26.716444 | 27.896744 |
| S  | 32.613750 | 30.523357 | 24.929960 |
| S  | 33.257252 | 25.900414 | 23.530390 |
| S  | 36.484337 | 28.118231 | 26.778795 |

24 generated by VMD

| Ca  | 18.231316 | 33.006516 | 34.105415 |
| Ca  | 23.145702 | 34.754021 | 35.746437 |
| Ca  | 23.353399 | 30.162739 | 32.969547 |
| Ca  | 22.814739 | 34.869438 | 30.364267 |
| Ca  | 24.969395 | 30.843735 | 27.838192 |
| Ca  | 27.443897 | 32.366096 | 31.192688 |
| Ca  | 29.090004 | 28.051819 | 29.774679 |
| Ca  | 30.657032 | 32.594048 | 27.513670 |
| Ca  | 30.446995 | 27.738266 | 24.663078 |
| Ca  | 33.630058 | 30.008873 | 28.381140 |
| Ca  | 34.620571 | 24.890228 | 26.746346 |
Ca 35.418041 28.939899 23.691071
S 21.260433 31.697113 35.628513
S 20.612478 35.655945 32.304422
S 21.891632 31.447079 29.832958
S 24.971336 33.578358 32.916424
S 25.907820 29.275644 30.415413
S 25.767569 34.066391 28.552830
S 28.448359 29.743816 26.660835
S 30.687019 31.185852 30.264574
S 31.988844 26.820904 27.967646
S 32.622120 30.711332 25.003387
S 33.337502 25.959337 23.464333
S 36.403751 27.932598 27.016142

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generated by VMD

Ca 18.409346 32.615089 33.690643
Ca 23.044781 34.919121 35.425049
Ca 23.363007 30.367867 32.824471
Ca 22.847118 35.162804 30.549955
Ca 25.206972 31.019388 28.119965
Ca 27.596548 32.365696 31.433815
Ca 29.166937 27.863659 29.725796
Ca 30.551481 32.416962 27.633934
Ca 30.271824 27.35493 25.042492
Ca 33.489899 29.741381 28.162865
Ca 34.992130 25.118538 26.795662
Ca 35.008270 28.888103 23.598942
S 21.356113 31.728214 35.445606
S 20.541052 35.144888 32.885464
S 22.016417 31.705536 29.878672
S 24.993944 33.549957 33.070919
S 25.984848 29.084332 30.561295
S 25.925774 34.084759 28.656364
S 28.235252 29.717810 26.715960
S 30.713732 30.863050 30.33403
S 32.123638 26.834730 27.797346
S 32.354706 30.689684 25.073503
S 33.145622 26.115322 23.644007
S 36.380566 28.198097 26.873936

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generated by VMD

Ca 18.569502 32.694023 34.092823
Ca 23.078819 34.876270 35.593269
Ca 23.376774 30.129898 32.906612
Ca 22.728796 34.638288 30.600750
Ca 25.129856 30.973957 27.866423
|  |  |  |
|---|---|---|
| Ca | 27.506975 | 32.655426 | 31.054428 |
| Ca | 29.074324 | 27.657543 | 29.513721 |
| Ca | 30.756041 | 32.350792 | 27.342489 |
| Ca | 30.275366 | 27.851685 | 24.798306 |
| Ca | 33.794025 | 30.050812 | 28.414696 |
| Ca | 34.502098 | 25.082550 | 26.804638 |
| Ca | 35.318016 | 28.710627 | 23.768339 |
| S  | 21.388227 | 31.700209 | 35.818516 |
| S  | 20.271456 | 35.922611 | 33.095238 |
| S  | 22.030653 | 31.414270 | 29.772720 |
| S  | 24.875807 | 33.351929 | 33.244118 |
| S  | 26.056358 | 29.403618 | 30.169865 |
| S  | 25.631390 | 34.361256 | 28.581936 |
| S  | 28.331451 | 29.895317 | 26.545921 |
| S  | 30.777451 | 30.938396 | 30.224449 |
| S  | 31.813423 | 26.906511 | 27.797276 |
| S  | 32.784367 | 30.703697 | 25.114632 |
| S  | 33.142006 | 25.940266 | 23.607737 |
| S  | 36.506836 | 28.027283 | 27.211132 |
| 24 | generated by VMD |
| Ca | 18.515383 | 32.732113 | 34.038364 |
| Ca | 23.211132 | 34.659821 | 35.823650 |
| Ca | 23.476231 | 30.346615 | 32.878067 |
| Ca | 22.468340 | 34.628265 | 30.550003 |
| Ca | 24.884232 | 31.084194 | 27.711632 |
| Ca | 27.694286 | 32.645058 | 30.741291 |
| Ca | 28.923660 | 27.788750 | 29.439667 |
| Ca | 30.936146 | 32.297401 | 27.518005 |
| Ca | 30.396690 | 28.085598 | 25.043705 |
| Ca | 33.984070 | 29.884010 | 28.608936 |
| Ca | 34.503181 | 25.375254 | 26.878311 |
| Ca | 35.309601 | 28.271427 | 23.702576 |
| S  | 21.514435 | 31.588093 | 35.944412 |
| S  | 20.469444 | 35.496147 | 33.539200 |
| S  | 21.914486 | 31.486485 | 29.744972 |
| S  | 24.862328 | 33.389668 | 32.756474 |
| S  | 25.955011 | 29.594425 | 30.281324 |
| S  | 25.428627 | 34.383553 | 28.056252 |
| S  | 28.289764 | 30.134552 | 26.569073 |
| S  | 30.665535 | 30.722473 | 30.193611 |
| S  | 31.846130 | 27.030807 | 28.107876 |
| S  | 33.010998 | 30.623066 | 25.052036 |
| S  | 33.031498 | 26.092714 | 23.552969 |
| S  | 36.428810 | 27.959518 | 27.207626 |
| 24 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.747107    | 32.763824    | 34.086231    |
| Ca      | 23.150309    | 34.767574    | 35.805317    |
| Ca      | 23.329268    | 30.337601    | 32.619438    |
| Ca      | 22.930592    | 34.972824    | 30.488430    |
| Ca      | 27.507874    | 32.545921    | 31.096844    |
| Ca      | 28.967278    | 37.61306     | 29.576828    |
| Ca      | 30.565445    | 32.92076     | 27.390295    |
| Ca      | 30.386671    | 27.836855    | 24.918486    |
| Ca      | 33.796150    | 30.091852    | 28.54477     |
| Ca      | 34.526058    | 24.927767    | 26.795658    |
| Ca      | 35.326084    | 28.880939    | 23.734467    |
| S       | 21.565523    | 31.579853    | 35.649857    |
| S       | 20.666491    | 35.595604    | 33.33723     |
| S       | 21.839815    | 31.682617    | 29.562222    |
| S       | 24.848927    | 33.385826    | 32.989136    |
| S       | 25.929054    | 29.483141    | 30.476568    |
| S       | 25.539034    | 34.139366    | 28.144352    |
| S       | 28.138920    | 29.671810    | 26.552145    |
| S       | 30.730453    | 30.882908    | 30.271042    |
| S       | 32.015202    | 26.925949    | 28.136347    |
| S       | 32.624329    | 30.700977    | 25.206398    |
| S       | 33.092850    | 26.203972    | 23.686459    |
| S       | 36.526581    | 28.129459    | 27.068859    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.301462    | 32.882278    | 34.031883    |
| Ca      | 23.293777    | 34.772423    | 35.582088    |
| Ca      | 23.020782    | 30.608795    | 32.947742    |
| Ca      | 22.822834    | 34.650730    | 30.587662    |
| Ca      | 25.055052    | 30.642519    | 28.051060    |
| Ca      | 27.692366    | 32.521988    | 30.099927    |
| Ca      | 28.924511    | 27.751163    | 29.649633    |
| Ca      | 30.647453    | 32.404827    | 27.330280    |
| Ca      | 30.643129    | 27.749374    | 24.690475    |
| Ca      | 33.728043    | 29.953896    | 28.131231    |
| Ca      | 34.553818    | 24.815784    | 26.773834    |
| Ca      | 35.423992    | 29.114431    | 23.775547    |
| S       | 21.247185    | 32.034401    | 35.739552    |
| S       | 20.406696    | 35.689308    | 33.529316    |
| S       | 21.735306    | 31.364985    | 29.600965    |
| S       | 24.695780    | 33.323875    | 32.872070    |
| S       | 25.958214    | 29.562180    | 30.574938    |
| S       | 25.766125    | 34.138985    | 28.675159    |
| S       | 28.225353    | 29.823168    | 26.683849    |
S       30.785416       30.920773       30.233084
S       31.976677       26.765350       27.939882
S       32.795582       30.808914       25.047913
S       33.486988       26.098095       23.479877
S       36.533493       27.901812       27.012747

24
generated by VMD
Ca       18.725594       32.393887       33.811779
Ca       23.322079       34.836246       35.698444
Ca       23.376787       30.527590       32.973270
Ca       22.878080       34.784245       30.605406
Ca       25.210308       30.979210       27.953644
Ca       27.487682       32.572590       31.019455
Ca       28.734846       27.821548       29.541656
Ca       30.657488       32.439415       27.482006
Ca       30.593285       27.847637       24.394753
Ca       33.648758       29.931303       28.219955
Ca       34.418999       25.013006       26.914131
Ca       35.393131       28.757893       24.044027
Ca       21.489307       31.766209       35.635868
S       20.425402       35.460983       33.392265
S       22.009699       31.660503       29.810459
S       24.997232       33.265476       32.998531
S       25.834274       29.543627       30.406836
S       25.553261       34.167988       28.340311
S       28.201843       29.890162       26.456718
S       30.616285       30.783737       30.265823
S       31.761694       27.055195       27.940716
S       32.788876       30.835476       25.000381
S       33.222862       25.820045       23.921265
S       36.372288       28.146114       27.112349

24
generated by VMD
Ca       18.409729       32.625183       33.943535
Ca       22.895658       34.911026       35.844601
Ca       23.442581       30.444965       32.929482
Ca       22.806166       34.836288       30.705938
Ca       24.977837       31.028452       27.845724
Ca       27.659040       32.707588       31.176525
Ca       28.886080       27.823032       29.617138
Ca       30.553898       32.377026       27.155502
Ca       30.483597       27.788221       24.433731
Ca       33.569767       30.004173       28.126797
Ca       34.506329       25.070892       26.844803
Ca       35.782112       28.633953       23.924397
S       21.410032       31.723888       35.909000
|     |           |           |           |
|-----|-----------|-----------|-----------|
| S   | 20.282869 | 35.520615 | 33.309010 |
| S   | 21.909214 | 31.601156 | 29.661669 |
| S   | 24.907944 | 33.471073 | 33.164177 |
| S   | 25.952990 | 29.608147 | 30.517937 |
| S   | 25.783667 | 34.268639 | 28.659191 |
| S   | 28.298172 | 29.724516 | 26.562550 |
| S   | 30.630514 | 30.802971 | 30.248428 |
| S   | 31.728508 | 26.755177 | 27.654358 |
| S   | 32.748512 | 30.615341 | 24.894299 |
| S   | 33.630257 | 25.840389 | 23.644356 |
| S   | 36.464581 | 28.117327 | 27.166962 |

24

generated by VMD

|     |           |           |           |
|-----|-----------|-----------|-----------|
| Ca  | 18.770573 | 32.769394 | 34.056648 |
| Ca  | 23.144423 | 35.033894 | 35.808666 |
| Ca  | 23.513069 | 30.449842 | 32.946587 |
| Ca  | 22.708948 | 34.506020 | 30.532909 |
| Ca  | 25.013699 | 30.792641 | 27.652363 |
| Ca  | 27.428080 | 32.548843 | 30.975346 |
| Ca  | 28.805910 | 27.855690 | 29.406998 |
| Ca  | 30.367010 | 32.321407 | 27.420410 |
| Ca  | 30.405493 | 28.014706 | 24.387241 |
| Ca  | 33.645008 | 29.984859 | 28.204168 |
| Ca  | 34.411968 | 24.924557 | 26.707495 |
| Ca  | 35.654034 | 28.913631 | 24.342978 |
| S   | 21.530300 | 31.810440 | 35.821079 |
| S   | 20.634281 | 35.660011 | 33.293083 |
| S   | 21.845490 | 31.320841 | 29.743237 |
| S   | 24.877594 | 33.483337 | 33.192085 |
| S   | 26.014202 | 29.531399 | 30.422106 |
| S   | 25.782822 | 34.085739 | 28.394556 |
| S   | 28.009750 | 29.756783 | 26.367184 |
| S   | 30.636112 | 30.893028 | 30.429367 |
| S   | 31.637558 | 26.975658 | 27.665319 |
| S   | 32.728168 | 30.708679 | 25.280869 |
| S   | 33.565857 | 26.045635 | 23.687317 |
| S   | 36.589733 | 27.913015 | 27.202023 |

24

generated by VMD

|     |           |           |           |
|-----|-----------|-----------|-----------|
| Ca  | 18.414005 | 32.740326 | 34.296043 |
| Ca  | 23.182367 | 34.793495 | 35.750355 |
| Ca  | 23.567924 | 30.524220 | 32.933186 |
| Ca  | 22.592651 | 34.529648 | 30.681990 |
| Ca  | 25.024746 | 31.041424 | 27.776833 |
| Ca  | 27.676266 | 32.663536 | 30.921370 |
| Ca  | 28.851364 | 27.883850 | 29.698318 |
| Ca    | 30.721022  | 32.510643  | 27.125347  |
|-------|------------|------------|------------|
| Ca    | 30.487030  | 27.774361  | 24.479811  |
| Ca    | 33.547882  | 29.984406  | 28.289612  |
| Ca    | 34.322517  | 24.885067  | 26.844631  |
| Ca    | 35.664703  | 28.880402  | 24.020588  |
| S     | 21.567812  | 31.579981  | 35.768764  |
| S     | 20.275364  | 35.528381  | 33.461433  |
| S     | 21.833763  | 31.500917  | 29.746788  |
| S     | 24.825731  | 33.436703  | 33.020176  |
| S     | 25.888023  | 29.689867  | 30.311125  |
| S     | 25.734495  | 34.218407  | 28.342026  |
| S     | 28.311119  | 29.806400  | 26.558041  |
| S     | 30.632271  | 31.112087  | 30.032627  |
| S     | 31.629414  | 26.814804  | 27.766256  |
| S     | 32.946342  | 30.611401  | 25.222681  |
| S     | 33.578972  | 25.973240  | 23.518387  |
| S     | 36.444241  | 27.816435  | 27.373648  |

24 generated by VMD

| Ca    | 30.721022  | 32.510643  | 27.125347  |
|-------|------------|------------|------------|
| Ca    | 30.487030  | 27.774361  | 24.479811  |
| Ca    | 33.547882  | 29.984406  | 28.289612  |
| Ca    | 34.322517  | 24.885067  | 26.844631  |
| Ca    | 35.664703  | 28.880402  | 24.020588  |
| S     | 21.567812  | 31.579981  | 35.768764  |
| S     | 20.275364  | 35.528381  | 33.461433  |
| S     | 21.833763  | 31.500917  | 29.746788  |
| S     | 24.825731  | 33.436703  | 33.020176  |
| S     | 25.888023  | 29.689867  | 30.311125  |
| S     | 25.734495  | 34.218407  | 28.342026  |
| S     | 28.311119  | 29.806400  | 26.558041  |
| S     | 30.632271  | 31.112087  | 30.032627  |
| S     | 31.629414  | 26.814804  | 27.766256  |
| S     | 32.946342  | 30.611401  | 25.222681  |
| S     | 33.578972  | 25.973240  | 23.518387  |
| S     | 36.444241  | 27.816435  | 27.373648  |

24 generated by VMD

| Ca    | 18.443775  | 32.861893  | 34.154846  |
|-------|------------|------------|------------|
| Ca    | 22.921490  | 35.103912  | 35.633492  |
| Ca    | 23.400314  | 30.460413  | 33.287365  |
| Ca    | 23.054750  | 34.342571  | 30.506207  |
| Ca    | 25.117905  | 30.536304  | 27.913845  |
| Ca    | 27.800840  | 32.702576  | 31.116676  |
| Ca    | 28.884348  | 28.041397  | 29.664499  |
| Ca    | 30.595066  | 32.377365  | 27.052612  |
| Ca    | 30.355549  | 27.940685  | 24.423275  |
| Ca    | 33.550949  | 29.860891  | 28.177223  |
| Ca    | 34.214729  | 24.915079  | 26.660912  |
| Ca    | 35.995228  | 29.120672  | 24.203739  |
| S     | 21.261929  | 31.838329  | 35.820061  |
| S     | 20.447433  | 35.719124  | 33.088940  |
| S     | 22.007143  | 31.048199  | 29.927801  |
| S     | 24.876287  | 33.461117  | 33.171531  |
| S     | 25.892370  | 29.460320  | 30.665981  |
| S     | 25.951134  | 33.960701  | 28.245403  |
| S     | 28.157307  | 29.912235  | 26.531099  |
| S     | 30.692118  | 30.832664  | 30.382341  |
| S     | 31.473812  | 26.909685  | 27.488747  |
| S     | 32.718563  | 30.791746  | 25.118193  |
| S     | 33.641090  | 26.408680  | 23.475914  |
| S     | 36.265881  | 27.693504  | 27.229084  |

24 generated by VMD

| Ca    | 18.443775  | 32.861893  | 34.154846  |
|-------|------------|------------|------------|
| Ca    | 18.630482  | 32.734005  | 34.366291  |
| Element | Values | Values | Values |
|---------|--------|--------|--------|
| Ca      | 23.212746 | 34.968979 | 35.773499 |
| Ca      | 23.317629 | 30.168926 | 32.906898 |
| Ca      | 22.642113 | 34.468655 | 30.369690 |
| Ca      | 25.114946 | 31.001213 | 27.707748 |
| Ca      | 27.675743 | 32.806267 | 31.096508 |
| Ca      | 29.044975 | 28.218597 | 29.788504 |
| Ca      | 30.686228 | 32.433071 | 27.346645 |
| Ca      | 33.592342 | 29.902763 | 28.193853 |
| Ca      | 34.112297 | 24.777142 | 26.655334 |
| Ca      | 35.766434 | 28.645033 | 24.037373 |
| S       | 21.573908 | 31.636635 | 35.726517 |
| S       | 20.457426 | 35.478004 | 33.312420 |
| S       | 21.899265 | 31.322815 | 29.472107 |
| S       | 24.802599 | 33.251701 | 32.926708 |
| S       | 26.010427 | 29.484638 | 30.670471 |
| S       | 25.730143 | 34.190952 | 28.354580 |
| S       | 28.208496 | 29.996723 | 26.591885 |
| S       | 30.668005 | 31.211281 | 30.302910 |
| S       | 31.547913 | 27.072090 | 27.554646 |
| S       | 32.715691 | 30.726719 | 25.126610 |
| S       | 33.420544 | 26.000790 | 23.646889 |
| S       | 36.449467 | 27.812876 | 27.396759 |

24

*generated by VMD*

| Element | Values | Values | Values |
|---------|--------|--------|--------|
| Ca      | 18.570551 | 32.684456 | 34.305984 |
| Ca      | 23.085703 | 34.744736 | 35.898621 |
| Ca      | 23.420448 | 30.307171 | 32.832245 |
| Ca      | 22.806301 | 34.633446 | 30.659714 |
| Ca      | 25.137173 | 31.150162 | 27.559870 |
| Ca      | 27.542736 | 32.940182 | 30.819628 |
| Ca      | 29.231054 | 28.169235 | 29.882481 |
| Ca      | 30.630152 | 32.590126 | 27.401747 |
| Ca      | 30.509813 | 28.144211 | 24.542070 |
| Ca      | 33.616146 | 29.859097 | 28.263309 |
| Ca      | 34.206997 | 24.842598 | 26.823509 |
| Ca      | 35.522640 | 28.660528 | 23.958101 |
| S       | 21.614641 | 31.467922 | 35.720932 |
| S       | 20.613117 | 35.546158 | 33.308147 |
| S       | 21.999878 | 31.405321 | 29.384672 |
| S       | 24.784653 | 33.122032 | 33.071426 |
| S       | 25.958761 | 29.485714 | 30.548717 |
| S       | 25.546541 | 33.983818 | 28.108793 |
| S       | 28.305576 | 29.804459 | 26.613895 |
| S       | 30.665422 | 31.469944 | 30.336903 |
| S       | 31.428583 | 27.053665 | 27.756954 |
S  32.811897  30.751343  25.100975
S  33.320992  25.812675  23.786711
S  36.390316  27.671045  27.254684

24
generated by VMD
Ca  18.653841  32.770321  33.960766
Ca  23.103121  34.652336  35.795193
Ca  23.392328  30.402618  32.787849
Ca  22.800085  34.654377  30.690845
Ca  25.027208  30.978722  27.795958
Ca  27.595510  32.908257  31.051292
Ca  29.048500  27.799904  29.802853
Ca  30.607248  32.363228  27.359070
Ca  30.310110  27.860453  24.607561
Ca  33.555237  29.932899  27.922779
Ca  34.457645  24.907333  27.053574
Ca  35.780357  28.796417  23.825193
S  21.434065  31.659508  35.604309
S  20.334324  35.513283  33.394791
S  21.946365  31.612024  29.694126
S  25.025404  33.355576  33.250053
S  25.949863  29.613775  30.345572
S  25.511379  34.283386  28.422508
S  28.196678  29.718208  26.526484
S  30.719440  31.004169  30.354561
S  31.580288  27.025505  27.650454
S  32.741169  30.687052  25.085873
S  33.477642  25.821808  23.774105
S  36.472347  27.978939  27.184296

24
generated by VMD
Ca  18.795656  32.356644  34.149487
Ca  22.884504  34.736065  35.687366
Ca  23.373873  30.562321  33.015327
Ca  22.760971  34.683414  30.488382
Ca  25.191858  30.827305  27.988419
Ca  27.674044  32.840187  31.129066
Ca  29.087780  27.996845  29.692532
Ca  30.640049  32.524933  27.301651
Ca  30.478512  28.238838  24.532114
Ca  33.524868  29.739643  28.359045
Ca  34.270008  24.796139  26.895287
Ca  35.489677  28.606550  23.881968
S  21.444040  31.610085  35.687412
S  20.311575  35.513283  33.394791
S  21.946365  31.612024  29.694126
S  25.025404  33.355576  33.250053
S  25.949863  29.613775  30.345572
S  25.511379  34.283386  28.422508
S  28.196678  29.718208  26.526484
S  30.719440  31.004169  30.354561
S  31.580288  27.025505  27.650454
S  32.741169  30.687052  25.085873
S  33.477642  25.821808  23.774105
S  36.472347  27.978939  27.184296

370
S   24.734472  33.498238  33.130592
S   26.072176  29.774179  30.567190
S   25.823975  34.191906  28.383759
S   28.169897  29.822464  26.623100
S   30.816475  31.142900  30.349316
S   31.487059  26.962427  27.541939
S   32.828373  30.825047  25.055382
S   33.438072  25.817842  23.567133
S   36.356026  27.801044  27.127216

24 generated by VMD
Ca  18.528721  32.804718  34.130379
Ca  23.056675  34.792801  35.269356
Ca  23.627865  30.301838  32.889862
Ca  22.819439  34.814201  30.532333
Ca  24.852718  30.619328  27.951822
Ca  27.701452  32.641602  31.200287
Ca  29.043686  27.777985  29.648577
Ca  30.606598  32.409637  27.569321
Ca  30.448168  28.083014  24.605751
Ca  33.714474  29.908607  28.311872
Ca  34.355408  24.865938  26.749298
Ca  35.285637  28.970722  23.955460
Ca  21.548277  31.717503  35.498177
S   20.317076  35.512703  33.021324
S   21.959480  31.396236  29.822533
S   25.058107  33.501781  33.056202
S   26.216314  29.662058  30.576771
S   25.707016  34.045227  28.380898
S   28.192396  29.812185  26.719221
S   30.740944  30.921181  30.450199
S   31.555088  27.030428  27.752554
S   32.683151  30.762844  25.339254
S   33.241508  26.049988  23.413635
S   36.459816  27.897545  27.094984

24 generated by VMD
Ca  18.468246  32.601662  34.607399
Ca  23.325041  34.784035  35.631737
Ca  23.260201  30.348921  32.719318
Ca  22.432884  34.707706  30.614452
Ca  25.109486  30.920193  27.851215
Ca  27.671310  32.834602  30.862692
Ca  28.965019  27.976749  29.575802
Ca  30.618776  32.468830  27.346788
Ca  30.579546  28.029896  24.503141
|   | Ca     | S      | Ca     | S     |
|---|--------|--------|--------|------|
| 1 | 33.51697 | 29.685167 | 28.330326 |
| 2 | 34.360786 | 24.767790 | 26.973473 |
| 3 | 35.763222 | 28.756104 | 24.132450 |
| 4 | 21.625946 | 31.626915 | 35.648506 |
| 5 | 20.343941 | 35.452942 | 33.577225 |
| 6 | 21.780531 | 31.564899 | 29.760859 |
| 7 | 24.987526 | 33.524185 | 32.854450 |
| 8 | 25.950493 | 29.609535 | 30.472263 |
| 9 | 25.460913 | 34.345222 | 28.217478 |
|10 | 28.395184 | 29.859562 | 26.514757 |
|11 | 30.464996 | 31.073044 | 30.212912 |
|12 | 31.623138 | 26.824343 | 27.496632 |
|13 | 32.918816 | 30.920406 | 25.112873 |
|14 | 33.591492 | 25.870136 | 23.671425 |
|15 | 36.505867 | 27.747206 | 27.251860 |

24 generated by VMD

|   | Ca     | S      | Ca     | S     |
|---|--------|--------|--------|------|
| 1 | 18.549307 | 32.336575 | 33.930206 |
| 2 | 22.895084 | 34.993942 | 35.738308 |
| 3 | 23.209860 | 30.428020 | 32.979866 |
| 4 | 22.752298 | 34.915440 | 30.712486 |
| 5 | 25.014265 | 30.917633 | 27.968464 |
| 6 | 27.750534 | 32.796192 | 31.348520 |
| 7 | 29.102104 | 28.242271 | 29.633732 |
| 8 | 30.704275 | 32.407494 | 27.127625 |
| 9 | 30.576653 | 27.693892 | 24.586834 |
|10 | 33.703484 | 29.912714 | 27.980381 |
|11 | 34.371979 | 24.738546 | 26.720013 |
|12 | 35.702866 | 28.784893 | 23.858414 |
|13 | 21.269241 | 31.744427 | 35.774208 |
|14 | 20.131428 | 35.375824 | 33.110481 |
|15 | 21.778358 | 31.516460 | 29.751505 |
|16 | 24.760670 | 33.407501 | 33.409958 |
|17 | 26.023855 | 29.772154 | 30.714499 |
|18 | 25.756832 | 34.275181 | 28.600582 |
|19 | 28.284929 | 29.961113 | 26.602854 |
|20 | 30.807346 | 31.106339 | 30.186834 |
|21 | 31.721863 | 26.833214 | 27.660732 |
|22 | 32.927788 | 30.654720 | 24.844217 |
|23 | 33.577820 | 25.817486 | 23.551653 |
|24 | 36.347164 | 27.668032 | 27.147627 |

24 generated by VMD

|   | Ca     | S      | Ca     | S     |
|---|--------|--------|--------|------|
| 1 | 18.530655 | 32.495899 | 33.920547 |
| 2 | 23.002932 | 34.906086 | 35.685638 |
| 3 | 23.519190 | 30.328394 | 32.911072 |
|   |   |   |
|---|---|---|
| Ca | 22.719837 | 34.645733 | 30.635498 |
| Ca | 25.116085 | 30.675251 | 27.770163 |
| Ca | 27.751732 | 28.083700 | 29.793228 |
| Ca | 30.526997 | 32.468349 | 27.420263 |
| Ca | 30.470295 | 27.915409 | 24.383202 |
| Ca | 33.659599 | 29.978680 | 28.166237 |
| Ca | 33.987610 | 24.771837 | 26.803810 |
| Ca | 35.670555 | 28.905895 | 24.069973 |
| S  | 21.538010 | 31.635857 | 35.671875 |
| S  | 20.250057 | 35.440517 | 33.289856 |
| S  | 22.156637 | 31.487129 | 29.676632 |
| S  | 25.066973 | 33.489056 | 33.189644 |
| S  | 26.243536 | 29.574097 | 30.728899 |
| S  | 25.615356 | 34.140774 | 28.340940 |
| S  | 28.235060 | 29.917164 | 26.444002 |
| S  | 30.730873 | 31.124928 | 30.250908 |
| S  | 31.534702 | 27.061308 | 27.925709 |
| S  | 32.849419 | 30.661619 | 25.045835 |
| S  | 33.484642 | 25.958324 | 23.412354 |
| S  | 36.195755 | 27.650307 | 27.260109 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.583666 | 32.108906 | 33.945850 |
| Ca | 23.117050 | 34.874298 | 35.717987 |
| Ca | 23.323318 | 30.327436 | 32.833252 |
| Ca | 22.908894 | 35.147316 | 30.514723 |
| Ca | 25.002539 | 31.046038 | 27.749447 |
| Ca | 27.633707 | 32.813328 | 31.165810 |
| Ca | 28.983540 | 27.866662 | 29.605354 |
| Ca | 30.738386 | 32.425503 | 27.414120 |
| Ca | 30.411819 | 28.054472 | 24.677620 |
| Ca | 33.704250 | 29.820587 | 28.252831 |
| Ca | 34.360966 | 24.861454 | 27.125433 |
| Ca | 35.355774 | 28.895710 | 23.580629 |
| S  | 21.604477 | 31.672142 | 35.657829 |
| S  | 20.283499 | 35.221748 | 33.203789 |
| S  | 21.830498 | 31.684546 | 29.693405 |
| S  | 25.016273 | 33.552834 | 33.064934 |
| S  | 25.955521 | 29.491333 | 30.544575 |
| S  | 25.757267 | 34.222649 | 28.329620 |
| S  | 28.309330 | 29.880280 | 26.726339 |
| S  | 30.676889 | 31.034796 | 30.379375 |
| S  | 31.749306 | 26.887098 | 27.965019 |
| S  | 32.736835 | 30.719639 | 25.069101 |
| S  | 33.284283 | 25.844910 | 23.830637 |
|     |  36.391949 | 27.826401 | 26.892355 |
|-----|------------|------------|------------|
| 24  | generated by VMD | Ca 18.504263 | 32.105545 | 33.929703 |
|     | Ca 22.973778 | 35.008801 | 35.551151 |
|     | Ca 23.478254 | 30.521381 | 32.912498 |
|     | Ca 22.758034 | 34.534893 | 30.679380 |
|     | Ca 25.100838 | 30.803564 | 27.859123 |
|     | Ca 27.940477 | 33.043884 | 31.146889 |
|     | Ca 28.857754 | 28.200878 | 29.768734 |
|     | Ca 30.677105 | 32.473785 | 27.417727 |
|     | Ca 30.328545 | 27.956882 | 24.522226 |
|     | Ca 33.744354 | 29.890718 | 28.204580 |
|     | Ca 34.095215 | 24.756973 | 26.673969 |
|     | Ca 35.762997 | 28.860119 | 23.942554 |
|     | S 21.354811  | 31.888430 | 35.653694 |
|     | S 20.257919  | 35.204483 | 32.981289 |
|     | S 21.976526  | 31.406946 | 29.703220 |
|     | S 25.033060  | 33.405296 | 33.313019 |
|     | S 26.283646  | 29.795002 | 30.852631 |
|     | S 25.731836  | 34.295551 | 28.439156 |
|     | S 28.046150  | 29.954933 | 26.657143 |
|     | S 30.831100  | 31.139227 | 30.226360 |
|     | S 31.567488  | 26.910831 | 27.798473 |
|     | S 32.683556  | 30.530945 | 25.167009 |
|     | S 33.334629  | 26.117468 | 23.407757 |
|     | S 36.397739  | 27.493483 | 27.131790 |
| 24  | generated by VMD | Ca 18.342545 | 32.024643 | 33.965260 |
|     | Ca 22.857773 | 35.210209 | 35.610435 |
|     | Ca 23.136505 | 30.626484 | 32.973454 |
|     | Ca 22.843143 | 34.625145 | 30.659233 |
|     | Ca 25.204544 | 30.788700 | 28.006245 |
|     | Ca 27.715855 | 32.815155 | 31.082561 |
|     | Ca 29.071640 | 28.191448 | 29.917473 |
|     | Ca 30.658615 | 32.412659 | 27.442966 |
|     | Ca 30.494560 | 28.116013 | 24.421638 |
|     | Ca 34.154465 | 29.985987 | 28.136417 |
|     | Ca 34.020615 | 24.601606 | 26.685448 |
|     | Ca 35.583946 | 28.728554 | 23.900043 |
|     | S 21.348431 | 32.071533 | 35.839569 |
|     | S 20.077831 | 35.120667 | 33.049004 |
|     | S 21.695732 | 31.405527 | 29.638990 |
|     | S 24.839420 | 33.375687 | 33.269047 |
|     | S 25.983078 | 29.919659 | 30.692066 |
|   |           |           |           |
|---|-----------|-----------|-----------|
| S | 25.866638 | 34.199039 | 28.599648 |
| S | 28.362827 | 29.780067 | 26.833843 |
| S | 30.950928 | 31.244186 | 30.367199 |
| S | 31.716799 | 27.030357 | 27.695854 |
| S | 33.069599 | 30.632801 | 25.115078 |
| S | 33.255836 | 26.024200 | 23.238903 |
| S | 36.468666 | 27.369690 | 26.799639 |

24 generated by VMD

| Ca |           |           |           |
|----|-----------|-----------|-----------|
| Ca | 18.719934 | 32.220089 | 33.747883 |
| Ca | 22.799486 | 35.163082 | 35.364498 |
| Ca | 23.311857 | 30.453178 | 33.062260 |
| Ca | 22.672649 | 34.873074 | 30.694136 |
| Ca | 25.010929 | 30.603573 | 28.047489 |
| Ca | 27.802675 | 32.798641 | 31.319723 |
| Ca | 29.138805 | 27.951361 | 29.749777 |
| Ca | 30.724216 | 32.373859 | 27.538698 |
| Ca | 30.360626 | 28.004955 | 24.630322 |
| Ca | 34.037048 | 29.890373 | 27.948032 |
| Ca | 34.168388 | 24.781506 | 26.510981 |
| Ca | 35.265041 | 29.023245 | 23.730322 |
| S  | 21.317955 | 31.970348 | 35.607464 |
| S  | 20.191395 | 35.355862 | 32.585163 |
| S  | 21.921814 | 31.600319 | 29.773746 |
| S  | 24.92755  | 33.364620 | 33.354298 |
| S  | 26.115154 | 29.552595 | 30.995918 |
| S  | 25.807257 | 34.182915 | 28.620264 |
| S  | 28.170956 | 29.775513 | 26.811554 |
| S  | 30.815952 | 31.049831 | 30.486631 |
| S  | 31.726241 | 27.046551 | 27.956123 |
| S  | 32.947079 | 30.535141 | 25.364691 |
| S  | 33.317951 | 26.077831 | 23.258093 |
| S  | 36.448692 | 27.651608 | 26.779278 |

24 generated by VMD

| Ca |           |           |           |
|----|-----------|-----------|-----------|
| Ca | 18.526724 | 32.051735 | 34.070644 |
| Ca | 22.857697 | 35.184273 | 35.499947 |
| Ca | 23.267351 | 30.489712 | 32.886135 |
| Ca | 22.679094 | 34.828217 | 30.356024 |
| Ca | 25.086996 | 30.805626 | 28.109724 |
| Ca | 27.741362 | 32.691788 | 31.081280 |
| Ca | 28.919044 | 27.974702 | 29.627186 |
| Ca | 30.575623 | 32.518305 | 27.442257 |
| Ca | 30.407215 | 28.106527 | 24.728577 |
| Ca | 33.777992 | 29.833313 | 28.183708 |
| Ca | 34.428787 | 24.588448 | 26.621096 |
|  | Ca     | 35.446354 | 28.926460 | 23.880653 |
|  | S      | 21.640608 | 31.960415 | 35.751263 |
|  | S      | 20.167221 | 35.349937 | 33.021957 |
|  | S      | 21.815672 | 31.375141 | 29.695593 |
|  | S      | 25.060423 | 33.522316 | 33.250172 |
|  | S      | 26.071253 | 29.583309 | 30.647793 |
|  | S      | 25.852343 | 34.286602 | 28.479633 |
|  | S      | 28.203644 | 30.114592 | 26.663532 |
|  | S      | 30.840088 | 30.939537 | 30.33652 |
|  | S      | 31.805809 | 26.785019 | 27.761599 |
|  | S      | 32.807735 | 30.716206 | 25.35136 |
|  | S      | 33.172882 | 26.104565 | 23.534496 |
|  | S      | 36.568111 | 27.560583 | 26.961567 |

24

generated by VMD

|  | Ca     | 19.084232 | 31.819149 | 34.140144 |
|  | Ca     | 23.003798 | 35.210926 | 32.97871 |
|  | Ca     | 23.293957 | 30.432768 | 32.904991 |
|  | Ca     | 22.758919 | 34.949890 | 30.410553 |
|  | Ca     | 25.146408 | 30.792044 | 27.993135 |
|  | Ca     | 27.752308 | 32.802212 | 30.869831 |
|  | Ca     | 28.866413 | 27.950644 | 29.848747 |
|  | Ca     | 30.670729 | 32.591919 | 27.533857 |
|  | Ca     | 30.221001 | 28.124754 | 24.551861 |
|  | Ca     | 33.764797 | 29.696890 | 28.188416 |
|  | Ca     | 33.957954 | 24.586426 | 26.632416 |
|  | Ca     | 35.606533 | 29.110481 | 24.275040 |
|  | S      | 21.855854 | 31.797081 | 35.918186 |
|  | S      | 20.279243 | 34.861664 | 32.769035 |
|  | S      | 22.025602 | 31.593369 | 29.684872 |
|  | S      | 25.058186 | 33.674030 | 33.222607 |
|  | S      | 26.095240 | 29.642887 | 30.637085 |
|  | S      | 25.620150 | 34.086185 | 28.241920 |
|  | S      | 27.982817 | 30.138695 | 26.608360 |
|  | S      | 30.759315 | 31.138763 | 30.304996 |
|  | S      | 31.490585 | 26.915285 | 27.775188 |
|  | S      | 32.769241 | 30.684441 | 25.469625 |
|  | S      | 33.320820 | 26.263260 | 23.489571 |
|  | S      | 36.335865 | 27.436214 | 27.171728 |

24

generated by VMD

|  | Ca     | 18.605679 | 32.104980 | 33.951214 |
|  | Ca     | 23.112823 | 34.980793 | 35.254593 |
|  | Ca     | 23.325579 | 30.609707 | 32.920715 |
|  | Ca     | 23.057781 | 34.867355 | 30.538845 |
|  | Ca     | 24.799681 | 30.557743 | 27.931406 |
| Ca  | 27.878016 | 32.772320 | 31.068733 |
|-----|-----------|-----------|-----------|
| Ca  | 28.992283 | 28.125343 | 29.942230 |
| Ca  | 30.391541 | 32.387733 | 27.585402 |
| Ca  | 30.257027 | 28.104061 | 24.548412 |
| Ca  | 33.806725 | 29.897820 | 27.921587 |
| Ca  | 34.043648 | 24.717075 | 26.767651 |
| Ca  | 35.736023 | 29.052353 | 24.189000 |
| S   | 21.457903 | 31.817366 | 35.734695 |
| S   | 20.478884 | 34.995239 | 32.756462 |
| S   | 22.017403 | 31.696270 | 29.660017 |
| S   | 25.172922 | 33.556015 | 33.161125 |
| S   | 26.088198 | 29.514509 | 31.006805 |
| S   | 25.745214 | 34.015450 | 28.464752 |
| S   | 28.044968 | 29.844444 | 26.906647 |
| S   | 30.811600 | 31.061008 | 30.181505 |
| S   | 31.442184 | 26.989882 | 27.669456 |
| S   | 32.618847 | 30.873672 | 25.107393 |
| S   | 33.334160 | 26.380413 | 23.404003 |
| S   | 36.501057 | 27.378515 | 27.037563 |

24

generated by VMD

| Ca  | 18.796913 | 32.123158 | 34.345108 |
|-----|-----------|-----------|-----------|
| Ca  | 22.975075 | 35.093525 | 35.440769 |
| Ca  | 23.373291 | 30.640308 | 33.000591 |
| Ca  | 22.587162 | 34.654800 | 30.530121 |
| Ca  | 25.014687 | 30.906929 | 27.840759 |
| Ca  | 27.708038 | 32.706799 | 30.948822 |
| Ca  | 29.081501 | 28.066071 | 29.851896 |
| Ca  | 30.775410 | 32.730213 | 27.463671 |
| Ca  | 30.433504 | 28.079609 | 24.709396 |
| Ca  | 33.673317 | 29.686934 | 28.124220 |
| Ca  | 33.956600 | 24.593224 | 26.638798 |
| Ca  | 35.935818 | 28.829117 | 24.105297 |
| S   | 21.819538 | 31.758286 | 35.723988 |
| S   | 20.116161 | 35.016434 | 33.111122 |
| S   | 21.793148 | 31.189112 | 29.648012 |
| S   | 24.960793 | 33.827244 | 33.068100 |
| S   | 25.870367 | 29.644478 | 30.479710 |
| S   | 25.571560 | 34.321091 | 28.343653 |
| S   | 28.203678 | 30.179155 | 26.749670 |
| S   | 30.865057 | 31.102631 | 30.310623 |
| S   | 31.551319 | 26.909733 | 27.803661 |
| S   | 32.948063 | 30.721199 | 25.092436 |
| S   | 33.335487 | 26.264511 | 23.448730 |
| S   | 36.373627 | 27.255505 | 27.160969 |

24
|   |   |   |
|---|---|---|
| Ca | 18.901714 | 32.078835 | 34.336189 |
| Ca | 22.808294 | 35.235580 | 35.353931 |
| Ca | 23.504715 | 30.423618 | 32.922283 |
| Ca | 22.465605 | 34.726410 | 30.335545 |
| Ca | 25.373774 | 30.631977 | 27.782524 |
| Ca | 27.569738 | 32.963219 | 31.177610 |
| Ca | 29.053131 | 28.066994 | 29.813942 |
| Ca | 30.680349 | 32.540428 | 27.552441 |
| Ca | 30.526558 | 28.099483 | 24.345177 |
| Ca | 33.568359 | 29.656651 | 28.213520 |
| Ca | 33.807430 | 24.847492 | 26.441586 |
| Ca | 35.729294 | 28.946201 | 24.265896 |
| S  | 21.849884 | 31.830257 | 35.850845 |
| S  | 20.217091 | 35.268379 | 33.145428 |
| S  | 22.006855 | 31.167803 | 29.657028 |
| S  | 24.870710 | 33.793053 | 33.006386 |
| S  | 26.131866 | 29.644758 | 30.646925 |
| S  | 25.551590 | 34.202454 | 28.442675 |
| S  | 28.441483 | 29.901600 | 26.683666 |
| S  | 30.680815 | 31.237942 | 30.416813 |
| S  | 31.501446 | 26.844044 | 27.732986 |
| S  | 32.867290 | 30.686665 | 25.315714 |
| S  | 33.286133 | 26.341270 | 23.244343 |
| S  | 36.325993 | 27.164976 | 27.256432 |

24

|   |   |   |
|---|---|---|
| Ca | 18.667461 | 32.251606 | 34.211067 |
| Ca | 22.939882 | 34.884613 | 35.497253 |
| Ca | 23.682169 | 30.445896 | 32.931358 |
| Ca | 22.641541 | 34.807236 | 30.576784 |
| Ca | 25.149595 | 30.926300 | 27.848841 |
| Ca | 27.666945 | 33.023300 | 31.088028 |
| Ca | 29.058502 | 27.886597 | 29.778702 |
| Ca | 30.570013 | 32.397583 | 27.255365 |
| Ca | 30.641073 | 27.791126 | 24.484009 |
| Ca | 33.274822 | 29.732765 | 28.235847 |
| Ca | 34.100853 | 24.607691 | 26.708702 |
| Ca | 35.852570 | 29.095926 | 24.137585 |
| S  | 21.595703 | 31.707386 | 35.821915 |
| S  | 20.272720 | 35.254059 | 33.162056 |
| S  | 21.971741 | 31.606178 | 29.939390 |
| S  | 25.077679 | 33.686119 | 33.150757 |
| S  | 26.029345 | 29.755829 | 30.457718 |
| S  | 25.725613 | 34.259731 | 28.221695 |
| S  | 28.134619 | 29.562775 | 26.558506 |
|    |   x   |   y   |   z   |
|----|-------|-------|-------|
| S  | 30.53 | 31.20 | 30.30 |
| S  | 31.47 | 26.76 | 27.08 |
| S  | 32.75 | 30.63 | 25.08 |
| S  | 33.71 | 26.43 | 23.49 |
| S  | 36.19 | 27.58 | 27.31 |
|    |       |       |       |
| Ca | 18.84 | 32.22 | 33.93 |
| Ca | 23.21 | 34.86 | 35.49 |
| Ca | 23.20 | 30.43 | 27.51 |
| Ca | 30.54 | 32.43 | 29.65 |
| Ca | 30.41 | 27.83 | 24.78 |
| Ca | 33.73 | 29.73 | 28.35 |
| Ca | 34.28 | 24.83 | 26.69 |
| Ca | 35.41 | 29.14 | 23.88 |
| S  | 21.52 | 31.67 | 35.68 |
| S  | 20.39 | 35.54 | 33.23 |
| S  | 21.88 | 31.72 | 29.65 |
| S  | 24.88 | 33.54 | 33.07 |
| S  | 25.97 | 29.58 | 30.45 |
| S  | 25.49 | 34.21 | 28.29 |
| S  | 28.29 | 29.52 | 26.84 |
| S  | 30.89 | 30.85 | 30.38 |
| S  | 31.78 | 26.87 | 28.06 |
| S  | 32.57 | 30.62 | 25.19 |
| S  | 33.30 | 26.25 | 23.52 |
| S  | 36.67 | 27.75 | 26.85 |

24 generated by VMD
|   |          |          |          |
|---|----------|----------|----------|
| S | 20.164700 | 35.537674 | 33.113064 |
| S | 22.002655 | 31.401787 | 29.851936 |
| S | 24.805412 | 33.476559 | 33.056694 |
| S | 26.314983 | 29.642059 | 30.672848 |
| S | 25.725433 | 34.248825 | 28.395687 |
| S | 28.440439 | 30.007454 | 26.698481 |
| S | 30.776039 | 31.108961 | 30.287052 |
| S | 31.610754 | 26.807076 | 27.745964 |
| S | 32.675774 | 30.794277 | 25.116423 |
| S | 33.406090 | 26.043991 | 23.489361 |
| S | 36.284107 | 27.452560 | 27.097858 |

24

generated by VMD

Ca 18.773153 32.263248 33.867756
Ca 23.119619 35.170334 35.433285
Ca 23.502815 30.506569 32.939240
Ca 22.916805 34.643135 30.565697
Ca 25.027870 30.653954 27.982681
Ca 27.793016 32.664104 31.065922
Ca 28.892319 28.035969 29.743809
Ca 30.605989 32.475517 27.441418
Ca 30.355595 28.114880 24.514860
Ca 33.496666 29.753412 28.174191
Ca 34.277225 25.029385 26.841644
Ca 35.614502 28.998880 24.390339
S 21.676910 31.872250 35.798019
S 20.256453 35.349121 33.044201
S 21.866312 31.456860 29.767427
S 25.098600 33.295830 33.130272
S 26.002975 29.541050 30.618475
S 25.749130 34.126987 28.334545
S 28.094776 29.893398 26.629848
S 30.777601 30.948231 30.215660
S 31.443871 26.847813 27.688358
S 32.671528 30.654861 25.085411
S 33.341793 26.405241 23.462223
S 36.364510 27.599056 27.204746

24

generated by VMD

Ca 18.495958 32.492813 34.005733
Ca 22.796188 35.033012 35.382370
Ca 23.331882 30.561769 33.205425
Ca 22.803967 34.877991 30.496956
Ca 25.073997 30.926321 27.953644
Ca 27.752502 32.626846 31.258461
Ca 28.968012 27.760685 29.757160
|   |      |      |      |
|---|------|------|------|
|   | 30.692907 | 32.153244 | 27.241631 |
|   | 30.391754 | 27.834309 | 24.505585 |
|   | 33.641136 | 29.812397 | 28.291631 |
|   | 34.585484 | 24.994678 | 26.615034 |
|   | 35.653725 | 28.985783 | 23.835989 |
| S | 21.218311 | 31.745777 | 35.867348 |
| S | 20.396742 | 35.573364 | 32.925854 |
| S | 21.977701 | 31.717527 | 29.903275 |
| S | 24.872639 | 33.465160 | 33.255413 |
| S | 25.949142 | 29.454269 | 30.629791 |
| S | 25.896702 | 34.208946 | 28.581455 |
| S | 28.130156 | 29.462574 | 26.766228 |
| S | 30.763918 | 30.869221 | 30.350576 |
| S | 31.830956 | 26.799232 | 27.698158 |
| S | 32.725739 | 30.678423 | 25.014460 |
| S | 33.393929 | 26.142302 | 23.344303 |
| S | 36.376648 | 28.123409 | 27.053625 |

24 generated by VMD

| Ca | 18.327629 | 32.586552 | 34.304287 |
| Ca | 22.976851 | 35.062557 | 35.512672 |
| Ca | 23.292318 | 30.559959 | 33.132889 |
| Ca | 22.780056 | 34.791832 | 30.502346 |
| Ca | 25.184286 | 30.907047 | 28.083038 |
| Ca | 27.717417 | 32.434616 | 30.961699 |
| Ca | 29.055645 | 27.751244 | 29.749035 |
| Ca | 30.742661 | 32.469826 | 27.482328 |
| Ca | 30.327265 | 28.084812 | 24.539246 |
| Ca | 33.557220 | 29.680984 | 28.485161 |
| Ca | 34.552166 | 24.976341 | 26.913883 |
| Ca | 35.680473 | 28.975994 | 23.590014 |
| S | 21.325579 | 31.868702 | 35.860622 |
| S | 20.490341 | 35.311150 | 32.935783 |
| S | 21.880838 | 31.633202 | 29.735413 |
| S | 24.993763 | 33.440224 | 33.213936 |
| S | 25.930637 | 29.330971 | 30.252328 |
| S | 25.695854 | 34.098759 | 28.251200 |
| S | 28.270744 | 29.743320 | 26.659029 |
| S | 30.704435 | 30.960655 | 30.239094 |
| S | 31.503735 | 26.804558 | 27.712187 |
| S | 32.805161 | 30.851250 | 25.060268 |
| S | 33.492790 | 26.135090 | 23.533997 |
| S | 36.432133 | 27.840410 | 26.956621 |

24 generated by VMD

| Ca | 18.046911 | 33.345024 | 34.427979 |
|   |   |   |   |
|---|---|---|---|
| Ca | 23.131376 | 34.922276 | 35.379486 |
| Ca | 23.280550 | 30.514700 | 33.121689 |
| Ca | 22.819408 | 34.664391 | 30.593979 |
| Ca | 25.175640 | 30.599678 | 27.958134 |
| Ca | 27.532417 | 32.330376 | 31.115234 |
| Ca | 28.923988 | 27.691212 | 30.050007 |
| Ca | 30.694138 | 32.254250 | 27.358595 |
| Ca | 33.740509 | 28.033209 | 24.511520 |
| Ca | 34.377254 | 25.129501 | 26.233536 |
| Ca | 35.658775 | 28.961521 | 23.782677 |
| S  | 21.174425 | 31.967354 | 35.731159 |
| S  | 20.366428 | 35.831615 | 33.006672 |
| S  | 22.125519 | 31.317722 | 29.738796 |
| S  | 24.841612 | 33.323486 | 33.126404 |
| S  | 25.895033 | 29.126087 | 30.670235 |
| S  | 25.651173 | 33.865776 | 28.234669 |
| S  | 28.262304 | 29.536644 | 26.953453 |
| S  | 30.711927 | 31.002417 | 30.338799 |
| S  | 31.754215 | 26.823166 | 27.735165 |
| S  | 32.949249 | 30.776274 | 25.223001 |
| S  | 33.429482 | 26.333557 | 23.389549 |
| S  | 36.695015 | 28.131418 | 26.889786 |

24

generated by VMD

| Ca | 18.743275 | 32.538040 | 33.961857 |
| Ca | 23.090305 | 34.777706 | 35.969395 |
| Ca | 23.475235 | 30.498127 | 32.874420 |
| Ca | 22.856792 | 34.757908 | 30.637756 |
| Ca | 24.871767 | 30.915182 | 27.704630 |
| Ca | 27.514540 | 32.668938 | 30.986839 |
| Ca | 29.151913 | 27.962847 | 29.825584 |
| Ca | 30.631775 | 32.386559 | 27.431437 |
| Ca | 30.454100 | 27.791157 | 24.754652 |
| Ca | 33.658718 | 30.013199 | 28.277767 |
| Ca | 34.469227 | 24.745390 | 26.902790 |
| Ca | 35.456913 | 28.880758 | 23.894314 |
| S  | 21.548061 | 31.509268 | 35.579914 |
| S  | 20.534691 | 35.652840 | 33.405128 |
| S  | 21.755733 | 31.715931 | 29.515499 |
| S  | 24.909634 | 33.288353 | 32.978447 |
| S  | 25.785702 | 29.456387 | 30.272614 |
| S  | 25.543224 | 34.242798 | 28.302240 |
| S  | 28.265961 | 29.678116 | 26.778496 |
| S  | 30.684040 | 31.252127 | 30.360882 |
| S  | 31.739872 | 27.020515 | 27.861126 |
|    | S        | 32.870014 | 30.957336 | 24.930012 |
|----|----------|-----------|-----------|-----------|
|    | S        | 33.389050 | 25.808437 | 23.711876 |
|    | S        | 36.319530 | 27.782122 | 27.019657 |

24

generated by VMD

|    | Ca       | 18.497353 | 32.897331 | 34.194302 |
|----|----------|-----------|-----------|-----------|
|    | Ca       | 23.173378 | 34.751060 | 35.738266 |
|    | Ca       | 23.269806 | 30.389709 | 32.809891 |
|    | Ca       | 22.597288 | 34.784985 | 30.624449 |
|    | Ca       | 24.950081 | 30.632021 | 27.893007 |
|    | Ca       | 27.712584 | 32.791924 | 31.039562 |
|    | Ca       | 29.014235 | 27.901817 | 29.842073 |
|    | Ca       | 30.545321 | 32.372929 | 27.333424 |
|    | Ca       | 30.743046 | 27.910025 | 24.440071 |
|    | Ca       | 33.553375 | 29.800930 | 28.290154 |
|    | Ca       | 34.401440 | 24.844967 | 26.875259 |
|    | Ca       | 35.662319 | 28.810307 | 23.755119 |
|    | S        | 21.373562 | 31.691719 | 35.425449 |
|    | S        | 20.506992 | 35.729935 | 33.394127 |
|    | S        | 21.760107 | 31.397158 | 29.598654 |
|    | S        | 24.744286 | 33.459797 | 33.095493 |
|    | S        | 26.018066 | 29.611383 | 30.801735 |
|    | S        | 25.567595 | 34.109367 | 28.574516 |
|    | S        | 28.271767 | 29.689140 | 26.747234 |
|    | S        | 30.686975 | 31.094831 | 30.253304 |
|    | S        | 31.660995 | 26.822582 | 27.646164 |
|    | S        | 32.879147 | 30.953671 | 25.036737 |
|    | S        | 33.648735 | 26.030125 | 23.590858 |
|    | S        | 36.478954 | 27.822330 | 26.940182 |

24

generated by VMD

|    | Ca       | 18.688356 | 32.925522 | 33.874039 |
|----|----------|-----------|-----------|-----------|
|    | Ca       | 23.121490 | 34.883682 | 35.889759 |
|    | Ca       | 23.417641 | 30.355255 | 32.876942 |
|    | Ca       | 22.732969 | 34.699127 | 30.821476 |
|    | Ca       | 24.979103 | 30.526093 | 27.789774 |
|    | Ca       | 27.453800 | 32.746574 | 30.870348 |
|    | Ca       | 29.185997 | 27.855011 | 29.950565 |
|    | Ca       | 30.595152 | 32.476124 | 27.405254 |
|    | Ca       | 30.423841 | 27.879421 | 24.614744 |
|    | Ca       | 33.599380 | 29.690994 | 28.013309 |
|    | Ca       | 34.496288 | 24.804655 | 26.815041 |
|    | Ca       | 35.665638 | 29.108435 | 23.937021 |
|    | S        | 21.232124 | 31.803003 | 35.620068 |
|    | S        | 20.545200 | 35.822762 | 33.343361 |
|    | S        | 21.843725 | 31.536358 | 29.479443 |
|  |  |  |  |
|---|---|---|---|
| S | 24.799206 | 33.240402 | 33.199589 |
| S | 26.190353 | 29.443245 | 30.632996 |
| S | 25.441214 | 34.051701 | 28.239393 |
| S | 28.188080 | 29.599007 | 26.856192 |
| S | 30.904173 | 31.191578 | 30.310877 |
| S | 31.484911 | 26.749596 | 27.666618 |
| S | 32.638363 | 30.864054 | 25.017300 |
| S | 33.573689 | 26.267298 | 23.640564 |
| S | 36.519352 | 27.784641 | 27.075390 |

24 generated by VMD

| Ca | 18.343922 | 32.611469 | 33.910954 |
| Ca | 22.786566 | 34.864017 | 35.649551 |
| Ca | 33.570059 | 30.531532 | 32.999126 |
| Ca | 22.905712 | 34.560776 | 30.645552 |
| Ca | 25.269508 | 30.699291 | 27.873402 |
| Ca | 27.697689 | 32.858921 | 31.226990 |
| Ca | 28.886368 | 28.129875 | 29.869535 |
| Ca | 30.773396 | 32.589035 | 27.539381 |
| Ca | 30.396152 | 27.734962 | 24.649853 |
| Ca | 33.481026 | 29.855236 | 28.065109 |
| Ca | 34.216152 | 24.889149 | 26.933270 |
| Ca | 35.635731 | 28.935007 | 23.844385 |
| S | 21.326530 | 31.657303 | 35.608437 |
| S | 20.303385 | 35.456821 | 33.079391 |
| S | 22.058220 | 31.416523 | 29.596401 |
| S | 25.094429 | 33.410011 | 33.296539 |
| S | 26.111742 | 29.660013 | 30.748371 |
| S | 25.783230 | 34.107151 | 28.501945 |
| S | 28.311909 | 29.938805 | 26.713085 |
| S | 30.826727 | 31.118549 | 30.140327 |
| S | 31.428949 | 26.856911 | 27.789188 |
| S | 32.599213 | 30.679441 | 24.936024 |
| S | 33.496151 | 25.953634 | 23.473305 |
| S | 36.415257 | 27.785595 | 26.849878 |

24 generated by VMD

| Ca | 18.422670 | 32.650879 | 34.251495 |
| Ca | 23.206421 | 34.981407 | 35.654385 |
| Ca | 23.309017 | 30.451473 | 32.880352 |
| Ca | 22.625330 | 34.513985 | 30.568254 |
| Ca | 25.033365 | 30.672047 | 27.979160 |
| Ca | 27.739464 | 32.628494 | 30.983433 |
| Ca | 29.069304 | 28.088398 | 29.903732 |
| Ca | 30.677576 | 32.520950 | 27.363152 |
| Ca | 30.456758 | 28.354713 | 24.594490 |
|   | Ca   | S         | S         |
|---|------|-----------|-----------|
|   |      |           |           |
| Ca| 33.511471 | 29.775955 | 28.082214 |
| Ca| 34.143269 | 24.802759 | 26.864441 |
| Ca| 35.728958 | 28.806578 | 24.086634 |
| S | 21.479300 | 31.760685 | 35.576103 |
| S | 20.441813 | 35.482193 | 33.226021 |
| S | 21.930502 | 31.312237 | 29.663582 |
| S | 25.016937 | 33.287949 | 33.114479 |
| S | 25.903780 | 29.395164 | 30.602737 |
| S | 25.581028 | 34.009472 | 28.317938 |
| S | 28.221233 | 30.009111 | 26.641808 |
| S | 30.989700 | 31.216415 | 30.153915 |
| S | 31.362598 | 27.081181 | 27.597713 |
| S | 33.020836 | 30.913391 | 24.908159 |
| S | 33.502739 | 26.078667 | 23.682873 |
| S | 36.345963 | 27.505993 | 27.242958 |

24 generated by VMD

|   | Ca   | S         | S         |
|---|------|-----------|-----------|
|   |      |           |           |
| Ca| 18.480082 | 32.693405 | 33.852379 |
| Ca| 23.051939 | 34.879990 | 35.747746 |
| Ca| 23.434864 | 30.319416 | 33.025345 |
| Ca| 22.813770 | 34.763626 | 30.364246 |
| Ca| 25.100321 | 30.586663 | 28.117914 |
| Ca| 27.615482 | 32.677193 | 31.137363 |
| Ca| 28.965662 | 27.850597 | 29.679699 |
| Ca| 30.522907 | 32.389793 | 27.495270 |
| Ca| 30.389534 | 28.006872 | 24.501633 |
| Ca| 33.472015 | 29.761400 | 28.208740 |
| Ca| 34.305546 | 24.841528 | 26.759472 |
| Ca| 35.803719 | 32.904200 | 23.938320 |
| S | 21.476555 | 31.727352 | 35.760254 |
| S | 20.545189 | 35.779919 | 33.083363 |
| S | 21.961878 | 31.340969 | 30.008041 |
| S | 25.096786 | 33.604053 | 33.003517 |
| S | 26.100986 | 32.401217 | 30.644228 |
| S | 25.552244 | 33.979599 | 28.173294 |
| S | 28.205902 | 29.702869 | 26.659954 |
| S | 30.724895 | 31.017420 | 30.287672 |
| S | 31.570103 | 27.034401 | 27.601883 |
| S | 32.731983 | 30.750437 | 25.173716 |
| S | 33.484890 | 26.362522 | 23.482336 |
| S | 36.312763 | 27.735582 | 27.233641 |

24 generated by VMD

|   | Ca   | S         | S         |
|---|------|-----------|-----------|
|   |      |           |           |
| Ca| 18.636335 | 32.643585 | 33.948612 |
| Ca| 22.990685 | 35.010605 | 35.645473 |
| Ca| 23.302250 | 30.388058 | 33.175034 |
|   |   |   |
|---|---|---|
| Ca | 22.689550 | 34.766899 | 30.421478 |
| Ca | 25.266834 | 30.504431 | 28.041473 |
| Ca | 27.617556 | 32.833939 | 30.837879 |
| Ca | 28.909845 | 27.813059 | 29.779434 |
| Ca | 30.695833 | 32.261715 | 27.505884 |
| Ca | 30.540531 | 28.112267 | 24.449684 |
| Ca | 33.650894 | 29.776070 | 28.189327 |
| Ca | 34.180592 | 24.938610 | 26.584240 |
| Ca | 35.649002 | 29.139217 | 24.040474 |
| S  | 21.296581 | 31.867405 | 35.281281 |
| S  | 20.452888 | 35.531872 | 33.130306 |
| S  | 22.060808 | 31.457003 | 29.847393 |
| S  | 24.894482 | 33.517002 | 33.212509 |
| S  | 26.080578 | 29.483738 | 30.931911 |
| S  | 25.562672 | 33.940979 | 28.113029 |
| S  | 28.12253 | 29.663185 | 26.835552 |
| S  | 30.810038 | 30.964874 | 30.251457 |
| S  | 31.533825 | 26.962839 | 27.508915 |
| S  | 32.892376 | 30.796516 | 25.136879 |
| S  | 33.479286 | 26.364674 | 23.455624 |
| S  | 36.404404 | 27.561493 | 27.145172 |

24
generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.442654 | 32.780075 | 33.985901 |
| Ca | 23.094982 | 35.327297 | 35.411530 |
| Ca | 23.719692 | 30.415321 | 33.056717 |
| Ca | 22.640675 | 34.578575 | 30.594353 |
| Ca | 24.991768 | 30.363304 | 28.013493 |
| Ca | 27.489002 | 32.513954 | 31.155411 |
| Ca | 29.045521 | 27.850677 | 29.799191 |
| Ca | 30.762732 | 32.496227 | 27.404827 |
| Ca | 30.634781 | 28.067528 | 24.531227 |
| Ca | 33.382347 | 29.677765 | 28.108795 |
| Ca | 33.982498 | 24.703091 | 26.479496 |
| Ca | 35.835262 | 29.188507 | 24.248177 |
| S  | 21.675892 | 32.033234 | 35.704006 |
| S  | 20.165253 | 35.456963 | 32.975384 |
| S  | 22.097126 | 31.231483 | 29.913015 |
| S  | 25.017508 | 33.692459 | 33.115242 |
| S  | 26.040689 | 29.314911 | 30.746094 |
| S  | 25.551382 | 33.864197 | 28.492126 |
| S  | 28.308468 | 29.743126 | 26.686829 |
| S  | 30.653221 | 31.047817 | 30.361771 |
| S  | 31.463062 | 26.865093 | 27.546835 |
| S  | 32.909924 | 30.950634 | 25.095884 |
| S  | 33.545269 | 26.583942 | 23.337692 |
Ca       18.486584       32.651890       34.030540
Ca       23.142052       35.359295       34.996117
Ca       23.376377       30.168428       33.196182
Ca       22.763514       34.588760       30.534283
Ca       24.980900       30.500912       28.049225
Ca       27.643101       32.528946       31.019476
Ca       29.120213       27.944630       29.938808
Ca       30.583900       32.405045       27.751934
Ca       30.452374       28.299416       24.337738
Ca       33.608856       29.719416       28.133144
Ca       33.961319       24.725792       26.464497
Ca       35.715256       29.190044       24.129490
S        21.546892       32.076763       35.773167
S        20.295460       35.492287       32.723080
S        21.938854       31.308159       30.103228
S        24.990513       33.371117       33.071945
S        25.993397       29.440525       30.844082
S        25.602013       33.871918       28.341007
S        28.353638       29.845810       26.912441
S        30.888935       30.984608       30.415012
S        31.467564       26.825014       27.580799
S        32.897232       31.046917       25.343372
S        33.507629       26.418865       23.428091
S        36.403442       27.535500       26.822346

S        18.868395       32.574150       34.194096
Ca       22.838747       35.472179       35.644150
Ca       23.506060       30.477785       33.001640
Ca       22.710785       34.662853       30.340281
Ca       25.230520       30.560295       27.953808
Ca       27.539684       32.724453       31.127491
Ca       28.988224       27.875641       29.616089
Ca       30.448856       32.544865       27.477795
Ca       30.693529       28.205420       24.155712
Ca       33.367714       29.777536       28.269211
Ca       33.965954       24.703327       26.272427
Ca       35.865788       28.963661       24.599970
S        21.824501       31.972786       36.072578
S        20.261662       35.330338       32.926392
S        22.091242       31.108879       29.830238
S        24.883366       33.559906       33.137188
S        26.010696       29.275269       30.683960
|     |       |       |       |
|-----|-------|-------|-------|
| S   | 25.524792 | 33.950981 | 28.263765 |
| S   | 28.371527 | 29.786156 | 26.704456 |
| S   | 30.644236 | 31.170147 | 30.345697 |
| S   | 31.481117 | 26.797499 | 27.407921 |
| S   | 32.944126 | 30.939327 | 25.169386 |
| S   | 33.525005 | 26.397156 | 23.329891 |
| S   | 36.133438 | 27.469452 | 27.415924 |

24 generated by VMD

| Ca  | 18.626663 | 32.695469 | 34.092903 |
| Ca  | 23.023445 | 35.166145 | 35.367046 |
| Ca  | 23.617632 | 30.545456 | 33.230934 |
| Ca  | 22.597443 | 34.587051 | 30.207619 |
| Ca  | 25.194302 | 30.644920 | 28.017841 |
| Ca  | 27.446060 | 32.513786 | 31.156874 |
| Ca  | 28.953098 | 27.605637 | 29.823368 |
| Ca  | 30.639980 | 32.263565 | 27.705269 |
| Ca  | 30.612915 | 28.519562 | 24.501415 |
| Ca  | 33.634132 | 29.580378 | 28.622023 |
| Ca  | 34.196213 | 25.083981 | 26.419428 |
| Ca  | 35.544350 | 29.156090 | 23.799870 |
| S   | 21.721163 | 32.032379 | 35.794342 |
| S   | 20.286461 | 35.600677 | 32.862526 |
| S   | 22.216213 | 31.197784 | 29.807091 |
| S   | 24.978302 | 33.755997 | 32.938526 |
| S   | 25.923252 | 29.270880 | 30.665337 |
| S   | 25.660927 | 33.858498 | 28.295326 |
| S   | 28.220299 | 29.596676 | 26.828592 |
| S   | 30.635633 | 30.797253 | 30.480303 |
| S   | 31.529064 | 26.741243 | 27.629349 |
| S   | 32.852139 | 30.896351 | 25.500484 |
| S   | 33.174774 | 26.273632 | 23.300713 |
| S   | 36.435574 | 27.916618 | 26.892849 |

24 generated by VMD

| Ca  | 18.765453 | 32.776241 | 34.079552 |
| Ca  | 23.008114 | 35.082870 | 35.163170 |
| Ca  | 23.436510 | 30.130699 | 33.352341 |
| Ca  | 22.773674 | 34.563023 | 30.332529 |
| Ca  | 25.186668 | 30.531569 | 28.110764 |
| Ca  | 27.598240 | 32.759750 | 31.033609 |
| Ca  | 28.932251 | 27.743649 | 29.802938 |
| Ca  | 30.702085 | 32.281033 | 27.374447 |
| Ca  | 30.602268 | 28.510880 | 24.396564 |
| Ca  | 33.410774 | 29.664230 | 28.643559 |
| Ca  | 34.108761 | 24.880722 | 26.413952 |
Ca       35.661205       29.203831       23.867
S        21.559914       32.206734       35.926807
S        20.355392       35.692726       32.853653
S        22.095322       31.117554       29.933071
S        24.813087       33.389854       33.058144
S        26.079607       29.425505       30.791826
S        25.709185       33.856178       28.161362
S        28.128593       29.771446       26.915157
S        30.640369       30.927380       30.481461
S        31.628223       32.815395       27.747540
S        32.830135       30.769825       25.307770
S        33.512066       26.494841       23.013783
S        36.182178       27.704165       27.178230

24 generated by VMD
Ca       18.272087       33.044693       34.395813
Ca       23.193817       34.967247       35.583809
Ca       23.539278       30.293434       32.905098
Ca       22.717434       34.388435       30.523396
Ca       25.112083       30.668354       27.881172
Ca       27.390223       32.779049       30.994875
Ca       29.063011       27.773987       29.861013
Ca       30.740833       32.324482       27.391603
Ca       30.603292       28.358017       24.601685
Ca       33.647636       29.909065       28.456894
Ca       33.971909       24.746685       26.649130
Ca       35.771637       28.955544       23.939255
S        21.503452       31.895058       35.696587
S        20.380287       35.714935       33.116356
S        22.087959       31.174774       29.835049
S        24.898785       33.435192       33.067631
S        26.054064       29.348392       30.538929
S        25.360300       33.849594       28.130779
S        28.324341       29.718981       26.799650
S        30.718842       31.003647       30.211073
S        31.587185       26.965517       27.857006
S        33.191376       30.848255       25.150379
S        33.253258       26.413818       23.217102
S        36.336990       27.722942       27.135735

24 generated by VMD
Ca       18.535801       32.628220       33.944901
Ca       23.042206       34.998562       35.364616
Ca       23.603909       30.445114       33.152828
Ca       22.576471       34.616371       30.508081
Ca       24.959011       30.868206       28.031376
Ca 27.393738 32.699146 31.139315
Ca 29.203356 27.894363 29.860119
Ca 30.697887 28.305086 24.677116
Ca 33.973572 29.786896 27.979141
Ca 34.048309 24.653784 26.360107
Ca 35.678764 28.879248 24.107271
S 21.531614 31.987392 35.626671
S 20.215668 35.465332 33.007755
S 22.062197 31.101814 29.834953
S 24.957302 33.575684 33.046768
S 26.073267 29.515835 30.704786
S 25.351191 34.075180 28.325840
S 28.278954 29.759567 26.886118
S 30.731194 30.966782 30.555798
S 31.627779 26.968470 27.759743
S 32.956642 30.849194 25.327747
S 33.299797 26.300983 23.374434
S 36.530769 27.375463 26.898979

24 generated by VMD
Ca 18.302856 32.996597 34.098602
Ca 23.221359 35.065613 35.672661
Ca 23.407421 30.428818 33.039486
Ca 22.696056 34.102436 30.438681
Ca 25.327814 30.889275 28.052235
Ca 27.793751 32.924644 30.970284
Ca 29.060932 27.937916 29.887867
Ca 30.711117 32.390064 27.250648
Ca 30.491369 28.155985 24.567146
Ca 33.730183 29.794863 28.251783
Ca 34.070076 24.694807 26.546793
Ca 35.555252 29.079487 24.018738
S 21.270290 31.858482 35.710667
S 20.459167 35.456650 33.046181
S 21.925812 31.070847 29.725527
S 24.847187 33.143753 32.961330
S 26.014992 29.629845 30.735481
S 25.599363 34.087460 28.331627
S 28.354027 29.751064 26.807125
S 30.747444 31.094706 30.246948
S 31.606022 26.860394 27.941090
S 32.969467 30.774925 25.267292
S 33.267399 26.396399 23.393383
S 36.290710 27.715042 26.978470

24
| Element | X1  | Y1  | Z1  |
|---------|-----|-----|-----|
| Ca      | 18.052719 | 33.487984 | 33.782215 |
| Ca      | 23.006203  | 35.342377  | 35.571190  |
| Ca      | 23.468412  | 30.415958  | 33.372879  |
| Ca      | 22.644718  | 33.721886  | 30.379356  |
| Ca      | 25.121731  | 30.859020  | 28.355146  |
| Ca      | 27.677965  | 32.725834  | 31.143297  |
| Ca      | 29.146406  | 27.876591  | 29.991474  |
| Ca      | 30.748154  | 32.195282  | 27.536213  |
| Ca      | 30.611540  | 28.305925  | 24.535339  |
| Ca      | 33.809990  | 29.904091  | 28.359819  |
| Ca      | 34.137589  | 24.782412  | 26.173853  |
| Ca      | 35.817432  | 29.019764  | 23.639942  |
| S       | 21.059368  | 32.114956  | 35.647285  |
| S       | 20.528536  | 35.498253  | 32.69705   |
| S       | 21.904930  | 30.955320  | 30.055889  |
| S       | 24.889965  | 33.191479  | 33.236225  |
| S       | 26.124784  | 29.546949  | 30.738682  |
| S       | 25.695082  | 33.917671  | 28.518965  |
| S       | 28.254557  | 29.573200  | 26.883257  |
| S       | 30.690269  | 30.897135  | 30.479403  |
| S       | 31.779110  | 27.009766  | 27.668461  |
| S       | 32.865707  | 30.904226  | 25.117542  |
| S       | 33.298187  | 26.353977  | 23.198723  |
| S       | 36.386673  | 27.699999  | 26.858189  |

24 generated by VMD

| Element | X1  | Y1  | Z1  |
|---------|-----|-----|-----|
| Ca      | 18.264561 | 33.074516 | 33.565929 |
| Ca      | 22.817770  | 35.135712  | 35.587025  |
| Ca      | 23.497543  | 30.352839  | 33.145840  |
| Ca      | 22.686581  | 34.373749  | 30.710018  |
| Ca      | 25.182415  | 30.847023  | 27.869591  |
| Ca      | 27.771032  | 32.746109  | 31.368080  |
| Ca      | 29.073418  | 27.908470  | 29.740498  |
| Ca      | 30.571451  | 32.442238  | 27.433197  |
| Ca      | 30.385263  | 27.798840  | 24.573132  |
| Ca      | 33.579449  | 29.995304  | 28.055580  |
| Ca      | 34.521965  | 24.868929  | 26.422649  |
| Ca      | 35.496628  | 28.874052  | 23.944153  |
| S       | 21.114403  | 31.869366  | 35.659760  |
| S       | 20.328468  | 35.699417  | 33.167847  |
| S       | 21.891214  | 31.239033  | 29.816517  |
| S       | 24.986040  | 33.302826  | 33.310272  |
| S       | 26.138382  | 29.465946  | 30.644003  |
| S       | 25.760696  | 34.194733  | 28.823967  |
| S       | 28.283552  | 29.665457  | 26.627554  |
S    30.861147   31.085299   30.207922
S    31.815151   26.774734   27.819895
S    32.700012   30.636524   25.108646
S    33.433266   25.980816   23.515495
S    36.559608   27.968117   26.830769
24
generated by VMD
Ca   18.207762   33.331249   33.643402
Ca   22.965977   35.159023   35.361286
Ca   23.342062   30.284046   33.298935
Ca   22.613457   34.577385   30.406460
Ca   25.293264   30.729397   28.327751
Ca   27.572956   32.636520   31.180363
Ca   29.264435   27.560730   29.806427
Ca   30.620193   32.353512   27.496502
Ca   30.344612   28.117580   24.946548
Ca   33.960426   29.812613   28.077164
Ca   34.307251   25.012323   26.214973
Ca   35.456879   29.197834   23.928127
S    21.122280   32.129234   35.550213
S    20.484375   35.770725   32.841770
S    22.175333   31.047264   30.057850
S    24.931637   33.284729   33.237587
S    26.129892   29.041113   30.749638
S    25.551842   33.628668   28.470526
S    28.385086   29.511677   26.947063
S    30.557867   30.909655   30.387674
S    31.928623   26.805573   27.795452
S    32.723545   30.750622   25.21202
S    33.126030   26.532028   23.312004
S    36.654285   27.782391   26.651184
24
generated by VMD
Ca   18.058990   32.950562   33.508308
Ca   22.828979   35.281517   35.465866
Ca   23.539370   30.222651   33.311939
Ca   22.753963   34.555260   30.453243
Ca   24.952480   30.748339   28.296764
Ca   27.698290   32.531883   31.285164
Ca   29.288841   27.798122   29.646328
Ca   30.722940   32.405270   27.532991
Ca   30.446411   28.145428   24.705153
Ca   33.932022   29.982061   27.920887
Ca   34.463276   24.751419   26.308624
Ca   35.563831   28.859898   23.744087
S    21.164618   31.970722   35.615700
|  |  |  |  |
|---|---|---|---|
| S  | 20.258961 | 35.826534 | 33.155876 |
| S  | 21.918528 | 31.215273 | 30.127636 |
| S  | 24.884411 | 33.505138 | 33.233070 |
| S  | 26.023190 | 29.274708 | 30.786606 |
| S  | 25.619452 | 33.968655 | 28.452091 |
| S  | 28.313480 | 29.760523 | 26.884254 |
| S  | 30.795170 | 30.987631 | 30.509768 |
| S  | 31.863169 | 26.913769 | 27.507082 |
| S  | 32.828541 | 30.833645 | 25.145144 |
| S  | 33.328842 | 26.076092 | 23.261250 |
| S  | 36.472336 | 27.734947 | 27.081930 |

24

generated by VMD

| Ca  | 18.242741 | 33.272217 | 33.714668 |
| Ca  | 23.003666 | 35.329475 | 35.222923 |
| Ca  | 23.510368 | 30.162405 | 33.467094 |
| Ca  | 22.546810 | 34.193584 | 30.405516 |
| Ca  | 25.092373 | 30.556572 | 28.300774 |
| Ca  | 27.588524 | 32.853642 | 31.213127 |
| Ca  | 29.207180 | 27.677773 | 29.793461 |
| Ca  | 30.616756 | 32.367672 | 27.797434 |
| Ca  | 30.606699 | 28.351669 | 24.483086 |
| Ca  | 33.729362 | 29.668543 | 28.247087 |
| Ca  | 34.389515 | 24.945776 | 25.858057 |
| Ca  | 35.719688 | 29.028152 | 23.959549 |
| S   | 21.043503 | 32.287308 | 35.684723 |
| S   | 20.413418 | 35.969791 | 32.848103 |
| S   | 21.824291 | 30.847687 | 30.392418 |
| S   | 24.790958 | 33.348221 | 33.080910 |
| S   | 26.109846 | 29.385923 | 30.982140 |
| S   | 25.569687 | 33.746758 | 28.340874 |
| S   | 28.344837 | 29.695406 | 26.912971 |
| S   | 30.830021 | 30.913229 | 30.357124 |
| S   | 31.614040 | 26.680021 | 27.516445 |
| S   | 33.035973 | 30.828016 | 25.400047 |
| S   | 33.330738 | 26.459026 | 23.140396 |
| S   | 36.562351 | 27.731182 | 26.821156 |

24

generated by VMD

| Ca  | 18.279991 | 33.350658 | 33.676357 |
| Ca  | 22.978874 | 35.313866 | 35.265491 |
| Ca  | 23.471491 | 30.187672 | 33.318604 |
| Ca  | 22.471567 | 34.337036 | 30.431475 |
| Ca  | 25.104893 | 30.643139 | 28.554338 |
| Ca  | 27.602156 | 32.739658 | 31.164108 |
| Ca  | 29.334530 | 27.583178 | 30.111971 |
| Ca     | 30.785149 | 32.287819 | 27.734856 |
|--------|-----------|-----------|-----------|
| Ca     | 30.362923 | 28.229630 | 24.705688 |
| Ca     | 33.896484 | 29.641088 | 28.086609 |
| Ca     | 34.352325 | 24.854704 | 25.953506 |
| Ca     | 35.514404 | 29.359035 | 23.759741 |
| S      | 21.111347 | 32.096958 | 35.360214 |
| S      | 20.446167 | 35.985939 | 32.815205 |
| S      | 21.931522 | 30.943554 | 30.146973 |
| S      | 24.718473 | 33.553101 | 33.081524 |
| S      | 26.066711 | 29.253563 | 30.984501 |
| S      | 25.535778 | 33.661568 | 28.276417 |
| S      | 28.345556 | 29.576744 | 27.154690 |
| S      | 30.801762 | 30.869452 | 30.575693 |
| S      | 31.844849 | 26.706123 | 27.630772 |
| S      | 32.943817 | 30.736683 | 25.380783 |
| S      | 33.272087 | 26.616474 | 23.084766 |
| S      | 36.547203 | 27.772406 | 26.685715 |

24 generated by VMD

| Ca     | 18.669323 | 33.382175 | 34.252251 |
|--------|-----------|-----------|-----------|
| Ca     | 23.509087 | 35.126656 | 35.421391 |
| Ca     | 23.509155 | 30.335644 | 33.051006 |
| Ca     | 22.528210 | 34.627548 | 30.344139 |
| Ca     | 24.901039 | 30.325687 | 27.817467 |
| Ca     | 27.403095 | 32.312195 | 30.886669 |
| Ca     | 28.875174 | 27.516529 | 29.554440 |
| Ca     | 30.364214 | 32.371941 | 27.822174 |
| Ca     | 30.563049 | 28.019733 | 24.342178 |
| Ca     | 33.477158 | 29.790781 | 28.487667 |
| Ca     | 34.546894 | 25.088821 | 26.389442 |
| Ca     | 35.528099 | 29.544992 | 24.370113 |
| S      | 21.742775 | 32.191383 | 35.839008 |
| S      | 20.742311 | 36.061443 | 33.158020 |
| S      | 21.954920 | 31.071297 | 29.889698 |
| S      | 25.026150 | 33.403755 | 32.728760 |
| S      | 25.846533 | 29.037109 | 30.401882 |
| S      | 25.274075 | 33.684753 | 28.195004 |
| S      | 28.209967 | 29.689816 | 26.717976 |
| S      | 30.508463 | 30.642233 | 30.525431 |
| S      | 31.717964 | 26.734692 | 27.575003 |
| S      | 32.737267 | 30.761726 | 25.637470 |
| S      | 33.573055 | 26.592808 | 23.318722 |
| S      | 36.512020 | 27.986324 | 27.214100 |

24 generated by VMD

| Ca     | 18.687174 | 33.131989 | 34.096741 |
|   |   |   |   |
|---|---|---|---|
| Ca | 23.568102 | 34.861912 | 35.121395 |
| Ca | 23.570930 | 30.427731 | 33.069748 |
| Ca | 22.486599 | 34.763130 | 30.541666 |
| Ca | 24.883982 | 27.481447 | 29.604595 |
| Ca | 27.419010 | 30.333607 | 28.134525 |
| Ca | 30.428852 | 32.77649  | 30.851666 |
| Ca | 33.577618 | 29.822424 | 28.339184 |
| Ca | 34.422909 | 24.911781 | 26.437710 |
| Ca | 35.790031 | 29.312191 | 24.415943 |
| Ca | 33.09580 | 28.418266 | 24.490330 |
| S  | 21.624651 | 32.128536 | 35.742828 |
| S  | 20.625355 | 35.901703 | 33.291862 |
| S  | 21.939167 | 31.244793 | 30.097099 |
| S  | 25.036148 | 33.501122 | 32.751266 |
| S  | 25.941118 | 29.014736 | 30.532557 |
| S  | 25.347250 | 33.823647 | 28.137768 |
| S  | 28.139580 | 29.638840 | 26.761934 |
| S  | 30.588181 | 30.708401 | 30.134502 |
| S  | 31.598764 | 26.848824 | 27.541412 |
| S  | 32.882336 | 30.948345 | 25.407923 |
| S  | 33.454163 | 26.700373 | 23.458603 |
| S  | 36.431767 | 27.783928 | 27.565035 |

24

generated by VMD

| Ca | 18.328815 | 33.112499 | 34.182846 |
| Ca | 23.261440 | 35.182976 | 35.150196 |
| Ca | 23.714724 | 30.244764 | 33.085434 |
| Ca | 22.512129 | 34.467701 | 30.554987 |
| Ca | 24.906227 | 30.539913 | 28.064350 |
| Ca | 27.461597 | 32.702133 | 30.912243 |
| Ca | 29.024403 | 27.490995 | 29.628941 |
| Ca | 30.695450 | 32.435642 | 27.735895 |
| Ca | 30.412281 | 28.228436 | 24.454844 |
| Ca | 33.670731 | 29.760399 | 28.482458 |
| Ca | 34.453224 | 25.066113 | 26.266968 |
| Ca | 35.677895 | 28.920116 | 23.997183 |
| S  | 21.446976 | 31.971182 | 35.502609 |
| S  | 20.545570 | 36.010433 | 33.347984 |
| S  | 21.908176 | 31.214489 | 29.847336 |
| S  | 25.000847 | 33.445946 | 32.986282 |
| S  | 25.929237 | 29.219372 | 30.550659 |
| S  | 25.536350 | 33.824631 | 28.277109 |
| S  | 28.305740 | 29.630831 | 26.876881 |
| S  | 30.545666 | 30.750603 | 30.520691 |
| S  | 31.763161 | 26.811960 | 27.651922 |
|   |               |               |               |
|---|---------------|---------------|---------------|
| S | 32.783669     | 30.851276     | 25.373436     |
| S | 33.339771     | 26.303864     | 23.380829     |
| S | 36.495911     | 28.113720     | 27.107933     |

24 generated by VMD

| Ca       |               |               |               |
|----------|---------------|---------------|---------------|
| Ca       | 18.174427     | 33.139133     | 34.039444     |
| Ca       | 23.448915     | 34.650246     | 35.549416     |
| Ca       | 23.626671     | 30.438292     | 33.084373     |
| Ca       | 22.464941     | 34.694790     | 30.587835     |
| Ca       | 25.023375     | 30.552467     | 27.978493     |
| Ca       | 27.251354     | 32.620220     | 30.976395     |
| Ca       | 29.082596     | 27.774149     | 29.628887     |
| Ca       | 30.578703     | 32.473934     | 27.542099     |
| Ca       | 30.449421     | 28.192223     | 24.623772     |
| Ca       | 33.727795     | 29.981930     | 28.377693     |
| Ca       | 34.472023     | 24.764736     | 26.428879     |
| Ca       | 35.608238     | 28.983284     | 24.055222     |
| S        | 21.464775     | 31.944031     | 35.278896     |
| S        | 20.562799     | 35.801220     | 33.434494     |
| S        | 22.019083     | 31.192507     | 29.847685     |
| S        | 25.133411     | 33.632992     | 32.947865     |
| S        | 25.967066     | 29.252399     | 30.588449     |
| S        | 25.309341     | 33.902832     | 28.155827     |
| S        | 28.278557     | 29.761568     | 26.778624     |
| S        | 30.562258     | 30.929443     | 30.425930     |
| S        | 31.855154     | 26.922123     | 27.830149     |
| S        | 32.840740     | 30.780766     | 25.379841     |
| S        | 33.316540     | 26.109077     | 23.360573     |
| S        | 36.501831     | 27.805681     | 27.039200     |

24 generated by VMD

| Ca       |               |               |               |
|----------|---------------|---------------|---------------|
| Ca       | 18.371616     | 33.315758     | 34.165550     |
| Ca       | 22.987032     | 35.092682     | 35.558773     |
| Ca       | 23.514683     | 30.161726     | 33.098824     |
| Ca       | 22.810886     | 34.494007     | 30.471506     |
| Ca       | 24.937571     | 30.306694     | 27.987232     |
| Ca       | 27.607916     | 32.554443     | 30.934309     |
| Ca       | 29.250654     | 27.660416     | 29.745157     |
| Ca       | 30.638945     | 32.437996     | 27.728640     |
| Ca       | 30.342293     | 28.151449     | 24.538103     |
| Ca       | 33.537472     | 29.865341     | 28.353594     |
| Ca       | 34.485462     | 24.918200     | 26.160404     |
| Ca       | 35.543980     | 29.072647     | 24.069393     |
| S        | 21.065607     | 31.706860     | 35.399956     |
| S        | 20.611523     | 35.951118     | 32.897522     |
| S        | 22.058271     | 31.002100     | 30.077248     |
|     | X       | Y       | Z       |
|-----|---------|---------|---------|
| S   | 25.058521 | 33.698410 | 33.094017 |
| S   | 26.143759 | 29.262070 | 30.618084 |
| S   | 25.610455 | 33.891018 | 28.247318 |
| S   | 28.315763 | 29.836267 | 26.832680 |
| S   | 30.851196 | 30.960539 | 30.429134 |
| S   | 31.712263 | 26.970501 | 27.819176 |
| S   | 32.671658 | 30.792803 | 25.243038 |
| S   | 33.272091 | 26.334635 | 23.423222 |
| S   | 36.320427 | 27.862362 | 27.047199 |

24 generated by VMD

| Ca  | X       | Y       | Z       |
|-----|---------|---------|---------|
| Ca  | 17.996702 | 33.186855 | 33.764614 |
| Ca  | 22.710493 | 35.164268 | 35.764366 |
| Ca  | 23.553049 | 30.332432 | 33.039589 |
| Ca  | 22.725336 | 34.522774 | 30.632404 |
| Ca  | 25.119158 | 30.641123 | 27.997152 |
| Ca  | 27.778427 | 32.503155 | 31.273989 |
| Ca  | 29.129972 | 27.928238 | 29.852551 |
| Ca  | 30.613285 | 32.338348 | 27.298782 |
| Ca  | 30.446934 | 27.895962 | 24.704941 |
| Ca  | 33.690014 | 30.043842 | 28.354280 |
| Ca  | 34.386028 | 25.015068 | 26.378326 |
| Ca  | 35.388611 | 28.772171 | 23.781099 |
| S   | 21.011177 | 31.787254 | 35.410255 |
| S   | 20.526760 | 35.892326 | 33.186043 |
| S   | 22.038919 | 31.230335 | 29.807667 |
| S   | 24.931175 | 33.428471 | 33.457661 |
| S   | 26.027363 | 29.367773 | 30.767773 |
| S   | 25.736637 | 33.880051 | 28.370461 |
| S   | 28.533489 | 29.641537 | 26.846388 |
| S   | 30.916267 | 30.986956 | 30.375540 |
| S   | 31.894888 | 26.927490 | 27.830833 |
| S   | 32.697479 | 30.726419 | 25.135359 |
| S   | 33.462921 | 26.027121 | 23.154270 |
| S   | 36.404972 | 28.060131 | 26.755760 |

24 generated by VMD
|   |        |        |        |
|---|--------|--------|--------|
| Ca| 33.440662 | 29.804886 | 28.248215 |
| Ca| 34.264851 | 24.686632 | 26.591141 |
| Ca| 35.672592 | 29.112692 | 23.754536 |
| S | 21.100155 | 31.735306 | 35.434742 |
| S | 20.782419 | 35.577431 | 33.091728 |
| S | 22.098272 | 31.258034 | 29.894629 |
| S | 24.996040 | 33.367535 | 33.394791 |
| S | 26.264311 | 29.635326 | 30.826698 |
| S | 25.603903 | 33.943089 | 28.309723 |
| S | 28.279854 | 29.633984 | 26.691906 |
| S | 30.735178 | 31.103840 | 30.30417 |
| S | 31.663883 | 26.719227 | 27.770815 |
| S | 32.737400 | 30.854145 | 25.015045 |
| S | 33.554546 | 26.076380 | 23.407158 |
| S | 36.215050 | 27.957836 | 27.069506 |

24

generated by VMD

|   |        |        |        |
|---|--------|--------|--------|
| Ca| 18.256849 | 32.907902 | 33.484657 |
| Ca| 22.779461 | 35.112076 | 35.914783 |
| Ca| 23.611158 | 30.141171 | 33.153687 |
| Ca| 22.935059 | 34.952583 | 30.478378 |
| Ca| 25.173271 | 30.488205 | 28.269232 |
| Ca| 27.663025 | 32.647923 | 30.993504 |
| Ca| 29.151327 | 27.894341 | 29.734514 |
| Ca| 30.594530 | 32.573887 | 27.438885 |
| Ca| 30.275204 | 28.042458 | 24.606983 |
| Ca| 33.700191 | 29.950327 | 28.113129 |
| Ca| 34.271431 | 24.769051 | 26.657745 |
| Ca| 35.603722 | 29.030891 | 23.962210 |
| S | 21.096909 | 31.690596 | 35.455856 |
| S | 20.465448 | 35.776382 | 33.064743 |
| S | 22.05187 | 31.262360 | 29.995947 |
| S | 25.021317 | 33.390823 | 33.204716 |
| S | 26.215021 | 29.327587 | 30.934021 |
| S | 25.652470 | 33.874321 | 28.319139 |
| S | 28.172977 | 29.860001 | 26.832664 |
| S | 30.861319 | 31.004917 | 30.221500 |
| S | 31.710258 | 26.851944 | 27.689285 |
| S | 32.691944 | 30.777498 | 25.010399 |
| S | 33.246864 | 26.109940 | 23.461063 |
| S | 36.512100 | 27.862896 | 26.943007 |

24

generated by VMD

|   |        |        |        |
|---|--------|--------|--------|
| Ca| 18.241419 | 33.075653 | 33.821373 |
| Ca| 22.921896 | 34.952900 | 35.883331 |
| Ca| 23.256779 | 30.245346 | 33.050556 |
| Element | X Coordination | Y Coordination | Z Coordination |
|---------|----------------|----------------|----------------|
| Ca      | 22.779501      | 34.694889      | 30.542038      |
| Ca      | 25.142340      | 30.696274      | 28.075424      |
| Ca      | 27.579365      | 32.696709      | 30.946308      |
| Ca      | 29.041576      | 27.953087      | 29.772339      |
| Ca      | 30.647243      | 32.349930      | 27.281862      |
| Ca      | 30.392979      | 28.041313      | 24.470520      |
| Ca      | 33.833931      | 29.906147      | 28.323772      |
| Ca      | 34.358768      | 25.104115      | 26.569092      |
| Ca      | 35.619247      | 28.605755      | 23.698673      |
| S       | 21.021151      | 31.778229      | 35.615635      |
| S       | 20.573143      | 35.899357      | 33.385300      |
| S       | 21.982914      | 31.393337      | 30.019142      |
| S       | 24.828480      | 33.220432      | 33.199940      |
| S       | 26.162460      | 29.342209      | 30.823036      |
| S       | 25.587301      | 33.863995      | 28.324551      |
| S       | 28.168947      | 29.714237      | 26.688534      |
| S       | 30.789951      | 31.063728      | 30.150871      |
| S       | 31.810745      | 26.941055      | 27.694845      |
| S       | 32.872910      | 30.529287      | 24.937454      |
| S       | 33.554897      | 26.261898      | 23.317883      |
| S       | 36.552044      | 27.970192      | 27.347572      |

24 generated by VMD

| Element | X Coordination | Y Coordination | Z Coordination |
|---------|----------------|----------------|----------------|
| Ca      | 18.434187      | 33.445824      | 33.789978      |
| Ca      | 23.043154      | 34.722103      | 35.816093      |
| Ca      | 23.281277      | 30.145821      | 33.101936      |
| Ca      | 22.955198      | 34.602627      | 30.542938      |
| Ca      | 24.797377      | 30.704720      | 27.875956      |
| Ca      | 27.773956      | 32.647888      | 30.752645      |
| Ca      | 29.146631      | 27.851233      | 29.972116      |
| Ca      | 30.443016      | 32.327011      | 27.269360      |
| Ca      | 30.247532      | 27.983299      | 24.751411      |
| Ca      | 33.675236      | 29.838564      | 28.344944      |
| Ca      | 34.339870      | 25.129322      | 26.585670      |
| Ca      | 35.561852      | 29.189213      | 23.882217      |
| S       | 21.084259      | 31.619186      | 35.542694      |
| S       | 20.864759      | 35.912609      | 33.157036      |
| S       | 21.973167      | 31.285965      | 29.863770      |
| S       | 25.013882      | 33.164631      | 33.251171      |
| S       | 26.127737      | 29.497311      | 30.854160      |
| S       | 25.444159      | 33.678524      | 27.884264      |
| S       | 28.277386      | 29.647652      | 26.891747      |
| S       | 30.868980      | 31.098125      | 30.272259      |
| S       | 31.773973      | 26.805077      | 27.837326      |
| S       | 32.716503      | 30.592043      | 25.129793      |
| S       | 33.375420      | 26.488747      | 23.400579      |
|          |                  |                  |                  |
|----------|------------------|------------------|------------------|
| S        | 36.500477        | 27.922483        | 27.169983        |
| Ca       | 18.217121        | 33.376324        | 33.308670        |
| Ca       | 22.761190        | 34.734821        | 35.704632        |
| Ca       | 23.421276        | 30.188889        | 33.113705        |
| Ca       | 22.992210        | 34.565777        | 30.628780        |
| Ca       | 25.344530        | 30.537605        | 28.174879        |
| Ca       | 27.761467        | 32.856373        | 31.402161        |
| Ca       | 29.069178        | 27.853024        | 30.103775        |
| Ca       | 30.704548        | 32.552586        | 27.347466        |
| Ca       | 30.276976        | 27.853092        | 24.627296        |
| Ca       | 33.524963        | 30.001930        | 28.003874        |
| Ca       | 34.386890        | 24.831497        | 26.648365        |
| Ca       | 35.517799        | 29.150631        | 23.626755        |
| S        | 20.860193        | 31.595078        | 29.300732        |
| S        | 20.674099        | 36.054184        | 33.042534        |
| S        | 22.123159        | 31.201946        | 29.882137        |
| S        | 24.965034        | 33.292839        | 33.390316        |
| S        | 26.510967        | 29.466713        | 31.351528        |
| S        | 25.607763        | 33.569260        | 28.322153        |
| S        | 28.290560        | 29.711246        | 26.823202        |
| S        | 30.909843        | 31.065727        | 30.134794        |
| S        | 31.655991        | 26.923710        | 27.835327        |
| S        | 32.568287        | 30.786804        | 24.807583        |
| S        | 33.394985        | 26.195854        | 23.343212        |
| S        | 36.181011        | 27.934151        | 27.016171        |

24 generated by VMD

|          |                  |                  |                  |
|----------|------------------|------------------|------------------|
| Ca       | 18.514526        | 33.102692        | 33.527527        |
| Ca       | 22.912926        | 34.541996        | 35.739559        |
| Ca       | 23.467894        | 30.258457        | 33.202415        |
| Ca       | 23.061773        | 34.606258        | 30.608133        |
| Ca       | 24.962347        | 30.831936        | 27.953381        |
| Ca       | 27.727932        | 32.749977        | 31.085806        |
| Ca       | 28.924654        | 27.804790        | 29.821838        |
| Ca       | 30.606182        | 32.428078        | 27.183737        |
| Ca       | 30.236668        | 28.071342        | 24.704762        |
| Ca       | 33.693687        | 30.052135        | 28.105482        |
| Ca       | 34.549065        | 24.872410        | 26.854691        |
| Ca       | 35.475182        | 28.981548        | 23.810997        |
| S        | 21.130615        | 31.534794        | 35.367821        |
| S        | 20.614727        | 35.756081        | 33.127014        |
| S        | 22.056503        | 31.483780        | 29.963423        |
| S        | 25.003212        | 33.305634        | 33.358986        |
| S        | 26.081856        | 29.481049        | 30.844612        |
|  | X      | Y      | Z      |
|---|--------|--------|--------|
| S | 25.781723 | 33.886860 | 28.249123 |
| S | 28.150169 | 29.805649 | 26.742203 |
| S | 30.688139 | 31.064016 | 30.048212 |
| S | 31.699158 | 26.977997 | 27.837112 |
| S | 32.749321 | 30.746273 | 25.020851 |
| S | 33.206120 | 31.064016 | 30.048212 |
| S | 36.425697 | 27.996603 | 27.046936 |

24 generated by VMD

| Ca  | X      | Y      | Z      |
|-----|--------|--------|--------|
| Ca  | 18.455521 | 33.041897 | 33.645893 |
| Ca  | 22.818016 | 34.612312 | 35.770817 |
| Ca  | 23.414654 | 30.043430 | 33.182125 |
| Ca  | 22.858137 | 34.722805 | 30.435268 |
| Ca  | 25.137964 | 30.639648 | 28.236906 |
| Ca  | 27.651691 | 32.888660 | 31.112535 |
| Ca  | 28.965836 | 27.762407 | 29.623260 |
| Ca  | 30.674530 | 32.379257 | 27.307581 |
| Ca  | 30.303669 | 28.056446 | 24.631153 |
| Ca  | 33.688457 | 30.024479 | 28.047157 |
| Ca  | 34.241688 | 24.912804 | 26.664658 |
| Ca  | 35.626785 | 28.929243 | 23.802261 |
| S   | 21.245369 | 31.529697 | 35.314690 |
| S   | 20.642906 | 35.949402 | 33.264870 |
| S   | 22.051140 | 31.296259 | 30.057861 |
| S   | 24.921673 | 33.483559 | 33.001881 |
| S   | 26.119146 | 29.402416 | 30.873837 |
| S   | 25.714390 | 34.017578 | 28.270258 |
| S   | 28.137211 | 29.784351 | 26.806149 |
| S   | 30.757055 | 31.105900 | 30.162867 |
| S   | 31.737999 | 27.049644 | 27.869678 |
| S   | 32.841667 | 30.746601 | 25.103844 |
| S   | 33.311993 | 26.096657 | 23.760492 |
| S   | 36.402420 | 27.824543 | 26.989441 |

24 generated by VMD

| Ca  | X      | Y      | Z      |
|-----|--------|--------|--------|
| Ca  | 18.268650 | 33.426792 | 33.784882 |
| Ca  | 22.872677 | 34.743084 | 35.483006 |
| Ca  | 23.352863 | 30.068584 | 33.024536 |
| Ca  | 22.717655 | 34.667419 | 30.619102 |
| Ca  | 25.079165 | 30.818016 | 28.188002 |
| Ca  | 27.843967 | 32.577442 | 30.998192 |
| Ca  | 29.240803 | 27.729836 | 30.020054 |
| Ca  | 30.682671 | 32.451118 | 27.232037 |
| Ca  | 30.257902 | 27.878677 | 24.668045 |
| Ca  | 33.863609 | 29.724533 | 28.186556 |
| Ca  | 34.551113 | 25.145737 | 26.392885 |
| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 35.313480 | 28.940083 | 24.009789 |
| S       | 20.865971  | 31.604944  | 35.289810  |
| S       | 20.404274  | 36.032356  | 33.086143  |
| S       | 21.978333  | 31.323910  | 29.943651  |
| S       | 24.938887  | 33.360153  | 33.274185  |
| S       | 26.309343  | 29.305391  | 30.935020  |
| S       | 25.706408  | 33.794750  | 28.369675  |
| S       | 28.260775  | 29.728329  | 27.039036  |
| S       | 31.088800  | 31.100071  | 30.245579  |
| S       | 31.864807  | 26.895124  | 27.730450  |
| S       | 32.579479  | 30.742100  | 25.050941  |
| S       | 33.128944  | 26.167971  | 23.489479  |
| S       | 36.549450  | 28.073620  | 26.879036  |

24

Generated by VMD

| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 18.364071 | 33.629208 | 33.807816 |
| Ca      | 23.018032 | 34.634983 | 35.700272 |
| Ca      | 23.415380 | 30.078583 | 33.184097 |
| Ca      | 22.675713 | 34.472824 | 30.756907 |
| Ca      | 25.125711 | 30.707104 | 28.068752 |
| Ca      | 27.648361 | 32.607006 | 31.019207 |
| Ca      | 28.765627 | 28.011173 | 29.475441 |
| Ca      | 30.659708 | 32.572216 | 26.925175 |
| Ca      | 30.444174 | 27.976650 | 24.814262 |
| Ca      | 33.958313 | 30.080658 | 27.844076 |
| Ca      | 34.346775 | 24.883949 | 26.871544 |
| Ca      | 35.947617 | 28.825630 | 23.948982 |
| S       | 21.060501 | 31.635288 | 35.274570 |
| S       | 20.781109 | 35.969349 | 33.521862 |
| S       | 21.849649 | 31.070820 | 29.985760 |
| S       | 25.025280 | 33.147034 | 33.272560 |
| S       | 25.922867 | 29.342512 | 30.768555 |
| S       | 25.447208 | 33.941586 | 28.244713 |
| S       | 28.012253 | 29.974323 | 26.615917 |
| S       | 30.649578 | 31.012264 | 29.987650 |
| S       | 31.842346 | 26.909758 | 27.942963 |
| S       | 32.912418 | 30.642925 | 25.052059 |
| S       | 33.239746 | 26.238117 | 23.633255 |
| S       | 36.607529 | 27.936066 | 27.223690 |

24

Generated by VMD

| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 18.651230 | 33.998714 | 33.527306 |
| Ca      | 23.386398 | 34.594120 | 35.829300 |
| Ca      | 23.391636 | 30.059534 | 33.119446 |
| Ca      | 22.557953 | 34.664841 | 30.866219 |
| Ca      | 24.788040 | 30.686773 | 28.047157 |
|    |      |      |      |
|----|------|------|------|
| Ca | 27.583458 | 32.628479 | 31.138435 |
| Ca | 29.122084 | 27.538549 | 29.498966 |
| Ca | 30.546513 | 32.180294 | 27.147163 |
| Ca | 30.464310 | 27.903053 | 24.582670 |
| Ca | 33.750874 | 30.138962 | 28.461870 |
| Ca | 34.766640 | 25.222908 | 26.654793 |
| Ca | 35.632427 | 29.053947 | 24.04193 |
| S  | 20.908957 | 31.783257 | 35.239212 |
| S  | 20.893700 | 36.048397 | 33.698006 |
| S  | 21.834354 | 31.070147 | 29.873457 |
| S  | 24.843990 | 33.368908 | 33.159737 |
| S  | 26.008640 | 29.298584 | 30.787701 |
| S  | 25.268919 | 33.861889 | 28.311745 |
| S  | 28.241137 | 29.467264 | 26.515581 |
| S  | 30.40734 | 30.917271 | 29.992016 |
| S  | 32.045921 | 27.181931 | 27.814415 |
| S  | 32.699192 | 30.420593 | 25.080395 |
| S  | 33.491539 | 26.156668 | 23.262623 |
| S  | 36.437405 | 28.054974 | 27.287594 |

24

generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 18.536070 | 33.622498 | 33.246231 |
| Ca | 23.147476 | 34.761078 | 35.762077 |
| Ca | 23.315466 | 30.181753 | 33.321491 |
| Ca | 22.885784 | 34.541367 | 30.437393 |
| Ca | 25.195286 | 30.145300 | 28.275982 |
| Ca | 27.681587 | 32.507072 | 31.157120 |
| Ca | 29.111816 | 27.782785 | 29.946793 |
| Ca | 30.384167 | 32.566643 | 27.517330 |
| Ca | 30.525721 | 28.091427 | 24.394497 |
| Ca | 33.575512 | 30.149181 | 28.279306 |
| Ca | 34.427643 | 24.945770 | 26.313244 |
| Ca | 35.432323 | 29.076138 | 23.923752 |
| S  | 20.978912 | 32.008751 | 35.540001 |
| S  | 20.829174 | 35.926460 | 32.962082 |
| S  | 22.085678 | 30.906448 | 30.034649 |
| S  | 24.755980 | 33.498566 | 33.135529 |
| S  | 26.174524 | 29.163559 | 30.999928 |
| S  | 25.757925 | 33.764023 | 28.427633 |
| S  | 28.187023 | 29.552015 | 26.844166 |
| S  | 30.705395 | 31.064381 | 30.257547 |
| S  | 31.722855 | 26.965290 | 27.782726 |
| S  | 32.742157 | 30.948296 | 25.114948 |
| S  | 33.440460 | 26.288399 | 23.123899 |
| S  | 36.121208 | 27.842884 | 27.138077 |
generated by VMD

Ca  18.276543  33.057079  33.765480
Ca  23.202141  34.469128  35.944546
Ca  23.383332  30.442537  32.843365
Ca  22.921394  34.515495  30.817368
Ca  24.805563  30.642586  28.013960
Ca  27.673685  32.902237  31.012703
Ca  28.799597  27.865747  29.641647
Ca  30.509478  32.267967  27.153961
Ca  30.446690  27.977760  24.710217
Ca  33.740517  30.276649  28.173542
Ca  34.464550  24.967188  26.830446
Ca  35.769089  28.655666  23.937588
S   21.106937  31.412979  35.420532
S   20.853718  35.690941  33.517822
S   21.914539  31.176601  29.756927
S   24.898680  33.761677  33.050865
S   26.203318  29.905622  30.665987
S   25.548710  34.180946  28.347370
S   28.023647  29.704798  26.715282
S   30.824982  30.936264  30.132202
S   31.687668  26.952950  27.706284
S   32.826318  30.627270  24.923353
S   33.495762  26.087200  23.468658
S   36.338169  27.822744  27.389977

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generated by VMD

Ca  18.278008  33.369556  33.441860
Ca  23.001207  34.386726  35.698860
Ca  23.493624  30.476789  33.049004
Ca  22.806873  34.426544  30.920874
Ca  24.963055  30.633667  28.097000
Ca  27.816143  32.714432  31.171036
Ca  29.057377  27.923218  29.790520
Ca  30.462980  32.506115  27.311258
Ca  30.429781  27.813972  24.565084
Ca  33.646538  30.119637  27.811446
Ca  34.555824  24.872894  26.772806
Ca  35.714230  28.971172  23.988363
S   21.061695  31.524754  35.355171
S   20.670174  35.846596  33.392838
S   21.957674  31.340786  29.987148
S   24.965975  33.645565  33.018478
S   26.155571  29.528149  30.779222
S   25.668880  34.012733  28.556581
S   28.031931  29.717464  26.706003
|   |   |   |   |
|---|---|---|---|
| S | 30.846031 | 31.034889 | 30.027004 |
| S | 31.698994 | 26.886353 | 27.716959 |
| S | 32.634655 | 30.631645 | 24.893929 |
| S | 34.75948 | 25.937222 | 23.485424 |
| S | 36.326851 | 27.979143 | 27.303158 |

24

-generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 18.435316 | 33.081833 | 33.445030 |
| Ca | 22.925501 | 34.861603 | 36.000072 |
| Ca | 23.373840 | 30.457397 | 32.952835 |
| Ca | 22.850510 | 34.513336 | 30.806955 |
| Ca | 25.060743 | 30.561047 | 28.200275 |
| Ca | 27.869419 | 32.771313 | 31.272614 |
| Ca | 29.076864 | 27.783464 | 29.922497 |
| Ca | 30.505854 | 32.395172 | 27.004101 |
| Ca | 30.40023 | 27.980293 | 24.416080 |
| Ca | 33.592411 | 30.161358 | 28.040510 |
| Ca | 34.398224 | 24.907089 | 26.543371 |
| Ca | 35.882404 | 28.866348 | 23.940990 |
| S | 20.893240 | 31.720852 | 35.441433 |
| S | 20.597622 | 35.852776 | 33.377869 |
| S | 21.821791 | 31.238997 | 29.801699 |
| S | 24.792038 | 33.683346 | 33.061390 |
| S | 26.089172 | 29.277882 | 30.855070 |
| S | 25.733490 | 34.002357 | 28.646338 |
| S | 28.170973 | 29.593655 | 26.860115 |
| S | 30.911835 | 30.986599 | 30.160221 |
| S | 31.749971 | 26.981985 | 27.769934 |
| S | 32.687103 | 30.661022 | 24.818378 |
| S | 33.527283 | 26.121304 | 23.419380 |
| S | 36.374321 | 27.839029 | 27.182892 |

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-generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 18.373117 | 32.702969 | 34.023544 |
| Ca | 23.100945 | 34.451149 | 36.027863 |
| Ca | 23.316288 | 30.559597 | 32.799610 |
| Ca | 22.954525 | 34.717636 | 30.814867 |
| Ca | 25.201401 | 30.981846 | 28.007591 |
| Ca | 27.633692 | 32.768269 | 31.024551 |
| Ca | 28.896351 | 28.021461 | 29.729321 |
| Ca | 30.525387 | 32.324051 | 27.331036 |
| Ca | 30.506807 | 27.844677 | 24.661215 |
| Ca | 33.662315 | 29.910055 | 27.921104 |
| Ca | 34.548500 | 25.171785 | 26.847830 |
| Ca | 35.870560 | 28.659283 | 24.050686 |
| S | 21.174240 | 31.413404 | 35.749310 |
|      |        |        |        |
|------|--------|--------|--------|
| S    | 20.523026 | 35.541893 | 33.257469 |
| S    | 21.909966 | 31.512613 | 29.640636 |
| S    | 24.869183 | 33.929771 | 33.062347 |
| S    | 26.035742 | 29.769817 | 30.598450 |
| S    | 25.414616 | 34.260063 | 28.221186 |
| S    | 28.145973 | 29.603008 | 26.705559 |
| S    | 30.693581 | 31.049618 | 30.128881 |
| S    | 31.676575 | 26.800922 | 27.735891 |
| S    | 32.783535 | 30.523869 | 24.924751 |
| S    | 33.465633 | 25.997700 | 23.488565 |
| S    | 36.438034 | 27.776585 | 27.187824 |

24

generated by VMD

|      |        |        |        |
|------|--------|--------|--------|
| Ca   | 18.372524 | 32.933231 | 33.646988 |
| Ca   | 22.783590 | 34.665520 | 35.853222 |
| Ca   | 23.405594 | 30.468872 | 32.908485 |
| Ca   | 22.696320 | 34.418907 | 30.659065 |
| Ca   | 25.347248 | 30.573112 | 28.398830 |
| Ca   | 27.850349 | 32.891777 | 31.121048 |
| Ca   | 29.092216 | 28.093224 | 29.743465 |
| Ca   | 30.586193 | 32.633980 | 27.168703 |
| Ca   | 30.347630 | 27.751259 | 24.477793 |
| Ca   | 33.755615 | 30.028118 | 27.863590 |
| Ca   | 34.183277 | 24.690182 | 26.591064 |
| Ca   | 35.594902 | 28.805477 | 24.098785 |
| S    | 21.100399 | 31.523849 | 35.394146 |
| S    | 20.551208 | 35.609043 | 33.430740 |
| S    | 22.036232 | 31.215229 | 29.885654 |
| S    | 24.696350 | 33.899429 | 32.898266 |
| S    | 26.211161 | 29.558586 | 31.108608 |
| S    | 25.819917 | 34.082409 | 28.443050 |
| S    | 28.170433 | 29.828987 | 26.821392 |
| S    | 30.856457 | 31.275202 | 30.034292 |
| S    | 31.684973 | 26.918829 | 27.667259 |
| S    | 32.853508 | 30.606184 | 25.092663 |
| S    | 33.446903 | 26.373564 | 23.289282 |
| S    | 36.376995 | 27.455013 | 27.342466 |

24

generated by VMD

|      |        |        |        |
|------|--------|--------|--------|
| Ca   | 18.381918 | 32.538536 | 33.773548 |
| Ca   | 22.990919 | 34.967918 | 35.836483 |
| Ca   | 23.613478 | 30.529625 | 33.088387 |
| Ca   | 22.842564 | 34.307625 | 30.720224 |
| Ca   | 25.076096 | 30.719017 | 27.861746 |
| Ca   | 27.683229 | 32.927490 | 31.252949 |
| Ca   | 29.003841 | 27.988661 | 29.760952 |
|    |        |        |        |
|----|--------|--------|--------|
| Ca | 30.579983 | 32.418056 | 27.232 |
| Ca | 30.656841 | 28.148701 | 24.359972 |
| Ca | 33.469940 | 29.912764 | 28.217842 |
| Ca | 34.045635 | 24.759434 | 26.669508 |
| Ca | 35.756889 | 28.894314 | 23.973137 |
| S  | 21.263416 | 31.629400 | 35.639252 |
| S  | 20.537540 | 35.473320 | 33.200195 |
| S  | 22.068684 | 31.250122 | 29.934488 |
| S  | 24.794317 | 34.019608 | 32.998711 |
| S  | 26.185837 | 29.657017 | 30.819454 |
| S  | 25.713089 | 33.979839 | 28.343304 |
| S  | 28.133202 | 29.674656 | 26.683374 |
| S  | 30.704098 | 31.046097 | 30.181679 |
| S  | 31.493519 | 27.040464 | 27.752888 |
| S  | 32.982819 | 30.636169 | 25.067238 |
| S  | 33.495445 | 26.208786 | 23.241203 |
| S  | 36.246716 | 27.572445 | 27.330696 |

24

| generated by VMD |
|------------------|
| Ca 18.311348 32.815376 34.224220 |
| Ca 22.820923 34.965736 35.847225 |
| Ca 23.269171 30.655752 32.953232 |
| Ca 22.612400 34.458721 30.769867 |
| Ca 25.179024 30.806576 28.007858 |
| Ca 27.647755 32.876244 30.995174 |
| Ca 29.126871 27.844570 29.728531 |
| Ca 30.886209 32.558800 27.434589 |
| Ca 30.501339 27.896465 24.598574 |
| Ca 33.817421 29.817860 28.036118 |
| Ca 34.366741 24.469860 26.447117 |
| Ca 35.813354 29.043839 23.998787 |
| S 21.256844 31.722607 35.819843 |
| S 20.291542 35.585693 33.235241 |
| S 21.783348 31.173618 29.755535 |
| S 24.591854 33.874580 32.968948 |
| S 26.107609 29.592905 30.736248 |
| S 25.618084 34.155167 28.302273 |
| S 28.450758 29.752197 26.690647 |
| S 30.626905 31.025457 30.199337 |
| S 31.845982 26.862087 27.713293 |
| S 32.751759 30.667130 25.114542 |
| S 33.482491 26.207455 23.390034 |
| S 36.560314 27.471333 26.972841 |

24

| generated by VMD |
|------------------|
| Ca 18.727440 32.430428 33.960297 |
|   |   |   |   |
|---|---|---|---|
| Ca | 23.246202 | 34.830891 | 35.748528 |
| Ca | 23.444080 | 34.447754 | 32.834015 |
| Ca | 22.813820 | 30.492754 | 32.834015 |
| Ca | 24.993847 | 30.787663 | 27.818970 |
| Ca | 27.679718 | 32.939983 | 30.814939 |
| Ca | 28.880943 | 27.935995 | 29.804756 |
| Ca | 30.642765 | 32.523140 | 27.454624 |
| Ca | 30.640244 | 27.931343 | 24.839330 |
| Ca | 33.591022 | 29.910545 | 28.229160 |
| Ca | 34.021698 | 24.596796 | 26.659698 |
| Ca | 35.613857 | 28.897848 | 24.050407 |
| S  | 21.474407 | 31.472910 | 35.526798 |
| S  | 20.593166 | 35.407692 | 33.319698 |
| S  | 21.937553 | 31.280628 | 29.667660 |
| S  | 24.709614 | 33.839401 | 32.895496 |
| S  | 26.034184 | 29.677113 | 30.610706 |
| S  | 25.620811 | 34.281471 | 28.390331 |
| S  | 28.247219 | 29.835159 | 26.659858 |
| S  | 30.791674 | 31.86153 | 30.277110 |
| S  | 31.744968 | 27.131157 | 28.048084 |
| S  | 32.702309 | 30.790756 | 25.038734 |
| S  | 33.442059 | 26.093529 | 23.447580 |
| S  | 36.138145 | 27.578918 | 27.138748 |

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generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 18.363277 | 32.692627 | 34.054939 |
| Ca | 23.224653 | 34.592133 | 35.676273 |
| Ca | 23.82854 | 30.404408 | 32.935104 |
| Ca | 23.141052 | 35.200447 | 30.490257 |
| Ca | 24.813078 | 30.459106 | 27.796535 |
| Ca | 27.670237 | 32.533051 | 31.032085 |
| Ca | 28.930971 | 28.129393 | 29.665436 |
| Ca | 30.480274 | 32.297272 | 27.503532 |
| Ca | 30.385832 | 27.819286 | 24.643532 |
| Ca | 33.690392 | 30.002705 | 28.286335 |
| Ca | 34.290203 | 24.907104 | 26.899651 |
| Ca | 35.562160 | 29.025236 | 23.825611 |
| S  | 21.326859 | 31.375952 | 35.541607 |
| S  | 20.723158 | 35.625141 | 33.065277 |
| S  | 22.026293 | 31.436825 | 29.879943 |
| S  | 24.960278 | 33.565262 | 33.110996 |
| S  | 26.052380 | 32.528698 | 30.718086 |
| S  | 25.746361 | 34.000782 | 28.202995 |
| S  | 28.027306 | 29.806538 | 26.657669 |
| S  | 30.884609 | 31.048269 | 30.320087 |
| S  | 31.688042 | 27.077112 | 28.003273 |
| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
|------|--------------|--------------|--------------|
| S    | 32.686008    | 30.726574    | 25.057613    |
| S    | 33.345791    | 26.065857    | 23.464092    |
| S    | 36.317879    | 27.980293    | 27.199198    |

generated by VMD

| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
|------|--------------|--------------|--------------|
| Ca   | 18.393667    | 32.863430    | 33.758858    |
| Ca   | 23.171028    | 34.874195    | 35.405243    |
| Ca   | 23.167503    | 30.320770    | 33.219902    |
| Ca   | 22.831663    | 35.056465    | 30.572376    |
| Ca   | 25.119314    | 30.559217    | 28.274477    |
| Ca   | 27.785625    | 32.559193    | 31.017338    |
| Ca   | 28.986134    | 27.842960    | 29.937088    |
| Ca   | 30.562355    | 32.333843    | 27.448612    |
| Ca   | 30.451546    | 28.059456    | 24.680157    |
| Ca   | 33.756706    | 29.911428    | 28.267036    |
| Ca   | 34.453644    | 24.886366    | 26.504332    |
| Ca   | 35.555607    | 29.029076    | 23.790564    |
| S    | 21.007000    | 31.759090    | 35.540607    |
| S    | 20.466305    | 35.734688    | 33.075508    |
| S    | 22.038841    | 31.535137    | 29.907619    |
| S    | 24.920534    | 33.556600    | 32.891335    |
| S    | 26.065130    | 29.079689    | 30.834127    |
| S    | 25.603485    | 33.808559    | 28.389637    |
| S    | 28.132545    | 29.688795    | 26.915464    |
| S    | 30.980602    | 30.971706    | 30.331970    |
| S    | 31.876289    | 26.918808    | 27.990734    |
| S    | 32.649746    | 30.752441    | 25.072380    |
| S    | 33.263077    | 26.294899    | 23.183853    |
| S    | 36.481750    | 27.924166    | 26.930794    |

generated by VMD

| Atom | X-Coordinate | Y-Coordinate | Z-Coordinate |
|------|--------------|--------------|--------------|
| Ca   | 18.542652    | 33.016754    | 33.724258    |
| Ca   | 23.033520    | 34.817364    | 35.619881    |
| Ca   | 23.428749    | 30.338661    | 33.125961    |
| Ca   | 22.886063    | 34.855621    | 30.203732    |
| Ca   | 25.103745    | 30.708311    | 27.913376    |
| Ca   | 27.707703    | 32.534050    | 31.043917    |
| Ca   | 28.811037    | 27.560120    | 29.806675    |
| Ca   | 30.484468    | 32.312016    | 27.559311    |
| Ca   | 30.480812    | 27.947504    | 25.511890    |
| Ca   | 33.805107    | 29.859116    | 28.380428    |
| Ca   | 34.338501    | 25.099705    | 26.146915    |
| Ca   | 35.189358    | 29.402050    | 23.586063    |
| S    | 21.175232    | 31.713741    | 35.707634    |
| S    | 20.634163    | 35.732430    | 32.828049    |
| S    | 22.147728    | 31.464729    | 29.891766    |
|  S  |  24.877258 |  33.616337 |  33.091900 |
|-----|------------|------------|------------|
|  S  |  25.949333 |  29.223118 |  30.677755 |
|  S  |  25.813370 |  33.798561 |  28.181850 |
|  S  |  28.283058 |  29.603012 |  26.734570 |
|  S  |  30.637518 |  30.734066 |  30.401081 |
|  S  |  32.296783 |  27.104242 |  28.468334 |
|  S  |  32.446106 |  30.635551 |  25.317608 |
|  S  |  33.131641 |  26.379360 |  23.496675 |
|  S  |  36.516144 |  27.843662 |  26.520422 |

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generated by VMD

|  Ca  |  18.585558 |  33.406704 |  33.774986 |
|-----|------------|------------|------------|
|  Ca  |  23.118690 |  34.830643 |  35.590141 |
|  Ca  |  23.394875 |  30.299829 |  33.025349 |
|  Ca  |  22.679680 |  34.658558 |  30.403769 |
|  Ca  |  25.051708 |  30.798885 |  28.197723 |
|  Ca  |  27.686733 |  32.467243 |  31.061516 |
|  Ca  |  28.982437 |  27.662947 |  29.872036 |
|  Ca  |  30.512302 |  32.400642 |  27.535238 |
|  Ca  |  30.357964 |  28.044802 |  24.657331 |
|  Ca  |  33.754314 |  29.948757 |  28.147928 |
|  Ca  |  34.719410 |  24.876215 |  26.785975 |
|  Ca  |  35.372635 |  29.115829 |  23.820831 |
|  S   |  21.214804 |  31.691643 |  35.523155 |
|  S   |  20.780348 |  35.848995 |  33.087143 |
|  S   |  21.865965 |  31.433027 |  29.949440 |
|  S   |  24.846199 |  33.299465 |  32.877243 |
|  S   |  25.834526 |  29.087437 |  30.573650 |
|  S   |  25.626196 |  33.924496 |  28.403286 |
|  S   |  28.192631 |  29.724243 |  26.896395 |
|  S   |  30.619286 |  30.865685 |  30.368002 |
|  S   |  31.919350 |  26.811356 |  27.973019 |
|  S   |  32.588303 |  30.855576 |  25.315245 |
|  S   |  33.389336 |  26.203342 |  23.495226 |
|  S   |  36.626774 |  28.043718 |  26.605419 |

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generated by VMD

|  Ca  |  18.281963 |  33.272804 |  33.994690 |
|-----|------------|------------|------------|
|  Ca  |  22.948349 |  34.854355 |  35.584663 |
|  Ca  |  23.269478 |  30.193474 |  32.992687 |
|  Ca  |  22.603706 |  34.594078 |  30.410801 |
|  Ca  |  25.333103 |  30.696468 |  28.047653 |
|  Ca  |  27.775879 |  32.705826 |  31.183319 |
|  Ca  |  29.222515 |  27.942953 |  29.802841 |
|  Ca  |  30.672018 |  32.589035 |  27.470884 |
|  Ca  |  30.510633 |  28.058685 |  24.699602 |
| Chemical | Value 1  | Value 2  | Value 3  |
|----------|---------|---------|---------|
| Ca       | 33.790230 | 29.955486 | 28.190769 |
| Ca       | 34.271557 | 24.807552 | 26.639088 |
| Ca       | 35.460197 | 35.728367 | 32.993916 |
| S        | 21.073467 | 31.750971 | 35.611145 |
| S        | 20.491621 | 35.728367 | 32.993916 |
| S        | 22.021305 | 31.77132  | 29.998013 |
| S        | 24.785442 | 33.399342 | 33.170097 |
| S        | 26.146950 | 29.416002 | 30.656494 |
| S        | 25.463333 | 33.82179  | 28.469299 |
| S        | 28.392691 | 29.849400 | 26.779163 |
| S        | 30.872066 | 31.160938 | 30.455029 |
| S        | 31.752867 | 26.843281 | 27.934193 |
| S        | 32.744869 | 30.592819 | 25.153347 |
| S        | 33.393440 | 27.186071 | 23.354332 |
| S        | 36.442314 | 27.678257 | 26.745712 |

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generated by VMD

| Chemical | Value 1  | Value 2  | Value 3  |
|----------|---------|---------|---------|
| Ca       | 18.516565 | 33.289871 | 34.180920 |
| Ca       | 23.155350 | 34.732529 | 35.875771 |
| Ca       | 23.352428 | 30.240120 | 32.869389 |
| Ca       | 22.336514 | 34.649590 | 30.513390 |
| Ca       | 25.146132 | 30.793264 | 27.900208 |
| Ca       | 27.487774 | 32.738075 | 30.928169 |
| Ca       | 29.015245 | 27.953907 | 29.637634 |
| Ca       | 30.717081 | 32.463936 | 27.615267 |
| Ca       | 30.447763 | 27.687889 | 24.629477 |
| Ca       | 33.900455 | 30.018444 | 28.240246 |
| Ca       | 34.513855 | 24.975796 | 26.744133 |
| Ca       | 35.520309 | 28.698849 | 23.724312 |
| S        | 21.123745 | 31.464621 | 35.553356 |
| S        | 20.661798 | 35.909985 | 33.554199 |
| S        | 21.882488 | 31.327805 | 29.719652 |
| S        | 24.729614 | 33.437599 | 33.124123 |
| S        | 26.000217 | 29.448437 | 30.497860 |
| S        | 25.316959 | 34.025139 | 28.189552 |
| S        | 28.329170 | 30.073715 | 26.572571 |
| S        | 30.829056 | 31.053013 | 30.297199 |
| S        | 31.779039 | 26.874384 | 28.007244 |
| S        | 32.822506 | 30.480316 | 25.125315 |
| S        | 33.577351 | 26.096027 | 23.449875 |
| S        | 36.558628 | 27.866756 | 26.990139 |

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generated by VMD

| Chemical | Value 1  | Value 2  | Value 3  |
|----------|---------|---------|---------|
| Ca       | 18.621941 | 33.739826 | 33.792797 |
| Ca       | 23.482639 | 34.922138 | 35.701599 |
| Ca       | 23.081289 | 30.154003 | 33.035370 |
|   | Ca     | S      | generated by VMD |
|---|--------|--------|------------------|
| Ca| 22.780581 | 34.440380 | 30.499233 |
| Ca| 24.834427 | 30.357855 | 28.053093 |
| Ca| 27.523008 | 32.301773 | 30.969255 |
| Ca| 28.928381 | 30.969255 | 29.730431 |
| Ca| 30.234024 | 32.481277 | 27.349215 |
| Ca| 30.612933 | 28.020218 | 24.676275 |
| Ca| 33.738701 | 29.942818 | 28.190296 |
| Ca| 34.412560 | 24.972261 | 26.567829 |
| Ca| 35.744698 | 29.340523 | 23.953572 |
| S | 21.221886 | 32.057190 | 35.801792 |
| S | 20.931679 | 36.073128 | 33.204395 |
| S | 21.810638 | 31.194471 | 29.872807 |
| S | 24.815420 | 33.050747 | 30.674942 |
| S | 25.856409 | 29.146223 | 28.202688 |
| S | 28.046940 | 29.667587 | 26.715000 |
| S | 30.537222 | 30.774864 | 30.241322 |
| S | 31.868362 | 27.029221 | 27.902920 |
| S | 32.804596 | 30.824989 | 25.253754 |
| S | 33.622424 | 26.393576 | 23.422783 |
| S | 36.628147 | 27.986313 | 27.061886 |
| Ca| 18.453665 | 33.197975 | 33.911911 |
| Ca| 23.219236 | 34.994667 | 35.912815 |
| Ca| 23.149754 | 30.165001 | 33.068581 |
| Ca| 22.869980 | 34.766304 | 30.446842 |
| Ca| 25.005508 | 30.506252 | 28.009653 |
| Ca| 27.489136 | 32.579277 | 31.006245 |
| Ca| 28.827393 | 27.706299 | 29.468990 |
| Ca| 30.344332 | 32.264305 | 27.189198 |
| Ca| 30.374895 | 27.925730 | 24.487156 |
| Ca| 33.891644 | 29.904686 | 28.046692 |
| Ca| 34.451336 | 25.048697 | 26.702442 |
| Ca| 35.823250 | 29.071480 | 24.033419 |
| S | 21.157618 | 31.927692 | 35.635139 |
| S | 20.891492 | 35.981152 | 33.390919 |
| S | 21.874731 | 31.258749 | 29.925745 |
| S | 24.831125 | 33.445847 | 33.202835 |
| S | 25.850847 | 29.269402 | 30.600136 |
| S | 25.742672 | 33.747906 | 28.339470 |
| S | 27.908371 | 29.750923 | 26.637117 |
| S | 30.577869 | 30.665543 | 30.180824 |
| S | 31.907238 | 26.994652 | 27.771849 |
| S | 32.645954 | 30.702866 | 25.158567 |
| S | 33.645058 | 26.368515 | 23.499023 |
|  |  |  |  |
|---|---|---|---|
| S | 36.806976 | 28.056095 | 27.314484 |
| 24 generated by VMD |
| Ca | 18.465466 | 33.108780 | 33.924938 |
| Ca | 22.996193 | 34.889740 | 35.558380 |
| Ca | 23.252621 | 30.040390 | 32.950668 |
| Ca | 22.882397 | 34.715389 | 30.271786 |
| Ca | 25.249598 | 30.888161 | 28.201111 |
| Ca | 27.725002 | 32.540981 | 31.104446 |
| Ca | 29.103479 | 27.645771 | 29.926767 |
| Ca | 30.351477 | 32.517086 | 27.544228 |
| Ca | 30.438902 | 28.022823 | 24.705975 |
| Ca | 33.506752 | 29.866650 | 28.028742 |
| Ca | 34.419991 | 24.966484 | 26.602818 |
| Ca | 35.507645 | 28.874514 | 23.956324 |
| S | 21.195353 | 31.669121 | 35.554695 |
| S | 20.590225 | 35.898071 | 33.146103 |
| S | 22.044140 | 31.432426 | 29.951797 |
| S | 24.829414 | 33.419521 | 32.914673 |
| S | 26.031191 | 29.233509 | 30.795999 |
| S | 25.784803 | 33.863483 | 28.229513 |
| S | 28.264343 | 29.661499 | 26.986206 |
| S | 30.842913 | 30.896065 | 30.365591 |
| S | 31.919012 | 27.023773 | 28.023396 |
| S | 32.523228 | 30.914745 | 24.978912 |
| S | 33.504047 | 26.286371 | 23.294411 |
| S | 36.291851 | 27.924713 | 26.918924 |
| 24 generated by VMD |
| Ca | 18.352507 | 33.340408 | 33.769505 |
| Ca | 23.142788 | 34.659454 | 35.581417 |
| Ca | 23.443863 | 30.142952 | 33.122608 |
| Ca | 22.878235 | 34.599010 | 30.364401 |
| Ca | 24.984756 | 30.607918 | 28.034824 |
| Ca | 27.658165 | 32.637253 | 31.082558 |
| Ca | 29.095146 | 27.894108 | 29.939671 |
| Ca | 30.335480 | 32.402252 | 27.593651 |
| Ca | 30.344643 | 27.821686 | 24.609406 |
| Ca | 33.678913 | 30.094723 | 28.160099 |
| Ca | 34.304604 | 24.835735 | 26.568203 |
| Ca | 35.494236 | 29.346085 | 24.177189 |
| S | 21.181595 | 31.663799 | 35.202141 |
| S | 20.952122 | 36.092083 | 33.037251 |
| S | 21.978851 | 31.106417 | 29.819883 |
| S | 24.940220 | 33.230690 | 33.285671 |
| S | 26.071323 | 29.549963 | 30.821453 |
414

S          25.764244       33.876915       28.303423
S          28.169695       29.552923       26.952015
S          30.886261       31.026497       30.430649
S          31.786421       26.901970       27.871552
S          32.339069       30.793516       24.983398
S          33.587959       26.203972       23.497688
S          36.348942       27.919712       26.731411

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generated by VMD

Ca         18.264658       33.392372       33.921623
Ca         23.003853       34.653992       35.878342
Ca         23.373087       30.344061       33.015709
Ca         22.690432       34.473980       30.414635
Ca         25.013353       30.746479       27.801748
Ca         27.747871       32.786659       31.149731
Ca         29.229158       27.992922       29.836605
Ca         30.580196       32.374542       27.366871
Ca         30.448460       27.699732       24.972952
Ca         33.583202       30.014040       28.097607
Ca         34.472725       24.785511       26.587337
Ca         35.582813       29.034742       23.801819
S          21.025528       31.620434       35.372536
S          20.818007       35.730820       33.255989
S          21.656670       31.134262       29.784843
S          25.020712       33.419407       33.058060
S          26.094448       29.538837       30.793028
S          25.671791       33.970291       28.298149
S          28.441124       29.861938       26.847963
S          30.779234       31.108789       30.481071
S          31.868095       26.843353       27.878181
S          32.543255       30.747917       25.058849
S          33.427017       26.227032       23.424454
S          36.384323       27.797920       26.841942

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generated by VMD

Ca         18.447329       33.324211       34.049389
Ca         23.087824       34.635262       35.682404
Ca         23.254499       30.241978       33.016396
Ca         22.860830       34.565544       30.610340
Ca         24.973446       30.678581       27.991825
Ca         27.533247       32.613564       31.046112
Ca         29.033718       27.931435       29.842625
Ca         30.576656       32.369022       27.324022
Ca         30.478817       27.608088       24.798607
Ca         33.796017       30.032999       27.999897
Ca         34.377655       25.055733       26.761189
|     |         |         |         |
|-----|---------|---------|---------|
| Ca  | 35.563072 | 29.006832 | 23.847610 |
| S   | 21.284145 | 31.624542 | 35.550861 |
| S   | 20.794865 | 35.937687 | 32.949741 |
| S   | 21.793419 | 31.394226 | 29.703547 |
| S   | 24.784225 | 33.129005 | 33.262169 |
| S   | 25.833220 | 29.454487 | 30.634850 |
| S   | 25.750059 | 34.013405 | 28.471062 |
| S   | 28.299599 | 29.704685 | 26.724686 |
| S   | 30.821354 | 31.088531 | 30.264883 |
| S   | 31.767088 | 26.989225 | 27.920040 |
| S   | 32.734909 | 30.656952 | 25.033937 |
| S   | 33.488777 | 26.252760 | 23.426411 |
| S   | 36.385319 | 27.991343 | 27.027451 |

24 generated by VMD

| Ca  | 18.575481 | 33.001228 | 33.835911 |
| Ca  | 22.700468 | 34.916267 | 35.796936 |
| Ca  | 23.324425 | 30.254768 | 32.967659 |
| Ca  | 22.599358 | 34.766159 | 30.535820 |
| Ca  | 25.145409 | 30.888477 | 27.935030 |
| Ca  | 27.829708 | 32.765144 | 31.153454 |
| Ca  | 28.981741 | 27.780142 | 29.748600 |
| Ca  | 30.414200 | 32.281036 | 27.383577 |
| Ca  | 30.423180 | 27.702326 | 24.702454 |
| Ca  | 33.600521 | 29.930799 | 27.828945 |
| Ca  | 34.324997 | 24.992672 | 26.891750 |
| Ca  | 35.821808 | 29.050409 | 23.949345 |
| S   | 21.322826 | 31.525612 | 35.678719 |
| S   | 20.327198 | 35.855644 | 33.249062 |
| S   | 21.966522 | 31.306805 | 29.848089 |
| S   | 24.748766 | 33.560959 | 33.231766 |
| S   | 26.163582 | 29.506996 | 30.703251 |
| S   | 26.011408 | 34.136131 | 28.573610 |
| S   | 28.210276 | 29.644163 | 26.642014 |
| S   | 30.783192 | 31.001644 | 30.229542 |
| S   | 31.708691 | 26.817793 | 27.725576 |
| S   | 32.642776 | 30.566879 | 24.907997 |
| S   | 33.616383 | 26.219032 | 23.493204 |
| S   | 36.477169 | 27.828949 | 26.927723 |

24 generated by VMD

| Ca  | 18.763939 | 32.401028 | 33.711460 |
| Ca  | 23.248802 | 34.725296 | 35.944370 |
| Ca  | 23.400295 | 30.550449 | 32.797272 |
| Ca  | 22.984064 | 34.495865 | 30.773838 |
| Ca  | 25.148151 | 31.028906 | 27.613394 |
|    |    |    |    |
|----|----|----|----|
| Ca | 27.796257 | 32.916153 | 31.120529 |
| Ca | 28.986090 | 28.048536 | 29.729568 |
| Ca | 30.276550 | 32.572472 | 27.053890 |
| Ca | 30.230246 | 27.646147 | 24.847193 |
| Ca | 33.606888 | 29.899178 | 27.894825 |
| Ca | 34.332627 | 24.885712 | 27.135008 |
| Ca | 35.483372 | 29.053896 | 24.031961 |
| S  | 21.446590 | 31.533064 | 35.462059 |
| S  | 20.643597 | 35.455936 | 33.382015 |
| S  | 22.041569 | 31.555914 | 29.343142 |
| S  | 24.919037 | 33.213516 | 33.294868 |
| S  | 25.996597 | 29.755600 | 30.447456 |
| S  | 25.849930 | 34.218536 | 28.421825 |
| S  | 28.038771 | 29.784649 | 26.560043 |
| S  | 30.622896 | 31.278198 | 30.115231 |
| S  | 31.633957 | 26.825275 | 28.054741 |
| S  | 32.564117 | 30.356672 | 25.114567 |
| S  | 33.294552 | 26.207640 | 23.836250 |
| S  | 36.410435 | 27.891438 | 27.254528 |

generated by VMD

|    |    |    |    |
|----|----|----|----|
| Ca | 18.566936 | 32.760941 | 33.844639 |
| Ca | 22.960190 | 34.793350 | 35.648399 |
| Ca | 23.370451 | 30.216822 | 33.040779 |
| Ca | 22.680096 | 34.732788 | 30.520554 |
| Ca | 25.072905 | 30.803387 | 28.027939 |
| Ca | 27.664827 | 32.779095 | 31.072735 |
| Ca | 29.022593 | 28.104410 | 29.870789 |
| Ca | 30.534744 | 32.506569 | 27.120598 |
| Ca | 30.444901 | 27.779000 | 24.441212 |
| Ca | 33.686226 | 29.705986 | 28.040279 |
| Ca | 34.227604 | 25.068947 | 26.943209 |
| Ca | 35.686600 | 28.974590 | 24.016541 |
| S  | 21.271254 | 31.539576 | 35.660553 |
| S  | 20.555225 | 35.644802 | 33.179459 |
| S  | 22.048962 | 31.445980 | 29.921673 |
| S  | 24.857433 | 33.348320 | 33.263496 |
| S  | 26.103937 | 29.610609 | 30.712292 |
| S  | 25.700140 | 34.119968 | 28.346464 |
| S  | 28.152374 | 29.804684 | 26.552177 |
| S  | 30.926989 | 31.066872 | 30.223488 |
| S  | 31.480453 | 26.894646 | 27.770245 |
| S  | 32.876114 | 30.679664 | 25.005066 |
| S  | 33.423981 | 26.250980 | 23.669220 |
| S  | 36.405056 | 27.669872 | 27.048262 |
|    |    |    |    |
|----|----|----|----|
| Ca | 18.619934 | 32.894878 | 34.088337 |
| Ca | 23.181046 | 34.786728 | 35.719311 |
| Ca | 23.358883 | 30.288586 | 32.869102 |
| Ca | 22.801214 | 34.879520 | 30.574163 |
| Ca | 24.957579 | 30.766335 | 27.852917 |
| Ca | 27.609766 | 32.639702 | 31.050854 |
| Ca | 29.018736 | 27.719059 | 29.813656 |
| Ca | 30.357269 | 32.080311 | 27.154480 |
| Ca | 30.178833 | 27.909742 | 24.674898 |
| Ca | 33.616867 | 29.975906 | 28.276535 |
| Ca | 34.522377 | 25.211483 | 26.742153 |
| Ca | 35.678253 | 28.938890 | 24.242596 |
| S  | 21.392406 | 31.624611 | 35.551456 |
| S  | 20.725468 | 35.758453 | 33.353111 |
| S  | 21.871950 | 31.631981 | 29.637753 |
| S  | 24.932386 | 33.445953 | 33.187267 |
| S  | 25.912737 | 29.388535 | 30.389259 |
| S  | 25.792471 | 34.163116 | 28.290409 |
| S  | 28.048897 | 29.280851 | 26.635418 |
| S  | 30.768847 | 30.819939 | 30.188549 |
| S  | 31.739029 | 26.977783 | 27.890400 |
| S  | 32.646885 | 30.568996 | 24.980314 |
| S  | 33.475849 | 26.482008 | 23.516140 |
| S  | 36.512325 | 28.066664 | 27.260948 |

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|    |    |    |    |
|----|----|----|----|
| Ca | 18.847054 | 32.484962 | 34.104485 |
| Ca | 23.093140 | 34.921837 | 35.927425 |
| Ca | 23.336676 | 30.420769 | 33.011726 |
| Ca | 22.824711 | 34.627449 | 30.362438 |
| Ca | 25.107096 | 30.747606 | 27.611938 |
| Ca | 27.748852 | 32.926014 | 31.263824 |
| Ca | 28.943180 | 28.240295 | 29.754818 |
| Ca | 30.361923 | 32.545258 | 27.146862 |
| Ca | 30.610455 | 27.867123 | 24.292976 |
| Ca | 33.480282 | 29.994635 | 28.168896 |
| Ca | 34.101101 | 24.798531 | 26.803738 |
| Ca | 35.479073 | 28.848866 | 24.330318 |
| S  | 21.346054 | 31.473814 | 35.736286 |
| S  | 20.700096 | 35.395111 | 33.315693 |
| S  | 21.926979 | 31.180967 | 29.738174 |
| S  | 24.912312 | 33.496017 | 33.119534 |
| S  | 26.024986 | 29.801365 | 30.651152 |
| S  | 25.876747 | 34.172596 | 28.340286 |
| S  | 28.152527 | 29.642586 | 26.374546 |
|   |   |   |
|---|---|---|
| **S** | 30.754129 | 31.327560 | 30.123938 |
| **S** | 31.466560 | 27.040146 | 27.588228 |
| **S** | 32.917725 | 30.638325 | 25.088444 |
| **S** | 33.736046 | 26.126440 | 23.305395 |
| **S** | 35.972301 | 27.581764 | 27.778938 |

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generated by VMD

| **Ca** | 18.875729 | 32.547951 | 33.921425 |
| **Ca** | 22.791502 | 35.236847 | 35.639320 |
| **Ca** | 23.258018 | 30.586847 | 33.106918 |
| **Ca** | 22.496761 | 34.424698 | 30.674078 |
| **Ca** | 25.233963 | 31.087593 | 27.870443 |
| **Ca** | 27.584642 | 32.740845 | 31.125225 |
| **Ca** | 29.080620 | 27.904131 | 29.957165 |
| **Ca** | 30.727423 | 32.391384 | 27.493942 |
| **Ca** | 30.487452 | 28.060385 | 24.569603 |
| **Ca** | 33.792740 | 29.841167 | 27.801052 |
| **Ca** | 34.083870 | 24.633606 | 26.673100 |
| **Ca** | 35.812004 | 28.746601 | 23.756096 |
| **S**  | 21.366001 | 31.777386 | 35.768009 |
| **S**  | 20.386803 | 35.549301 | 33.139584 |
| **S**  | 21.955460 | 31.128775 | 29.595142 |
| **S**  | 24.723818 | 33.291019 | 33.318829 |
| **S**  | 26.034683 | 29.725452 | 30.723427 |
| **S**  | 25.455605 | 34.245346 | 28.435936 |
| **S**  | 28.327284 | 29.661711 | 26.798431 |
| **S**  | 30.699509 | 31.148756 | 30.360313 |
| **S**  | 31.583597 | 27.039700 | 27.691521 |
| **S**  | 33.012768 | 30.773588 | 25.003855 |
| **S**  | 33.514999 | 26.243690 | 23.363640 |
| **S**  | 36.434807 | 27.513268 | 27.153006 |

24

generated by VMD

| **Ca** | 18.774693 | 32.386951 | 34.052616 |
| **Ca** | 23.126278 | 34.792847 | 35.437325 |
| **Ca** | 23.352627 | 30.314089 | 32.958832 |
| **Ca** | 22.638430 | 34.597786 | 30.612606 |
| **Ca** | 25.036352 | 30.948151 | 27.958807 |
| **Ca** | 27.703398 | 32.870934 | 30.887897 |
| **Ca** | 29.141312 | 28.198793 | 29.887154 |
| **Ca** | 30.495958 | 32.447269 | 27.043650 |
| **Ca** | 30.296032 | 28.025362 | 24.535828 |
| **Ca** | 33.736038 | 29.751616 | 28.038765 |
| **Ca** | 33.926353 | 24.853880 | 26.707125 |
| **Ca** | 35.843075 | 28.905090 | 24.231245 |
| **S**  | 21.370104 | 31.572592 | 35.646412 |
S  20.622145  35.745163  33.285641  
S  21.944878  31.229822  29.868483  
S  24.797426  33.424229  33.035088  
S  26.019108  29.655182  30.579288  
S  25.623571  34.268730  28.397240  
S  28.041498  29.762535  26.748230  
S  30.896269  31.094072  30.218235  
S  31.638172  27.017847  27.702805  
S  32.815258  30.588013  25.173737  
S  33.516453  26.307228  23.504650  
S  36.364594  27.541813  27.428371  

24  generated by VMD
Ca  18.878170  32.712868  34.106895  
Ca  23.114126  34.920620  35.391846  
Ca  23.390947  30.231541  32.981270  
Ca  22.913157  34.765327  30.595043  
Ca  25.007191  30.840279  27.956200  
Ca  27.498459  32.452045  31.013538  
Ca  28.942526  27.973516  29.859386  
Ca  30.660862  32.629635  27.343044  
Ca  30.429859  27.968575  24.736963  
Ca  33.385464  29.768581  27.942472  
Ca  34.293762  24.815144  26.866459  
Ca  35.653450  29.120041  24.158764  
S  21.509073  31.582254  35.462685  
S  20.805950  35.772739  33.153740  
S  21.981718  31.425360  29.750160  
S  24.785412  33.373478  33.108593  
S  25.911041  29.202761  30.735729  
S  25.559639  33.825306  28.254383  
S  28.263823  29.840179  26.793846  
S  30.734360  31.125956  30.155487  
S  31.527071  27.121750  27.617592  
S  32.624523  30.948454  24.975224  
S  33.496441  26.222313  23.688702  
S  36.353020  27.661276  27.292007  

24  generated by VMD
Ca  18.360813  32.657028  33.995213  
Ca  22.864517  34.917549  35.636337  
Ca  23.352619  30.379177  32.854286  
Ca  22.642696  34.841267  30.716021  
Ca  24.986301  31.139112  27.820997  
Ca  27.854870  32.729771  31.237312  
Ca  29.002720  27.817562  29.945324
|   | Ca     | S     |
|---|--------|-------|
| 1 | 30.420494 | 32.266632 | 27.253529 |
| 2 | 30.465286 | 27.856232 | 24.553291 |
| 3 | 33.790524 | 24.929852 | 26.804829 |
| 4 | 34.306614 | 28.790506 | 23.833122 |
| 5 | 35.836723 | 29.918591 | 27.931528 |
| 6 | 34.306614 | 24.929852 | 26.804829 |
| 7 | 35.836723 | 28.790506 | 23.833122 |
| 8 | 36.527496 | 31.029423 | 30.266775 |
| 9 | 31.701962 | 34.111328 | 28.359474 |
| 10 | 32.811169 | 30.598310 | 24.903488 |
| 11 | 33.600010 | 26.208574 | 23.254381 |
| 12 | 36.527496 | 27.799927 | 26.981548 |

24 generated by VMD

|   | Ca     | S     |
|---|--------|-------|
| 1 | 18.539745 | 32.786777 | 34.026466 |
| 2 | 22.939493 | 34.870251 | 35.597382 |
| 3 | 23.266321 | 30.414433 | 32.946868 |
| 4 | 22.610510 | 34.728127 | 30.634621 |
| 5 | 25.009882 | 30.787754 | 27.877138 |
| 6 | 27.777155 | 32.792953 | 31.128826 |
| 7 | 29.088457 | 27.846631 | 29.708443 |
| 8 | 30.609585 | 32.396454 | 27.410801 |
| 9 | 30.365238 | 27.980232 | 24.690950 |
| 10 | 33.933529 | 29.943050 | 28.075567 |
| 11 | 34.361351 | 24.730927 | 26.759008 |
| 12 | 35.669685 | 28.931263 | 23.626034 |

24 generated by VMD

|   | Ca     | S     |
|---|--------|-------|
| 1 | 18.607355 | 32.470062 | 33.889420 |
Ca  23.163826  34.964195  35.541832
Ca  23.138227  30.376268  32.658558
Ca  22.897856  34.783131  30.715977
Ca  25.075008  31.403034  27.837681
Ca  27.695160  32.394119  31.227230
Ca  28.921820  27.802629  29.769520
Ca  30.598867  32.203308  27.180662
Ca  30.227633  34.783131  29.599449
Ca  33.766392  30.171045  28.175491
Ca  34.611465  24.936764  26.983330
Ca  35.556400  28.961872  23.726135
S   21.324497  31.712402  35.564503
S   20.457518  35.565216  33.089287
S   22.045132  31.835037  29.599449
S   24.993414  33.289875  33.348259
S   25.903437  29.432224  30.827766
S   25.685543  34.084030  28.588549
S   27.985794  29.600113  26.711761
S   30.758446  30.831127  30.161980
S   31.920750  26.934528  27.988815
S   32.618893  30.715033  24.964354
S   33.385452  25.960396  23.674847
S   36.381142  28.061756  26.878992

24 generated by VMD
Ca  18.560581  32.870140  33.871948
Ca  23.207420  34.631443  35.760540
Ca  23.307394  30.440712  32.750362
Ca  23.163826  34.812725  30.651335
Ca  24.919340  30.817955  27.803787
Ca  27.624130  32.654404  30.793158
Ca  28.921820  27.976242  29.982040
Ca  30.598867  32.435410  27.357552
Ca  30.545893  27.838888  24.566063
Ca  33.629704  29.937321  28.429169
Ca  34.550381  24.963636  26.984409
Ca  35.239998  29.140289  23.633516
S   21.277420  31.713074  35.644222
S   20.635805  35.642021  33.205227
S   21.832443  31.705757  29.704256
S   25.055971  33.082233  33.147652
S   25.967621  29.344704  30.723385
S   25.705641  33.823608  28.165964
S   28.237577  29.646040  26.727310
S   30.629732  31.084629  30.288401
S   31.816538  26.800684  27.939743
|     |        |        |        |
|-----|--------|--------|--------|
| S   | 32.649464 | 30.82751 | 25.118231 |
| S   | 33.359455 | 26.043657 | 23.588448 |
| S   | 36.271622 | 28.051758 | 27.103306 |

24

generated by VMD

|     |        |        |        |
|-----|--------|--------|--------|
| Ca  | 18.669544 | 33.022125 | 33.994072 |
| Ca  | 23.136698 | 34.841862 | 35.633614 |
| Ca  | 23.054535 | 30.307882 | 32.789341 |
| Ca  | 22.765060 | 34.566055 | 30.745697 |
| Ca  | 24.973133 | 30.967243 | 27.865978 |
| Ca  | 27.810808 | 32.496338 | 31.096531 |
| Ca  | 29.020170 | 27.833412 | 29.798847 |
| Ca  | 30.602716 | 32.382351 | 27.210407 |
| Ca  | 30.501797 | 27.869314 | 24.451633 |
| Ca  | 33.596497 | 29.972290 | 27.987469 |
| Ca  | 34.488892 | 24.992210 | 27.199734 |
| Ca  | 35.596008 | 28.972389 | 23.902431 |
| S   | 21.295219 | 31.731194 | 35.584679 |
| S   | 20.545649 | 35.682041 | 33.094311 |
| S   | 21.850849 | 31.713999 | 29.678875 |
| S   | 25.001869 | 33.155956 | 33.382000 |
| S   | 26.048031 | 29.243023 | 30.710316 |
| S   | 25.611893 | 33.937164 | 28.475048 |
| S   | 28.187231 | 29.763422 | 26.725580 |
| S   | 30.888906 | 30.975891 | 30.224937 |
| S   | 31.552702 | 26.990641 | 27.648495 |
| S   | 32.638855 | 30.811783 | 24.950500 |
| S   | 33.474762 | 25.972109 | 23.624716 |
| S   | 36.408230 | 28.099346 | 27.164856 |

24

generated by VMD

|     |        |        |        |
|-----|--------|--------|--------|
| Ca  | 18.334635 | 32.712036 | 34.090641 |
| Ca  | 22.908865 | 34.928837 | 35.849792 |
| Ca  | 23.292215 | 30.593742 | 32.862717 |
| Ca  | 22.557079 | 34.502129 | 30.567287 |
| Ca  | 25.051468 | 30.798660 | 27.928009 |
| Ca  | 27.642818 | 32.916317 | 31.072348 |
| Ca  | 29.234863 | 28.105484 | 29.688190 |
| Ca  | 30.600964 | 32.417728 | 27.481081 |
| Ca  | 30.451494 | 28.021818 | 24.631496 |
| Ca  | 34.061543 | 29.803883 | 27.692017 |
| Ca  | 34.356728 | 24.672083 | 26.872147 |
| Ca  | 35.837547 | 28.814232 | 24.061962 |
| S   | 21.207653 | 31.747553 | 35.643105 |
| S   | 20.505033 | 35.589058 | 33.373543 |
| S   | 21.707815 | 31.431801 | 29.630951 |
| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 33.650696 | 30.074936 | 28.115133 |
| Ca      | 34.540718 | 24.840414 | 27.059919 |
| Ca      | 35.598114 | 28.935928 | 23.810024 |
| S       | 21.315567 | 31.629841 | 35.426910 |
| S       | 20.446293 | 35.822651 | 33.579971 |
| S       | 21.730412 | 31.617657 | 29.527815 |
| S       | 24.843563 | 33.168610 | 33.316761 |
| S       | 25.975851 | 29.446196 | 30.531162 |
| S       | 25.54640 | 34.180885 | 28.469490 |
| S       | 28.213213 | 29.804504 | 26.681419 |
| S       | 30.761816 | 31.272657 | 30.150797 |
| S       | 31.743618 | 26.901665 | 27.910175 |
| S       | 32.747925 | 30.510460 | 24.931187 |
| S       | 33.508595 | 25.822491 | 23.598927 |
| S       | 36.489323 | 27.900349 | 27.125130 |

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generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 18.632195 | 32.161663 | 33.815174 |
| Ca      | 23.035404 | 34.684277 | 35.831173 |
| Ca      | 23.034348 | 30.205923 | 32.685745 |
| Ca      | 23.012381 | 35.081799 | 30.624222 |
| Ca      | 25.203590 | 31.135473 | 27.959538 |
| Ca      | 27.675148 | 32.766037 | 31.080687 |
| Ca      | 29.181787 | 28.311144 | 30.041458 |
| Ca      | 30.522917 | 32.582909 | 26.835770 |
| Ca      | 30.301100 | 27.664303 | 24.697489 |
| Ca      | 33.563961 | 29.872738 | 27.754589 |
| Ca      | 34.401840 | 24.794746 | 27.156160 |
| Ca      | 35.501331 | 28.847977 | 23.969387 |
| S       | 21.395777 | 31.355122 | 35.672298 |
| S       | 20.403580 | 35.380947 | 33.314678 |
| S       | 21.968864 | 31.814327 | 29.573078 |
| S       | 24.770802 | 33.173744 | 33.174259 |
| S       | 25.909134 | 29.819330 | 30.564240 |
| S       | 25.983358 | 34.472519 | 28.433018 |
| S       | 28.196001 | 29.706993 | 26.834091 |
| S       | 30.967819 | 31.415485 | 30.308605 |
| S       | 31.573177 | 26.875586 | 27.949928 |
| S       | 32.588348 | 30.551361 | 24.849844 |
| S       | 33.435478 | 25.984028 | 23.872284 |
| S       | 36.461704 | 27.641609 | 26.942343 |

24

generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 18.776512 | 32.266800 | 34.045101 |
| Ca      | 22.796680 | 34.738518 | 35.848804 |
| Ca      | 23.286106 | 30.534647 | 32.773205 |
| Element | x | y | z |
|---------|---|---|---|
| Ca      | 22.774036  | 34.889801  | 30.530481  |
| Ca      | 25.120461  | 30.866156  | 27.626850  |
| Ca      | 27.726967  | 32.986500  | 31.387234  |
| Ca      | 28.914473  | 28.057447  | 29.783123  |
| Ca      | 30.729155  | 32.478138  | 26.944992  |
| Ca      | 30.340485  | 32.478138  | 26.944992  |
| Ca      | 33.703587  | 29.920567  | 28.006365  |
| Ca      | 34.400372  | 24.699339  | 27.116486  |
| Ca      | 35.499752  | 28.937208  | 23.849035  |
| S       | 21.370306  | 31.457722  | 35.813637  |
| S       | 20.413717  | 35.457150  | 33.349876  |
| S       | 22.153753  | 31.612907  | 29.349751  |
| S       | 24.706539  | 33.451324  | 33.091892  |
| S       | 26.023432  | 29.728411  | 30.775816  |
| S       | 25.841976  | 34.316330  | 28.588886  |
| S       | 28.329697  | 29.840260  | 26.549053  |
| S       | 30.796156  | 31.262280  | 30.457214  |
| S       | 31.539272  | 26.827608  | 27.783943  |
| S       | 32.685925  | 30.385160  | 24.941740  |
| S       | 33.735777  | 26.011538  | 23.708227  |
| S       | 36.417149  | 27.793201  | 27.013893  |

24

generated by VMD
|   | X   | Y   | Z   |
|---|-----|-----|-----|
| S | 36.538979 | 27.939362 | 27.106796 |
| Ca | 18.358105 | 32.521759 | 33.787117 |
| Ca | 22.621014 | 34.824409 | 35.505692 |
| Ca | 23.362940 | 30.248230 | 32.955433 |
| Ca | 22.948160 | 35.050735 | 30.561567 |
| Ca | 24.947836 | 30.717163 | 28.182480 |
| Ca | 27.916685 | 32.845837 | 31.389786 |
| Ca | 29.135460 | 27.978645 | 29.838139 |
| Ca | 30.610777 | 32.345753 | 27.201618 |
| Ca | 30.166151 | 27.597252 | 24.586441 |
| Ca | 33.724304 | 29.734543 | 27.841106 |
| Ca | 34.219841 | 24.957954 | 26.763170 |
| Ca | 35.681847 | 28.980247 | 23.801802 |
| S | 21.059483 | 31.421728 | 35.563789 |
| S | 20.293678 | 35.653877 | 32.920387 |
| S | 21.922203 | 31.647430 | 30.023960 |
| S | 24.901222 | 33.689377 | 33.289360 |
| S | 26.236904 | 29.679028 | 30.861897 |
| S | 26.023502 | 34.141663 | 28.739574 |
| S | 28.260277 | 29.779640 | 26.705124 |
| S | 30.762686 | 31.149797 | 30.233665 |
| S | 31.922647 | 26.846163 | 27.803646 |
| S | 32.583027 | 30.413639 | 24.980179 |
| S | 33.389729 | 26.156849 | 23.461809 |
| S | 36.671532 | 27.918331 | 26.942305 |

24

generated by VMD

|   | X   | Y   | Z   |
|---|-----|-----|-----|
| Ca | 18.175434 | 32.583275 | 33.661346 |
| Ca | 22.842667 | 34.736992 | 35.740929 |
| Ca | 23.279558 | 30.361263 | 32.810635 |
| Ca | 23.070534 | 34.969345 | 30.741817 |
| Ca | 24.869823 | 30.744368 | 27.932182 |
| Ca | 27.871014 | 33.084145 | 31.382166 |
| Ca | 29.054995 | 28.232788 | 29.859825 |
| Ca | 30.564865 | 32.440254 | 27.157677 |
| Ca | 30.435200 | 27.593258 | 24.678404 |
| Ca | 33.665085 | 30.004974 | 27.887091 |
| Ca | 34.321426 | 24.851192 | 26.704067 |
| Ca | 35.654320 | 28.674141 | 23.923035 |
| S | 21.102724 | 31.447060 | 35.479481 |
| S | 20.358589 | 35.462696 | 33.210510 |
| S | 21.891308 | 31.724550 | 29.692041 |
| S | 24.843954 | 33.300056 | 33.532063 |
| S | 26.228844 | 29.676521 | 30.976875 |
|   |          |          |          |
|---|----------|----------|----------|
| S | 25.937014 | 34.058792 | 28.663212 |
| S | 28.191183 | 29.868073 | 26.614433 |
| S | 31.028334 | 31.331696 | 30.142138 |
| S | 31.696884 | 27.007912 | 27.823183 |
| S | 32.674671 | 30.435619 | 24.844702 |
| S | 33.426781 | 25.679609 | 23.557735 |
| S | 36.534859 | 28.031479 | 26.924475 |

24
generated by VMD

| Ca |          |          |          |
|----|----------|----------|----------|
| Ca | 18.481083 | 33.126644 | 33.771626 |
| Ca | 22.956078 | 34.772034 | 35.899368 |
| Ca | 23.401608 | 30.288687 | 32.869167 |
| Ca | 22.879484 | 34.394188 | 30.680998 |
| Ca | 25.127882 | 30.776962 | 27.880192 |
| Ca | 27.650276 | 32.611938 | 31.101559 |
| Ca | 29.054642 | 28.227337 | 29.972115 |
| Ca | 30.661457 | 32.475281 | 27.261431 |
| Ca | 30.338499 | 27.826809 | 24.678509 |
| Ca | 33.656162 | 29.978201 | 28.168831 |
| Ca | 34.334145 | 24.922678 | 26.670029 |
| Ca | 35.620049 | 28.844002 | 23.878513 |
| S  | 21.188175 | 31.568556 | 35.532707 |
| S  | 20.743174 | 35.772415 | 33.207512 |
| S  | 21.914913 | 31.282166 | 29.725784 |
| S  | 24.798758 | 33.170872 | 33.294235 |
| S  | 26.079443 | 29.705879 | 30.547005 |
| S  | 25.778564 | 34.042709 | 28.393993 |
| S  | 28.218716 | 29.747925 | 26.688881 |
| S  | 30.721264 | 31.226240 | 30.191841 |
| S  | 31.691282 | 27.003464 | 28.008759 |
| S  | 32.521744 | 30.555233 | 24.965654 |
| S  | 33.471142 | 26.049950 | 23.576714 |
| S  | 36.431484 | 27.929878 | 26.974663 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 35.513760 | 28.654673 | 23.656536 |
| S       | 21.022835  | 31.255070  | 35.494926  |
| S       | 20.051823  | 35.378890  | 32.990959  |
| S       | 22.088068  | 31.426098  | 29.662804  |
| S       | 24.941389  | 33.286961  | 33.309113  |
| S       | 26.457123  | 29.932777  | 30.806036  |
| S       | 25.768652  | 34.317890  | 28.396055  |
| S       | 28.492731  | 30.114204  | 26.870560  |
| S       | 31.036949  | 31.584929  | 30.274284  |
| S       | 31.538963  | 26.941605  | 27.889048  |
| S       | 32.725510  | 30.65856   | 24.942205  |
| S       | 33.041187  | 25.864487  | 23.702854  |
| S       | 36.412693  | 27.27496   | 26.587051  |

24 generated by VMD

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 18.013880  | 32.832115  | 34.259552  |
| Ca      | 22.692816  | 34.554756  | 35.784134  |
| Ca      | 23.408815  | 30.163565  | 32.916553  |
| Ca      | 22.779030  | 34.808956  | 30.686550  |
| Ca      | 25.368708  | 31.009693  | 28.005119  |
| Ca      | 27.790764  | 32.886826  | 31.075111  |
| Ca      | 29.362452  | 28.228884  | 29.691059  |
| Ca      | 30.702385  | 32.713871  | 27.120060  |
| Ca      | 30.420017  | 27.51183   | 24.707823  |
| Ca      | 33.486507  | 29.970797  | 28.084072  |
| Ca      | 34.236420  | 24.689980  | 26.922287  |
| Ca      | 35.510227  | 28.764240  | 23.852943  |
| S       | 21.221664  | 31.312124  | 35.389610  |
| S       | 20.287605  | 35.499725  | 33.312088  |
| S       | 22.061970  | 31.507124  | 29.606503  |
| S       | 25.000912  | 33.388153  | 33.317890  |
| S       | 26.147062  | 29.738995  | 30.694763  |
| S       | 25.693296  | 34.244392  | 28.315706  |
| S       | 28.653210  | 30.043711  | 26.659908  |
| S       | 30.798210  | 31.624352  | 30.179333  |
| S       | 31.726032  | 26.814963  | 27.888943  |
| S       | 32.703403  | 30.583981  | 24.911463  |
| S       | 33.358051  | 25.766235  | 23.602501  |
| S       | 36.296627  | 27.641724  | 26.953655  |

24 generated by VMD

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 18.175894  | 32.913715  | 34.207588  |
| Ca      | 23.057648  | 34.275105  | 35.695038  |
| Ca      | 23.373436  | 30.229338  | 32.989449  |
| Ca      | 22.800674  | 34.968391  | 30.542961  |
| Ca      | 25.339718  | 31.065870  | 27.939503  |
|   | Ca       | S        | 24 |
|---|----------|----------|----|
|Ca| 27.686255| 33.019501| 31.078510 |
|Ca| 29.287573| 27.976433| 29.689932 |
|Ca| 30.732826| 32.627716| 27.215157 |
|Ca| 30.045708| 27.921313| 25.012520 |
|Ca| 33.646820| 30.002800| 28.243067 |
|Ca| 34.619526| 24.797413| 26.698919 |
|Ca| 35.339664| 28.626682| 23.815620 |
|S | 21.076338| 31.162540| 35.49664  |
|S | 20.430277| 35.468189| 33.131744 |
|S | 22.213669| 31.532526| 29.651417 |
|S | 24.737993| 33.327705| 33.153999 |
|S | 26.277309| 29.732471| 30.577297 |
|S | 25.827070| 34.358532| 28.360409 |
|S | 28.406565| 29.936916| 26.707224 |
|S | 30.917507| 31.500164| 30.179363 |
|S | 31.766050| 26.901466| 28.012891 |
|S | 32.435635| 30.448347| 25.085882 |
|S | 33.039341| 25.676048| 23.751663 |
|S | 36.450886| 27.960047| 26.894529 |

24 generated by VMD

|   | Ca       | S        | 24 |
|---|----------|----------|----|
|Ca| 18.092279| 33.073826| 34.200485 |
|Ca| 22.664064| 34.319180| 35.286629 |
|Ca| 23.463326| 30.290174| 33.226944 |
|Ca| 22.615826| 34.807533| 30.690329 |
|Ca| 25.343636| 31.159336| 28.119173 |
|Ca| 27.938612| 32.977058| 31.241623 |
|Ca| 29.165956| 29.968744| 29.584805 |
|Ca| 30.730793| 32.625847| 27.498875 |
|Ca| 30.417772| 27.680286| 24.676064 |
|Ca| 33.670742| 30.032904| 28.099728 |
|Ca| 34.654266| 24.706211| 26.817183 |
|Ca| 35.338650| 28.579414| 23.517288 |
|S | 20.973940| 31.181709| 35.230221 |
|S | 20.090101| 35.503922| 33.055126 |
|S | 22.230000| 31.428185| 29.929649 |
|S | 24.772884| 33.670242| 33.340927 |
|S | 26.292381| 29.760082| 30.613682 |
|S | 25.937428| 34.408222| 28.681793 |
|S | 28.469276| 30.063786| 26.701775 |
|S | 30.910435| 31.229080| 30.175766 |
|S | 31.754444| 26.815536| 28.013968 |
|S | 32.520210| 30.576551| 24.828487 |
|S | 33.321171| 25.549877| 23.631731 |
|S | 36.352001| 27.892359| 26.777821 |
generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 18.155962 | 33.238022 | 34.441826 |
| Ca | 22.992966 | 34.365456 | 35.611977 |
| Ca | 23.453835 | 30.342724 | 32.925159 |
| Ca | 22.659737 | 34.822163 | 30.529724 |
| Ca | 25.037415 | 30.847673 | 27.789761 |
| Ca | 27.703396 | 32.737297 | 31.102352 |
| Ca | 28.971228 | 27.797020 | 29.606770 |
| Ca | 30.683052 | 32.523651 | 27.461605 |
| Ca | 30.609055 | 27.652649 | 24.944702 |
| Ca | 33.726009 | 30.022003 | 28.279331 |
| Ca | 34.407372 | 25.015884 | 26.977203 |
| Ca | 35.350662 | 28.934532 | 23.516357 |
| S  | 21.213215 | 31.277733 | 35.271042 |
| S  | 20.620098 | 35.724224 | 33.264343 |
| S  | 21.955467 | 31.476479 | 29.775757 |
| S  | 24.974291 | 33.532146 | 33.000530 |
| S  | 25.906284 | 29.533405 | 30.451090 |
| S  | 25.744518 | 34.216393 | 28.445152 |
| S  | 28.359268 | 29.825062 | 26.651630 |
| S  | 30.785929 | 31.071365 | 30.197805 |
| S  | 31.967501 | 26.875496 | 28.383924 |
| S  | 32.628376 | 30.536753 | 25.042646 |
| S  | 33.401436 | 25.912991 | 23.505575 |
| S  | 36.413033 | 28.018936 | 26.761993 |

24

generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 18.097569 | 33.025925 | 34.434837 |
| Ca | 22.941210 | 34.197556 | 35.738792 |
| Ca | 23.289684 | 30.204918 | 32.589714 |
| Ca | 22.811489 | 35.066753 | 30.645947 |
| Ca | 25.292503 | 31.215961 | 27.922829 |
| Ca | 27.776363 | 32.994995 | 31.173630 |
| Ca | 29.201187 | 28.032978 | 29.619156 |
| Ca | 30.567419 | 32.401505 | 27.206215 |
| Ca | 30.449310 | 27.322323 | 24.943203 |
| Ca | 33.657482 | 30.087086 | 28.252346 |
| Ca | 34.646973 | 25.034004 | 27.021584 |
| Ca | 35.196564 | 28.674284 | 23.476673 |
| S  | 21.015299 | 31.027246 | 35.209835 |
| S  | 20.448193 | 35.630913 | 33.440559 |
| S  | 21.974190 | 31.619328 | 29.646748 |
| S  | 24.897041 | 33.477268 | 33.143433 |
| S  | 26.203506 | 29.839632 | 30.448376 |
| S  | 25.824560 | 34.476913 | 28.538158 |
| S  | 28.415520 | 29.774887 | 26.630096 |
S  30.675547  31.249382  30.194832
S  31.893822  26.934986  28.196019
S  32.514751  30.356342  24.981693
S  33.469929  25.614090  23.688438
S  36.459957  28.040791  26.796013

24
generated by VMD
Ca  18.142498  33.075047  34.400604
Ca  22.673515  34.573174  35.597935
Ca  23.565886  30.362673  32.987064
Ca  22.720476  34.824242  30.549961
Ca  25.193579  30.782619  27.931784
Ca  27.626539  32.827698  31.113556
Ca  29.072504  28.092598  29.829609
Ca  30.694956  32.424271  27.379290
Ca  30.440022  27.760733  24.591074
Ca  33.887478  29.937695  28.092052
Ca  34.510685  24.641773  26.701145
Ca  35.534176  28.778656  23.716503
S  21.052282  31.227077  35.430141
S  20.246464  35.668049  33.158287
S  22.057650  31.411407  29.767828
S  24.816032  33.561771  33.276882
S  26.222921  29.795940  30.612682
S  25.821671  34.281296  28.533848
S  28.298412  29.858639  26.655199
S  30.783823  31.233051  30.295727
S  31.833754  26.916454  27.950974
S  32.688034  30.625969  24.945738
S  33.243820  25.894093  23.499073
S  36.592953  27.745157  26.923084

24
generated by VMD
Ca  18.059361  33.119930  34.476418
Ca  23.094509  34.363213  35.743553
Ca  23.483292  30.337948  32.905636
Ca  22.732893  34.834229  30.556494
Ca  25.216650  30.906219  27.800365
Ca  27.586365  32.777119  31.083836
Ca  29.119989  28.016243  29.632685
Ca  30.515175  32.382053  27.238522
Ca  30.305849  27.575377  24.588118
Ca  33.669216  29.991467  28.263771
Ca  34.581409  24.851799  26.903404
Ca  35.453976  28.898174  23.894890
S  21.149048  31.139807  35.412334
|  |  |  |  |
|---|---|---|---|
| S | 20.542810 | 35.671600 | 33.298256 |
| S | 21.992119 | 31.534138 | 29.729454 |
| S | 24.937895 | 33.656578 | 33.143616 |
| S | 26.082903 | 29.721779 | 30.471039 |
| S | 25.693903 | 34.332447 | 28.275200 |
| S | 28.451128 | 29.821808 | 26.681595 |
| S | 30.600252 | 31.170595 | 30.214546 |
| S | 31.906225 | 26.908817 | 27.984436 |
| S | 32.719791 | 30.394817 | 25.107824 |
| S | 33.269993 | 25.878105 | 23.417175 |
| S | 36.555233 | 28.015778 | 27.116875 |

24 generated by VMD

| Ca | 18.087049 | 33.316044 | 34.539284 |
| Ca | 22.874523 | 34.442509 | 35.634926 |
| Ca | 23.415615 | 30.326935 | 32.960644 |
| Ca | 22.706985 | 34.822529 | 30.344851 |
| Ca | 25.054466 | 30.615616 | 27.959267 |
| Ca | 27.452078 | 32.820656 | 30.948940 |
| Ca | 29.419138 | 28.147757 | 29.666960 |
| Ca | 30.844391 | 32.387863 | 27.469086 |
| Ca | 30.347994 | 27.946413 | 24.793224 |
| Ca | 33.949631 | 29.833830 | 27.993687 |
| Ca | 34.450527 | 24.716175 | 26.760269 |
| Ca | 35.405430 | 28.937986 | 23.772568 |
| S | 20.973471 | 31.292582 | 35.524006 |
| S | 20.450768 | 35.725266 | 33.355400 |
| S | 21.962526 | 31.459892 | 29.829136 |
| S | 24.732609 | 33.578953 | 33.126823 |
| S | 26.032812 | 29.502167 | 30.508675 |
| S | 25.609823 | 34.017670 | 28.124432 |
| S | 28.576365 | 29.932320 | 26.760456 |
| S | 30.821239 | 31.240509 | 30.402607 |
| S | 31.801413 | 26.919607 | 27.903973 |
| S | 32.898392 | 30.617041 | 25.218822 |
| S | 33.178581 | 26.017048 | 23.656906 |
| S | 36.674137 | 27.682709 | 26.685118 |

24 generated by VMD

| Ca | 18.137011 | 33.110817 | 34.481712 |
| Ca | 22.700569 | 34.425018 | 35.731560 |
| Ca | 23.380106 | 30.235420 | 32.794868 |
| Ca | 22.960703 | 35.007729 | 30.475227 |
| Ca | 25.247978 | 30.732550 | 28.114342 |
| Ca | 27.713400 | 32.799747 | 31.203491 |
| Ca | 29.195044 | 28.114235 | 29.901848 |
| Element | Value 1 | Value 2 | Value 3 |
|---------|---------|---------|---------|
| Ca      | 30.627745 | 32.420815 | 27.326649 |
| Ca      | 30.426508 | 27.713959 | 24.814198 |
| Ca      | 33.886169 | 24.771528 | 26.849258 |
| Ca      | 35.500729 | 28.815414 | 23.710293 |
| S       | 20.822821 | 31.205698 | 35.250504 |
| S       | 20.462341 | 35.678204 | 33.157681 |
| S       | 22.055109 | 31.711903 | 29.690746 |
| S       | 24.850317 | 33.448586 | 33.397472 |
| S       | 26.077290 | 29.787062 | 30.770542 |
| S       | 25.822165 | 34.056389 | 28.339462 |
| S       | 28.178736 | 29.619564 | 26.607517 |
| S       | 30.855402 | 31.270947 | 30.149408 |
| S       | 31.847652 | 26.944773 | 27.997608 |
| S       | 32.577423 | 30.592875 | 24.903080 |
| S       | 33.509659 | 25.995125 | 23.624746 |
| S       | 36.537331 | 27.861042 | 26.841415 |

24 generated by VMD

| Element | Value 1 | Value 2 | Value 3 |
|---------|---------|---------|---------|
| Ca      | 18.072079 | 33.376747 | 34.365784 |
| Ca      | 22.960619 | 34.355701 | 35.711269 |
| Ca      | 23.292252 | 30.379946 | 32.928043 |
| Ca      | 22.864414 | 34.978146 | 30.475124 |
| Ca      | 25.025028 | 30.744186 | 28.040405 |
| Ca      | 27.698761 | 32.689209 | 31.022799 |
| Ca      | 29.228329 | 28.035694 | 29.942867 |
| Ca      | 30.726933 | 32.325027 | 27.244963 |
| Ca      | 30.372604 | 27.711487 | 24.634043 |
| Ca      | 33.758793 | 29.836258 | 28.106632 |
| Ca      | 34.486382 | 24.999348 | 26.471905 |
| Ca      | 35.714779 | 28.880997 | 23.894341 |
| S       | 20.933340 | 31.489975 | 35.614098 |
| S       | 20.494476 | 35.580063 | 33.195839 |
| S       | 21.809603 | 31.450117 | 29.922237 |
| S       | 24.814022 | 33.586784 | 33.064053 |
| S       | 25.955736 | 29.536804 | 30.639233 |
| S       | 25.657930 | 34.112103 | 28.388227 |
| S       | 28.212040 | 29.573139 | 26.765995 |
| S       | 30.817471 | 31.256538 | 30.227753 |
| S       | 31.923664 | 26.766327 | 27.751619 |
| S       | 32.851494 | 30.644878 | 24.983932 |
| S       | 33.385754 | 25.995674 | 23.468746 |
| S       | 36.663467 | 27.994900 | 27.080158 |

24 generated by VMD

| Element | Value 1 | Value 2 | Value 3 |
|---------|---------|---------|---------|
| Ca      | 18.242359 | 33.321095 | 34.307320 |
| Ca     | 22.768747 | 34.420189 | 35.500301 |
|--------|-----------|-----------|-----------|
| Ca     | 23.372002 | 30.370346 | 33.130119 |
| Ca     | 22.953970 | 35.054256 | 30.352615 |
| Ca     | 24.944180 | 30.752663 | 28.026665 |
| Ca     | 27.841541 | 32.731773 | 31.027225 |
| Ca     | 28.887447 | 27.681540 | 29.833004 |
| Ca     | 30.377615 | 32.093437 | 27.467426 |
| Ca     | 30.434126 | 29.981949 | 28.175591 |
| Ca     | 34.577511 | 25.080688 | 26.774586 |
| Ca     | 35.433140 | 29.099871 | 23.785358 |
| S      | 20.925583 | 31.242306 | 35.407078 |
| S      | 20.643776 | 35.678543 | 33.020855 |
| S      | 22.135393 | 31.674541 | 29.999823 |
| S      | 24.938282 | 33.684597 | 33.177071 |
| S      | 26.034798 | 29.507900 | 30.805321 |
| S      | 25.819138 | 33.986675 | 28.183266 |
| S      | 28.151411 | 29.521685 | 26.719696 |
| S      | 30.920879 | 30.786993 | 30.396072 |
| S      | 31.885952 | 26.982437 | 27.809071 |
| S      | 32.528233 | 30.758114 | 25.043861 |
| S      | 33.487556 | 26.094528 | 23.497356 |
| S      | 36.583851 | 27.955624 | 26.813984 |

24

generated by VMD

| Ca     | 18.314098 | 33.223816 | 33.705574 |
|--------|-----------|-----------|-----------|
| Ca     | 23.081705 | 34.354115 | 35.936569 |
| Ca     | 23.456917 | 30.486473 | 32.931202 |
| Ca     | 23.140539 | 34.786278 | 30.615404 |
| Ca     | 24.799118 | 30.541557 | 27.896561 |
| Ca     | 27.800905 | 32.598911 | 30.980705 |
| Ca     | 29.001347 | 28.025484 | 29.810074 |
| Ca     | 30.514509 | 32.292088 | 27.178858 |
| Ca     | 30.494637 | 27.798721 | 24.674271 |
| Ca     | 33.636497 | 30.026634 | 28.296085 |
| Ca     | 34.340260 | 24.826628 | 26.895641 |
| Ca     | 35.643433 | 29.090729 | 23.951855 |
| S      | 20.864738 | 31.458221 | 35.379223 |
| S      | 20.955938 | 35.720123 | 33.561272 |
| S      | 21.957199 | 31.386330 | 29.904236 |
| S      | 25.005108 | 33.564000 | 33.183578 |
| S      | 26.069241 | 29.477434 | 30.670536 |
| S      | 25.608210 | 33.894714 | 28.099056 |
| S      | 28.038977 | 29.748962 | 26.631466 |
| S      | 30.799364 | 31.134468 | 30.126633 |
| S      | 31.720322 | 26.929373 | 27.930521 |
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| S | 32.526920 | 30.798624 | 24.754990 |
| S | 33.562569 | 26.118471 | 23.819416 |
| S | 36.387520 | 28.017515 | 27.006353 |

24 generated by VMD

| Ca  | 18.075336 | 33.724937 | 33.714931 |
|-----|-----------|-----------|-----------|
| Ca  | 23.112925 | 34.285477 | 35.879486 |
| Ca  | 23.127003 | 30.326136 | 32.806381 |
| Ca  | 22.941345 | 34.731560 | 30.549679 |
| Ca  | 25.331043 | 30.478958 | 28.218599 |
| Ca  | 27.772493 | 32.806492 | 31.112823 |
| Ca  | 29.323269 | 27.891878 | 29.899126 |
| Ca  | 30.395451 | 32.489944 | 27.547884 |
| Ca  | 30.563902 | 27.827847 | 24.687395 |
| Ca  | 33.531269 | 30.039770 | 28.056007 |
| Ca  | 34.613777 | 24.827335 | 27.048771 |
| Ca  | 35.246391 | 29.034582 | 23.58362 |
| S   | 20.657051 | 31.432304 | 35.149361 |
| S   | 21.068134 | 35.765385 | 33.420074 |
| S   | 21.998701 | 31.186909 | 29.882835 |
| S   | 24.847385 | 33.373985 | 32.932388 |
| S   | 26.260826 | 29.511354 | 30.825005 |
| S   | 25.661919 | 33.899662 | 28.257294 |
| S   | 28.200960 | 29.744274 | 26.912746 |
| S   | 30.875957 | 31.142452 | 30.302402 |
| S   | 32.027851 | 27.057583 | 27.880852 |
| S   | 32.459717 | 30.781895 | 24.925331 |
| S   | 33.326656 | 26.045710 | 23.572231 |
| S   | 36.300632 | 27.893597 | 26.774605 |

24 generated by VMD

| Ca  | 18.657795 | 33.587200 | 33.734722 |
|-----|-----------|-----------|-----------|
| Ca  | 23.028072 | 34.127968 | 35.866898 |
| Ca  | 23.154816 | 30.345640 | 33.016907 |
| Ca  | 22.875402 | 34.998936 | 30.686829 |
| Ca  | 25.005074 | 30.708485 | 28.006268 |
| Ca  | 27.422060 | 32.732807 | 30.978453 |
| Ca  | 29.167076 | 27.861145 | 29.765251 |
| Ca  | 30.305769 | 32.485374 | 27.193031 |
| Ca  | 30.472195 | 27.506729 | 24.559250 |
| Ca  | 33.526936 | 30.081594 | 27.870075 |
| Ca  | 34.873093 | 24.931770 | 26.969339 |
| Ca  | 35.481941 | 29.034328 | 23.928791 |
| S   | 20.806982 | 31.269238 | 35.303047 |
| S   | 21.108047 | 36.158966 | 33.612694 |
| S   | 21.963457 | 31.622126 | 29.965046 |
|  |  |  |  |
|---|---|---|---|
| S | 24.874502 | 33.255589 | 33.272102 |
| S | 25.902163 | 29.437895 | 26.572887 |
| S | 28.215172 | 31.162186 | 28.330311 |
| S | 30.592749 | 31.162186 | 27.867916 |
| S | 32.424477 | 30.493345 | 24.919422 |
| S | 33.753288 | 26.007011 | 23.748718 |
| S | 36.559624 | 28.206245 | 27.143179 |

24 generated by VMD

| Ca | 18.302649 | 33.652500 | 33.802307 |
| Ca | 23.217846 | 34.068733 | 35.700447 |
| Ca | 23.282333 | 30.351435 | 33.145737 |
| Ca | 23.075369 | 34.851471 | 30.103786 |
| Ca | 25.161766 | 30.446112 | 28.368195 |
| Ca | 27.821669 | 32.599712 | 31.191866 |
| Ca | 29.147875 | 27.809895 | 30.049229 |
| Ca | 30.349628 | 32.542191 | 27.373409 |
| Ca | 30.423931 | 27.800936 | 24.614954 |
| Ca | 33.585930 | 30.169685 | 27.952152 |
| Ca | 34.260605 | 24.852772 | 26.826328 |
| Ca | 35.477821 | 29.281826 | 23.867125 |
| S | 20.751688 | 31.409540 | 35.306808 |
| S | 21.051479 | 35.694035 | 33.149185 |
| S | 22.088354 | 31.361513 | 29.913767 |
| S | 24.791613 | 33.572544 | 33.089458 |
| S | 26.213072 | 29.307842 | 30.956036 |
| S | 25.909222 | 33.815430 | 28.209133 |
| S | 28.096418 | 29.624645 | 26.555382 |
| S | 30.755917 | 31.148767 | 30.238262 |
| S | 31.802591 | 27.040699 | 27.787970 |
| S | 32.457813 | 30.731682 | 25.025770 |
| S | 33.365570 | 26.137617 | 23.635998 |
| S | 36.328865 | 28.028461 | 27.076767 |

24 generated by VMD

| Ca | 18.529898 | 33.520458 | 33.832359 |
| Ca | 23.093575 | 33.904900 | 35.727921 |
| Ca | 23.309738 | 30.248631 | 33.088245 |
| Ca | 22.889660 | 34.980518 | 30.394030 |
| Ca | 24.981787 | 30.693996 | 28.133863 |
| Ca | 27.732840 | 32.683800 | 31.079235 |
| Ca | 29.134209 | 27.914240 | 29.636707 |
| Ca | 30.638939 | 32.535984 | 27.299572 |
| Ca | 30.408838 | 27.626905 | 24.901199 |
| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 33.800694 | 30.102119 | 27.969618 |
| Ca      | 34.669346 | 24.860159 | 26.990173 |
| Ca      | 35.359852 | 28.984419 | 23.734257 |
| S       | 20.778284 | 31.145391 | 35.241585 |
| S       | 20.848185 | 35.771141 | 33.418030 |
| S       | 21.895685 | 28.984419 | 23.734257 |
| S       | 24.856928 | 33.580250 | 33.121906 |
| S       | 25.682529 | 34.210560 | 28.290499 |
| S       | 28.125656 | 29.906864 | 26.596910 |
| S       | 30.680420 | 31.173744 | 30.058533 |
| S       | 31.970188 | 27.068611 | 27.842880 |
| S       | 32.512756 | 30.583139 | 24.928055 |
| S       | 33.325996 | 25.745310 | 23.720551 |
| S       | 36.392094 | 28.04628 | 27.181713 |

24 generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 18.556633 | 33.449955 | 33.877312 |
| Ca      | 23.296219 | 33.977528 | 35.960552 |
| Ca      | 23.372723 | 30.332298 | 32.789104 |
| Ca      | 22.407900 | 34.839947 | 30.323978 |
| Ca      | 25.183905 | 30.605658 | 28.189594 |
| Ca      | 27.564516 | 32.630230 | 31.077019 |
| Ca      | 29.019659 | 27.989708 | 29.820583 |
| Ca      | 30.602663 | 32.517403 | 27.321730 |
| Ca      | 30.455664 | 27.725885 | 24.680073 |
| Ca      | 33.515816 | 30.068127 | 28.297638 |
| Ca      | 34.662918 | 25.015562 | 26.985207 |
| Ca      | 35.399017 | 28.892429 | 23.690701 |
| S       | 21.067524 | 31.180517 | 35.126625 |
| S       | 21.072550 | 35.851967 | 33.696510 |
| S       | 21.988089 | 31.417297 | 29.605827 |
| S       | 24.875614 | 33.815807 | 32.903500 |
| S       | 26.168680 | 29.587420 | 30.775753 |
| S       | 25.538986 | 33.889961 | 28.128090 |
| S       | 28.405609 | 29.916525 | 26.752811 |
| S       | 30.590767 | 31.121946 | 30.301521 |
| S       | 31.714949 | 26.864241 | 27.893381 |
| S       | 32.694195 | 30.697077 | 25.085434 |
| S       | 33.225327 | 25.828104 | 23.692551 |
| S       | 36.340099 | 28.044628 | 27.181713 |

24 generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 18.131577 | 33.768997 | 33.887085 |
| Ca      | 23.129181 | 33.813995 | 35.781944 |
| Ca      | 23.462185 | 30.263386 | 32.940346 |
Ca 22.810337  34.972088  30.557173
Ca 25.162537  30.531523  27.927032
Ca 27.690536  32.569397  30.983312
Ca 29.216692  27.787144  29.865393
Ca 30.484974  32.636230  27.310545
Ca 30.475094  27.643433  24.956303
Ca 33.561813  29.970911  28.239002
Ca 34.772449  25.116156  27.042377
Ca 35.143517  28.899691  23.397850
S  20.643467  31.451998  34.971760
S  20.903812  35.902767  33.697807
S  21.993910  31.430161  29.731342
S  24.994410  33.495205  33.150406
S  26.084906  29.380653  30.564079
S  25.703274  34.052177  28.234745
S  28.508923  29.737705  26.816706
S  30.779587  31.245201  30.252304
S  31.982119  26.734034  28.157864
S  32.534958  30.679451  24.944208
S  33.275726  25.878145  23.848917
S  36.274036  28.339577  26.681570

24 generated by VMD
Ca 18.455301  33.259304  33.161568
Ca 23.113535  33.591801  35.760330
Ca 23.261597  30.120949  32.852318
Ca 22.996973  34.815742  30.599125
Ca 25.147346  31.151909  27.973246
Ca 27.968353  32.940414  31.139406
Ca 29.248152  28.090532  29.839344
Ca 30.506157  32.644981  27.321186
Ca 30.160975  27.561153  25.070666
Ca 33.693932  30.313732  28.090984
Ca 34.680733  25.090967  27.140800
Ca 34.804951  28.530533  23.380434
S  20.821365  31.007904  34.809727
S  21.014927  35.719418  33.604580
S  21.981316  31.673033  29.630354
S  25.079472  33.393448  33.227276
S  26.153297  29.643333  30.798908
S  25.848385  34.159973  28.453869
S  28.301365  29.759342  26.853302
S  30.895729  31.397970  30.186394
S  32.024643  27.065859  28.377169
S  32.326462  30.553265  24.868538
S  32.989491  25.484203  24.083401
S  36.245613  28.330288  26.717766

24
generated by VMD
Ca  18.278477  33.609528  33.130592
Ca  23.106754  33.771736  35.941608
Ca  23.510578  30.155937  32.863762
Ca  22.936333  34.747997  30.627827
Ca  25.222670  31.008133  27.703823
Ca  27.778748  33.018738  31.430445
Ca  29.076086  27.949974  29.825500
Ca  30.100988  32.625290  27.548153
Ca  30.457233  27.632980  25.100834
Ca  33.612774  30.059998  28.160261
Ca  34.860058  25.032356  27.151691
Ca  34.919685  28.670626  23.158741
S   20.524017  31.129795  34.526218
S   21.159904  35.595055  33.514862
S   22.174351  31.330801  29.893280
S   25.026476  33.559335  33.307919
S   26.482735  29.841343  31.074600
S   25.775873  34.195511  28.491213
S   28.050447  29.791389  26.764759
S   30.674915  31.161592  30.111120
S   32.144283  26.965792  28.433104
S   32.469578  30.648067  24.674429
S   33.096306  25.544144  23.991081
S   36.280800  28.261370  26.514225

24
generated by VMD
Ca  18.449081  33.553486  33.103470
Ca  22.731220  34.000874  35.946747
Ca  23.514576  30.051886  32.996975
Ca  22.608706  34.726368  30.497709
Ca  25.392282  30.928156  27.996473
Ca  27.773603  32.930935  31.331440
Ca  29.070868  27.868349  29.771011
Ca  30.556610  32.753540  27.369556
Ca  30.607647  27.719288  24.956709
Ca  33.564117  30.022274  28.143440
Ca  34.684681  25.007351  27.061138
Ca  34.699459  28.649733  23.222630
S   20.732323  31.178164  35.013981
S   20.865124  35.772659  33.487373
S   22.225975  31.335962  29.786310
S   24.785330  33.604782  33.255924
S   26.478235  29.605762  30.895752
|    |   |   |   |
|----|---|---|---|
| S  | 25.680017 | 34.168301 | 28.573338 |
| S  | 28.514834 | 29.841629 | 26.843475 |
| S  | 30.859232 | 31.143982 | 30.196402 |
| S  | 32.117908 | 27.037106 | 28.231331 |
| S  | 32.607857 | 30.765060 | 24.705061 |
| S  | 32.912296 | 25.581091 | 23.975269 |
| S  | 36.261013 | 28.053331 | 26.578560 |
| Ca | 18.621862 | 33.804539 | 33.144318 |
| Ca | 22.866060 | 34.242519 | 35.870945 |
| Ca | 23.576561 | 30.310295 | 32.874241 |
| Ca | 22.836070 | 34.569828 | 30.659176 |
| Ca | 25.037529 | 30.512051 | 28.065514 |
| Ca | 27.675737 | 32.628281 | 31.268063 |
| Ca | 29.121767 | 27.828993 | 29.750347 |
| Ca | 30.344810 | 32.435028 | 27.639606 |
| Ca | 33.720070 | 30.084110 | 28.249626 |
| Ca | 34.598888 | 24.952042 | 26.766907 |
| Ca | 35.079441 | 28.845345 | 23.592148 |
| S  | 20.848549 | 31.417618 | 34.855423 |
| S  | 20.870903 | 35.941547 | 33.474201 |
| S  | 22.127695 | 30.930904 | 30.014166 |
| S  | 24.879589 | 33.731369 | 33.267670 |
| S  | 26.255157 | 29.598988 | 30.654659 |
| S  | 25.545437 | 34.088699 | 28.506762 |
| S  | 28.345791 | 29.865011 | 26.767231 |
| S  | 30.837725 | 31.016798 | 30.250016 |
| S  | 32.019154 | 26.908334 | 28.096548 |
| S  | 32.492554 | 30.807875 | 24.880375 |
| S  | 33.247971 | 25.950739 | 23.780516 |
| S  | 36.470444 | 28.155659 | 26.580606 |

24 generated by VMD

| Ca  | 18.659447 | 33.525085 | 33.046360 |
| Ca  | 22.850206 | 33.919212 | 36.128708 |
| Ca  | 23.367453 | 30.355892 | 32.907475 |
| Ca  | 23.114359 | 34.531731 | 31.015356 |
| Ca  | 24.630234 | 30.696207 | 27.638716 |
| Ca  | 27.723387 | 32.971775 | 31.268375 |
| Ca  | 29.015839 | 28.123287 | 29.678825 |
| Ca  | 30.596334 | 32.645287 | 27.133865 |
| Ca  | 30.415556 | 27.479746 | 24.847424 |
| Ca  | 33.605675 | 30.089302 | 28.087276 |
| Ca  | 34.580250 | 24.985790 | 27.274271 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 35.123058    | 28.702431    | 23.632       |
| S       | 20.884634    | 31.234081    | 34.94868     |
| S       | 21.076941    | 35.594143    | 33.53704     |
| S       | 21.916502    | 31.155956    | 29.850079    |
| S       | 24.963177    | 33.613415    | 33.308990    |
| S       | 26.305519    | 29.806593    | 30.635681    |
| S       | 25.663914    | 34.279999    | 28.591206    |
| S       | 28.216278    | 29.875187    | 26.566713    |
| S       | 30.982378    | 31.266476    | 30.186739    |
| S       | 31.949806    | 27.013937    | 28.069551    |
| S       | 32.384968    | 30.678921    | 24.789864    |
| S       | 33.259827    | 25.653898    | 23.966972    |
| S       | 36.434292    | 28.101690    | 26.829084    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.263704    | 33.489639    | 33.189152    |
| Ca      | 22.744732    | 34.444427    | 35.856079    |
| Ca      | 23.438673    | 30.201797    | 33.194260    |
| Ca      | 23.171921    | 34.604733    | 30.705427    |
| Ca      | 24.727995    | 30.464441    | 27.777628    |
| Ca      | 27.78307     | 32.876770    | 31.492371    |
| Ca      | 29.152494    | 27.970482    | 29.722084    |
| Ca      | 30.650965    | 32.466209    | 27.455265    |
| Ca      | 30.384188    | 27.731192    | 24.756382    |
| Ca      | 33.766125    | 30.053967    | 27.977234    |
| Ca      | 34.613632    | 25.029224    | 26.808945    |
| Ca      | 35.113201    | 28.637108    | 23.506935    |
| S       | 20.712782    | 31.514278    | 34.957619    |
| S       | 20.746651    | 35.779217    | 33.173897    |
| S       | 22.073488    | 31.107590    | 29.923866    |
| S       | 24.952888    | 33.680882    | 33.518333    |
| S       | 26.248062    | 29.453697    | 31.131075    |
| S       | 25.865677    | 33.924618    | 28.631950    |
| S       | 28.334299    | 29.883516    | 26.687622    |
| S       | 30.875626    | 31.063660    | 30.318790    |
| S       | 31.959908    | 27.092304    | 27.754683    |
| S       | 32.555592    | 30.905550    | 24.855644    |
| S       | 33.057804    | 25.782248    | 23.699841    |
| S       | 36.521294    | 28.142523    | 26.844898    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.186222    | 33.500561    | 33.370262    |
| Ca      | 22.706841    | 34.627571    | 35.852955    |
| Ca      | 23.275061    | 30.234257    | 33.219601    |
| Ca      | 22.518478    | 34.468292    | 30.685753    |
| Ca      | 25.204872    | 30.493954    | 27.832455    |
|   |       |       |       |
|---|-------|-------|-------|
| Ca | 27.852951 | 32.898186 | 31.492939 |
| Ca | 29.139591  | 28.026821  | 29.883665  |
| Ca | 30.683731  | 32.542305  | 27.398315  |
| Ca | 30.546852  | 27.935492  | 24.749132  |
| Ca | 33.690674  | 29.810883  | 27.914082  |
| Ca | 34.450977  | 24.860792  | 26.629097  |
| Ca | 35.416710  | 28.875122  | 23.564362  |
| S  | 20.700233  | 31.748255  | 35.214542  |
| S  | 20.544865  | 35.827690  | 33.185413  |
| S  | 22.203226  | 30.900431  | 30.011051  |
| S  | 24.969444  | 33.518028  | 33.282921  |
| S  | 26.308357  | 29.587276  | 31.314604  |
| S  | 25.856117  | 34.038944  | 28.593655  |
| S  | 28.376400  | 29.517729  | 26.721066  |
| S  | 30.811310  | 31.301819  | 30.291672  |
| S  | 31.688871  | 27.078205  | 27.629890  |
| S  | 32.757584  | 30.790920  | 24.968666  |
| S  | 33.293766  | 25.931311  | 23.431326  |
| S  | 36.536728  | 27.785231  | 26.702621  |

24 generated by VMD

|   |       |       |       |
|---|-------|-------|-------|
| Ca | 18.563166  | 33.676746  | 33.304539  |
| Ca | 23.184872  | 34.421974  | 36.112007  |
| Ca | 23.344913  | 30.289394  | 32.944252  |
| Ca | 22.926849  | 34.255077  | 30.923193  |
| Ca | 24.831867  | 30.372215  | 27.558418  |
| Ca | 27.553442  | 32.681351  | 30.999683  |
| Ca | 29.121958  | 28.080568  | 29.875971  |
| Ca | 30.602667  | 32.718513  | 27.33534  |
| Ca | 30.310827  | 27.928034  | 24.61953  |
| Ca | 33.614990  | 29.984791  | 28.009300  |
| Ca | 34.303432  | 24.949793  | 26.867613  |
| Ca | 35.695225  | 28.762751  | 24.017288  |
| S  | 20.857182  | 31.760162  | 35.363060  |
| S  | 21.145823  | 35.751694  | 33.571114  |
| S  | 21.971048  | 30.879623  | 29.857473  |
| S  | 24.839479  | 33.510307  | 33.200554  |
| S  | 25.998066  | 29.405834  | 30.617207  |
| S  | 25.522617  | 33.753860  | 28.478165  |
| S  | 28.304188  | 29.958282  | 26.597244  |
| S  | 30.978014  | 31.312214  | 29.981915  |
| S  | 31.626661  | 27.099995  | 27.903402  |
| S  | 32.565430  | 30.771049  | 24.987295  |
| S  | 33.301037  | 25.952988  | 23.717106  |
| S  | 36.556381  | 28.022842  | 27.099747  |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.137102 | 33.299900 | 33.960579 |
| Ca      | 23.244324 | 34.609581 | 35.742359 |
| Ca      | 23.187527 | 30.350882 | 33.009014 |
| Ca      | 23.072411 | 34.387470 | 30.675434 |
| Ca      | 24.560490 | 30.401720 | 27.535309 |
| Ca      | 27.863668 | 32.626244 | 31.126675 |
| Ca      | 28.966358 | 27.921566 | 29.799318 |
| Ca      | 30.574938 | 32.493855 | 27.466244 |
| Ca      | 30.419413 | 28.243919 | 24.694483 |
| Ca      | 33.801170 | 29.948895 | 28.254326 |
| Ca      | 34.514862 | 24.83395  | 26.916672 |
| Ca      | 35.665016 | 28.971008 | 23.660885 |
| S       | 21.067171 | 31.710306 | 35.537628 |
| S       | 20.746494 | 35.759861 | 33.363022 |
| S       | 21.754320 | 31.182039 | 29.781073 |
| S       | 25.044342 | 33.536499 | 32.949177 |
| S       | 26.021023 | 29.535351 | 30.669376 |
| S       | 25.708889 | 33.775993 | 28.297768 |
| S       | 28.192553 | 29.690626 | 26.686403 |
| S       | 30.901136 | 31.088037 | 30.216726 |
| S       | 31.713858 | 27.032372 | 28.043867 |
| S       | 32.834347 | 30.929679 | 24.968815 |
| S       | 33.198711 | 26.221352 | 23.603456 |
| S       | 36.529957 | 27.758419 | 26.981487 |

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| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.353985 | 33.044365 | 33.594357 |
| Ca      | 23.274376 | 34.119160 | 35.771927 |
| Ca      | 23.430906 | 30.266933 | 32.918701 |
| Ca      | 22.887484 | 34.589817 | 30.756588 |
| Ca      | 24.735901 | 30.666513 | 27.603800 |
| Ca      | 27.904793 | 32.900688 | 30.871777 |
| Ca      | 29.218937 | 28.587524 | 29.934519 |
| Ca      | 30.568214 | 32.791031 | 26.873833 |
| Ca      | 30.512625 | 27.885370 | 24.635006 |
| Ca      | 33.710602 | 29.947105 | 28.170017 |
| Ca      | 33.865730 | 24.809523 | 27.066887 |
| Ca      | 35.543930 | 28.757614 | 24.074575 |
| S       | 20.958723 | 31.274017 | 35.147198 |
| S       | 20.703655 | 35.597580 | 33.661133 |
| S       | 22.047678 | 31.003056 | 30.008039 |
| S       | 25.066658 | 33.474834 | 33.202503 |
| S       | 26.382526 | 29.707483 | 30.858908 |
| S       | 25.501017 | 34.027321 | 28.340298 |
| S       | 28.316839 | 30.055660 | 26.513702 |
|   | X     | Y     | Z     |
|---|-------|-------|-------|
| S | 31.010130 | 31.660566 | 30.049061 |
| S | 31.400936 | 26.976994  | 27.928614 |
| S | 32.817623 | 30.567844  | 25.000273 |
| S | 33.154247 | 25.970146  | 23.706928 |
| S | 36.352543 | 27.619789  | 27.258625 |

24 generated by VMD

| Ca | 18.320192 | 32.951550 | 33.626934 |
| Ca | 23.156755 | 34.544506 | 35.767532 |
| Ca | 23.409250 | 29.958294 | 32.906487 |
| Ca | 22.981983 | 34.870560 | 30.683672 |
| Ca | 24.996887 | 30.720270 | 27.683777 |
| Ca | 27.594286 | 32.738201 | 31.197304 |
| Ca | 28.990822 | 28.557816 | 29.924931 |
| Ca | 30.560436 | 32.631512 | 27.352571 |
| Ca | 30.350145 | 27.806623 | 24.525591 |
| Ca | 33.568531 | 30.071850 | 28.268490 |
| Ca | 34.168205 | 24.920643 | 26.823166 |
| Ca | 35.336163 | 28.579398 | 23.890696 |
| S  | 21.108648 | 31.411411 | 35.273422 |
| S  | 20.803122 | 35.683338 | 33.350346 |
| S  | 22.178785 | 31.360294 | 29.793650 |
| S  | 25.058388 | 33.239822 | 33.174122 |
| S  | 26.376581 | 29.550629 | 30.803020 |
| S  | 25.607475 | 33.920696 | 28.392132 |
| S  | 28.377419 | 29.765583 | 26.695002 |
| S  | 30.823320 | 31.353004 | 30.277161 |
| S  | 31.480516 | 27.070396 | 27.831621 |
| S  | 32.649837 | 30.704456 | 24.757879 |
| S  | 33.232601 | 25.875944 | 23.849657 |
| S  | 36.589710 | 28.014706 | 27.090893 |

24 generated by VMD

| Ca | 18.409128 | 32.926102 | 33.615711 |
| Ca | 23.326010 | 34.201874 | 35.872810 |
| Ca | 23.588627 | 30.278322 | 32.579247 |
| Ca | 23.296772 | 34.555523 | 30.683048 |
| Ca | 24.874620 | 30.643137 | 27.645306 |
| Ca | 27.791363 | 32.836647 | 31.205599 |
| Ca | 29.184856 | 28.552219 | 29.770172 |
| Ca | 30.350847 | 32.761738 | 26.959522 |
| Ca | 30.320276 | 27.826004 | 24.466536 |
| Ca | 33.320091 | 30.191660 | 28.254782 |
| Ca | 33.836071 | 25.042543 | 27.104273 |
| Ca | 35.368713 | 28.532238 | 24.187710 |
| S  | 21.180103 | 31.266493 | 35.096249 |
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24

generated by VMD

Ca  18.121712  33.106953  33.434002
Ca  22.665562  34.403225  35.761597
Ca  23.410866  30.155474  33.100014
Ca  23.243187  34.572514  30.495909
Ca  25.040508  30.316803  27.918476
Ca  27.734106  32.975674  31.416023
Ca  29.540916  28.410519  30.025288
Ca  30.446314  32.954113  27.586346
Ca  30.470732  27.939377  24.777285
Ca  33.583740  30.104630  28.170746
Ca  33.968369  24.878237  26.525665
Ca  35.340912  28.418774  23.543430
S   20.844183  31.337780  35.070423
S   20.722569  35.499043  32.996372
S   22.144342  31.295757  29.736950
S   25.086130  33.381649  33.389420
S   26.581314  29.724663  31.193750
S   25.859592  33.927105  28.408590
S   28.468925  29.982723  26.973358
S   30.796915  31.744343  30.309126
S   31.764650  27.040808  26.199703
S   32.792221  30.632593  24.760342
S   32.897549  25.777914  23.405117
S   36.194740  27.719364  26.742119

24

generated by VMD

Ca  18.250031  33.036259  33.512074
Ca  22.969757  34.386448  35.992958
Ca  23.531023  30.248016  32.827728
Ca  22.807060  34.765694  30.576101
Ca  24.963989  30.365046  27.784513
Ca  27.909286  32.884148  31.417316
Ca  29.393324  28.378025  29.889091
|   | Value1 | Value2 | Value3 |
|---|--------|--------|--------|
| Ca | 30.522243 | 32.786362 | 27.362213 |
| Ca | 30.518614 | 27.834293 | 24.602297 |
| Ca | 33.514980 | 30.066574 | 28.335720 |
| Ca | 34.148834 | 24.951389 | 26.863438 |
| Ca | 35.310345 | 28.603218 | 23.631405 |
| S  | 21.006836 | 31.388359 | 35.039108 |
| S  | 20.718929 | 35.748543 | 33.32695 |
| S  | 22.181597 | 31.172028 | 29.721302 |
| S  | 24.999651 | 33.658203 | 33.219475 |
| S  | 26.527344 | 29.415710 | 30.961597 |
| S  | 25.799011 | 33.891743 | 28.476208 |
| S  | 28.337723 | 29.839182 | 26.672939 |
| S  | 30.940495 | 31.493799 | 30.367750 |
| S  | 31.450304 | 27.063604 | 27.961287 |
| S  | 32.612309 | 30.608021 | 24.979378 |
| S  | 33.200779 | 25.740143 | 23.359518 |
| S  | 36.105648 | 27.975222 | 27.053936 |

24 generated by VMD

|   | Value1 | Value2 | Value3 |
|---|--------|--------|--------|
| Ca | 18.218632 | 33.145798 | 33.753563 |
| Ca | 28.082167 | 34.284081 | 35.753471 |
| Ca | 28.495621 | 30.224751 | 32.931698 |
| Ca | 22.957691 | 34.857281 | 30.442986 |
| Ca | 24.760221 | 30.377165 | 27.728495 |
| Ca | 28.039644 | 32.695667 | 31.057405 |
| Ca | 29.311996 | 28.262705 | 29.988121 |
| Ca | 30.624275 | 32.538811 | 27.392632 |
| Ca | 30.457151 | 27.804773 | 24.494038 |
| Ca | 33.613178 | 29.919548 | 28.163933 |
| Ca | 34.247147 | 24.783907 | 26.869915 |
| Ca | 35.294899 | 29.060818 | 23.855705 |
| S  | 20.905914 | 31.563797 | 35.134869 |
| S  | 20.599777 | 35.789574 | 33.473572 |
| S  | 21.934303 | 31.270061 | 29.718925 |
| S  | 25.064632 | 33.416470 | 33.031837 |
| S  | 26.296988 | 29.523716 | 31.037628 |
| S  | 25.710014 | 33.867245 | 28.445602 |
| S  | 28.358425 | 29.704473 | 26.698097 |
| S  | 31.151171 | 31.512938 | 30.366444 |
| S  | 31.648533 | 26.968681 | 27.965990 |
| S  | 32.520489 | 30.800127 | 25.024967 |
| S  | 33.167744 | 26.063749 | 23.650242 |
| S  | 36.259457 | 27.863892 | 26.959900 |

24 generated by VMD

|   | Value1 | Value2 | Value3 |
|---|--------|--------|--------|
| Ca | 18.466349 | 33.528683 | 33.550461 |
Ca       23.219524       34.276207       35.965416
Ca       23.085672       29.916721       32.943775
Ca       23.130941       34.723919       30.531349
Ca       24.841921       30.482077       27.419910
Ca       27.701427       32.580635       31.005907
Ca       29.115917       28.540033       29.929214
Ca       30.440672       32.550896       27.487059
Ca       30.412008       27.727110       24.731991
Ca       33.636795       30.158840       28.020386
Ca       34.307934       24.992798       27.035450
Ca       35.474724       29.016666       23.773853
S        20.910898       31.635717       35.426674
S        21.179386       35.911968       33.650463
S        21.921080       31.180767       29.705700
S        24.969534       32.991322       33.103409
S        26.253450       29.417364       30.752789
S        25.649523       33.675617       28.216267
S        28.217754       29.703957       26.658089
S        30.913147       31.630444       30.171577
S        31.547184       27.094723       28.109875
S        32.550930       30.749483       25.057510
S        33.322285       25.986156       23.696835
S        36.450962       27.827932       26.996101
24
-generated by VMD
Ca       18.593884       33.493958       33.614994
Ca       23.096180       34.670628       35.742355
Ca       23.444113       29.881409       32.945705
Ca       22.764490       34.697536       30.524294
Ca       25.002848       30.470564       28.008307
Ca       27.640535       32.657074       30.945629
Ca       29.388851       28.061096       29.924168
Ca       30.606857       32.687897       27.473274
Ca       30.468124       27.967138       24.606155
Ca       33.476811       29.874941       28.357813
Ca       34.289482       24.912773       26.742641
Ca       35.566559       29.172228       23.763950
S        20.996649       31.570030       35.294189
S        20.768854       36.127968       33.374168
S        21.909502       31.110485       29.898996
S        24.923183       33.229294       32.955265
S        26.588387       29.316662       31.126812
S        25.476454       33.728127       28.214777
S        28.241388       29.885220       26.819637
S        30.712019       31.222063       30.247017
S        31.597057       26.848904       27.812050
|   |          |          |          |
|---|----------|----------|----------|
| S | 32.609753 | 30.766951 | 25.014864 |
| S | 33.335945 | 26.086838 | 23.468067 |
| S | 36.220432 | 27.860233 | 27.068211 |

24

generated by VMD

| Ca |          |          |          |
|----|----------|----------|----------|
| Ca | 18.372238 | 32.971394 | 33.579582 |
| Ca | 22.986494 | 34.822060 | 35.526649 |
| Ca | 23.645334 | 30.282957 | 33.081703 |
| Ca | 22.719124 | 34.636845 | 30.459038 |
| Ca | 24.747543 | 30.417006 | 27.933736 |
| Ca | 27.889544 | 32.923630 | 31.194370 |
| Ca | 29.289570 | 28.077145 | 29.944733 |
| Ca | 30.391535 | 32.289395 | 27.555066 |
| Ca | 30.469765 | 27.917019 | 24.522398 |
| Ca | 33.599495 | 29.747841 | 28.264572 |
| Ca | 34.208511 | 24.819664 | 26.407455 |
| Ca | 35.597366 | 29.337385 | 24.023611 |
| S  | 21.158985 | 31.559368 | 35.352158 |
| S  | 20.696632 | 36.058643 | 33.158318 |
| S  | 21.917175 | 31.316002 | 29.920616 |
| S  | 24.967060 | 33.617226 | 33.026283 |
| S  | 26.451963 | 29.576044 | 31.076010 |
| S  | 25.520100 | 33.734234 | 28.396149 |
| S  | 28.130745 | 29.384897 | 26.878479 |
| S  | 30.936890 | 31.158878 | 30.434483 |
| S  | 31.599230 | 26.843239 | 27.840033 |
| S  | 32.507256 | 30.684624 | 25.272121 |
| S  | 33.545738 | 26.484962 | 23.243771 |
| S  | 36.371662 | 27.645048 | 26.849167 |

24

generated by VMD

| Ca |          |          |          |
|----|----------|----------|----------|
| Ca | 18.651306 | 33.238979 | 33.191151 |
| Ca | 23.065481 | 34.938831 | 35.612156 |
| Ca | 23.535805 | 30.251255 | 33.115795 |
| Ca | 22.766872 | 34.589504 | 30.324162 |
| Ca | 24.890034 | 30.245092 | 28.041687 |
| Ca | 27.675911 | 32.561901 | 31.287872 |
| Ca | 29.174107 | 27.901854 | 29.962891 |
| Ca | 30.318161 | 32.218723 | 27.667158 |
| Ca | 30.557783 | 28.001432 | 24.512154 |
| Ca | 33.705032 | 30.006397 | 28.443798 |
| Ca | 34.152081 | 24.872578 | 26.471098 |
| Ca | 35.460777 | 29.297541 | 23.711460 |
| S  | 21.184696 | 31.701447 | 35.340530 |
| S  | 20.964294 | 35.947609 | 33.153240 |
| S  | 21.874020 | 31.113506 | 29.978086 |
|   |       |       |       |
|---|-------|-------|-------|
| S | 24.868387 | 33.642666 | 32.997238 |
| S | 26.353754 | 29.498440 | 31.237789 |
| S | 25.611801 | 33.721565 | 28.450459 |
| S | 28.063732 | 29.587883 | 26.770073 |
| S | 30.809158 | 30.889069 | 30.519707 |
| S | 31.694023 | 26.992069 | 27.891655 |
| S | 32.632862 | 30.919680 | 25.252613 |
| S | 33.414959 | 26.263714 | 23.134665 |
| S | 36.294994 | 27.898281 | 26.872662 |

24

generated by VMD

| Ca |       |       |       |
|----|-------|-------|-------|
| Ca | 18.551088 | 33.121105 | 33.655804 |
| Ca | 22.945581 | 35.038708 | 35.649693 |
| Ca | 23.485901 | 30.363338 | 33.242973 |
| Ca | 22.647629 | 34.457092 | 30.324966 |
| Ca | 24.853926 | 30.405901 | 27.902878 |
| Ca | 27.839050 | 32.835686 | 31.173428 |
| Ca | 29.213690 | 27.938425 | 29.837719 |
| Ca | 30.518156 | 32.249580 | 27.547256 |
| Ca | 30.484932 | 28.078070 | 24.430481 |
| Ca | 33.710644 | 29.934202 | 28.303059 |
| Ca | 34.055126 | 24.870205 | 26.258568 |
| Ca | 35.555382 | 29.303593 | 23.947536 |
| S  | 21.152460 | 31.902092 | 35.591843 |
| S  | 20.594862 | 35.894909 | 32.966297 |
| S  | 21.838427 | 30.962442 | 29.857832 |
| S  | 24.921108 | 33.474564 | 33.175316 |
| S  | 26.356819 | 29.536549 | 31.174168 |
| S  | 25.824581 | 33.572983 | 28.417267 |
| S  | 28.204880 | 29.529953 | 26.722752 |
| S  | 30.833357 | 31.035774 | 30.495377 |
| S  | 31.569241 | 26.885057 | 27.637552 |
| S  | 32.810970 | 30.774363 | 25.320503 |
| S  | 33.384136 | 26.420757 | 23.203598 |
| S  | 36.368137 | 27.714710 | 27.103180 |

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generated by VMD

| Ca |       |       |       |
|----|-------|-------|-------|
| Ca | 18.424053 | 33.243382 | 33.654999 |
| Ca | 23.036150 | 34.877556 | 35.831886 |
| Ca | 23.500164 | 30.213717 | 32.971420 |
| Ca | 22.879299 | 34.322021 | 30.595921 |
| Ca | 24.771437 | 30.363127 | 27.715389 |
| Ca | 27.755566 | 32.851280 | 31.131660 |
| Ca | 29.283039 | 28.261488 | 29.804573 |
| Ca | 30.422022 | 32.531807 | 27.399059 |
| Ca | 30.385244 | 28.109447 | 24.425888 |
| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 33.532433| 29.959042| 28.241848|
| Ca      | 34.068405| 24.756193| 26.557980|
| Ca      | 35.636021| 28.921162| 24.220856|
| S       | 21.146610| 31.775240| 35.634205|
| S       | 20.978951| 35.855179| 33.101555|
| S       | 21.734703| 30.969225| 29.765211|
| S       | 24.866299| 33.265804| 33.174278|
| S       | 26.516268| 29.320469| 30.917099|
| S       | 25.686947| 33.653965| 28.349676|
| S       | 28.134541| 29.853733| 26.665684|
| S       | 30.947557| 31.427250| 30.274727|
| S       | 31.496138| 26.927523| 27.821337|
| S       | 32.712299| 30.878456| 25.175552|
| S       | 33.431114| 26.335581| 23.384403|
| S       | 36.374874| 27.627401| 27.124798|

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generated by VMD

| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 18.367184| 33.041821| 33.704006|
| Ca      | 23.191523| 34.673870| 35.522621|
| Ca      | 23.309460| 30.082033| 33.016716|
| Ca      | 22.952530| 34.608555| 30.594788|
| Ca      | 24.781845| 30.375740| 27.752907|
| Ca      | 27.874439| 32.662949| 31.099102|
| Ca      | 29.129475| 28.519125| 30.010693|
| Ca      | 30.556728| 32.568001| 27.301640|
| Ca      | 30.473152| 28.111973| 24.711781|
| Ca      | 33.609695| 29.927279| 27.912119|
| Ca      | 33.976456| 24.788204| 26.694283|
| Ca      | 35.524254| 29.048306| 24.174580|
| S       | 21.015186| 31.653692| 35.386742|
| S       | 20.827694| 35.727516| 33.186081|
| S       | 22.031513| 31.900112| 29.701759|
| S       | 25.043541| 33.227859| 33.157181|
| S       | 26.267246| 29.224745| 30.926750|
| S       | 25.865505| 33.758400| 28.392834|
| S       | 28.224895| 29.904465| 26.842609|
| S       | 31.016140| 31.432627| 30.276228|
| S       | 31.613562| 27.197584| 28.081598|
| S       | 32.499981| 30.841784| 24.948826|
| S       | 33.323902| 26.111958| 23.569664|
| S       | 36.244125| 27.621578| 26.974604|

24

generated by VMD

| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 18.229324| 33.449871| 33.929543|
| Ca      | 23.168215| 34.332928| 35.785751|
| Ca      | 23.614473| 29.910728| 32.798630|
Ca     22.791859  34.566063  30.780270
Ca     24.955650  30.541794  27.645458
Ca     27.787212  32.785400  31.100124
Ca     29.408350  28.444084  29.740788
Ca     30.292768  32.660164  27.192234
Ca     30.500610  27.956627  24.440498
Ca     33.376087  29.962734  28.073385
Ca     34.155243  24.848648  27.044773
Ca     35.573082  28.806309  24.121414
S      21.125795  31.522032  35.202251
S      20.705782  35.851959  33.411324
S      22.087433  31.222900  29.609436
S      24.994066  33.285328  33.92181
S      26.457201  29.418907  30.874912
S      25.670633  33.969810  28.354458
S      28.308176  29.726755  26.667439
S      30.831450  31.664198  30.107086
S      31.366322  26.943117  27.858486
S      32.557472  30.664452  25.011024
S      33.512508  25.962704  23.538626
S      36.250343  27.802563  27.259947

generated by VMD

Ca     18.385414  33.245377  34.122704
Ca     23.176720  34.655190  35.566135
Ca     23.359221  30.100746  32.574306
Ca     22.805500  34.664642  30.751217
Ca     24.678658  30.651871  27.646328
Ca     27.859041  32.550606  30.996902
Ca     28.986517  28.383556  30.014238
Ca     30.564871  32.627663  27.058661
Ca     30.502823  27.896095  24.659672
Ca     33.704773  30.089506  28.108231
Ca     34.079441  24.830074  26.914665
Ca     35.684448  28.974934  24.067173
S      21.308456  31.623720  35.397675
S      20.603127  35.727524  33.436272
S      21.757036  31.352291  29.612072
S      24.986074  33.024517  33.298389
S      26.172733  29.312416  30.772221
S      25.713163  33.875572  28.477505
S      28.137562  29.882168  26.768806
S      30.956589  31.394955  30.018589
S      31.712534  27.007328  28.066486
S      32.692127  30.673258  24.907887
S      33.579456  26.104050  23.571957
|   |   |   |
|---|---|---|
| S | 36.313789 | 27.651966 | 27.131729 |

24

generated by VMD

| Ca | 18.349186 | 32.728447 | 33.771996 |
| Ca | 22.965534 | 34.493027 | 35.607178 |
| Ca | 23.423714 | 30.179924 | 32.802505 |
| Ca | 23.107216 | 34.83843  | 30.597729 |
| Ca | 24.934465 | 30.461054 | 27.819336 |
| Ca | 27.840580 | 32.770897 | 31.129715 |
| Ca | 29.169407 | 28.560829 | 29.975821 |
| Ca | 30.617256 | 32.607147 | 27.067909 |
| Ca | 30.367800 | 27.892181 | 24.614170 |
| Ca | 33.715641 | 30.065771 | 27.913803 |
| Ca | 33.869662 | 24.856506 | 26.891026 |
| Ca | 35.590271 | 28.819340 | 24.127514 |

| S  | 21.118612 | 31.455366 | 35.56244 |
| S  | 20.516451 | 35.530834 | 33.167927 |
| S  | 21.904770 | 31.719194 | 29.613613 |
| S  | 24.964714 | 33.314304 | 33.336414 |
| S  | 26.302383 | 29.502352 | 30.932547 |
| S  | 25.855970 | 33.806744 | 28.610085 |
| S  | 28.242895 | 29.736589 | 26.658535 |
| S  | 31.013297 | 31.572151 | 30.251579 |
| S  | 31.599598 | 27.111618 | 28.099726 |
| S  | 32.619236 | 30.645802 | 24.887108 |
| S  | 33.269867 | 25.971443 | 23.443415 |
| S  | 36.269287 | 27.664616 | 27.064137 |

24

generated by VMD

| Ca | 18.296114 | 32.656773 | 33.736835 |
| Ca | 23.189018 | 34.368423 | 35.671478 |
| Ca | 23.561653 | 30.026814 | 32.750351 |
| Ca | 22.857464 | 34.782604 | 30.732437 |
| Ca | 24.854681 | 31.006371 | 27.672810 |
| Ca | 28.078581 | 32.812508 | 31.005882 |
| Ca | 29.260166 | 28.594259 | 29.966719 |
| Ca | 30.564568 | 32.831371 | 27.139137 |
| Ca | 30.216366 | 27.822277 | 24.744093 |
| Ca | 33.536533 | 29.874771 | 27.981056 |
| Ca | 34.009926 | 24.734737 | 27.165867 |
| Ca | 35.390555 | 28.685959 | 24.033669 |
| S  | 21.327202 | 31.237064 | 35.306335 |
| S  | 20.544561 | 35.526066 | 33.243122 |
| S  | 21.872694 | 31.375673 | 29.659155 |
| S  | 25.100309 | 33.256039 | 33.161270 |
| S  | 26.437153 | 29.526587 | 30.827396 |
|    | 25.607862 | 34.086632 | 28.475811 |
|----|----------|----------|-----------|
| S  | 28.247391| 30.128941| 26.705685 |
| S  | 31.129488| 31.780516| 30.055588 |
| S  | 31.412374| 27.137783| 28.108097 |
| S  | 32.628735| 30.581272| 24.968407 |
| S  | 33.394054| 25.967449| 23.684418 |
| S  | 36.194160| 27.499159| 27.144363 |

24

*generated by VMD*

| Ca | 18.370424 | 32.897743 | 33.393902 |
| Ca | 22.924303 | 34.641922 | 35.779778 |
| Ca | 23.637157 | 30.275791 | 32.762310 |
| Ca | 22.679712 | 34.591206 | 30.925335 |
| Ca | 24.888239 | 30.660196 | 27.948431 |
| Ca | 27.772148 | 32.951702 | 31.245495 |
| Ca | 29.172840 | 28.314468 | 29.958340 |
| Ca | 30.534281 | 32.574883 | 27.225449 |
| Ca | 30.441149 | 27.777073 | 24.511543 |
| Ca | 33.527287 | 29.945074 | 27.781168 |
| Ca | 33.943386 | 24.641611 | 26.861477 |
| Ca | 35.848640 | 28.941523 | 24.040825 |
| S  | 21.228626 | 31.615116 | 35.281773 |
| S  | 20.474449 | 35.593628 | 33.350571 |
| S  | 22.046429 | 31.178410 | 29.760750 |
| S  | 24.922728 | 33.675247 | 33.291016 |
| S  | 26.394878 | 29.706665 | 31.135296 |
| S  | 25.600849 | 33.941032 | 28.673481 |
| S  | 28.252172 | 29.719284 | 26.737196 |
| S  | 30.737139 | 31.381042 | 30.081703 |
| S  | 31.573706 | 27.052904 | 28.001816 |
| S  | 32.750488 | 30.627844 | 24.835985 |
| S  | 33.610249 | 26.242346 | 23.403837 |
| S  | 36.388836 | 27.353321 | 26.952595 |

24

*generated by VMD*

| Ca | 18.430099 | 32.845306 | 33.855072 |
| Ca | 23.063906 | 34.602695 | 35.523621 |
| Ca | 23.482445 | 30.134644 | 32.656311 |
| Ca | 22.940359 | 34.574879 | 30.801653 |
| Ca | 24.927414 | 30.902025 | 27.802029 |
| Ca | 27.778446 | 32.752220 | 31.063591 |
| Ca | 29.538452 | 28.473181 | 29.878681 |
| Ca | 30.427101 | 32.473499 | 27.217825 |
| Ca | 30.363890 | 27.733791 | 24.548038 |
| Ca | 33.480114 | 30.034348 | 28.311344 |
| Ca | 33.832634 | 24.861576 | 26.812252 |
|    |      |      |      |
|----|------|------|------|
| Ca | 35.19173 | 28.932369 | 23.995394 |
| S  | 21.310867 | 31.562155 | 35.227337 |
| S  | 20.613525 | 35.672451 | 33.212563 |
| S  | 21.947771 | 31.179449 | 29.845394 |
| S  | 25.041311 | 33.325993 | 33.079300 |
| S  | 26.509079 | 29.543640 | 31.045567 |
| S  | 25.655291 | 33.878197 | 28.521744 |
| S  | 28.301352 | 29.767117 | 26.702408 |
| S  | 30.907383 | 31.526339 | 30.290321 |
| S  | 31.343958 | 27.096199 | 27.893265 |
| S  | 32.701664 | 30.641319 | 24.934277 |
| S  | 33.320419 | 26.184341 | 23.427664 |
| S  | 36.083332 | 27.602304 | 27.294384 |

24 generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 18.395172 | 32.779884 | 33.688553 |
| Ca | 22.848722 | 34.355965 | 35.509426 |
| Ca | 23.694559 | 30.001137 | 33.119892 |
| Ca | 22.950134 | 34.725391 | 30.538776 |
| Ca | 25.026962 | 30.590820 | 27.815264 |
| Ca | 27.950140 | 33.076180 | 30.842480 |
| Ca | 29.634233 | 28.730145 | 29.949825 |
| Ca | 30.576548 | 32.744938 | 27.177660 |
| Ca | 30.414740 | 28.040699 | 24.670300 |
| Ca | 33.561337 | 29.950863 | 27.982357 |
| Ca | 33.361362 | 24.744129 | 26.796759 |
| Ca | 35.645176 | 28.852802 | 24.154099 |
| S  | 21.122013 | 31.248634 | 35.539452 |
| S  | 20.506130 | 35.448772 | 33.022980 |
| S  | 22.150969 | 31.124302 | 30.059628 |
| S  | 25.036964 | 33.486298 | 33.145996 |
| S  | 26.560268 | 29.603310 | 30.960930 |
| S  | 25.817755 | 33.809223 | 28.097996 |
| S  | 28.355352 | 30.110695 | 26.794785 |
| S  | 31.059565 | 31.665289 | 30.255390 |
| S  | 31.253178 | 26.982342 | 28.046246 |
| S  | 32.756031 | 30.698193 | 25.074028 |
| S  | 33.147804 | 26.286991 | 23.496929 |
| S  | 35.894909 | 27.243073 | 27.200310 |

24 generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 18.191675 | 32.975697 | 33.728497 |
| Ca | 22.714331 | 34.916660 | 35.666962 |
| Ca | 23.729860 | 30.190674 | 33.132889 |
| Ca | 22.783871 | 34.448669 | 30.409676 |
| Ca | 25.106602 | 30.457678 | 27.877186 |
|       | 455  | 27.914371 | 32.875401 | 31.135712 |
|-------|------|------------|------------|------------|
| Ca    | 455  | 29.672508  | 28.422722  | 29.975586  |
| Ca    | 455  | 30.449018  | 28.007298  | 24.479670  |
| Ca    | 455  | 33.405472  | 29.813854  | 28.392307  |
| Ca    | 455  | 33.703777  | 24.752037  | 26.419756  |
| Ca    | 455  | 35.597965  | 28.890141  | 23.783251  |
| S     | 455  | 21.150082  | 31.536091  | 35.287811  |
| S     | 455  | 20.442928  | 35.540379  | 32.799309  |
| S     | 455  | 22.087172  | 31.025372  | 29.932362  |
| S     | 455  | 24.969646  | 33.538239  | 33.323799  |
| S     | 455  | 26.574043  | 29.695530  | 31.245415  |
| S     | 455  | 25.688597  | 33.720490  | 28.299877  |
| S     | 455  | 28.596663  | 29.864059  | 26.927288  |
| S     | 455  | 31.049255  | 31.447994  | 30.386431  |
| S     | 455  | 31.470903  | 26.905190  | 27.970016  |
| S     | 455  | 32.526089  | 30.858829  | 25.098251  |
| S     | 455  | 33.136318  | 26.303856  | 23.143560  |
| S     | 455  | 36.065311  | 27.388348  | 26.996395  |

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|       | 24   | 18.445730 | 32.938465 | 33.912575 |
|-------|------|------------|------------|------------|
| Ca    | 24   | 22.986374  | 34.643005  | 35.614006  |
| Ca    | 24   | 23.577402  | 29.976011  | 33.071423  |
| Ca    | 24   | 22.695210  | 34.514469  | 30.621212  |
| Ca    | 24   | 25.018909  | 30.890774  | 27.842285  |
| Ca    | 24   | 27.735989  | 32.896709  | 30.975065  |
| Ca    | 24   | 29.353130  | 28.571333  | 30.022758  |
| Ca    | 24   | 30.709042  | 32.454323  | 27.208059  |
| Ca    | 24   | 30.274166  | 27.976852  | 24.412838  |
| Ca    | 24   | 33.683746  | 29.933371  | 28.011135  |
| Ca    | 24   | 33.778461  | 24.698313  | 26.677794  |
| Ca    | 24   | 35.828194  | 28.818768  | 24.249908  |
| S     | 24   | 21.213934  | 31.406017  | 35.420998  |
| S     | 24   | 20.407084  | 35.706890  | 33.216507  |
| S     | 24   | 21.999514  | 31.104362  | 29.810181  |
| S     | 24   | 25.002674  | 33.408695  | 33.191795  |
| S     | 24   | 26.411716  | 29.594978  | 30.927155  |
| S     | 24   | 25.522392  | 34.005188  | 28.265995  |
| S     | 24   | 28.290941  | 29.986084  | 26.767170  |
| S     | 24   | 30.979315  | 31.501846  | 30.179968  |
| S     | 24   | 31.321653  | 26.931086  | 27.935699  |
| S     | 24   | 32.794659  | 30.656109  | 24.989336  |
| S     | 24   | 33.427395  | 26.219193  | 23.471600  |
| S     | 24   | 36.262390  | 27.467207  | 27.144619  |
| Element | x1    | y1    | z1    |
|---------|-------|-------|-------|
| Ca      | 18.430740 | 32.290344 | 33.991249 |
| Ca      | 23.068897  | 34.786312 | 35.395309  |
| Ca      | 23.746172  | 30.167625 | 32.817394  |
| Ca      | 22.720697  | 34.583385 | 30.629408  |
| Ca      | 24.914772  | 30.877216 | 27.794498  |
| Ca      | 27.963205  | 32.970634 | 31.023426  |
| Ca      | 29.332346  | 28.676094 | 30.082478  |
| Ca      | 30.634018  | 32.691574 | 27.241020  |
| Ca      | 30.254957  | 27.962898 | 24.688274  |
| Ca      | 33.557426  | 29.782324 | 28.271727  |
| Ca      | 33.553101  | 25.003824 | 26.603958  |
| Ca      | 35.668896  | 28.640905 | 24.007895  |
| S       | 21.499323  | 31.370937 | 35.149788  |
| S       | 20.397320  | 35.389236 | 33.051048  |
| S       | 21.988182  | 31.083668 | 29.881081  |
| S       | 25.091089  | 33.473927 | 33.078114  |
| S       | 26.357794  | 29.764280 | 30.846659  |
| S       | 25.584015  | 34.022064 | 28.377096  |
| S       | 28.587301  | 30.157717 | 26.913265  |
| S       | 31.063805  | 31.604691 | 30.306847  |
| S       | 31.242771  | 26.901293 | 28.058334  |
| S       | 32.800846  | 30.470888 | 25.129425  |
| S       | 33.162086  | 26.304405 | 23.342102  |
| S       | 36.100201  | 27.323761 | 27.259666  |

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| Element | x1    | y1    | z1    |
|---------|-------|-------|-------|
| Ca      | 18.656908 | 32.348366 | 34.236183 |
| Ca      | 23.078156  | 34.632000 | 35.230759  |
| Ca      | 23.868465  | 30.236393 | 32.964321  |
| Ca      | 22.826487  | 34.847294 | 30.768200  |
| Ca      | 24.813351  | 30.648386 | 27.608107  |
| Ca      | 27.930895  | 32.891254 | 31.021782  |
| Ca      | 29.487865  | 28.722334 | 29.713026  |
| Ca      | 30.572290  | 32.787834 | 26.854477  |
| Ca      | 30.394785  | 27.799206 | 24.506929  |
| Ca      | 33.474339  | 29.650135 | 28.480385  |
| Ca      | 33.269176  | 24.784597 | 26.797808  |
| Ca      | 35.567570  | 29.110533 | 24.536146  |
| S       | 21.634228  | 31.230209 | 35.310017  |
| S       | 20.379627  | 35.129097 | 32.929585  |
| S       | 22.012329  | 31.187378 | 30.021843  |
| S       | 25.244720  | 33.603092 | 33.211357  |
| S       | 26.531740  | 29.647694 | 30.706383  |
| S       | 25.586630  | 34.091228 | 28.263706  |
| S       | 28.340145  | 30.012169 | 26.430456  |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| S       | 31.002157    | 31.703873    | 29.969387    |
| S       | 31.078156    | 27.069584    | 28.061245    |
| S       | 32.776279    | 30.511669    | 25.162258    |
| S       | 33.454884    | 26.549849    | 23.528248    |
| S       | 35.738884    | 27.109186    | 27.627399    |

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| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.588684    | 31.814171    | 33.660954    |
| Ca      | 22.933388    | 34.613712    | 35.502106    |
| Ca      | 23.522511    | 30.043615    | 32.924362    |
| Ca      | 23.047579    | 34.859566    | 30.594202    |
| Ca      | 25.294334    | 30.653547    | 27.696138    |
| Ca      | 27.928661    | 32.739830    | 31.407772    |
| Ca      | 29.477766    | 28.998901    | 29.958141    |
| Ca      | 30.777143    | 33.002319    | 26.582901    |
| Ca      | 30.304178    | 27.852001    | 24.518385    |
| Ca      | 33.401848    | 29.923597    | 28.330528    |
| Ca      | 33.272915    | 24.677219    | 26.859823    |
| Ca      | 35.427231    | 28.866182    | 24.241718    |
| S       | 21.442955    | 31.427380    | 35.594349    |
| S       | 20.281189    | 35.202526    | 32.860714    |
| S       | 22.216782    | 31.397240    | 29.814032    |
| S       | 25.146709    | 33.492496    | 33.358215    |
| S       | 26.637774    | 29.646603    | 31.011637    |
| S       | 25.862688    | 33.926201    | 28.554062    |
| S       | 28.518974    | 30.291647    | 26.537933    |
| S       | 31.209013    | 32.046417    | 29.765217    |
| S       | 30.927990    | 27.036842    | 28.015423    |
| S       | 32.760605    | 30.423378    | 25.076666    |
| S       | 33.194866    | 26.007511    | 23.518936    |
| S       | 35.544273    | 27.357105    | 27.555851    |

*Generated by VMD*
|    |        |        |        |
|----|--------|--------|--------|
| S  | 20.18798 | 34.982479 | 33.178730 |
| S  | 22.015722 | 31.538330 | 29.740026 |
| S  | 25.191153 | 33.372540 | 33.437653 |
| S  | 26.451574 | 29.921452 | 30.774229 |
| S  | 25.872452 | 34.278614 | 28.584423 |
| S  | 28.433844 | 30.196783 | 26.391455 |
| S  | 30.946751 | 32.026134 | 29.627728 |
| S  | 31.266182 | 26.998869 | 28.321762 |
| S  | 32.916534 | 30.330009 | 24.927292 |
| S  | 33.449894 | 25.810211 | 23.551981 |
| S  | 35.682365 | 27.346626 | 27.508556 |

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generated by VMD

|    |        |        |        |
|----|--------|--------|--------|
| Ca | 18.642275 | 31.715710 | 33.990475 |
| Ca | 22.983633 | 34.450851 | 35.652397 |
| Ca | 23.547304 | 30.326742 | 32.703365 |
| Ca | 22.598154 | 35.039429 | 30.845112 |
| Ca | 25.167393 | 30.963612 | 27.505348 |
| Ca | 27.851221 | 33.150402 | 31.276962 |
| Ca | 29.365767 | 28.940620 | 29.649559 |
| Ca | 30.874107 | 32.839256 | 26.170113 |
| Ca | 30.347326 | 27.731258 | 24.725433 |
| Ca | 33.231335 | 29.913498 | 28.547110 |
| Ca | 33.522717 | 24.490788 | 27.152042 |
| Ca | 35.775723 | 28.630495 | 24.156597 |
| S  | 21.597082 | 31.010195 | 35.845917 |
| S  | 20.283083 | 34.790787 | 33.162441 |
| S  | 22.112934 | 31.714075 | 29.582260 |
| S  | 25.018553 | 33.517868 | 33.245144 |
| S  | 26.572742 | 29.884827 | 30.772579 |
| S  | 25.925165 | 34.378075 | 28.527412 |
| S  | 28.408123 | 30.181566 | 26.330708 |
| S  | 31.107864 | 32.083012 | 29.741043 |
| S  | 31.090780 | 26.885145 | 28.209606 |
| S  | 32.795567 | 30.489380 | 24.968569 |
| S  | 33.215111 | 25.975424 | 23.679039 |
| S  | 35.686089 | 27.197033 | 27.500824 |

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generated by VMD

|    |        |        |        |
|----|--------|--------|--------|
| Ca | 18.757412 | 31.687386 | 34.212982 |
| Ca | 22.968927 | 34.224701 | 35.827816 |
| Ca | 23.701105 | 30.223774 | 32.578026 |
| Ca | 22.863468 | 35.003246 | 30.618942 |
| Ca | 24.931641 | 31.089314 | 27.301779 |
| Ca | 27.885118 | 33.161308 | 31.047556 |
| Ca | 29.482695 | 29.156649 | 29.628496 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 30.729294 | 32.787533 | 26.282042 |
| Ca      | 30.452217 | 27.893064 | 24.789520 |
| Ca      | 33.295990 | 29.932423 | 28.535250 |
| Ca      | 33.116226 | 24.569553 | 27.289978 |
| Ca      | 35.743149 | 28.324728 | 24.311970 |
| S       | 21.853357 | 30.857079 | 35.549370 |
| S       | 20.376026 | 34.763103 | 33.196846 |
| S       | 22.051176 | 31.658932 | 29.650513 |
| S       | 24.968599 | 33.472198 | 33.377350 |
| S       | 26.643532 | 29.862066 | 30.602837 |
| S       | 25.805897 | 34.451988 | 28.339659 |
| S       | 28.373171 | 30.191338 | 26.375118 |
| S       | 31.107107 | 32.174488 | 29.767185 |
| S       | 31.048635 | 27.207119 | 28.215534 |
| S       | 32.759945 | 30.507504 | 25.004055 |
| S       | 33.104614 | 25.943356 | 23.760765 |
| S       | 35.700752 | 27.157185 | 27.676437 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 18.449579 | 32.426720 | 33.437061 |
| Ca      | 22.799271 | 34.372314 | 35.823009 |
| Ca      | 23.759752 | 30.115168 | 32.720619 |
| Ca      | 22.767076 | 34.837563 | 30.752956 |
| Ca      | 25.052042 | 31.053207 | 27.691956 |
| Ca      | 27.864977 | 32.880737 | 31.567009 |
| Ca      | 29.459047 | 28.759861 | 30.129223 |
| Ca      | 30.785330 | 32.704647 | 26.309341 |
| Ca      | 30.409925 | 27.504992 | 24.865873 |
| Ca      | 33.265430 | 29.794355 | 28.486568 |
| Ca      | 33.756939 | 24.868345 | 26.927422 |
| Ca      | 35.447723 | 28.780712 | 23.616055 |
| S       | 21.400475 | 31.229263 | 35.370869 |
| S       | 20.313511 | 35.443764 | 33.106468 |
| S       | 22.127441 | 31.556902 | 29.775799 |
| S       | 24.868797 | 33.330914 | 33.230721 |
| S       | 26.663725 | 29.740982 | 30.885380 |
| S       | 25.889702 | 34.150509 | 28.758942 |
| S       | 28.449974 | 29.936443 | 26.710928 |
| S       | 31.113991 | 31.826237 | 29.778919 |
| S       | 31.357601 | 26.810108 | 28.283966 |
| S       | 32.681324 | 30.460194 | 24.981434 |
| S       | 33.146286 | 25.929417 | 23.480480 |
| S       | 35.890163 | 27.786711 | 27.249020 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 18.213303 | 32.483040 | 33.651989 |
| Element | X Coordination | Y Coordination | Z Coordination |
|---------|----------------|----------------|---------------|
| Ca      | 22.728077      | 34.629288      | 35.624283     |
| Ca      | 23.630890      | 30.295483      | 32.804840     |
| Ca      | 22.618330      | 34.748219      | 30.749317     |
| Ca      | 25.071054      | 30.885157      | 27.817255     |
| Ca      | 28.020264      | 32.963341      | 31.478304     |
| Ca      | 29.403006      | 28.880180      | 30.024784     |
| Ca      | 30.912210      | 32.707550      | 26.633965     |
| Ca      | 30.402048      | 27.611309      | 24.768246     |
| Ca      | 33.656124      | 29.651363      | 28.419228     |
| Ca      | 33.973846      | 24.796207      | 26.781965     |
| Ca      | 35.457203      | 28.738791      | 23.602232     |
| S       | 21.259636      | 31.233101      | 35.280025     |
| S       | 20.127766      | 35.394478      | 33.128735     |
| S       | 21.826300      | 31.318575      | 29.768536     |
| S       | 24.916679      | 33.571629      | 33.347168     |
| S       | 26.407812      | 29.718678      | 30.937065     |
| S       | 25.769173      | 34.204884      | 28.873531     |
| S       | 28.436821      | 30.032978      | 26.706266     |
| S       | 31.369564      | 31.603212      | 30.126556     |
| S       | 31.470596      | 26.950653      | 28.130558     |
| S       | 32.746868      | 30.497967      | 24.855545     |
| S       | 33.134769      | 25.936071      | 23.487492     |
| S       | 36.167698      | 27.447903      | 26.942066     |

24 points generated by VMD

| Element | X Coordination | Y Coordination | Z Coordination |
|---------|----------------|----------------|---------------|
| Ca      | 18.435038      | 32.532921      | 33.926220     |
| Ca      | 22.901978      | 34.499958      | 35.562202     |
| Ca      | 23.656349      | 30.261276      | 32.783363     |
| Ca      | 22.887794      | 34.512531      | 30.817053     |
| Ca      | 25.032705      | 30.598238      | 27.627262     |
| Ca      | 27.941101      | 32.938038      | 31.322607     |
| Ca      | 29.363436      | 29.204727      | 29.672012     |
| Ca      | 30.543058      | 33.153320      | 26.232651     |
| Ca      | 30.505219      | 27.520226      | 24.812529     |
| Ca      | 33.644165      | 29.598627      | 28.615658     |
| Ca      | 33.524609      | 24.811775      | 26.823914     |
| Ca      | 35.576176      | 28.802595      | 23.973822     |
| S       | 21.371944      | 31.312845      | 35.387207     |
| S       | 20.340021      | 35.163345      | 32.963146     |
| S       | 22.054895      | 31.434944      | 29.769989     |
| S       | 24.966194      | 33.218029      | 33.424568     |
| S       | 26.497663      | 29.637667      | 30.733158     |
| S       | 25.907204      | 34.079819      | 28.944435     |
| S       | 28.235193      | 30.213173      | 26.475965     |
| S       | 31.166836      | 32.048363      | 29.636309     |
| S       | 31.289213      | 26.900524      | 28.336863     |
|  |  |  |  |
|---|---|---|---|
| S | 32.745972 | 30.486135 | 25.208538 |
| S | 33.108150 | 26.045509 | 23.624058 |
| S | 36.025066 | 27.325485 | 27.266502 |

generated by VMD

| Ca | 18.452780 | 32.315834 | 33.493160 |
| Ca | 22.650877 | 34.596661 | 35.484146 |
| Ca | 23.789972 | 29.926252 | 32.909977 |
| Ca | 23.184015 | 34.558067 | 30.813026 |
| Ca | 25.243635 | 30.724506 | 27.892982 |
| Ca | 28.200197 | 32.778244 | 31.647324 |
| Ca | 29.525873 | 29.296593 | 29.977116 |
| Ca | 30.576221 | 33.032700 | 26.092522 |
| Ca | 30.288345 | 27.746319 | 24.817291 |
| Ca | 33.635101 | 29.856218 | 28.389700 |
| Ca | 33.283634 | 24.880024 | 27.046354 |
| Ca | 35.385857 | 28.759321 | 23.969570 |
| S | 21.188604 | 31.061232 | 35.280716 |
| S | 20.445366 | 35.379784 | 32.783859 |
| S | 22.260384 | 31.339367 | 29.633202 |
| S | 24.954615 | 33.117184 | 33.469688 |
| S | 29.600449 | 29.592171 | 30.946354 |
| S | 26.206017 | 33.850857 | 28.815763 |
| S | 28.493752 | 30.173061 | 26.666630 |
| S | 31.199728 | 32.362572 | 29.684715 |
| S | 31.030594 | 27.167620 | 28.421383 |
| S | 32.628258 | 30.380070 | 24.931152 |
| S | 32.807346 | 26.151278 | 23.467365 |
| S | 35.688435 | 27.254128 | 27.306070 |

generated by VMD

| Ca | 18.653547 | 32.495914 | 33.528439 |
| Ca | 22.908236 | 34.753841 | 35.625488 |
| Ca | 23.586655 | 30.086384 | 32.831657 |
| Ca | 22.834555 | 34.627815 | 30.686472 |
| Ca | 25.122421 | 30.708256 | 27.908104 |
| Ca | 27.906437 | 32.637222 | 31.511612 |
| Ca | 29.580706 | 28.813072 | 29.845448 |
| Ca | 30.373367 | 32.654095 | 26.259415 |
| Ca | 30.195784 | 27.897034 | 24.629860 |
| Ca | 33.755981 | 29.677942 | 28.589767 |
| Ca | 33.683540 | 24.926632 | 26.751858 |
| Ca | 35.524590 | 28.903349 | 24.078732 |
| S | 21.248655 | 31.466293 | 35.350494 |
| S | 20.591349 | 35.551056 | 32.984241 |
| S | 22.122601 | 31.182501 | 29.722403 |
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generated by VMD

Ca  18.623346  32.442780  33.825745
Ca  22.828203  34.797100  35.578510
Ca  23.718729  29.987026  32.881130
Ca  22.602486  34.589783  30.694000
Ca  25.254730  30.583206  27.798267
Ca  27.425280  32.721428  31.415413
Ca  29.790110  28.913103  29.967438
Ca  30.576841  32.869759  26.217699
Ca  30.475695  34.543941  24.690142
Ca  33.615570  29.717123  28.687445
Ca  33.566830  24.543941  26.527122
Ca  35.682728  28.817886  24.069878
S   21.446228  31.463604  35.664219
S   20.461250  35.462292  33.142765
S   22.083790  31.244473  29.672857
S   25.010258  33.522896  33.338257
S   26.232691  29.610409  30.588137
S   25.718079  34.132137  28.618223
S   28.563398  29.899609  26.603781
S   30.741327  32.125343  29.830303
S   31.429579  26.850615  28.147306
S   32.917549  30.516071  25.341425
S   33.055996  26.267803  23.335014
S   35.899323  27.179287  27.304962

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generated by VMD

Ca  18.489599  32.737823  33.741074
Ca  23.026079  34.625729  35.146637
Ca  23.848446  30.032164  33.078838
Ca  22.807676  34.372837  30.734875
Ca  25.029602  30.699156  27.698757
Ca  27.771072  32.710659  31.378958
Ca  29.522457  29.009535  29.901314
Ca  30.510092  32.818667  26.300751
Ca  30.350828  27.981789  24.682537
| Element | Value 1      | Value 2      | Value 3      |
|---------|--------------|--------------|--------------|
| Ca      | 33.632431    | 29.544598    | 28.794403    |
| Ca      | 33.264881    | 25.090879    | 26.734131    |
| Ca      | 35.701721    | 28.808411    | 23.962421    |
| S       | 21.344505    | 31.371820    | 35.562332    |
| S       | 20.443291    | 35.566559    | 32.814220    |
| S       | 22.100639    | 30.979218    | 29.961086    |
| S       | 25.114035    | 33.388927    | 33.385769    |
| S       | 28.364735    | 30.076500    | 26.567163    |
| S       | 30.950354    | 31.874508    | 29.875978    |
| S       | 31.314497    | 26.951170    | 28.271095    |
| S       | 32.785263    | 30.524323    | 25.345615    |
| S       | 33.092777    | 26.337032    | 23.325481    |
| S       | 35.968262    | 27.403904    | 27.227528    |

Generated by VMD

| Element | Value 1      | Value 2      | Value 3      |
|---------|--------------|--------------|--------------|
| Ca      | 18.452147    | 32.324749    | 33.453468    |
| Ca      | 22.721090    | 34.813293    | 35.307835    |
| Ca      | 23.903843    | 30.017092    | 33.145393    |
| Ca      | 22.778540    | 34.286156    | 30.591583    |
| Ca      | 25.357714    | 30.602348    | 28.071516    |
| Ca      | 27.952459    | 32.856068    | 31.445925    |
| Ca      | 29.827616    | 29.182468    | 29.956715    |
| Ca      | 30.547480    | 32.898167    | 26.296896    |
| Ca      | 30.401108    | 27.735550    | 24.941961    |
| Ca      | 33.616581    | 29.591692    | 28.626263    |
| Ca      | 32.836876    | 25.050621    | 26.556370    |
| Ca      | 35.681915    | 28.727695    | 23.861713    |
| S       | 21.291157    | 31.492579    | 35.379635    |
| S       | 20.241161    | 35.295761    | 32.760414    |
| S       | 22.271662    | 31.068995    | 29.866360    |
| S       | 25.087769    | 33.302979    | 33.431320    |
| S       | 26.546463    | 29.500114    | 30.874382    |
| S       | 25.959295    | 34.223293    | 28.676567    |
| S       | 28.656158    | 30.150627    | 26.865879    |
| S       | 31.061115    | 32.047318    | 29.952005    |
| S       | 31.253540    | 26.996761    | 28.438152    |
| S       | 32.787701    | 30.517097    | 25.170311    |
| S       | 32.832409    | 26.493114    | 23.032818    |
| S       | 35.660583    | 27.125484    | 27.236526    |

Generated by VMD

| Element | Value 1      | Value 2      | Value 3      |
|---------|--------------|--------------|--------------|
| Ca      | 18.450308    | 32.591118    | 33.437294    |
| Ca      | 22.835505    | 34.865311    | 35.455788    |
| Ca      | 23.663029    | 29.767284    | 33.020233    |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 22.847326    | 34.398392    | 30.693230    |
| Ca      | 25.131796    | 30.696239    | 27.975992    |
| Ca      | 27.98241     | 32.877586    | 31.32767     |
| Ca      | 29.882248    | 29.017904    | 29.844070    |
| Ca      | 30.564327    | 33.017155    | 26.277296    |
| Ca      | 30.212027    | 27.930033    | 24.965672    |
| Ca      | 33.761494    | 29.437492    | 28.785578    |
| Ca      | 33.405323    | 24.733021    | 26.687210    |
| Ca      | 35.376522    | 28.959322    | 23.818473    |
| S       | 21.261820    | 31.555199    | 35.335526    |
| S       | 20.303633    | 35.377922    | 32.923641    |
| S       | 21.996824    | 31.004574    | 29.846264    |
| S       | 25.061243    | 33.231152    | 33.286686    |
| S       | 26.550711    | 29.531973    | 30.785936    |
| S       | 25.749588    | 34.144176    | 28.906734    |
| S       | 28.432253    | 30.212519    | 26.826736    |
| S       | 31.249252    | 32.080154    | 29.692394    |
| S       | 31.232168    | 26.773212    | 28.230391    |
| S       | 32.795784    | 30.530191    | 25.289719    |
| S       | 32.993099    | 26.248470    | 23.426781    |
| S       | 35.981575    | 27.319668    | 27.105391    |

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| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.417294    | 32.419479    | 33.877102    |
| Ca      | 22.908022    | 34.521725    | 35.481766    |
| Ca      | 23.745190    | 29.927748    | 32.783112    |
| Ca      | 22.901052    | 34.604927    | 30.792809    |
| Ca      | 24.960911    | 30.784351    | 27.699337    |
| Ca      | 27.936430    | 33.076221    | 31.229286    |
| Ca      | 29.611746    | 29.210258    | 29.661119    |
| Ca      | 30.723890    | 32.910275    | 25.933025    |
| Ca      | 30.311136    | 27.674017    | 24.752289    |
| Ca      | 33.428711    | 29.672321    | 28.702280    |
| Ca      | 33.545448    | 24.688280    | 26.905975    |
| Ca      | 35.672169    | 28.735355    | 23.943890    |
| S       | 21.458025    | 31.042793    | 35.337669    |
| S       | 20.258532    | 35.388481    | 33.210148    |
| S       | 22.093578    | 31.345551    | 29.827332    |
| S       | 25.011250    | 33.216019    | 33.410858    |
| S       | 26.546152    | 29.635342    | 30.762098    |
| S       | 25.930136    | 34.310406    | 28.779350    |
| S       | 28.298050    | 30.138124    | 26.464348    |
| S       | 31.124540    | 32.111961    | 29.534353    |
| S       | 31.078659    | 26.971859    | 28.289139    |
| S       | 32.770012    | 30.332943    | 25.415057    |
| S       | 32.991032    | 26.182674    | 23.734566    |
|   |     |     |     |     |
|---|-----|-----|-----|-----|
| S | 35.997219 | 27.398907 | 27.413712 |     |
| Ca | 18.173723 | 32.846848 | 34.006718 |     |
| Ca | 22.772888 | 34.648239 | 35.604706 |     |
| Ca | 23.652283 | 30.149570 | 33.052055 |     |
| Ca | 22.678164 | 34.371563 | 30.752758 |     |
| Ca | 25.218689 | 30.841080 | 27.799797 |     |
| Ca | 27.715374 | 32.893898 | 31.476181 |     |
| Ca | 29.797174 | 29.214205 | 29.671915 |     |
| Ca | 30.556671 | 33.016541 | 26.217163 |     |
| Ca | 30.510715 | 27.534985 | 24.685814 |     |
| Ca | 33.732231 | 29.693962 | 28.658575 |     |
| Ca | 33.302395 | 25.017025 | 26.709938 |     |
| Ca | 35.588638 | 28.665508 | 23.900606 |     |
| S | 21.124657 | 31.331261 | 35.381157 |     |
| S | 20.433191 | 35.405029 | 32.959240 |     |
| S | 22.180910 | 31.067104 | 29.839863 |     |
| S | 24.858646 | 33.201710 | 33.531364 |     |
| S | 26.558083 | 29.542591 | 30.618601 |     |
| S | 25.900354 | 34.072586 | 28.949484 |     |
| S | 28.509069 | 29.955940 | 26.393333 |     |
| S | 31.022865 | 32.080421 | 29.662079 |     |
| S | 31.264839 | 26.981815 | 28.226339 |     |
| S | 33.033306 | 30.355892 | 25.178249 |     |
| S | 33.057590 | 26.098602 | 23.352386 |     |
| S | 36.077560 | 27.313656 | 27.311655 |     |

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| Ca | 18.216576 | 32.240288 | 34.139404 |
| Ca | 22.753645 | 34.531677 | 35.639256 |
| Ca | 23.479645 | 30.235901 | 32.792427 |
| Ca | 22.863855 | 34.607674 | 30.606823 |
| Ca | 25.064510 | 30.853376 | 27.617493 |
| Ca | 27.765217 | 32.831085 | 31.061586 |
| Ca | 29.693951 | 29.291960 | 29.772125 |
| Ca | 31.066616 | 33.231037 | 26.421432 |
| Ca | 30.425484 | 27.967913 | 24.734344 |
| Ca | 33.973034 | 29.681705 | 28.693510 |
| Ca | 33.603168 | 24.688812 | 26.912659 |
| Ca | 35.129906 | 28.379040 | 23.960253 |
| S | 21.371939 | 31.276777 | 35.550880 |
| S | 20.433626 | 35.160515 | 33.250389 |
| S | 21.937407 | 31.191360 | 29.536972 |
| S | 24.996332 | 33.287144 | 33.178135 |
| S | 26.493441 | 29.433969 | 30.526230 |
|   | S           | Ca          | S           | Ca          | S           | Ca          |
|---|-------------|-------------|-------------|-------------|-------------|-------------|
| S | 25.843035   | 18.547935   | 30.351658   | 35.826492   | 33.582890   | 30.826492   |
| S | 28.559292   | 23.197306   | 32.315024   | 29.035925   | 32.684834   | 30.368353   |
| S | 31.178568   | 23.924805   | 36.339768   | 25.932045   | 33.264061   | 30.285751   |
| S | 31.394402   | 22.676416   | 32.973953   | 30.029587   | 33.630714   | 27.658073   |
| S | 32.973953   | 24.877890   | 32.476940   | 30.884708   | 33.661091   | 32.715191   |
| S | 32.476940   | 27.658073   | 36.025467   | 32.715191   | 33.826068   | 29.117756   |
|   | 30.826492   | 29.642437   | 32.973953   | 29.117756   | 35.383446   | 30.042233   |
|   | 33.582890   | 30.638330   | 36.025467   | 33.042233   | 35.383446   | 30.884708   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|   | 33.582890   | 30.285751   | 32.973953   | 27.987507   | 35.383446   | 32.715191   |
|    | 35.706184 | 28.501326 | 24.013039 |
|----|-----------|-----------|-----------|
| S  | 20.976343 | 31.355314 | 34.923252 |
| S  | 20.477558 | 35.462959 | 33.733772 |
| S  | 22.159559 | 31.270380 | 29.846685 |
| S  | 25.134417 | 33.025726 | 33.420464 |
| S  | 26.166882 | 29.366962 | 30.418390 |
| S  | 25.821592 | 34.545921 | 29.157299 |
| S  | 28.337038 | 30.083738 | 26.464054 |
| S  | 30.759438 | 32.095753 | 29.277895 |
| S  | 31.593872 | 26.993828 | 28.446580 |
| S  | 32.922028 | 30.166641 | 25.020061 |
| S  | 33.010365 | 25.930603 | 23.702497 |
| S  | 36.051800 | 27.786142 | 27.496338 |

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| Ca  | 18.724928 | 33.460178 | 33.148891 |
|-----|-----------|-----------|-----------|
| Ca  | 22.824331 | 34.332138 | 36.136982 |
| Ca  | 23.538923 | 29.822392 | 32.818172 |
| Ca  | 22.905405 | 34.486290 | 30.984783 |
| Ca  | 25.254383 | 30.635664 | 27.854168 |
| Ca  | 27.576420 | 32.576477 | 31.487473 |
| Ca  | 29.710810 | 29.084309 | 29.412535 |
| Ca  | 30.281023 | 32.731335 | 25.778618 |
| Ca  | 30.239311 | 27.793955 | 24.778500 |
| Ca  | 33.463413 | 29.968390 | 28.531765 |
| Ca  | 34.071857 | 24.990625 | 27.251162 |
| Ca  | 35.472145 | 28.627171 | 24.003716 |
| S   | 21.141188 | 31.471582 | 35.040047 |
| S   | 20.717800 | 35.842823 | 33.761185 |
| S   | 22.246073 | 31.127417 | 29.715862 |
| S   | 25.021526 | 32.947014 | 33.509212 |
| S   | 26.294153 | 29.238979 | 30.530634 |
| S   | 25.967682 | 34.193645 | 29.069763 |
| S   | 28.281504 | 29.810825 | 26.238033 |
| S   | 30.588987 | 32.012489 | 29.268476 |
| S   | 31.438648 | 26.878368 | 28.255768 |
| S   | 32.672340 | 30.252581 | 25.152290 |
| S   | 33.099529 | 25.998026 | 23.804493 |
| S   | 36.187664 | 28.017405 | 27.407526 |

24 generated by VMD

| Ca  | 18.419260 | 33.029320 | 33.161263 |
|-----|-----------|-----------|-----------|
| Ca  | 22.703785 | 34.187366 | 36.102551 |
| Ca  | 23.720661 | 29.974243 | 32.873844 |
| Ca  | 22.996410 | 34.599133 | 30.909344 |
| Ca  | 25.112078 | 30.930193 | 27.746353 |
|   |   |   |
|---|---|---|
| Ca | 27.886017 | 32.786140 | 31.552317 |
| Ca | 29.708853 | 29.176956 | 29.657393 |
| Ca | 30.120424 | 32.818760 | 25.965242 |
| Ca | 30.207308 | 27.504461 | 24.859280 |
| Ca | 33.631184 | 29.824997 | 28.553221 |
| Ca | 33.872978 | 29.824997 | 28.553221 |
| S  | 20.893461 | 31.190041 | 35.014259 |
| S  | 20.683926 | 35.529858 | 33.566566 |
| S  | 22.265905 | 31.469383 | 29.700401 |
| S  | 25.063383 | 33.082165 | 33.702106 |
| S  | 26.365576 | 29.620846 | 30.845802 |
| S  | 26.139050 | 34.164722 | 28.722858 |
| S  | 28.300163 | 29.797562 | 26.357569 |
| S  | 30.814541 | 32.096207 | 29.413363 |
| S  | 31.367147 | 26.912563 | 28.376928 |
| S  | 32.600407 | 30.252502 | 25.015079 |
| S  | 33.254974 | 25.843832 | 23.801904 |
| S  | 36.097153 | 27.923624 | 27.178061 |

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|   |   |   |
|---|---|---|
| Ca | 18.363678 | 33.027790 | 33.156544 |
| Ca | 22.888863 | 34.198936 | 35.716564 |
| Ca | 23.848644 | 29.853765 | 32.819462 |
| Ca | 22.804855 | 34.427013 | 30.973843 |
| Ca | 24.950319 | 31.018257 | 27.912163 |
| Ca | 28.223089 | 32.871777 | 31.537468 |
| Ca | 29.607979 | 29.476917 | 29.777374 |
| Ca | 30.258368 | 33.049133 | 25.756920 |
| Ca | 30.203331 | 27.441681 | 24.842085 |
| Ca | 33.395889 | 29.837250 | 28.582062 |
| Ca | 33.831699 | 24.690008 | 27.106632 |
| Ca | 35.401707 | 28.626617 | 23.90898 |
| S  | 21.116335 | 31.190168 | 34.706001 |
| S  | 20.586926 | 35.451084 | 33.522770 |
| S  | 22.135513 | 31.227314 | 29.908195 |
| S  | 25.172501 | 32.957939 | 33.534405 |
| S  | 26.637737 | 29.422796 | 30.672779 |
| S  | 26.035946 | 34.298206 | 28.994322 |
| S  | 28.281584 | 30.064722 | 26.446056 |
| S  | 30.973011 | 32.282520 | 29.512489 |
| S  | 31.270889 | 26.978926 | 28.216576 |
| S  | 32.583363 | 30.329161 | 25.116428 |
| S  | 33.017921 | 25.814886 | 23.745674 |
| S  | 36.129852 | 27.763145 | 27.392298 |
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.379578     | 33.209969     | 33.369713     |
| Ca      | 22.876154     | 34.512802     | 30.894825     |
| Ca      | 23.620903     | 29.653004     | 32.923126     |
| Ca      | 22.926880     | 34.512802     | 30.894825     |
| Ca      | 25.114595     | 31.090942     | 27.800175     |
| Ca      | 27.903585     | 32.700588     | 31.416134     |
| Ca      | 29.527891     | 29.202663     | 29.736538     |
| Ca      | 30.466164     | 32.800819     | 25.994301     |
| Ca      | 30.072552     | 27.608143     | 24.857988     |
| Ca      | 33.618927     | 29.830381     | 28.443779     |
| Ca      | 33.874825     | 25.047642     | 27.229391     |
| Ca      | 35.549812     | 28.645527     | 23.789373     |
| S       | 20.943100     | 31.110947     | 34.885593     |
| S       | 20.657110     | 35.852867     | 33.434883     |
| S       | 22.092667     | 31.198788     | 29.98510      |
| S       | 24.971302     | 32.976437     | 33.462204     |
| S       | 26.560644     | 29.476404     | 30.676319     |
| S       | 25.988260     | 34.087779     | 28.865479     |
| S       | 28.264009     | 30.101391     | 26.484848     |
| S       | 31.155846     | 32.011440     | 29.690220     |
| S       | 31.388672     | 26.990198     | 28.340612     |
| S       | 32.571182     | 30.310928     | 24.960979     |
| S       | 32.989983     | 25.806940     | 23.870535     |
| S       | 36.205441     | 27.914524     | 27.129295     |

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| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 18.492331     | 32.892189     | 33.054497     |
| Ca      | 22.792418     | 34.202660     | 35.805649     |
| Ca      | 23.738836     | 29.716143     | 32.780346     |
| Ca      | 23.130371     | 34.620213     | 30.987516     |
| Ca      | 24.748335     | 31.040815     | 27.685303     |
| Ca      | 27.943314     | 32.773979     | 31.505470     |
| Ca      | 29.225334     | 29.271044     | 29.931145     |
| Ca      | 30.445797     | 32.965130     | 26.154238     |
| Ca      | 30.079552     | 27.765802     | 24.899895     |
| Ca      | 33.760197     | 29.837029     | 28.334393     |
| Ca      | 33.963734     | 25.046789     | 27.363245     |
| Ca      | 35.377834     | 28.445198     | 23.729439     |
| S       | 21.141052     | 31.164330     | 35.095051     |
| S       | 20.680443     | 35.701706     | 33.111767     |
| S       | 22.083559     | 31.285763     | 29.867250     |
| S       | 25.111979     | 33.021778     | 33.607735     |
| S       | 26.351318     | 29.390972     | 30.663437     |
| S       | 26.017805     | 34.090477     | 28.942375     |
| S       | 28.182840     | 30.172852     | 26.591646     |
|   |        |        |        |
|---|--------|--------|--------|
| S | 31.060247 | 31.944304 | 29.697748 |
| S | 31.557835 | 26.994284 | 28.296944 |
| S | 32.555588 | 30.330982 | 24.956472 |
| S | 32.927151 | 25.749731 | 23.866203 |
| S | 36.352268 | 27.875895 | 27.012285 |

24 generated by VMD

| Ca | 18.425108 | 32.898701 | 33.606007 |
| Ca | 22.828663 | 34.335411 | 35.411861 |
| Ca | 23.615173 | 29.843811 | 32.780487 |
| Ca | 23.001411 | 34.368786 | 30.854006 |
| Ca | 25.087761 | 31.083776 | 27.693710 |
| Ca | 27.840458 | 32.745735 | 31.528492 |
| Ca | 29.336243 | 29.391674 | 29.944510 |
| Ca | 30.632574 | 32.773384 | 26.102154 |
| Ca | 30.261578 | 27.707773 | 24.903803 |
| Ca | 33.757454 | 29.862337 | 28.508703 |
| Ca | 33.570110 | 24.936701 | 27.084377 |
| Ca | 35.390354 | 28.688820 | 23.663595 |
| S  | 21.243086 | 31.041897 | 35.099277 |
| S  | 20.602526 | 35.685143 | 33.050079 |
| S  | 22.123241 | 31.250704 | 29.810940 |
| S  | 25.128490 | 32.971954 | 33.545204 |
| S  | 26.461201 | 29.484388 | 30.798176 |
| S  | 25.994036 | 34.035305 | 28.840679 |
| S  | 28.220716 | 30.077602 | 26.605995 |
| S  | 31.049061 | 31.973423 | 29.691319 |
| S  | 31.478079 | 27.117687 | 28.394365 |
| S  | 32.652905 | 30.395318 | 25.112478 |
| S  | 32.905262 | 25.952688 | 23.729822 |
| S  | 36.115829 | 27.678814 | 27.179985 |

24 generated by VMD

| Ca | 18.369898 | 32.711311 | 33.732584 |
| Ca | 22.717806 | 34.235912 | 35.541538 |
| Ca | 23.810806 | 29.924730 | 32.892277 |
| Ca | 22.862667 | 34.703491 | 30.886541 |
| Ca | 24.867323 | 30.992367 | 27.732004 |
| Ca | 27.840624 | 32.981991 | 31.399742 |
| Ca | 29.595116 | 29.269211 | 29.588902 |
| Ca | 30.523411 | 32.884098 | 26.253174 |
| Ca | 30.217316 | 27.578825 | 24.842031 |
| Ca | 33.662342 | 29.774223 | 28.544859 |
| Ca | 34.029343 | 24.542673 | 27.008770 |
| Ca | 35.577690 | 28.624807 | 23.740236 |
| S  | 21.035803 | 31.033409 | 35.066742 |
|   | S        | 20.566288 | 35.704926 | 33.274338 |
|---|----------|-----------|-----------|-----------|
| S | 22.031235| 31.335674 | 30.015013 |
| S | 24.880695| 33.349037 | 33.438622 |
| S | 26.551563| 29.550039 | 30.570196 |
| S | 25.900658| 34.225460 | 28.905001 |
| S | 28.298279| 30.111958 | 26.287006 |
| S | 31.137774| 32.123482 | 29.818300 |
| S | 31.523865| 26.873440 | 27.347734 |
| S | 32.475208| 30.322092 | 25.309391 |
| S | 33.037876| 25.777142 | 23.594158 |
| S | 36.206371| 27.669752 | 27.150171 |

24

generated by VMD

|   | Ca       | 18.545155 | 32.692501 | 33.859844 |
|---|----------|-----------|-----------|-----------|
| Ca| 18.328299| 33.281006 | 33.514370 |
| Ca| 22.852341| 34.025490 | 36.062588 |
| Ca| 23.858299| 30.029613 | 32.662113 |
| Ca| 22.918671| 34.390793 | 30.816116 |
| Ca| 25.100998| 31.028481 | 27.701412 |
| Ca| 28.028597| 32.997456 | 31.546162 |
| Ca| 29.655119| 30.001493 | 29.729671 |

24

generated by VMD
| Element | Ca   | S    |
|---------|------|------|
|         | 30.080481 | 32.751583 | 25.896152 |
|         | 30.049559  | 27.498684  | 24.920914  |
|         | 33.674519  | 29.991756  | 28.617302  |
|         | 33.913292  | 24.897209  | 27.042654  |
|         | 35.218369  | 28.616619  | 24.121700  |
|         | 21.049360  | 31.071886  | 34.653229  |
|         | 20.879032  | 35.594826  | 33.525429  |
|         | 22.144192  | 31.161985  | 29.728249  |
|         | 25.036131  | 32.895855  | 33.485497  |
|         | 26.753527  | 29.723518  | 30.745821  |
|         | 25.863550  | 34.165363  | 28.791992  |
|         | 28.150345  | 29.907932  | 26.290104  |
|         | 31.115927  | 32.257156  | 29.437099  |
|         | 31.416723  | 26.910904  | 28.305511  |
|         | 32.553391  | 30.432547  | 25.019957  |
|         | 33.193157  | 26.035212  | 23.694319  |
|         | 35.886227  | 27.632679  | 27.631693  |

24 generated by VMD

| Element | Ca   | S    |
|---------|------|------|
|         | 18.457024 | 33.908432 |
|         | 22.959183 | 35.824234 |
|         | 23.777889 | 32.802532 |
|         | 22.903708 | 30.710716 |
|         | 25.213600 | 27.531273 |
|         | 28.072052 | 31.383579 |
|         | 29.537416 | 29.763926 |
|         | 30.403495 | 25.802990 |
|         | 30.409286 | 24.919731 |
|         | 33.352974 | 28.398306 |
|         | 33.575634 | 27.182177 |
|         | 35.648396 | 24.256571 |
|         | 21.133600 | 35.154922 |
|         | 20.694113 | 33.444893 |
|         | 21.963196 | 29.737328 |
|         | 25.009594 | 33.310814 |
|         | 26.626560 | 30.677954 |
|         | 25.955383 | 28.675154 |
|         | 28.178360 | 26.412718 |
|         | 30.995794 | 29.296194 |
|         | 31.074249 | 28.365475 |
|         | 32.635525 | 24.933533 |
|         | 33.218449 | 23.956289 |
|         | 35.964233 | 27.490345 |

24 generated by VMD

| Element | Ca   | S    |
|---------|------|------|
|         | 18.457024 | 33.836666 |
| Ca   | 22.910089 | 34.062492 | 35.972973 |
|------|-----------|-----------|-----------|
| Ca   | 23.792818 | 29.818565 | 32.737049 |
| Ca   | 22.835045 | 34.508705 | 30.824198 |
| Ca   | 25.029444 | 30.960821 | 27.722609 |
| Ca   | 28.073750 | 32.966190 | 31.487497 |
| Ca   | 29.374254 | 29.051430 | 29.768059 |
| Ca   | 30.433163 | 32.738480 | 25.853191 |
| Ca   | 30.399137 | 27.587826 | 24.536482 |
| Ca   | 33.350571 | 29.927174 | 28.475231 |
| Ca   | 33.738991 | 24.842657 | 27.282461 |
| Ca   | 35.547325 | 28.646761 | 24.143524 |
| S    | 21.016363 | 30.914009 | 34.875900 |
| S    | 20.782965 | 35.616577 | 33.408943 |
| S    | 22.021099 | 31.296574 | 29.759012 |
| S    | 24.998198 | 33.078899 | 33.375793 |
| S    | 26.617039 | 29.708090 | 30.818333 |
| S    | 25.914089 | 34.242149 | 28.839882 |
| S    | 28.241915 | 29.996902 | 26.376154 |
| S    | 31.066799 | 32.405117 | 29.406425 |
| S    | 31.158493 | 27.067608 | 28.138504 |
| S    | 32.672371 | 30.375648 | 24.914040 |
| S    | 33.292854 | 25.890129 | 23.810406 |
| S    | 35.996277 | 27.566418 | 27.576702 |

generated by VMD

| Ca   | 18.392349 | 32.620934 | 33.616634 |
|------|-----------|-----------|-----------|
| Ca   | 22.836918 | 34.097672 | 35.745422 |
| Ca   | 23.790819 | 30.264128 | 32.852638 |
| Ca   | 22.985466 | 34.507660 | 30.873335 |
| Ca   | 25.135275 | 31.287066 | 27.649204 |
| Ca   | 27.996681 | 32.915665 | 31.495743 |
| Ca   | 29.423845 | 28.875500 | 29.551600 |
| Ca   | 30.275045 | 32.770351 | 25.876377 |
| Ca   | 30.393158 | 27.557816 | 24.680664 |
| Ca   | 33.412292 | 29.927042 | 28.526865 |
| Ca   | 34.019176 | 24.670162 | 27.170731 |
| Ca   | 35.290653 | 28.738413 | 24.127172 |
| S    | 21.026539 | 30.983978 | 35.114670 |
| S    | 20.664913 | 35.445621 | 33.509441 |
| S    | 22.024820 | 31.473007 | 29.834406 |
| S    | 24.989996 | 33.251915 | 33.340294 |
| S    | 26.598059 | 29.696823 | 30.763481 |
| S    | 26.176462 | 34.366177 | 28.781607 |
| S    | 28.212622 | 29.920013 | 26.420237 |
| S    | 31.014950 | 32.088615 | 29.438158 |
| S    | 31.272696 | 26.807562 | 28.167559 |
|  | X   | Y   | Z   |
|---|-----|-----|-----|
| S | 32.686039 | 30.408730 | 24.947910 |
| S | 33.125713 | 25.769026 | 23.955830 |
| S | 35.975544 | 27.856192 | 27.500069 |

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generated by VMD

| Ca | X   | Y   | Z   |
|----|-----|-----|-----|
| Ca | 18.449457 | 33.052002 | 34.158928 |
| Ca | 23.023962 | 34.152214 | 35.951038 |
| Ca | 23.672379 | 25.769026 | 23.955830 |
| Ca | 22.768394 | 30.630800 | 32.640766 |
| Ca | 27.810018 | 32.854380 | 30.798676 |
| Ca | 29.302742 | 31.052691 | 27.335325 |
| Ca | 29.084431 | 31.259735 |
| Ca | 30.252693 | 32.883362 | 26.033209 |
| Ca | 30.376408 | 25.588232 | 25.060728 |
| Ca | 33.601315 | 29.704172 | 28.657026 |
| Ca | 34.31732 | 24.853170 | 27.299644 |
| Ca | 35.502708 | 28.623539 | 24.049660 |
| Ca | 21.115992 | 31.023693 | 35.244141 |
| Ca | 20.905592 | 35.669365 | 33.647655 |
| Ca | 21.929682 | 31.488043 | 29.575951 |
| Ca | 25.07457 | 33.147457 | 33.433376 |
| Ca | 26.212572 | 29.600819 | 30.313932 |
| Ca | 25.889915 | 34.209633 | 28.870218 |
| Ca | 28.177790 | 30.071430 | 26.165659 |
| Ca | 30.878063 | 31.682335 | 29.303043 |
| Ca | 31.605192 | 26.864429 | 28.227322 |
| Ca | 32.646851 | 30.435303 | 25.140007 |
| Ca | 33.260330 | 25.676136 | 23.958284 |
| Ca | 36.215405 | 27.987244 | 27.376545 |

generated by VMD

| Ca | X   | Y   | Z   |
|----|-----|-----|-----|
| Ca | 18.408714 | 32.985455 | 33.682819 |
| Ca | 22.789522 | 34.250427 | 36.106300 |
| Ca | 23.587742 | 29.895678 | 32.583569 |
| Ca | 22.833992 | 34.617779 | 30.917036 |
| Ca | 24.977528 | 31.081892 | 27.614723 |
| Ca | 27.814901 | 32.818733 | 31.445961 |
| Ca | 29.526979 | 28.907730 | 29.412670 |
| Ca | 30.287518 | 32.826939 | 25.864603 |
| Ca | 30.554775 | 27.704124 | 24.844095 |
| Ca | 33.512280 | 29.668983 | 28.237411 |
| Ca | 34.329224 | 24.689680 | 27.323448 |
| Ca | 35.244255 | 28.646111 | 24.021650 |
| S  | 21.060946 | 31.145380 | 35.035187 |
| S  | 20.643499 | 35.835236 | 33.673386 |
| S  | 21.922928 | 31.490717 | 29.892704 |
| S     | 24.925390 | 33.003368 | 33.578735 |
|-------|-----------|-----------|-----------|
| S     | 26.344563 | 29.653191 | 30.651886 |
| S     | 28.231472 | 29.967316 | 26.170273 |
| S     | 30.916166 | 31.917564 | 29.382040 |
| S     | 31.952733 | 26.845047 | 28.341711 |
| S     | 32.142841 | 25.760698 | 24.064871 |
| S     | 36.452332 | 27.867687 | 27.355177 |

24 generated by VMD

| Ca    | 18.359135 | 32.967720 | 33.963177 |
|-------|-----------|-----------|-----------|
| Ca    | 22.587521 | 34.301212 | 35.700905 |
| Ca    | 23.926929 | 29.865093 | 32.703354 |
| Ca    | 22.881887 | 34.835522 | 30.762623 |
| Ca    | 25.063633 | 31.007586 | 27.821505 |
| Ca    | 27.845272 | 32.754959 | 31.570755 |
| Ca    | 29.697704 | 28.798531 | 29.402903 |
| Ca    | 30.184292 | 32.997841 | 26.015081 |
| Ca    | 30.451935 | 27.450869 | 24.766100 |
| Ca    | 33.414719 | 29.774975 | 28.606853 |
| Ca    | 34.099197 | 24.675322 | 27.191887 |
| Ca    | 35.244827 | 28.875580 | 23.963335 |
| S     | 21.157543 | 30.997499 | 34.862366 |
| S     | 20.659927 | 35.669403 | 33.359936 |
| S     | 22.122047 | 31.491533 | 29.839260 |
| S     | 24.985716 | 33.303600 | 33.507984 |
| S     | 26.680283 | 29.471886 | 30.679733 |
| S     | 25.949818 | 34.268219 | 28.873661 |
| S     | 28.241299 | 29.957447 | 26.262438 |
| S     | 30.952044 | 32.075081 | 29.625961 |
| S     | 31.455284 | 26.763268 | 28.136574 |
| S     | 32.484161 | 30.423880 | 25.114305 |
| S     | 33.184231 | 25.766357 | 23.782284 |
| S     | 36.090675 | 27.806675 | 27.427101 |

24 generated by VMD

| Ca    | 17.931396 | 33.066544 | 34.198082 |
|-------|-----------|-----------|-----------|
| Ca    | 22.907003 | 34.510479 | 35.957790 |
| Ca    | 23.702175 | 30.287788 | 32.795967 |
| Ca    | 22.845238 | 34.497425 | 31.053495 |
| Ca    | 25.217560 | 30.773663 | 27.379726 |
| Ca    | 27.855959 | 32.734314 | 31.418751 |
| Ca    | 29.210852 | 28.754374 | 29.504477 |
| Ca    | 30.103342 | 32.904728 | 25.825727 |
| Ca    | 30.644701 | 27.650412 | 24.653553 |
| Element | Value 1       | Value 2       | Value 3       |
|---------|---------------|---------------|---------------|
| Ca      | 33.381676     | 29.645182     | 28.849796     |
| Ca      | 34.046383     | 24.757355     | 27.061531     |
| Ca      | 35.532452     | 28.519094     | 24.085749     |
| S       | 21.206024     | 31.489372     | 35.162422     |
| S       | 20.453199     | 35.519394     | 33.400013     |
| S       | 22.107193     | 31.546785     | 29.796843     |
| S       | 25.123100     | 33.143375     | 33.640022     |
| S       | 26.407270     | 29.487461     | 30.493834     |
| S       | 25.822969     | 34.047951     | 28.829945     |
| S       | 28.346153     | 29.620853     | 26.105946     |
| S       | 31.009104     | 31.944881     | 29.412128     |
| S       | 31.499653     | 26.739235     | 28.148035     |
| S       | 32.742527     | 30.490431     | 25.140182     |
| S       | 33.511902     | 25.923555     | 23.640247     |
| S       | 36.112228     | 27.828465     | 27.385761     |

24 generated by VMD

| Element | Value 1       | Value 2       | Value 3       |
|---------|---------------|---------------|---------------|
| Ca      | 18.122307     | 32.803768     | 33.949139     |
| Ca      | 22.893097     | 34.143795     | 35.733170     |
| Ca      | 23.786015     | 30.058073     | 32.692444     |
| Ca      | 22.923031     | 34.801151     | 31.135090     |
| Ca      | 24.883734     | 30.975109     | 27.609707     |
| Ca      | 27.870745     | 32.851833     | 31.419189     |
| Ca      | 29.617741     | 29.169235     | 29.665657     |
| Ca      | 30.169245     | 32.878902     | 25.862864     |
| Ca      | 30.618258     | 27.703650     | 24.822441     |
| Ca      | 33.615204     | 29.892475     | 28.666492     |
| Ca      | 33.722912     | 24.603781     | 27.244175     |
| Ca      | 35.407120     | 28.530647     | 23.717823     |
| S       | 21.096518     | 31.094971     | 34.980732     |
| S       | 20.543150     | 35.435562     | 33.450581     |
| S       | 22.098465     | 31.640821     | 29.727251     |
| S       | 25.062035     | 33.093578     | 33.419689     |
| S       | 26.586720     | 29.568203     | 30.611515     |
| S       | 25.825474     | 34.251125     | 28.928734     |
| S       | 28.184078     | 29.831802     | 26.271393     |
| S       | 30.970898     | 32.218811     | 29.410627     |
| S       | 31.380312     | 26.939728     | 28.306562     |
| S       | 32.771973     | 30.606913     | 25.282188     |
| S       | 33.452732     | 25.598907     | 23.758732     |
| S       | 36.118294     | 27.607227     | 27.273848     |

24 generated by VMD

| Element | Value 1       | Value 2       | Value 3       |
|---------|---------------|---------------|---------------|
| Ca      | 18.553371     | 32.996162     | 34.185444     |
| Ca      | 22.863825     | 34.207325     | 35.847763     |
| Ca      | 23.871298     | 29.864712     | 32.562920     |

476
Ca   22.873276  34.774715  30.806301
Ca   24.894785  30.968525  27.541039
Ca   27.944624  32.682922  31.549475
Ca   29.326580  29.301514  29.666500
Ca   30.088448  32.723297  25.884129
Ca   30.570009  27.510979  24.887499
Ca   33.416172  29.658104  28.672182
Ca   34.122265  24.887001  27.269697
Ca   35.456921  28.787006  24.040958
S    21.185381  30.946543  34.875431
S    20.876669  35.759064  33.512188
S    22.015038  31.653004  29.572582
S    25.005957  33.098946  33.466743
S    26.507072  29.472855  30.389776
S    25.922029  34.076653  28.749268
S    28.139406  29.829672  26.323198
S    30.836819  31.982780  29.404795
S    31.507616  26.734747  28.340231
S    32.576443  30.557100  25.160381
S    33.181648  25.757271  23.766485
S    35.984383  28.070524  27.465057

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generated by VMD

Ca   18.349218  32.918484  34.126106
Ca   23.039263  34.183887  35.750217
Ca   23.481869  29.858974  32.524788
Ca   22.892231  34.676746  30.981165
Ca   24.987566  31.142427  27.442770
Ca   27.773291  32.738365  31.085629
Ca   29.317984  29.099087  29.555313
Ca   30.261608  32.691792  25.670589
Ca   30.406469  27.620831  24.943491
Ca   33.612247  30.008877  28.488813
Ca   33.904224  24.867620  27.551676
Ca   35.609421  28.745985  24.034790
S    21.367231  31.035358  35.296726
S    20.646107  35.611221  33.683884
S    21.859022  31.627541  29.843977
S    25.066999  33.012730  33.464622
S    26.290670  29.467030  30.292658
S    26.026466  34.352341  28.919140
S    28.151878  29.948988  26.174961
S    30.841288  31.903803  29.174139
S    31.475965  26.732124  28.260113
S    32.825817  30.474049  25.093822
S    33.293488  25.870377  23.986404
|  |  |  |  |
|---|---|---|---|
| S  | 36.239662 | 27.711388 | 27.597729 |
| 24 | generated by VMD |
| Ca | 18.136816 | 32.785622 | 34.357117 |
| Ca | 22.811243 | 34.238358 | 35.980755 |
| Ca | 23.735172 | 30.229065 | 32.377872 |
| Ca | 22.748274 | 34.906502 | 30.870396 |
| Ca | 25.007626 | 30.962757 | 27.513597 |
| Ca | 28.054304 | 32.727089 | 31.590801 |
| Ca | 29.496643 | 28.876852 | 29.441784 |
| Ca | 30.244822 | 32.902168 | 25.839947 |
| Ca | 30.447939 | 27.710373 | 24.683327 |
| Ca | 33.306145 | 29.766605 | 28.629478 |
| Ca | 34.065712 | 24.735550 | 27.361822 |
| Ca | 35.557522 | 28.731730 | 24.056381 |
| S  | 21.351799 | 31.015076 | 35.156471 |
| S  | 20.566116 | 35.397747 | 33.471443 |
| S  | 21.922804 | 31.664587 | 29.581213 |
| S  | 25.211170 | 33.455700 | 33.367435 |
| S  | 26.713657 | 29.463867 | 30.425056 |
| S  | 25.939587 | 34.136932 | 28.952011 |
| S  | 28.248356 | 29.780468 | 26.192810 |
| S  | 30.782433 | 32.054695 | 29.306608 |
| S  | 31.348709 | 26.776533 | 28.162560 |
| S  | 32.672207 | 30.349190 | 25.123384 |
| S  | 33.334778 | 25.819412 | 23.920620 |
| S  | 36.016323 | 27.813122 | 27.577160 |
| 24 | generated by VMD |
| Ca | 18.466103 | 33.267113 | 34.016621 |
| Ca | 23.117161 | 34.278351 | 35.700291 |
| Ca | 23.743011 | 29.733225 | 32.698555 |
| Ca | 22.902422 | 34.463093 | 30.972801 |
| Ca | 24.897348 | 30.866428 | 27.678082 |
| Ca | 27.966122 | 32.527359 | 31.661671 |
| Ca | 29.530031 | 29.081194 | 29.316301 |
| Ca | 30.309010 | 32.854656 | 25.738558 |
| Ca | 30.187967 | 27.828617 | 24.496391 |
| Ca | 33.488224 | 29.758965 | 28.566160 |
| Ca | 33.949749 | 25.035473 | 27.370827 |
| Ca | 35.518486 | 28.555847 | 24.115292 |
| S  | 21.134817 | 31.208923 | 35.018581 |
| S  | 20.563427 | 35.723656 | 33.277145 |
| S  | 21.971918 | 31.388561 | 29.739912 |
| S  | 25.050819 | 32.840702 | 33.566956 |
| S  | 26.464462 | 29.441082 | 30.535254 |
|     | x       | y       | z       |
|-----|---------|---------|---------|
| S   | 26.018822 | 34.013527 | 28.930031 |
| S   | 28.189392 | 30.081327 | 26.149769 |
| S   | 30.990322 | 32.215878 | 29.476665 |
| S   | 32.662334 | 30.458578 | 25.037800 |
| S   | 33.244816 | 25.913322 | 24.034819 |
| S   | 36.095150 | 27.901529 | 27.628441 |

24

generated by VMD

|     | x       | y       | z       |
|-----|---------|---------|---------|
| Ca  | 18.285452 | 33.127968 | 34.256401 |
| Ca  | 22.914211 | 34.437714 | 35.641510 |
| Ca  | 23.842707 | 29.792313 | 32.798950 |
| Ca  | 22.938612 | 34.738377 | 31.057465 |
| Ca  | 24.813240 | 30.695156 | 27.590004 |
| Ca  | 27.824575 | 32.697235 | 31.240776 |
| Ca  | 29.543133 | 28.841545 | 29.434484 |
| Ca  | 30.021799 | 32.892986 | 25.940744 |
| Ca  | 30.375647 | 29.908072 | 24.417576 |
| Ca  | 33.488976 | 29.664003 | 28.620714 |
| Ca  | 34.180771 | 24.771160 | 27.441057 |
| Ca  | 35.527493 | 28.868475 | 24.145206 |
| S   | 21.090414 | 31.244616 | 34.926682 |
| S   | 20.542072 | 35.670593 | 33.394829 |
| S   | 22.201292 | 31.430971 | 29.812824 |
| S   | 25.058352 | 32.975456 | 33.592857 |
| S   | 26.349670 | 29.477745 | 30.438894 |
| S   | 26.046244 | 34.304924 | 28.997341 |
| S   | 28.180447 | 29.941452 | 26.237740 |
| S   | 30.883463 | 32.023296 | 29.391342 |
| S   | 31.301826 | 26.804369 | 27.991220 |
| S   | 32.601940 | 30.626051 | 25.184912 |
| S   | 33.391739 | 25.686926 | 23.989346 |
| S   | 36.315945 | 27.678669 | 27.397419 |

24

generated by VMD

|     | x       | y       | z       |
|-----|---------|---------|---------|
| Ca  | 18.067755 | 32.802952 | 33.831680 |
| Ca  | 22.814713 | 34.461777 | 35.848679 |
| Ca  | 23.697140 | 30.058880 | 32.800983 |
| Ca  | 23.030981 | 34.730953 | 30.799839 |
| Ca  | 24.864267 | 30.930073 | 27.714291 |
| Ca  | 27.929090 | 32.715500 | 31.462685 |
| Ca  | 29.505877 | 29.167265 | 29.523647 |
| Ca  | 30.640215 | 32.773407 | 25.924360 |
| Ca  | 30.286077 | 27.788494 | 24.927301 |
| Ca  | 33.693626 | 29.719078 | 28.608822 |
| Ca  | 34.003799 | 25.002874 | 27.337715 |
| Ca   | 35.349930 | 28.472672 | 23.810196 |
| S    | 21.056705 | 31.096237 | 35.221420 |
| S    | 20.486649 | 35.322281 | 33.269497 |
| S    | 22.145760 | 31.406269 | 29.815975 |
| S    | 25.015020 | 33.263165 | 33.608482 |
| S    | 26.554802 | 29.515402 | 30.541164 |
| S    | 26.195927 | 34.081062 | 28.855061 |
| S    | 28.056833 | 30.090460 | 26.251431 |
| S    | 30.949614 | 31.904381 | 29.417681 |
| S    | 31.347326 | 26.982754 | 28.119408 |
| S    | 32.625351 | 30.580151 | 25.295933 |
| S    | 33.197433 | 25.794979 | 23.774328 |
| S    | 36.205196 | 27.638969 | 27.179474 |

24 generated by VMD

| Ca   | 18.244385 | 32.799450 | 33.617142 |
| S    | 21.686077 | 34.198723 | 35.862896 |
| S    | 23.901482 | 30.043871 | 32.801884 |
| S    | 22.851219 | 34.704494 | 30.794735 |
| S    | 24.906929 | 30.829308 | 27.784439 |
| S    | 27.736485 | 32.851913 | 31.579435 |
| S    | 29.495625 | 29.404457 | 29.742081 |
| S    | 30.594828 | 32.862606 | 25.823923 |
| S    | 30.175423 | 27.759741 | 24.818993 |
| S    | 33.721840 | 29.611465 | 28.473993 |
| S    | 33.715813 | 25.051743 | 27.162121 |
| S    | 35.482052 | 28.603626 | 23.998667 |

24 generated by VMD

| Ca   | 18.459097 | 32.893196 | 34.260864 |
| S    | 22.972300 | 34.409130 | 35.875504 |
| S    | 23.659630 | 30.029358 | 32.717335 |
| S    | 22.784502 | 34.503441 | 30.763527 |
| S    | 24.902941 | 31.005814 | 27.533546 |
|   | Ca       | 32.865345 | 31.243603 |
|---|----------|-----------|-----------|
|   | Ca       | 29.169994 | 29.668695 |
|   | Ca       | 32.661118 | 25.736984 |
|   | Ca       | 27.725492 | 24.997841 |
|   | Ca       | 29.661533 | 28.676517 |
|   | Ca       | 24.629005 | 27.037865 |
|   | Ca       | 29.007601 | 24.086761 |
|   | S        | 31.182623 | 35.325531 |
|   | S        | 35.518547 | 33.304512 |
|   | S        | 31.381445 | 29.518267 |
|   | S        | 33.111412 | 33.403313 |
|   | S        | 29.504925 | 30.396036 |
|   | S        | 34.185413 | 28.678223 |
|   | S        | 29.785606 | 26.370617 |
|   | S        | 31.918419 | 29.367245 |
|   | S        | 26.811255 | 28.300632 |
|   | S        | 30.673756 | 25.495281 |
|   | S        | 26.072086 | 23.673607 |
|   | S        | 27.593544 | 27.507732 |

24 generated by VMD

|   | Ca       | 33.306736 | 34.414513 |
|---|----------|-----------|-----------|
|   | Ca       | 34.467949 | 35.637329 |
|   | Ca       | 30.200020 | 32.900162 |
|   | Ca       | 34.517212 | 30.747015 |
|   | Ca       | 30.710123 | 27.554230 |
|   | Ca       | 32.643013 | 31.127298 |
|   | Ca       | 28.904726 | 29.948006 |
|   | Ca       | 32.627495 | 26.136166 |
|   | Ca       | 27.711502 | 24.816719 |
|   | Ca       | 29.646183 | 28.710705 |
|   | Ca       | 25.089741 | 26.699293 |
|   | Ca       | 28.949150 | 24.056623 |
|   | S        | 31.337519 | 35.276165 |
|   | S        | 35.669811 | 33.154205 |
|   | S        | 31.193981 | 29.713570 |
|   | S        | 33.189865 | 33.223511 |
|   | S        | 29.270012 | 30.613876 |
|   | S        | 34.027939 | 28.727360 |
|   | S        | 29.753693 | 26.597519 |
|   | S        | 31.539917 | 29.579782 |
|   | S        | 26.841112 | 28.082693 |
|   | S        | 30.512758 | 25.230503 |
|   | S        | 26.362999 | 23.510370 |
|   | S        | 27.826593 | 27.482430 |
|   | 18.430593 | 33.297329 | 34.298714 |
|---|------------|------------|------------|
| Ca| 23.171093  | 34.385582  | 35.836559  |
| Ca| 23.473097  | 29.970922  | 32.736256  |
| Ca| 22.928919  | 34.291374  | 30.697536  |
| Ca| 25.076908  | 30.848434  | 27.474852  |
| Ca| 27.818636  | 32.536125  | 31.252110  |
| Ca| 29.375444  | 29.137766  | 29.626862  |
| Ca| 30.193245  | 32.791828  | 26.015751  |
| Ca| 30.465506  | 27.570122  | 24.959652  |
| Ca| 33.701515  | 29.678267  | 28.634983  |
| Ca| 33.685875  | 25.077106  | 27.022701  |
| Ca| 35.566010  | 29.041155  | 24.082985  |
| S | 21.303267  | 31.353098  | 35.385372  |
| S | 20.753614  | 35.628517  | 33.179493  |
| S | 22.030405  | 31.279713  | 29.439693  |
| S | 24.959911  | 32.908646  | 33.233814  |
| S | 26.271301  | 29.297770  | 30.719072  |
| S | 26.012455  | 34.041710  | 28.692127  |
| S | 28.22969   | 29.814529  | 26.334343  |
| S | 30.90369   | 31.870440  | 29.495148  |
| S | 31.456781  | 26.881237  | 28.356432  |
| S | 32.815243  | 30.494871  | 25.225485  |
| S | 32.957184  | 26.332916  | 23.726624  |
| S | 36.147022  | 27.770596  | 27.513500  |

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|   | 18.357452 | 33.218323 | 33.950409 |
|---|------------|------------|------------|
| Ca| 22.836920  | 34.520794  | 35.864292  |
| Ca| 23.682281  | 29.917368  | 33.049095  |
| Ca| 22.972103  | 34.219936  | 30.777670  |
| Ca| 25.048012  | 30.739384  | 27.666645  |
| Ca| 27.841585  | 32.792995  | 31.452145  |
| Ca| 29.401470  | 29.192965  | 29.572720  |
| Ca| 30.261013  | 32.762047  | 25.741278  |
| Ca| 30.485655  | 27.732662  | 24.850079  |
| Ca| 33.609936  | 29.733696  | 28.663321  |
| Ca| 33.301498  | 25.023144  | 26.999155  |
| Ca| 35.747311  | 28.880106  | 24.059843  |
| S | 21.135561  | 31.303833  | 35.179642  |
| S | 20.89422   | 35.599430  | 33.212994  |
| S | 21.993103  | 31.037857  | 29.759571  |
| S | 24.913929  | 33.139179  | 33.524338  |
| S | 26.480854  | 29.419279  | 30.659784  |
| S | 26.12957   | 33.846088  | 28.897163  |
| S | 28.292147  | 29.711910  | 26.200659  |
|   |   |   |   |
|---|---|---|---|
| S | 30.928667 | 32.116055 | 29.163198 |
| S | 31.258310 | 26.920002 | 28.258011 |
| S | 32.931938 | 30.576645 | 25.240505 |
| S | 33.252575 | 26.339073 | 23.635147 |
| S | 35.962830 | 27.557306 | 27.562408 |

24
generated by VMD

| Ca | 18.398781 | 33.079224 | 33.866299 |
| Ca | 22.993177 | 34.245247 | 35.725227 |
| Ca | 23.603275 | 29.684713 | 32.848286 |
| Ca | 22.922293 | 34.225433 | 30.706158 |
| Ca | 25.027779 | 31.095514 | 27.702507 |
| Ca | 27.950386 | 33.009537 | 31.331047 |
| Ca | 29.594337 | 29.508259 | 29.669550 |
| Ca | 30.300797 | 32.914536 | 25.862242 |
| Ca | 30.202950 | 27.702015 | 24.734303 |
| Ca | 33.761986 | 29.761351 | 28.658039 |
| Ca | 33.706913 | 24.778196 | 27.040752 |
| Ca | 35.423721 | 28.652294 | 24.236858 |
| Ca | 21.253433 | 31.109112 | 35.283344 |
| Ca | 20.803549 | 35.543777 | 33.088825 |
| Ca | 21.952831 | 31.151493 | 29.913427 |
| Ca | 25.009769 | 32.780750 | 33.369152 |
| Ca | 26.528011 | 29.506163 | 30.507317 |
| Ca | 26.051725 | 34.088699 | 28.843679 |
| Ca | 28.152357 | 30.146706 | 26.408800 |
| Ca | 31.044655 | 32.303905 | 29.369478 |
| Ca | 31.279282 | 26.988010 | 28.254843 |
| Ca | 32.790005 | 30.469473 | 25.084805 |
| Ca | 33.011253 | 26.121117 | 23.681927 |
| Ca | 35.956795 | 27.434551 | 27.753155 |

24
generated by VMD

| Ca | 18.259338 | 33.199387 | 33.631393 |
| Ca | 22.752953 | 34.325779 | 35.900810 |
| Ca | 23.704793 | 29.846203 | 32.900993 |
| Ca | 22.952810 | 34.320704 | 30.794495 |
| Ca | 25.103798 | 30.890820 | 27.520197 |
| Ca | 28.147558 | 32.640762 | 31.454426 |
| Ca | 29.457235 | 29.301970 | 29.652813 |
| Ca | 30.148411 | 32.867302 | 26.041555 |
| Ca | 30.228172 | 27.721676 | 24.705605 |
| Ca | 33.697746 | 29.729610 | 28.710655 |
| Ca | 33.850105 | 24.913965 | 27.221588 |
| Ca | 35.245789 | 28.757244 | 23.929422 |
| S | 21.152039 | 31.339809 | 35.094112 |
|  |  |  |  |
|---|---|---|---|
| S | 20.812382 | 35.605534 | 33.224564 |
| S | 22.116127 | 31.028465 | 29.799118 |
| S | 25.102694 | 33.007301 | 33.400120 |
| S | 26.536182 | 29.500366 | 30.673092 |
| S | 26.056772 | 34.024097 | 28.917126 |
| S | 28.234360 | 29.954599 | 26.312757 |
| S | 31.017921 | 32.049171 | 29.450415 |
| S | 32.697506 | 30.597967 | 25.254002 |
| S | 33.026043 | 26.073963 | 23.917921 |
| S | 36.165653 | 27.648357 | 27.284168 |

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generated by VMD

| Ca | 18.421116 | 33.198406 | 33.487953 |
| Ca | 22.685556 | 34.348526 | 35.837578 |
| Ca | 23.864676 | 29.858799 | 32.935322 |
| Ca | 23.006483 | 34.543739 | 30.828135 |
| Ca | 24.944569 | 31.039814 | 27.768780 |
| Ca | 27.964828 | 32.746738 | 31.420866 |
| Ca | 29.623799 | 28.867979 | 29.587534 |
| Ca | 30.128370 | 32.700127 | 25.831427 |
| Ca | 30.329941 | 27.519169 | 24.782465 |
| Ca | 33.645802 | 29.659590 | 28.589794 |
| Ca | 33.880657 | 25.117531 | 27.000372 |
| Ca | 35.450470 | 28.860500 | 23.893654 |
| S | 21.119154 | 31.159714 | 34.963905 |
| S | 20.508911 | 35.769405 | 33.223400 |
| S | 22.102930 | 31.286179 | 30.024471 |
| S | 25.087694 | 33.076618 | 33.514805 |
| S | 26.385248 | 29.482506 | 30.789349 |
| S | 26.068291 | 34.135700 | 29.014351 |
| S | 28.289001 | 29.740879 | 26.385025 |
| S | 31.049337 | 32.057884 | 29.379208 |
| S | 31.325432 | 26.720026 | 28.386196 |
| S | 32.636311 | 30.343618 | 25.176992 |
| S | 33.146816 | 26.100983 | 23.618612 |
| S | 36.051979 | 27.965591 | 27.499794 |

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generated by VMD

| Ca | 18.320852 | 33.299484 | 33.467445 |
| Ca | 22.734570 | 34.349968 | 35.865273 |
| Ca | 23.831568 | 30.001173 | 33.077709 |
| Ca | 22.906143 | 34.387981 | 30.632450 |
| Ca | 25.062092 | 30.691742 | 27.854557 |
| Ca | 27.861984 | 32.656612 | 31.698366 |
| Ca | 29.461029 | 29.136221 | 29.818659 |
|   | Ca       | 30.38842 | 33.025021 | 26.026962 |
|---|----------|----------|-----------|-----------|
|   | Ca       | 30.328478| 27.615751 | 24.739702 |
|   | Ca       | 33.511017| 29.700981 | 28.526991 |
|   | Ca       | 33.753010| 24.892094 | 26.964737 |
|   | Ca       | 35.536888| 28.899498 | 23.893927 |
| S | 20.939430| 31.306875| 35.094395 |
| S | 20.659035| 35.694275| 33.038155 |
| S | 22.039635| 30.950319| 30.026955 |
| S | 25.062923| 33.471222| 33.456852 |
| S | 26.531750| 29.288134| 30.763521 |
| S | 26.093111| 33.929829| 28.989582 |
| S | 28.310904| 29.956835| 26.543478 |
| S | 31.002949| 31.837002| 29.475042 |
| S | 31.403074| 26.842415| 28.080151 |
| S | 32.778206| 30.558706| 25.093466 |
| S | 33.177555| 26.081966| 23.564640 |
| S | 36.025017| 27.725924| 27.247036 |

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generated by VMD

|   | Ca       | 18.409014| 33.016365| 33.798927 |
|---|----------|----------|-----------|-----------|
|   | Ca       | 22.902506| 34.387764| 35.789448 |
|   | Ca       | 23.950613| 29.883547| 33.013096 |
|   | Ca       | 22.756592| 34.406250| 30.728914 |
|   | Ca       | 24.973619| 31.034203| 27.556692 |
|   | Ca       | 27.856026| 32.791016| 31.299341 |
|   | Ca       | 29.618652| 29.113876| 29.588261 |
|   | Ca       | 30.230804| 32.808517| 25.984623 |
|   | Ca       | 30.353558| 27.762331| 24.933411 |
|   | Ca       | 33.516087| 29.692474| 28.651739 |
|   | Ca       | 33.689869| 24.788357| 27.009163 |
|   | Ca       | 35.547012| 28.976671| 24.191441 |
| S | 21.198526| 31.129175| 35.118286 |
| S | 20.683168| 35.738853| 33.334961 |
| S | 22.205761| 31.107740| 30.012390 |
| S | 25.121998| 33.241211| 33.280609 |
| S | 26.516232| 29.465721| 30.531639 |
| S | 25.832790| 34.220379| 28.840675 |
| S | 28.093306| 29.793325| 26.302465 |
| S | 30.867327| 31.998112| 29.353683 |
| S | 31.209188| 26.759842| 28.190680 |
| S | 32.810059| 30.517239| 25.209446 |
| S | 33.251377| 26.100929| 23.673492 |
| S | 36.125965| 27.566185| 27.546650 |

24

generated by VMD

|   | Ca       | 18.474161| 33.107414| 33.482708 |
| Element | X1     | Y1     | Z1     |
|---------|--------|--------|--------|
| Ca      | 23.028353 | 34.396858 | 36.008106 |
| Ca      | 23.976866 | 29.875698 | 32.905510 |
| Ca      | 22.811100 | 34.327442 | 30.779324 |
| Ca      | 24.775925 | 30.917341 | 27.599686 |
| Ca      | 27.542692 | 32.760185 | 31.211210 |
| Ca      | 29.705666 | 29.225269 | 29.721470 |
| Ca      | 30.346102 | 32.726616 | 26.213120 |
| Ca      | 30.193899 | 27.796875 | 24.902641 |
| Ca      | 33.770527 | 29.534657 | 28.734127 |
| Ca      | 33.859505 | 25.037956 | 27.029819 |
| Ca      | 35.385044 | 28.796984 | 24.017765 |
| S       | 21.377935 | 31.291332 | 35.126804 |
| S       | 20.752289 | 35.766098 | 33.416115 |
| S       | 21.962770 | 30.973713 | 29.852745 |
| S       | 24.955742 | 33.214169 | 33.304146 |
| S       | 26.388783 | 29.410320 | 30.362761 |
| S       | 25.801443 | 34.116714 | 28.584389 |
| S       | 28.152042 | 30.160873 | 26.488745 |
| S       | 31.005873 | 31.933277 | 29.694242 |
| S       | 31.420517 | 26.782780 | 28.152996 |
| S       | 32.805542 | 30.264433 | 25.338482 |
| S       | 33.009296 | 26.165628 | 23.632114 |
| S       | 36.217876 | 27.717373 | 27.380997 |

24 generated by VMD

| Element | X1     | Y1     | Z1     |
|---------|--------|--------|--------|
| Ca      | 18.261497 | 32.612816 | 34.017982 |
| Ca      | 22.860008 | 34.365360 | 35.967060 |
| Ca      | 23.994045 | 30.064827 | 32.935524 |
| Ca      | 22.743011 | 34.643539 | 30.607189 |
| Ca      | 25.044649 | 30.872074 | 27.595642 |
| Ca      | 27.655979 | 32.952843 | 31.323624 |
| Ca      | 29.789495 | 29.271606 | 29.680721 |
| Ca      | 30.385237 | 32.698158 | 25.816019 |
| Ca      | 30.497471 | 27.850288 | 24.936670 |
| Ca      | 33.733681 | 29.686436 | 28.765577 |
| Ca      | 33.427494 | 24.819838 | 26.938829 |
| Ca      | 35.563744 | 28.585609 | 24.066486 |
| S       | 21.229256 | 31.228371 | 35.104366 |
| S       | 20.536921 | 35.408287 | 33.358887 |
| S       | 22.032280 | 31.206863 | 29.751305 |
| S       | 25.105036 | 33.301445 | 33.306362 |
| S       | 26.443264 | 29.618193 | 30.484978 |
| S       | 25.800255 | 34.107689 | 28.680138 |
| S       | 28.355671 | 30.067562 | 26.550415 |
| S       | 31.078701 | 32.017826 | 29.459747 |
| S       | 31.378334 | 26.870531 | 28.250965 |
S  32.898293  30.491421  25.419876
S  33.010788  26.177723  23.504210
S  35.894917  27.380693  27.417530

24 generated by VMD
Ca  18.389040  33.158859  34.423073
Ca  22.846525  34.259754  35.796188
Ca  23.991282  30.106491  32.862854
Ca  22.656269  34.686096  30.948704
Ca  24.846449  30.724226  27.464962
Ca  27.706675  32.735600  30.964931
Ca  29.505945  29.129910  29.594883
Ca  30.096037  32.778763  25.951134
Ca  30.489729  27.857990  24.736767
Ca  33.572800  29.632046  28.759155
Ca  33.839458  24.584734  26.965521
Ca  35.753338  28.912613  24.330635
S  21.447872  31.124397  35.078968
S  20.462330  35.825439  33.405701
S  22.231995  31.182287  30.024040
S  25.212883  33.192841  33.190781
S  26.386011  29.395500  30.405491
S  25.476999  34.224388  28.545954
S  28.124456  29.890499  26.328262
S  30.910257  31.836292  29.461132
S  31.478045  26.921410  27.914860
S  32.837887  30.661648  25.384497
S  33.426880  26.204933  23.604700
S  36.030910  27.273378  27.796867

24 generated by VMD
Ca  18.469564  32.969254  34.093010
Ca  22.986155  34.483456  35.640076
Ca  24.074957  30.092024  32.749672
Ca  22.797819  34.866127  30.852360
Ca  24.711004  30.601376  27.695234
Ca  27.722681  32.579567  31.431675
Ca  29.586859  28.847305  29.470774
Ca  30.175238  32.966999  26.156239
Ca  30.389553  27.569212  24.632814
Ca  33.494373  29.624020  28.728767
Ca  33.847286  24.781069  27.107656
Ca  35.699165  29.105015  24.174370
S  21.336426  31.286135  34.956738
S  20.577557  35.746414  33.413715
S  21.969706  31.396151  29.967262
|   | S        | 25.089167       | 33.478325       | 33.288406 |
|---|----------|-----------------|-----------------|-----------|
| S | 26.346222 | 29.308640       | 30.502972       |           |
| S | 25.674330 | 33.863529       | 28.814058       |           |
| S | 28.338251 | 29.900330       | 26.309666       |           |
| S | 30.873606 | 31.762486       | 29.589539       |           |
| S | 31.317253 | 26.684654       | 28.060062       |           |
| S | 32.671028 | 30.478096       | 25.198648       |           |
| S | 33.518936 | 26.153484       | 23.587776       |           |
| S | 36.052868 | 27.756420       | 27.518501       |           |

24 generated by VMD

| Ca |   | 18.610355       | 33.276062       | 34.360149 |
| Ca |   | 23.072153       | 34.424023       | 35.742950 |
| Ca |   | 23.731464       | 29.851860       | 32.806709 |
| Ca |   | 22.823399       | 34.381775       | 30.695534 |
| Ca |   | 24.748796       | 30.744682       | 27.355726 |
| Ca |   | 27.806353       | 32.377953       | 31.301968 |
| Ca |   | 29.513624       | 29.115513       | 29.391094 |
| Ca |   | 29.947182       | 32.769115       | 25.81243 |
| Ca |   | 30.620390       | 27.676262       | 24.792938 |
| Ca |   | 33.773373       | 29.658846       | 28.776230 |
| Ca |   | 33.722504       | 24.726078       | 27.020370 |
| Ca |   | 35.551304       | 29.134651       | 24.402342 |
| S  |   | 21.231834       | 31.399628       | 35.124374 |
| S  |   | 20.966593       | 35.994102       | 33.542351 |
| S  |   | 21.933727       | 31.140652       | 29.887764 |
| S  |   | 25.111307       | 33.071030       | 33.328217 |
| S  |   | 26.306356       | 29.234455       | 30.227978 |
| S  |   | 25.780043       | 33.933357       | 28.671246 |
| S  |   | 28.121767       | 29.767225       | 26.210636 |
| S  |   | 30.757200       | 32.044193       | 29.412655 |
| S  |   | 31.424112       | 26.960688       | 28.322426 |
| S  |   | 32.744598       | 30.728462       | 25.376394 |
| S  |   | 33.524113       | 26.341232       | 23.720287 |
| S  |   | 35.897484       | 27.548199       | 27.658463 |

24 generated by VMD

| Ca |   | 18.712324       | 32.914700       | 34.333336 |
| Ca |   | 23.105356       | 34.026882       | 35.808479 |
| Ca |   | 24.018932       | 30.172009       | 32.567207 |
| Ca |   | 22.622742       | 34.836170       | 30.661022 |
| Ca |   | 24.936443       | 30.845882       | 27.361391 |
| Ca |   | 27.674484       | 32.644344       | 31.180061 |
| Ca |   | 29.364119       | 28.904079       | 29.745859 |
| Ca |   | 30.232014       | 32.868969       | 26.071323 |
| Ca |   | 30.432056       | 27.657503       | 24.789753 |
| Element | X Coord 1 | Y Coord 1 | Z Coord 1 | X Coord 2 | Y Coord 2 | Z Coord 2 |
|---------|-----------|-----------|-----------|-----------|-----------|-----------|
| Ca      | 33.515575 | 29.671875 | 28.865002 |           |           |           |
| Ca      | 33.927536 | 25.022621 | 27.158215 |           |           |           |
| Ca      | 35.427738 | 28.795219 | 24.048313 |           |           |           |
| S       | 21.363981 | 30.930832 | 34.965698 |           |           |           |
| S       | 20.850168 | 35.684845 | 33.720375 |           |           |           |
| S       | 22.171459 | 31.468937 | 29.701914 |           |           |           |
| S       | 25.137636 | 33.449162 | 32.980942 |           |           |           |
| S       | 26.342529 | 29.248119 | 30.311420 |           |           |           |
| S       | 25.696667 | 34.183857 | 28.663425 |           |           |           |
| S       | 28.210209 | 29.916449 | 26.361526 |           |           |           |
| S       | 30.736713 | 31.998257 | 29.543751 |           |           |           |
| S       | 31.286011 | 26.798454 | 28.358534 |           |           |           |
| S       | 32.669441 | 30.477964 | 25.284657 |           |           |           |
| S       | 33.339134 | 26.066422 | 23.839529 |           |           |           |
| S       | 35.946819 | 27.716499 | 27.618345 |           |           |           |

24 generated by VMD

| Element | X Coord | Y Coord | Z Coord |
|---------|---------|---------|---------|
| Ca      | 18.596045 | 32.980690 | 34.267059 |
| Ca      | 23.154875 | 34.050148 | 35.837101 |
| Ca      | 23.648022 | 29.864723 | 32.522774 |
| Ca      | 22.929256 | 34.808697 | 31.008900 |
| Ca      | 24.594406 | 31.061726 | 27.367079 |
| Ca      | 27.698877 | 32.645615 | 31.145470 |
| Ca      | 29.288090 | 29.275700 | 29.505810 |
| Ca      | 30.482933 | 32.761162 | 25.858425 |
| Ca      | 30.331984 | 27.640593 | 24.801502 |
| Ca      | 33.650856 | 29.591549 | 28.789406 |
| Ca      | 34.038872 | 25.471905 | 27.469685 |
| Ca      | 35.587349 | 28.527874 | 24.056347 |
| S       | 21.430698 | 31.080929 | 35.050804 |
| S       | 20.993408 | 35.675335 | 33.734856 |
| S       | 21.759096 | 31.512581 | 29.784998 |
| S       | 25.089104 | 33.066231 | 33.355980 |
| S       | 26.215939 | 29.446606 | 30.251925 |
| S       | 25.525322 | 34.150417 | 28.504745 |
| S       | 28.088097 | 29.966568 | 26.131195 |
| S       | 30.841305 | 31.815754 | 29.324066 |
| S       | 31.343130 | 26.722843 | 28.272863 |
| S       | 32.837906 | 30.246704 | 25.298950 |
| S       | 33.217442 | 25.952961 | 23.918243 |
| S       | 36.376991 | 27.982780 | 27.681873 |

24 generated by VMD

| Element | X Coord | Y Coord | Z Coord |
|---------|---------|---------|---------|
| Ca      | 18.608803 | 33.066334 | 33.797276 |
| Ca      | 23.111713 | 34.208534 | 36.139435 |
| Ca      | 23.538000 | 29.890963 | 32.654011 |
| Element | X Value | Y Value | Z Value |
|---------|---------|---------|---------|
| Ca      | 22.995434 | 34.886650 | 30.836948 |
| Ca      | 24.715710 | 30.862581 | 27.302261 |
| Ca      | 27.551931 | 32.586517 | 25.972515 |
| Ca      | 29.246014 | 28.991610 | 29.743134 |
| Ca      | 30.410477 | 32.586517 | 25.972515 |
| Ca      | 30.159182 | 27.669077 | 24.942074 |
| Ca      | 33.551514 | 29.763660 | 28.529415 |
| Ca      | 34.102413 | 25.212315 | 27.382950 |
| Ca      | 35.581818 | 28.717436 | 23.926733 |
| S       | 21.317600 | 31.182295 | 35.319588 |
| S       | 20.947088 | 35.757004 | 33.739529 |
| S       | 22.152355 | 31.578348 | 29.699503 |
| S       | 25.027386 | 33.257240 | 33.311333 |
| S       | 26.105211 | 29.211792 | 30.310116 |
| S       | 25.629076 | 34.177948 | 28.549751 |
| S       | 28.148577 | 29.829205 | 26.242920 |
| S       | 30.695225 | 31.684748 | 29.506098 |
| S       | 31.567036 | 27.010658 | 28.240704 |
| S       | 32.649139 | 30.231979 | 25.110979 |
| S       | 33.433693 | 26.102161 | 23.890905 |
| S       | 36.474648 | 27.955338 | 27.485537 |

24 generated by VMD

| Element | X Value | Y Value | Z Value |
|---------|---------|---------|---------|
| Ca      | 18.561207 | 32.606064 | 34.349102 |
| Ca      | 22.910061 | 34.665802 | 35.727657 |
| Ca      | 23.687531 | 29.983891 | 32.678692 |
| Ca      | 22.945534 | 34.873871 | 30.507538 |
| Ca      | 24.882843 | 30.669044 | 27.639008 |
| Ca      | 27.660267 | 32.645077 | 31.107180 |
| Ca      | 29.355469 | 28.751829 | 29.741383 |
| Ca      | 30.493923 | 32.831722 | 26.210020 |
| Ca      | 30.159279 | 28.026669 | 25.032575 |
| Ca      | 33.720337 | 29.469000 | 28.718901 |
| Ca      | 33.807594 | 24.789160 | 26.896603 |
| Ca      | 35.680641 | 28.921253 | 24.113871 |
| S       | 21.510719 | 31.271042 | 35.314444 |
| S       | 20.576088 | 35.719898 | 33.351456 |
| S       | 21.956268 | 31.233250 | 29.822479 |
| S       | 25.015617 | 33.483566 | 33.058735 |
| S       | 26.257237 | 29.195431 | 30.443436 |
| S       | 25.631037 | 34.088207 | 28.495647 |
| S       | 28.168953 | 29.921019 | 26.396568 |
| S       | 31.122072 | 31.708733 | 29.571884 |
| S       | 31.463003 | 26.778387 | 28.260561 |
| S       | 32.826363 | 30.668949 | 25.405199 |
| S       | 33.111694 | 26.491076 | 23.647678 |
|   |       |       |       |
|---|-------|-------|-------|
| S | 36.216316 | 27.507128 | 27.411795 |
| 24 | generated by VMD |
| Ca | 18.813881 | 32.748043 | 33.795437 |
| Ca | 22.915003 | 34.396870 | 36.031021 |
| Ca | 23.706886 | 30.079926 | 32.635216 |
| Ca | 22.907181 | 34.722675 | 30.770836 |
| Ca | 24.765127 | 30.853386 | 27.542439 |
| Ca | 27.646187 | 32.450245 | 31.304346 |
| Ca | 29.367756 | 28.895084 | 29.563675 |
| Ca | 30.285433 | 32.735176 | 25.990807 |
| Ca | 30.376991 | 27.544331 | 24.883942 |
| Ca | 33.558750 | 29.909904 | 28.772572 |
| Ca | 33.863628 | 24.981247 | 27.122883 |
| Ca | 35.656132 | 28.692104 | 24.043049 |
| S  | 21.435032 | 31.112200 | 35.299492 |
| S  | 20.883858 | 35.595554 | 33.450077 |
| S  | 22.003721 | 31.518936 | 29.779915 |
| S  | 25.124252 | 33.481411 | 33.419022 |
| S  | 26.066956 | 29.500591 | 30.497213 |
| S  | 25.874773 | 34.204926 | 28.627928 |
| S  | 28.064892 | 29.846306 | 26.271208 |
| S  | 30.622139 | 31.745596 | 29.564301 |
| S  | 31.501312 | 26.926842 | 28.274620 |
| S  | 32.829414 | 30.307930 | 25.124924 |
| S  | 33.384785 | 26.126705 | 23.641037 |
| S  | 36.065849 | 27.924053 | 27.534115 |
| 24 | generated by VMD |
| Ca | 18.643219 | 32.965565 | 34.092194 |
| Ca | 23.203800 | 34.340092 | 35.681870 |
| Ca | 23.609905 | 29.714046 | 32.768940 |
| Ca | 23.056961 | 34.820129 | 30.756124 |
| Ca | 24.946016 | 30.862862 | 27.447647 |
| Ca | 27.790462 | 32.493935 | 31.269806 |
| Ca | 29.241711 | 29.281490 | 29.460419 |
| Ca | 30.156578 | 32.942631 | 25.857647 |
| Ca | 30.443663 | 27.698513 | 24.635389 |
| Ca | 33.418285 | 29.796856 | 28.762379 |
| Ca | 33.854919 | 24.947411 | 27.454876 |
| Ca | 35.481651 | 28.798752 | 24.187902 |
| S  | 21.326571 | 31.047144 | 35.414642 |
| S  | 20.914322 | 35.588398 | 33.556168 |
| S  | 22.020344 | 31.413170 | 29.886093 |
| S  | 25.115177 | 33.170914 | 33.241814 |
| S  | 26.211643 | 29.258303 | 30.292253 |
|  |  |  |  |
|---|---|---|---|
| S  | 25.878786 | 34.065575 | 28.773527 |
| S  | 28.076540 | 30.030157 | 26.116356 |
| S  | 30.750698 | 31.988487 | 29.377008 |
| S  | 31.186607 | 26.894192 | 28.172901 |
| S  | 32.849552 | 30.501953 | 25.227116 |
| S  | 33.650539 | 25.796944 | 23.767012 |
| S  | 35.892059 | 27.882565 | 27.739716 |

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generated by VMD

| Ca  | 18.378691 | 32.568962 | 33.689964 |
| Ca  | 22.790073 | 34.200123 | 35.773079 |
| Ca  | 23.700817 | 30.033165 | 32.812267 |
| Ca  | 22.856312 | 34.780022 | 30.500132 |
| Ca  | 25.212177 | 31.018158 | 27.686724 |
| Ca  | 27.831177 | 32.727074 | 31.669470 |
| Ca  | 29.542789 | 29.031431 | 29.808609 |
| Ca  | 30.652924 | 32.998047 | 26.412189 |
| Ca  | 30.257532 | 27.724007 | 24.962921 |
| Ca  | 33.727966 | 29.600803 | 28.54458 |
| Ca  | 33.979057 | 24.800022 | 27.147013 |
| Ca  | 35.126934 | 28.668373 | 23.63036 |
| S   | 21.212055 | 31.089184 | 35.260506 |
| S   | 20.506054 | 35.592171 | 33.268131 |
| S   | 21.977749 | 31.386555 | 29.679272 |
| S   | 24.837296 | 33.608562 | 33.175114 |
| S   | 26.373201 | 29.480320 | 30.670132 |
| S   | 26.009510 | 34.205166 | 28.785933 |
| S   | 28.265720 | 30.091145 | 26.516449 |
| S   | 31.219290 | 31.711292 | 29.889706 |
| S   | 31.522099 | 26.942785 | 28.304953 |
| S   | 32.590332 | 30.536867 | 24.997206 |
| S   | 33.025219 | 25.695217 | 23.823923 |
| S   | 36.125031 | 27.810570 | 26.928875 |

24

generated by VMD

| Ca  | 18.219810 | 32.367668 | 33.727665 |
| Ca  | 23.043646 | 34.164589 | 35.556183 |
| Ca  | 23.880121 | 30.020554 | 32.583393 |
| Ca  | 22.860413 | 34.865208 | 30.904337 |
| Ca  | 24.930990 | 31.024719 | 27.631115 |
| Ca  | 28.023838 | 33.045227 | 31.319181 |
| Ca  | 29.450598 | 29.275402 | 29.781845 |
| Ca  | 30.613874 | 32.943111 | 26.180098 |
| Ca  | 30.275803 | 27.674820 | 24.780128 |
| Ca  | 33.500778 | 29.804756 | 28.610558 |
| Ca  | 33.822674 | 24.599743 | 27.454174 |


|     |      |      |      |
|-----|------|------|------|
| Ca  | 35.229195 | 28.629829 | 23.856684 |
| S   | 21.354961 | 30.924768 | 35.107033 |
| S   | 20.422379 | 35.294109 | 33.487015 |
| S   | 22.028580 | 31.428869 | 29.632637 |
| S   | 25.230429 | 33.373585 | 33.379650 |
| S   | 26.577538 | 29.466932 | 30.541422 |
| S   | 25.877365 | 34.390442 | 28.815678 |
| S   | 28.255646 | 30.169350 | 26.358637 |
| S   | 31.270195 | 31.937748 | 29.624786 |
| S   | 31.192329 | 27.033403 | 28.206505 |
| S   | 32.858978 | 30.487194 | 25.163202 |
| S   | 33.005318 | 25.590382 | 23.940563 |
| S   | 35.794617 | 27.787630 | 27.297543 |

24 generated by VMD

|     |      |      |      |
|-----|------|------|------|
| Ca  | 18.419487 | 32.697594 | 33.785511 |
| Ca  | 22.641298 | 34.132912 | 35.836819 |
| Ca  | 23.579697 | 29.795330 | 32.654980 |
| Ca  | 22.836151 | 34.652905 | 30.817001 |
| Ca  | 25.066187 | 30.997375 | 27.737902 |
| Ca  | 28.021584 | 32.988464 | 31.592785 |
| Ca  | 29.527699 | 29.514416 | 29.690203 |
| Ca  | 30.329733 | 32.901985 | 25.910278 |
| Ca  | 30.314131 | 27.577543 | 24.908829 |
| Ca  | 33.793179 | 29.668484 | 28.496284 |
| Ca  | 33.808842 | 24.722080 | 27.119854 |
| Ca  | 35.390831 | 28.483000 | 23.962164 |
| S   | 21.173233 | 30.860815 | 35.240852 |
| S   | 20.560066 | 35.583565 | 33.391708 |
| S   | 22.031754 | 31.503815 | 29.652349 |
| S   | 24.904282 | 33.253376 | 33.288834 |
| S   | 26.703215 | 29.719410 | 30.720093 |
| S   | 25.897331 | 34.184536 | 28.764221 |
| S   | 28.166859 | 30.169926 | 26.361565 |
| S   | 31.222855 | 32.106747 | 29.467785 |
| S   | 31.438154 | 26.964588 | 28.316799 |
| S   | 32.838123 | 30.490143 | 25.078661 |
| S   | 32.952324 | 25.823763 | 23.835941 |
| S   | 36.103012 | 27.507292 | 27.308506 |

24 generated by VMD

|     |      |      |      |
|-----|------|------|------|
| Ca  | 18.555477 | 32.590458 | 33.757030 |
| Ca  | 23.121429 | 34.175438 | 35.935196 |
| Ca  | 23.654110 | 29.925804 | 32.788414 |
| Ca  | 22.924036 | 34.739140 | 30.740055 |
| Ca  | 24.792252 | 30.711365 | 27.523066 |
| Element | Value 1     | Value 2     | Value 3     |
|---------|------------|------------|------------|
| Ca      | 27.848072  | 32.782810  | 31.230850  |
| Ca      | 29.443020  | 29.445183  | 29.948914  |
| Ca      | 30.466625  | 32.854465  | 25.963352  |
| Ca      | 30.552204  | 27.585249  | 24.814388  |
| Ca      | 33.653816  | 29.779678  | 28.658106  |
| Ca      | 33.416275  | 24.970011  | 27.079357  |
| Ca      | 35.569511  | 28.592018  | 24.004616  |
| S       | 21.299397  | 31.170092  | 35.179310  |
| S       | 20.662622  | 35.614044  | 33.610271  |
| S       | 21.975266  | 31.485857  | 29.656082  |
| S       | 24.921488  | 33.250721  | 33.138927  |
| S       | 26.479372  | 29.422606  | 30.597689  |
| S       | 25.727621  | 33.978298  | 28.570509  |
| S       | 28.214779  | 30.090580  | 26.566860  |
| S       | 31.094488  | 32.050011  | 29.506184  |
| S       | 31.381020  | 26.978992  | 28.311031  |
| S       | 32.859455  | 30.436546  | 25.340212  |
| S       | 33.162899  | 26.087360  | 23.590014  |
| S       | 35.944771  | 27.583328  | 27.429632  |

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generated by VMD

| Element | Value 1     | Value 2     | Value 3     |
|---------|------------|------------|------------|
| Ca      | 18.486151  | 32.675953  | 34.070110  |
| Ca      | 23.225630  | 33.993881  | 35.752377  |
| Ca      | 23.524969  | 29.859833  | 32.306705  |
| Ca      | 22.849056  | 35.065514  | 31.077024  |
| Ca      | 24.947189  | 30.945461  | 27.535666  |
| Ca      | 27.876122  | 32.664410  | 31.338598  |
| Ca      | 29.499231  | 29.264816  | 29.637859  |
| Ca      | 30.356201  | 32.780075  | 25.819292  |
| Ca      | 30.327370  | 27.694468  | 24.945187  |
| Ca      | 33.654545  | 29.854584  | 28.546680  |
| Ca      | 33.935719  | 24.872278  | 27.479122  |
| Ca      | 35.390621  | 28.576515  | 23.986681  |
| S       | 21.451302  | 30.993105  | 34.901257  |
| S       | 20.485313  | 35.683990  | 33.656040  |
| S       | 21.809206  | 31.632582  | 29.699425  |
| S       | 24.962349  | 33.051823  | 33.267395  |
| S       | 26.474144  | 29.548237  | 30.570774  |
| S       | 25.752968  | 34.327347  | 28.750763  |
| S       | 28.200577  | 30.122959  | 26.428486  |
| S       | 30.972059  | 32.018875  | 29.392790  |
| S       | 31.380775  | 26.860741  | 28.255844  |
| S       | 32.668602  | 30.356342  | 25.134823  |
| S       | 33.318478  | 25.724998  | 23.930563  |
| S       | 36.171459  | 27.731308  | 27.456625  |

24
|   |       |       |       |
|---|-------|-------|-------|
| Ca| 18.604645 | 32.253216 | 33.767487 |
| Ca| 23.256182  | 34.000244  | 36.012066  |
| Ca| 23.870838  | 30.335474  | 32.394730  |
| Ca| 23.027317  | 34.713898  | 30.843939  |
| Ca| 24.756100  | 30.820744  | 37.509842  |
| Ca| 29.611838  | 32.905315  | 31.227962  |
| Ca| 29.313807  | 29.247700  | 29.627661  |
| Ca| 30.131977  | 32.867233  | 25.874359  |
| Ca| 30.228027  | 27.660255  | 24.806915  |
| Ca| 33.609634  | 29.676357  | 28.493656  |
| Ca| 33.673122  | 24.736425  | 27.336626  |
| Ca| 35.381176  | 28.834946  | 24.393007  |
| S | 21.681107  | 30.878445  | 35.025536  |
| S | 20.741207  | 35.263107  | 33.667221  |
| S | 21.959688  | 31.814287  | 29.476252  |
| S | 25.287025  | 33.282318  | 33.238968  |
| S | 26.280476  | 29.623951  | 30.650509  |
| S | 25.877979  | 34.245239  | 28.633650  |
| S | 28.036057  | 30.034180  | 26.310596  |
| S | 30.875322  | 32.164162  | 29.357422  |
| S | 31.082603  | 27.151207  | 28.276493  |
| S | 32.718315  | 30.292053  | 25.120918  |
| S | 33.309677  | 25.871315  | 24.027086  |
| S | 36.096115  | 27.627983  | 27.866722  |

24

|   |       |       |       |
|---|-------|-------|-------|
| Ca| 18.941296 | 32.422901 | 34.222111 |
| Ca| 23.435669  | 34.148190  | 35.695366  |
| Ca| 23.480040  | 30.073711  | 32.393661  |
| Ca| 22.827394  | 34.787056  | 30.774628  |
| Ca| 24.678423  | 31.151295  | 27.532166  |
| Ca| 27.902359  | 32.636703  | 31.126757  |
| Ca| 29.221544  | 29.115599  | 29.507441  |
| Ca| 30.319294  | 32.742054  | 25.803417  |
| Ca| 30.324623  | 27.795849  | 24.894590  |
| Ca| 33.573372  | 29.847328  | 28.685524  |
| Ca| 33.834122  | 24.939812  | 27.455658  |
| Ca| 35.673939  | 28.662804  | 24.277958  |
| S | 21.636562  | 30.989138  | 35.369793  |
| S | 20.876032  | 35.456650  | 33.652134  |
| S | 21.648628  | 31.894161  | 29.518768  |
| S | 25.021744  | 33.010368  | 33.161701  |
| S | 26.170124  | 29.588341  | 30.436941  |
| S | 25.789719  | 34.137917  | 28.632259  |
| S | 27.996319  | 30.097340  | 26.244083  |
|   |    |    |    |
|---|----|----|----|
| S | 30.848244 | 31.763966 | 29.315346 |
| S | 31.312647 | 26.822422 | 28.281099 |
| S | 32.625317 | 30.561535 | 25.169374 |
| S | 33.405983 | 25.854877 | 24.009798 |
| S | 36.176662 | 27.800064 | 27.779493 |

24

generated by VMD

| Ca | 18.589314 | 32.398598 | 34.213562 |
| Ca | 23.225594 | 34.053093 | 35.873707 |
| Ca | 23.589170 | 30.341768 | 32.657692 |
| Ca | 22.807810 | 34.718620 | 30.759598 |
| Ca | 24.511831 | 30.862219 | 27.467051 |
| Ca | 27.948521 | 32.999672 | 31.064419 |
| Ca | 29.436413 | 29.171299 | 29.461815 |
| Ca | 30.440542 | 32.779892 | 25.883265 |
| Ca | 30.437332 | 27.630306 | 24.782969 |
| Ca | 33.519947 | 29.459837 | 28.752249 |
| Ca | 33.880283 | 24.750736 | 27.286154 |
| Ca | 35.805466 | 28.829510 | 24.074886 |
| S  | 21.623751 | 30.978451 | 35.327290 |
| S  | 20.567272 | 35.326767 | 33.770950 |
| S  | 21.863602 | 31.603846 | 29.573488 |
| S  | 25.128864 | 33.336628 | 33.263878 |
| S  | 26.306957 | 29.732584 | 30.368711 |
| S  | 25.790468 | 34.209259 | 28.430885 |
| S  | 27.993280 | 30.242737 | 26.246120 |
| S  | 31.053352 | 32.165001 | 29.417282 |
| S  | 31.014847 | 26.762131 | 28.318626 |
| S  | 32.788086 | 30.461906 | 25.316824 |
| S  | 33.492268 | 25.910168 | 23.847771 |
| S  | 35.905136 | 27.574995 | 27.780876 |

24

generated by VMD

| Ca | 18.483658 | 32.472034 | 34.002651 |
| Ca | 23.105925 | 34.129345 | 35.893200 |
| Ca | 23.549118 | 30.096336 | 32.717911 |
| Ca | 22.934256 | 34.746376 | 30.652166 |
| Ca | 24.765553 | 30.889851 | 27.461468 |
| Ca | 27.913536 | 32.820339 | 30.971169 |
| Ca | 29.475525 | 29.201481 | 29.598045 |
| Ca | 30.706369 | 32.892162 | 25.898899 |
| Ca | 30.356657 | 28.068710 | 25.361757 |
| Ca | 33.695023 | 29.767448 | 28.642004 |
| Ca | 33.619759 | 24.692131 | 27.371889 |
| Ca | 35.474342 | 28.583496 | 23.895176 |
| S  | 21.317696 | 30.942339 | 35.433617 |
S  20.695663  35.360630  33.533226
S  21.876583  31.432028  29.667080
S  25.070341  33.304604  33.243484
S  26.337122  29.443308  30.361498
S  25.796394  34.144913  28.516985
S  28.265087  30.384886  26.325535
S  31.146330  31.874275  29.399603
S  31.306946  26.971647  28.467625
S  32.918335  30.637287  25.093380
S  32.959595  25.889688  23.978582
S  35.950237  27.554745  27.452362

24

generated by VMD

Ca  18.519678  32.537731  33.647083
Ca  22.876284  34.036934  35.991730
Ca  23.632702  29.976795  32.579254
Ca  22.962177  34.837662  30.657984
Ca  24.806244  30.986664  27.647226
Ca  27.888533  32.820438  31.390934
Ca  29.403547  29.399693  29.764488
Ca  30.436399  32.996422  26.033287
Ca  30.362259  27.714712  25.116417
Ca  33.850079  29.529114  28.459042
Ca  33.793884  25.034016  27.435299
Ca  35.155426  28.443531  23.594950
S  21.364635  30.972729  35.138645
S  20.515995  35.278374  33.407925
S  21.972422  31.769468  29.611477
S  24.980337  33.130390  33.338482
S  26.428555  29.547829  30.537830
S  26.075951  34.187107  28.828039
S  28.180145  30.230659  26.440674
S  31.217899  31.997333  29.514433
S  31.279860  27.089108  28.520283
S  32.830902  30.473091  25.139538
S  33.099056  25.550739  24.056244
S  36.087151  27.757116  27.08835

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generated by VMD

Ca  18.454567  32.618252  33.449730
Ca  22.732027  33.961605  35.930702
Ca  23.619953  29.987251  32.463913
Ca  22.969629  34.866325  30.593767
Ca  24.887190  30.842846  27.925007
Ca  28.050076  32.928364  31.575945
Ca  29.573402  29.218424  29.820457
| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 30.476515 | 32.801647 | 26.149452 |
| Ca      | 30.044697 | 27.714085 | 25.165758 |
| Ca      | 33.777641 | 29.550686 | 28.324383 |
| Ca      | 33.678677 | 24.914528 | 27.268955 |
| Ca      | 35.338604 | 28.645985 | 23.722313 |
| S       | 21.169239 | 30.936363 | 35.012283 |
| S       | 20.552031 | 35.484020 | 33.528618 |
| S       | 22.089558 | 31.452360 | 29.440845 |
| S       | 24.984528 | 33.462505 | 33.210266 |
| S       | 26.616911 | 29.728275 | 30.957577 |
| S       | 25.929079 | 34.206394 | 28.847992 |
| S       | 28.249256 | 30.153860 | 26.540277 |
| S       | 31.352585 | 31.867664 | 29.672386 |
| S       | 31.452272 | 27.078714 | 28.412777 |
| S       | 32.529236 | 30.315844 | 24.969578 |
| S       | 33.034241 | 25.773556 | 23.967220 |
| S       | 36.158020 | 27.905067 | 26.989853 |

24 generated by VMD

| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 18.330635 | 32.866394 | 33.407085 |
| Ca      | 22.961514 | 33.830513 | 36.033440 |
| Ca      | 23.604166 | 30.054132 | 32.570141 |
| Ca      | 22.958973 | 34.954582 | 30.665865 |
| Ca      | 24.796194 | 30.788441 | 27.905125 |
| Ca      | 28.042561 | 32.791531 | 31.224718 |
| Ca      | 29.593800 | 28.941742 | 29.649824 |
| Ca      | 30.626026 | 32.968075 | 26.215881 |
| Ca      | 30.201000 | 27.711128 | 24.928688 |
| Ca      | 33.505634 | 29.547068 | 28.324215 |
| Ca      | 34.192978 | 25.120621 | 27.462454 |
| Ca      | 35.280521 | 28.544567 | 23.639832 |
| S       | 21.230951 | 31.174435 | 35.069016 |
| S       | 20.705288 | 35.502899 | 33.499638 |
| S       | 21.943321 | 31.362793 | 29.713806 |
| S       | 25.058735 | 33.321968 | 33.205803 |
| S       | 26.501879 | 29.410336 | 30.774349 |
| S       | 26.600179 | 34.183861 | 28.829645 |
| S       | 28.318119 | 30.121616 | 26.497580 |
| S       | 31.138798 | 31.963406 | 29.607018 |
| S       | 31.118315 | 26.770290 | 28.280277 |
| S       | 32.657955 | 30.459347 | 25.173710 |
| S       | 33.030285 | 25.761822 | 24.017525 |
| S       | 35.920586 | 28.148460 | 27.244387 |

24 generated by VMD

| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 18.452820 | 32.697380 | 33.506348 |
|  |  |  |  |
|---|---|---|---|
| Ca | 23.018747 | 34.111603 | 36.005409 |
| Ca | 23.687658 | 29.887829 | 32.741238 |
| Ca | 22.874508 | 34.664314 | 30.876682 |
| Ca | 24.886545 | 30.589285 | 27.590361 |
| Ca | 28.067656 | 32.904743 | 31.203043 |
| Ca | 29.487684 | 29.416191 | 29.473721 |
| Ca | 30.684372 | 33.158104 | 26.222660 |
| Ca | 30.347738 | 27.834078 | 24.790077 |
| Ca | 33.588699 | 29.430847 | 28.627506 |
| Ca | 33.716526 | 25.116756 | 27.508766 |
| Ca | 35.368633 | 28.312965 | 23.820555 |
| S  | 21.278547 | 30.994106 | 35.215332 |
| S  | 20.615141 | 35.462624 | 33.590637 |
| S  | 22.108011 | 31.174240 | 29.702444 |
| S  | 24.981968 | 33.353668 | 33.419773 |
| S  | 26.582895 | 29.718967 | 30.477684 |
| S  | 25.723602 | 34.148895 | 28.724777 |
| S  | 28.264309 | 30.326160 | 26.142761 |
| S  | 31.238937 | 32.095612 | 29.518499 |
| S  | 31.060095 | 27.010033 | 28.216858 |
| S  | 32.813179 | 30.495037 | 25.164097 |
| S  | 33.086250 | 25.602467 | 23.988232 |
| S  | 35.785606 | 27.794132 | 27.412537 |

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generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 18.475233 | 32.866997 | 33.528408 |
| Ca | 22.868490 | 34.201065 | 36.052490 |
| Ca | 23.552931 | 29.714197 | 32.748848 |
| Ca | 22.869270 | 34.686630 | 30.720367 |
| Ca | 24.846949 | 30.912609 | 27.742907 |
| Ca | 27.847687 | 32.662373 | 31.552212 |
| Ca | 29.509256 | 29.385090 | 29.665861 |
| Ca | 30.518984 | 33.088966 | 25.943359 |
| Ca | 30.318710 | 27.859808 | 24.670727 |
| Ca | 33.702488 | 29.539135 | 28.364614 |
| Ca | 33.835838 | 25.043247 | 27.643358 |
| Ca | 35.522461 | 28.364960 | 23.818581 |
| S  | 21.129770 | 31.092194 | 35.376545 |
| S  | 20.647457 | 35.600273 | 33.376945 |
| S  | 21.924456 | 31.411093 | 29.835049 |
| S  | 24.980001 | 33.088184 | 33.350727 |
| S  | 26.569323 | 29.480038 | 30.512432 |
| S  | 25.887915 | 34.205627 | 28.962664 |
| S  | 28.170189 | 30.286274 | 26.296329 |
| S  | 31.048466 | 32.050976 | 29.378185 |
| S  | 31.376297 | 26.926289 | 28.035570 |
S  32.728287  30.410765  24.985020
S  33.151028  25.742725  24.072943
S  36.238533  27.680553  27.305964

24

generated by VMD

Ca  18.625767  32.303482  34.000641
Ca  22.829401  34.111717  35.968163
Ca  23.581499  29.897343  32.817001
Ca  22.939671  34.887283  30.501678
Ca  24.864799  31.012699  27.591015
Ca  27.798622  32.915298  31.281925
Ca  29.460749  29.520903  29.634249
Ca  30.736145  33.093388  26.033949
Ca  30.433733  27.880497  24.969135
Ca  33.529881  29.408054  28.480062
Ca  33.641506  24.853912  27.442223
Ca  35.387184  28.503754  23.853756
S  21.586412  30.907696  35.455681
S  20.477253  35.158928  33.185257
S  22.216286  31.311180  29.788029
S  24.920853  33.542648  33.307510
S  26.348530  29.599180  30.513426
S  25.770515  34.337986  28.672834
S  28.454161  30.365147  26.309893
S  31.240391  32.128532  29.474937
S  30.922287  26.845177  27.913845
S  32.977425  30.588211  25.120649
S  33.094639  25.656582  24.034079
S  35.882088  27.470440  27.590080

24

generated by VMD

Ca  18.631813  31.906593  34.112179
Ca  22.959347  34.186546  36.015816
Ca  23.898176  30.209990  32.658649
Ca  22.857718  34.868404  30.734896
Ca  24.778755  31.024317  27.313549
Ca  28.084782  32.982407  31.084471
Ca  29.252245  29.190205  29.176243
Ca  30.984222  33.062229  25.867836
Ca  30.359612  28.016327  24.983971
Ca  33.529350  29.318363  28.951662
Ca  35.588802  25.082256  27.503189
Ca  35.493717  28.221760  23.964546
S  21.723547  30.908226  35.540718
S  20.487278  34.807243  33.446754
S  21.944504  31.378632  29.842756
S  25.061695  33.771263  33.069603
S  26.378281  29.596169  28.563381
S  25.710350  34.279320  28.563381
S  28.285725  30.601139  25.990871
S  31.220093  32.241554  29.438753
S  30.736462  26.882458  23.979830
S  35.782875  27.739201  27.749336

24

generated by VMD
Ca  18.601509  32.111145  33.881866
Ca  22.750910  33.973858  35.926609
Ca  23.852131  30.157417  32.760372
Ca  22.580841  34.917633  30.552624
Ca  24.840452  30.929352  27.653786
Ca  27.959093  33.125435  31.260609
Ca  29.520462  29.104588  29.609488
Ca  30.993801  33.074673  26.085644
Ca  30.261787  27.801785  24.602737
Ca  33.740242  29.253170  28.674480
Ca  33.599995  24.970524  27.456577
Ca  35.433437  28.212086  23.872070
Ca  21.536922  30.860559  35.324436
S  20.273739  35.252087  33.515938
S  22.114258  31.465799  29.783455
S  24.851322  33.655357  33.152042
S  26.606678  29.687857  30.490271
S  25.871178  34.347137  28.748510
S  28.347935  30.287277  26.382797
S  31.176994  32.431084  29.627117
S  30.942696  27.017948  28.145864
S  32.897675  30.318686  25.231453
S  32.950993  25.786324  23.732176
S  36.014999  27.558304  27.469189

24

generated by VMD
Ca  18.650196  32.233315  34.068260
Ca  23.024422  34.274059  35.596695
Ca  23.921806  30.221375  32.837170
Ca  22.733137  34.821827  30.536942
Ca  24.835533  31.048906  27.449741
Ca  27.785986  32.755466  31.456059
Ca  29.407251  28.996704  29.308172
Ca  30.688143  32.948830  26.158558
Ca  30.369101  27.958950  24.718298
|   | Ca   | S     | Ca   |
|---|------|-------|------|
|   | 33.530891 | 29.277576 | 28.693932 |
|   | 33.625957 | 24.977886 | 27.380009 |
| S | 35.484734 | 31.106140 | 35.439110 |
|   | 20.315807 | 35.195663 | 33.313068 |
| S | 22.106886 | 31.212738 | 30.022942 |
|   | 25.016125 | 33.867653 | 33.184967 |
| S | 26.417809 | 29.551868 | 30.498642 |
|   | 25.873486 | 34.262356 | 28.631556 |
| S | 28.316290 | 30.399021 | 26.144642 |
|   | 30.923225 | 31.710159 | 29.534895 |
| S | 30.904371 | 26.655159 | 27.980892 |
|   | 32.823500 | 30.273785 | 25.251301 |
| S | 33.151237 | 25.912542 | 23.892538 |
|   | 36.008759 | 27.878193 | 27.639751 |

24

generated by VMD

|   | Ca   | S     | Ca   |
|---|------|-------|------|
|   | 18.398088 | 32.451469 | 34.341393 |
|   | 23.003849 | 34.621429 | 35.473125 |
| Ca | 23.648260 | 29.990414 | 32.869274 |
|   | 22.776180 | 34.591652 | 30.673149 |
| Ca | 24.891113 | 30.798874 | 27.498663 |
|   | 27.790352 | 32.802433 | 31.234735 |
| Ca | 29.442139 | 29.107475 | 29.651325 |
|   | 30.778263 | 33.114414 | 26.370186 |
| Ca | 30.346716 | 28.086494 | 24.587854 |
|   | 33.548786 | 29.417721 | 28.645739 |
| Ca | 33.587227 | 24.970379 | 27.382103 |
|   | 35.696274 | 28.711788 | 23.857071 |
| S | 21.662807 | 31.350651 | 35.653797 |
|   | 20.385370 | 35.435097 | 33.216202 |
| S | 22.013157 | 31.131386 | 29.721655 |
|   | 24.953926 | 33.310688 | 33.288940 |
| S | 26.238344 | 29.489414 | 30.346710 |
|   | 25.906845 | 34.106773 | 28.729303 |
| S | 28.433954 | 30.383644 | 26.404734 |
|   | 30.988588 | 31.696287 | 29.709898 |
| S | 30.891872 | 26.758865 | 27.868376 |
|   | 33.002907 | 30.445808 | 25.151505 |
| S | 33.346458 | 25.847076 | 23.831381 |
|   | 35.988541 | 27.679808 | 27.432964 |

24

generated by VMD

|   | Ca   | S     | Ca   |
|---|------|-------|------|
|   | 18.884190 | 32.732594 | 34.163635 |
|   | 22.799644 | 34.477047 | 35.749660 |
| Ca | 23.486717 | 30.178341 | 32.791512 |
| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 22.804731| 34.690361| 30.524006|
| Ca      | 25.098181| 30.785271| 27.809202|
| Ca      | 27.651968| 32.685696| 31.299786|
| Ca      | 29.638029| 29.007473| 29.462269|
| Ca      | 30.606354| 33.055939| 26.323738|
| Ca      | 30.387600| 28.001268| 24.566170|
| Ca      | 33.734829| 29.372581| 28.813322|
| Ca      | 33.756916| 24.969509| 27.215796|
| Ca      | 35.280346| 28.707314| 23.823202|
| S       | 21.498724| 31.210255| 35.673794|
| S       | 20.557629| 35.259392| 33.055851|
| S       | 22.062094| 30.961864| 29.712643|
| S       | 24.865503| 33.452698| 33.206173|
| S       | 26.209843| 29.543495| 30.507994|
| S       | 26.006691| 34.184620| 28.595102|
| S       | 28.260208| 30.400063| 26.288033|
| S       | 30.934174| 31.732693| 29.654633|
| S       | 31.099766| 26.723019| 27.961506|
| S       | 32.990108| 30.573133| 25.518999|
| S       | 32.962978| 25.753998| 23.763786|
| S       | 36.142845| 27.841433| 27.458435|

24 generated by VMD

| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 18.877825| 32.860668| 34.208149|
| Ca      | 22.854321| 34.397694| 35.668167|
| Ca      | 23.740259| 30.242893| 32.638405|
| Ca      | 22.802292| 34.787125| 30.260372|
| Ca      | 24.953300| 30.724163| 27.674316|
| Ca      | 27.648439| 32.538155| 31.507248|
| Ca      | 29.367172| 28.636356| 29.440575|
| Ca      | 30.473133| 32.943787| 26.628769|
| Ca      | 30.249542| 27.850885| 24.662304|
| Ca      | 33.430435| 29.298370| 28.758137|
| Ca      | 33.980701| 25.161709| 26.904127|
| Ca      | 35.597267| 29.044167| 23.861492|
| S       | 21.889072| 31.385630| 35.694134|
| S       | 20.488255| 35.484428| 32.964165|
| S       | 21.916796| 31.285408| 29.693319|
| S       | 24.985619| 33.804001| 32.945137|
| S       | 26.280680| 29.369459| 30.858860|
| S       | 25.824074| 33.871357| 28.654884|
| S       | 28.403404| 29.990543| 26.318344|
| S       | 30.891695| 31.330334| 30.144360|
| S       | 31.006792| 26.645653| 27.970192|
| S       | 32.698040| 30.523745| 25.436968|
| S       | 33.342735| 25.998791| 23.697903|
|  |   |   |   |
|---|---|---|---|
| S | 36.018204 | 28.124718 | 27.349705 |
| 24 | generated by VMD |
| Ca | 18.727835 | 32.944992 | 34.101143 |
| Ca | 22.924854 | 34.342278 | 35.836197 |
| Ca | 23.635464 | 29.962318 | 32.696198 |
| Ca | 22.766378 | 34.603657 | 30.732836 |
| Ca | 24.948225 | 30.684687 | 27.560753 |
| Ca | 27.812114 | 32.543918 | 31.435629 |
| Ca | 29.369003 | 28.975540 | 29.338085 |
| Ca | 30.582863 | 32.912033 | 26.246069 |
| Ca | 30.539320 | 27.827026 | 24.550365 |
| Ca | 33.530655 | 29.484856 | 28.814077 |
| Ca | 33.893093 | 25.073338 | 27.425936 |
| Ca | 35.427059 | 28.939251 | 23.882866 |
| S  | 21.444281 | 31.406366 | 35.648544 |
| S  | 20.571161 | 35.705673 | 33.295311 |
| S  | 21.944141 | 31.142403 | 29.678808 |
| S  | 24.908413 | 33.427979 | 33.249992 |
| S  | 26.238350 | 29.446304 | 30.686527 |
| S  | 25.771982 | 34.039177 | 28.624802 |
| S  | 28.424791 | 30.287727 | 26.058050 |
| S  | 30.815847 | 31.647026 | 29.677521 |
| S  | 31.077705 | 26.729897 | 27.997587 |
| S  | 32.897503 | 30.540112 | 25.244516 |
| S  | 33.421242 | 25.807701 | 23.945896 |
| S  | 36.047691 | 27.825676 | 27.212337 |
| 24 | generated by VMD |
| Ca | 18.809040 | 32.754421 | 34.076080 |
| Ca | 22.859383 | 34.588840 | 35.537155 |
| Ca | 23.843882 | 29.987904 | 32.743385 |
| Ca | 22.883980 | 34.570339 | 30.424080 |
| Ca | 24.950689 | 30.697166 | 27.654299 |
| Ca | 27.734573 | 32.645031 | 31.420979 |
| Ca | 29.411404 | 28.798065 | 29.604254 |
| Ca | 30.602264 | 32.965286 | 26.609869 |
| Ca | 30.316849 | 27.969784 | 24.585861 |
| Ca | 33.440777 | 29.281086 | 28.897589 |
| Ca | 33.862785 | 25.243698 | 27.196026 |
| Ca | 35.501652 | 28.885624 | 23.666241 |
| S  | 21.772974 | 31.396992 | 35.639210 |
| S  | 20.389919 | 35.615467 | 33.070763 |
| S  | 21.973623 | 31.125156 | 29.885956 |
| S  | 24.917830 | 33.500526 | 33.047222 |
| S  | 26.419857 | 29.324871 | 30.520836 |
| S   | 25.885096 | 34.100822 | 28.596767 |
|-----|-----------|-----------|-----------|
| S   | 28.304224 | 30.262880 | 26.346558 |
| S   | 30.958521 | 31.523874 | 29.935154 |
| S   | 30.757019 | 26.571968 | 27.955399 |
| S   | 32.797443 | 30.457123 | 25.614304 |
| S   | 33.272953 | 25.968739 | 23.688389 |
| S   | 36.053268 | 28.064339 | 27.223644 |

24 generated by VMD

| Ca  | 18.612511 | 32.236374 | 33.982567 |
|-----|-----------|-----------|-----------|
| Ca  | 23.195446 | 34.436081 | 35.657375 |
| Ca  | 23.864326 | 30.143890 | 32.603611 |
| Ca  | 22.834616 | 34.955441 | 30.483194 |
| Ca  | 24.738022 | 30.742601 | 27.479940 |
| Ca  | 27.772133 | 32.589584 | 31.313715 |
| Ca  | 29.582090 | 28.875023 | 29.465097 |
| Ca  | 30.587576 | 33.000271 | 26.502558 |
| Ca  | 30.420782 | 27.969530 | 24.635929 |
| Ca  | 33.495750 | 29.440037 | 28.783232 |
| Ca  | 33.626743 | 25.047947 | 27.625221 |
| Ca  | 35.292915 | 28.855228 | 23.746014 |
| S   | 21.687572 | 31.239365 | 35.538158 |
| S   | 20.528843 | 35.389343 | 33.300381 |
| S   | 21.974308 | 31.283827 | 29.729441 |
| S   | 25.161652 | 33.489595 | 33.084675 |
| S   | 26.370119 | 29.394876 | 30.411558 |
| S   | 25.829912 | 34.036411 | 28.643250 |
| S   | 28.369732 | 30.408245 | 26.258497 |
| S   | 31.136765 | 31.777737 | 29.747635 |
| S   | 30.867172 | 26.727028 | 28.086994 |
| S   | 32.842705 | 30.555532 | 25.563820 |
| S   | 33.109894 | 25.762993 | 23.925713 |
| S   | 35.818451 | 27.947716 | 27.371483 |

24 generated by VMD

| Ca  | 18.779442 | 32.339493 | 34.203987 |
|-----|-----------|-----------|-----------|
| Ca  | 23.175287 | 34.663010 | 35.629578 |
| Ca  | 23.656532 | 30.020792 | 32.714722 |
| Ca  | 22.669518 | 34.789124 | 30.503754 |
| Ca  | 25.007298 | 30.957561 | 27.632431 |
| Ca  | 27.730156 | 32.510586 | 31.450960 |
| Ca  | 29.346788 | 29.032642 | 29.532684 |
| Ca  | 30.398914 | 33.039677 | 26.370911 |
| Ca  | 30.405180 | 27.989555 | 24.314781 |
| Ca  | 33.554585 | 29.315557 | 28.648491 |
| Ca  | 33.820042 | 24.911854 | 27.269392 |
|   |     Ca      |     S        |     S      |
|---|------------|-------------|-----------|
| 1| 35.423340  | 28.796055   | 24.149183 |
| 2| 21.790897  | 31.256901   | 24.188816 |
| 3| 20.458145  | 31.348957   | 29.751682 |
| 4| 25.000504  | 33.425529   | 33.035950 |
| 5| 26.393097  | 29.550646   | 30.701502 |
| 6| 25.642296  | 34.016235   | 28.729794 |
| 7| 28.314854  | 30.265339   | 26.108509 |
| 8| 31.012577  | 31.664108   | 29.674507 |
| 9| 30.94218   | 26.826565   | 27.758892 |
|10| 33.016090  | 30.530397   | 25.468303 |
|11| 33.406021  | 25.825657   | 23.885071 |
|12| 35.958279  | 27.772091   | 27.632721 |

24

generated by VMD

|   |     Ca      |     S        |     S      |
|---|------------|-------------|-----------|
| 1| 18.449722  | 32.142670   | 34.053448 |
| 2| 23.00456   | 34.455894   | 35.758698 |
| 3| 23.723270  | 30.116806   | 32.875954 |
| 4| 23.103294  | 33.908350   | 30.924347 |
| 5| 24.72646   | 30.733631   | 27.613457 |
| 6| 27.751110  | 32.915115   | 30.922302 |
| 7| 29.526943  | 28.926495   | 29.477085 |
| 8| 30.722401  | 32.988419   | 26.109573 |
| 9| 30.314421  | 28.065271   | 24.451490 |
|10| 33.506191  | 29.292990   | 28.667288 |
|11| 33.823856  | 24.964912   | 27.387627 |
|12| 35.70077   | 28.605656   | 24.105904 |

24

generated by VMD

|   |     Ca      |     S        |     S      |
|---|------------|-------------|-----------|
| 1| 18.429512  | 32.248383   | 34.194443 |
| 2| 23.160336  | 34.370888   | 35.720215 |
| 3| 23.762270  | 30.222256   | 32.781342 |
| 4| 22.814370  | 34.745934   | 30.794804 |
| 5| 24.729191  | 30.791420   | 27.511002 |
| Ca     | 27.989819 | 32.795937 | 31.201752 |
|--------|-----------|-----------|-----------|
| Ca     | 29.351379 | 29.149151 | 29.573868 |
| Ca     | 30.787884 | 33.125145 | 26.089466 |
| Ca     | 30.258980 | 28.034241 | 24.573204 |
| Ca     | 33.609802 | 29.471127 | 28.731453 |
| Ca     | 33.571278 | 24.984949 | 27.486923 |
| Ca     | 35.471302 | 28.491913 | 24.070019 |
| S      | 21.478462 | 31.205145 | 35.584644 |
| S      | 20.319633 | 35.159176 | 33.233547 |
| S      | 21.910305 | 31.385748 | 29.670803 |
| S      | 25.075912 | 33.399578 | 33.203175 |
| S      | 26.542034 | 29.447365 | 30.380850 |
| S      | 25.799908 | 34.144650 | 28.692871 |
| S      | 28.301514 | 30.430098 | 26.166824 |
| S      | 31.178764 | 31.837826 | 29.463398 |
| S      | 30.885479 | 26.718048 | 28.035173 |
| S      | 33.122932 | 30.667530 | 25.262020 |
| S      | 33.122055 | 25.820591 | 23.986948 |
| S      | 36.019470 | 27.652966 | 27.531273 |

Generated by VMD

| Ca     | 18.615562 | 32.633312 | 34.037033 |
|--------|-----------|-----------|-----------|
| Ca     | 23.150940 | 34.187973 | 35.597534 |
| Ca     | 23.703751 | 29.923038 | 32.807228 |
| Ca     | 23.146751 | 34.734787 | 30.576139 |
| Ca     | 24.792116 | 30.697174 | 27.472696 |
| Ca     | 27.870811 | 32.831940 | 31.003490 |
| Ca     | 29.339993 | 29.211639 | 29.667591 |
| Ca     | 30.517883 | 33.208633 | 26.110065 |
| Ca     | 30.087267 | 27.899324 | 24.550997 |
| Ca     | 33.585194 | 29.304268 | 28.722191 |
| Ca     | 33.542847 | 25.220331 | 27.447208 |
| Ca     | 35.603668 | 28.731228 | 24.099981 |
| S      | 21.549414 | 31.121937 | 35.528763 |
| S      | 20.649143 | 35.269115 | 33.086227 |
| S      | 22.031273 | 31.295506 | 30.064716 |
| S      | 25.198366 | 33.290943 | 33.351227 |
| S      | 26.329149 | 29.380451 | 30.532299 |
| S      | 25.828352 | 34.037735 | 28.536549 |
| S      | 28.324295 | 30.341751 | 26.240318 |
| S      | 30.993443 | 31.905193 | 29.494780 |
| S      | 30.856220 | 26.752647 | 28.066273 |
| S      | 32.841599 | 30.500889 | 25.306728 |
| S      | 33.177788 | 26.089870 | 23.900883 |
| S      | 35.984299 | 27.730370 | 27.739117 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.695700    | 32.182304    | 34.445389    |
| Ca      | 22.726871    | 34.443974    | 35.623108    |
| Ca      | 23.836216    | 30.169106    | 32.714058    |
| Ca      | 22.792715    | 34.622147    | 30.631264    |
| Ca      | 24.976189    | 30.956638    | 27.430595    |
| Ca      | 27.788540    | 32.913330    | 31.416800    |
| Ca      | 29.579288    | 29.239128    | 29.513626    |
| Ca      | 30.676138    | 33.197060    | 26.124363    |
| Ca      | 30.359623    | 28.045889    | 24.775791    |
| Ca      | 33.600121    | 29.166489    | 28.534309    |
| Ca      | 33.498165    | 24.683851    | 27.316200    |
| Ca      | 35.646500    | 28.628075    | 24.040016    |
| S       | 21.894588    | 31.153061    | 35.637482    |
| S       | 20.092148    | 34.898209    | 33.041855    |
| S       | 21.932079    | 31.206373    | 29.705582    |
| S       | 24.958241    | 33.661633    | 33.265728    |
| S       | 26.469906    | 29.777840    | 30.310898    |
| S       | 25.962643    | 34.335209    | 28.683369    |
| S       | 28.319933    | 30.458366    | 26.233778    |
| S       | 31.263042    | 31.911476    | 29.563929    |
| S       | 30.828758    | 26.803051    | 28.087282    |
| S       | 32.948387    | 30.572229    | 25.391994    |
| S       | 33.174797    | 25.878666    | 23.899147    |
| S       | 35.699478    | 27.395927    | 27.553478    |
|   |   |   |   |
|---|---|---|---|
| S | 30.983772 | 31.820335 | 29.569139 |
| S | 30.702057 | 26.885620 | 28.035192 |
| S | 32.900951 | 30.323975 | 25.239666 |
| S | 33.272675 | 26.018589 | 24.082500 |
| S | 35.869278 | 27.706818 | 27.72885  |

24 generated by VMD

| Ca | 18.612625 | 32.244926 | 34.210670 |
|----|-----------|-----------|-----------|
| Ca | 23.077829 | 34.467072 | 35.682178 |
| Ca | 23.661140 | 30.172302 | 32.915554 |
| Ca | 22.981144 | 34.930927 | 30.649637 |
| Ca | 24.775337 | 30.813650 | 27.368748 |
| Ca | 27.663990 | 32.673187 | 31.302679 |
| Ca | 29.144915 | 29.106159 | 29.518951 |
| Ca | 30.613113 | 32.741081 | 26.262415 |
| Ca | 30.258699 | 28.056160 | 24.397043 |
| Ca | 33.562805 | 29.422859 | 28.750387 |
| Ca | 33.523827 | 25.233400 | 27.357906 |
| Ca | 35.893295 | 28.518118 | 24.225758 |
| S  | 21.631451 | 31.288063 | 35.797020 |
| S  | 20.446367 | 35.204735 | 33.141731 |
| S  | 22.115931 | 31.389435 | 29.877544 |
| S  | 25.004341 | 33.657440 | 33.255726 |
| S  | 26.189495 | 29.436201 | 30.435457 |
| S  | 25.928230 | 33.893883 | 26.816631 |
| S  | 28.143351 | 30.120449 | 26.074120 |
| S  | 30.988411 | 31.726959 | 29.736980 |
| S  | 31.125687 | 26.982641 | 27.704838 |
| S  | 33.082886 | 30.363523 | 25.248327 |
| S  | 33.135197 | 26.039379 | 23.882767 |
| S  | 36.160007 | 27.817474 | 27.526997 |

24 generated by VMD

| Ca | 18.722851 | 32.046963 | 34.363155 |
|----|-----------|-----------|-----------|
| Ca | 23.373287 | 34.671501 | 35.618179 |
| Ca | 23.747704 | 30.294476 | 32.666153 |
| Ca | 22.844431 | 35.139259 | 30.761753 |
| Ca | 24.542904 | 30.766769 | 27.372505 |
| Ca | 27.568876 | 32.467842 | 31.074005 |
| Ca | 29.222551 | 28.863308 | 29.346788 |
| Ca | 30.537966 | 32.768185 | 26.388916 |
| Ca | 30.465866 | 27.928217 | 24.783327 |
| Ca | 33.546104 | 29.441441 | 28.967186 |
| Ca | 33.952702 | 24.791512 | 27.145420 |
| Ca | 35.837265 | 28.722475 | 24.103409 |
| S  | 21.954002 | 31.392212 | 35.728279 |
S  20.495354  35.243382  33.250828
S  21.795977  31.583389  29.712345
S  25.148308  33.745331  33.198410
S  25.966911  29.327026  30.177849
S  25.566202  34.156208  28.526991
S  28.001707  30.241550  26.147182
S  30.694581  31.461344  29.768597
S  31.319996  26.756947  26.067057
S  32.838348  30.588541  25.610723
S  33.331200  25.927620  23.676081
S  36.244915  27.974640  27.484924

24 generated by VMD
Ca  18.872404  31.852070  34.414181
Ca  22.836343  34.679958  35.627647
Ca  23.654299  30.342167  32.597206
Ca  22.862684  35.109646  30.814507
Ca  24.782055  30.873455  27.171640
Ca  27.656708  32.502243  31.013028
Ca  28.834833  29.009308  29.526781
Ca  30.599464  32.888523  26.468081
Ca  30.428034  27.756470  24.551964
Ca  33.472477  29.366507  28.752476
Ca  33.611851  25.036242  27.384022
Ca  35.716721  28.905273  24.211926
S  22.118946  31.310272  35.748535
S  20.377190  35.156956  33.378483
S  21.866268  31.740250  29.843969
S  25.170940  33.589512  32.930145
S  25.974495  29.270451  30.043953
S  25.694839  34.163231  28.545471
S  28.246260  30.216862  26.170609
S  30.780807  31.487026  29.767809
S  31.111624  26.804283  28.161633
S  32.862022  30.513231  25.415941
S  33.462517  25.836823  23.893040
S  36.206295  27.889256  27.509697

24 generated by VMD
Ca  18.796606  32.139725  33.806458
Ca  23.314770  34.596958  35.493595
Ca  23.808596  30.156332  32.597061
Ca  22.883663  34.978355  30.553463
Ca  24.934486  30.595814  27.432243
Ca  27.776190  32.573727  31.267811
Ca  29.179064  29.023544  29.866690
| Element | X1      | Y1      | Z1      |
|---------|---------|---------|---------|
| Ca      | 30.420612 | 33.137810 | 26.393570 |
| Ca      | 30.371704 | 28.174099 | 24.898895 |
| Ca      | 33.576870 | 29.404911 | 28.909489 |
| Ca      | 33.633591 | 24.844702 | 27.199814 |
| Ca      | 35.222237 | 28.946554 | 24.084141 |
| S       | 21.918022 | 31.312490 | 35.591576 |
| S       | 20.498627 | 35.307842 | 33.187538 |
| S       | 22.068443 | 31.433598 | 29.756536 |
| S       | 25.139778 | 33.447464 | 32.988220 |
| S       | 26.192251 | 29.050606 | 30.544998 |
| S       | 25.907726 | 33.962524 | 28.534508 |
| S       | 28.195103 | 30.185955 | 26.405369 |
| S       | 30.940449 | 31.674465 | 29.724407 |
| S       | 31.012999 | 26.876392 | 28.133766 |
| S       | 32.913673 | 30.685829 | 25.479330 |
| S       | 33.005936 | 25.955956 | 23.811487 |
| S       | 36.008659 | 27.834448 | 27.279102 |

24 generated by VMD

| Element | X1      | Y1      | Z1      |
|---------|---------|---------|---------|
| Ca      | 19.001904 | 32.037704 | 34.014488 |
| Ca      | 22.974230 | 35.079979 | 35.042408 |
| Ca      | 23.912003 | 30.270390 | 33.012619 |
| Ca      | 22.855221 | 34.501293 | 30.208328 |
| Ca      | 24.818417 | 30.504959 | 27.667339 |
| Ca      | 27.686211 | 32.613487 | 31.437286 |
| Ca      | 29.291773 | 29.016113 | 29.747320 |
| Ca      | 30.519211 | 33.119488 | 26.788841 |
| Ca      | 30.366879 | 28.360764 | 24.710232 |
| Ca      | 33.631264 | 29.189386 | 28.868849 |
| Ca      | 33.426704 | 24.863708 | 26.756464 |
| Ca      | 35.358624 | 29.055851 | 24.104473 |
| S       | 21.873425 | 31.766382 | 35.821964 |
| S       | 20.468287 | 35.025864 | 32.686623 |
| S       | 21.981245 | 31.104744 | 29.896381 |
| S       | 25.010019 | 33.539139 | 33.006485 |
| S       | 26.321407 | 29.298758 | 30.656519 |
| S       | 25.941032 | 33.877689 | 28.686821 |
| S       | 28.204220 | 30.413631 | 26.419312 |
| S       | 31.067871 | 31.502741 | 30.063667 |
| S       | 30.933083 | 26.822992 | 27.925446 |
| S       | 32.914627 | 30.690773 | 25.769161 |
| S       | 33.083172 | 26.258179 | 23.458883 |
| S       | 36.079308 | 27.385973 | 27.190136 |

24 generated by VMD

| Element | X1      | Y1      | Z1      |
|---------|---------|---------|---------|
| Ca      | 18.898592 | 31.938715 | 34.132267 |
Ca  23.031620  34.802330  35.508598
Ca  23.648516  30.213055  32.875710
Ca  22.906933  34.710171  30.285032
Ca  24.775623  30.843182  27.518698
Ca  27.718407  32.556084  31.414505
Ca  29.099422  29.022388  29.644560
Ca  30.849989  33.003250  26.443005
Ca  30.363081  28.024673  24.509792
Ca  33.469227  29.469452  28.680229
Ca  33.505367  24.970627  27.217396
Ca  35.705048  28.813053  23.975460
S   21.935028  31.559540  35.915291
S   20.495899  34.962212  33.025723
S   22.018679  31.344173  29.751286
S   24.933800  33.638557  33.064594
S   26.150362  29.259144  30.589375
S   25.998686  34.115822  28.582150
S   28.201445  30.485680  26.336979
S   30.879013  31.547216  30.001505
S   30.954687  26.747307  27.913149
S   32.843216  30.572067  25.268007
S   33.261154  26.128174  23.846518
S   36.076138  27.573116  27.440220

24

Ca  18.529253  32.214054  34.121975
Ca  23.081369  34.847538  35.590992
Ca  23.620571  30.276377  32.869419
Ca  22.703339  34.872536  30.488548
Ca  24.917315  30.803785  27.536091
Ca  27.868753  32.563103  31.239714
Ca  29.171347  28.988941  29.632200
Ca  30.683041  32.894966  26.738817
Ca  30.558287  27.836082  24.687685
Ca  33.474068  29.202778  28.420897
Ca  33.883598  24.876656  27.375252
Ca  35.444595  29.050888  23.889048
S   21.702393  31.492157  35.784786
S   20.349728  35.055294  33.068859
S   22.108185  31.504835  29.655128
S   25.154011  33.594315  33.169327
S   26.229927  29.298954  30.674850
S   25.725004  34.054592  28.619047
S   28.294708  30.340906  26.328625
S   30.962038  31.398823  29.839060
S   30.913668  26.643112  27.668121

generated by VMD
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| S       | 32.820419    | 30.616661    | 25.362764    |
| S       | 33.340111    | 26.027903    | 23.876521    |
| S       | 36.184311    | 27.844822    | 27.304256    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.591492    | 32.302086    | 33.998417    |
| Ca      | 23.028887    | 35.032745    | 35.776202    |
| Ca      | 23.624893    | 30.326606    | 32.865215    |
| Ca      | 22.705935    | 34.727737    | 30.734808    |
| Ca      | 24.781418    | 30.664236    | 27.608826    |
| Ca      | 27.790438    | 32.538712    | 31.270990    |
| Ca      | 29.298344    | 28.918381    | 29.736347    |
| Ca      | 30.550545    | 32.909138    | 26.588083    |
| Ca      | 30.330612    | 28.082035    | 24.604465    |
| Ca      | 33.786919    | 28.980198    | 28.665184    |
| Ca      | 33.881413    | 24.927788    | 27.110855    |
| Ca      | 35.681137    | 29.024534    | 23.837341    |
| S       | 21.560259    | 31.677193    | 35.599487    |
| S       | 20.376175    | 35.197514    | 33.006287    |
| S       | 21.936691    | 31.342691    | 29.590195    |
| S       | 25.078602    | 33.574158    | 33.309803    |
| S       | 26.281738    | 29.333130    | 30.634617    |
| S       | 25.622211    | 34.018417    | 28.703157    |
| S       | 28.062878    | 30.227648    | 26.623535    |
| S       | 31.123707    | 31.309795    | 29.672398    |
| S       | 31.226280    | 26.555092    | 27.906376    |
| S       | 32.743073    | 30.583092    | 25.282803    |
| S       | 33.200096    | 26.338888    | 23.803226    |
| S       | 36.456245    | 27.708670    | 27.210026    |

24 generated by VMD
|   |        |        |        |
|---|--------|--------|--------|
| S | 25.165344 | 33.499725 | 32.981762 |
| S | 26.241932 | 29.255177 | 30.609692 |
| S | 25.776623 | 33.772484 | 28.541565 |
| S | 28.416620 | 30.397572 | 26.448757 |
| S | 30.841705 | 31.487740 | 29.852905 |
| S | 31.317379 | 26.849138 | 28.240191 |
| S | 32.897026 | 30.663700 | 25.474268 |
| S | 33.046429 | 26.123238 | 23.741077 |
| S | 35.958790 | 27.590773 | 27.090849 |

24

generated by VMD

| Ca |        |        |        |
|----|--------|--------|--------|
| Ca | 18.712753 | 32.235752 | 33.896873 |
| Ca | 23.390121 | 34.728615 | 35.502316 |
| Ca | 23.415335 | 30.114202 | 32.805370 |
| Ca | 22.882469 | 34.909695 | 30.739693 |
| Ca | 24.918030 | 30.789562 | 27.583614 |
| Ca | 27.877840 | 32.595089 | 31.185200 |
| Ca | 29.019608 | 28.888552 | 29.479042 |
| Ca | 30.542114 | 33.005013 | 26.540573 |
| Ca | 30.325134 | 27.996674 | 24.622259 |
| Ca | 33.607132 | 29.436531 | 28.688360 |
| Ca | 33.896343 | 24.901402 | 27.257317 |
| Ca | 35.699383 | 28.876165 | 23.925755 |
| S  | 21.634220 | 31.508982 | 35.760895 |
| S  | 20.317009 | 35.269150 | 33.226818 |
| S  | 22.029287 | 31.291040 | 29.716593 |
| S  | 25.069786 | 33.487656 | 33.057724 |
| S  | 26.222338 | 29.382202 | 30.655689 |
| S  | 25.663124 | 34.101223 | 28.774559 |
| S  | 28.211407 | 30.260075 | 26.335615 |
| S  | 30.897160 | 31.538059 | 29.716311 |
| S  | 31.095469 | 26.762127 | 27.970390 |
| S  | 32.759048 | 30.498516 | 25.312351 |
| S  | 33.377453 | 25.976690 | 23.888844 |
| S  | 36.157482 | 27.747120 | 27.297953 |

24

generated by VMD

| Ca |        |        |        |
|----|--------|--------|--------|
| Ca | 18.725601 | 31.931263 | 33.801094 |
| Ca | 23.155153 | 34.828239 | 35.630264 |
| Ca | 23.630035 | 30.141598 | 32.771809 |
| Ca | 22.985664 | 34.832474 | 30.519306 |
| Ca | 24.650532 | 30.791153 | 27.573713 |
| Ca | 27.829769 | 32.783401 | 31.469734 |
| Ca | 29.232822 | 29.133362 | 29.529949 |
| Ca | 30.486519 | 32.983704 | 26.400278 |
| Ca | 30.250893 | 27.988468 | 24.606363 |
Ca  33.567299  29.396000  28.684834
Ca  33.636276  25.011503  27.224861
Ca  35.616493  35.011490  33.138016
S   21.613125  31.537165  35.818588
S   20.649139  31.452209  29.755623
S   25.077493  33.171700  33.179676
S   26.276691  34.792227  30.687134
S   25.950430  34.171021  28.510818
S   28.067795  32.79736  26.211235
S   30.996880  31.573151  29.789846
S   31.190996  26.954468  28.000483
S   32.807659  30.472595  25.225773
S   33.234238  26.109781  23.931484
S   36.228371  30.279736  26.211235

generated by VMD
Ca  18.567608  32.229691  33.859112
Ca  22.673151  34.579952  35.458740
Ca  23.692177  30.256680  32.922634
Ca  22.829479  34.695343  30.481831
Ca  24.971470  30.683720  27.758039
Ca  28.018429  32.844330  31.621807
Ca  29.554512  29.117626  29.753059
Ca  28.07659  30.472595  25.225773
Ca  33.576435  29.294188  28.568691
Ca  33.724854  24.716370  27.005539
Ca  35.353127  28.824396  23.890396
S   21.452057  31.413712  35.634117
S   20.402279  35.181438  32.811943
S   22.160442  31.357780  29.819363
S   25.034630  33.513119  33.211834
S   26.441818  29.461697  30.903835
S   25.927519  34.04872  28.680826
S   28.241825  30.252365  26.485519
S   31.061226  31.710850  29.675014
S   31.204674  26.773666  27.894068
S   32.745956  30.602074  25.318502
S   33.176666  26.287455  23.761377
S   36.043747  27.408371  27.230833

generated by VMD
Ca  18.896147  31.923147  33.922009
Ca  23.090042  34.657234  35.487049
Ca  23.621822  30.374615  32.609741
| Element | X1    | Y1    | Z1    | X2    | Y2    | Z2    |
|---------|-------|-------|-------|-------|-------|-------|
| Ca      | 22.737274 | 34.766582 | 30.613045 |
| Ca      | 24.832150  | 30.789410  | 27.696651 |
| Ca      | 27.911198  | 32.830746  | 31.065079 |
| Ca      | 29.296207  | 28.990170  | 29.932507 |
| Ca      | 30.766476  | 32.887440  | 26.554506 |
| Ca      | 30.317680  | 28.224205  | 24.567816 |
| Ca      | 33.442444  | 29.422363  | 28.765438 |
| Ca      | 33.677834  | 24.775089  | 27.152832 |
| Ca      | 35.402740  | 28.817268  | 23.994738 |
| S       | 21.860870  | 31.434948  | 35.606346 |
| S       | 20.460415  | 35.148346  | 33.139465 |
| S       | 21.995298  | 31.458118  | 29.553314 |
| S       | 25.053343  | 33.327568  | 33.117992 |
| S       | 26.256426  | 29.451611  | 30.706921 |
| S       | 25.732292  | 34.062412  | 28.533842 |
| S       | 28.339184  | 30.162804  | 26.623241 |
| S       | 31.019201  | 31.651672  | 29.844187 |
| S       | 31.095528  | 26.743389  | 27.992060 |
| S       | 32.987503  | 26.069033  | 23.757210 |
| S       | 35.948166  | 27.681808  | 27.362322 |

24 generated by VMD

| Element | X1    | Y1    | Z1    | X2    | Y2    | Z2    |
|---------|-------|-------|-------|-------|-------|-------|
| Ca      | 18.864140  | 31.930950  | 33.945992 |
| Ca      | 22.916840  | 34.784924  | 35.584042 |
| Ca      | 23.679092  | 30.198977  | 32.851646 |
| Ca      | 22.891659  | 34.801506  | 30.452297 |
| Ca      | 24.833466  | 30.699184  | 27.790329 |
| Ca      | 27.915562  | 32.807865  | 31.036041 |
| Ca      | 29.587921  | 28.907661  | 29.674358 |
| Ca      | 30.564531  | 33.193222  | 26.492783 |
| Ca      | 30.218212  | 28.157032  | 24.939903 |
| Ca      | 33.776543  | 29.434593  | 28.790714 |
| Ca      | 33.783310  | 24.664719  | 26.841852 |
| Ca      | 35.254711  | 28.689005  | 23.968689 |
| S       | 21.580788  | 31.413830  | 35.528648 |
| S       | 20.484806  | 34.942734  | 32.907398 |
| S       | 22.074600  | 31.463053  | 29.637646 |
| S       | 25.080008  | 33.383392  | 33.121151 |
| S       | 26.301266  | 29.593515  | 30.705133 |
| S       | 25.796566  | 34.156155  | 28.430557 |
| S       | 28.254070  | 30.414028  | 26.536844 |
| S       | 31.033772  | 31.636570  | 29.960915 |
| S       | 31.215862  | 26.709143  | 28.132635 |
| S       | 32.858597  | 30.732327  | 25.599386 |
| S       | 32.695919  | 26.060818  | 23.704487 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.472137    | 32.059994    | 34.009865    |
| Ca      | 23.244495    | 34.442886    | 35.516418    |
| Ca      | 23.975212    | 30.175081    | 32.745960    |
| Ca      | 22.784662    | 34.832489    | 30.852791    |
| Ca      | 24.869024    | 30.852432    | 27.663124    |
| Ca      | 27.603188    | 32.802814    | 30.852943    |
| Ca      | 29.700794    | 29.023605    | 29.408009    |
| Ca      | 30.741745    | 33.117210    | 26.242552    |
| Ca      | 30.055893    | 28.113533    | 24.861168    |
| Ca      | 33.713394    | 29.403450    | 28.918873    |
| Ca      | 33.893330    | 24.602787    | 27.038189    |
| Ca      | 35.557045    | 28.526484    | 23.992283    |
| S       | 21.619877    | 31.104626    | 35.534466    |
| S       | 20.270868    | 35.176140    | 33.448353    |
| S       | 21.864281    | 31.500401    | 29.808290    |
| S       | 25.068291    | 33.574001    | 33.134712    |
| S       | 26.195581    | 29.541306    | 30.254456    |
| S       | 25.518864    | 34.328312    | 28.512873    |
| S       | 28.348034    | 30.496504    | 26.310673    |
| S       | 31.075039    | 31.949726    | 29.573135    |
| S       | 31.285515    | 26.861158    | 28.352966    |
| S       | 32.922119    | 30.398880    | 25.471029    |
| S       | 32.832897    | 26.051104    | 23.994137    |
| S       | 36.107765    | 27.365150    | 27.442820    |

24 generated by VMD
| S    | 25.805462 | 34.117432 | 28.585735 |
|------|-----------|-----------|-----------|
| S    | 28.093193 | 30.238964 | 26.325140 |
| S    | 31.004681 | 31.902460 | 29.564728 |
| S    | 31.327034 | 26.787437 | 28.140804 |
| S    | 32.880196 | 30.552870 | 25.372120 |
| S    | 33.048676 | 26.037441 | 23.895157 |
| S    | 36.068985 | 27.519926 | 27.698917 |

24

generated by VMD

| Ca   | 18.501928 | 32.300331 | 34.171234 |
|------|-----------|-----------|-----------|
| Ca   | 22.905296 | 34.596718 | 35.753365 |
| Ca   | 23.714083 | 30.278320 | 32.597507 |
| Ca   | 22.643299 | 34.617569 | 30.60691 |
| Ca   | 24.699394 | 30.751701 | 27.721447 |
| Ca   | 27.702778 | 32.560074 | 31.148890 |
| Ca   | 29.533663 | 29.139252 | 29.582550 |
| Ca   | 30.629751 | 33.147789 | 26.097675 |
| Ca   | 30.237848 | 28.078316 | 24.667233 |
| Ca   | 33.774475 | 29.402191 | 28.662050 |
| Ca   | 33.659050 | 24.697926 | 27.245205 |
| Ca   | 35.598400 | 28.716747 | 24.179487 |
| S    | 21.624041 | 31.182487 | 35.557392 |
| S    | 20.595240 | 35.255829 | 33.324020 |
| S    | 21.943316 | 31.539749 | 29.736443 |
| S    | 25.115084 | 33.409386 | 33.198425 |
| S    | 26.274040 | 29.444790 | 30.438055 |
| S    | 25.733356 | 34.213478 | 28.668074 |
| S    | 28.248735 | 30.423672 | 26.330166 |
| S    | 31.066870 | 31.742142 | 29.532045 |
| S    | 31.219976 | 26.868488 | 27.954882 |
| S    | 32.863625 | 30.591480 | 25.315248 |
| S    | 33.130718 | 25.896954 | 24.051643 |
| S    | 36.305103 | 27.444641 | 27.400333 |

24

generated by VMD

| Ca   | 18.621613 | 32.155624 | 34.063629 |
|------|-----------|-----------|-----------|
| Ca   | 23.063911 | 34.468163 | 35.785244 |
| Ca   | 23.373833 | 30.205704 | 32.781044 |
| Ca   | 22.740435 | 34.589199 | 30.659628 |
| Ca   | 24.896275 | 30.860126 | 27.522072 |
| Ca   | 27.930567 | 32.980804 | 31.326015 |
| Ca   | 29.231991 | 29.236305 | 29.699989 |
| Ca   | 30.743172 | 32.864323 | 26.131845 |
| Ca   | 30.440073 | 27.946518 | 24.777657 |
| Ca   | 33.611271 | 29.412968 | 28.689413 |
| Ca   | 33.547291 | 24.809269 | 27.131613 |
|   | Ca  |   | S   |   | S   |   | S   |   | S   |   | S   |   |
|---|-----|---|-----|---|-----|---|-----|---|-----|---|-----|---|
|   | 35.607353 | 28.607208 | 23.939310 |
| S | 21.612629 | 31.315697 | 35.539047 |
| S | 20.413960 | 35.171032 | 33.200554 |
| S | 21.968157 | 31.267359 | 29.677454 |
| S | 25.102680 | 33.497860 | 33.264622 |
| S | 26.294697 | 29.589256 | 30.642252 |
| S | 25.781904 | 34.201012 | 28.558918 |
| S | 28.242470 | 30.324684 | 26.247408 |
| S | 30.997072 | 31.854679 | 29.640781 |
| S | 31.228727 | 26.857559 | 28.241781 |
| S | 32.979763 | 30.501677 | 25.361471 |
| S | 33.112755 | 26.127014 | 23.776432 |
| S | 36.173481 | 27.455973 | 27.281919 |

24 generated by VMD

| Ca | 18.448383 | 32.465538 | 34.159134 |
| Ca | 23.145149 | 34.451572 | 35.830986 |
| Ca | 23.570740 | 30.239927 | 32.684574 |
| Ca | 22.808125 | 34.828133 | 30.848877 |
| Ca | 24.750143 | 30.761648 | 27.501984 |
| Ca | 27.821985 | 32.702927 | 30.919840 |
| Ca | 29.399918 | 28.859570 | 29.547680 |
| Ca | 30.626007 | 32.902504 | 26.376009 |
| Ca | 30.545631 | 27.834621 | 24.903767 |
| Ca | 33.734978 | 29.685104 | 28.879341 |
| Ca | 34.026688 | 24.582273 | 27.050833 |
| Ca | 35.566349 | 28.732548 | 23.853697 |
| S | 21.526047 | 31.322018 | 35.350468 |
| S | 20.286797 | 35.281372 | 33.567326 |
| S | 21.902346 | 31.596375 | 29.693285 |
| S | 25.081867 | 33.395340 | 33.263950 |
| S | 26.171125 | 29.644253 | 30.460957 |
| S | 25.495865 | 34.273994 | 28.474123 |
| S | 28.261333 | 30.152912 | 26.260389 |
| S | 30.909391 | 31.745331 | 29.676849 |
| S | 31.403133 | 26.854012 | 28.274658 |
| S | 32.854435 | 30.571682 | 25.338953 |
| S | 33.141953 | 25.822323 | 23.774536 |
| S | 36.241581 | 27.594040 | 27.247864 |

24 generated by VMD

| Ca | 18.583199 | 32.292618 | 33.962521 |
| Ca | 22.979992 | 34.507698 | 35.850216 |
| Ca | 23.831554 | 30.225266 | 32.748722 |
| Ca | 22.938581 | 34.697002 | 30.625992 |
| Ca | 24.945587 | 30.658295 | 27.313683 |
|     |     |     |     |
|-----|-----|-----|-----|
| Ca  | 27.899574 | 33.067566 | 31.355652 |
| Ca  | 29.338219 | 29.090366 | 29.334457 |
| Ca  | 30.351727 | 33.168610 | 26.439589 |
| Ca  | 30.415386 | 27.819256 | 24.830841 |
| Ca  | 33.538589 | 29.687202 | 28.794485 |
| Ca  | 33.700005 | 24.379917 | 27.194309 |
| Ca  | 35.344597 | 28.875980 | 23.894897 |
|     |     |     |     |
| S   | 21.740410 | 31.286278 | 35.441200 |
| S   | 20.459961 | 35.197723 | 33.312462 |
| S   | 22.021238 | 31.233337 | 29.562775 |
| S   | 25.205116 | 33.204262 | 33.425846 |
| S   | 26.372669 | 29.558437 | 30.502596 |
| S   | 25.833450 | 34.214878 | 28.420452 |
| S   | 28.335442 | 30.313744 | 26.160078 |
| S   | 30.968946 | 32.002628 | 29.786171 |
| S   | 31.141903 | 26.884342 | 28.141880 |
| S   | 32.772423 | 30.677708 | 25.452812 |
| S   | 33.163616 | 25.726059 | 23.919880 |
| S   | 35.837906 | 27.530895 | 27.468559 |

24

generated by VMD

|     |     |     |     |
|-----|-----|-----|-----|
| Ca  | 18.548332 | 32.065937 | 34.124092 |
| Ca  | 22.951237 | 34.514332 | 35.813915 |
| Ca  | 23.600216 | 30.409929 | 32.635941 |
| Ca  | 22.678810 | 34.911942 | 30.614895 |
| Ca  | 24.889824 | 30.783436 | 27.531090 |
| Ca  | 27.900833 | 33.065033 | 31.193703 |
| Ca  | 29.454624 | 29.065796 | 29.866585 |
| Ca  | 30.577492 | 32.745312 | 26.440033 |
| Ca  | 30.429213 | 27.673920 | 24.735357 |
| Ca  | 33.552441 | 29.600080 | 28.766853 |
| Ca  | 33.579983 | 24.609249 | 26.990076 |
| Ca  | 35.526535 | 28.892405 | 23.956661 |
|     |     |     |     |
| S   | 21.651070 | 31.283340 | 35.582664 |
| S   | 20.390316 | 35.023891 | 33.245346 |
| S   | 22.001205 | 31.630466 | 29.587423 |
| S   | 24.985233 | 33.573685 | 33.222263 |
| S   | 26.236835 | 29.604015 | 30.503414 |
| S   | 25.676994 | 34.234409 | 28.446472 |
| S   | 28.319771 | 30.010366 | 26.452963 |
| S   | 31.209373 | 31.749382 | 29.952576 |
| S   | 31.301075 | 26.749344 | 28.204063 |
| S   | 32.884800 | 30.607162 | 25.268345 |
| S   | 33.267544 | 26.112003 | 23.660507 |
| S   | 36.106319 | 27.384672 | 27.144794 |

24
| Element | X1    | Y1    | Z1    | X2    | Y2    | Z2    |
|---------|-------|-------|-------|-------|-------|-------|
| Ca      | 18.681067 | 31.982658 | 33.691101 | 23.282349 | 34.429150 | 35.915646 |
| Ca      | 23.581436 | 30.104771 | 32.675606 | 22.920681 | 34.756279 | 30.745968 |
| Ca      | 24.966412 | 30.778957 | 27.405056 | 28.145321 | 32.807053 | 31.232685 |
| Ca      | 29.270054 | 29.378113 | 29.631182 | 30.396486 | 33.176079 | 26.120871 |
| Ca      | 30.118870 | 27.855061 | 24.992516 | 30.144002 | 29.633249 | 28.582470 |
| Ca      | 33.649815 | 24.642490 | 27.343544 | 35.426018 | 28.792942 | 24.225348 |
| S       | 21.396013 | 31.307808 | 35.394638 | 20.549278 | 35.145119 | 33.507423 |
| S       | 20.400179 | 31.395927 | 29.589645 | 25.155319 | 33.374290 | 33.185619 |
| S       | 26.387444 | 29.574432 | 30.591191 | 25.817497 | 34.086464 | 28.614601 |
| S       | 28.226103 | 30.497612 | 26.270739 | 31.093678 | 31.858700 | 29.410568 |
| S       | 31.123507 | 26.911514 | 28.203316 | 32.744755 | 30.409896 | 25.118153 |
| S       | 33.120102 | 25.908791 | 23.890318 | 36.583636 | 29.959949 | 28.495438 |
| S       | 36.213580 | 27.493385 | 27.601822 | 33.653851 | 24.778662 | 27.710793 |
| Ca      | 18.593784 | 31.990993 | 33.732082 | 22.885252 | 34.251450 | 35.955856 |
| Ca      | 23.682232 | 30.096310 | 32.527843 | 22.955242 | 34.927940 | 30.883183 |
| Ca      | 25.076817 | 31.146021 | 27.425861 | 28.158836 | 32.812508 | 31.389038 |
| Ca      | 29.531626 | 29.431580 | 29.487968 | 30.555502 | 33.161385 | 26.174141 |
| Ca      | 30.409260 | 27.499088 | 24.902456 | 33.583836 | 29.959949 | 28.489456 |
| Ca      | 33.653851 | 24.778662 | 27.710793 | 34.893307 | 28.470322 | 23.999275 |
| S       | 21.452044 | 30.960030 | 35.313461 | 20.399221 | 35.150032 | 33.339039 |
| S       | 22.101746 | 31.559290 | 29.591122 | 25.068260 | 33.279572 | 33.385483 |
| S       | 26.400887 | 29.438232 | 30.321117 | 26.102287 | 34.387589 | 28.870167 |
| S       | 28.283829 | 30.403435 | 26.332355 | 24.356352 | 35.259435 | 33.596646 |
S       30.924503       32.180939       29.419979
S       31.399944       27.120476       28.284704
S       32.696545       30.364363       25.113749
S       33.043011       25.477989       23.832680
S       35.867630       27.451668       27.458244

24 generated by VMD
Ca      18.510063       31.750870       33.737877
Ca      22.702061       34.692081       35.760307
Ca      23.936775       30.386700       32.922058
Ca      22.854755       34.630756       30.654762
Ca      25.162895       31.002954       27.771313
Ca      27.934311       33.081017       31.470123
Ca      29.524363       28.858561       29.550438
Ca      30.580126       33.043022       26.277779
Ca      30.437130       27.827675       24.394396
Ca      33.414375       29.632511       28.743809
Ca      33.618000       24.530638       27.083080
Ca      35.456871       28.735229       24.046074
S       21.435385       31.383690       35.612408
S       20.217447       35.154770       33.051300
S       22.249557       31.334576       29.677458
S       25.099710       33.524349       33.380901
S       26.449024       29.725506       30.777992
S       26.076740       34.287750       28.850163
S       28.266148       30.151192       26.307981
S       30.998383       31.856293       29.629086
S       30.897221       26.855801       27.876034
S       32.717712       30.546261       25.179958
S       33.214165       25.799694       23.746416
S       35.966774       27.508169       27.438293

24 generated by VMD
Ca      18.714699       32.041767       33.759560
Ca      22.825222       34.754616       35.641941
Ca      23.763655       30.270306       32.768620
Ca      22.942932       34.561562       30.899899
Ca      25.074963       30.895206       27.691360
Ca      27.889435       32.793266       31.289570
Ca      29.483440       29.094421       29.463228
Ca      30.569941       32.959290       26.100792
Ca      30.369133       27.905327       24.718321
Ca      33.451057       29.612480       28.751413
Ca      33.588264       24.937565       27.209036
Ca      35.468140       28.755499       24.035952
S       21.641285       31.417055       35.572025
|    |   S   |   S   |   S   |
|----|-------|-------|-------|
|    | 20.405920 | 35.213257 | 33.096680 |
|    | 22.320091 | 31.266399 | 29.638233 |
|    | 25.085754 | 33.329838 | 33.511520 |
|    | 26.222649 | 29.414227 | 30.590343 |
|    | 26.088768 | 34.229267 | 28.815426 |
|    | 28.290974 | 30.152233 | 26.251965 |
|    | 30.884155 | 31.741074 | 29.587465 |
|    | 30.884254 | 26.842075 | 27.975166 |
|    | 32.824547 | 30.572186 | 25.108082 |
|    | 33.221359 | 25.865223 | 23.841522 |
|    | 35.709381 | 27.675905 | 27.621922 |

24

generated by VMD

|    |   Ca   |   Ca   |   Ca   |
|----|--------|--------|--------|
|    | 18.782814 | 31.976753 | 34.221901 |
|    | 23.173073 | 34.541382 | 35.699917 |
|    | 23.569241 | 30.369152 | 32.908421 |
|    | 22.802681 | 34.601582 | 30.250801 |
|    | 25.001375 | 30.957478 | 27.651402 |
|    | 27.840969 | 32.831814 | 31.044916 |
|    | 29.480509 | 29.170450 | 29.714083 |
|    | 30.486069 | 32.955517 | 26.240145 |
|    | 30.474613 | 27.977531 | 24.519444 |
|    | 33.336411 | 29.417236 | 28.820927 |
|    | 33.403820 | 24.911469 | 27.075983 |
|    | 35.558037 | 28.677250 | 24.208027 |
|    | 21.797665 | 31.352493 | 35.628265 |
|    | 20.426273 | 34.946609 | 33.274841 |
|    | 21.981318 | 31.435410 | 29.668638 |
|    | 24.987926 | 33.415108 | 32.960155 |
|    | 26.301781 | 29.632473 | 30.566860 |
|    | 26.039127 | 34.135525 | 28.628574 |
|    | 28.372307 | 30.183363 | 26.418421 |
|    | 30.955925 | 31.837065 | 29.734501 |
|    | 30.865299 | 26.769945 | 27.979336 |
|    | 32.909309 | 30.670757 | 25.514528 |
|    | 33.329811 | 26.005943 | 23.659924 |
|    | 35.843689 | 27.527748 | 27.550058 |

24

generated by VMD

|    |   Ca   |   Ca   |   Ca   |
|----|--------|--------|--------|
|    | 18.636641 | 32.225601 | 34.218395 |
|    | 23.116104 | 34.905056 | 35.719681 |
|    | 23.670933 | 30.459700 | 32.663017 |
|    | 22.566286 | 34.545448 | 30.664173 |
|    | 24.881603 | 30.758022 | 27.382343 |
|    | 27.698528 | 32.790890 | 31.283627 |
|    | 29.363029 | 29.000210 | 29.604580 |
| Ca      | 30.595259 | 32.871548 | 26.568653 |
|---------|-----------|-----------|-----------|
| Ca      | 30.569916 | 27.968838 | 24.639172 |
| Ca      | 33.589027 | 29.410049 | 28.924074 |
| Ca      | 33.649174 | 24.763964 | 27.077873 |
| Ca      | 35.630726 | 28.814350 | 23.859299 |
| S       | 21.822460 | 31.416334 | 35.640266 |
| S       | 20.435089 | 35.205097 | 33.417892 |
| S       | 22.007320 | 31.358131 | 29.621012 |
| S       | 25.000191 | 33.519241 | 33.068977 |
| S       | 26.208776 | 29.507133 | 30.490540 |
| S       | 25.606113 | 33.995861 | 28.476912 |
| S       | 28.322289 | 30.141857 | 26.202742 |
| S       | 30.894577 | 31.647413 | 29.881084 |
| S       | 31.211926 | 26.731520 | 28.135155 |
| S       | 32.896317 | 30.667339 | 25.482311 |
| S       | 33.291866 | 26.123833 | 23.548382 |
| S       | 36.055984 | 27.472622 | 27.369997 |

24 generated by VMD

| Ca      | 18.798981 | 32.154472 | 34.416824 |
|---------|-----------|-----------|-----------|
| Ca      | 22.846039 | 34.894901 | 35.835724 |
| Ca      | 23.608389 | 30.346920 | 32.712204 |
| Ca      | 22.633654 | 34.570026 | 30.716158 |
| Ca      | 24.841190 | 31.015072 | 27.482010 |
| Ca      | 27.601410 | 32.834663 | 31.012316 |
| Ca      | 29.406370 | 28.952145 | 29.644190 |
| Ca      | 30.429428 | 32.758202 | 26.176752 |
| Ca      | 30.671721 | 27.900124 | 24.548317 |
| Ca      | 33.553436 | 29.328232 | 28.821842 |
| Ca      | 33.704453 | 24.913664 | 27.023493 |
| Ca      | 35.698460 | 28.765762 | 24.145737 |
| S       | 21.896832 | 31.430086 | 35.643723 |
| S       | 20.252155 | 35.227917 | 33.464298 |
| S       | 21.818348 | 31.442926 | 29.641706 |
| S       | 24.995657 | 33.429413 | 33.198208 |
| S       | 26.046841 | 29.596273 | 30.255192 |
| S       | 25.838615 | 34.438381 | 28.613827 |
| S       | 28.295902 | 29.893780 | 26.334206 |
| S       | 30.948933 | 31.479658 | 29.647518 |
| S       | 31.168749 | 26.676998 | 28.023964 |
| S       | 33.007359 | 30.627462 | 25.321646 |
| S       | 33.376057 | 26.167549 | 23.770599 |
| S       | 36.281097 | 27.455427 | 27.489605 |

24 generated by VMD

| Ca      | 18.875330 | 31.749687 | 34.237770 |
| Element | $x_1$ | $x_2$ | $x_3$ |
|---------|-------|-------|-------|
| Ca      | 22.763912 | 34.683620 | 35.933258 |
| Ca      | 23.877743 | 30.379189  | 32.681324  |
| Ca      | 22.671055 | 34.705059  | 30.662176  |
| Ca      | 25.055107 | 31.042038  | 27.496777  |
| Ca      | 27.693333 | 33.036812  | 31.230177  |
| Ca      | 29.580452 | 29.125513  | 29.437681  |
| Ca      | 30.411480 | 32.879906  | 26.156013  |
| Ca      | 33.459801 | 29.403332  | 28.784561  |
| Ca      | 33.515579 | 24.669664  | 27.314228  |
| Ca      | 35.599243 | 28.551836  | 24.148632  |
| S       | 21.867123 | 31.161573  | 35.351059  |
| S       | 20.360643 | 34.969551  | 33.522686  |
| S       | 22.110043 | 31.307995  | 29.389587  |
| S       | 25.004833 | 33.651787  | 33.408222  |
| S       | 26.416542 | 29.904289  | 30.457779  |
| S       | 25.777702 | 34.501877  | 28.702339  |
| S       | 28.297043 | 30.089771  | 26.085897  |
| S       | 30.757107 | 31.913269  | 29.583656  |
| S       | 31.000137 | 26.912258  | 28.091805  |
| S       | 32.982315 | 30.527548  | 25.337399  |
| S       | 33.194103 | 25.983414  | 23.790010  |
| S       | 35.966080 | 27.246565  | 27.609049  |

24 generated by VMD

| Element | $x_1$ | $x_2$ | $x_3$ |
|---------|-------|-------|-------|
| Ca      | 18.779114 | 31.691187  | 33.631084  |
| Ca      | 22.751549 | 34.607433  | 35.845177  |
| Ca      | 23.743523 | 30.275337  | 32.816570  |
| Ca      | 22.917206 | 34.484795  | 30.738827  |
| Ca      | 25.355110 | 31.163662  | 27.467651  |
| Ca      | 27.839081 | 33.038902  | 31.532631  |
| Ca      | 29.644508 | 29.141739  | 29.560633  |
| Ca      | 30.394100 | 32.733944  | 26.253700  |
| Ca      | 30.290520 | 27.866882  | 24.594065  |
| Ca      | 33.53946  | 29.674500  | 28.793627  |
| Ca      | 33.464020 | 24.751892  | 27.203365  |
| Ca      | 35.404446 | 28.444328  | 23.829628  |
| S       | 21.476051 | 31.200039  | 35.403149  |
| S       | 20.340813 | 35.113617  | 33.199230  |
| S       | 22.000843 | 31.378283  | 29.601177  |
| S       | 25.06829  | 33.692902  | 33.505672  |
| S       | 26.498440 | 29.878933  | 30.772114  |
| S       | 26.055267 | 34.350422  | 28.808565  |
| S       | 28.445885 | 30.91570   | 26.242481  |
| S       | 30.854498 | 32.046116  | 29.716335  |
| S       | 31.166569 | 26.957668  | 28.119329  |
|     |          |          |          |
|-----|----------|----------|----------|
| S   | 32.741577| 30.414219| 25.235214|
| S   | 33.068874| 25.84763| 23.63499 |
| S   | 35.891365| 27.456930| 27.435286|

24 generated by VMD

|     |          |          |          |
|-----|----------|----------|----------|
| Ca  | 18.609989| 32.084534| 33.775928|
| Ca  | 22.705029| 34.638931| 35.961292|
| Ca  | 23.594149| 30.287582| 32.520531|
| Ca  | 23.015688| 34.569855| 30.790977|
| Ca  | 25.242752| 31.040180| 27.641203|
| Ca  | 27.832647| 32.633236| 31.746223|
| Ca  | 29.378551| 29.063747| 29.660275|
| Ca  | 30.540182| 33.076107| 25.855152|
| Ca  | 30.280731| 27.756166| 24.536793|
| Ca  | 33.383041| 29.376829| 28.447449|
| Ca  | 33.785812| 25.071430| 27.402506|
| Ca  | 35.666241| 28.543104| 23.882847|
| S   | 21.393169| 31.335789| 35.508980|
| S   | 20.586260| 35.124802| 33.297455|
| S   | 22.270790| 31.426960| 29.678762|
| S   | 25.023071| 33.598133| 33.321606|
| S   | 26.281118| 29.506624| 30.730360|
| S   | 26.154030| 34.154739| 28.896307|
| S   | 28.363853| 30.002819| 26.180704|
| S   | 30.884380| 31.949455| 29.533085|
| S   | 30.780331| 26.810095| 28.153568|
| S   | 32.870121| 30.317915| 25.055164|
| S   | 33.237282| 25.955681| 23.879454|
| S   | 35.840897| 27.975256| 27.483381|

24 generated by VMD

|     |          |          |          |
|-----|----------|----------|----------|
| Ca  | 18.696911| 31.852699| 33.649017|
| Ca  | 22.959772| 34.668381| 35.934860|
| Ca  | 23.594139| 30.350529| 32.789917|
| Ca  | 22.861771| 34.899879| 30.522793|
| Ca  | 24.929893| 30.900925| 27.626940|
| Ca  | 27.844051| 32.719570| 31.358269|
| Ca  | 29.479750| 28.931454| 29.769382|
| Ca  | 30.518894| 32.846985| 26.191494|
| Ca  | 30.259430| 27.750378| 24.698067|
| Ca  | 33.533222| 29.404829| 28.596136|
| Ca  | 33.777813| 24.909491| 27.065220|
| Ca  | 35.518879| 28.676592| 23.966475|
| S   | 21.516710| 31.340466| 35.554916|
| S   | 20.360348| 35.226215| 33.399475|
| S   | 22.246143| 31.441706| 29.618935|
|    |       |       |       |
|----|-------|-------|-------|
| S  | 24.982628 | 33.613888 | 33.177216 |
| S  | 26.283691  | 29.531952 | 30.632412 |
| S  | 26.031111  | 34.360573 | 28.774927 |
| S  | 28.154900  | 30.230404 | 26.336880 |
| S  | 30.941513  | 31.658764 | 29.829441 |
| S  | 31.168530  | 26.698133 | 28.108540 |
| S  | 32.772991  | 30.548883 | 25.165485 |
| S  | 33.190674  | 25.810276 | 23.735365 |
| S  | 36.096401  | 27.927076 | 27.437838 |
| 24 | generated by VMD |
| Ca | 18.842209  | 31.945272 | 33.834351 |
| Ca | 23.077431  | 34.444401 | 36.001255 |
| Ca | 23.588455  | 30.158081 | 32.556229 |
| Ca | 22.985592  | 34.777878 | 30.633156 |
| Ca | 24.928761  | 30.905327 | 27.601488 |
| Ca | 27.971628  | 32.907215 | 31.644871 |
| Ca | 29.299789  | 29.134129 | 29.541252 |
| Ca | 30.549042  | 32.890671 | 26.006981 |
| Ca | 30.439838  | 27.932104 | 24.454020 |
| Ca | 33.466778  | 29.521715 | 28.668198 |
| Ca | 33.522812  | 24.936474 | 27.487289 |
| Ca | 35.546261  | 28.484737 | 24.107382 |
| S  | 21.669441  | 31.220005 | 35.376091 |
| S  | 20.561863  | 35.057999 | 33.429810 |
| S  | 21.924557  | 31.395744 | 29.616272 |
| S  | 25.090778  | 33.435772 | 33.242725 |
| S  | 26.345888  | 29.597347 | 30.533718 |
| S  | 25.943459  | 34.180923 | 28.725159 |
| S  | 28.329861  | 30.206623 | 26.104584 |
| S  | 30.942211  | 32.196747 | 29.535492 |
| S  | 30.793236  | 26.955502 | 28.007267 |
| S  | 32.807533  | 30.597713 | 25.164751 |
| S  | 33.192524  | 25.684732 | 24.005619 |
| S  | 35.900013  | 27.732855 | 27.662102 |

24

|    |       |       |       |
|----|-------|-------|-------|
| Ca | 18.673824  | 31.712597 | 34.097538 |
| Ca | 22.842514  | 34.391945 | 35.730339 |
| Ca | 23.682858  | 30.127029 | 32.737602 |
| Ca | 22.669897  | 34.818066 | 30.745867 |
| Ca | 25.009186  | 31.287880 | 27.618118 |
| Ca | 27.984589  | 33.171059 | 31.229652 |
| Ca | 29.481300  | 29.235241 | 29.381714 |
| Ca | 30.629040  | 32.855995 | 25.671619 |
| Ca | 30.245567  | 27.965815 | 24.636204 |
|   | 18.506512 | 31.973270 | 34.067596 |
|---|---|---|---|
| Ca | Ca | Ca | Ca |
| 18.506512 | 31.973270 | 34.067596 | 34.067596 |
| 22.845783 | 34.341297 | 35.820621 | 35.820621 |
| 23.645905 | 30.464088 | 32.71243 | 32.71243 |
| 22.680401 | 34.718765 | 30.71836 | 30.71836 |
| 25.252575 | 30.916138 | 27.579697 | 27.579697 |
| 27.946947 | 33.225082 | 31.232437 | 31.232437 |
| 29.507923 | 29.057589 | 29.551147 | 29.551147 |
| 30.984907 | 32.849319 | 25.910501 | 25.910501 |
| 30.417500 | 27.982256 | 24.622532 | 24.622532 |
| 33.569717 | 29.478086 | 28.914040 | 28.914040 |
| 33.459549 | 24.919241 | 27.004667 | 27.004667 |
| 35.459396 | 28.252367 | 24.146645 | 24.146645 |
| 21.341633 | 30.955172 | 35.547516 | 35.547516 |
| 20.285730 | 34.999836 | 33.559971 | 33.559971 |
| 22.097969 | 31.209442 | 29.722927 | 29.722927 |
| 24.881210 | 33.796124 | 33.070930 | 33.070930 |
| 26.461226 | 29.935898 | 30.647463 | 30.647463 |
| 25.763603 | 34.324604 | 28.766539 | 28.766539 |
| 28.373665 | 30.324471 | 26.250137 | 26.250137 |
| 31.204863 | 31.990007 | 29.536533 | 29.536533 |
| 31.146732 | 26.912590 | 28.102322 | 28.102322 |
| 33.018944 | 30.324453 | 25.224039 | 25.224039 |
| 32.916336 | 25.807753 | 23.657841 | 23.657841 |
| 35.951012 | 27.542282 | 27.574104 | 27.574104 |
| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 22.806585 | 34.742928 | 30.612896 |
| Ca      | 25.016876 | 31.136526 | 27.258858 |
| Ca      | 28.019382 | 32.789978 | 31.266590 |
| Ca      | 29.359680 | 29.101982 | 29.525301 |
| Ca      | 30.767494 | 32.904911 | 25.887829 |
| Ca      | 30.335798 | 27.985771 | 24.683590 |
| Ca      | 33.151218 | 29.729988 | 28.790623 |
| Ca      | 33.566650 | 24.871189 | 27.180626 |
| Ca      | 35.637447 | 28.322472 | 24.453094 |
| S       | 21.574009 | 30.921165 | 35.526279 |
| S       | 20.619795 | 34.988678 | 33.96198 |
| S       | 22.128159 | 31.233080 | 29.551908 |
| S       | 24.962021 | 33.526070 | 33.165886 |
| S       | 26.495079 | 29.695065 | 30.443119 |
| S       | 25.948662 | 34.378822 | 28.663099 |
| S       | 28.229265 | 30.177250 | 26.213181 |
| S       | 31.041626 | 32.099861 | 29.542091 |
| S       | 30.960434 | 27.117735 | 28.063850 |
| S       | 32.967079 | 30.486839 | 25.239202 |
| S       | 33.107288 | 25.656330 | 23.908587 |
| S       | 35.746342 | 27.734871 | 27.657679 |

24 generated by VMD

| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 18.340351 | 32.340862 | 33.885921 |
| Ca      | 22.784929 | 34.455456 | 36.052559 |
| Ca      | 23.673573 | 30.220921 | 32.664711 |
| Ca      | 22.936937 | 34.538803 | 30.706406 |
| Ca      | 25.066307 | 31.049217 | 27.472683 |
| Ca      | 28.041847 | 33.038528 | 31.463804 |
| Ca      | 29.593075 | 29.096766 | 29.493088 |
| Ca      | 30.424828 | 32.822853 | 26.161999 |
| Ca      | 30.345169 | 27.979706 | 24.586159 |
| Ca      | 33.611649 | 29.699871 | 28.639042 |
| Ca      | 33.783283 | 24.671198 | 27.295650 |
| Ca      | 35.317135 | 28.523418 | 24.028973 |
| S       | 21.251293 | 31.163494 | 35.182884 |
| S       | 20.561462 | 35.125534 | 33.266827 |
| S       | 22.132103 | 31.056953 | 29.725876 |
| S       | 25.076527 | 33.628979 | 33.362206 |
| S       | 26.507439 | 29.722876 | 30.662964 |
| S       | 25.983517 | 34.352394 | 28.840443 |
| S       | 28.307224 | 29.942104 | 26.297401 |
| S       | 31.160969 | 31.957533 | 29.590105 |
| S       | 31.091049 | 26.790592 | 27.932018 |
| S       | 32.802910 | 30.617437 | 25.210657 |
| S       | 32.832535 | 25.889965 | 24.028864 |
|   | 36.093849 | 27.614582 | 27.388815 |
|---|-----------|-----------|-----------|

**24**

generated by VMD

|   | 18.563135 | 32.324993 | 33.976772 |
|---|-----------|-----------|-----------|
| Ca| 22.887167 | 34.363705 | 35.883873 |
| Ca| 23.420341 | 30.275442 | 32.460243 |
| Ca| 22.859226 | 34.581482 | 30.788656 |
| Ca| 25.051647 | 31.049374 | 27.467508 |
| Ca| 27.979012 | 32.857674 | 31.440865 |
| Ca| 29.506016 | 29.217047 | 29.447254 |
| Ca| 30.691517 | 32.821846 | 26.157129 |
| Ca| 30.315985 | 27.769915 | 24.683392 |
| Ca| 33.519836 | 29.898146 | 28.830530 |
| Ca| 33.833775 | 24.881350 | 27.256836 |
| Ca| 35.215126 | 28.412767 | 23.931198 |
| S | 21.414621 | 30.949356 | 35.353271 |
| S | 20.576199 | 35.217751 | 33.511440 |
| S | 22.030695 | 31.153503 | 29.684334 |
| S | 24.900997 | 33.495033 | 33.156380 |
| S | 26.484838 | 29.842115 | 30.516064 |
| S | 26.008228 | 34.433891 | 28.790504 |
| S | 28.345364 | 30.233297 | 26.212574 |
| S | 31.133644 | 31.958309 | 29.675524 |
| S | 31.155827 | 26.803587 | 28.185816 |
| S | 32.938538 | 30.435839 | 25.246099 |
| S | 32.882763 | 25.509577 | 23.882198 |
| S | 36.005630 | 27.814047 | 27.401579 |

**24**

generated by VMD

|   | 18.403950 | 32.568764 | 33.341839 |
|---|-----------|-----------|-----------|
| Ca| 22.818840 | 34.266914 | 35.862904 |
| Ca| 23.508387 | 30.095781 | 32.760452 |
| Ca| 23.043211 | 34.524372 | 30.758392 |
| Ca| 25.174480 | 30.872066 | 27.71945 |
| Ca| 27.987862 | 32.760246 | 31.525003 |
| Ca| 29.344334 | 29.330959 | 29.968699 |
| Ca| 30.666769 | 32.835499 | 26.180397 |
| Ca| 30.397602 | 27.581112 | 25.032024 |
| Ca| 33.613548 | 29.753187 | 28.520214 |
| Ca| 33.682518 | 25.191122 | 27.227089 |
| Ca| 35.186378 | 28.403358 | 23.560217 |
| S | 21.017572 | 31.192158 | 35.386234 |
| S | 20.518078 | 35.408531 | 33.301792 |
| S | 22.191013 | 31.304539 | 29.654335 |
| S | 25.119337 | 33.465946 | 33.348095 |
| S | 26.399580 | 29.564236 | 30.892010 |
S   26.138924  34.042755  28.767174
S   28.378632  30.097553  26.414232
S   31.104141  31.858841  29.815126
S   31.137753  26.965551  28.176107
S   32.769882  30.510050  25.081989
S   33.089779  25.799530  23.509579
S   36.027542  27.906984  27.144176
24 generated by VMD
Ca  18.520721  32.778339  33.705193
Ca  23.310369  34.025429  36.018188
Ca  23.410782  30.112768  32.703228
Ca  22.926239  34.742538  30.774885
Ca  24.876369  30.838642  27.671762
Ca  27.728968  32.865570  31.168438
Ca  29.234787  28.994862  29.824892
Ca  30.583813  33.004105  26.066244
Ca  30.304989  27.682089  24.726524
Ca  33.623833  29.543640  28.246874
Ca  34.191292  24.937151  27.555473
Ca  35.358067  28.645771  23.782398
S   21.165508  31.191290  35.091141
S   20.776730  35.486061  33.714165
S   21.938822  31.490643  29.567102
S   24.965107  33.332245  33.303341
S   26.123684  29.545895  30.631290
S   25.802856  34.148499  28.739796
S   28.449764  30.055443  26.466629
S   30.820656  31.793667  29.657185
S   31.291862  26.776926  28.084122
S   32.825050  30.501408  25.104576
S   33.269978  25.774338  24.002993
S   36.219753  28.032734  27.333603
24 generated by VMD
Ca  18.654732  32.489979  33.718609
Ca  23.013533  34.176765  35.968395
Ca  23.569313  29.942097  32.797264
Ca  22.964376  34.604527  30.533806
Ca  24.912529  30.867701  27.611172
Ca  28.028572  32.875809  31.464987
Ca  29.315128  29.365032  29.767874
Ca  30.623760  33.124050  26.212965
Ca  30.297817  27.998682  24.853548
Ca  33.576881  29.387056  28.610130
Ca  33.622066  25.123068  27.385204
|  | Ca     |  | S      |  | S      |  |
|---|---|---|---|---|---|---|
| Ca | 35.431015 | 28.571890 | 23.715185 |
| S  | 21.321041 | 31.084044 | 35.265301 |
| S  | 20.698082 | 35.386501 | 33.149895 |
| S  | 21.929363 | 30.048882 | 29.597795 |
| S  | 24.982643 | 33.443161 | 33.149895 |
| S  | 26.363098 | 29.637037 | 30.594440 |
| S  | 25.895636 | 34.312668 | 28.770443 |
| S  | 28.296196 | 30.243042 | 26.383694 |
| S  | 31.270508 | 31.870670 | 29.506182 |
| S  | 31.194828 | 26.759306 | 28.373196 |
| S  | 32.759613 | 30.422369 | 25.192955 |
| S  | 32.916187 | 25.719177 | 23.958208 |
| S  | 36.083153 | 27.840578 | 27.232912 |

24 generated by VMD

| Ca     |  | S      |  | S      |  |
|---|---|---|---|---|---|
| Ca | 18.381844 | 32.882309 | 33.583908 |
| Ca | 23.085260 | 34.251190 | 36.036385 |
| Ca | 23.456144 | 29.985716 | 32.703793 |
| Ca | 23.005501 | 34.916653 | 30.878578 |
| Ca | 25.041719 | 30.861252 | 27.793232 |
| Ca | 27.837254 | 32.725868 | 31.460751 |
| Ca | 29.624599 | 28.970343 | 29.595051 |
| Ca | 30.510090 | 32.750702 | 26.116867 |
| Ca | 30.485371 | 27.485294 | 24.556423 |
| Ca | 33.316341 | 29.758682 | 28.587601 |
| Ca | 34.114376 | 25.148724 | 27.598885 |
| Ca | 35.262535 | 28.691723 | 23.540817 |
| S  | 21.014118 | 31.227398 | 35.059475 |
| S  | 20.609295 | 35.419113 | 33.647968 |
| S  | 22.208183 | 31.508572 | 29.628191 |
| S  | 24.866161 | 33.362423 | 33.405083 |
| S  | 26.334618 | 29.411001 | 30.664600 |
| S  | 26.132719 | 34.204918 | 28.925726 |
| S  | 28.460089 | 29.968046 | 26.238998 |
| S  | 30.852310 | 31.903212 | 29.628380 |
| S  | 31.177800 | 26.673542 | 28.183659 |
| S  | 32.552986 | 30.409483 | 25.021702 |
| S  | 33.510246 | 25.555799 | 23.902060 |
| S  | 35.880573 | 28.228069 | 27.181911 |

24 generated by VMD

| Ca     |  | S      |  | S      |  |
|---|---|---|---|---|---|
| Ca | 18.510311 | 32.396084 | 33.711311 |
| Ca | 22.906513 | 34.265762 | 35.919094 |
| Ca | 23.714310 | 30.088243 | 32.795486 |
| Ca | 22.925934 | 34.933144 | 30.761385 |
| Ca | 25.142727 | 31.002296 | 27.522087 |

532
| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 27.760906 | 32.679207 | 31.500195 |
| Ca      | 29.643147 | 29.132427 | 29.602001 |
| Ca      | 30.586262 | 32.876289 | 25.947859 |
| Ca      | 30.154922 | 27.888199 | 24.509106 |
| Ca      | 33.599312 | 29.516146 | 28.442631 |
| Ca      | 33.872025 | 24.927813 | 27.598614 |
| Ca      | 35.383575 | 28.520294 | 23.800049 |
| S       | 21.200697 | 31.061174 | 35.498474 |
| S       | 20.482822 | 35.137596 | 33.378574 |
| S       | 22.306660 | 31.411734 | 29.735586 |
| S       | 24.954660 | 33.558788 | 33.368759 |
| S       | 26.260555 | 29.530167 | 30.421019 |
| S       | 26.123085 | 34.388153 | 28.845453 |
| S       | 28.356457 | 30.019941 | 26.335495 |
| S       | 30.874619 | 32.078915 | 29.624020 |
| S       | 31.020439 | 26.967411 | 28.052752 |
| S       | 32.817513 | 30.364159 | 25.058971 |
| S       | 33.084711 | 25.720297 | 24.016653 |
| S       | 36.042110 | 27.835781 | 27.494473 |

generated by VMD

| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 18.459290 | 32.939758 | 33.680344 |
| Ca      | 23.079121 | 34.333294 | 35.996929 |
| Ca      | 23.743458 | 29.930126 | 32.857487 |
| Ca      | 23.121700 | 34.854942 | 30.838144 |
| Ca      | 24.957237 | 30.923561 | 27.639400 |
| Ca      | 27.685806 | 32.454372 | 31.273479 |
| Ca      | 29.516319 | 29.068174 | 29.422569 |
| Ca      | 30.246344 | 32.871346 | 25.845528 |
| Ca      | 30.447598 | 27.767309 | 24.650003 |
| Ca      | 33.411381 | 29.766090 | 28.516197 |
| Ca      | 34.049049 | 24.972622 | 27.523647 |
| Ca      | 35.516487 | 28.735796 | 24.030897 |
| S       | 21.092125 | 31.107864 | 35.397129 |
| S       | 20.773455 | 35.548706 | 33.513466 |
| S       | 22.121258 | 31.378927 | 29.920029 |
| S       | 25.096117 | 33.201401 | 33.325691 |
| S       | 26.223980 | 29.317310 | 30.349350 |
| S       | 26.097511 | 34.190578 | 28.863894 |
| S       | 28.119530 | 30.009060 | 26.076553 |
| S       | 30.684521 | 31.824957 | 29.495068 |
| S       | 31.095928 | 26.828346 | 27.975979 |
| S       | 32.777630 | 30.553181 | 25.040474 |
| S       | 33.412205 | 25.609560 | 24.168526 |
| S       | 35.992001 | 28.112698 | 27.539259 |

24
| Element | X1    | Y1    | Z1    |
|---------|-------|-------|-------|
| Ca      | 18.665146 | 32.520531 | 33.981701 |
| Ca      | 23.087936 | 34.437870 | 35.677265 |
| Ca      | 23.871490 | 30.081757 | 32.799084 |
| Ca      | 22.865974 | 34.888641 | 30.587826 |
| Ca      | 24.977077 | 30.933664 | 27.723680 |
| Ca      | 27.468105 | 32.439888 | 31.230400 |
| Ca      | 29.493101 | 28.901438 | 29.586092 |
| Ca      | 30.417583 | 33.021324 | 26.449978 |
| Ca      | 30.334248 | 28.045301 | 24.826038 |
| Ca      | 33.544273 | 29.328985 | 28.650591 |
| Ca      | 33.989803 | 25.123028 | 27.289711 |
| Ca      | 35.364731 | 28.624289 | 23.823435 |
| S       | 21.643280 | 31.168568 | 35.398994 |
| S       | 20.647030 | 35.552044 | 33.333126 |
| S       | 22.027000 | 31.403297 | 29.696135 |
| S       | 25.118504 | 33.298874 | 32.993011 |
| S       | 26.214317 | 29.243271 | 30.357918 |
| S       | 25.771072 | 34.368584 | 28.511280 |
| S       | 28.216314 | 30.071438 | 26.407314 |
|   |   |   |
|---|---|---|
| S | 30.790503 | 31.691832 | 29.842970 |
| S | 31.147781 | 26.751066 | 28.098972 |
| S | 32.865921 | 30.583487 | 25.411505 |
| S | 33.123077 | 25.742487 | 23.894939 |
| S | 36.075752 | 28.078377 | 27.368029 |

24

generated by VMD

| Ca | 18.704498 | 32.355930 | 33.890564 |
| Ca | 22.956356 | 33.878105 | 35.849949 |
| Ca | 23.622496 | 30.142288 | 32.652950 |
| Ca | 23.158524 | 34.877853 | 30.917044 |
| Ca | 25.045235 | 31.096230 | 27.414721 |
| Ca | 27.592991 | 32.867077 | 31.365271 |
| Ca | 29.605995 | 29.329060 | 29.596178 |
| Ca | 30.669258 | 32.920277 | 26.015686 |
| Ca | 30.169441 | 27.766466 | 24.949606 |
| Ca | 33.523842 | 29.661833 | 28.569210 |
| Ca | 34.011089 | 25.037565 | 27.648312 |
| Ca | 35.209240 | 28.357529 | 23.637321 |
| S | 21.107342 | 30.914333 | 35.302025 |
| S | 20.635881 | 35.459198 | 33.488819 |
| S | 22.104565 | 31.462841 | 29.555508 |
| S | 24.933891 | 33.241608 | 33.229015 |
| S | 26.359558 | 29.711983 | 30.251797 |
| S | 26.080595 | 34.302017 | 28.895752 |
| S | 28.481817 | 30.225700 | 26.155880 |
| S | 30.960529 | 31.932291 | 29.573135 |
| S | 31.098671 | 26.858341 | 28.473347 |
| S | 32.657078 | 30.332067 | 25.085546 |
| S | 32.986492 | 25.580299 | 24.290079 |
| S | 36.044624 | 27.989096 | 27.132374 |

24

generated by VMD

| Ca | 18.527037 | 32.469589 | 33.896809 |
| Ca | 23.010225 | 34.105530 | 36.004238 |
| Ca | 23.609856 | 30.315231 | 32.563805 |
| Ca | 23.100037 | 34.712967 | 30.818577 |
| Ca | 24.849522 | 31.082336 | 27.408836 |
| Ca | 28.030849 | 32.832081 | 31.437849 |
| Ca | 29.124819 | 29.376507 | 29.731800 |
| Ca | 30.450821 | 32.657612 | 26.112270 |
| Ca | 30.238022 | 27.758343 | 24.869049 |
| Ca | 33.695999 | 29.470825 | 28.619179 |
| Ca | 33.889706 | 25.248989 | 27.506901 |
| Ca | 35.466309 | 28.626930 | 23.508797 |
| S | 21.284760 | 30.961102 | 35.372128 |
| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| S    | 20.669575 | 35.379517 | 33.358257 |
| S    | 21.995510  | 31.344580  | 29.540429  |
| S    | 24.930279  | 33.414757  | 33.065819  |
| S    | 26.313372  | 29.670074  | 30.461029  |
| S    | 25.990314  | 34.045403  | 28.720116  |
| S    | 28.225273  | 30.060570  | 26.422335  |
| S    | 31.100418  | 31.785782  | 29.577530  |
| S    | 31.173904  | 26.799671  | 28.470699  |
| S    | 32.914562  | 30.300661  | 25.219151  |
| S    | 32.969963  | 25.984783  | 24.088732  |
| S    | 36.158943  | 27.896240  | 27.165699  |

24 generated by VMD

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| Ca   | 18.286230 | 32.549564 | 33.580418 |
| Ca   | 23.194147 | 33.898399 | 35.870823 |
| Ca   | 23.682457 | 30.209558 | 32.475094 |
| Ca   | 22.881550 | 34.734917 | 30.944023 |
| Ca   | 24.996964 | 31.123196 | 27.633038 |
| Ca   | 28.016640 | 32.968338 | 31.577864 |
| Ca   | 29.589960 | 29.179277 | 29.733980 |
| Ca   | 30.371407 | 32.790688 | 26.113274 |
| Ca   | 30.223328 | 27.674997 | 24.807585 |
| Ca   | 33.647236 | 29.573881 | 28.550900 |
| Ca   | 33.785042 | 25.212603 | 27.694363 |
| Ca   | 35.434330 | 28.534090 | 23.600368 |
| S    | 21.213352 | 31.072289 | 34.902134 |
| S    | 20.670958 | 35.343014 | 33.652012 |
| S    | 21.949039 | 31.388004 | 29.628269 |
| S    | 24.932270 | 33.337879 | 33.200397 |
| S    | 26.595509 | 29.754963 | 30.767597 |
| S    | 25.989113 | 34.299690 | 28.847307 |
| S    | 28.184893 | 29.918430 | 26.392971 |
| S    | 31.046276 | 31.935017 | 29.484886 |
| S    | 30.974949 | 26.806400 | 28.271627 |
| S    | 32.856503 | 30.285128 | 25.044306 |
| S    | 33.145447 | 25.706526 | 23.973469 |
| S    | 36.052414 | 28.003212 | 27.193310 |

24 generated by VMD

| Atom | X      | Y      | Z      |
|------|--------|--------|--------|
| Ca   | 18.518715 | 32.597050 | 33.751690 |
| Ca   | 23.159969 | 34.280090 | 36.182663 |
| Ca   | 23.405663 | 30.408493 | 32.705341 |
| Ca   | 23.049091 | 34.531898 | 30.823782 |
| Ca   | 24.991924 | 31.054764 | 27.571859 |
| Ca   | 27.955753 | 32.665173 | 31.379942 |
| Ca   | 29.059383 | 28.979515 | 29.716808 |
|   | Ca     | S      |
|---|--------|--------|
| 1 | 30.507900 | 32.692760 | 26.108967 |
| 2 | 30.306189 | 27.571478 | 24.575230 |
| 3 | 33.626228 | 28.834755 | 23.985296 |
| 4 | 33.848747 | 25.359844 | 27.505602 |
| 5 | 35.602764 | 28.834755 | 23.985296 |
| 6 | 21.275478 | 31.185516 | 35.383842 |
| 7 | 20.845562 | 35.477089 | 33.604946 |
| 8 | 22.056671 | 31.351248 | 29.605192 |
| 9 | 24.802431 | 33.490952 | 33.163891 |
| 10 | 26.303444 | 29.585712 | 30.621906 |
| 11 | 25.849226 | 34.102722 | 28.588867 |
| 12 | 28.098845 | 30.077559 | 26.149870 |
| 13 | 30.832647 | 31.562998 | 29.538582 |
| 14 | 26.303444 | 29.585712 | 30.621906 |
| 15 | 25.849226 | 34.102722 | 28.588867 |

24

24

generated by VMD
|  | Ca   | 34.11259 | 36.095261 | 22.964161 | 23.429420 | 23.859983 | 29.339525 | 30.550398 | 34.216980 | 35.715668 | 21.072304 | 20.908028 | 21.798206 | 24.960936 | 26.297043 | 25.830002 | 28.228455 | 30.852440 | 31.129402 | 32.95630 | 33.432220 | 35.912216 | 18.486216 | 23.285925 | 23.531628 | 22.968859 | 24.727764 | 27.967022 | 29.076637 | 30.501719 | 30.360920 | 33.575226 | 34.102921 | 35.631508 | 21.172859 | 20.951773 | 21.793583 | 24.986326 | 26.254919 | 25.835228 | 28.045532 | 30.972759 | 31.103046 |
|  | 30.051311 | 32.672714 | 28.984491 | 32.794323 | 27.808037 | 29.597168 | 25.069021 | 32.794323 | 34.153923 | 29.942085 | 31.729649 | 35.717674 | 31.330364 | 33.268822 | 29.641140 | 34.153923 | 29.942085 | 31.729649 | 26.778954 | 30.572435 | 25.667627 | 28.058861 | 32.949669 | 34.077927 | 30.226665 | 34.366730 | 30.924091 | 32.602322 | 29.071863 | 32.959946 | 27.856853 | 29.366335 | 25.150442 | 28.730118 | 31.159939 | 35.427990 | 31.401611 | 33.484837 | 29.479000 | 34.088188 | 30.032177 | 31.649796 | 26.754572 | 27.968323 |
|   | X Position 1 | X Position 2 | X Position 3 |
|---|--------------|--------------|--------------|
| S | 32.897224    | 30.624651    | 25.269085    |
| S | 33.312630    | 25.887377    | 24.122681    |
| S | 36.177803    | 28.027004    | 27.484060    |

24 generated by VMD

| Ca | 18.600992   | 33.215134   | 34.173492   |
| Ca | 22.977695   | 34.101433   | 35.896980   |
| Ca | 23.723118   | 29.777756   | 32.641670   |
| Ca | 22.807789   | 34.530590   | 30.702335   |
| Ca | 24.740957   | 30.721035   | 27.515018   |
| Ca | 27.835892   | 32.929672   | 31.008848   |
| Ca | 29.367981   | 29.319693   | 29.509464   |
| Ca | 30.551090   | 32.889450   | 25.895506   |
| Ca | 30.245066   | 27.950974   | 24.821615   |
| Ca | 33.493050   | 29.209412   | 28.495434   |
| Ca | 33.847969   | 25.029974   | 27.620316   |
| Ca | 35.612286   | 28.689659   | 24.106928   |
| S  | 21.176659   | 30.878778   | 35.131310   |
| S  | 21.109848   | 35.691414   | 33.880619   |
| S  | 21.852867   | 31.313812   | 29.899921   |
| S  | 25.030369   | 33.213158   | 33.000271   |
| S  | 26.301308   | 29.408520   | 30.411989   |
| S  | 25.622417   | 34.156662   | 28.522396   |
| S  | 28.089783   | 30.204853   | 26.316612   |
| S  | 31.022245   | 31.815331   | 29.448755   |
| S  | 31.233603   | 26.774839   | 27.900303   |
| S  | 32.872578   | 30.635237   | 25.351337   |
| S  | 33.211372   | 25.813122   | 24.086212   |
| S  | 36.393036   | 28.029612   | 27.602736   |

24 generated by VMD

| Ca | 18.638676   | 33.119720   | 33.752651   |
| Ca | 23.014019   | 33.965912   | 36.169621   |
| Ca | 23.587078   | 30.061371   | 32.614403   |
| Ca | 23.207527   | 34.534805   | 30.840107   |
| Ca | 24.959927   | 30.665464   | 27.603685   |
| Ca | 27.799101   | 33.095665   | 31.435020   |
| Ca | 29.241531   | 29.221855   | 29.792118   |
| Ca | 30.468895   | 32.902168   | 25.865759   |
| Ca | 30.410179   | 27.766647   | 24.773251   |
| Ca | 33.332024   | 29.663622   | 28.738153   |
| Ca | 34.102757   | 24.880356   | 27.292759   |
| Ca | 35.464584   | 28.627542   | 23.921513   |
| S  | 21.031069   | 31.039747   | 35.111137   |
| S  | 21.143267   | 35.771786   | 33.783394   |
| S  | 21.750832   | 31.166214   | 29.541180   |
| S        | 24.933735 | 33.257351 | 33.132114 |
| S        | 26.446682 | 29.433023 | 30.668314 |
| S        | 25.700285 | 33.912888 | 28.485632 |
| S        | 28.304718 | 29.945396 | 26.394199 |
| S        | 30.792477 | 32.136600 | 29.529335 |
| S        | 31.225590 | 26.830750 | 28.022963 |
| S        | 32.830883 | 30.581808 | 25.340052 |
| S        | 33.237968 | 25.736946 | 23.772734 |
| S        | 36.096245 | 27.982368 | 27.359949 |

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generated by VMD

| Ca       | 18.616821 | 33.043602 | 33.538818 |
| Ca       | 22.826515 | 34.032635 | 35.971264 |
| Ca       | 23.656252 | 29.904156 | 33.029938 |
| Ca       | 23.173134 | 34.588242 | 30.923435 |
| Ca       | 25.036251 | 30.781975 | 27.369726 |
| Ca       | 27.910986 | 32.606964 | 31.536297 |
| Ca       | 29.219749 | 29.266203 | 29.617090 |
| Ca       | 30.108154 | 33.014458 | 25.916428 |
| Ca       | 30.444994 | 27.723446 | 24.817209 |
| Ca       | 33.523125 | 29.667271 | 28.480278 |
| Ca       | 33.959103 | 25.241110 | 27.550749 |
| Ca       | 35.257698 | 28.594948 | 23.723686 |
| Ca       | 20.913078 | 30.981422 | 34.993374 |
| S        | 21.044691 | 35.853745 | 33.617950 |
| Ca       | 22.201286 | 31.342878 | 29.847504 |
| S        | 25.024967 | 33.288452 | 33.417542 |
| S        | 26.339874 | 29.457653 | 30.549009 |
| S        | 26.027561 | 33.948273 | 28.639227 |
| S        | 28.241211 | 30.052038 | 26.120089 |
| S        | 30.871456 | 31.887136 | 29.447479 |
| S        | 31.181873 | 26.699999 | 28.057035 |
| S        | 32.787563 | 30.536060 | 25.274788 |
| S        | 33.199547 | 25.526800 | 24.131212 |
| S        | 36.154114 | 28.260538 | 27.369932 |

24

generated by VMD

| Ca       | 18.336861 | 33.329010 | 33.727661 |
| Ca       | 22.979446 | 33.994408 | 36.286282 |
| Ca       | 23.697666 | 30.068796 | 32.931194 |
| Ca       | 22.840141 | 34.444717 | 30.840141 |
| Ca       | 24.964064 | 30.708729 | 27.550177 |
| Ca       | 27.721836 | 32.784279 | 30.957649 |
| Ca       | 29.403168 | 28.913473 | 29.527504 |
| Ca       | 30.214214 | 32.970909 | 25.932850 |
| Ca       | 30.687483 | 27.740406 | 24.733166 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 33.475704 | 29.618858 | 28.834412 |
| Ca      | 34.122433 | 24.933077 | 27.364004 |
| Ca      | 35.245163 | 28.914906 | 23.775562 |
| S       | 20.944853 | 31.227989 | 35.174961 |
| S       | 20.970228 | 35.766548 | 33.697617 |
| S       | 22.107964 | 31.329861 | 29.892532 |
| S       | 25.12496  | 33.320961 | 33.74920 |
| S       | 26.273228 | 29.489914 | 30.529552 |
| S       | 25.693506 | 34.174408 | 28.622364 |
| S       | 28.189959 | 30.028778 | 26.108040 |
| S       | 30.685472 | 31.785202 | 29.324799 |
| S       | 31.309860 | 26.663940 | 28.182814 |
| S       | 32.996635 | 30.512665 | 25.436707 |
| S       | 33.486568 | 25.553455 | 23.885990 |
| S       | 36.249138 | 28.024752 | 27.249142 |

generated by VMD

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 18.680611 | 33.003670 | 33.721157 |
| Ca      | 22.813446 | 34.323692 | 35.918724 |
| Ca      | 23.699825 | 29.745068 | 33.165646 |
| Ca      | 23.425686 | 34.639015 | 30.683744 |
| Ca      | 24.961704 | 30.717918 | 27.603050 |
| Ca      | 27.819366 | 32.722355 | 31.302200 |
| Ca      | 29.241331 | 29.122105 | 29.345697 |
| Ca      | 30.277021 | 32.839302 | 25.813560 |
| Ca      | 30.192242 | 27.66835  | 24.677261 |
| Ca      | 33.369450 | 29.391197 | 28.571327 |
| Ca      | 34.032619 | 25.268297 | 27.451464 |
| Ca      | 35.737041 | 29.028187 | 24.125919 |
| S       | 21.006351 | 31.186981 | 35.166412 |
| S       | 21.130119 | 35.927841 | 33.235630 |
| S       | 22.077415 | 31.276644 | 30.078669 |
| S       | 25.047455 | 33.119820 | 33.460983 |
| S       | 26.290421 | 29.365232 | 30.773951 |
| S       | 25.971611 | 33.936058 | 28.741215 |
| S       | 27.958691 | 29.933229 | 26.130667 |
| S       | 30.826639 | 31.843225 | 29.169889 |
| S       | 31.017086 | 26.667456 | 27.990881 |
| S       | 32.750172 | 30.220993 | 25.166031 |
| S       | 33.460983 | 26.296577 | 23.921127 |
| S       | 36.105789 | 28.065311 | 27.567608 |

generated by VMD

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 18.436588 | 33.271450 | 33.730587 |
| Ca      | 22.997868 | 34.025955 | 35.921768 |
| Ca      | 23.775696 | 29.775278 | 32.665565 |
| Ca   | 22.890417 | 34.521484 | 30.930275 |
|------|-----------|-----------|-----------|
| Ca   | 24.853973 | 30.832645 | 27.577213 |
| Ca   | 27.928303 | 32.526237 | 31.591579 |
| Ca   | 29.380714 | 29.228884 | 29.343895 |
| Ca   | 30.223639 | 32.701252 | 25.702698 |
| Ca   | 30.242731 | 27.727453 | 24.726677 |
| Ca   | 33.498356 | 29.684244 | 28.748667 |
| Ca   | 33.920692 | 25.077072 | 27.431211 |
| Ca   | 35.679173 | 28.782854 | 24.129089 |
| S    | 21.079666 | 31.190825 | 35.064358 |
| S    | 21.020519 | 35.894768 | 33.729839 |
| S    | 21.924526 | 31.123625 | 29.924374 |
| S    | 25.120911 | 33.304955 | 33.230068 |
| S    | 26.529045 | 29.477592 | 30.592354 |
| S    | 25.921387 | 34.073875 | 28.926712 |
| S    | 27.901348 | 29.922585 | 26.143795 |
| S    | 30.824459 | 32.079308 | 29.084499 |
| S    | 31.149574 | 26.850380 | 28.065327 |
| S    | 32.785461 | 30.389309 | 25.188444 |
| S    | 33.493355 | 25.792601 | 23.855124 |
| S    | 36.141640 | 28.045519 | 27.635963 |

24 generated by VMD

| Ca   | 18.500305 | 33.366840 | 33.280167 |
|------|-----------|-----------|-----------|
| Ca   | 22.728153 | 34.337761 | 35.917633 |
| Ca   | 23.649769 | 29.945772 | 33.011436 |
| Ca   | 23.079659 | 34.615128 | 30.663185 |
| Ca   | 25.115650 | 30.692894 | 27.756569 |
| Ca   | 27.935913 | 32.639053 | 31.684961 |
| Ca   | 29.347813 | 29.035429 | 29.731237 |
| Ca   | 30.083681 | 32.633083 | 25.983561 |
| Ca   | 30.261992 | 27.582123 | 24.824863 |
| Ca   | 33.424164 | 29.553812 | 28.532927 |
| Ca   | 34.100197 | 25.174337 | 27.077948 |
| Ca   | 35.647961 | 28.923117 | 23.689968 |
| S    | 20.784168 | 31.431952 | 35.110409 |
| S    | 21.031528 | 35.887405 | 33.449463 |
| S    | 22.042454 | 31.188705 | 29.941477 |
| S    | 25.041283 | 33.064095 | 33.506546 |
| S    | 26.482779 | 29.424118 | 30.832956 |
| S    | 25.998135 | 33.842560 | 28.895969 |
| S    | 28.085489 | 29.654287 | 26.403587 |
| S    | 30.919680 | 31.787598 | 29.458494 |
| S    | 31.159258 | 26.611732 | 28.064964 |
| S    | 32.734261 | 30.556019 | 25.142212 |
| S    | 33.523071 | 25.989086 | 23.725227 |
|  |  |  |  |
|---|---|---|---|
| S  | 36.042637 | 28.363182 | 27.254305 |
| Ca | 18.294733 | 33.088753 | 33.414619 |
| Ca | 22.925106 | 34.256172 | 36.035347 |
| Ca | 23.809250 | 29.982330 | 32.764122 |
| Ca | 23.170275 | 34.554165 | 30.912054 |
| Ca | 24.911739 | 30.961372 | 27.729027 |
| Ca | 27.919933 | 32.759163 | 31.568796 |
| Ca | 29.382980 | 29.043629 | 29.500183 |
| Ca | 30.312111 | 32.917797 | 25.915012 |
| Ca | 30.202072 | 27.622219 | 24.610069 |
| Ca | 33.495407 | 29.630552 | 28.519590 |
| Ca | 34.101963 | 25.367319 | 27.446491 |
| Ca | 35.454338 | 28.497160 | 23.813618 |
| S  | 20.957470 | 31.131332 | 35.052891 |
| S  | 20.820940 | 35.636177 | 33.349030 |
| S  | 22.018467 | 31.286755 | 29.890785 |
| S  | 25.164919 | 33.012432 | 33.487686 |
| S  | 26.473866 | 29.314919 | 30.757385 |
| S  | 26.106352 | 34.138954 | 28.895206 |
| S  | 28.148508 | 30.006290 | 26.263103 |
| S  | 30.776855 | 32.024429 | 29.515289 |
| S  | 31.123627 | 26.812635 | 28.189722 |
| S  | 32.838215 | 30.429308 | 25.071825 |
| S  | 33.174305 | 25.570308 | 23.823187 |
| S  | 36.137558 | 28.255838 | 27.414974 |

generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 18.366215 | 33.036255 | 33.742069 |
| Ca | 22.893162 | 34.291828 | 35.960049 |
| Ca | 23.872869 | 29.994904 | 33.041492 |
| Ca | 22.879955 | 34.545658 | 30.871521 |
| Ca | 24.911192 | 30.746609 | 27.587713 |
| Ca | 27.859818 | 32.779552 | 31.481731 |
| Ca | 29.150478 | 29.315132 | 29.692936 |
| Ca | 30.591398 | 32.931519 | 25.916565 |
| Ca | 30.443325 | 28.036358 | 24.714230 |
| Ca | 33.674946 | 29.360662 | 28.582972 |
| Ca | 33.792629 | 25.051060 | 27.319824 |
| Ca | 35.826954 | 28.579458 | 23.740503 |
| S  | 21.119629 | 31.168831 | 35.144272 |
| S  | 20.655155 | 35.605606 | 33.350811 |
| S  | 22.049055 | 31.126619 | 29.808561 |
| S  | 25.064037 | 33.321770 | 33.541687 |
| S  | 26.325993 | 29.309546 | 30.726984 |
|   |   |   |   |
|---|---|---|---|
| S | 25.716175 | 33.946362 | 28.688654 |
| S | 28.205845 | 30.212297 | 26.234978 |
| S | 30.898630 | 31.890034 | 29.425453 |
| S | 31.118546 | 26.936163 | 28.216881 |
| S | 32.969513 | 30.351479 | 24.904758 |
| S | 33.188271 | 25.911394 | 23.810312 |
| S | 36.146240 | 27.850990 | 27.435068 |

24

generated by VMD

| Ca | 18.368275 | 32.637096 | 33.254913 |
| Ca | 22.752934 | 34.128639 | 36.161037 |
| Ca | 23.547096 | 30.275803 | 32.930595 |
| Ca | 23.123795 | 34.841370 | 30.868923 |
| Ca | 25.040575 | 30.616837 | 27.719584 |
| Ca | 28.095589 | 32.852470 | 31.289761 |
| Ca | 29.403727 | 29.135567 | 29.708084 |
| Ca | 30.477890 | 32.920036 | 26.119884 |
| Ca | 30.513212 | 27.729195 | 24.590530 |
| Ca | 33.515900 | 29.515045 | 28.459795 |
| Ca | 33.964546 | 25.076202 | 27.469284 |
| Ca | 35.492821 | 28.664383 | 23.574730 |
| S | 20.946741 | 31.191816 | 35.380184 |
| S | 20.507908 | 35.565678 | 33.471191 |
| S | 21.944508 | 31.431454 | 30.037294 |
| S | 25.155359 | 33.428207 | 33.312263 |
| S | 26.438637 | 29.361446 | 30.608326 |
| S | 26.011757 | 34.119308 | 28.754984 |
| S | 28.255816 | 30.072498 | 26.249781 |
| S | 31.054028 | 31.887028 | 29.584099 |
| S | 31.056202 | 26.719391 | 28.288118 |
| S | 32.778389 | 30.315226 | 25.089649 |
| S | 33.357399 | 25.718750 | 23.827377 |
| S | 35.916958 | 28.096552 | 27.189653 |

24

generated by VMD

| Ca | 18.564219 | 32.718433 | 33.328770 |
| Ca | 23.118479 | 34.193966 | 36.037575 |
| Ca | 23.686451 | 29.937685 | 32.923088 |
| Ca | 23.263300 | 34.835403 | 30.629581 |
| Ca | 24.980129 | 30.752602 | 27.560226 |
| Ca | 27.825369 | 32.633438 | 31.419161 |
| Ca | 29.352917 | 29.163639 | 29.668667 |
| Ca | 30.414738 | 32.803043 | 25.971699 |
| Ca | 30.217369 | 27.612812 | 24.543333 |
| Ca | 33.374466 | 29.668777 | 28.476248 |
| Ca | 33.775406 | 25.350496 | 27.645397 |
| Ca   | 35.385216 | 28.733206 | 23.996559 |
| S    | 21.127577 | 31.022053 | 35.291214 |
| S    | 20.791941 | 35.598221 | 33.485916 |
| S    | 22.121489 | 31.458981 | 29.856441 |
| S    | 25.044323 | 33.229877 | 33.359299 |
| S    | 26.350548 | 29.312214 | 30.562033 |
| S    | 26.076593 | 34.044266 | 28.696764 |
| S    | 28.287657 | 30.128565 | 26.310059 |
| S    | 31.023321 | 31.914450 | 29.574287 |
| S    | 31.085676 | 26.845158 | 28.142145 |
| S    | 32.631023 | 30.346195 | 25.014793 |
| S    | 33.138721 | 25.878845 | 24.024624 |
| S    | 36.083107 | 28.117777 | 27.422213 |

24 generated by VMD

| Ca   | 18.309444 | 33.132191 | 33.731194 |
| Ca   | 23.190262 | 34.202835 | 36.072968 |
| Ca   | 23.667057 | 29.841581 | 32.943268 |
| Ca   | 23.126202 | 34.597954 | 30.963619 |
| Ca   | 24.949600 | 30.898529 | 27.488909 |
| Ca   | 27.723339 | 32.712852 | 31.108290 |
| Ca   | 29.173029 | 29.216061 | 29.496340 |
| Ca   | 30.484888 | 32.781387 | 25.742237 |
| Ca   | 30.314402 | 27.799223 | 24.627087 |
| Ca   | 33.500404 | 29.698343 | 28.522606 |
| Ca   | 33.986713 | 25.064697 | 27.593861 |
| Ca   | 35.512253 | 28.592731 | 24.128637 |
| S    | 21.103811 | 31.196377 | 35.34532 |
| S    | 20.900391 | 35.623966 | 33.614456 |
| S    | 22.048120 | 31.264076 | 29.848797 |
| S    | 25.073217 | 32.893753 | 33.426651 |
| S    | 26.221823 | 29.345053 | 30.328955 |
| S    | 25.859020 | 34.105312 | 28.603039 |
| S    | 28.172771 | 30.118561 | 26.164089 |
| S    | 30.800371 | 31.912588 | 29.241962 |
| S    | 31.367838 | 26.854824 | 28.041288 |
| S    | 32.822578 | 30.596382 | 25.165554 |
| S    | 33.222363 | 25.896358 | 24.135784 |
| S    | 36.190140 | 27.954422 | 27.605019 |

24 generated by VMD

| Ca   | 18.288836 | 33.252296 | 33.983433 |
| Ca   | 23.184013 | 34.358788 | 35.926708 |
| Ca   | 23.528122 | 29.942162 | 32.810825 |
| Ca   | 22.999868 | 34.528790 | 30.715984 |
| Ca   | 24.867125 | 30.677937 | 27.530722 |
|   |   |   |
|---|---|---|
| Ca | 27.926228 | 32.599571 | 31.533283 |
| Ca | 29.443096 | 29.164146 | 29.579628 |
| Ca | 30.475374 | 32.716469 | 25.813366 |
| Ca | 30.351141 | 27.733250 | 24.674887 |
| Ca | 33.466019 | 29.636261 | 28.757088 |
| Ca | 33.965542 | 24.996086 | 27.233046 |
| Ca | 35.874458 | 28.786398 | 23.928051 |
| S  | 20.989025 | 31.354481 | 35.355244 |
| S  | 20.881615 | 35.624958 | 33.660198 |
| S  | 21.835854 | 31.268143 | 29.824554 |
| S  | 25.049679 | 33.023445 | 33.234074 |
| S  | 26.377598 | 29.342812 | 30.618328 |
| S  | 25.831482 | 34.038460 | 28.616737 |
| S  | 28.128212 | 29.832691 | 26.219254 |
| S  | 30.794548 | 32.007103 | 29.378172 |
| S  | 31.086330 | 26.957348 | 28.058311 |
| S  | 32.930138 | 30.403162 | 25.250793 |
| S  | 33.493912 | 26.046463 | 23.730450 |
| S  | 35.951839 | 28.008902 | 27.506893 |

24

generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.413044 | 33.082439 | 33.692604 |
| Ca | 22.960308 | 34.053070 | 35.961655 |
| Ca | 23.685038 | 29.926325 | 32.868732 |
| Ca | 23.072680 | 34.839649 | 30.878567 |
| Ca | 24.920162 | 30.556328 | 27.611837 |
| Ca | 27.749138 | 32.593346 | 31.300356 |
| Ca | 29.723770 | 29.199633 | 29.452835 |
| Ca | 30.207943 | 32.942795 | 25.759920 |
| Ca | 30.344034 | 27.832565 | 24.773293 |
| Ca | 33.680454 | 29.695242 | 28.764645 |
| Ca | 33.854980 | 25.171951 | 27.288708 |
| Ca | 35.487530 | 28.625156 | 24.037329 |
| S  | 21.152428 | 31.131096 | 35.229179 |
| S  | 20.874428 | 35.805370 | 33.614323 |
| S  | 22.059238 | 31.321327 | 29.837326 |
| S  | 25.019272 | 33.078819 | 33.415428 |
| S  | 26.355246 | 29.521481 | 30.549358 |
| S  | 25.698723 | 33.965317 | 28.547827 |
| S  | 28.211851 | 29.956097 | 26.197828 |
| S  | 30.894302 | 32.048939 | 29.302124 |
| S  | 31.136253 | 26.782513 | 28.144627 |
| S  | 33.089653 | 30.387846 | 25.342703 |
| S  | 33.135712 | 25.873165 | 23.851885 |
| S  | 35.993820 | 27.909502 | 27.516941 |
|   |   |   |
|---|---|---|
| Ca | 547.359104 | 33.045845 | 34.181881 |
| Ca | 22.946350 | 34.113396 | 35.817852 |
| Ca | 23.597775 | 29.762272 | 32.608879 |
| Ca | 23.018723 | 34.836288 | 30.865005 |
| Ca | 27.762396 | 32.816235 | 31.182930 |
| Ca | 29.439003 | 29.110809 | 29.663296 |
| Ca | 30.460350 | 32.821404 | 25.851547 |
| Ca | 30.437782 | 27.35235 | 24.670269 |
| Ca | 33.516304 | 29.961517 | 28.83554 |
| Ca | 33.668388 | 25.135174 | 27.213667 |
| Ca | 35.440514 | 28.460899 | 24.077568 |
| S | 21.091770 | 31.031849 | 35.049274 |
| S | 20.815881 | 35.620090 | 33.657066 |
| S | 22.061642 | 31.353382 | 29.765205 |
| S | 25.068539 | 32.988712 | 33.436546 |
| S | 26.559813 | 29.377853 | 30.367817 |
| S | 25.878736 | 34.132168 | 28.719788 |
| S | 28.319683 | 30.059937 | 26.242540 |
| S | 31.102587 | 32.297672 | 29.320560 |
| S | 31.216705 | 26.978722 | 28.227173 |
| S | 32.844009 | 30.396729 | 25.210285 |
| S | 33.315367 | 25.668209 | 23.89532 |
| S | 33.012526 | 27.860054 | 27.544485 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.237583 | 32.784645 | 34.293125 |
| Ca | 23.092653 | 34.307968 | 35.852859 |
| Ca | 23.665207 | 30.224167 | 32.626465 |
| Ca | 22.911062 | 34.333939 | 30.938189 |
| Ca | 25.069666 | 30.915638 | 27.539867 |
| Ca | 28.014351 | 33.010872 | 31.217113 |
| Ca | 29.425758 | 29.222269 | 29.674778 |
| Ca | 30.569632 | 32.862991 | 25.820374 |
| Ca | 30.479145 | 27.733505 | 24.544182 |
| Ca | 33.282536 | 29.650923 | 28.755207 |
| Ca | 33.627792 | 25.000357 | 27.137163 |
| Ca | 35.772274 | 28.519276 | 24.257351 |
| S | 21.241016 | 31.040836 | 35.149803 |
| S | 20.864925 | 35.355026 | 33.645618 |
| S | 21.998531 | 31.263420 | 29.558720 |
| S | 24.984812 | 32.916763 | 33.236534 |
| S | 26.527031 | 29.677155 | 30.551970 |
| S | 25.675579 | 34.298634 | 28.632210 |
| S | 28.328491 | 30.016705 | 26.310324 |
|   |      |      |      |
|---|------|------|------|
| S | 30.982018 | 32.283077 | 29.337847 |
| S | 31.052925 | 26.872564 | 28.248686 |
| S | 32.831833 | 30.430336 | 25.149227 |
| S | 33.259285 | 25.890600 | 23.806435 |
| S | 35.825897 | 27.688410 | 27.656025 |

24 generated by VMD

| Ca |      |      |      |
|----|------|------|------|
| Ca | 18.204973 | 32.676048 | 33.999130 |
| Ca | 23.078533 | 34.296906 | 35.719585 |
| Ca | 23.750755 | 30.425423 | 32.832745 |
| Ca | 22.832375 | 34.223686 | 30.842770 |
| Ca | 24.996777 | 31.006371 | 27.543913 |
| Ca | 28.036060 | 32.899296 | 31.301701 |
| Ca | 29.362362 | 29.114410 | 29.487043 |
| Ca | 30.676556 | 32.914757 | 25.938793 |
| Ca | 30.346119 | 27.728220 | 24.613523 |
| Ca | 33.331238 | 29.898396 | 28.749065 |
| Ca | 33.448982 | 24.961819 | 27.047562 |
| Ca | 35.711639 | 28.556337 | 24.293068 |
| S  | 21.315357 | 31.197044 | 35.452831 |
| S  | 20.638599 | 35.153008 | 33.367729 |
| S  | 22.023224 | 31.109436 | 29.709223 |
| S  | 25.221024 | 33.043335 | 33.295277 |
| S  | 26.471201 | 29.758217 | 30.634605 |
| S  | 25.870388 | 34.220222 | 28.735106 |
| S  | 28.250568 | 30.212410 | 26.317923 |
| S  | 31.171335 | 32.137962 | 29.350462 |
| S  | 30.990820 | 26.878752 | 28.054226 |
| S  | 32.876968 | 30.352789 | 25.082422 |
| S  | 33.258522 | 25.943150 | 23.806046 |
| S  | 35.855633 | 27.591991 | 27.765345 |

24 generated by VMD

| Ca |      |      |      |
|----|------|------|------|
| Ca | 18.355869 | 32.692940 | 34.091122 |
| Ca | 23.059469 | 34.604332 | 35.779629 |
| Ca | 23.612309 | 30.389790 | 32.821030 |
| Ca | 22.945415 | 34.311295 | 30.750847 |
| Ca | 25.010698 | 30.850666 | 27.753187 |
| Ca | 28.000103 | 33.047356 | 31.476303 |
| Ca | 29.494120 | 28.842579 | 29.429955 |
| Ca | 30.469917 | 32.877113 | 25.987595 |
| Ca | 30.397141 | 27.815742 | 24.525286 |
| Ca | 33.479584 | 29.686169 | 28.743572 |
| Ca | 33.618664 | 24.615589 | 26.937710 |
| Ca | 35.701302 | 28.794565 | 24.343433 |
| S  | 21.347252 | 31.353922 | 35.506596 |
|   | S       | Ca       |
|---|---------|----------|
|   | 20.541767 | 35.171074 | 33.267876 |
|   | 21.817442 | 31.104942 | 29.631874 |
|   | 24.900646 | 33.109673 | 31.97350  |
|   | 26.446777 | 29.716927 | 30.731730 |
|   | 28.874552 | 34.254395 | 28.704281 |
| S | 28.354530 | 30.028385 | 26.310049 |
|   | 31.073528 | 32.077305 | 29.490814 |
|   | 31.248943 | 26.727760 | 27.888325 |
| S | 32.775677 | 30.539030 | 25.245478 |
|   | 33.202419 | 26.092041 | 23.667812 |
| S | 35.991901 | 27.596498 | 27.658199 |

24

generated by VMD

|   | Ca       | S       |
|---|----------|---------|
|   | 18.421307 | 32.09689 |
| Ca| 23.148617 | 35.742126|
| Ca| 23.572401 | 32.744129|
| Ca| 22.876617 | 30.857134|
| Ca| 25.005905 | 27.828884|
| Ca| 27.757446 | 31.304201|
| Ca| 29.473408 | 29.653465|
| Ca| 32.522720 | 26.227100|
| Ca| 30.463297 | 24.619313|
| Ca| 33.578323 | 28.410660|
| Ca| 33.821693 | 27.070301|
| Ca| 35.518978 | 24.054657|
| S | 21.190022 | 35.287788|
| S | 20.683334 | 33.269028|
| S | 21.970144 | 29.810417|
| S | 25.028580 | 33.298298|
| S | 26.450916 | 30.813211|
| S | 25.949413 | 28.679247|
| S | 28.205288 | 26.356680|
| S | 30.898827 | 29.669783|
| S | 31.159193 | 28.182121|
| S | 32.907829 | 25.186474|
| S | 33.178650 | 23.571697|
| S | 35.937134 | 27.643776|

24

generated by VMD

|   | Ca       | S       | Ca       | S       |
|---|----------|---------|----------|---------|
|   | 18.063103| 32.657162| 33.756840|
| Ca| 22.814850| 33.965157| 35.742226|
| Ca| 23.417530| 30.151768| 32.745544|
| Ca| 22.684153| 34.984219| 31.048683|
| Ca| 25.082306| 31.040176| 27.937952|
| Ca| 28.019466| 32.892696| 31.338633|
| Ca| 29.547733| 29.090731| 29.737507|
| Element | Ca1 | Ca2 | Ca3 | Ca4 |
|---------|-----|-----|-----|-----|
| Ca      | 30.773108 | 30.195475 | 34.011669 | 35.775238 |
|         | 32.480762 | 27.595327 | 24.861610 | 28.360632 |
|         | 25.810490 | 24.730995 | 27.213493 | 23.834087 |

| Element | S1 | S2 | S3 | S4 |
|---------|----|----|----|----|
| S       | 20.825048 | 20.486435 | 21.921413 | 24.889425 |
|         | 30.937193 | 35.489983 | 31.548899 | 33.495274 |
|         | 35.113335 | 33.548187 | 30.000538 | 33.290138 |

24

generated by VMD

| Element | Ca1 | Ca2 | Ca3 | Ca4 |
|---------|-----|-----|-----|-----|
| Ca      | 18.639870 | 22.845211 | 23.565022 | 23.009319 |
|         | 32.561440 | 34.219193 | 29.873446 | 34.674744 |
|         | 33.813091 | 35.675655 | 32.615227 | 30.881186 |

| Element | S1 | S2 | S3 | S4 |
|---------|----|----|----|----|
| S       | 21.199606 | 24.942516 | 23.912296 | 29.91047 |
|         | 30.979282 | 32.910645 | 32.149422 | 31.440147 |
|         | 29.796245 | 29.410645 | 30.311165 | 32.796650 |
|         | 29.373000 | 29.981243 | 29.960243 | 25.831512 |

24

generated by VMD

| Element | Ca1 | Ca2 | Ca3 | Ca4 |
|---------|-----|-----|-----|-----|
| Ca      | 18.465992 | 22.845211 | 23.565022 | 23.009319 |
|         | 32.440132 | 34.219193 | 29.873446 | 34.674744 |

24

generated by VMD
| Element | X1      | Y1      | Z1      |
|---------|---------|---------|---------|
| Ca      | 22.841515 | 34.136127 | 36.078751 |
| Ca      | 23.393414 | 30.162312 | 32.621773 |
| Ca      | 23.236031 | 34.780304 | 30.980227 |
| Ca      | 25.087227 | 31.158472 | 27.573597 |
| Ca      | 28.026476 | 32.740402 | 31.695107 |
| Ca      | 29.224337 | 29.409966 | 29.555620 |
| Ca      | 30.488428 | 32.599533 | 25.522331 |
| Ca      | 33.561287 | 29.791718 | 28.408646 |
| Ca      | 33.625038 | 25.199640 | 27.475243 |
| Ca      | 35.471478 | 28.447224 | 24.131588 |
| S       | 21.081673 | 30.974150 | 35.242950 |
| S       | 20.591684 | 35.432739 | 33.471542 |
| S       | 22.059986 | 31.628740 | 29.727562 |
| S       | 25.078308 | 33.208847 | 33.430088 |
| S       | 26.474628 | 29.580410 | 30.622166 |
| S       | 26.104828 | 34.295425 | 28.850359 |
| S       | 28.132509 | 29.870846 | 26.125681 |
| S       | 30.800915 | 32.032150 | 29.261761 |
| S       | 31.298559 | 26.916559 | 28.096048 |
| S       | 32.721935 | 30.291561 | 25.068907 |
| S       | 33.364376 | 25.616022 | 24.014050 |
| S       | 36.206730 | 28.080736 | 27.427950 |

24 generated by VMD

| Element | X1      | Y1      | Z1      |
|---------|---------|---------|---------|
| Ca      | 18.735455 | 32.310356 | 33.872379 |
| Ca      | 23.128159 | 33.651039 | 36.046043 |
| Ca      | 23.649147 | 30.292421 | 32.486710 |
| Ca      | 23.165974 | 35.073830 | 30.869928 |
| Ca      | 24.853914 | 30.961622 | 27.501440 |
| Ca      | 28.055130 | 32.907288 | 31.101486 |
| Ca      | 29.389534 | 29.084154 | 29.489454 |
| Ca      | 30.55157  | 32.917519 | 25.511957 |
| Ca      | 30.199480 | 27.533230 | 24.833197 |
| Ca      | 33.242371 | 29.869469 | 28.842369 |
| Ca      | 33.852764 | 24.636890 | 27.462208 |
| Ca      | 35.445660 | 28.765015 | 24.410282 |
| S       | 21.333813 | 30.495926 | 35.173996 |
| S       | 20.850822 | 35.243031 | 33.651146 |
| S       | 22.048672 | 31.782612 | 29.744537 |
| S       | 25.256573 | 33.494019 | 33.290939 |
| S       | 26.541573 | 29.850021 | 30.349783 |
| S       | 25.890789 | 34.368111 | 28.488113 |
| S       | 27.914791 | 29.947342 | 26.326380 |
| S       | 31.060644 | 32.374180 | 29.080246 |
| S       | 31.213289 | 27.022738 | 28.296358 |
|   |   |   |   |
|---|---|---|---|
| S | 32.598957 | 30.266329 | 25.166622 |
| S | 33.341518 | 25.870153 | 24.027826 |
| S | 35.895847 | 27.582685 | 27.916626 |

24

generated by VMD

| Ca | 18.817898 | 32.471397 | 33.900440 |
| Ca | 23.104033 | 33.905563 | 36.044125 |
| Ca | 23.631479 | 29.890394 | 32.553196 |
| Ca | 22.679472 | 34.741829 | 30.657980 |
| Ca | 24.918083 | 31.054831 | 27.530931 |
| Ca | 27.799032 | 32.959316 | 31.332466 |
| Ca | 29.553473 | 29.549385 | 29.446388 |
| Ca | 30.380062 | 32.871498 | 25.623388 |
| Ca | 30.294376 | 27.798435 | 24.844397 |
| Ca | 33.652821 | 29.988432 | 28.497328 |
| Ca | 33.479393 | 24.619244 | 27.477224 |
| Ca | 35.663776 | 28.470892 | 24.477373 |
| S | 21.475285 | 30.748409 | 35.289040 |
| S | 20.928375 | 35.391403 | 33.834675 |
| S | 22.074394 | 31.491503 | 29.655863 |
| S | 24.860416 | 33.096981 | 32.226997 |
| S | 26.477449 | 29.659815 | 30.522709 |
| S | 25.914305 | 34.410637 | 28.619558 |
| S | 28.094555 | 30.172150 | 26.033487 |
| S | 30.958717 | 32.303112 | 29.140018 |
| S | 31.086447 | 27.133499 | 28.285995 |
| S | 32.873306 | 30.369289 | 24.979727 |
| S | 33.180302 | 25.766008 | 24.053406 |
| S | 35.862640 | 27.436005 | 27.912962 |

24

generated by VMD

| Ca | 18.436552 | 32.764820 | 34.320057 |
| Ca | 23.027035 | 33.941490 | 35.954437 |
| Ca | 23.579084 | 29.936642 | 32.608593 |
| Ca | 23.060163 | 34.788208 | 31.005493 |
| Ca | 24.806499 | 31.107634 | 27.477919 |
| Ca | 27.836279 | 32.831284 | 31.218397 |
| Ca | 29.284292 | 29.444124 | 29.264927 |
| Ca | 30.532446 | 32.851051 | 25.557867 |
| Ca | 30.338602 | 27.650909 | 24.537411 |
| Ca | 33.581329 | 29.815218 | 28.379738 |
| Ca | 33.906284 | 24.725080 | 27.674950 |
| Ca | 35.665997 | 28.692303 | 24.618486 |
| S | 21.186962 | 30.787867 | 35.322051 |
| S | 20.754002 | 35.398224 | 33.875076 |
| S | 21.975292 | 31.449100 | 29.734306 |
|     | 25.226185 | 33.270237 | 33.326099 |
|-----|-----------|-----------|-----------|
| S   | 26.408081 | 29.652575 | 30.342171 |
| S   | 25.793804 | 34.325588 | 28.645645 |
| S   | 28.142963 | 30.050823 | 25.871759 |
| S   | 30.626499 | 32.354202 | 29.112103 |
| S   | 31.189392 | 26.967756 | 28.085304 |
| S   | 32.810562 | 30.171350 | 24.986618 |
| S   | 33.418392 | 25.800446 | 24.118147 |
| S   | 36.133396 | 27.523129 | 27.902382 |

|     | 24 generated by VMD |
|-----|---------------------|
| Ca  | 18.306068 32.640289 34.049400 |
| Ca  | 22.982666 34.308220 36.000084 |
| Ca  | 23.668465 30.000973 32.789860 |
| Ca  | 24.429191 34.542870 30.830755 |
| Ca  | 24.857462 31.147955 27.438641 |
| Ca  | 27.864342 33.041103 31.259142 |
| Ca  | 29.255913 29.364315 29.488440 |
| Ca  | 30.513332 32.852264 25.770000 |
| Ca  | 30.586990 27.833727 24.736671 |
| Ca  | 33.472275 29.766432 28.550148 |
| Ca  | 33.709541 24.545620 27.218630 |
| Ca  | 35.685284 28.641172 24.280981 |
| S   | 21.202122 31.012579 35.566483 |
| S   | 20.675473 35.416458 33.716919 |
| S   | 22.018341 31.392853 29.845671 |
| S   | 25.014027 33.090919 33.274235 |
| S   | 26.409159 29.626293 30.473206 |
| S   | 25.796173 34.228859 28.536922 |
| S   | 28.132740 30.087500 26.127983 |
| S   | 30.840599 32.133926 29.183441 |
| S   | 31.380962 26.926191 28.230692 |
| S   | 32.890011 30.522356 24.979343 |
| S   | 33.510422 25.787127 23.849594 |
| S   | 36.045319 27.390028 27.742832 |

|     | 24 generated by VMD |
|-----|---------------------|
| Ca  | 18.508659 32.491234 33.859875 |
| Ca  | 22.813677 34.243332 35.779003 |
| Ca  | 23.592831 29.945398 32.755302 |
| Ca  | 22.962879 34.682777 30.764309 |
| Ca  | 25.160484 31.011820 27.588665 |
| Ca  | 28.023058 32.702911 31.509251 |
| Ca  | 29.346298 29.332983 29.445168 |
| Ca  | 30.528448 32.805161 25.959705 |
| Ca  | 30.214790 27.786350 24.857252 |
|   |   |   |   |
|---|---|---|---|
| Ca | 33.713402 | 24.788544 | 27.502726 |
| Ca | 35.250347 | 28.607090 | 24.094410 |
| S  | 21.147446 | 30.989464 | 35.434280 |
| S  | 20.462111 | 35.367432 | 33.266209 |
| S  | 22.230160 | 31.271366 | 29.725653 |
| S  | 25.119583 | 33.200058 | 33.425514 |
| S  | 26.471100 | 29.478334 | 30.678539 |
| S  | 26.262062 | 34.373611 | 28.687189 |
| S  | 28.179522 | 30.265343 | 26.150196 |
| S  | 30.957050 | 32.106617 | 29.291094 |
| S  | 31.265209 | 27.196558 | 28.199219 |
| S  | 32.795120 | 30.510622 | 25.020779 |
| S  | 32.859985 | 25.906042 | 24.010695 |
| S  | 36.084011 | 27.385204 | 27.589905 |

24

generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 18.590656 | 32.881630 | 33.360783 |
| Ca | 22.908932 | 34.511532 | 35.635517 |
| Ca | 23.749210 | 29.716862 | 33.115261 |
| Ca | 22.903412 | 34.500191 | 30.727661 |
| Ca | 25.124054 | 31.061832 | 27.802547 |
| Ca | 27.980591 | 32.483059 | 31.497627 |
| Ca | 29.218271 | 29.206175 | 29.712559 |
| Ca | 30.274986 | 32.827209 | 25.794651 |
| Ca | 30.346672 | 27.929914 | 24.575985 |
| Ca | 33.576584 | 29.859518 | 28.418533 |
| Ca | 33.668419 | 24.838318 | 27.277599 |
| Ca | 35.549282 | 28.966309 | 24.266710 |
| S  | 21.186239 | 31.338806 | 35.296043 |
| S  | 20.807751 | 35.716484 | 33.146721 |
| S  | 22.107306 | 31.14738 | 30.133066 |
| S  | 25.120064 | 32.955536 | 33.490273 |
| S  | 26.443771 | 29.443207 | 30.880486 |
| S  | 26.058960 | 33.977947 | 28.889244 |
| S  | 28.039108 | 29.910648 | 26.278290 |
| S  | 30.753551 | 31.832369 | 29.264200 |
| S  | 31.254082 | 27.034246 | 28.024244 |
| S  | 32.781853 | 30.558727 | 24.967546 |
| S  | 33.383636 | 26.099880 | 23.712101 |
| S  | 35.892677 | 27.534945 | 27.672422 |

24

generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 18.741863 | 32.825745 | 33.536861 |
| Ca | 22.870777 | 34.696632 | 35.758965 |
| Ca | 23.662949 | 29.744251 | 32.754890 |
|    | 555 | 42x745 | 200x745 | 34x730 | 27.786976 | 32.634468 | 31.365170 |
|----|-----|-------|---------|--------|-----------|-----------|-----------|
| Ca | 22.872486 | 34.591179 | 30.689156 | Ca | 24.945189 | 30.741016 | 27.703375 |
| Ca | 30.367371 | 27.852131 | 24.867847 | Ca | 33.524582 | 29.621164 | 28.508938 |
| Ca | 33.751465 | 24.908997 | 27.133408 | Ca | 35.625175 | 28.875273 | 24.150326 |
| S  | 21.351032 | 31.197712 | 35.370094 | S  | 20.769512 | 35.712284 | 33.423023 |
| S  | 21.975510 | 31.351847 | 30.026840 | S  | 25.044550 | 33.061615 | 33.226555 |
| S  | 26.403011 | 29.211605 | 30.757256 | S  | 25.867777 | 34.042145 | 28.737213 |
| S  | 28.059776 | 30.057608 | 26.415596 | S  | 30.938835 | 31.845613 | 29.404634 |
| S  | 31.273121 | 26.871773 | 28.083794 | S  | 32.848396 | 30.532831 | 25.213768 |
| S  | 33.182362 | 26.176672 | 23.755224 | S  | 36.171425 | 27.661367 | 27.485073 |

Ca 18.494322 33.210136 33.817020
Ca 23.059628 34.455276 35.795361
Ca 23.650558 30.020151 32.879929
Ca 22.989159 34.635212 30.771889
Ca 24.808117 30.689974 27.506107
Ca 27.631786 32.489784 31.416603
Ca 29.306038 29.161171 29.652063
Ca 30.111988 32.626770 26.009720
Ca 30.517498 27.773731 24.831291
Ca 33.613579 29.886841 28.753267
Ca 33.783321 24.960318 27.161179
Ca 35.613075 28.921911 24.015562
S  21.225018 31.211451 35.278545
S  20.896858 35.759464 33.451317
S  22.078325 31.228767 29.888483
S  25.069685 33.181019 33.368584
S  26.316374 29.194582 30.521381
S  25.743414 33.973240 28.601000
S  28.186119 29.808094 26.247566
S  30.741009 31.845264 29.535879
S  31.503857 26.902889 28.195517
S  32.940681 30.533684 25.326815
S  33.186615 26.141142 23.512550

24 generated by VMD
|  |  |  |  |
|---|---|---|---|
| S | 36.253067 | 27.689104 | 27.402420 |
| 24 | | | |
| generated by VMD | | | |
| Ca | 18.460632 | 32.840118 | 33.658096 |
| Ca | 22.767868 | 34.169075 | 35.871529 |
| Ca | 23.831905 | 29.971220 | 32.732109 |
| Ca | 23.239929 | 34.780495 | 30.929821 |
| Ca | 24.721626 | 30.811531 | 27.497215 |
| Ca | 27.784639 | 32.778992 | 31.813955 |
| Ca | 29.386615 | 29.533096 | 29.659592 |
| Ca | 30.393270 | 32.821831 | 25.752266 |
| Ca | 30.356907 | 27.760065 | 24.702440 |
| Ca | 33.817417 | 29.693155 | 28.553112 |
| Ca | 33.739788 | 24.788380 | 27.554794 |
| Ca | 35.267567 | 28.716158 | 23.926329 |
| S | 21.331413 | 30.867081 | 34.933697 |
| S | 20.723850 | 35.715851 | 33.460644 |
| S | 22.053200 | 31.369520 | 29.834949 |
| S | 24.885590 | 33.236610 | 33.490376 |
| S | 26.443390 | 29.389145 | 30.437696 |
| S | 25.947086 | 33.862328 | 28.788992 |
| S | 28.221394 | 30.010254 | 26.237015 |
| S | 30.879663 | 32.120338 | 29.431641 |
| S | 31.427322 | 27.067911 | 28.314497 |
| S | 32.847198 | 30.438240 | 25.129890 |
| S | 33.010014 | 25.874718 | 23.977184 |
| S | 36.179771 | 27.683929 | 27.252165 |

|  |  |  |  |
|---|---|---|---|
| generated by VMD | | | |
| Ca | 18.338394 | 32.626064 | 33.446152 |
| Ca | 22.818552 | 34.172176 | 35.920643 |
| Ca | 23.512699 | 30.085152 | 32.880066 |
| Ca | 23.091175 | 34.854504 | 30.596706 |
| Ca | 25.047853 | 30.877827 | 27.729156 |
| Ca | 27.917976 | 32.694016 | 31.571182 |
| Ca | 29.566078 | 29.183067 | 29.715595 |
| Ca | 30.281334 | 32.909912 | 25.979929 |
| Ca | 30.503281 | 27.862907 | 24.792248 |
| Ca | 33.664932 | 29.650499 | 28.504705 |
| Ca | 33.706928 | 24.802336 | 27.234085 |
| Ca | 35.443474 | 28.905020 | 23.724522 |
| S | 21.047478 | 31.208191 | 35.324177 |
| S | 20.705158 | 35.592739 | 33.320919 |
| S | 22.094570 | 31.274574 | 30.050385 |
| S | 25.012747 | 33.327156 | 33.293903 |
| S | 26.521946 | 29.570908 | 30.835712 |
|   |   |   |   |
|---|---|---|---|
| S | 26.018585 | 34.029671 | 28.701466 |
| S | 28.138466 | 29.934078 | 26.337729 |
| S | 30.906307 | 31.914766 | 29.542116 |
| S | 31.321060 | 26.853733 | 28.283512 |
| S | 32.730782 | 30.531296 | 25.134178 |
| S | 33.246593 | 25.805075 | 23.858540 |
| S | 36.083591 | 27.634338 | 27.162390 |

24 generated by VMD

| Ca | 18.340551 | 32.775879 | 33.176308 |
| Ca | 22.760986 | 34.030796 | 36.054821 |
| Ca | 23.319447 | 29.949102 | 32.919235 |
| Ca | 23.057056 | 34.680130 | 30.877148 |
| Ca | 25.081690 | 31.205330 | 27.609989 |
| Ca | 28.019844 | 32.785046 | 31.605268 |
| Ca | 29.249313 | 29.383823 | 29.795132 |
| Ca | 30.388470 | 32.759468 | 25.889708 |
| Ca | 30.421181 | 27.616655 | 24.952740 |
| Ca | 33.765942 | 29.682388 | 28.295286 |
| Ca | 34.030090 | 24.871838 | 27.585348 |
| Ca | 35.332596 | 28.464630 | 23.365181 |
| S | 20.700743 | 31.091843 | 35.339531 |
| S | 20.726143 | 35.556454 | 33.452995 |
| S | 22.056974 | 31.501217 | 29.761770 |
| S | 24.933413 | 33.201828 | 33.572998 |
| S | 26.320637 | 29.543140 | 30.648170 |
| S | 26.192139 | 34.149284 | 29.063766 |
| S | 28.309214 | 30.031096 | 26.351955 |
| S | 31.261829 | 32.016312 | 29.457993 |
| S | 31.473511 | 26.970478 | 28.336723 |
| S | 32.538315 | 30.360266 | 24.706205 |
| S | 33.336494 | 25.679052 | 24.158054 |
| S | 36.103439 | 27.994009 | 26.963753 |

24 generated by VMD

| Ca | 18.530704 | 32.824760 | 33.142998 |
| Ca | 22.726765 | 33.995663 | 36.159439 |
| Ca | 23.523207 | 30.098658 | 32.866653 |
| Ca | 23.057068 | 34.794090 | 30.803522 |
| Ca | 24.950285 | 30.831297 | 27.585293 |
| Ca | 27.888241 | 32.699417 | 31.606707 |
| Ca | 29.279718 | 29.214445 | 29.688534 |
| Ca | 30.352600 | 32.796257 | 25.715176 |
| Ca | 30.385197 | 27.530418 | 24.897060 |
| Ca | 33.795734 | 29.793226 | 28.366589 |
| Ca | 33.966049 | 24.979937 | 27.504456 |
| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 35.368607| 28.847893| 23.719610|
| S       | 20.94898 | 31.127472| 35.263691|
| S       | 20.967758| 35.72192 | 33.619024|
| S       | 22.144989| 31.521667| 29.610437|
| S       | 25.078529| 33.31341 | 33.623783|
| S       | 26.214363| 29.487467| 30.739515|
| S       | 26.002872| 34.069519| 28.800482|
| S       | 28.169170| 29.803911| 26.485764|
| S       | 30.768597| 31.806278| 29.360762|
| S       | 31.469036| 26.891081| 28.314535|
| S       | 32.560806| 30.38477 | 24.954546|
| S       | 33.302433| 25.854492| 23.987558|
| S       | 36.268501| 27.885035| 27.127083|

24 generated by VMD

| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 18.503986| 32.846973| 33.285347|
| Ca      | 22.952084| 34.126427| 35.972061|
| Ca      | 23.311417| 30.033365| 32.902882|
| Ca      | 23.172619| 34.856270| 31.083532|
| Ca      | 24.952045| 30.996586| 27.605602|
| Ca      | 27.845409| 32.723770| 31.576775|
| Ca      | 29.416750| 29.116760| 29.683601|
| Ca      | 30.186821| 32.575809| 25.832422|
| Ca      | 30.485373| 27.577547| 24.819820|
| Ca      | 33.673340| 29.726456| 28.332200|
| Ca      | 34.008938| 24.962908| 27.520716|
| Ca      | 35.762428| 28.754513| 23.580122|
| S       | 20.827343| 31.250471| 35.380020|
| S       | 20.693493| 35.708725| 33.608673|
| S       | 22.073353| 31.440496| 29.797373|
| S       | 24.941059| 33.386337| 33.469833|
| S       | 26.167969| 29.329994| 30.567272|
| S       | 26.132305| 34.073830| 29.019978|
| S       | 28.208012| 29.649618| 26.260326|
| S       | 30.832863| 31.922886| 29.396776|
| S       | 31.213203| 26.923834| 28.324478|
| S       | 32.685490| 30.393682| 24.803877|
| S       | 33.521202| 25.923279| 24.012697|
| S       | 36.147156| 27.999510| 27.102699|

24 generated by VMD

| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 18.692015| 33.105350| 33.180313|
| Ca      | 23.206001| 34.132378| 36.185925|
| Ca      | 23.724287| 29.925789| 32.722538|
| Ca      | 23.271755| 34.616749| 30.918507|
| Ca      | 24.881161| 30.759497| 27.449781|
| Element | Value1   | Value2   | Value3   |
|---------|----------|----------|----------|
| Ca      | 27.591698| 32.553047| 31.411495|
| Ca      | 29.379025| 29.315479| 29.460678|
| Ca      | 30.051039| 32.761909| 25.738556|
| Ca      | 30.272243| 27.714554| 24.976236|
| Ca      | 33.563244| 29.716433| 28.495052|
| Ca      | 33.867191| 25.279524| 27.551888|
| Ca      | 35.666901| 28.831581| 23.988937|
| S       | 20.976536| 31.280123| 35.325359|
| S       | 21.089670| 35.574791| 33.757919|
| S       | 22.303707| 31.474096| 29.795818|
| S       | 25.242373| 32.867165| 33.460590|
| S       | 26.172228| 29.268541| 30.399693|
| S       | 26.067730| 33.883583| 28.674469|
| S       | 27.961433| 29.890747| 26.167093|
| S       | 30.626762| 32.025826| 29.152531|
| S       | 31.124832| 27.171360| 28.217476|
| S       | 32.637054| 30.201448| 25.154821|
| S       | 33.298676| 25.874168| 24.204563|
| S       | 36.052509| 28.075819| 27.549770|

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generated by VMD

| Element | Value1   | Value2   | Value3   |
|---------|----------|----------|----------|
| Ca      | 18.574001| 33.381470| 33.434998|
| Ca      | 22.900120| 33.719402| 36.201611|
| Ca      | 23.767204| 30.333107| 32.687634|
| Ca      | 23.248465| 34.820545| 30.812447|
| Ca      | 24.903458| 30.741272| 27.534231|
| Ca      | 27.694538| 32.381714| 31.402233|
| Ca      | 29.247341| 29.010679| 29.623375|
| Ca      | 29.944725| 32.686462| 25.881327|
| Ca      | 30.397057| 27.427092| 25.014416|
| Ca      | 33.574287| 29.703100| 28.452251|
| Ca      | 34.312237| 25.169102| 27.489134|
| Ca      | 35.108765| 29.087891| 23.883160|
| S       | 21.111876| 31.241217| 35.087669|
| S       | 21.114258| 35.641808| 33.623562|
| S       | 22.164061| 31.785824| 29.661472|
| S       | 25.274290| 33.074677| 33.237686|
| S       | 26.184040| 29.188040| 30.539143|
| S       | 26.024061| 33.937996| 28.639967|
| S       | 27.963213| 29.658634| 26.300592|
| S       | 30.715912| 31.774002| 29.460096|
| S       | 31.419640| 26.933506| 28.353502|
| S       | 32.489853| 30.363745| 25.299355|
| S       | 33.362732| 25.919985| 24.002542|
| S       | 36.223953| 28.318758| 27.317629|
| Element | X Position  | Y Position  | Z Position  |
|---------|-------------|-------------|-------------|
| Ca      | 18.578918   | 33.565697   | 33.399193   |
| Ca      | 23.116476   | 33.853836   | 36.210323   |
| Ca      | 23.847744   | 29.924061   | 32.481102   |
| Ca      | 22.975277   | 34.719002   | 31.164459   |
| Ca      | 24.773195   | 30.919653   | 27.486572   |
| Ca      | 27.580744   | 32.442139   | 31.291664   |
| Ca      | 29.476971   | 28.953888   | 29.588280   |
| Ca      | 30.075428   | 32.582092   | 25.951893   |
| Ca      | 30.205528   | 27.358566   | 25.027418   |
| Ca      | 33.644917   | 29.815178   | 28.528728   |
| Ca      | 34.274208   | 25.327618   | 27.848499   |
| Ca      | 35.245113   | 28.922514   | 23.829662   |
| S       | 21.069965   | 31.335203   | 34.714870   |
| S       | 21.066090   | 35.835457   | 33.886192   |
| S       | 22.062458   | 31.479607   | 29.784973   |
| S       | 25.139774   | 32.951275   | 33.513634   |
| S       | 26.080044   | 29.234270   | 30.129440   |
| S       | 25.922684   | 34.279022   | 28.907242   |
| S       | 28.096430   | 29.860619   | 26.109192   |
| Element | X Coordinate | Y Coordinate | Z Coordinate |
|---------|--------------|--------------|--------------|
| S       | 30.708183    | 31.732233    | 29.417622    |
| S       | 31.452848    | 26.741539    | 28.304211    |
| S       | 32.522270    | 30.229937    | 24.949865    |
| S       | 33.385006    | 25.770578    | 24.234886    |
| S       | 36.419754    | 28.466076    | 27.180138    |

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generated by VMD

| Element | X Coordinate | Y Coordinate | Z Coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.730118    | 33.161438    | 33.404148    |
| Ca      | 23.128193    | 33.746311    | 36.068329    |
| Ca      | 23.681374    | 29.692440    | 32.646179    |
| Ca      | 22.929119    | 34.709518    | 30.857143    |
| Ca      | 25.017330    | 31.114641    | 27.412683    |
| Ca      | 27.643335    | 32.796021    | 31.215075    |
| Ca      | 29.477570    | 29.193918    | 29.515251    |
| Ca      | 30.165142    | 32.942005    | 25.853388    |
| Ca      | 30.030087    | 27.654202    | 25.208494    |
| Ca      | 33.630035    | 29.486914    | 28.433029    |
| Ca      | 34.039551    | 25.177654    | 27.822681    |
| Ca      | 35.291012    | 28.648172    | 23.771122    |
| S       | 21.131710    | 30.830551    | 35.006775    |
| S       | 21.120350    | 35.645065    | 33.940136    |
| S       | 22.210058    | 31.447283    | 29.677078    |
| S       | 25.031368    | 33.192215    | 33.420177    |
| S       | 26.255562    | 29.489645    | 30.238916    |
| S       | 25.829365    | 34.419853    | 28.688719    |
| S       | 28.196918    | 30.028004    | 26.050608    |
| S       | 30.869530    | 31.865646    | 29.340834    |
| S       | 31.378613    | 26.803387    | 28.583611    |
| S       | 32.549679    | 30.371742    | 25.100704    |
| S       | 33.202927    | 25.715025    | 24.524454    |
| S       | 36.181099    | 28.168476    | 27.160540    |

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generated by VMD

| Element | X Coordinate | Y Coordinate | Z Coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 18.305099    | 33.025352    | 33.232822    |
| Ca      | 22.630600    | 34.020115    | 35.973129    |
| Ca      | 23.582287    | 29.986538    | 32.746742    |
| Ca      | 22.978455    | 34.700066    | 30.834415    |
| Ca      | 25.165348    | 31.048233    | 27.834864    |
| Ca      | 28.006348    | 32.720074    | 31.615952    |
| Ca      | 29.455183    | 29.201015    | 29.876177    |
| Ca      | 30.512283    | 32.821121    | 26.069584    |
| Ca      | 30.076191    | 27.530149    | 24.998888    |
| Ca      | 33.744087    | 29.857868    | 28.356094    |
| Ca      | 34.019772    | 25.169060    | 27.627264    |
| Ca      | 35.099953    | 28.496376    | 23.292336    |
| S       | 20.832197    | 30.962982    | 34.853004    |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| S       | 20.827341  | 35.631039  | 33.495716  |
| S       | 22.153276  | 31.385197  | 29.714550  |
| S       | 24.959246  | 33.274704  | 33.515430  |
| S       | 26.313818  | 29.317080  | 30.576292  |
| S       | 26.216541  | 34.251335  | 29.048126  |
| S       | 28.391487  | 29.999378  | 26.645235  |
| S       | 31.043041  | 31.910282  | 29.59064   |
| S       | 31.465731  | 26.982895  | 28.242880  |
| S       | 32.678524  | 30.416149  | 24.887337  |
| S       | 33.031361  | 25.500971  | 24.021021  |
| S       | 36.231949  | 28.092051  | 26.883091  |

24 generated by VMD

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Ca      | 18.270350  | 33.009037  | 33.680496  |
| Ca      | 22.823669  | 33.641289  | 35.883499  |
| Ca      | 23.580664  | 29.969826  | 32.561890  |
| Ca      | 22.978504  | 34.895901  | 31.030245  |
| Ca      | 24.929279  | 31.276007  | 27.469421  |
| Ca      | 28.040321  | 32.811272  | 31.380554  |
| Ca      | 29.312412  | 29.214912  | 29.903702  |
| Ca      | 30.270878  | 32.825104  | 26.066910  |
| Ca      | 30.237114  | 27.496723  | 25.087801  |
| Ca      | 33.744244  | 29.650475  | 28.434326  |
| Ca      | 34.196991  | 25.270840  | 27.735386  |
| Ca      | 35.112690  | 28.401871  | 23.477793  |
| S       | 20.951260  | 30.816399  | 34.767170  |
| S       | 20.892208  | 35.558510  | 33.803062  |
| S       | 22.169264  | 31.604044  | 29.569063  |
| S       | 25.019466  | 33.077816  | 33.309380  |
| S       | 26.185034  | 29.516245  | 30.403809  |
| S       | 25.960308  | 34.465805  | 28.808969  |
| S       | 28.193798  | 29.968800  | 26.550617  |
| S       | 31.181274  | 32.028816  | 29.480402  |
| S       | 31.635201  | 27.049911  | 28.470852  |
| S       | 32.595589  | 30.150307  | 24.981476  |
| S       | 33.009296  | 25.524727  | 24.226967  |
| S       | 36.430195  | 28.075415  | 26.856272  |

24 generated by VMD

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Ca      | 18.410686  | 33.021183  | 33.242779  |
| Ca      | 22.968107  | 33.550407  | 36.095573  |
| Ca      | 23.503902  | 30.292738  | 32.394848  |
| Ca      | 22.946188  | 34.611614  | 31.008900  |
| Ca      | 24.755772  | 31.083973  | 27.538576  |
| Ca      | 28.169649  | 32.984596  | 31.401201  |
| Ca      | 29.482744  | 29.300978  | 29.980776  |
|   |       |       |       |
|---|-------|-------|-------|
| Ca| 30.536175 | 32.779564 | 26.059254 |
| Ca| 30.094196 | 27.612614 | 24.996632 |
| Ca| 33.652683 | 29.649445 | 28.422523 |
| Ca| 34.031685 | 25.185246 | 27.679638 |
| Ca| 35.090408 | 28.454758 | 23.484699 |
| S | 20.897930 | 30.776505 | 34.774242 |
| S | 20.855087 | 35.417763 | 33.903606 |
| S | 21.877348 | 31.194460 | 29.517380 |
| S | 25.064703 | 33.534409 | 33.284721 |
| S | 26.426105 | 29.853476 | 30.669397 |
| S | 25.900509 | 34.155197 | 28.690430 |
| S | 28.176781 | 30.115360 | 26.715115 |
| S | 31.337662 | 31.925920 | 29.537172 |
| S | 31.461742 | 26.886499 | 28.464077 |
| S | 32.718864 | 30.405148 | 25.078381 |
| S | 32.934711 | 25.639555 | 24.126108 |
| S | 36.426338 | 27.868601 | 26.870838 |

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generated by VMD

|   |       |       |       |
|---|-------|-------|-------|
| Ca| 18.159412 | 33.288292 | 33.640198 |
| Ca| 23.198475 | 33.312965 | 36.143421 |
| Ca| 23.376625 | 30.136795 | 32.343994 |
| Ca| 22.993851 | 34.637978 | 31.044447 |
| Ca| 24.910339 | 30.944221 | 27.555326 |
| Ca| 28.035019 | 33.073673 | 31.187832 |
| Ca| 29.623558 | 29.412350 | 29.860641 |
| Ca| 30.224731 | 32.491512 | 25.849524 |
| Ca| 30.182072 | 27.692945 | 24.976519 |
| Ca| 33.751781 | 29.607906 | 28.463280 |
| Ca| 34.070221 | 25.212681 | 27.711618 |
| Ca| 35.314728 | 28.628881 | 23.768526 |
| S | 20.751507 | 31.035660 | 34.740211 |
| S | 21.101322 | 35.442307 | 34.129555 |
| S | 21.932789 | 31.464554 | 29.378305 |
| S | 25.004713 | 33.311413 | 33.285503 |
| S | 26.445034 | 29.764513 | 30.570272 |
| S | 25.771561 | 34.208717 | 28.725618 |
| S | 28.094666 | 29.802860 | 26.490683 |
| S | 31.224533 | 31.926254 | 29.370571 |
| S | 31.573570 | 26.922161 | 28.409048 |
| S | 32.588501 | 30.358761 | 25.035145 |
| S | 33.090904 | 25.682320 | 24.172218 |
| S | 36.300201 | 27.940361 | 27.087574 |

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generated by VMD

|   |       |       |       |
|---|-------|-------|-------|
| Ca| 18.310867 | 33.132690 | 33.380013 |
| Element | Value1  | Value2  | Value3  |
|---------|---------|---------|---------|
| Ca      | 23.056171 | 33.163872 | 36.140594 |
| Ca      | 23.474077 | 29.942038 | 32.721626 |
| Ca      | 22.913380 | 34.947800 | 30.780329 |
| Ca      | 25.101910 | 31.258650 | 27.579542 |
| Ca      | 27.960163 | 33.014156 | 31.354723 |
| Ca      | 29.412700 | 32.481647 | 29.984249 |
| Ca      | 30.419382 | 32.677498 | 25.606844 |
| Ca      | 30.068190 | 27.478933 | 24.883915 |
| Ca      | 33.542248 | 29.712730 | 28.376551 |
| Ca      | 34.217186 | 25.201162 | 27.778467 |
| Ca      | 35.294617 | 28.247322 | 23.683235 |
| S       | 20.762848 | 30.712570 | 34.775650 |
| S       | 21.122331 | 35.484283 | 34.049911 |
| S       | 22.075012 | 31.575218 | 29.667866 |
| S       | 25.108250 | 33.174309 | 33.298048 |
| S       | 26.501790 | 29.652197 | 30.620058 |
| S       | 25.778000 | 34.493866 | 28.692627 |
| S       | 28.236284 | 30.000227 | 26.568977 |
| S       | 30.971966 | 32.090775 | 29.345669 |
| S       | 31.429245 | 26.853025 | 28.239769 |
| S       | 32.689831 | 30.312408 | 24.917261 |
| S       | 33.066475 | 25.504772 | 24.200611 |
| S       | 36.198078 | 28.221405 | 27.293499 |

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generated by VMD

| Element | Value1  | Value2  | Value3  |
|---------|---------|---------|---------|
| Ca      | 18.675388 | 32.940132 | 33.506462 |
| Ca      | 22.965965 | 33.580109 | 36.193222 |
| Ca      | 23.633520 | 29.882315 | 32.630318 |
| Ca      | 22.829079 | 34.779438 | 30.905647 |
| Ca      | 24.932468 | 31.100311 | 27.493572 |
| Ca      | 27.935390 | 33.139030 | 31.284084 |
| Ca      | 29.292217 | 29.512814 | 29.592279 |
| Ca      | 30.545937 | 32.959557 | 25.625122 |
| Ca      | 30.248608 | 27.632544 | 24.926277 |
| Ca      | 33.469955 | 29.763176 | 28.311275 |
| Ca      | 33.879402 | 24.989470 | 27.817438 |
| Ca      | 35.373276 | 28.406315 | 23.899616 |
| S       | 20.940571 | 30.606243 | 34.899624 |
| S       | 20.979391 | 35.536057 | 34.250614 |
| S       | 22.159885 | 31.358109 | 29.547747 |
| S       | 24.956371 | 33.245522 | 33.392017 |
| S       | 26.480522 | 29.805906 | 30.475842 |
| S       | 25.768181 | 34.347229 | 28.646652 |
| S       | 28.205505 | 29.980066 | 26.206169 |
| S       | 31.082401 | 32.156517 | 29.282858 |
| S       | 31.263180 | 26.972370 | 28.325722 |
|    |      |      |      |
|----|------|------|------|
| S  | 32.668114 | 30.390961 | 24.949276 |
| S  | 33.278732 | 25.503349 | 24.301001 |
| S  | 36.155937 | 27.712582 | 27.471096 |

24 generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 18.506599 | 33.295944 | 33.529648 |
| Ca | 23.278452 | 33.329597 | 36.361420 |
| Ca | 23.478790 | 29.973604 | 32.431168 |
| Ca | 22.739521 | 34.751762 | 30.983374 |
| Ca | 24.977058 | 30.912697 | 27.632685 |
| Ca | 27.915691 | 33.000397 | 31.083817 |
| Ca | 29.288963 | 29.422224 | 29.681328 |
| Ca | 30.481716 | 32.747704 | 25.855427 |
| Ca | 30.288422 | 27.778049 | 24.673496 |
| Ca | 33.504204 | 29.654377 | 28.415501 |
| Ca | 34.047462 | 25.179808 | 27.990992 |
| Ca | 35.495647 | 28.370676 | 23.845200 |
| S  | 20.970158 | 30.802750 | 34.838188 |
| S  | 21.043571 | 35.612297 | 34.226494 |
| S  | 21.967012 | 31.464203 | 29.588924 |
| S  | 25.048893 | 33.254517 | 33.201431 |
| S  | 26.455318 | 29.636478 | 30.732445 |
| S  | 25.617569 | 34.262718 | 28.568466 |
| S  | 28.175188 | 29.980536 | 26.350998 |
| S  | 30.926428 | 31.942524 | 29.157398 |
| S  | 31.221348 | 26.893345 | 28.052410 |
| S  | 32.735409 | 30.430552 | 25.000740 |
| S  | 33.320374 | 25.536997 | 24.361961 |
| S  | 36.236267 | 28.066210 | 27.376572 |

24 generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 18.520042 | 33.455933 | 33.575537 |
| Ca | 23.122654 | 33.335205 | 36.136539 |
| Ca | 23.508488 | 29.766144 | 32.525990 |
| Ca | 23.182072 | 34.616478 | 30.838184 |
| Ca | 24.912327 | 31.016834 | 27.486277 |
| Ca | 27.923172 | 33.069687 | 31.279972 |
| Ca | 29.326294 | 29.799002 | 29.836718 |
| Ca | 30.159813 | 32.769302 | 25.723442 |
| Ca | 30.267128 | 27.747700 | 24.918425 |
| Ca | 33.610153 | 29.826941 | 28.542828 |
| Ca | 33.901070 | 25.302368 | 27.821148 |
| Ca | 35.161362 | 28.265144 | 23.819307 |
| S  | 20.851055 | 30.709938 | 34.749752 |
| S  | 21.449142 | 35.438774 | 33.944450 |
| S  | 22.020861 | 31.480938 | 29.523954 |
S  25.092371  32.869026  33.340137
S  26.428263  29.406776  30.444410
S  25.988728  34.147812  28.623344
S  28.088909  29.928057  26.419836
S  30.955193  32.247139  29.290907
S  31.370337  27.124620  28.341131
S  32.670337  30.356354  25.144131
S  32.926117  25.532703  24.293530
S  36.282753  28.088026  27.320051

24
generated by VMD
Ca  18.352821  32.917042  33.717945
Ca  23.036505  33.412018  36.202599
Ca  23.325050  30.161026  32.379333
Ca  23.033562  34.736435  30.941154
Ca  24.922733  31.263401  27.499056
Ca  28.058155  32.986534  31.223831
Ca  29.263664  29.415607  29.732203
Ca  30.528555  32.630611  25.754642
Ca  30.132946  27.491882  25.057522
Ca  33.665482  29.720881  28.427057
Ca  33.986031  25.198294  27.800056
Ca  35.274551  28.384125  23.713837
S  20.984385  30.702108  34.973900
S  20.997528  35.356003  34.034760
S  21.941780  31.570171  29.527826
S  25.141607  33.191658  33.189995
S  26.373833  29.716480  30.477909
S  25.821945  34.444016  28.566387
S  28.052887  29.976305  26.317696
S  31.199888  32.049759  29.341877
S  31.387783  27.025707  28.411831
S  32.859901  30.449671  25.083031
S  33.089366  25.503414  24.430092
S  36.281776  27.996971  27.135534

24
generated by VMD
Ca  18.597744  33.039246  33.590416
Ca  22.999454  33.416611  36.199978
Ca  23.647697  29.986040  32.792713
Ca  22.893364  34.648338  30.954775
Ca  25.015917  31.147316  27.614105
Ca  27.841982  33.123676  31.080376
Ca  29.245911  29.156126  29.625849
Ca  30.536648  32.672249  25.832340
Ca  30.337145  27.728193  24.718283
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 33.426964 | 29.752642 | 28.602428 |
| Ca      | 34.028450 | 25.003317 | 27.716595 |
| Ca      | 35.561996 | 28.338921 | 23.947847 |
| S       | 21.109365 | 30.889378 | 34.870033 |
| S       | 20.921515 | 35.484634 | 33.991533 |
| S       | 22.028061 | 31.270193 | 29.732811 |
| S       | 25.047531 | 33.384533 | 33.395439 |
| S       | 26.398132 | 28.552400 | 30.557945 |
| S       | 25.701935 | 34.432152 | 28.485244 |
| S       | 28.189758 | 29.948173 | 26.194069 |
| S       | 30.960049 | 32.079292 | 29.325098 |
| S       | 31.107193 | 29.935041 | 28.121286 |
| S       | 32.771500 | 30.382826 | 24.999399 |
| S       | 33.204708 | 25.695187 | 24.202868 |
| S       | 36.147003 | 27.934061 | 27.379873 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 18.345398 | 33.158798 | 33.312954 |
| Ca      | 22.852440 | 34.059647 | 36.028694 |
| Ca      | 23.859510 | 29.959309 | 32.819878 |
| Ca      | 22.853289 | 34.371246 | 31.133269 |
| Ca      | 24.874523 | 30.868023 | 27.574192 |
| Ca      | 27.803230 | 33.018902 | 31.259472 |
| Ca      | 29.735031 | 29.075851 | 29.774876 |
| Ca      | 30.519918 | 32.896729 | 25.933384 |
| Ca      | 30.261030 | 27.852245 | 24.721502 |
| Ca      | 33.734268 | 29.608984 | 28.565029 |
| Ca      | 33.895351 | 24.978382 | 27.357866 |
| Ca      | 35.474094 | 28.375359 | 23.782112 |
| S       | 20.987467 | 31.081054 | 34.972008 |
| S       | 20.619274 | 35.672859 | 33.800289 |
| S       | 22.155157 | 31.200323 | 29.757660 |
| S       | 25.009144 | 33.201023 | 33.552391 |
| S       | 26.328951 | 29.675604 | 30.667648 |
| S       | 25.567619 | 34.263443 | 28.589500 |
| S       | 28.434349 | 30.153458 | 26.479984 |
| S       | 30.908939 | 31.990894 | 29.561420 |
| S       | 31.308258 | 26.907681 | 28.160139 |
| S       | 32.959541 | 30.436241 | 25.065653 |
| S       | 32.971485 | 25.637283 | 23.861965 |
| S       | 36.261787 | 27.857622 | 27.207792 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 18.535795 | 33.466850 | 33.131775 |
| Ca      | 22.856144 | 34.086563 | 36.086014 |
| Ca      | 23.607639 | 29.824833 | 32.818760 |
| Ca   | 22.915134 | 34.469429 | 31.011440 |
|------|-----------|-----------|-----------|
| Ca   | 24.851292 | 30.883434 | 27.685375 |
| Ca   | 27.894567 | 32.717781 | 31.564213 |
| Ca   | 29.523815 | 29.028254 | 29.815617 |
| Ca   | 30.151442 | 32.579361 | 26.016899 |
| Ca   | 30.317802 | 27.467075 | 24.708076 |
| Ca   | 33.773663 | 29.608091 | 28.294464 |
| Ca   | 34.149593 | 25.087297 | 27.612635 |
| Ca   | 35.409451 | 28.829708 | 23.576668 |
| S    | 20.805592 | 31.462585 | 34.704189 |
| S    | 20.725761 | 35.824825 | 33.632282 |
| S    | 22.012737 | 31.396431 | 29.864151 |
| S    | 25.045822 | 32.981010 | 33.777859 |
| S    | 26.330566 | 29.491564 | 30.680380 |
| S    | 25.948986 | 34.164337 | 28.959299 |
| S    | 28.272816 | 29.802261 | 26.390804 |
| S    | 30.987108 | 31.757551 | 29.431046 |
| S    | 31.281666 | 26.719971 | 28.092482 |
| S    | 32.598919 | 30.508001 | 24.936241 |
| S    | 33.321491 | 25.878334 | 24.163897 |
| S    | 36.402336 | 28.264509 | 26.984867 |

generated by VMD

| Ca   | 18.521839 | 33.078369 | 33.906723 |
|------|-----------|-----------|-----------|
| Ca   | 23.228344 | 34.143723 | 36.126217 |
| Ca   | 23.537594 | 30.008053 | 32.538807 |
| Ca   | 22.854626 | 34.673779 | 30.984905 |
| Ca   | 24.649895 | 30.815348 | 27.487471 |
| Ca   | 27.789213 | 32.750229 | 31.173916 |
| Ca   | 29.392872 | 29.237377 | 29.629524 |
| Ca   | 30.250792 | 32.613991 | 25.888489 |
| Ca   | 30.326664 | 27.855831 | 24.737026 |
| Ca   | 33.790810 | 29.507280 | 28.673386 |
| Ca   | 33.858124 | 25.068333 | 27.666595 |
| Ca   | 35.459652 | 28.669853 | 23.885960 |
| S    | 21.079205 | 31.055090 | 35.109726 |
| S    | 21.008415 | 35.641418 | 33.868130 |
| S    | 21.933590 | 31.584826 | 29.560656 |
| S    | 25.058208 | 33.039684 | 33.350822 |
| S    | 26.287760 | 29.553354 | 30.341255 |
| S    | 25.584995 | 34.104065 | 28.517391 |
| S    | 28.099476 | 29.829256 | 26.201038 |
| S    | 30.972992 | 31.739977 | 29.466106 |
| S    | 31.337540 | 26.957232 | 28.052799 |
| S    | 32.813431 | 30.397266 | 25.215475 |
| S    | 33.348015 | 25.908012 | 24.197327 |
|      | S    | Ca    | Ca    |
|------|------|-------|-------|
|      | 36.536049 | 28.067657 | 27.360313 |

24

generated by VMD

|      | S    | Ca    | Ca    |
|------|------|-------|-------|
|      | 21.191837 | 31.339214 | 35.050682 |
|      | 20.832947 | 35.607216 | 33.705688 |
|      | 21.867666 | 31.242132 | 29.669266 |
|      | 25.074553 | 33.056770 | 33.390381 |
|      | 26.295610 | 29.564091 | 30.410887 |
|      | 25.584766 | 34.088928 | 28.601919 |
|      | 28.263885 | 29.879435 | 26.283737 |
|      | 31.118513 | 31.893688 | 29.552116 |
|      | 31.235394 | 26.930326 | 28.114342 |
|      | 32.869022 | 30.496490 | 25.286840 |
|      | 32.998562 | 25.871460 | 23.907993 |
|      | 36.346809 | 28.051437 | 27.330538 |

24

generated by VMD

|      | S    | Ca    | Ca    |
|------|------|-------|-------|
|      | 18.536819 | 32.510551 | 33.379936 |
|      | 22.727541 | 34.227596 | 36.007271 |
|      | 23.913950 | 30.025013 | 32.642204 |
|      | 22.994225 | 34.779140 | 31.099972 |
|      | 24.773708 | 30.947414 | 27.386871 |
|      | 27.682894 | 32.748802 | 31.646339 |
|      | 29.665405 | 29.437777 | 29.676527 |
|      | 30.342310 | 32.680618 | 26.269066 |
|      | 30.068012 | 27.592140 | 24.814608 |
|      | 33.680645 | 29.349796 | 28.453953 |
|      | 33.907066 | 25.209957 | 27.834404 |
|      | 35.332264 | 28.468029 | 23.640354 |
|      | 21.412216 | 31.075890 | 34.953541 |
|      | 20.344585 | 35.565628 | 33.363125 |
|      | 22.030861 | 31.712345 | 29.718201 |
|      | 25.126863 | 33.112213 | 33.558998 |
|      | 26.561867 | 29.707016 | 30.341480 |
|     |     |     |
|-----|-----|-----|
| S   | 25.812616 | 34.199196 | 28.889362 |
| S   | 28.203106 | 30.293671 | 26.322702 |
| S   | 31.544216 | 31.804750 | 29.548071 |
| S   | 31.273096 | 26.765169 | 28.131008 |
| S   | 32.412991 | 30.352781 | 25.019646 |
| S   | 33.135914 | 25.737926 | 24.094086 |
| S   | 36.236885 | 27.996628 | 27.148325 |

24 generated by VMD

|     |     |     |
|-----|-----|-----|
| Ca  | 18.347401 | 32.782372 | 33.515602 |
| Ca  | 23.017651 | 33.901058 | 35.957020 |
| Ca  | 23.687668 | 29.794044 | 32.472115 |
| Ca  | 23.217512 | 34.568001 | 31.237411 |
| Ca  | 24.840485 | 31.031601 | 27.472389 |
| Ca  | 27.611900 | 33.058670 | 31.030874 |
| Ca  | 29.339516 | 29.631376 | 29.785719 |
| Ca  | 30.530781 | 32.738457 | 25.803780 |
| Ca  | 30.276543 | 27.504383 | 25.042347 |
| Ca  | 33.624962 | 29.407692 | 28.631680 |
| Ca  | 33.815521 | 25.224705 | 27.592644 |
| Ca  | 35.434498 | 28.474482 | 23.645378 |
| S   | 21.151520 | 30.932650 | 35.107193 |
| S   | 20.742123 | 35.482685 | 33.620564 |
| S   | 22.048977 | 31.605240 | 29.667231 |
| S   | 25.030239 | 32.932381 | 33.598358 |
| S   | 26.564161 | 29.887415 | 30.397568 |
| S   | 25.739912 | 34.302628 | 28.699705 |
| S   | 28.047401 | 30.185850 | 26.484520 |
| S   | 31.228971 | 32.111820 | 29.408535 |
| S   | 31.291599 | 26.901863 | 28.301970 |
| S   | 32.666901 | 30.223791 | 25.111025 |
| S   | 33.109100 | 25.707630 | 24.213671 |
| S   | 36.354721 | 27.909229 | 27.142735 |

24 generated by VMD

|     |     |     |
|-----|-----|-----|
| Ca  | 18.803579 | 33.450317 | 33.725224 |
| Ca  | 23.040550 | 33.893211 | 36.320988 |
| Ca  | 23.704935 | 29.938643 | 32.519794 |
| Ca  | 22.951691 | 34.417648 | 30.952343 |
| Ca  | 24.809179 | 30.781708 | 27.256870 |
| Ca  | 27.744003 | 32.778419 | 31.210150 |
| Ca  | 29.237726 | 29.343155 | 29.643639 |
| Ca  | 30.301088 | 32.970261 | 26.083437 |
| Ca  | 30.163507 | 27.601807 | 24.884674 |
| Ca  | 33.527405 | 29.759619 | 28.493078 |
| Ca  | 34.189701 | 25.130840 | 27.648829 |
|    | Ca   | S    | S    |
|----|------|------|------|
|    | 35.328781 | 28.630112 | 24.005386 |
| S  | 21.147293  | 31.204578  | 34.985573  |
| S  | 21.065575  | 35.810783  | 33.786728  |
| S  | 21.917835  | 31.506454  | 29.502970  |
| S  | 25.033550  | 32.865208  | 33.554108  |
| S  | 26.221256  | 29.317772  | 30.265633  |
| S  | 25.714632  | 33.820961  | 28.639071  |
| S  | 28.211266  | 30.086107  | 26.273939  |
| S  | 30.966534  | 31.886162  | 29.397591  |
| S  | 31.395081  | 26.826311  | 28.154545  |
| S  | 32.683506  | 30.625700  | 25.126751  |
| S  | 33.318832  | 25.570646  | 24.137709  |
| S  | 36.242542  | 28.083591  | 27.370998  |
|    | generated by VMD |
| Ca | 18.594671  | 33.349442  | 33.502178  |
| Ca | 22.987000  | 33.631058  | 36.030251  |
| Ca | 23.604702  | 29.709148  | 32.587627  |
| Ca | 23.030777  | 34.458393  | 31.227325  |
| Ca | 24.843430  | 30.952995  | 27.370934  |
| Ca | 27.911129  | 32.843864  | 31.193985  |
| Ca | 29.398714  | 29.402794  | 29.590984  |
| Ca | 30.452126  | 32.790726  | 25.941156  |
| Ca | 30.101233  | 27.760597  | 24.907806  |
| Ca | 33.560612  | 29.864405  | 28.511898  |
| Ca | 33.978088  | 25.376110  | 27.956066  |
| Ca | 35.113655  | 28.234392  | 23.840719  |
| S  | 21.002901  | 31.007099  | 34.704994  |
| S  | 21.134022  | 35.710899  | 33.680580  |
| S  | 21.992516  | 31.507671  | 29.790424  |
| S  | 25.077972  | 32.600048  | 33.556946  |
| S  | 26.468325  | 29.543819  | 30.372221  |
| S  | 25.905262  | 34.221321  | 28.685602  |
| S  | 28.123962  | 30.236843  | 26.105938  |
| S  | 31.012932  | 32.024284  | 29.494064  |
| S  | 31.549309  | 27.129162  | 28.327244  |
| S  | 32.545559  | 30.430115  | 25.033600  |
| S  | 33.063667  | 25.537136  | 24.418011  |
| S  | 36.267494  | 27.990299  | 27.105946  |
|    | generated by VMD |
| Ca | 18.446053  | 32.868767  | 33.023804  |
| Ca | 22.777422  | 33.884583  | 35.723843  |
| Ca | 23.827543  | 29.767048  | 32.494209  |
| Ca | 23.378101  | 34.892410  | 31.211109  |
| Ca | 24.780140  | 30.915352  | 27.584122  |
| Element | Value 1    | Value 2    | Value 3    |
|---------|------------|------------|------------|
| Ca      | 27.982466  | 32.877426  | 31.346397  |
| Ca      | 29.442987  | 29.210907  | 25.034533  |
| Ca      | 30.666285  | 32.738853  | 26.093224  |
| Ca      | 29.985298  | 27.427082  | 25.034533  |
| Ca      | 33.384590  | 29.877449  | 28.506863  |
| Ca      | 34.130547  | 29.125267  | 27.807613  |
| Ca      | 34.842941  | 28.693535  | 23.53674   |
| S       | 21.150537  | 30.808880  | 34.789227  |
| S       | 20.787800  | 35.747875  | 33.349121  |
| S       | 22.372433  | 31.829201  | 30.051758  |
| S       | 24.967913  | 32.888458  | 33.637196  |
| S       | 26.585728  | 29.437691  | 30.382988  |
| S       | 26.036438  | 34.072540  | 28.89175   |
| S       | 28.093784  | 30.162937  | 26.44235   |
| S       | 31.244453  | 32.072121  | 29.672623  |
| S       | 31.328957  | 27.035282  | 28.358109  |
| S       | 32.183308  | 30.268969  | 25.095364  |
| S       | 33.209023  | 25.512196  | 24.207672  |
| S       | 36.115280  | 28.183987  | 26.905912  |

24

generated by VMD

| Element | Value 1    | Value 2    | Value 3    |
|---------|------------|------------|------------|
| Ca      | 18.388336  | 32.973373  | 33.581253  |
| Ca      | 23.028244  | 33.725685  | 35.93952   |
| Ca      | 23.515484  | 29.807144  | 32.527740  |
| Ca      | 22.962200  | 34.908409  | 31.181646  |
| Ca      | 24.681259  | 31.317242  | 27.516495  |
| Ca      | 27.839851  | 32.839630  | 31.036968  |
| Ca      | 29.590319  | 29.163975  | 29.715317  |
| Ca      | 30.582567  | 32.796696  | 26.051571  |
| Ca      | 30.258602  | 27.600281  | 25.088388  |
| Ca      | 33.814819  | 29.744696  | 28.426725  |
| Ca      | 34.199272  | 24.997559  | 27.873400  |
| Ca      | 35.013416  | 28.401146  | 23.595592  |
| S       | 21.050318  | 30.819437  | 34.815319  |
| S       | 20.692951  | 35.578899  | 33.721188  |
| S       | 21.843685  | 31.757992  | 29.825542  |
| S       | 25.107182  | 32.901104  | 33.425030  |
| S       | 26.377115  | 29.447987  | 30.39975   |
| S       | 25.778412  | 34.549572  | 28.675282  |
| S       | 28.170452  | 30.248665  | 26.411373  |
| S       | 31.207546  | 31.771124  | 29.363218  |
| S       | 31.590405  | 27.025614  | 28.308502  |
| S       | 32.667473  | 30.442646  | 25.004187  |
| S       | 33.088604  | 25.370144  | 24.488182  |
| S       | 36.271549  | 28.111006  | 26.973225  |

24
generated by VMD

Ca  18.316473  32.955124  33.660969
Ca  22.895828  33.955124  35.791828
Ca  23.675093  29.882492  32.655979
Ca  22.896721  34.460274  31.158987
Ca  22.893623  33.955124  34.32343
Ca  27.967575  32.982449  31.418709
Ca  29.408360  29.533876  29.690645
Ca  30.372650  32.982449  30.003164
Ca  30.332453  29.853962  28.536663
Ca  33.728340  25.073608  27.890556
Ca  35.079937  28.399452  23.557051
S   21.026436  30.979820  34.737469
S   20.841867  35.496429  33.499622
S   22.116779  31.454557  29.551182
S   25.127655  32.868305  33.792530
S   26.516321  29.549377  30.518936
S   26.063679  34.204639  28.932501
S   28.338598  30.187328  26.205360
S   31.092609  32.088364  29.586725
S   31.369499  26.984005  28.142776
S   32.564911  30.403999  25.047192
S   33.117504  25.02104  24.366783
S   36.202713  27.824606  27.079884

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generated by VMD

Ca  18.249588  32.769508  33.618156
Ca  23.004211  33.988449  35.899879
Ca  23.593685  30.092056  32.415634
Ca  23.045021  34.512733  31.276560
Ca  24.723183  31.068718  27.451395
Ca  27.977964  32.912842  31.429291
Ca  29.475130  29.638798  29.578018
Ca  30.591450  33.007927  25.874309
Ca  30.094055  27.458338  24.965935
Ca  33.694916  29.533791  28.321163
Ca  33.989021  25.207153  27.778051
Ca  35.311573  28.450283  23.885496
S   21.096128  30.874256  34.953720
S   20.637941  35.533897  33.426308
S   21.988998  31.715836  29.60542
S   25.103512  32.866859  33.740746
S   26.402790  29.694046  30.253502
S   25.818100  34.053970  29.070709
S   28.320408  30.249430  26.316294
|    | 31.328583 | 32.002731 | 29.306093 |
|----|-----------|-----------|-----------|
| S  | 31.389666 | 26.931017 | 28.288572 |
| S  | 32.674828 | 30.134836 | 24.902340 |
| S  | 32.886887 | 25.577061 | 24.366034 |
| S  | 36.322426 | 28.025602 | 27.158344 |

24

generated by VMD

|    | 18.268311 | 32.959602 | 33.970940 |
|----|-----------|-----------|-----------|
| Ca | 23.194744 | 33.957581 | 35.941963 |
| Ca | 23.507187 | 29.900249 | 32.229465 |
| Ca | 22.941219 | 34.533340 | 31.123329 |
| Ca | 24.708941 | 30.998486 | 27.420458 |
| Ca | 28.010250 | 32.998734 | 31.078320 |
| Ca | 29.408825 | 29.418961 | 29.575276 |
| Ca | 30.499153 | 32.940155 | 25.940228 |
| Ca | 30.237961 | 27.537163 | 25.063810 |
| Ca | 33.704605 | 29.674046 | 28.535137 |
| Ca | 34.088264 | 24.908272 | 27.639137 |
| Ca | 35.257202 | 28.462124 | 23.780596 |
| Ca | 36.343715 | 27.923952 | 27.238117 |

24

generated by VMD

|    | 18.512218 | 33.108765 | 33.948856 |
|----|-----------|-----------|-----------|
| Ca | 23.190199 | 34.148533 | 35.909592 |
| Ca | 23.604736 | 30.017429 | 32.439556 |
| Ca | 22.910023 | 34.629829 | 31.150522 |
| Ca | 24.727571 | 30.876907 | 27.275452 |
| Ca | 27.772331 | 32.741600 | 31.199604 |
| Ca | 29.420755 | 29.074465 | 29.480581 |
| Ca | 30.284149 | 32.987789 | 26.037554 |
| Ca | 30.297911 | 27.749218 | 24.801392 |
| Ca | 33.551113 | 29.664867 | 28.595711 |
| Ca | 34.147308 | 25.053677 | 27.829193 |
| Ca | 35.298252 | 28.707317 | 23.866283 |
| S  | 21.219501 | 31.049080 | 34.997475 |
|    | S          | Ca         | S          |
|----|------------|------------|------------|
|    | 20.972898  | 35.638294  | 33.687050  |
|    | 22.059500  | 31.594389  | 29.676521  |
|    | 25.178589  | 32.876347  | 33.447365  |
|    | 26.207539  | 29.456791  | 30.301056  |
|    | 25.805180  | 34.077175  | 28.681164  |
|    | 28.068832  | 30.117481  | 26.199055  |
|    | 30.935183  | 31.687166  | 29.389006  |
|    | 31.428864  | 26.740299  | 28.246040  |
|    | 32.565533  | 30.393826  | 25.092018  |
|    | 33.313725  | 25.782650  | 24.274527  |
|    | 36.248077  | 28.126146  | 27.414490  |

24 generated by VMD

|    | S          | Ca         | S          |
|----|------------|------------|------------|
|    | 18.398607  | 32.893311  | 33.908356  |
|    | 22.998558  | 34.119297  | 36.037910  |
|    | 23.526516  | 30.028091  | 32.562794  |
|    | 23.022192  | 34.797428  | 30.860062  |
|    | 24.651127  | 30.912861  | 27.377640  |
|    | 27.943966  | 32.841675  | 31.288414  |
|    | 29.133667  | 29.077744  | 29.808645  |
|    | 30.644077  | 32.743134  | 26.063381  |
|    | 30.263901  | 27.657803  | 24.919449  |
|    | 33.623581  | 29.675310  | 28.559370  |
|    | 34.190838  | 25.114090  | 27.689430  |
|    | 35.386902  | 28.673485  | 23.589695  |
|    | 21.075171  | 31.007465  | 35.270123  |
|    | 20.816206  | 35.539593  | 33.597893  |
|    | 22.006638  | 31.763874  | 29.528978  |
|    | 25.013323  | 33.059052  | 33.387604  |
|    | 26.207741  | 29.498390  | 30.457430  |
|    | 25.877028  | 34.203487  | 28.586374  |
|    | 28.138842  | 30.055141  | 26.387299  |
|    | 31.014610  | 31.688942  | 29.758894  |
|    | 31.494076  | 26.802486  | 28.141285  |
|    | 32.643559  | 30.375990  | 25.030756  |
|    | 33.279850  | 25.593893  | 24.074516  |
|    | 36.369118  | 28.177561  | 27.053726  |

24 generated by VMD

|    | Ca         | S          | Ca         |
|----|------------|------------|------------|
|    | 18.532646  | 32.718491  | 33.742199  |
|    | 23.212872  | 34.100838  | 35.922829  |
|    | 23.759407  | 29.827927  | 32.435089  |
|    | 22.784355  | 34.471291  | 30.878216  |
|    | 24.850250  | 30.979385  | 27.569843  |
|    | 27.999384  | 32.853188  | 31.216364  |
|    | 29.558969  | 29.320305  | 29.488907  |
|    | Ca     | S       | 576  |
|----|--------|---------|------|
| Ca | 30.464334 | 32.946159 | 25.890779 |
| Ca | 30.207443 | 27.634026 | 24.838425 |
| Ca | 33.664558 | 24.963484 | 27.634941 |
| Ca | 35.296238 | 28.735100 | 24.000753 |
| S  | 21.502878 | 31.052320 | 35.999999 |
| S  | 20.632843 | 35.491714 | 33.717335 |
| S  | 21.969435 | 31.454884 | 29.528471 |
| S  | 25.003498 | 32.995785 | 33.360836 |
| S  | 26.415491 | 29.630329 | 30.484814 |
| S  | 25.830265 | 34.312813 | 28.823997 |
| S  | 28.243515 | 30.232780 | 26.210205 |
| S  | 31.131926 | 32.181767 | 29.379585 |
| S  | 31.159660 | 27.030302 | 28.293003 |
| S  | 32.707394 | 30.409769 | 25.105427 |
| S  | 33.021461 | 25.626038 | 23.989082 |
| S  | 36.015369 | 27.674303 | 27.531841 |

24 generated by VMD

|    | Ca     | S       | 576  |
|----|--------|---------|------|
| Ca | 18.437443 | 32.434326 | 34.134392 |
| Ca | 22.865921 | 34.369102 | 35.964432 |
| Ca | 23.462559 | 30.048321 | 32.671791 |
| Ca | 23.033249 | 34.649513 | 31.042492 |
| Ca | 24.894596 | 31.293846 | 27.325642 |
| Ca | 27.896387 | 32.975628 | 31.243034 |
| Ca | 29.402107 | 29.304188 | 29.589485 |
| Ca | 30.312624 | 32.845970 | 25.841999 |
| Ca | 30.430061 | 27.718102 | 24.707758 |
| Ca | 33.700333 | 29.590551 | 28.633095 |
| Ca | 33.845837 | 24.951324 | 27.510864 |
| Ca | 35.582867 | 28.420452 | 24.021454 |
| S  | 21.411481 | 31.014677 | 35.252892 |
| S  | 20.540813 | 35.336201 | 33.692158 |
| S  | 21.886829 | 31.638134 | 29.590349 |
| S  | 24.946451 | 32.944519 | 33.350143 |
| S  | 26.334555 | 29.638794 | 30.456184 |
| S  | 25.746910 | 34.410210 | 28.682478 |
| S  | 28.268749 | 30.083004 | 26.213772 |
| S  | 31.138519 | 32.151543 | 29.300449 |
| S  | 31.229031 | 26.848549 | 28.168644 |
| S  | 32.875496 | 30.355515 | 25.208160 |
| S  | 33.236153 | 25.561964 | 23.866856 |
| S  | 36.238411 | 27.715553 | 27.471523 |

24 generated by VMD

|    | Ca     | S       | 576  |
|----|--------|---------|------|
| Ca | 18.465174 | 32.862629 | 34.322803 |
|   | Ca    | S     | Ca    | S     | Ca    | S     | Ca    | S     | Ca    | S     | Ca    | S     | Ca    | S     | Ca    | S     | Ca    | S     | Ca    | S     | Ca    | S     | Ca    | S     |
|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
|   | 23.258816 | 33.961399 | 36.181053 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 23.427799 | 30.142456 | 32.212410 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 22.966560 | 34.733482 | 30.944218 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 24.749031 | 30.825047 | 27.251343 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 27.909950 | 32.839874 | 31.183678 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 29.214886 | 29.442242 | 29.565058 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 30.485207 | 32.695992 | 25.728601 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 30.181477 | 27.606136 | 24.860706 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 33.532372 | 29.703728 | 28.701611 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 33.847561 | 25.198769 | 27.600615 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 35.677151 | 28.580399 | 24.165867 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 21.433987 | 31.052631 | 35.135368 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 20.940239 | 35.475555 | 33.973404 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 21.944363 | 31.504961 | 29.413113 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 25.027651 | 32.870605 | 33.265869 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 26.377028 | 29.663736 | 30.341711 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 25.760143 | 34.105003 | 28.460369 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 28.110788 | 30.113850 | 26.117025 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 30.990761 | 31.872139 | 29.336231 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 31.098265 | 26.890381 | 28.229580 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 32.840477 | 30.287138 | 25.190228 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 33.293419 | 25.780315 | 24.173616 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|   | 36.186913 | 28.091471 | 27.585588 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |

24

generated by VMD
|     |        |        |        |
|-----|--------|--------|--------|
| S   | 32.797531 | 30.373577 | 25.109653 |
| S   | 33.141808 | 25.797329 | 23.996674  |
| S   | 36.329063 | 27.800573 | 27.269215  |

24 generated by VMD

|     |        |        |        |
|-----|--------|--------|--------|
| Ca  | 19.005539 | 32.226768 | 34.000473 |
| Ca  | 23.440121 | 34.355072 | 35.737541 |
| Ca  | 23.103170 | 30.210320 | 32.145245 |
| Ca  | 22.754126 | 34.834961 | 30.950474 |
| Ca  | 24.626436 | 30.873947 | 27.358580 |
| Ca  | 27.833206 | 32.851292 | 31.082172 |
| Ca  | 29.185438 | 29.026138 | 29.775196 |
| Ca  | 30.493584 | 32.648945 | 26.127945 |
| Ca  | 30.371059 | 27.720549 | 24.920105 |
| Ca  | 33.465134 | 29.733097 | 28.875130 |
| Ca  | 34.146904 | 24.993271 | 27.266743 |
| Ca  | 35.637745 | 28.605606 | 23.878551 |
| S   | 21.640102 | 31.163589 | 35.236286 |
| S   | 20.717445 | 35.420799 | 33.746799 |
| S   | 21.989479 | 31.858349 | 29.485716 |
| S   | 25.075134 | 33.146217 | 33.35567 |
| S   | 26.065662 | 29.632572 | 30.485500 |
| S   | 25.710426 | 34.191235 | 28.560175 |
| S   | 28.101110 | 29.895214 | 26.509565 |
| S   | 30.879961 | 31.801935 | 29.634995 |
| S   | 31.350418 | 26.824398 | 28.347445 |
| S   | 32.814960 | 30.354885 | 25.293335 |
| S   | 33.060879 | 25.922899 | 23.840702 |
| S   | 36.251930 | 28.008041 | 27.345810 |

24 generated by VMD

|     |        |        |        |
|-----|--------|--------|--------|
| Ca  | 18.360756 | 32.493809 | 33.733276 |
| Ca  | 22.846952 | 34.050922 | 36.023151 |
| Ca  | 23.602339 | 30.358185 | 32.594765 |
| Ca  | 22.867111 | 34.937386 | 30.681559 |
| Ca  | 24.772549 | 30.770824 | 27.718231 |
| Ca  | 27.808472 | 32.888699 | 31.257366 |
| Ca  | 29.666698 | 29.229202 | 29.752659 |
| Ca  | 30.559402 | 32.873154 | 26.078735 |
| Ca  | 30.588406 | 27.819300 | 24.965466 |
| Ca  | 33.815388 | 29.627436 | 28.763943 |
| Ca  | 33.782635 | 24.857279 | 26.992329 |
| Ca  | 35.458771 | 28.394562 | 23.640676 |
| S   | 21.318686 | 31.000343 | 35.330280 |
| S   | 20.546146 | 35.446960 | 33.555748 |
| S   | 21.919151 | 31.650997 | 29.693657 |
|     |     |     |     |
|-----|-----|-----|-----|
| S   | 24.927433 | 33.433804 | 33.248974 |
| S   | 26.375343 | 29.633842 | 30.674585 |
| S   | 25.598560 | 34.051487 | 28.564726 |
| S   | 28.296829 | 30.082687 | 26.508600 |
| S   | 30.983252 | 31.944611 | 29.595039 |
| S   | 31.580154 | 26.904278 | 28.403028 |
| S   | 33.003838 | 30.404095 | 25.339924 |
| S   | 32.923344 | 25.769497 | 23.661282 |
| S   | 36.117790 | 27.676662 | 27.162041 |

24

generated by VMD

|     |     |     |     |
|-----|-----|-----|-----|
| Ca  | 18.379120 | 32.401680 | 33.536655 |
| Ca  | 22.857008 | 34.191353 | 35.686512 |
| Ca  | 23.684460 | 30.201355 | 32.507809 |
| Ca  | 22.756733 | 34.794605 | 30.903849 |
| Ca  | 24.775307 | 30.725521 | 27.810419 |
| Ca  | 27.995335 | 33.003014 | 31.438387 |
| Ca  | 29.481649 | 29.498577 | 29.963806 |
| Ca  | 30.636200 | 32.999561 | 26.170061 |
| Ca  | 30.313042 | 27.809122 | 24.964613 |
| Ca  | 33.914047 | 29.466539 | 28.600424 |
| Ca  | 33.716846 | 24.879538 | 27.215534 |
| Ca  | 35.250237 | 28.564531 | 23.570873 |
| Ca  | 21.246239 | 31.014511 | 34.995422 |
| S   | 20.451130 | 35.305626 | 33.471638 |
| S   | 21.963858 | 31.650862 | 29.502167 |
| S   | 24.910156 | 33.258553 | 33.353809 |
| S   | 26.536325 | 29.668032 | 30.851986 |
| S   | 25.699816 | 34.150555 | 28.864471 |
| S   | 28.328011 | 30.227224 | 26.654007 |
| S   | 31.407320 | 32.180283 | 29.560276 |
| S   | 31.463768 | 26.838833 | 28.309067 |
| S   | 32.651611 | 30.369440 | 25.290314 |
| S   | 32.963413 | 25.721985 | 23.867161 |
| S   | 36.338306 | 27.378817 | 26.850767 |

24

generated by VMD

|     |     |     |     |
|-----|-----|-----|-----|
| Ca  | 18.384161 | 33.157288 | 33.749893 |
| Ca  | 23.113319 | 33.922272 | 35.777523 |
| Ca  | 23.592005 | 29.938057 | 32.491989 |
| Ca  | 23.03926 | 34.364136 | 31.061148 |
| Ca  | 24.736359 | 30.578060 | 27.789246 |
| Ca  | 28.060974 | 33.024010 | 31.221621 |
| Ca  | 29.297651 | 29.380295 | 29.744295 |
| Ca  | 30.549091 | 32.791782 | 25.916531 |
| Ca  | 30.338013 | 27.785770 | 24.747494 |
|   | 33.529934  | 29.672211 | 28.681906 |
|---|------------|------------|------------|
| Ca| 33.778904  | 25.334246  | 27.333248  |
| Ca| 35.524548  | 28.644260  | 23.815434  |
| S | 21.188101  | 31.162550  | 34.836460  |
| S | 20.792658  | 35.635990  | 33.492832  |
| S | 21.848820  | 31.418039  | 29.593307  |
| S | 25.206057  | 32.903202  | 33.476353  |
| S | 26.532246  | 29.474752  | 30.766899  |
| S | 25.816238  | 33.859238  | 28.749605  |
| S | 28.140776  | 30.051897  | 26.388493  |
| S | 31.141794  | 32.179779  | 29.484833  |
| S | 31.022652  | 27.169418  | 28.408144  |
| S | 32.818661  | 30.332928  | 25.256666  |
| S | 33.172504  | 25.884224  | 23.944574  |
| S | 36.100700  | 27.635561  | 27.211531  |

24

generated by VMD

|   | 18.655499  | 31.947725  | 33.708202  |
|---|------------|------------|------------|
| Ca| 22.820175  | 34.124336  | 35.920624  |
| Ca| 23.820978  | 30.232386  | 32.758236  |
| Ca| 22.985023  | 34.740063  | 30.931734  |
| Ca| 24.981886  | 31.119574  | 27.502563  |
| Ca| 27.954498  | 33.183327  | 31.356735  |
| Ca| 29.574577  | 29.596123  | 29.388092  |
| Ca| 30.409256  | 32.920036  | 25.591797  |
| Ca| 30.262564  | 27.855827  | 24.950203  |
| Ca| 33.319050  | 29.550961  | 28.711723  |
| Ca| 33.838608  | 24.691471  | 27.369904  |
| Ca| 35.365059  | 28.530472  | 24.314579  |
| S | 21.543400  | 30.904587  | 35.176598  |
| S | 20.431599  | 35.072002  | 33.476280  |
| S | 22.259584  | 31.471870  | 29.695591  |
| S | 25.231838  | 33.364586  | 33.480854  |
| S | 26.564568  | 29.785591  | 30.538420  |
| S | 25.934822  | 34.371750  | 28.748260  |
| S | 28.098225  | 30.208563  | 26.096361  |
| S | 30.890907  | 32.452934  | 29.178064  |
| S | 30.982727  | 26.881954  | 28.057423  |
| S | 32.798084  | 30.321547  | 25.408554  |
| S | 33.113720  | 25.683540  | 23.892487  |
| S | 35.883377  | 27.288895  | 27.686749  |

24

generated by VMD

|   | 18.506262  | 32.591190  | 33.656757  |
|---|------------|------------|------------|
| Ca| 23.185108  | 34.130310  | 36.111607  |
| Ca| 23.496574  | 29.884903  | 32.725700  |
| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 23.104267 | 34.610218 | 30.867050 |
| Ca      | 24.838959 | 30.856306 | 27.468143 |
| Ca      | 27.791233 | 32.854946 | 31.381207 |
| Ca      | 29.223316 | 29.465542 | 29.457756 |
| Ca      | 30.604412 | 32.842030 | 25.730124 |
| Ca      | 30.442684 | 27.697357 | 24.571194 |
| Ca      | 33.293610 | 29.678183 | 28.584312 |
| S       | 21.267502 | 31.240858 | 35.385704 |
| S       | 20.818199 | 35.383812 | 33.569500 |
| S       | 22.123848 | 31.245934 | 29.721600 |
| S       | 25.055744 | 32.925453 | 33.507217 |
| S       | 26.322998 | 29.579872 | 30.503113 |
| S       | 26.006744 | 34.171776 | 28.680756 |
| S       | 28.142170 | 30.172401 | 26.096806 |
| S       | 31.081615 | 32.457176 | 29.369200 |
| S       | 30.983646 | 27.234930 | 28.235058 |
| S       | 32.679039 | 30.424015 | 24.992306 |
| S       | 33.318054 | 25.800028 | 24.044575 |
| S       | 36.043011 | 27.430872 | 27.588924 |

24 generated by VMD

| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 18.509304 | 32.772240 | 33.634476 |
| Ca      | 23.250811 | 34.217121 | 36.013454 |
| Ca      | 23.829149 | 30.040962 | 32.895920 |
| Ca      | 23.058887 | 34.324173 | 30.929771 |
| Ca      | 24.858124 | 30.826374 | 27.439495 |
| Ca      | 27.811708 | 32.897125 | 31.116404 |
| Ca      | 29.480186 | 29.707376 | 29.407049 |
| Ca      | 30.451988 | 33.047424 | 25.726536 |
| Ca      | 30.273182 | 27.839380 | 24.652803 |
| Ca      | 33.388741 | 29.542465 | 28.951714 |
| Ca      | 33.792091 | 24.786133 | 27.328754 |
| Ca      | 35.332458 | 28.865093 | 24.299660 |
| S       | 21.399822 | 31.267529 | 35.352276 |
| S       | 20.907495 | 35.439713 | 33.428833 |
| S       | 22.089521 | 31.021082 | 29.711571 |
| S       | 25.085835 | 32.895248 | 33.489120 |
| S       | 26.409229 | 29.434347 | 30.292801 |
| S       | 25.793493 | 34.026299 | 28.643511 |
| S       | 28.338085 | 30.279430 | 25.967855 |
| S       | 30.844484 | 32.318981 | 29.364313 |
| S       | 30.956250 | 27.003704 | 28.196793 |
| S       | 32.634537 | 30.503426 | 25.462608 |
| S       | 33.155594 | 25.824955 | 24.076893 |
|  | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| S | 36.065666 | 27.419432 | 27.557402 |
| Ca | 18.518166 | 32.517166 | 33.808102 |
| Ca | 23.074354 | 34.200737 | 35.877960 |
| Ca | 23.779543 | 29.935429 | 32.666515 |
| Ca | 23.010542 | 34.520844 | 31.065369 |
| Ca | 24.940506 | 30.971022 | 27.481209 |
| Ca | 27.718027 | 33.033607 | 31.082304 |
| Ca | 29.398800 | 29.670851 | 29.575983 |
| Ca | 30.265522 | 33.043507 | 25.942669 |
| Ca | 30.309292 | 27.379585 | 24.715412 |
| Ca | 33.273598 | 24.973173 | 27.187189 |
| Ca | 35.513252 | 28.694693 | 23.884485 |
| S | 21.471737 | 31.165037 | 35.198811 |
| S | 20.589146 | 35.466553 | 33.472771 |
| S | 22.081577 | 31.462772 | 29.683445 |
| S | 25.086025 | 33.155243 | 33.532772 |
| S | 26.437651 | 29.610800 | 30.399935 |
| S | 25.803570 | 34.125526 | 28.781530 |
| S | 28.167915 | 30.295286 | 26.230852 |
| S | 30.996111 | 32.371162 | 29.391319 |
| S | 31.002140 | 26.868921 | 28.272848 |
| S | 32.576687 | 30.221207 | 25.563423 |
| S | 33.584297 | 25.765062 | 23.852753 |
| S | 36.192223 | 27.529501 | 27.441917 |

24 generated by VMD

|  | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| Ca | 18.578003 | 32.605717 | 33.770550 |
| Ca | 22.935669 | 34.633423 | 35.865425 |
| Ca | 23.834023 | 30.062626 | 32.914490 |
| Ca | 22.925478 | 34.583988 | 30.828838 |
| Ca | 24.792519 | 30.686924 | 27.513170 |
| Ca | 27.831781 | 32.794147 | 31.234606 |
| Ca | 29.470966 | 29.095053 | 29.554014 |
| Ca | 30.409664 | 32.883564 | 26.072403 |
| Ca | 30.419796 | 28.190807 | 24.833767 |
| Ca | 33.536327 | 29.647665 | 28.681528 |
| Ca | 33.688465 | 24.645947 | 27.118275 |
| Ca | 35.460693 | 28.746365 | 24.077171 |
| S | 21.481590 | 31.274876 | 35.441765 |
| S | 20.572269 | 35.453140 | 33.178963 |
| S | 21.998734 | 31.292446 | 29.768988 |
| S | 25.090778 | 33.224331 | 33.256821 |
| S | 26.400715 | 29.361364 | 30.645830 |
| S     | 25.856955 | 33.920856 | 28.615694 |
|-------|-----------|-----------|-----------|
| S     | 28.197575 | 30.120174 | 26.322681 |
| S     | 30.966768 | 32.081409 | 29.577267 |
| S     | 31.053345 | 26.874233 | 28.088772 |
| S     | 32.812870 | 30.583086 | 25.544176 |
| S     | 33.364765 | 26.062006 | 23.653988 |
| S     | 36.040340 | 27.475901 | 27.380859 |

24 generated by VMD

| Ca    | 18.252827 | 33.079624 | 33.844017 |
|-------|-----------|-----------|-----------|
| Ca    | 22.890112 | 34.475605 | 36.068184 |
| Ca    | 23.483124 | 30.013535 | 32.823994 |
| Ca    | 22.834236 | 34.471626 | 30.928349 |
| Ca    | 25.012468 | 30.784094 | 27.716682 |
| Ca    | 27.637012 | 32.805931 | 31.219927 |
| Ca    | 29.658144 | 29.129936 | 29.635029 |
| Ca    | 30.485376 | 32.747101 | 26.034542 |
| Ca    | 30.673836 | 27.878067 | 24.589901 |
| Ca    | 33.545479 | 29.860241 | 28.456177 |
| Ca    | 33.985458 | 24.726509 | 27.011374 |
| Ca    | 35.581184 | 28.646004 | 23.927464 |
| S     | 20.907232 | 31.502922 | 35.365929 |
| S     | 20.696440 | 35.735245 | 33.562508 |
| S     | 21.988846 | 31.175264 | 29.793482 |
| S     | 24.857576 | 33.032555 | 33.424381 |
| S     | 26.334251 | 29.506622 | 30.731354 |
| S     | 25.853575 | 34.051903 | 28.753233 |
| S     | 28.287231 | 29.919867 | 26.386707 |
| S     | 30.931419 | 31.963491 | 29.542048 |
| S     | 31.302979 | 26.887676 | 28.023542 |
| S     | 32.804890 | 30.651421 | 25.177982 |
| S     | 33.628704 | 25.684891 | 23.478867 |
| S     | 36.079971 | 27.569939 | 27.444351 |

24 generated by VMD

| Ca    | 18.531628 | 33.109570 | 33.956753 |
|-------|-----------|-----------|-----------|
| Ca    | 23.460182 | 34.391937 | 35.616650 |
| Ca    | 23.527597 | 30.154560 | 32.487801 |
| Ca    | 22.845081 | 34.089722 | 31.116568 |
| Ca    | 24.889332 | 30.670872 | 27.620075 |
| Ca    | 27.772758 | 32.619209 | 31.194654 |
| Ca    | 29.653893 | 29.134392 | 29.405724 |
| Ca    | 29.959129 | 32.915207 | 25.758640 |
| Ca    | 30.485064 | 27.889484 | 24.786381 |
| Ca    | 33.696232 | 29.706354 | 28.690161 |
| Ca    | 33.675709 | 24.702179 | 27.133160 |
|  | Ca     | S      | Ca     |
|---|--------|--------|--------|
|  | 35.619274 | 29.021563 | 24.341900 |
|  | 21.465290  | 31.337521 | 35.259537 |
|  | 20.829468  | 35.674885 | 33.279411 |
|  | 21.904451  | 31.376879 | 29.759624 |
|  | 25.175627  | 32.808884 | 33.588696 |
|  | 26.269955  | 29.515991 | 30.390587 |
|  | 25.591869  | 34.015800 | 28.872871 |
|  | 28.134956  | 29.952229 | 26.224079 |
|  | 30.896711  | 32.128174 | 29.283766 |
|  | 31.189606  | 26.877754 | 28.205654 |
|  | 32.712349  | 30.534727 | 25.296360 |
|  | 33.473061  | 26.164268 | 23.905167 |
|  | 35.960274  | 27.507919 | 27.765863 |

24 generated by VMD

|  | Ca     | S      | Ca     |
|---|--------|--------|--------|
|  | 18.424637 | 33.300583 | 34.153072 |
|  | 23.033436 | 34.513802 | 36.048458 |
|  | 23.729134 | 30.129601 | 32.818233 |
|  | 22.684574 | 34.472458 | 30.826775 |
|  | 24.779034 | 30.656429 | 27.554905 |
|  | 27.613163 | 32.489937 | 31.328026 |
|  | 29.391434 | 30.013037 | 29.540350 |
|  | 30.291656 | 32.647942 | 26.154858 |
|  | 30.487541 | 27.839439 | 24.514080 |
|  | 33.756058 | 29.669720 | 28.740414 |
|  | 33.984913 | 24.779903 | 27.124165 |
|  | 35.572891 | 29.061085 | 24.014778 |
|  | 21.095505 | 31.474398 | 35.288563 |
|  | 20.916985 | 35.682941 | 33.632416 |
|  | 21.939602 | 31.336655 | 29.615379 |
|  | 25.120885 | 33.048409 | 33.296741 |
|  | 26.188835 | 30.239471 | 30.368473 |
|  | 25.640942 | 34.089684 | 28.547329 |
|  | 28.110855 | 29.727470 | 26.327841 |
|  | 30.773792 | 32.033424 | 29.430603 |
|  | 31.405933 | 26.919123 | 28.077353 |
|  | 32.883617 | 30.541157 | 25.328470 |
|  | 33.630577 | 26.018206 | 23.771183 |
|  | 36.257820 | 27.615080 | 27.437536 |

24 generated by VMD

|  | Ca     | S      | Ca     |
|---|--------|--------|--------|
|  | 18.372952 | 32.646027 | 34.220116 |
|  | 23.169950 | 34.489822 | 35.884995 |
|  | 23.588793 | 30.150181 | 32.788631 |
|  | 22.641754 | 34.542656 | 30.756649 |
|  | 24.929344 | 30.871742 | 27.634052 |
| Element | X1   | Y1   | Z1   | X2   | Y2   | Z2   |
|---------|------|------|------|------|------|------|
| Ca      | 27.648512 | 32.971630 | 30.927317 | 29.455154 | 29.045631 | 29.533051 |
| Ca      | 30.538904 | 32.620846 | 25.740141 | 30.689287 | 27.967430 | 24.640995 |
| Ca      | 33.567215 | 29.472845 | 28.827848 | 35.567215 | 29.472845 | 28.827848 |
| Ca      | 30.689287 | 27.967430 | 24.640995 | 33.567215 | 29.472845 | 28.827848 |
| Ca      | 33.843581 | 24.538456 | 27.117020 | 25.538927 | 27.967430 | 24.640995 |
| Ca      | 36.618641 | 32.595310 | 33.800140 | 18.518641 | 32.595310 | 33.800140 |
| Ca      | 29.539154 | 29.045631 | 29.533051 | 30.538904 | 32.620846 | 25.740141 |
| Ca      | 33.567215 | 29.472845 | 28.827848 | 33.567215 | 29.472845 | 28.827848 |
| Ca      | 30.689287 | 27.967430 | 24.640995 | 33.567215 | 29.472845 | 28.827848 |
| Ca      | 33.843581 | 24.538456 | 27.117020 | 25.538927 | 27.967430 | 24.640995 |

24 generated by VMD
| Element | X1  | Y1  | Z1  |
|---------|-----|-----|-----|
| Ca      | 18.821516 | 32.102486 | 34.212284 |
| Ca      | 23.319918 | 34.241776 | 35.797314 |
| Ca      | 23.707932 | 30.297308 | 32.575314 |
| Ca      | 22.681946 | 34.680485 | 30.802402 |
| Ca      | 24.755569 | 30.869232 | 27.386818 |
| Ca      | 27.690027 | 32.866238 | 31.055428 |
| Ca      | 29.418667 | 29.033489 | 29.436131 |
| Ca      | 30.359058 | 32.957214 | 26.090466 |
| Ca      | 30.223738 | 27.761917 | 24.632706 |
| Ca      | 33.389763 | 29.808496 | 28.740091 |
| Ca      | 33.655273 | 24.671581 | 27.277281 |
| Ca      | 35.786964 | 28.710943 | 24.498663 |
| S       | 21.878321 | 31.035686 | 35.496838 |
| S       | 20.593521 | 35.349285 | 33.624065 |
| S       | 22.002995 | 31.504208 | 29.557051 |
| S       | 25.084869 | 33.528946 | 33.266891 |
| S       | 26.175747 | 29.696619 | 30.218964 |
| S       | 25.724518 | 34.364258 | 28.542702 |
| S       | 28.200853 | 30.108025 | 26.125824 |
| S       | 30.968519 | 32.033234 | 29.507690 |
| S       | 30.992912 | 26.906250 | 28.031984 |
| S       | 32.748322 | 30.498873 | 25.291161 |
| S       | 33.417988 | 25.977787 | 23.957987 |
| S       | 36.121159 | 27.295681 | 27.813999 |

24 generated by VMD

| Element | X1  | Y1  | Z1  |
|---------|-----|-----|-----|
| Ca      | 18.700558 | 32.808270 | 33.901386 |
| Ca      | 22.991241 | 34.240532 | 35.820755 |
| Ca      | 23.691832 | 30.079803 | 32.705372 |
| Ca      | 22.809072 | 34.691509 | 30.825924 |
| Ca      | 24.970608 | 30.618690 | 27.833530 |
| Ca      | 27.699715 | 32.948048 | 31.311611 |
| Ca      | 29.643753 | 28.870350 | 29.519081 |
| Ca      | 30.272299 | 32.716316 | 26.018333 |
| Ca      | 30.343237 | 27.702614 | 24.625553 |
| Ca      | 33.563435 | 29.588593 | 28.748661 |
| Ca      | 34.062691 | 24.711449 | 27.061954 |
| Ca      | 35.460854 | 29.095070 | 24.156113 |
| S       | 21.551964 | 31.223639 | 35.371155 |
| S       | 20.420868 | 35.760941 | 33.249035 |
| S       | 22.050632 | 31.419262 | 29.670521 |
| S       | 24.802711 | 33.321609 | 33.298046 |
| S       | 26.362207 | 29.579765 | 30.605167 |
| S       | 25.917393 | 34.217781 | 28.721533 |
| S       | 28.325924 | 29.976135 | 26.381128 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| S       | 30.823410 | 31.858517 | 29.669559 |
| S       | 31.308659 | 26.703123 | 28.065189 |
| S       | 32.769428 | 30.435720 | 25.204634 |
| S       | 33.286064 | 26.047890 | 23.704916 |
| S       | 35.891483 | 27.684479 | 27.470879 |

24 generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.297768 | 32.647369 | 33.910767 |
| Ca      | 22.818428 | 34.640636 | 35.888470 |
| Ca      | 23.604895 | 30.121231 | 32.887329 |
| Ca      | 22.978519 | 34.593922 | 30.687994 |
| Ca      | 25.032867 | 30.925423 | 27.651779 |
| Ca      | 27.760735 | 32.773148 | 31.291977 |
| Ca      | 29.661512 | 28.597137 | 29.585825 |
| Ca      | 30.410215 | 32.858276 | 26.183985 |
| Ca      | 30.434910 | 27.845016 | 24.515551 |
| Ca      | 33.388195 | 29.617512 | 28.731621 |
| Ca      | 34.028198 | 24.770313 | 27.161282 |
| Ca      | 35.457897 | 28.906927 | 23.903782 |
| S       | 21.263515 | 31.503746 | 35.676147 |
| S       | 20.510265 | 35.487793 | 33.252697 |
| S       | 22.124804 | 31.393322 | 29.849031 |
| S       | 25.128094 | 33.135651 | 33.395790 |
| S       | 26.298103 | 29.536686 | 30.357456 |
| S       | 25.852787 | 34.214371 | 28.693840 |
| S       | 28.270685 | 29.994637 | 26.350286 |
| S       | 30.817368 | 31.866390 | 29.566345 |
| S       | 31.274750 | 26.688225 | 27.940212 |
| S       | 32.789993 | 30.432705 | 25.241203 |
| S       | 33.344604 | 26.003363 | 23.844658 |
| S       | 36.170910 | 27.746296 | 27.372032 |

24 generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.374937 | 32.663593 | 33.964504 |
| Ca      | 22.268564 | 34.444580 | 35.941620 |
| Ca      | 23.667599 | 30.123266 | 32.688794 |
| Ca      | 22.852131 | 34.364555 | 30.872265 |
| Ca      | 24.897738 | 30.908371 | 27.401001 |
| Ca      | 27.741383 | 32.529503 | 31.085428 |
| Ca      | 29.514446 | 29.000893 | 29.527246 |
| Ca      | 30.534275 | 33.008091 | 26.222870 |
| Ca      | 30.274807 | 27.768234 | 24.721724 |
| Ca      | 33.433548 | 29.875412 | 28.795094 |
| Ca      | 33.857605 | 24.691544 | 27.281641 |
| Ca      | 35.660942 | 28.648373 | 24.028168 |
| S       | 21.529984 | 31.458988 | 35.356308 |
|    |       |       |       |
|----|-------|-------|-------|
| S  | 20.770535 | 35.688335 | 33.557755 |
| S  | 21.867363 | 31.240370 | 29.644791 |
| S  | 25.030588 | 32.987087 | 33.351482 |
| S  | 26.146740 | 29.468647 | 30.457497 |
| S  | 25.738338 | 34.111717 | 28.562527 |
| S  | 28.365051 | 30.115566 | 26.299505 |
| S  | 30.854225 | 31.992027 | 29.553526 |
| S  | 31.238041 | 26.954042 | 28.118160 |
| S  | 32.833363 | 30.619343 | 25.165091 |
| S  | 33.345264 | 25.930370 | 23.785284 |
| S  | 35.922600 | 27.707123 | 27.557835 |

24 generated by VMD

| Ca |       |       |       |
|----|-------|-------|-------|
| Ca | 18.444542 | 33.015835 | 33.773724 |
| Ca | 23.082008 | 34.252396 | 36.045143 |
| Ca | 23.650154 | 30.022823 | 32.956699 |
| Ca | 22.768276 | 34.521755 | 30.815609 |
| Ca | 24.774300 | 30.873596 | 27.624386 |
| Ca | 27.642595 | 32.562824 | 31.298241 |
| Ca | 29.300362 | 29.100452 | 29.351120 |
| Ca | 30.588589 | 32.817657 | 25.941639 |
| Ca | 30.495647 | 27.950180 | 24.711943 |
| Ca | 33.599091 | 29.858994 | 28.577337 |
| Ca | 33.940498 | 24.788845 | 27.471195 |
| Ca | 35.726357 | 28.401333 | 24.041746 |
| S  | 21.301315 | 31.213396 | 35.379169 |
| S  | 20.747347 | 35.560822 | 33.505699 |
| S  | 21.956100 | 31.288395 | 29.920076 |
| S  | 25.148636 | 33.214127 | 33.453091 |
| S  | 26.151428 | 29.443808 | 30.494896 |
| S  | 25.688869 | 34.220470 | 28.688534 |
| S  | 28.147217 | 30.207336 | 25.953480 |
| S  | 30.711182 | 31.866123 | 29.454254 |
| S  | 31.386627 | 27.024357 | 28.083426 |
| S  | 32.904663 | 30.533115 | 25.048962 |
| S  | 33.449211 | 25.927555 | 23.914711 |
| S  | 36.114979 | 27.633842 | 27.434961 |

24 generated by VMD

| Ca |       |       |       |
|----|-------|-------|-------|
| Ca | 18.733582 | 33.387051 | 33.433945 |
| Ca | 23.040842 | 34.554947 | 35.976017 |
| Ca | 23.793938 | 29.815094 | 32.967834 |
| Ca | 22.986015 | 34.415779 | 30.643042 |
| Ca | 24.911884 | 30.679432 | 27.645128 |
| Ca | 27.836044 | 32.594398 | 31.323259 |
| Ca | 29.398804 | 29.042233 | 29.680450 |
|   | Ca   |            |            |      |
|---|------|------------|------------|------|
|   | 30.194759 | 32.899643 | 26.244892 |
|   | 30.305401 | 27.751369 | 24.600760 |
|   | 33.513138 | 29.702703 | 28.565716 |
|   | 33.897957 | 25.053257 | 27.133945 |
|   | 35.373428 | 29.006115 | 24.244511 |
| S | 21.236675 | 31.399189 | 35.280678 |
| S | 20.943829 | 35.591946 | 33.217979 |
| S | 21.933849 | 31.010817 | 29.778313 |
| S | 25.187332 | 33.083961 | 33.325569 |
| S | 26.421329 | 29.173712 | 30.727619 |
| S | 25.865505 | 33.971397 | 28.857300 |
| S | 28.132437 | 29.977402 | 26.127327 |
| S | 30.764397 | 31.889965 | 29.620495 |
| S | 31.182278 | 26.917038 | 28.114773 |
| S | 32.614952 | 30.336773 | 25.271919 |
| S | 33.361927 | 26.235569 | 23.656521 |
| S | 36.089775 | 27.810246 | 27.502159 |

24 generated by VMD

|   | Ca   |            |            |      |
|---|------|------------|------------|------|
|   | 18.169773 | 33.135651 | 33.643402 |
|   | 23.017096 | 34.391647 | 35.746498 |
|   | 23.625011 | 30.089767 | 33.027306 |
|   | 22.986917 | 34.882595 | 30.785513 |
|   | 24.812027 | 30.608072 | 27.691641 |
|   | 28.018414 | 32.785400 | 31.338074 |
|   | 29.415380 | 28.736988 | 29.664188 |
|   | 30.148743 | 32.727165 | 26.053982 |
|   | 30.353199 | 27.797577 | 24.647196 |
|   | 33.638172 | 29.567141 | 28.686764 |
|   | 34.181404 | 25.077244 | 27.073092 |
|   | 35.586132 | 28.962177 | 24.006021 |
| S | 20.928871 | 31.304935 | 35.307392 |
| S | 20.696480 | 35.588692 | 33.311661 |
| S | 22.119387 | 31.269705 | 30.058245 |
| S | 25.125885 | 33.271938 | 33.466370 |
| S | 26.400120 | 29.563698 | 30.786097 |
| S | 25.848999 | 33.896523 | 28.593636 |
| S | 28.026628 | 29.841908 | 26.413860 |
| S | 30.956297 | 31.766165 | 29.469538 |
| S | 31.332355 | 26.534733 | 27.917347 |
| S | 32.716019 | 30.485058 | 25.233654 |
| S | 33.365368 | 26.248997 | 23.622688 |
| S | 36.251320 | 27.766281 | 27.395912 |

24 generated by VMD

|   | Ca   |            |            |      |
|---|------|------------|------------|------|
|   | 18.528000 | 33.287464 | 33.825748 |
| Element | X-coordinate 1 | X-coordinate 2 | X-coordinate 3 |
|---------|----------------|----------------|----------------|
| Ca      | 22.892651      | 34.041458      | 36.018532      |
| Ca      | 23.531454      | 30.066601      | 32.803349      |
| Ca      | 22.889877      | 35.002380      | 30.716541      |
| Ca      | 24.887566      | 30.449162      | 27.651508      |
| Ca      | 27.566273      | 32.601273      | 31.305521      |
| Ca      | 29.510891      | 28.909462      | 29.718477      |
| Ca      | 30.215839      | 32.809433      | 25.894520      |
| Ca      | 30.567390      | 27.604160      | 24.784725      |
| Ca      | 33.708649      | 29.711075      | 28.562078      |
| Ca      | 34.152672      | 24.994652      | 26.973251      |
| Ca      | 35.77973       | 28.791901      | 23.928139      |
| S       | 21.093023      | 31.193693      | 35.539299      |
| S       | 20.696571      | 35.859802      | 33.501419      |
| S       | 21.971321      | 31.498924      | 29.845135      |
| S       | 24.862862      | 33.429863      | 33.294487      |
| S       | 26.184105      | 29.415573      | 30.604401      |
| S       | 25.731083      | 33.953377      | 28.764090      |
| S       | 28.180515      | 29.753386      | 26.482414      |
| S       | 30.958347      | 31.766407      | 29.330997      |
| S       | 31.362156      | 26.720131      | 28.263500      |
| S       | 32.951195      | 30.417646      | 25.103762      |
| S       | 33.330765      | 26.197914      | 23.521931      |
| S       | 36.168816      | 27.824266      | 27.506231      |

24 generated by VMD

| Element | X-coordinate 1 | X-coordinate 2 | X-coordinate 3 |
|---------|----------------|----------------|----------------|
| Ca      | 18.250170      | 33.081154      | 33.993492      |
| Ca      | 23.092640      | 34.359844      | 35.672279      |
| Ca      | 23.649673      | 29.870148      | 32.851200      |
| Ca      | 22.907740      | 34.681541      | 30.847137      |
| Ca      | 24.900818      | 30.691135      | 27.705921      |
| Ca      | 27.907637      | 32.449612      | 31.325340      |
| Ca      | 29.638103      | 28.813803      | 29.417133      |
| Ca      | 30.405453      | 32.709015      | 25.806108      |
| Ca      | 30.223377      | 28.039721      | 24.481052      |
| Ca      | 33.610863      | 29.612177      | 28.584640      |
| Ca      | 34.024494      | 25.214287      | 27.253202      |
| Ca      | 35.615490      | 28.791250      | 24.213507      |
| S       | 21.130070      | 31.440254      | 35.461563      |
| S       | 20.758636      | 35.627754      | 33.333019      |
| S       | 22.059372      | 31.283318      | 29.810724      |
| S       | 25.178904      | 33.156742      | 33.289143      |
| S       | 26.361826      | 29.337250      | 30.705544      |
| S       | 25.778919      | 34.152546      | 28.737467      |
| S       | 28.187895      | 29.913830      | 26.372379      |
| S       | 30.727186      | 31.863499      | 29.391665      |
| S       | 31.024191      | 26.814528      | 27.974831      |
|   | 32.964497 | 30.422884 | 25.216553 |
|---|-----------|-----------|-----------|
|  S | 33.280617 | 26.137066 | 23.776852 |
|  S | 36.041367 | 27.836639 | 27.717495 |

24

generated by VMD

|   | 18.535053 | 33.125145 | 33.421070 |
|---|-----------|-----------|-----------|
|  Ca| 23.160355 | 34.278114 | 35.984451 |
|  Ca| 23.524811 | 30.058464 | 32.661148 |
|  Ca| 22.749704 | 34.523026 | 30.789406 |
|  Ca| 24.915142 | 30.591200 | 27.751955 |
|  Ca| 27.562796 | 32.689278 | 31.189552 |
|  Ca| 29.700771 | 29.069920 | 29.610970 |
|  Ca| 30.294466 | 32.591759 | 25.922739 |
|  Ca| 30.210623 | 27.877254 | 25.138868 |
|  Ca| 33.830799 | 29.755455 | 28.832500 |
|  Ca| 33.974167 | 24.811275 | 26.974659 |
|  Ca| 35.571777 | 28.752686 | 23.875479 |
|  S | 21.193647 | 31.320269 | 35.228271 |
|  S | 20.924660 | 35.780411 | 33.646400 |
|  S | 21.910282 | 31.284416 | 29.792830 |
|  S | 24.998394 | 33.222286 | 33.358990 |
|  S | 26.314512 | 29.467384 | 30.583174 |
|  S | 25.693270 | 34.035164 | 28.685501 |
|  S | 28.032087 | 29.752542 | 26.391142 |
|  S | 30.802605 | 31.932549 | 29.638233 |
|  S | 31.392111 | 26.973230 | 28.369736 |
|  S | 32.955368 | 30.622948 | 25.386475 |
|  S | 33.176315 | 26.128580 | 23.554256 |
|  S | 36.296375 | 27.656733 | 27.152222 |

24

generated by VMD

|   | 18.311787 | 33.077988 | 33.449669 |
|---|-----------|-----------|-----------|
|  Ca| 22.989653 | 33.943653 | 35.993622 |
|  Ca| 23.745827 | 29.779617 | 32.787140 |
|  Ca| 23.135971 | 34.882801 | 30.830879 |
|  Ca| 24.845612 | 30.787445 | 27.771320 |
|  Ca| 27.942492 | 32.702278 | 31.421043 |
|  Ca| 29.536398 | 29.155819 | 29.638006 |
|  Ca| 30.132437 | 32.958603 | 25.889183 |
|  Ca| 30.441191 | 27.547951 | 24.932320 |
|  Ca| 33.509819 | 29.968195 | 28.565908 |
|  Ca| 34.065617 | 24.973396 | 27.280207 |
|  Ca| 35.317589 | 28.566534 | 23.922665 |
|  S | 21.012405 | 31.035522 | 35.005817 |
|  S | 20.851154 | 35.777210 | 33.583847 |
|  S | 21.960007 | 31.457832 | 29.858059 |
generated by VMD

Ca  18.522758  32.826111  33.602062
Ca  23.033100  33.906769  36.051262
Ca  23.757477  29.994713  32.781776
Ca  22.801718  34.785408  30.660398
Ca  25.086193  30.781214  27.780014
Ca  27.538143  33.039169  31.167490
Ca  29.701298  29.247814  29.629673
Ca  30.440506  32.920547  25.672688
Ca  30.176880  27.634377  24.941334
Ca  33.581978  29.673428  28.672724
Ca  33.88981  24.790514  27.129787
Ca  35.413509  28.555479  24.121171
Ca  21.263889  30.934109  34.866619
Ca  20.789541  35.605507  33.808350
Ca  22.133137  31.288647  29.699646
Ca  24.905483  33.345184  33.312241
Ca  26.484936  29.687862  30.744793
Ca  25.789639  34.333920  28.783838
Ca  28.393017  29.972733  26.401512
Ca  30.863129  31.983255  29.236589
Ca  31.389267  26.828983  28.291267
Ca  32.755451  30.466980  25.225458
Ca  32.920372  25.975851  23.697329
Ca  36.089657  27.721481  27.661734

24

generated by VMD

Ca  18.473530  32.670567  33.546860
Ca  22.970341  34.216843  35.816727
Ca  23.680752  30.064869  32.651939
Ca  22.841873  34.681492  30.895754
Ca  25.109589  31.067062  27.560242
Ca  27.943138  32.794373  31.314535
Ca  29.677269  29.276230  29.687157
Ca  30.223341  32.854565  25.878180
Ca  30.368603  27.718592  24.881535
|  |  |  |  |
|---|---|---|---|
| Ca | 33.495926 | 29.830265 | 28.705574 |
| Ca | 33.771160 | 24.826031 | 27.307245 |
| Ca | 35.348137 | 28.477482 | 33.581825 |
| S  | 21.199356 | 30.908108 | 35.124451 |
| S  | 20.660580 | 35.477482 | 33.581825 |
| S  | 22.095089 | 31.371433 | 29.691996 |
| S  | 25.194496 | 33.163937 | 33.416763 |
| S  | 26.434031 | 29.446312 | 30.600491 |
| S  | 25.750420 | 34.454796 | 28.892616 |
| S  | 28.351265 | 30.105911 | 26.403391 |
| S  | 30.871431 | 32.125198 | 29.392735 |
| S  | 31.348248 | 26.936798 | 28.413982 |
| S  | 32.709328 | 30.494539 | 25.158211 |
| S  | 33.111870 | 25.734711 | 23.843887 |
| S  | 36.090218 | 27.601851 | 27.364765 |

24

generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 18.321358 | 32.579090 | 33.724728 |
| Ca | 23.181616 | 33.991600 | 36.143093 |
| Ca | 23.618130 | 30.003422 | 32.604408 |
| Ca | 22.874470 | 34.858948 | 30.979467 |
| Ca | 24.965000 | 31.189316 | 27.428911 |
| Ca | 27.901779 | 32.746964 | 31.316334 |
| Ca | 29.447325 | 29.349274 | 29.483576 |
| Ca | 30.277027 | 32.759201 | 25.760597 |
| Ca | 30.421318 | 27.605255 | 24.866272 |
| Ca | 33.545261 | 29.933428 | 28.503180 |
| Ca | 33.909332 | 24.712713 | 27.655094 |
| Ca | 35.473450 | 28.496428 | 23.907253 |
| S  | 21.303879 | 31.012278 | 35.218632 |
| S  | 20.758589 | 35.378990 | 33.845894 |
| S  | 22.033239 | 31.587467 | 29.637405 |
| S  | 25.119053 | 33.228230 | 33.481472 |
| S  | 26.117411 | 29.732700 | 30.299892 |
| S  | 25.854549 | 34.347755 | 28.780336 |
| S  | 28.203426 | 29.844318 | 26.113081 |
| S  | 30.667084 | 32.091736 | 29.106096 |
| S  | 31.398310 | 26.894184 | 28.330540 |
| S  | 32.927711 | 30.500793 | 25.101763 |
| S  | 33.354919 | 25.668093 | 24.105171 |
| S  | 36.045769 | 27.787909 | 27.546848 |

24

generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 18.190838 | 32.640045 | 33.558563 |
| Ca | 22.956551 | 34.263512 | 35.998383 |
| Ca | 23.705843 | 30.256878 | 32.657612 |
Ca  22.932335  34.768478  30.926447
Ca  24.972233  30.961977  27.809483
Ca  27.929535  32.776421  31.413374
Ca  29.771042  29.173231  29.580351
Ca  30.044947  32.608246  25.820488
Ca  30.220091  27.584785  24.700874
Ca  33.584751  29.793274  28.584921
Ca  33.883148  24.741314  27.220158
Ca  35.478508  28.776770  23.966770
S   21.264944  31.112698  35.014854
S   20.472288  35.309891  33.703430
S   22.17731   31.623238  29.565300
S   25.112701  33.38455  33.412617
S   26.392639  29.587833  30.741673
S   26.160978  34.309464  28.928101
S   28.131233  29.608519  26.397327
S   30.770592  32.108681  29.208126
S   31.279350  26.950483  28.306568
S   32.793251  30.369358  25.127951
S   33.374043  26.046503  23.866920
S   36.120461  27.589949  27.429737

generated by VMD
Ca  18.380272  32.831108  33.819210
Ca  23.170349  33.975780  35.773182
Ca  23.621597  29.970081  32.439297
Ca  23.104828  34.740788  30.904875
Ca  24.922550  30.892508  27.694525
Ca  28.032331  32.810692  31.328373
Ca  29.613682  29.398140  29.719257
Ca  30.091776  32.659863  25.700306
Ca  30.176292  27.548431  25.026428
Ca  33.619148  29.917376  28.640862
Ca  33.729919  24.902769  27.404995
Ca  35.378716  28.836771  24.224197
S   21.292797  30.951805  34.992550
S   20.950981  35.445370  33.496670
S   22.029751  31.546978  29.486921
S   25.152443  32.979256  33.387482
S   26.525232  29.499117  30.612120
S   26.012424  34.306664  28.642056
S   28.166080  29.802883  26.245680
S   30.739727  32.201332  29.261950
S   31.243116  26.961330  28.385311
S   32.667145  30.351381  25.237480
S   33.105938  25.994156  23.871838
|    |    |    |    |
|----|----|----|----|
| S  | 35.992973 | 27.775471 | 27.444469 |
| 24 | generated by VMD |
| Ca | 18.415890  | 32.798290  | 33.987835  |
| Ca | 22.862595  | 33.938663  | 36.054440  |
| Ca | 23.830805  | 29.806849  | 32.625858  |
| Ca | 23.054386  | 34.529144  | 30.998955  |
| Ca | 24.995541  | 31.150751  | 27.487539  |
| Ca | 27.682863  | 33.062223  | 31.409485  |
| Ca | 29.732956  | 29.470263  | 29.374350  |
| Ca | 30.385143  | 32.936092  | 25.568251  |
| Ca | 30.324070  | 27.688244  | 24.691193  |
| Ca | 33.523956  | 29.748854  | 28.524151  |
| Ca | 33.642422  | 24.625011  | 27.660803  |
| Ca | 35.546867  | 28.537506  | 24.239971  |
| S  | 21.226604  | 30.866047  | 35.118515  |
| S  | 20.694519  | 35.452816  | 33.813618  |
| S  | 22.218990  | 31.353697  | 29.698009  |
| S  | 25.157209  | 33.113564  | 33.485287  |
| S  | 26.377062  | 29.749771  | 30.310104  |
| S  | 25.735189  | 34.383476  | 28.617981  |
| S  | 28.285496  | 30.028044  | 26.071087  |
| S  | 30.805399  | 32.368874  | 29.169603  |
| S  | 31.135460  | 27.037661  | 28.242821  |
| S  | 32.815735  | 30.498180  | 24.974865  |
| S  | 33.275822  | 25.707691  | 24.128157  |
| S  | 35.995094  | 27.444279  | 27.696289  |
| 24 | generated by VMD |
| Ca | 18.290054  | 32.930294  | 33.925011  |
| Ca | 23.057676  | 33.913509  | 36.122448  |
| Ca | 23.678722  | 29.991966  | 32.594627  |
| Ca | 23.042572  | 34.463646  | 30.937199  |
| Ca | 25.101152  | 31.016693  | 27.585873  |
| Ca | 27.876162  | 33.212105  | 31.130413  |
| Ca | 29.794914  | 29.411371  | 29.452850  |
| Ca | 30.188211  | 32.711189  | 25.736927  |
| Ca | 30.195093  | 27.612144  | 24.661385  |
| Ca | 33.673416  | 29.912405  | 28.577627  |
| Ca | 33.701073  | 24.828468  | 27.527390  |
| Ca | 35.539951  | 28.478596  | 24.241312  |
| S  | 21.088642  | 30.784546  | 34.959492  |
| S  | 20.889736  | 35.386887  | 33.896576  |
| S  | 22.101227  | 31.482161  | 29.605156  |
| S  | 25.012955  | 32.981766  | 33.476593  |
| S  | 26.520756  | 29.811588  | 30.479443  |
|   |   |   |   |
|---|---|---|---|
| S | 25.847303 | 34.269493 | 28.702768 |
| S | 28.275930 | 29.945896 | 25.986000 |
| S | 30.853296 | 32.318047 | 29.219742 |
| S | 31.080517 | 27.121691 | 28.163666 |
| S | 32.798649 | 30.367216 | 25.115541 |
| S | 33.204323 | 25.769714 | 24.160091 |
| S | 35.907776 | 27.578648 | 27.681908 |

24

generated by VMD

| Ca | 18.541821 | 32.847759 | 34.028229 |
| Ca | 22.796553 | 33.753784 | 36.190777 |
| Ca | 23.708538 | 29.923218 | 32.667076 |
| Ca | 22.987244 | 34.920513 | 30.997078 |
| Ca | 24.897324 | 31.115242 | 27.392345 |
| Ca | 28.008379 | 32.904228 | 31.149822 |
| Ca | 29.437832 | 29.404268 | 29.476484 |
| Ca | 30.119957 | 32.860432 | 25.582317 |
| Ca | 30.309059 | 27.643612 | 24.568985 |
| Ca | 33.631626 | 29.680449 | 28.426126 |
| Ca | 35.584743 | 24.756548 | 27.747032 |
| Ca | 35.634911 | 28.587315 | 24.453909 |
| S | 21.315065 | 30.814190 | 35.372375 |
| S | 20.796974 | 35.263672 | 33.618050 |
| S | 21.979469 | 31.566137 | 29.743303 |
| S | 25.061375 | 33.065201 | 33.417736 |
| S | 26.667387 | 29.633612 | 30.340742 |
| S | 25.851562 | 34.281010 | 28.569572 |
| S | 28.172312 | 30.147299 | 25.993763 |
| S | 30.944994 | 32.164604 | 28.969402 |
| S | 31.078529 | 27.098017 | 28.067604 |
| S | 32.854595 | 30.497564 | 24.867325 |
| S | 33.206253 | 25.739309 | 24.332207 |
| S | 36.133560 | 27.632055 | 27.967756 |

24

generated by VMD

| Ca | 18.483036 | 33.092701 | 34.245846 |
| Ca | 22.824886 | 33.478432 | 36.101337 |
| Ca | 23.597584 | 29.918114 | 32.355263 |
| Ca | 22.967960 | 34.985039 | 30.789738 |
| Ca | 24.903271 | 31.220284 | 27.633942 |
| Ca | 28.001707 | 32.911041 | 31.320122 |
| Ca | 29.590137 | 29.189293 | 29.594465 |
| Ca | 30.275091 | 32.584175 | 25.638229 |
| Ca | 30.272219 | 27.524612 | 24.726715 |
| Ca | 33.486366 | 29.916878 | 28.578733 |
| Ca | 33.924980 | 24.894835 | 27.605711 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 35.444202 | 28.463797 | 24.045307 |
| S       | 21.157028 | 30.769087 | 35.030445 |
| S       | 20.694448 | 35.440353 | 33.673134 |
| S       | 21.858559 | 31.712973 | 29.547205 |
| S       | 24.980501 | 33.223904 | 33.386715 |
| S       | 26.631519 | 29.737574 | 30.537117 |
| S       | 25.887749 | 34.325237 | 28.788345 |
| S       | 28.292725 | 29.802284 | 26.305706 |
| S       | 31.080599 | 32.252075 | 29.142694 |
| S       | 31.233070 | 26.846542 | 28.182493 |
| S       | 32.684769 | 30.276802 | 24.987604 |
| S       | 33.273781 | 25.819677 | 24.082737 |
| S       | 36.173897 | 27.914364 | 27.640425 |

24

generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.071085 | 32.909378 | 34.188183 |
| Ca      | 23.061039 | 33.275871 | 36.224781 |
| Ca      | 23.507034 | 30.017822 | 32.452251 |
| Ca      | 23.048168 | 34.909809 | 30.967394 |
| Ca      | 25.054914 | 31.216793 | 27.342381 |
| Ca      | 27.998089 | 33.176537 | 31.559156 |
| Ca      | 29.308640 | 29.694632 | 29.662079 |
| Ca      | 30.363010 | 32.523254 | 25.327633 |
| Ca      | 30.373716 | 27.562140 | 24.915190 |
| Ca      | 33.664005 | 29.773472 | 28.346073 |
| Ca      | 33.696369 | 25.060663 | 28.092289 |
| Ca      | 35.460236 | 28.362272 | 23.819529 |
| S       | 20.902344 | 30.458061 | 34.870567 |
| S       | 20.767727 | 35.193367 | 33.881001 |
| S       | 22.173721 | 31.739667 | 29.551352 |
| S       | 24.993525 | 33.242157 | 33.325657 |
| S       | 26.326382 | 29.880297 | 30.431534 |
| S       | 26.075218 | 34.558838 | 28.760128 |
| S       | 28.284861 | 29.888342 | 26.227539 |
| S       | 31.096239 | 32.207119 | 29.127680 |
| S       | 31.407322 | 27.151981 | 28.432503 |
| S       | 32.710114 | 30.289518 | 24.813499 |
| S       | 33.123444 | 25.422747 | 24.223030 |
| S       | 36.252892 | 27.791092 | 27.398628 |

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generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 18.431614 | 32.737785 | 34.386845 |
| Ca      | 23.028900 | 33.250927 | 36.140579 |
| Ca      | 23.763901 | 30.200424 | 32.295643 |
| Ca      | 22.999685 | 34.983307 | 30.804674 |
| Ca      | 24.902746 | 31.155729 | 27.378765 |
| Chemical Element | X Position | Y Position | Z Position |
|------------------|------------|------------|------------|
| Ca               | 28.013027  | 33.236885  | 31.233315  |
| Ca               | 29.407398  | 29.581623  | 29.594368  |
| Ca               | 30.071180  | 32.611149  | 25.498325  |
| Ca               | 30.262516  | 27.739012  | 24.915426  |
| Ca               | 33.630985  | 29.782907  | 28.652712  |
| Ca               | 33.614899  | 24.807899  | 27.589508  |
| Ca               | 35.524078  | 28.505899  | 24.279232  |
| S                | 21.308868  | 30.438486  | 34.859730  |
| S                | 20.898865  | 35.155357  | 33.916367  |
| S                | 22.034904  | 31.561687  | 29.570694  |
| S                | 25.157551  | 33.464134  | 33.186058  |
| S                | 26.548521  | 29.874352  | 30.494595  |
| S                | 25.727200  | 34.435272  | 28.361698  |
| S                | 27.919292  | 29.874710  | 26.286085  |
| S                | 31.046463  | 32.267555  | 28.963316  |
| S                | 31.308235  | 27.047760  | 28.406349  |
| S                | 32.849869  | 30.454687  | 25.219292  |
| S                | 33.275436  | 25.765715  | 24.091892  |
| S                | 35.993927  | 27.366760  | 27.814554  |

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-generated by VMD-

| Chemical Element | X Position | Y Position | Z Position |
|------------------|------------|------------|------------|
| Ca               | 18.382977  | 32.722649  | 34.349953  |
| Ca               | 23.031847  | 33.334190  | 36.227028  |
| Ca               | 23.779999  | 30.222298  | 32.345060  |
| Ca               | 22.919296  | 34.694736  | 31.055691  |
| Ca               | 24.834557  | 31.063892  | 27.495684  |
| Ca               | 28.077663  | 33.372757  | 31.233709  |
| Ca               | 29.391615  | 29.410496  | 29.446350  |
| Ca               | 30.184608  | 32.485634  | 25.439463  |
| Ca               | 30.318535  | 27.662743  | 24.885572  |
| Ca               | 33.479996  | 29.850286  | 28.761127  |
| Ca               | 33.575150  | 24.627064  | 27.510439  |
| Ca               | 35.604103  | 28.550236  | 24.347679  |
| S                | 21.438402  | 30.639397  | 34.874393  |
| S                | 20.825115  | 35.145954  | 33.940514  |
| S                | 22.151421  | 31.474623  | 29.443285  |
| S                | 24.964405  | 33.482841  | 33.081760  |
| S                | 26.741337  | 30.135046  | 30.454947  |
| S                | 25.874372  | 34.626419  | 28.556540  |
| S                | 28.099178  | 29.573483  | 26.022078  |
| S                | 30.835474  | 32.445053  | 28.987831  |
| S                | 31.162525  | 27.038712  | 28.364029  |
| S                | 32.827522  | 30.484873  | 25.300255  |
| S                | 33.411106  | 25.827187  | 23.986223  |
| S                | 35.808861  | 27.429451  | 27.830080  |

24
Ca | 18.165176 | 33.188957 | 34.160782
---|-----------|-----------|-----------
Ca | 23.072706 | 33.513550 | 36.100861
Ca | 23.450733 | 30.028173 | 32.285019
Ca | 22.991638 | 34.644512 | 30.869549
Ca | 25.044022 | 30.734426 | 27.648205
Ca | 28.112427 | 33.011456 | 31.515585
Ca | 29.513237 | 29.494032 | 29.770515
Ca | 30.157822 | 32.938202 | 25.744808
Ca | 30.457912 | 27.468082 | 24.921627
Ca | 33.522064 | 29.794718 | 28.522696
Ca | 33.507339 | 24.943705 | 27.514574
Ca | 35.594357 | 28.638012 | 23.806103
S  | 20.873638 | 30.854141 | 34.687157
S  | 20.868595 | 35.409714 | 33.794228
S  | 22.065973 | 31.369759 | 29.457224
S  | 25.051174 | 33.299210 | 33.152672
S  | 26.668634 | 29.736246 | 30.969091
S  | 26.046757 | 34.119125 | 28.640438
S  | 28.290154 | 29.968872 | 26.418217
S  | 31.050760 | 32.280579 | 29.332672
S  | 31.185659 | 27.053362 | 28.453733
S  | 32.708260 | 30.396267 | 24.954662
S  | 33.226250 | 25.733343 | 23.865685
S  | 36.094719 | 27.681585 | 27.353960

24

Ca | 18.256577 | 32.698360 | 33.410866
Ca | 23.086708 | 33.595520 | 35.716068
Ca | 23.919632 | 30.092953 | 32.925339
Ca | 22.819340 | 34.569626 | 30.817318
Ca | 25.152992 | 31.069723 | 27.596466
Ca | 28.148491 | 33.093094 | 31.347586
Ca | 29.523230 | 29.306417 | 29.646681
Ca | 30.328979 | 32.912140 | 25.742262
Ca | 30.280300 | 27.650135 | 25.019009
Ca | 33.547955 | 29.981960 | 28.586590
Ca | 33.295204 | 24.761337 | 27.390532
Ca | 35.248779 | 28.504478 | 24.041187
S  | 20.963017 | 30.652683 | 34.765778
S  | 20.749805 | 35.248333 | 33.744877
S  | 22.201067 | 31.276218 | 29.929558
S  | 25.147963 | 33.483910 | 33.317406
S  | 26.707952 | 29.862606 | 30.664801
S  | 25.968353 | 34.325363 | 28.752239
S  | 28.373745 | 30.030876 | 26.373344
generated by VMD

S  31.265907  32.517838  29.382233
S  31.166218  27.162136  28.003100
S  32.604347  30.459356  25.127033
S  33.149178  25.629875  27.545795
24

Ca  18.366684  32.592171  33.581043
Ca  22.945364  33.459763  36.039818
Ca  23.896114  29.838413  32.520302
Ca  22.804253  34.666580  30.992664
Ca  25.046230  31.330343  27.734951
Ca  28.050430  33.249924  31.230278
Ca  29.480602  29.593325  29.582766
Ca  30.564331  32.803024  25.458458
Ca  30.290705  27.763117  24.865906
Ca  33.327080  29.879827  28.584850
Ca  33.431614  24.834736  27.844074
Ca  35.615440  28.134924  23.912327
Ca  21.244154  30.612675  34.720509
S  20.686226  35.227833  34.117233
S  22.058142  31.364805  29.707315
S  25.162834  33.312691  33.437801
S  25.714682  34.524971  28.701099
S  28.345200  30.189493  26.263847
S  30.966555  32.444836  29.013563
S  32.943855  30.208309  25.085991
S  33.118393  25.465256  24.111816
S  35.834499  27.612225  27.552357

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generated by VMD

Ca  18.591202  32.435867  33.371655
Ca  23.110649  33.392338  36.148430
Ca  23.947863  30.182430  32.601051
Ca  22.853458  34.800442  30.928143
Ca  24.999214  30.970245  27.698187
Ca  28.127337  33.196655  31.322878
Ca  29.486643  29.464365  29.580641
Ca  30.546837  32.886787  25.421127
Ca  30.379738  27.673050  24.747313
Ca  33.291397  29.948076  28.695854
Ca  33.284126  24.664555  27.494600
Ca  35.617157  28.179178  24.159641
S  21.295874  30.388367  34.801861
S  20.615242       35.132858       33.795963
S  21.915215       31.613646       29.861698
S  25.126848       33.558014       33.441883
S  26.852108       30.054451       30.671707
S  25.713737       34.380436       28.686249
S  28.160309       30.070686       26.235420
S  30.984018       32.774025       29.031080
S  31.042137       27.145948       28.373629
S  32.788651       30.336046       25.167795
S  33.146465       25.610312       24.006401
S  35.843822       27.441242       27.697737

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generated by VMD
Ca  18.572510       32.572319       33.673538
Ca  23.406052       33.158855       35.941250
Ca  23.893385       29.977034       32.723572
Ca  22.516361       34.831974       30.813313
Ca  24.903353       31.185957       27.410112
Ca  27.955456       33.300278       31.116394
Ca  29.391544       29.483875       29.546919
Ca  30.788246       32.788876       25.283882
Ca  30.264742       27.786934       24.830566
Ca  33.329659       29.907711       28.565029
Ca  33.422951       24.832899       27.752333
Ca  35.607708       28.085749       24.321194
S  21.390717       30.317415       34.797604
S  20.926201       35.030048       34.208508
S  21.968843       31.435095       29.708397
S  25.115814       33.485405       33.301079
S  26.766937       30.011827       30.494341
S  25.530228       34.511864       28.633627
S  28.188070       30.486773       26.198437
S  30.966747       32.700668       29.040989
S  30.920055       27.164742       28.397629
S  32.982231       30.380989       25.069613
S  33.110031       25.564070       24.256624
S  35.802223       27.298729       27.855122

24

generated by VMD
Ca  18.681984       32.775978       34.066837
Ca  23.263741       33.373405       36.186535
Ca  23.654615       30.083437       32.409111
Ca  22.724628       34.875763       30.881157
Ca  24.878716       31.142477       27.388620
Ca  27.852161       33.087875       31.181883
Ca  29.495914       29.254126       29.662756
|   |   |   |
|---|---|---|
| Ca | 30.609032 | 33.073643 | 25.553764 |
| Ca | 30.662411 | 27.724920 | 24.877588 |
| Ca | 33.574120 | 24.777252 | 27.574041 |
| Ca | 35.541641 | 28.236187 | 24.203825 |
| S  | 21.467850 | 30.484314 | 35.162350 |
| S  | 20.940968 | 35.304638 | 33.928375 |
| S  | 24.782742 | 33.3061076 | 33.206757 |
| S  | 26.540274 | 29.791214 | 30.295627 |
| S  | 25.625847 | 34.352669 | 28.571226 |
| S  | 28.370031 | 30.158829 | 26.030882 |
| S  | 30.959698 | 32.431213 | 29.219503 |
| S  | 31.168324 | 27.127253 | 28.460890 |
| S  | 32.885815 | 30.371550 | 25.113451 |
| S  | 33.221615 | 25.362171 | 24.039795 |
| S  | 35.775032 | 27.581331 | 27.756012 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.471596 | 33.087032 | 33.429173 |
| Ca | 22.945505 | 33.526306 | 36.269691 |
| Ca | 23.627678 | 29.797565 | 32.506924 |
| Ca | 22.978489 | 34.676029 | 30.859207 |
| Ca | 25.011003 | 31.055454 | 27.563625 |
| Ca | 27.992962 | 32.936516 | 31.138947 |
| Ca | 29.614855 | 29.423637 | 29.743336 |
| Ca | 30.828325 | 32.789696 | 25.783384 |
| Ca | 30.163393 | 27.508556 | 24.880037 |
| Ca | 33.384056 | 30.075344 | 28.372293 |
| Ca | 33.664303 | 24.851137 | 27.664625 |
| Ca | 35.372158 | 28.450624 | 24.005342 |
| S  | 21.014412 | 30.800823 | 34.878117 |
| S  | 20.851879 | 35.379040 | 33.946442 |
| S  | 22.094902 | 31.252140 | 29.789444 |
| S  | 25.118561 | 33.254471 | 33.309483 |
| S  | 26.571663 | 29.685520 | 30.661448 |
| S  | 25.871048 | 34.185356 | 28.518856 |
| S  | 28.391106 | 30.314880 | 26.417612 |
| S  | 31.049370 | 32.399734 | 29.332947 |
| S  | 31.223135 | 27.098553 | 28.368887 |
| S  | 32.542633 | 30.323494 | 24.931850 |
| S  | 33.034573 | 25.736177 | 24.062466 |
| S  | 35.902416 | 27.692028 | 27.505939 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 18.501114 | 32.768379 | 33.503841 |
| Element | X1  | X2  | X3  |
|---------|-----|-----|-----|
| Ca      | 23.042473 | 33.454865 | 36.188320 |
| Ca      | 23.594501  | 30.094030  | 32.648926  |
| Ca      | 23.145817  | 34.589485  | 30.821226  |
| Ca      | 24.848158  | 31.095711  | 27.573919  |
| Ca      | 27.73502   | 32.936356  | 31.245621  |
| Ca      | 29.521626  | 29.425114  | 29.810825  |
| Ca      | 30.835403  | 32.864212  | 25.814888  |
| Ca      | 30.181938  | 27.731430  | 24.640640  |
| Ca      | 33.406368  | 29.946909  | 28.379789  |
| Ca      | 33.776310  | 24.905043  | 27.612452  |
| Ca      | 35.16083   | 28.043287  | 23.976255  |
| S       | 21.171562  | 30.674946  | 34.940937  |
| S       | 20.952875  | 35.326427  | 33.865337  |
| S       | 21.958172  | 31.367149  | 29.684845  |
| S       | 25.001129  | 33.423943  | 33.245422  |
| S       | 26.608208  | 29.780043  | 30.611378  |
| S       | 25.777895  | 34.169380  | 28.579222  |
| S       | 28.423534  | 30.335039  | 26.389593  |
| S       | 30.979942  | 32.529182  | 29.529585  |
| S       | 31.046097  | 27.077000  | 28.334631  |
| S       | 32.790006  | 30.303560  | 25.000322  |
| S       | 32.940231  | 25.617685  | 24.039803  |
| S       | 35.923176  | 27.840845  | 27.502317  |

24 generated by VMD

| Element | X1  | X2  | X3  |
|---------|-----|-----|-----|
| Ca      | 18.682396 | 33.184063 | 33.508404 |
| Ca      | 22.911884 | 33.260040 | 36.201851 |
| Ca      | 23.727110 | 29.795753 | 32.645454 |
| Ca      | 22.767561 | 34.784203 | 30.906792 |
| Ca      | 25.153187 | 31.034233 | 27.584784 |
| Ca      | 27.862093 | 32.917564 | 31.33851  |
| Ca      | 29.628407 | 29.304527 | 29.563452 |
| Ca      | 30.669983 | 33.036469 | 25.443638 |
| Ca      | 30.342047 | 27.740686 | 24.746973 |
| Ca      | 33.422039 | 30.142822 | 28.615776 |
| Ca      | 33.788872 | 24.675516 | 27.446157 |
| Ca      | 35.385612 | 28.083544 | 24.24027  |
| S       | 21.115917 | 30.701385 | 34.934906 |
| S       | 20.950958 | 35.340347 | 34.001831 |
| S       | 22.179218 | 31.385628 | 29.827135 |
| S       | 24.864788 | 33.221008 | 33.264980 |
| S       | 26.688984 | 29.706568 | 30.502098 |
| S       | 25.835247 | 34.248489 | 28.591343 |
| S       | 28.302645 | 30.371658 | 26.176981 |
| S       | 30.882153 | 32.683868 | 29.175299 |
| S       | 31.243977 | 27.172422 | 28.412901 |
|     |       |       |       |
|-----|-------|-------|-------|
| S   | 32.675919 | 30.248741 | 24.941921 |
| S   | 32.910934 | 25.462666 | 24.100410 |
| S   | 35.728127 | 27.797806 | 27.771099 |

24 generated by VMD

| Ca  |       |       |       |
|-----|-------|-------|-------|
| Ca  | 18.453140 | 33.178741 | 33.658264 |
| Ca  | 23.299078 | 33.459587 | 35.986385 |
| Ca  | 23.657211 | 29.887775 | 32.691841 |
| Ca  | 22.873219 | 34.577793 | 30.981762 |
| Ca  | 24.918520 | 30.998579 | 27.472708 |
| Ca  | 27.704727 | 32.850258 | 31.070499 |
| Ca  | 29.447762 | 29.409151 | 29.620052 |
| Ca  | 30.804840 | 33.011658 | 25.723621 |
| Ca  | 30.158333 | 27.565323 | 24.806906 |
| Ca  | 33.513092 | 30.080019 | 28.586231 |
| Ca  | 33.647560 | 24.888264 | 27.607195 |
| Ca  | 35.409767 | 28.411360 | 24.098660 |
| S   | 20.953674 | 30.771156 | 34.781418 |
| S   | 21.124680 | 35.424255 | 33.999084 |
| S   | 22.213985 | 31.304461 | 29.772493 |
| S   | 25.161448 | 33.250233 | 33.341274 |
| S   | 26.541924 | 29.641769 | 30.667282 |
| S   | 25.447035 | 34.150345 | 28.495329 |
| S   | 28.410101 | 30.339947 | 26.248795 |
| S   | 30.933538 | 32.296349 | 29.329113 |
| S   | 31.301006 | 27.115913 | 28.320427 |
| S   | 32.737701 | 30.314657 | 24.959660 |
| S   | 33.119545 | 25.629601 | 23.993301 |
| S   | 35.888115 | 27.742834 | 27.727770 |

24 generated by VMD

| Ca  |       |       |       |
|-----|-------|-------|-------|
| Ca  | 18.454239 | 33.029488 | 33.796303 |
| Ca  | 23.407768 | 33.393589 | 35.965469 |
| Ca  | 23.380224 | 30.004017 | 32.334209 |
| Ca  | 22.829927 | 34.494812 | 31.163292 |
| Ca  | 24.977730 | 31.069637 | 27.678692 |
| Ca  | 27.941719 | 33.153187 | 31.147800 |
| Ca  | 29.424454 | 29.676495 | 29.768843 |
| Ca  | 30.800053 | 32.847813 | 25.674479 |
| Ca  | 30.224232 | 27.665443 | 24.965984 |
| Ca  | 33.500549 | 29.919783 | 28.603264 |
| Ca  | 33.589268 | 25.077759 | 27.514317 |
| Ca  | 35.649620 | 28.115498 | 23.929838 |
| S   | 21.064522 | 30.802248 | 34.768112 |
| S   | 20.992561 | 35.123444 | 34.175583 |
| S   | 21.957760 | 31.207245 | 29.558355 |
|   |   |   |
|---|---|---|
| S | 25.087669 | 33.254997 | 33.013744 |
| S | 26.684166 | 29.829897 | 30.667677 |
| S | 25.464067 | 34.428505 | 28.506033 |
| S | 28.383621 | 30.282106 | 26.250757 |
| S | 30.982883 | 32.252411 | 29.263517 |
| S | 31.244659 | 27.083477 | 28.489033 |
| S | 32.755066 | 30.209412 | 25.064497 |
| S | 33.034451 | 25.705627 | 23.933821 |
| S | 35.888824 | 27.673183 | 27.706453 |

24 generated by VMD

| Ca | 18.333923 | 32.430126 | 33.902363 |
| Ca | 23.056049 | 33.657799 | 36.137615 |
| Ca | 23.673992 | 30.005766 | 32.534943 |
| Ca | 22.936825 | 34.895390 | 30.906366 |
| Ca | 24.968807 | 31.121723 | 27.554869 |
| Ca | 27.648447 | 33.115936 | 31.308167 |
| Ca | 29.527140 | 29.555204 | 29.487705 |
| Ca | 30.746002 | 32.603760 | 25.545839 |
| Ca | 30.293697 | 27.544008 | 24.700386 |
| Ca | 33.563183 | 30.048138 | 28.610733 |
| Ca | 33.699688 | 24.859659 | 27.493542 |
| Ca | 35.665657 | 28.109825 | 24.042068 |
| S | 21.126759 | 30.726654 | 34.976967 |
| S | 20.713377 | 35.280296 | 34.103168 |
| S | 22.053127 | 31.647516 | 29.632090 |
| S | 25.140759 | 33.274368 | 33.289028 |
| S | 26.586441 | 29.893442 | 30.589375 |
| S | 25.851330 | 34.394234 | 28.487402 |
| S | 28.233242 | 30.072001 | 26.186014 |
| S | 30.890987 | 32.384087 | 29.310368 |
| S | 31.317101 | 27.146578 | 28.301884 |
| S | 32.762901 | 30.214069 | 25.127256 |
| S | 33.057961 | 25.688204 | 23.961021 |
| S | 35.872669 | 27.631220 | 27.750839 |

24 generated by VMD

| Ca | 18.180252 | 32.576954 | 33.377766 |
| Ca | 22.937521 | 34.202885 | 36.200325 |
| Ca | 23.760859 | 30.162573 | 32.747475 |
| Ca | 22.854942 | 34.792595 | 30.705097 |
| Ca | 25.137371 | 30.621950 | 27.870520 |
| Ca | 27.762100 | 32.895653 | 31.669827 |
| Ca | 29.638645 | 29.285593 | 29.580372 |
| Ca | 30.523327 | 32.773411 | 25.663235 |
| Ca | 30.437061 | 27.600103 | 24.632332 |
|   | Ca    | S     | S     |
|---|-------|-------|-------|
|  1 | 33.499523 | 29.633005 | 28.557348 |
|  2 | 33.482307 | 24.840294 | 27.258533 |
|  3 | 35.749226 | 35.244644 | 33.689743 |
|  4 | 21.112288 | 31.233894 | 35.039082 |
|  5 | 20.511494 | 35.244644 | 33.689743 |
|  6 | 22.298828 | 31.320137 | 29.808168 |
|  7 | 24.980373 | 33.611183 | 33.329865 |
|  8 | 26.828777 | 29.711084 | 31.096228 |
|  9 | 25.883865 | 34.144257 | 28.887327 |
| 10 | 28.310459 | 29.942787 | 26.221172 |
| 11 | 30.767616 | 32.209728 | 29.433563 |
| 12 | 30.926193 | 26.857553 | 28.101568 |
| 13 | 32.878189 | 30.478237 | 25.079353 |
| 14 | 33.301693 | 25.915516 | 23.684099 |
| 15 | 35.957203 | 27.590837 | 27.389675 |

24

generated by VMD

|   | Ca    | S     | S     |
|---|-------|-------|-------|
|  1 | 18.457687 | 32.539677 | 33.713978 |
|  2 | 22.901024 | 33.614616 | 35.908642 |
|  3 | 23.715811 | 29.967196 | 32.610611 |
|  4 | 23.106647 | 34.813263 | 30.688259 |
|  5 | 25.022537 | 30.821486 | 27.713308 |
|  6 | 27.995720 | 33.276184 | 31.357780 |
|  7 | 29.454365 | 29.674454 | 29.773445 |
|  8 | 30.485401 | 32.809570 | 25.670263 |
|  9 | 30.258671 | 27.864969 | 24.711304 |
| 10 | 33.515030 | 29.908909 | 28.529224 |
| 11 | 33.340115 | 24.817583 | 27.553308 |
| 12 | 35.324062 | 28.352728 | 24.056473 |
| 13 | 21.094921 | 30.534271 | 34.886894 |
| 14 | 20.799681 | 35.177460 | 33.668316 |
| 15 | 22.200455 | 31.400620 | 29.647879 |
| 16 | 25.087284 | 33.221416 | 33.353310 |
| 17 | 26.733212 | 29.955414 | 30.951832 |
| 18 | 26.013538 | 34.074265 | 28.449959 |
| 19 | 28.361935 | 30.265182 | 26.430714 |
| 20 | 31.309204 | 32.467636 | 29.318350 |
| 21 | 31.068712 | 27.182203 | 28.347271 |
| 22 | 32.890259 | 30.505333 | 25.097763 |
| 23 | 32.905037 | 25.684309 | 23.895905 |
| 24 | 35.678776 | 27.371340 | 27.605267 |

24

generated by VMD

|   | Ca    | S     | S     |
|---|-------|-------|-------|
|  1 | 18.399685 | 33.231754 | 33.592487 |
|  2 | 23.086803 | 33.716675 | 36.078659 |
|  3 | 23.801392 | 30.127735 | 32.808887 |

606
| Periodic Table | X-coordinates | Y-coordinates | Z-coordinates |
|---------------|---------------|---------------|---------------|
| Ca            | 23.037560     | 34.711964     | 30.847761     |
| Ca            | 24.801964     | 30.641403     | 27.596064     |
| Ca            | 28.079109     | 32.787613     | 31.140625     |
| Ca            | 29.289059     | 29.376801     | 29.605413     |
| Ca            | 30.156124     | 32.604950     | 25.781889     |
| Ca            | 30.328594     | 27.837868     | 24.819111     |
| Ca            | 33.656231     | 29.901293     | 28.602827     |
| Ca            | 33.625206     | 24.876793     | 27.355566     |
| Ca            | 35.553162     | 28.634222     | 24.062031     |
| S             | 20.907873     | 30.834789     | 35.076954     |
| S             | 20.988167     | 35.588158     | 33.806507     |
| S             | 22.059185     | 31.315540     | 29.792063     |
| S             | 24.972672     | 33.385750     | 33.224014     |
| S             | 26.532791     | 29.514643     | 30.665279     |
| S             | 25.814339     | 33.911453     | 28.554428     |
| S             | 28.068733     | 29.944178     | 26.262392     |
| S             | 31.044052     | 32.191605     | 29.232100     |
| S             | 31.389517     | 26.998268     | 28.219460     |
| S             | 32.696236     | 30.449240     | 25.312265     |
| S             | 33.294342     | 26.113567     | 23.981213     |
| S             | 36.137215     | 27.603731     | 27.522072     |

24 generated by VMD

| Periodic Table | X-coordinates | Y-coordinates | Z-coordinates |
|---------------|---------------|---------------|---------------|
| Ca            | 18.490559     | 33.046883     | 33.606606     |
| Ca            | 23.078970     | 33.518517     | 36.323265     |
| Ca            | 23.908665     | 30.375780     | 32.530201     |
| Ca            | 22.920876     | 34.728661     | 31.106262     |
| Ca            | 24.704655     | 30.861347     | 27.554043     |
| Ca            | 27.963303     | 33.039528     | 31.219566     |
| Ca            | 29.372173     | 29.259623     | 29.622221     |
| Ca            | 30.234900     | 32.463005     | 25.774967     |
| Ca            | 30.167669     | 27.435507     | 24.939281     |
| Ca            | 33.605072     | 29.798391     | 28.746334     |
| Ca            | 33.940010     | 24.916647     | 27.365107     |
| Ca            | 35.743176     | 28.732443     | 24.000265     |
| S             | 21.151939     | 30.947920     | 34.832905     |
| S             | 20.888641     | 35.442791     | 33.948544     |
| S             | 22.003122     | 31.377354     | 29.627832     |
| S             | 24.873882     | 33.548550     | 33.187553     |
| S             | 26.482372     | 29.827971     | 30.429033     |
| S             | 25.527142     | 34.217979     | 28.663973     |
| S             | 27.970678     | 29.791466     | 26.238398     |
| S             | 31.208458     | 32.134899     | 29.239792     |
| S             | 31.291597     | 26.861294     | 28.521250     |
| S             | 32.705200     | 30.175238     | 25.187721     |
| S             | 33.215797     | 26.114136     | 23.764256     |
S       36.271263       27.684151       27.510689

24 generated by VMD
Ca      18.530394       32.655968       33.859505
Ca      23.173119       33.734116       36.185192
Ca      23.708233       30.237293       32.452057
Ca      22.725595       34.580791       30.940062
Ca      24.789696       31.049488       27.374332
Ca      27.994720       33.227989       31.185940
Ca      29.514008       29.579773       29.734716
Ca      30.499115       32.625153       25.666594
Ca      30.261709       27.876829       24.938902
Ca      33.694267       29.777140       28.549908
Ca      33.526371       24.807947       27.389795
Ca      35.567490       28.459417       24.231293
S       21.240587       30.707577       35.094189
S       20.944000       35.129555       33.887108
S       21.828320       31.316580       29.465055
S       24.935123       33.500137       33.083462
S       26.550837       29.928623       30.481188
S       25.621170       34.281723       28.690437
S       28.357973       30.036219       26.399622
S       31.033117       32.218246       29.182577
S       31.320881       27.005011       28.395185
S       32.838524       30.273752       25.166716
S       33.060841       25.971542       23.978878
S       36.004002       27.319143       27.607361

24 generated by VMD
Ca      18.532198       33.120049       33.730896
Ca      23.478683       33.491039       36.123631
Ca      23.865707       30.126728       32.343735
Ca      23.046795       34.615910       31.116886
Ca      24.729702       30.925772       27.297924
Ca      28.117088       32.962166       31.053827
Ca      29.401333       29.423220       29.577534
Ca      30.034710       32.470512       25.614487
Ca      30.278305       27.553192       24.825539
Ca      33.464527       29.953669       28.655481
Ca      33.679157       24.830812       27.542479
Ca      35.541210       28.853331       24.438444
S       21.307764       30.767868       34.739891
S       21.042179       35.397255       34.187786
S       21.867310       31.250883       29.687510
S       25.133839       33.216949       33.248867
S       26.507004       29.674086       30.351954
S    25.662041  34.253975  28.571854
S    27.986219  29.891169  26.068336
S    30.907127  32.567936  29.085768
S    31.124889  27.226051  28.454540
S    32.725628  30.326845  25.173735
S    33.343678  25.959450  24.097273
S    35.942883  27.441172  27.951714

24

generated by VMD

Ca   18.555361  33.111790  33.597721
Ca   23.165684  33.715878  36.051064
Ca   23.734798  30.162603  32.427803
Ca   22.995790  34.378757  31.090796
Ca   24.838676  31.097244  27.475502
Ca   27.939501  32.921753  31.344017
Ca   29.462656  29.394911  29.426516
Ca   30.050026  32.756599  25.769699
Ca   30.290407  27.512703  24.878073
Ca   33.655487  29.857977  28.556667
Ca   33.858002  24.793631  27.494959
Ca   35.259300  28.835083  24.228710
S    21.183937  30.933964  34.908993
S    20.986118  35.437687  33.936153
S    21.932537  31.395479  29.595131
S    25.102310  33.354050  33.255863
S    26.467415  29.534754  30.383957
S    25.912039  34.119484  28.913025
S    28.001047  29.933031  26.153194
S    30.930521  32.126823  29.207363
S    31.435684  27.119875  28.408730
S    32.600567  30.288601  24.955244
S    33.245457  25.807064  24.085747
S    36.116776  27.710348  27.795137

24

generated by VMD

Ca   18.436607  33.178894  33.940296
Ca   22.897640  33.594627  36.136482
Ca   23.478626  30.294069  32.406044
Ca   23.186619  34.698212  30.929947
Ca   24.867245  30.967453  27.719585
Ca   28.175156  32.791725  31.473921
Ca   29.567446  29.206100  29.520084
Ca   29.854393  32.657127  25.609909
Ca   30.453003  27.454168  24.912893
Ca   33.551205  29.366578  28.445930
Ca   33.797218  24.963327  27.451769
|   | X     | Y     | Z     |
|---|-------|-------|-------|
| Ca| 35.492710 | 28.879271 | 24.169571 |
| S | 20.860987  | 30.771315  | 34.796356  |
| S | 21.074440  | 35.623547  | 33.865993  |
| S | 22.093140  | 31.568756  | 29.572674  |
| S | 24.954990  | 33.414009  | 33.369228  |
| S | 26.579437  | 29.489479  | 30.606236  |
| S | 25.926105  | 34.142986  | 28.679180  |
| S | 27.927099  | 29.497068  | 26.289293  |
| S | 31.133860  | 32.316200  | 29.057650  |
| S | 31.386349  | 27.010710  | 28.217150  |
| S | 32.447113  | 30.275303  | 25.246994  |
| S | 33.526524  | 25.839678  | 23.929792  |
| S | 36.052097  | 27.699495  | 27.596703  |

24 generated by VMD

|   | X     | Y     | Z     |
|---|-------|-------|-------|
| Ca| 18.346964  | 32.976418  | 33.254658  |
| Ca| 22.920605  | 33.762764  | 35.997776  |
| Ca| 23.606098  | 29.909292  | 32.589600  |
| Ca| 23.032253  | 34.979523  | 30.976620  |
| Ca| 24.952354  | 30.981812  | 27.859196  |
| Ca| 28.136185  | 32.784031  | 31.548115  |
| Ca| 29.535748  | 29.360365  | 29.790806  |
| Ca| 30.145384  | 32.511047  | 25.604479  |
| Ca| 30.095512  | 27.679033  | 24.952351  |
| Ca| 33.692829  | 29.818081  | 28.451048  |
| Ca| 34.188507  | 24.873510  | 27.510113  |
| Ca| 35.232143  | 28.739355  | 23.818142  |
| S | 20.759949  | 30.936527  | 34.883083  |
| S | 20.632542  | 35.782352  | 33.655510  |
| S | 22.213575  | 31.508467  | 29.701569  |
| S | 25.000229  | 33.258842  | 33.403141  |
| S | 26.594650  | 29.416578  | 30.784092  |
| S | 26.000792  | 34.292557  | 28.940308  |
| S | 28.106655  | 29.739372  | 26.524273  |
| S | 31.030281  | 32.014061  | 29.308661  |
| S | 31.532085  | 27.041882  | 28.367903  |
| S | 32.574478  | 30.322439  | 24.941153  |
| S | 33.148434  | 25.872774  | 23.917463  |
| S | 36.241714  | 27.738958  | 27.160049  |

24 generated by VMD

|   | X     | Y     | Z     |
|---|-------|-------|-------|
| Ca| 18.324596  | 33.473499  | 33.575294  |
| Ca| 23.216461  | 33.619877  | 36.170738  |
| Ca| 23.337837  | 29.995920  | 32.760883  |
| Ca| 23.136898  | 34.510117  | 30.538490  |
| Ca| 25.072189  | 30.832016  | 27.726454  |
Ca  27.781586  32.374939  31.473114
Ca  29.649004  32.856939  29.591499
Ca  30.257694  27.618677  24.816723
Ca  33.512199  29.897800  28.303692
Ca  33.967414  25.124769  27.628639
Ca  35.295052  28.824671  23.815977
S   20.806282  31.085354  34.955368
S   21.174419  35.999991  33.659283
S   22.168938  31.394430  29.630894
S   25.093218  33.293198  33.260403
S   26.401073  29.308044  30.802130
S   26.127863  33.876022  28.724937
S   28.178339  29.972795  26.532944
S   30.896929  32.164368  29.316704
S   31.196144  26.929068  28.337276
S   32.648487  30.328966  25.050276
S   33.224518  25.858101  23.964085
S   35.927494  28.056194  27.441463

24

generated by VMD
Ca  18.496021  33.536739  33.347076
Ca  22.794682  33.884407  35.977749
Ca  23.535931  29.929838  32.601810
Ca  22.934813  34.506351  30.937176
Ca  24.903929  30.913017  27.870674
Ca  27.981436  32.764595  31.595123
Ca  29.572144  29.138754  29.882055
Ca  30.231655  32.659588  25.879740
Ca  30.188049  27.620380  24.975414
Ca  33.604717  29.460678  28.292133
Ca  34.347237  24.942513  27.157127
Ca  35.498672  28.879599  23.835531
S   20.809362  31.172398  34.755783
S   20.978600  35.784492  33.669147
S   21.944069  31.141216  29.915318
S   24.953436  33.270424  33.168518
S   26.618853  29.478148  30.716248
S   25.926506  34.030228  28.913120
S   28.180717  29.896013  26.596130
S   31.032352  32.140945  29.422323
S   31.261452  26.864429  28.463964
S   32.525200  30.237230  24.993160
S   33.342445  26.080622  23.831810
S   36.057816  27.968355  27.142918

24
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 18.447287 | 33.074352 | 33.234871 |
| Ca      | 22.797501 | 34.070713 | 36.106064 |
| Ca      | 23.718224 | 29.981579 | 32.877003 |
| Ca      | 23.014381 | 34.752350 | 30.659101 |
| Ca      | 24.890808 | 30.531057 | 27.827721 |
| Ca      | 27.913242 | 32.823860 | 31.658249 |
| Ca      | 29.502129 | 29.084480 | 29.690107 |
| Ca      | 30.250172 | 32.392105 | 25.743586 |
| Ca      | 30.283789 | 29.971046 | 24.901440 |
| Ca      | 33.667492 | 29.495583 | 28.627846 |
| Ca      | 33.905010 | 25.001524 | 26.961140 |
| Ca      | 35.521202 | 28.828966 | 23.962358 |
| S       | 21.178257 | 31.129173 | 34.900784 |
| S       | 20.555321 | 35.841343 | 33.474789 |
| S       | 22.001827 | 31.355028 | 30.025734 |
| S       | 25.216194 | 33.503555 | 33.358620 |
| S       | 26.714645 | 29.511114 | 30.953924 |
| S       | 26.013962 | 33.787895 | 28.561754 |
| S       | 27.956327 | 29.461014 | 26.446339 |
| S       | 30.873726 | 32.113602 | 29.374470 |
| S       | 31.369167 | 26.885418 | 28.270466 |
| S       | 32.836342 | 30.674376 | 25.345938 |
| S       | 33.077370 | 26.291481 | 23.574207 |
| S       | 36.015667 | 27.738403 | 27.403517 |

24  generated by VMD
| Ca      | 18.340979 | 32.898533 | 33.438076 |
| Ca      | 22.706211 | 33.876434 | 35.949955 |
| Ca      | 23.603931 | 30.190207 | 33.081562 |
| Ca      | 23.013075 | 34.922920 | 30.678368 |
| Ca      | 25.060839 | 30.644295 | 27.784286 |
| Ca      | 28.068937 | 32.913231 | 31.480736 |
| Ca      | 29.516541 | 29.102539 | 29.769333 |
| Ca      | 30.152187 | 32.317982 | 25.616722 |
| Ca      | 30.305408 | 28.032721 | 24.809732 |
| Ca      | 33.536003 | 29.313562 | 28.569170 |
| Ca      | 33.998383 | 24.927595 | 27.186092 |
| Ca      | 35.747326 | 28.903151 | 23.872650 |
| S       | 20.830294 | 30.985485 | 35.431572 |
| S       | 20.685944 | 35.517517 | 33.381886 |
| S       | 22.339373 | 31.441271 | 29.970367 |
| S       | 24.866802 | 33.711411 | 33.378452 |
| S       | 26.724562 | 29.660595 | 30.941097 |
| S       | 26.048107 | 34.062916 | 28.669497 |
| S       | 28.059666 | 29.629753 | 26.511351 |
|      |      |      |      |
|------|------|------|------|
| S    | 30.919804 | 32.142967 | 29.220215 |
| S    | 31.006527 | 26.745478 | 28.113348 |
| S    | 32.902489 | 30.460859 | 25.084326 |
| S    | 33.393700 | 26.185371 | 23.643244 |
| S    | 35.893005 | 27.713232 | 27.357977 |

24 generated by VMD

|      |      |      |      |
|------|------|------|------|
| Ca   | 18.446560 | 33.121655 | 33.622990 |
| Ca   | 23.143818 | 33.658188 | 35.901283 |
| Ca   | 23.727589 | 30.123871 | 32.822598 |
| Ca   | 22.976288 | 34.825157 | 30.619701 |
| Ca   | 25.028313 | 30.633472 | 27.784935 |
| Ca   | 27.756344 | 33.071960 | 31.452648 |
| Ca   | 29.348747 | 29.060989 | 29.704390 |
| Ca   | 30.307049 | 32.406036 | 25.789619 |
| Ca   | 30.321749 | 27.738489 | 24.772982 |
| Ca   | 33.513123 | 29.857834 | 28.826912 |
| Ca   | 33.861053 | 24.892027 | 27.129610 |
| Ca   | 35.817600 | 28.760817 | 23.801098 |
| S    | 20.988361 | 30.858250 | 34.991474 |
| S    | 20.885925 | 35.617088 | 33.595963 |
| S    | 22.039944 | 31.370766 | 29.958384 |
| S    | 24.892117 | 33.519073 | 33.489048 |
| S    | 26.579777 | 29.695841 | 30.839968 |
| S    | 25.743122 | 34.119789 | 28.493202 |
| S    | 28.081722 | 29.719349 | 26.447613 |
| S    | 30.867805 | 32.278679 | 29.395441 |
| S    | 31.214279 | 26.870028 | 28.228788 |
| S    | 32.919815 | 30.363844 | 25.306339 |
| S    | 33.175270 | 25.994389 | 23.570133 |
| S    | 36.083549 | 27.742477 | 27.394863 |

24 generated by VMD

|      |      |      |      |
|------|------|------|------|
| Ca   | 18.579872 | 33.259117 | 33.171516 |
| Ca   | 22.916040 | 34.237267 | 36.035458 |
| Ca   | 23.607651 | 29.872786 | 32.894398 |
| Ca   | 23.043758 | 34.720886 | 30.692177 |
| Ca   | 24.924816 | 30.824808 | 27.715773 |
| Ca   | 27.971329 | 32.729248 | 31.624920 |
| Ca   | 29.354086 | 28.961327 | 29.803452 |
| Ca   | 30.141993 | 32.407249 | 25.656540 |
| Ca   | 30.427710 | 27.745216 | 24.900696 |
| Ca   | 33.632442 | 29.810011 | 28.615545 |
| Ca   | 34.025455 | 24.928745 | 27.068802 |
| Ca   | 35.655384 | 28.964128 | 23.737804 |
| S    | 20.988869 | 31.251965 | 34.990192 |
|   |          |          |          |
|---|----------|----------|----------|
| S | 20.870422 | 35.930817 | 33.654823 |
| S | 21.970591 | 31.277740 | 29.918112 |
| S | 24.933952 | 33.121239 | 33.355705 |
| S | 26.339148 | 29.440184 | 30.996317 |
| S | 25.911392 | 34.065578 | 28.802483 |
| S | 28.169643 | 29.383110 | 26.496536 |
| S | 30.670929 | 31.644930 | 29.357586 |
| S | 31.573139 | 26.980122 | 28.381437 |
| S | 32.700371 | 30.631628 | 25.056158 |
| S | 33.133884 | 26.187134 | 23.671249 |
| S | 36.177124 | 29.342331 |

24

generated by VMD

|   |          |          |          |
|---|----------|----------|----------|
| Ca| 18.564863 | 33.356937 | 33.230820 |
| Ca| 23.214485 | 34.140350 | 35.991043 |
| Ca| 23.712173 | 29.809893 | 32.835148 |
| Ca| 22.991787 | 34.457664 | 30.845098 |
| Ca| 24.853941 | 30.663378 | 27.596176 |
| Ca| 27.860830 | 32.536835 | 31.365812 |
| Ca| 29.29076  | 29.181486 | 29.612970 |
| Ca| 29.992750 | 32.679474 | 25.824709 |
| Ca| 30.273832 | 27.943413 | 24.870968 |
| Ca| 33.643364 | 29.716877 | 28.586838 |
| Ca| 33.889343 | 24.957005 | 27.396027 |
| Ca| 35.745010 | 28.859371 | 23.998516 |
| S | 21.006870 | 31.359653 | 35.088715 |
| S | 20.826126 | 35.740940 | 33.763477 |
| S | 21.998550 | 31.258932 | 29.842094 |
| S | 25.166260 | 33.054596 | 33.375553 |
| S | 26.447025 | 29.350231 | 30.762157 |
| S | 25.772535 | 34.056255 | 28.605074 |
| S | 28.034760 | 29.812065 | 26.410156 |
| S | 30.907177 | 31.982197 | 29.342297 |
| S | 31.265463 | 26.964693 | 28.253534 |
| S | 32.764400 | 30.501394 | 25.138756 |
| S | 33.174278 | 26.192875 | 23.897755 |
| S | 36.322105 | 27.723547 | 27.306379 |
#cluster_I_amoeba_trj.xyz

24 generated by VMD

| Element | X               | Y               | Z               |
|---------|-----------------|-----------------|-----------------|
| Ca      | 25.543577       | 29.011038       | 30.804272       |
| Ca      | 26.682152       | 30.365072       | 35.730659       |
| Ca      | 30.076239       | 28.366810       | 35.154945       |
| Ca      | 30.321184       | 33.367218       | 33.759338       |
| Ca      | 33.506248       | 29.655655       | 31.695606       |
| Ca      | 33.140263       | 30.476910       | 35.793125       |
| Ca      | 36.820084       | 27.071972       | 35.045879       |
| Ca      | 36.831272       | 31.576668       | 34.534275       |
| Ca      | 39.763645       | 28.132481       | 31.258093       |
| Ca      | 39.939034       | 30.186451       | 35.817661       |
| Ca      | 45.316982       | 26.738081       | 33.813873       |
| Ca      | 43.167465       | 29.614475       | 34.383205       |
| S       | 26.587788       | 27.088457       | 35.598965       |
| S       | 27.118244       | 34.015423       | 35.420288       |
| S       | 30.495308       | 30.111883       | 32.615459       |
| S       | 30.195469       | 31.274843       | 36.530834       |
| S       | 33.497520       | 27.631973       | 34.195450       |
| S       | 33.675613       | 32.924797       | 32.936005       |
| S       | 36.733498       | 29.116968       | 32.159924       |
| S       | 36.401905       | 29.724556       | 36.977905       |
| S       | 40.336926       | 27.043495       | 34.601097       |
| S       | 40.431664       | 31.235022       | 33.006760       |
| S       | 43.252098       | 27.917688       | 31.130278       |
| S       | 44.599712       | 27.743448       | 37.066776       |

24 generated by VMD

| Element | X               | Y               | Z               |
|---------|-----------------|-----------------|-----------------|
| Ca      | 25.651463       | 28.621279       | 30.739601       |
| Ca      | 26.754364       | 30.391479       | 35.894775       |
| Ca      | 30.374775       | 28.601618       | 35.084789       |
| Ca      | 30.177670       | 33.443569       | 33.814049       |
| Ca      | 33.389942       | 29.612503       | 31.507538       |
| Ca      | 33.231182       | 30.599585       | 35.776825       |
| Ca      | 36.836853       | 27.044014       | 35.127335       |
| Ca      | 36.913380       | 31.632021       | 34.632828       |
| Ca      | 39.632359       | 28.141754       | 31.601833       |
| Ca      | 39.974636       | 30.088774       | 36.158936       |
| Ca      | 45.262001       | 26.828438       | 33.563694       |
| Ca      | 43.061501       | 29.545240       | 34.247833       |
| S       | 27.030430       | 27.218561       | 35.380993       |
| S       | 26.920759       | 33.822948       | 35.186237       |
| S       | 30.449875       | 30.415291       | 32.625237       |
| S       | 30.132750       | 31.371574       | 36.588543       |
| S   | 33.514160 | 27.667479 | 34.200794 |
| S   | 33.697727 | 32.864967 | 33.097759 |
| S   | 36.730930 | 29.197613 | 32.006054 |
| S   | 36.600109 | 29.636461 | 37.052216 |
| S   | 40.200569 | 27.022779 | 34.514595 |
| S   | 40.270638 | 31.199377 | 33.080322 |
| S   | 43.134670 | 27.722523 | 31.142277 |
| S   | 44.491089 | 27.701590 | 37.005638 |

24 generated by VMD

| Ca  | 25.336937 | 28.530123 | 30.306284 |
| Ca  | 26.575768 | 30.443096 | 35.526051 |
| Ca  | 30.068983 | 28.448408 | 35.144032 |
| Ca  | 30.329233 | 33.283031 | 34.013645 |
| Ca  | 33.469028 | 29.767080 | 31.915442 |
| Ca  | 33.286789 | 30.479074 | 36.069801 |
| Ca  | 36.829411 | 27.240545 | 35.196732 |
| Ca  | 36.621689 | 31.841259 | 34.695290 |
| Ca  | 39.712196 | 28.130985 | 31.566132 |
| Ca  | 40.094036 | 30.268642 | 36.023056 |
| Ca  | 45.063652 | 26.513979 | 33.332962 |
| Ca  | 43.405197 | 29.583679 | 34.088833 |
| S   | 26.829811 | 27.124975 | 35.211792 |
| S   | 26.975140 | 33.900478 | 34.986099 |
| S   | 30.428663 | 30.343508 | 32.566353 |
| S   | 29.828827 | 31.154930 | 36.592468 |
| S   | 33.547520 | 27.740358 | 34.504322 |
| S   | 33.642151 | 32.983181 | 33.370216 |
| S   | 36.756157 | 29.345358 | 32.245060 |
| S   | 36.753445 | 29.871172 | 37.243275 |
| S   | 40.326878 | 26.981958 | 34.797127 |
| S   | 40.663811 | 31.124052 | 32.986057 |
| S   | 43.112381 | 27.509184 | 30.910206 |
| S   | 44.776184 | 27.782341 | 36.765175 |

24 generated by VMD

| Ca  | 25.275015 | 28.551502 | 30.116447 |
| Ca  | 26.458231 | 30.429998 | 35.691212 |
| Ca  | 30.184448 | 28.325745 | 35.201820 |
| Ca  | 30.474100 | 33.391243 | 33.845554 |
| Ca  | 33.700054 | 29.702295 | 31.946457 |
| Ca  | 33.307224 | 30.600090 | 36.042690 |
| Ca  | 36.700893 | 27.097723 | 35.319012 |
| Ca  | 36.753506 | 31.885906 | 34.852371 |
| Ca  | 39.745937 | 28.138908 | 31.425545 |
| Ca  | 39.950027 | 30.066223 | 36.074146 |
|   | Ca      | S        |   |
|---|---------|----------|---|
| 1| 45.139557 | 26.603376 | 33.196789 |
| 2| 43.101734 | 29.664917 | 34.008259 |
| 3| 26.771421 | 27.271011 | 35.188023 |
| 4| 27.055223 | 33.881493 | 34.850849 |
| 5| 30.621283 | 30.245232 | 32.727768 |
| 6| 29.956907 | 31.227072 | 36.591026 |
| 7| 33.437515 | 27.675661 | 34.472370 |
| 8| 33.851032 | 32.956230 | 33.376804 |
| 9| 36.765522 | 29.172226 | 32.434639 |
|10| 36.637997 | 29.841309 | 37.174225 |
|11| 40.339661 | 27.065208 | 34.786743 |
|12| 40.122757 | 31.141666 | 33.066555 |
|13| 43.102535 | 27.670914 | 31.015944 |
|14| 44.981346 | 27.785450 | 36.624527 |

generated by VMD

|   | Ca      | S        |   |
|---|---------|----------|---|
| 25| 25.639225 | 28.721746 | 30.585066 |
| 26| 26.734243 | 30.479088 | 35.695774 |
| 27| 30.283176 | 28.233746 | 35.395374 |
| 28| 30.428490 | 33.254677 | 33.834290 |
| 29| 33.454479 | 29.837414 | 31.664530 |
| 30| 33.239861 | 30.448931 | 35.822891 |
| 31| 36.655231 | 27.000492 | 35.018845 |
| 32| 36.708809 | 31.738201 | 34.585087 |
| 33| 39.645180 | 28.237867 | 31.217520 |
| 34| 39.754997 | 30.120275 | 36.118347 |
| 35| 45.199131 | 26.630611 | 33.523338 |
| 36| 43.186535 | 29.639505 | 34.125950 |
| 37| 26.860065 | 27.103882 | 35.391766 |
| 38| 27.080660 | 34.013466 | 35.025772 |
| 39| 30.580471 | 30.248169 | 32.715115 |
| 40| 30.075937 | 31.290623 | 36.583168 |
| 41| 33.492908 | 27.744804 | 34.135490 |
| 42| 33.824547 | 32.977180 | 33.296017 |
| 43| 36.634270 | 29.183542 | 32.243542 |
| 44| 36.421535 | 29.667088 | 37.124947 |
| 45| 40.155750 | 27.119797 | 34.719631 |
| 46| 40.305767 | 31.236401 | 32.983017 |
| 47| 43.083378 | 27.575008 | 31.228312 |
| 48| 44.989388 | 27.888897 | 36.996986 |

generated by VMD

|   | Ca      | S        |   |
|---|---------|----------|---|
| 24| 25.474010 | 28.966080 | 30.690479 |
| 25| 26.741701 | 30.465824 | 35.746578 |
| 26| 29.990398 | 28.439085 | 35.330086 |
| 27| 30.435297 | 33.289703 | 33.613293 |
| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 33.619751 | 29.625248 | 31.805351 |
| Ca      | 33.253517 | 30.381058 | 35.942734 |
| Ca      | 36.776989 | 27.041557 | 35.170681 |
| Ca      | 36.819778 | 31.815849 | 34.735477 |
| Ca      | 39.776012 | 28.093279 | 31.522749 |
| Ca      | 39.852272 | 30.126976 | 36.040260 |
| Ca      | 45.418545 | 26.735882 | 33.079979 |
| Ca      | 43.203865 | 29.665268 | 34.228584 |
| S       | 36.573275 | 27.184576 | 35.225285 |
| S       | 27.161587 | 33.979813 | 34.680935 |
| S       | 30.518703 | 29.940897 | 32.599583 |
| S       | 29.995636 | 31.393427 | 36.578583 |
| S       | 33.474491 | 27.690952 | 34.343407 |
| S       | 33.693291 | 32.754040 | 33.516575 |
| S       | 36.700558 | 29.210815 | 32.463207 |
| S       | 36.409901 | 29.601337 | 37.116016 |
| S       | 40.223690 | 27.132601 | 34.707684 |
| S       | 40.304470 | 31.197170 | 33.072674 |
| S       | 43.194546 | 27.860357 | 31.085077 |
| S       | 44.821575 | 27.799568 | 36.735397 |

24 generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 25.466194 | 28.898205 | 30.404013 |
| Ca      | 26.661327 | 30.44921  | 35.693245 |
| Ca      | 30.111536 | 28.360598 | 35.300209 |
| Ca      | 30.229511 | 33.219700 | 33.982529 |
| Ca      | 33.513149 | 29.626354 | 31.680315 |
| Ca      | 33.455132 | 30.682289 | 35.885895 |
| Ca      | 36.877079 | 27.220165 | 35.108521 |
| Ca      | 36.812668 | 31.979252 | 34.500095 |
| Ca      | 39.631557 | 27.938175 | 31.358606 |
| Ca      | 39.965988 | 30.086239 | 36.206421 |
| Ca      | 45.154579 | 26.663534 | 33.193794 |
| Ca      | 43.214550 | 29.570265 | 34.388481 |
| S       | 26.769581 | 27.189959 | 35.491821 |
| S       | 27.051130 | 33.776951 | 34.922352 |
| S       | 30.500603 | 30.027807 | 32.608173 |
| S       | 30.020338 | 31.362658 | 36.697918 |
| S       | 33.495468 | 27.768456 | 34.338619 |
| S       | 33.532021 | 32.755058 | 33.166492 |
| S       | 36.844120 | 29.376635 | 32.097389 |
| S       | 36.579174 | 29.753759 | 36.956646 |
| S       | 40.320141 | 26.977262 | 34.844379 |
| S       | 40.434853 | 31.154263 | 33.216606 |
| S       | 43.124897 | 27.890770 | 31.128801 |
| S       | 44.668251 | 27.668171 | 36.859364 |
|  |  |  |
|---|---|---|
| Ca | 25.587973 | 28.587589 | 30.459394 |
| Ca | 26.462828 | 30.315685 | 35.632206 |
| Ca | 30.159529 | 28.506901 | 35.224094 |
| Ca | 30.106806 | 33.415909 | 33.794224 |
| Ca | 33.462605 | 29.47918 | 31.859169 |
| Ca | 33.244240 | 30.713512 | 35.859730 |
| Ca | 36.934467 | 27.034735 | 35.632206 |
| Ca | 36.999119 | 31.794876 | 34.630447 |
| Ca | 39.805466 | 28.314884 | 31.727745 |
| Ca | 40.121704 | 30.354931 | 36.410286 |
| Ca | 45.028992 | 26.180120 | 33.053242 |
| Ca | 43.162155 | 29.510363 | 34.301388 |
| S  | 26.700300 | 27.148720 | 35.385777 |
| S  | 26.916765 | 33.806335 | 34.864643 |
| S  | 30.352470 | 30.152220 | 32.629143 |
| S  | 29.947212 | 31.423326 | 36.535000 |
| S  | 33.506058 | 27.745268 | 34.466259 |
| S  | 33.522938 | 32.915684 | 33.084194 |
| S  | 36.698811 | 29.306187 | 32.422451 |
| S  | 36.718258 | 29.891981 | 37.068665 |
| S  | 40.375957 | 27.119057 | 34.861553 |
| S  | 40.514549 | 31.294683 | 33.184738 |
| S  | 43.223251 | 28.019485 | 31.070292 |
| S  | 44.881393 | 27.364023 | 36.430687 |

24 generated by VMD

| Ca | 25.966328 | 29.169573 | 30.864616 |
| Ca | 26.503403 | 30.233929 | 35.465000 |
| Ca | 30.131878 | 28.487442 | 35.513515 |
| Ca | 30.203333 | 33.412319 | 33.861477 |
| Ca | 33.567329 | 29.615499 | 31.680689 |
| Ca | 33.180576 | 30.736036 | 35.836639 |
| Ca | 36.674061 | 27.053656 | 35.071030 |
| Ca | 36.840927 | 31.649729 | 34.466408 |
| Ca | 39.893517 | 28.124033 | 31.527245 |
| Ca | 39.756413 | 29.887043 | 35.992416 |
| Ca | 45.340359 | 26.530317 | 33.277702 |
| Ca | 43.097355 | 29.636227 | 34.341351 |
| S  | 26.933615 | 26.989824 | 35.584312 |
| S  | 26.977375 | 33.763515 | 34.682209 |
| S  | 30.528944 | 30.255575 | 32.815609 |
| S  | 29.747484 | 31.411322 | 36.657101 |
| S  | 33.558399 | 27.818844 | 34.465248 |
| S  | 33.595848 | 32.851364 | 33.016399 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| S       | 36.867039    | 29.197010    | 32.092773    |
| S       | 36.338364    | 29.712183    | 37.177460    |
| S       | 40.263321    | 27.001713    | 34.664200    |
| S       | 40.271145    | 31.217804    | 33.185520    |
| S       | 43.327362    | 27.989368    | 31.111031    |
| S       | 44.869511    | 27.647062    | 36.680820    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.193361    | 28.697708    | 30.493044    |
| Ca      | 26.521442    | 30.548035    | 35.606068    |
| Ca      | 30.210526    | 28.432856    | 35.062523    |
| Ca      | 30.127010    | 33.426147    | 33.782997    |
| Ca      | 33.338699    | 29.378578    | 31.772230    |
| Ca      | 33.373806    | 30.530081    | 35.862183    |
| Ca      | 36.99126     | 27.087465    | 35.139095    |
| Ca      | 36.966450    | 31.812511    | 34.617329    |
| Ca      | 39.706108    | 28.279051    | 31.747080    |
| Ca      | 39.930107    | 30.070576    | 36.227173    |
| Ca      | 45.575588    | 26.524090    | 32.967007    |
| Ca      | 43.157978    | 29.660475    | 34.331806    |
| S       | 26.755880    | 27.179979    | 35.247208    |
| S       | 26.844191    | 34.023392    | 35.178730    |
| S       | 30.400536    | 30.290625    | 32.545944    |
| S       | 29.977133    | 31.390972    | 36.428932    |
| S       | 33.564053    | 27.722742    | 34.540871    |
| S       | 33.605011    | 32.863388    | 33.214359    |
| S       | 36.758553    | 29.190506    | 32.380630    |
| S       | 36.500343    | 29.688599    | 37.183018    |
| S       | 40.351437    | 26.915342    | 34.697289    |
| S       | 40.404922    | 31.177166    | 33.067673    |
| S       | 43.213291    | 27.728868    | 31.220049    |
| S       | 44.978374    | 27.772230    | 36.717430    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.356691    | 28.828083    | 30.764761    |
| Ca      | 26.769947    | 30.271372    | 35.669907    |
| Ca      | 30.037163    | 28.168877    | 35.114201    |
| Ca      | 30.236519    | 33.410732    | 33.586212    |
| Ca      | 33.496254    | 29.782274    | 31.797150    |
| Ca      | 33.184601    | 30.740076    | 35.740471    |
| Ca      | 36.772018    | 27.089384    | 35.123024    |
| Ca      | 36.772820    | 31.725569    | 34.545494    |
| Ca      | 39.947433    | 28.135294    | 31.303892    |
| Ca      | 39.334983    | 29.931288    | 36.128635    |
| Ca      | 45.320702    | 26.489740    | 33.360191    |
| Ca      | 43.109661    | 29.663740    | 34.245331    |
| S     | 26.712448 | 27.137058 | 35.603230 |
|-------|-----------|-----------|-----------|
| S     | 27.051146 | 34.006268 | 35.100021 |
| S     | 30.423407 | 30.219965 | 32.728443 |
| S     | 29.995224 | 31.255646 | 36.656395 |
| S     | 33.443470 | 27.694515 | 34.195374 |
| S     | 33.612881 | 33.038441 | 33.167137 |
| S     | 36.823875 | 29.266758 | 32.288509 |
| S     | 36.414921 | 29.745499 | 36.955631 |
| S     | 40.430035 | 27.072958 | 34.702171 |
| S     | 40.387482 | 31.179783 | 33.081463 |
| S     | 43.459885 | 27.790417 | 31.256413 |
| S     | 44.723938 | 27.747698 | 36.916676 |

24

generated by VMD

| Ca    | 25.523659 | 28.850798 | 30.800568 |
|-------|-----------|-----------|-----------|
| Ca    | 26.857409 | 30.555492 | 35.321575 |
| Ca    | 30.251207 | 28.384878 | 35.468819 |
| Ca    | 30.510740 | 33.104721 | 33.855965 |
| Ca    | 33.554123 | 29.643145 | 31.964062 |
| Ca    | 33.412033 | 30.416500 | 35.678848 |
| Ca    | 36.816292 | 26.946383 | 34.944103 |
| Ca    | 36.784149 | 31.508640 | 34.608158 |
| Ca    | 39.701855 | 28.245520 | 31.758528 |
| Ca    | 39.879333 | 30.359991 | 36.244423 |
| Ca    | 45.266857 | 26.370466 | 32.922787 |
| Ca    | 42.992096 | 29.773445 | 34.368755 |
| S     | 26.775116 | 27.424410 | 35.371246 |
| S     | 27.196111 | 33.993984 | 34.955574 |
| S     | 30.456432 | 30.009901 | 32.668636 |
| S     | 30.092123 | 31.326443 | 36.610245 |
| S     | 33.523525 | 27.483366 | 34.260566 |
| S     | 33.697464 | 32.786095 | 32.918652 |
| S     | 36.680714 | 29.196789 | 32.252422 |
| S     | 36.442680 | 29.589088 | 37.016495 |
| S     | 40.397606 | 27.213305 | 34.772793 |
| S     | 40.158703 | 31.381493 | 33.161526 |
| S     | 42.970070 | 28.104687 | 31.281702 |
| S     | 44.510117 | 27.721836 | 36.818699 |

24

generated by VMD

| Ca    | 25.185520 | 28.722759 | 31.170053 |
|-------|-----------|-----------|-----------|
| Ca    | 26.733662 | 30.322393 | 35.189785 |
| Ca    | 30.332537 | 28.041594 | 34.940113 |
| Ca    | 30.176884 | 33.368942 | 33.935905 |
| Ca    | 33.629807 | 29.892023 | 31.907425 |
| Ca    | 33.304264 | 30.588505 | 35.882954 |
| Ca   | 36.826054 | 26.997978 | 35.058712 |
| Ca   | 36.891792 | 32.043453 | 34.635704 |
| Ca   | 39.764324 | 28.102087 | 31.647148 |
| Ca   | 40.106491 | 30.406837 | 36.186981 |
| Ca   | 45.124210 | 26.188812 | 33.179840 |
| Ca   | 43.135300 | 29.407169 | 34.375832 |
| S    | 26.818771 | 27.175955 | 35.599773 |
| S    | 26.781919 | 33.783337 | 34.808937 |
| S    | 30.605747 | 30.341955 | 32.635933 |
| S    | 29.923803 | 31.156471 | 36.418636 |
| S    | 33.532742 | 27.607861 | 34.079304 |
| S    | 33.721550 | 33.117249 | 33.178429 |
| S    | 36.674534 | 29.331518 | 32.200096 |
| S    | 36.674469 | 29.943914 | 37.013245 |
| S    | 40.174610 | 27.132332 | 34.891068 |
| S    | 40.378578 | 31.317263 | 33.123943 |
| S    | 43.057220 | 27.779566 | 31.188616 |
| S    | 44.879009 | 27.621475 | 36.782261 |

24 generated by VMD

| Ca   | 25.454596 | 28.285635 | 31.100883 |
| Ca   | 26.930210 | 30.326054 | 35.321838 |
| Ca   | 30.166731 | 28.470720 | 35.178471 |
| Ca   | 30.345770 | 33.406380 | 34.005531 |
| Ca   | 33.648052 | 30.047266 | 31.983231 |
| Ca   | 33.396912 | 30.585987 | 35.735172 |
| Ca   | 36.501816 | 27.226973 | 34.918476 |
| Ca   | 37.109791 | 31.604370 | 34.359360 |
| Ca   | 39.740414 | 28.136658 | 31.362335 |
| Ca   | 39.895058 | 29.900967 | 36.169350 |
| Ca   | 45.054787 | 26.627205 | 33.589973 |
| Ca   | 43.186058 | 29.603750 | 34.393013 |
| S    | 26.818264 | 27.268702 | 35.672722 |
| S    | 26.664673 | 33.862495 | 35.158363 |
| S    | 30.721806 | 30.413984 | 32.589043 |
| S    | 30.014563 | 31.293940 | 36.590317 |
| S    | 33.396343 | 27.738199 | 34.113590 |
| S    | 33.797951 | 33.081020 | 33.048405 |
| S    | 36.582214 | 29.158039 | 31.926720 |
| S    | 36.438118 | 29.636665 | 36.916553 |
| S    | 40.206104 | 26.910000 | 34.453274 |
| S    | 40.377583 | 31.003540 | 33.039062 |
| S    | 43.275059 | 28.018425 | 31.397848 |
| S    | 44.711086 | 27.784433 | 37.007195 |

24 generated by VMD
| Element | X1 Value | X2 Value | Y Value |
|---------|----------|----------|---------|
| Ca      | 25.763092| 28.323503| 31.170458|
| Ca      | 26.643414| 30.420692| 35.390858|
| Ca      | 30.011023| 28.391819| 35.285629|
| Ca      | 30.467834| 33.383675| 33.796307|
| Ca      | 33.671364| 30.110834| 32.060322|
| Ca      | 33.115166| 30.298826| 35.790604|
| Ca      | 36.748688| 26.968014| 34.711502|
| Ca      | 36.727955| 31.666002| 34.667469|
| Ca      | 39.792847| 28.204824| 31.276003|
| Ca      | 39.853508| 30.061958| 36.148773|
| Ca      | 45.194748| 26.532055| 33.295975|
| Ca      | 43.278431| 29.489544| 34.339485|
| S       | 26.666840| 27.282387| 36.044224|
| S       | 26.838411| 33.970802| 34.537819|
| S       | 30.615391| 30.329439| 32.699692|
| S       | 29.790270| 31.320858| 36.436203|
| S       | 33.377148| 27.702328| 34.154285|
| S       | 33.887245| 33.217709| 33.294781|
| S       | 36.708817| 29.267609| 32.031860|
| S       | 36.399689| 29.475758| 36.940182|
| S       | 40.430065| 27.127518| 34.707527|
| S       | 40.350681| 31.263273| 33.215256|
| S       | 43.450428| 27.940811| 31.101839|
| S       | 44.650948| 27.641209| 36.933590|

24 generated by VMD

| Element | X1 Value | X2 Value | Y Value |
|---------|----------|----------|---------|
| Ca      | 25.808136| 28.082979| 31.051392|
| Ca      | 26.717648| 30.333055| 35.295528|
| Ca      | 30.346163| 28.269308| 35.106297|
| Ca      | 30.262505| 33.374241| 33.976200|
| Ca      | 33.655857| 30.418633| 32.025841|
| Ca      | 33.132507| 30.849052| 35.785439|
| Ca      | 36.751102| 26.969646| 34.776672|
| Ca      | 36.765011| 31.613333| 34.576294|
| Ca      | 39.657314| 28.102926| 31.290247|
| Ca      | 39.755013| 30.091406| 36.164719|
| Ca      | 45.524963| 26.341560| 33.216904|
| Ca      | 42.999550| 29.438377| 34.538795|
| S       | 27.024445| 27.316601| 36.023052|
| S       | 26.832630| 33.982750| 34.963161|
| S       | 30.598633| 30.383947| 32.579090|
| S       | 29.822021| 31.217113| 36.439991|
| S       | 33.559628| 27.940819| 33.994907|
| S       | 33.656376| 33.289246| 33.327129|
| S       | 36.526535| 29.282330| 31.892033|
| S       | 36.301178| 29.573750| 36.856186|
|   |   |   |
|---|---|---|
| S | 40.231525 | 27.008036 | 34.480728 |
| S | 40.343807 | 31.007250 | 33.112816 |
| S | 43.228851 | 27.667017 | 31.435471 |
| S | 44.932487 | 27.838005 | 37.121773 |

24

generated by VMD

| Ca | 25.421293 | 28.427105 | 31.306923 |
| Ca | 26.467857 | 30.146599 | 35.538090 |
| Ca | 30.226906 | 28.488647 | 35.144215 |
| Ca | 30.151928 | 33.423534 | 33.825104 |
| Ca | 33.768211 | 30.216791 | 31.612730 |
| Ca | 33.233196 | 30.821768 | 35.660984 |
| Ca | 36.637173 | 26.985352 | 34.739128 |
| Ca | 37.114445 | 31.632523 | 34.561264 |
| Ca | 39.860291 | 28.033550 | 31.440077 |
| Ca | 39.997234 | 30.196388 | 36.291744 |
| Ca | 45.073479 | 26.383652 | 33.497196 |
| Ca | 43.134285 | 29.404556 | 34.393410 |
| S | 26.912598 | 26.823984 | 35.783798 |
| S | 26.790403 | 33.766788 | 34.883625 |
| S | 30.486698 | 30.475986 | 32.623592 |
| S | 29.799004 | 31.300068 | 36.558517 |
| S | 33.572136 | 28.126663 | 34.070492 |
| S | 33.642120 | 33.207253 | 33.120007 |
| S | 36.750004 | 29.323957 | 32.026718 |
| S | 36.504509 | 29.695446 | 36.977448 |
| S | 40.267761 | 27.076138 | 34.799545 |
| S | 40.568874 | 31.003164 | 33.125011 |
| S | 43.308846 | 27.798054 | 31.037790 |
| S | 44.744595 | 27.633474 | 37.013382 |

24

generated by VMD

| Ca | 25.665710 | 28.606060 | 31.242432 |
| Ca | 26.656761 | 30.414566 | 35.509815 |
| Ca | 30.156225 | 27.958830 | 35.240448 |
| Ca | 30.093494 | 33.346008 | 34.134136 |
| Ca | 33.532539 | 29.997122 | 31.502958 |
| Ca | 33.224415 | 30.670523 | 35.453701 |
| Ca | 36.709015 | 27.106266 | 34.811378 |
| Ca | 36.801647 | 31.809336 | 34.562294 |
| Ca | 39.949795 | 27.975937 | 31.327030 |
| Ca | 39.898232 | 30.249775 | 36.134785 |
| Ca | 45.433952 | 26.418591 | 33.487125 |
| Ca | 43.070129 | 29.457153 | 34.586384 |
| S | 26.970461 | 27.277008 | 35.753372 |
| S | 26.647242 | 34.090660 | 35.210251 |
|   |   |   |   |
|---|---|---|---|
| S | 30.510139 | 30.412069 | 32.668037 |
| S | 29.862778 | 31.221132 | 36.563889 |
| S | 33.445259 | 27.808809 | 33.951542 |
| S | 33.696354 | 33.071625 | 32.912018 |
| S | 36.720619 | 29.274693 | 31.978893 |
| S | 36.464424 | 29.577190 | 36.825836 |
| S | 40.271996 | 26.840630 | 34.619225 |
| S | 40.494820 | 31.197144 | 33.042126 |
| S | 43.280212 | 27.746397 | 31.459293 |
| 24 | generated by VMD |
| Ca | 25.721395 | 28.759590 | 31.214787 |
| Ca | 26.637594 | 30.196716 | 35.304035 |
| Ca | 30.060555 | 28.132273 | 35.192905 |
| Ca | 30.290348 | 33.356720 | 33.995834 |
| Ca | 33.589386 | 30.014137 | 31.740940 |
| Ca | 33.302715 | 30.514080 | 35.683514 |
| Ca | 36.484200 | 27.044233 | 34.907478 |
| Ca | 36.964756 | 32.001125 | 34.286606 |
| Ca | 39.873726 | 28.329353 | 31.297009 |
| Ca | 39.997574 | 30.294765 | 36.136093 |
| Ca | 45.188080 | 26.217569 | 33.395542 |
| Ca | 43.086857 | 29.303867 | 34.458050 |
| S | 26.729824 | 27.057215 | 35.888432 |
| S | 26.984730 | 33.737698 | 34.984627 |
| S | 30.581455 | 30.244476 | 32.745022 |
| S | 29.923439 | 31.186207 | 36.521866 |
| S | 33.360477 | 27.690525 | 34.080822 |
| S | 33.693893 | 33.133949 | 33.083817 |
| S | 36.749729 | 29.428894 | 32.032822 |
| S | 36.445053 | 29.841690 | 36.746891 |
| S | 40.004711 | 27.208460 | 34.690475 |
| S | 40.584602 | 31.203930 | 33.151806 |
| S | 43.165474 | 27.683031 | 31.448549 |
| S | 45.013348 | 27.810837 | 37.042805 |

24

|   |   |   |   |
|---|---|---|---|
| generated by VMD |
| Ca | 25.708481 | 28.468876 | 31.099573 |
| Ca | 26.648304 | 30.333481 | 35.334671 |
| Ca | 30.168709 | 28.387434 | 35.249897 |
| Ca | 30.221958 | 33.453949 | 34.087021 |
| Ca | 33.787827 | 30.134762 | 31.908749 |
| Ca | 33.031513 | 30.363266 | 35.823235 |
| Ca | 36.595230 | 26.906721 | 34.996582 |
| Ca | 36.838387 | 31.759855 | 34.466618 |
|   | Ca       | 39.849445 | 27.895073 | 31.379923 |
|---|----------|-----------|-----------|-----------|
|   | Ca       | 39.911964 | 27.162012 | 35.717094 |
|   | Ca       | 45.134800 | 26.596083 | 33.358738 |
|   | S        | 26.814030 | 34.084286 | 34.917809 |
|   | S        | 30.685789 | 30.490337 | 32.628220 |
|   | S        | 29.720892 | 31.231470 | 36.507133 |
|   | S        | 33.526484 | 27.857485 | 34.116726 |
|   | S        | 33.815716 | 33.110275 | 33.016029 |
|   | S        | 36.771141 | 29.063000 | 32.145992 |
|   | S        | 36.389969 | 29.732580 | 36.928829 |
|   | S        | 40.307518 | 26.900761 | 34.747589 |
|   | S        | 40.341072 | 30.891281 | 33.057404 |
|   | S        | 43.308456 | 28.162804 | 31.179195 |
|   | S        | 44.943146 | 27.776592 | 36.793507 |
|---|----------|-----------|-----------|-----------|
|   | generated by VMD |
|   | Ca       | 25.619213 | 28.665211 | 31.123430 |
|   | Ca       | 26.513298 | 30.461033 | 35.233295 |
|   | Ca       | 30.141130 | 28.441250 | 35.107506 |
|   | Ca       | 30.047691 | 33.498199 | 34.030384 |
|   | Ca       | 33.646389 | 29.424551 | 31.731991 |
|   | Ca       | 33.258858 | 30.633724 | 35.619701 |
|   | Ca       | 36.728226 | 26.769009 | 34.777916 |
|   | Ca       | 36.915524 | 31.588921 | 34.663986 |
|   | Ca       | 39.843376 | 28.042648 | 31.310701 |
|   | Ca       | 39.961517 | 30.058657 | 36.166645 |
|   | Ca       | 45.271996 | 26.606304 | 33.586964 |
|   | Ca       | 43.362374 | 29.671989 | 34.268585 |
|   | S        | 26.770788 | 27.398876 | 35.776966 |
|   | S        | 26.723024 | 34.017311 | 35.141441 |
|   | S        | 30.571796 | 30.404745 | 32.651165 |
|   | S        | 29.848757 | 31.399805 | 36.624344 |
|   | S        | 33.478439 | 27.634691 | 34.351337 |
|   | S        | 33.664192 | 32.860096 | 33.032898 |
|   | S        | 36.923054 | 29.163616 | 32.105461 |
|   | S        | 36.337368 | 29.570171 | 36.896046 |
|   | S        | 40.245750 | 26.993143 | 34.626106 |
|   | S        | 40.522171 | 31.078449 | 33.193703 |
|   | S        | 43.339695 | 28.227196 | 31.079876 |
|   | S        | 44.797935 | 27.781851 | 36.930237 |

|   | generated by VMD |
|   | Ca       | 25.645117 | 28.908596 | 31.047632 |
|   | Ca       | 26.478809 | 30.702682 | 35.283543 |
|   | Ca         | S        |
|---|------------|----------|
|   |            | generated by VMD |
| Ca | 30.393497  | 28.229891 | 35.091278 |
| Ca | 30.165339  | 33.507576 | 34.024349 |
| Ca | 33.541195  | 29.488173 | 31.955448 |
| Ca | 33.166996  | 30.560839 | 35.898960 |
| Ca | 36.847855  | 27.096735 | 34.898556 |
| Ca | 36.739383  | 31.277746 | 34.308270 |
| Ca | 39.972698  | 28.315113 | 31.080160 |
| Ca | 39.684364  | 30.196518 | 36.127087 |
| Ca | 45.479595  | 26.532455 | 33.192451 |
| Ca | 42.985397  | 29.583517 | 34.659924 |
| S  | 27.132542  | 27.473019 | 35.725075 |
| S  | 26.619566  | 34.161194 | 34.874310 |
| S  | 30.537916  | 30.162376 | 32.666203 |
| S  | 29.927422  | 31.397287 | 36.643646 |
| S  | 33.668446  | 27.516212 | 34.457798 |
| S  | 33.513336  | 32.686855 | 33.236942 |
| S  | 36.774124  | 29.055586 | 31.839361 |
| S  | 36.378315  | 29.546507 | 37.053078 |
| S  | 40.363602  | 27.009741 | 34.469139 |
| S  | 40.251122  | 31.206686 | 33.085770 |
| S  | 43.392193  | 28.051601 | 31.436901 |
| S  | 44.774605  | 27.724445 | 36.974827 |

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|     |          |          |          |
|-----|----------|----------|----------|
| S   | 43.537354| 28.030930| 31.208054|
| S   | 44.574760| 27.457638| 36.783508|

24 generated by VMD

| Ca  |          |          |          |
|-----|----------|----------|----------|
|     | 25.746574| 28.914110| 30.821339|
| Ca  | 26.733522| 30.424055| 35.167171|
| Ca  | 30.060244| 28.113544| 35.207748|
| Ca  | 30.340805| 33.060593| 34.042927|
| Ca  | 33.635765| 29.604179| 31.896118|
| Ca  | 33.050369| 30.736826| 36.051937|
| Ca  | 36.535748| 27.141806| 34.953129|
| Ca  | 36.997948| 31.795540| 34.379436|
| Ca  | 39.873913| 28.241350| 31.422277|
| Ca  | 39.796459| 30.299026| 36.320019|
| Ca  | 45.835674| 26.118204| 32.584805|
| Ca  | 42.995472| 29.581131| 34.413036|
| S   | 26.789196| 27.347105| 35.460751|
| S   | 26.737650| 33.900909| 34.688671|
| S   | 30.523718| 30.180958| 32.737484|
| S   | 29.830343| 31.227222| 36.687347|
| S   | 33.384903| 27.847099| 34.655022|
| S   | 33.788372| 32.760612| 33.20389|
| S   | 36.716331| 29.177790| 32.254299|
| S   | 36.442036| 29.887892| 37.153141|
| S   | 40.168343| 27.207792| 34.846401|
| S   | 40.450443| 31.075157| 33.139385|
| S   | 43.282589| 27.977541| 31.231585|
| S   | 44.717899| 27.771009| 36.714230|

24 generated by VMD

| Ca  |          |          |          |
|-----|----------|----------|----------|
|     | 25.902443| 28.984468| 30.990562|
| Ca  | 26.576286| 30.185703| 35.372879|
| Ca  | 30.233732| 28.373644| 35.066528|
| Ca  | 30.029514| 33.441544| 33.938332|
| Ca  | 33.605549| 29.796664| 31.799353|
| Ca  | 32.987434| 30.653231| 35.774639|
| Ca  | 36.803505| 26.855652| 35.102627|
| Ca  | 36.893482| 31.754166| 34.278065|
| Ca  | 39.858295| 27.998268| 31.491261|
| Ca  | 39.969852| 30.220858| 36.290245|
| Ca  | 45.637936| 26.256857| 32.933273|
| Ca  | 42.977577| 29.526855| 34.465534|
| S   | 27.061512| 27.095945| 35.613895|
| S   | 26.675535| 33.984924| 34.931484|
| S   | 30.525078| 30.354052| 32.637375|
| S   | 29.661999| 31.350040| 36.508705|
|   | 33.483616 | 27.994366 | 34.354252 |
|---|----------|----------|----------|
| S | 33.655884 | 32.920712 | 33.306702 |
| S | 36.672859 | 29.076994 | 32.270844 |
| S | 36.419231 | 29.703909 | 36.911697 |
| S | 40.284378 | 27.070810 | 34.809643 |
| S | 40.394787 | 30.986891 | 33.229782 |
| S | 43.194309 | 27.843702 | 31.311596 |
| S | 44.929977 | 27.958172 | 36.641445 |

24

generated by VMD

| Ca | 25.888592 | 29.142992 | 30.961086 |
|----|----------|----------|----------|
| Ca | 26.151703 | 30.435757 | 35.143562 |
| Ca | 30.370556 | 28.082533 | 35.143013 |
| Ca | 30.306429 | 33.317005 | 33.862030 |
| Ca | 33.687992 | 30.145216 | 32.038151 |
| Ca | 32.950935 | 30.590885 | 35.796665 |
| Ca | 36.673199 | 26.895350 | 35.312222 |
| Ca | 36.775242 | 31.517693 | 34.421799 |
| Ca | 39.765408 | 28.053005 | 31.422884 |
| Ca | 39.828785 | 30.121872 | 36.232773 |
| Ca | 45.984585 | 26.209822 | 32.460606 |
| Ca | 43.025730 | 29.835470 | 34.346710 |
| S  | 26.959650 | 27.249519 | 35.687943 |
| S  | 26.892122 | 33.852371 | 34.757133 |
| S  | 30.539011 | 30.339827 | 32.580070 |
| S  | 29.583466 | 31.235744 | 36.380711 |
| S  | 33.526993 | 27.844753 | 34.589367 |
| S  | 33.635765 | 30.399865 | 33.276558 |
| S  | 36.671566 | 28.875006 | 32.409199 |
| S  | 36.470020 | 29.663067 | 37.130871 |
| S  | 40.190948 | 26.959719 | 34.805164 |
| S  | 40.218231 | 31.130074 | 33.118984 |
| S  | 43.306503 | 27.832726 | 31.308184 |
| S  | 45.030449 | 28.021000 | 36.845001 |

24

generated by VMD

| Ca  | 25.596405 | 28.838768 | 31.110109 |
|-----|-----------|-----------|-----------|
| Ca  | 26.634735 | 30.343794 | 35.349964 |
| Ca  | 30.413189 | 28.261412 | 34.978550 |
| Ca  | 29.973501 | 33.298241 | 33.942368 |
| Ca  | 33.639378 | 30.016422 | 31.604879 |
| Ca  | 33.078793 | 30.820480 | 35.574509 |
| Ca  | 36.757271 | 27.060610 | 35.175396 |
| Ca  | 36.699783 | 31.427073 | 34.305397 |
| Ca  | 39.830421 | 27.961050 | 31.531034 |
| Ca  | 39.695347 | 30.202148 | 36.459034 |
Ca  45.824062      25.710848      32.657368
Ca  42.999508      29.637175      34.460648
S   27.259758      27.089584      35.613693
S   26.675461      33.705391      35.108837
S   30.521212      30.452402      32.551083
S   29.885136      31.332321      36.530834
S   33.570915      28.207901      34.167915
S   33.541275      33.293987      33.178772
S   36.680439      29.023138      32.068821
S   36.176075      29.632616      37.174263
S   40.050087      27.020555      34.927784
S   40.403084      31.144672      33.263363
S   43.288181      27.714439      31.540922
S   45.239906      28.196398      36.755154

24 generated by VMD

Ca  25.723148      29.246895      31.408081
Ca  26.393238      30.043562      35.582058
Ca  30.176304      28.338381      35.184551
Ca  30.244102      33.328781      33.657570
Ca  33.938564      29.949406      33.342449
Ca  32.918022      30.707642      35.688747
Ca  36.481331      27.219845      35.220001
Ca  36.835587      31.649664      34.371197
Ca  40.069801      28.087973      31.481314
Ca  39.995895      30.272810      36.233009
Ca  45.789455      25.330761      32.758133
Ca  42.959164      29.930838      34.580177
S   26.896955      26.986225      35.765057
S   26.658037      33.342560      34.839771
S   30.737368      30.317938      32.593212
S   29.642107      31.355593      36.544968
S   33.506771      27.993408      34.224651
S   33.679173      33.117149      33.180988
S   36.830097      29.098370      32.206379
S   36.279697      30.028234      37.075653
S   40.161457      27.022032      34.783188
S   40.282524      31.255793      33.219963
S   43.424362      27.928350      31.441862
S   44.810753      27.839182      36.647789

24 generated by VMD

Ca  25.814104      29.245781      31.497210
Ca  26.374388      30.376047      35.631596
Ca  30.374714      28.107674      35.405258
Ca  30.234346      33.351978      33.710445
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 33.636181 | 29.910744 | 31.446903 |
| Ca      | 33.068878 | 30.590759 | 35.580692 |
| Ca      | 36.592690 | 26.680923 | 34.897232 |
| Ca      | 36.785938 | 31.513481 | 34.962733 |
| Ca      | 39.909691 | 28.444981 | 31.481636 |
| Ca      | 39.703926 | 30.270370 | 36.121544 |
| Ca      | 45.943863 | 25.830408 | 33.019096 |
| Ca      | 42.957088 | 29.754250 | 34.509758 |
| S       | 26.874748 | 37.155947 | 35.771687 |
| S       | 26.880684 | 33.683987 | 34.778275 |
| S       | 30.558107 | 30.331873 | 32.736721 |
| S       | 29.813349 | 31.313423 | 36.516327 |
| S       | 33.475178 | 29.935743 | 33.973705 |
| S       | 33.749596 | 33.081600 | 33.032417 |
| S       | 36.735233 | 29.116777 | 31.947132 |
| S       | 36.293884 | 29.379932 | 36.807159 |
| S       | 40.188293 | 27.043833 | 34.805710 |
| S       | 40.257420 | 31.334646 | 33.245110 |
| S       | 43.182247 | 27.693247 | 31.675039 |
| S       | 45.029362 | 28.243048 | 36.943344 |
| S       | 24.768248 | 29.607000 | 31.345032 |
| S       | 26.476688 | 30.295021 | 35.712795 |
| S       | 30.242443 | 28.373795 | 35.429134 |
| S       | 30.102142 | 33.304630 | 33.506100 |
| S       | 33.680206 | 29.709560 | 31.803612 |
| S       | 33.105263 | 30.516155 | 35.747040 |
| S       | 36.743984 | 26.832775 | 34.941334 |
| S       | 36.769073 | 31.445997 | 34.509228 |
| S       | 39.966293 | 28.425480 | 31.625814 |
| S       | 39.757698 | 30.183924 | 36.254917 |
| S       | 46.207542 | 25.606520 | 32.826759 |
| S       | 42.912422 | 29.838236 | 34.548252 |
| S       | 26.790627 | 27.209187 | 35.486134 |
| S       | 26.623238 | 33.757717 | 34.696781 |
| S       | 30.522938 | 30.029848 | 32.680313 |
| S       | 29.877199 | 31.552063 | 36.318459 |
| S       | 33.475494 | 27.691412 | 34.217041 |
| S       | 33.568024 | 32.865780 | 32.986973 |
| S       | 36.751720 | 29.120485 | 32.201920 |
| S       | 36.242561 | 29.439796 | 37.075321 |
| S       | 40.358982 | 27.240585 | 34.707867 |
| S       | 40.170055 | 31.297520 | 33.362831 |
| S       | 43.316456 | 27.846905 | 31.496555 |
| S       | 45.090294 | 28.201067 | 36.550465 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.74838 | 29.743004 | 31.419502 |
| Ca      | 26.569382 | 30.530163 | 35.770153 |
| Ca      | 30.238682 | 28.344492 | 35.276058 |
| Ca      | 30.225878 | 33.221066 | 33.767452 |
| Ca      | 30.225878 | 33.221066 | 33.767452 |
| Ca      | 33.610832 | 29.429796 | 31.516674 |
| Ca      | 33.106907 | 30.450468 | 35.618984 |
| Ca      | 36.753101 | 26.833483 | 34.867374 |
| Ca      | 36.626053 | 31.293442 | 34.356213 |
| Ca      | 39.98712 | 28.638149 | 31.395241 |
| Ca      | 39.717720 | 30.226933 | 36.432755 |
| Ca      | 45.602173 | 25.906546 | 32.778927 |
| Ca      | 42.798046 | 29.629360 | 34.785198 |
| S       | 26.978085 | 27.369486 | 35.706108 |
| S       | 26.928064 | 33.590508 | 34.660904 |
| S       | 30.372162 | 29.997524 | 32.550747 |
| S       | 30.046917 | 31.517797 | 36.565350 |
| S       | 33.476604 | 27.765280 | 34.239647 |
| S       | 33.454674 | 32.728325 | 32.955559 |
| S       | 36.787827 | 28.923944 | 32.064194 |
| S       | 36.361378 | 29.418650 | 36.835899 |
| S       | 40.208126 | 27.003229 | 34.540398 |
| S       | 40.389538 | 31.288334 | 33.256516 |
| S       | 43.314625 | 28.089298 | 31.543131 |
| S       | 45.129608 | 28.452112 | 37.127754 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.709061 | 29.448326 | 31.524754 |
| Ca      | 26.421961 | 30.340435 | 35.840439 |
| Ca      | 30.142338 | 28.131418 | 35.209534 |
| Ca      | 30.051107 | 33.352520 | 33.579681 |
| Ca      | 33.492321 | 29.555771 | 31.612839 |
| Ca      | 33.217709 | 30.556700 | 35.389427 |
| Ca      | 36.846775 | 27.143909 | 34.855350 |
| Ca      | 36.720043 | 31.702150 | 34.668476 |
| Ca      | 39.939518 | 28.289337 | 31.535896 |
| Ca      | 39.694138 | 30.114136 | 36.331059 |
| Ca      | 45.898945 | 25.753233 | 32.779392 |
| Ca      | 42.728340 | 29.672878 | 34.394772 |
| S       | 26.752857 | 27.337185 | 35.771893 |
| S       | 26.889870 | 33.528137 | 34.844288 |
| S       | 30.588810 | 30.158787 | 32.631351 |
| S       | 30.031160 | 31.347403 | 36.262836 |
| S       | 33.588726 | 27.708313 | 34.096386 |
| S       | 33.486637 | 32.967827 | 32.858391 |
|      |        |        |        |
|------|--------|--------|--------|
| S    | 36.849251 | 29.292217 | 32.099178 |
| S    | 36.347412 | 29.609341 | 36.893593 |
| S    | 40.229992 | 27.101042 | 34.912838 |
| S    | 40.307896 | 31.420044 | 33.358379 |
| S    | 43.501595 | 27.951941 | 31.560404 |
| S    | 44.997471 | 27.908409 | 37.019489 |

24 generated by VMD

| Ca   | 25.491787 | 29.108128 | 31.553621 |
| Ca   | 26.621441 | 30.466900 | 35.816463 |
| Ca   | 30.410749 | 28.020596 | 35.394978 |
| Ca   | 30.244648 | 33.219120 | 33.775177 |
| Ca   | 33.685146 | 29.644108 | 31.422272 |
| Ca   | 33.009480 | 30.630806 | 35.559601 |
| Ca   | 36.652485 | 27.275291 | 34.748024 |
| Ca   | 36.685558 | 31.644756 | 34.363243 |
| Ca   | 40.123096 | 28.526031 | 31.595491 |
| Ca   | 39.676991 | 30.111500 | 36.154758 |
| Ca   | 45.652325 | 25.512064 | 32.968975 |
| Ca   | 42.768948 | 29.593832 | 34.613346 |
| S    | 27.043785 | 27.342503 | 35.740124 |
| S    | 26.990227 | 33.668091 | 34.820393 |
| S    | 30.498991 | 30.082336 | 32.758057 |
| S    | 30.021399 | 31.145456 | 36.578564 |
| S    | 33.547630 | 27.922785 | 33.932301 |
| S    | 33.602451 | 33.126400 | 32.838184 |
| S    | 36.875374 | 29.276058 | 31.846050 |
| S    | 36.129765 | 29.579069 | 36.807247 |
| S    | 40.255108 | 27.134827 | 34.647404 |
| S    | 40.343128 | 31.308975 | 33.376994 |
| S    | 43.499916 | 27.950306 | 31.654804 |
| S    | 44.603458 | 28.101450 | 37.065022 |

24 generated by VMD

| Ca   | 25.255638 | 29.525738 | 31.227728 |
| Ca   | 26.684513 | 30.472473 | 35.805790 |
| Ca   | 30.344017 | 28.216206 | 35.162189 |
| Ca   | 29.910351 | 33.013275 | 33.815990 |
| Ca   | 33.561008 | 29.480639 | 31.506672 |
| Ca   | 33.278156 | 30.526970 | 35.839764 |
| Ca   | 36.706985 | 27.052805 | 34.928795 |
| Ca   | 36.914879 | 31.444107 | 34.498184 |
| Ca   | 40.021225 | 28.437656 | 31.555546 |
| Ca   | 39.738998 | 30.083380 | 36.269070 |
| Ca   | 45.541874 | 25.597794 | 32.999584 |
| Ca   | 42.843029 | 29.967005 | 34.426460 |
|    | 27.042900 | 27.324535 | 35.573097 |
|----|-----------|-----------|-----------|
|    | 26.758669 | 33.847431 | 34.604286 |
|    | 30.475182 | 30.141930 | 32.569756 |
|    | 30.047409 | 31.385931 | 36.571400 |
|    | 33.501556 | 27.739330 | 34.140072 |
|    | 33.670727 | 32.842030 | 33.083668 |
|    | 36.872810 | 29.250599 | 32.038960 |
|    | 36.450573 | 29.438114 | 36.986355 |
|    | 40.243313 | 27.033918 | 34.658756 |
|    | 40.167797 | 31.240135 | 33.391941 |
|    | 43.432144 | 27.887577 | 31.371164 |
|    | 44.970230 | 28.441879 | 37.005459 |

**24**

generated by VMD

|    | 25.204191 | 29.869038 | 31.453264 |
|----|-----------|-----------|-----------|
|    | 26.748924 | 30.648304 | 35.682251 |
|    | 30.166977 | 28.114597 | 35.270123 |
|    | 30.159851 | 32.969757 | 33.741364 |
|    | 33.468528 | 29.239485 | 31.692759 |
|    | 33.099102 | 30.354916 | 35.622112 |
|    | 36.882553 | 27.124462 | 34.686039 |
|    | 36.611626 | 31.459059 | 34.234455 |
|    | 39.963459 | 28.578712 | 31.508776 |
|    | 39.795238 | 30.146023 | 36.376198 |
|    | 45.671840 | 25.656254 | 32.754124 |
|    | 42.922657 | 29.873547 | 34.827908 |
|    | 26.819548 | 27.347408 | 35.497959 |
|    | 27.131237 | 33.884525 | 34.850594 |
|    | 30.339893 | 29.773413 | 32.530949 |
|    | 30.259420 | 31.329435 | 36.500454 |
|    | 33.529179 | 27.555323 | 34.312756 |
|    | 33.581268 | 32.533817 | 32.805878 |
|    | 36.761925 | 29.272055 | 31.937502 |
|    | 36.544373 | 29.651583 | 36.832439 |
|    | 40.307537 | 27.007105 | 34.657105 |
|    | 40.280609 | 31.510063 | 33.359669 |
|    | 43.316483 | 28.157217 | 31.755207 |
|    | 45.050713 | 28.333235 | 37.140930 |

**24**

generated by VMD

|    | 25.156592 | 29.538927 | 31.525862 |
|----|-----------|-----------|-----------|
|    | 26.714329 | 30.438644 | 35.542919 |
|    | 30.371803 | 28.348476 | 35.219517 |
|    | 30.089306 | 33.290123 | 33.626831 |
|    | 33.608589 | 29.364361 | 31.836407 |
|    | 33.261795 | 30.405354 | 35.721889 |
Ca  36.763119  27.022652  34.702877
Ca  36.689034  31.418701  34.507824
Ca  40.083458  28.620611  31.587431
Ca  39.740868  29.813927  36.341808
Ca  45.504990  25.729424  32.792572
Ca  42.889606  29.919470  32.624683
S   26.721643  27.353954  35.651875
S   27.038450  33.801983  34.553703
S   30.552460  30.056166  32.525459
S   30.037392  31.464645  36.333122
S   33.465828  27.522869  34.405693
S   33.689457  32.660683  33.028179
S   36.741596  29.216429  32.189144
S   36.457367  29.323975  36.983162
S   40.243523  26.980541  34.648109
S   40.346340  31.471800  33.276875
S   43.344494  28.170372  31.393465
S   44.912502  28.457314  37.011391

24 generated by VMD

Ca  25.051680  29.807219  31.355331
Ca  26.613205  30.684952  35.700863
Ca  30.217382  28.079132  35.340160
Ca  30.203876  33.084805  33.352642
Ca  33.503555  29.313263  31.985476
Ca  33.089504  30.363592  35.995983
Ca  36.864922  27.096804  34.810177
Ca  36.668831  31.819595  34.578732
Ca  40.302284  28.728685  31.367405
Ca  39.845169  29.980984  36.168484
Ca  45.454956  25.222980  32.930107
Ca  43.221146  29.812243  34.474056
S   26.533720  27.295443  35.504169
S   26.886736  33.653103  34.357185
S   30.274019  29.781570  32.682449
S   30.090708  31.381351  36.320698
S   33.423412  27.456234  34.643166
S   33.543304  32.626087  33.180939
S   36.856445  29.433054  32.119987
S   36.353226  29.568213  36.980110
S   40.524948  27.307322  34.374458
S   40.238594  31.552601  33.466377
S   43.613201  28.072447  31.367594
S   45.058990  28.269737  36.974133

24 generated by VMD
|   |   |   |   |
|---|---|---|---|
| Ca | 25.262333 | 29.541014 | 31.467386 |
| Ca | 26.515196 | 30.395527 | 35.577084 |
| Ca | 30.162548 | 28.277168 | 35.371979 |
| Ca | 30.342354 | 33.376190 | 33.460476 |
| Ca | 33.449631 | 29.393497 | 31.557241 |
| Ca | 33.181602 | 30.503008 | 35.767807 |
| Ca | 36.781189 | 26.888714 | 34.775440 |
| Ca | 36.667000 | 31.581993 | 34.689240 |
| Ca | 40.187805 | 28.596987 | 31.799747 |
| Ca | 39.755409 | 29.815456 | 36.189186 |
| Ca | 45.564724 | 25.566372 | 32.795197 |
| Ca | 42.992710 | 30.057755 | 34.388298 |
| S  | 26.367420 | 27.331640 | 35.945877 |
| S  | 27.101364 | 33.652901 | 34.409897 |
| S  | 30.422024 | 30.003580 | 32.694180 |
| S  | 30.021296 | 31.416471 | 36.353790 |
| S  | 33.428040 | 27.593821 | 34.331547 |
| S  | 33.810162 | 32.700974 | 33.054493 |
| S  | 36.794743 | 29.278963 | 32.036373 |
| S  | 36.350639 | 29.293060 | 36.918030 |
| S  | 40.408329 | 27.037899 | 34.544056 |
| S  | 40.232185 | 31.603895 | 33.477905 |
| S  | 43.685848 | 28.219278 | 31.543365 |
| S  | 44.949310 | 28.265282 | 36.882092 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 25.234249 | 29.446613 | 31.610840 |
| Ca | 26.479998 | 30.675402 | 35.632397 |
| Ca | 30.167809 | 28.334595 | 35.244625 |
| Ca | 30.293312 | 33.098343 | 33.619572 |
| Ca | 33.546623 | 29.379419 | 31.519087 |
| Ca | 33.062325 | 30.261600 | 35.640438 |
| Ca | 36.853184 | 26.830486 | 34.720963 |
| Ca | 36.507843 | 31.314419 | 34.559200 |
| Ca | 40.020031 | 28.588009 | 31.537659 |
| Ca | 39.772671 | 30.370432 | 36.301594 |
| Ca | 45.578114 | 25.826220 | 32.775429 |
| Ca | 43.098145 | 29.870081 | 34.793915 |
| S  | 26.895510 | 27.576422 | 35.949696 |
| S  | 27.131395 | 33.927383 | 34.585617 |
| S  | 30.424076 | 29.990101 | 32.490555 |
| S  | 29.998648 | 31.446970 | 36.506016 |
| S  | 33.498154 | 27.445507 | 34.058804 |
| S  | 33.663715 | 32.563843 | 33.028057 |
| S  | 36.731445 | 29.205822 | 31.923294 |
| S  | 36.289265 | 29.225224 | 36.939304 |
S  40.455986  27.227467  34.528461
S  40.296818  31.441725  33.364109
S  43.522797  28.259108  31.583595
S  44.911777  28.086252  37.117527

24

generated by VMD

Ca  25.034821  29.756403  31.744808
Ca  26.707724  30.658232  35.633171
Ca  29.958029  28.210957  35.471542
Ca  30.354130  33.174007  33.453583
Ca  33.804173  29.436371  31.469194
Ca  33.140190  30.394194  35.752396
Ca  36.989990  26.929853  34.875050
Ca  36.444874  31.163965  34.485386
Ca  39.975132  28.572905  31.455450
Ca  39.653469  30.030653  36.453175
Ca  45.304169  25.713871  32.612038
Ca  42.945152  29.888700  34.779293
S  26.538359  27.376413  35.871758
S  27.188749  33.593231  34.164818
S  30.693787  29.946011  32.676769
S  30.134317  31.316828  36.465469
S  33.630386  27.795525  34.211800
S  33.853333  32.683571  32.932831
S  36.790806  29.092281  31.861284
S  36.277103  29.257826  36.980125
S  40.562538  27.168694  34.611851
S  40.086697  31.333002  33.502392
S  43.411507  28.609076  31.448053
S  44.954426  28.288792  37.118492

24

generated by VMD

Ca  25.220814  30.023285  31.776192
Ca  26.645958  30.582714  35.736446
Ca  30.176224  28.333069  35.237907
Ca  30.327669  33.240238  33.609699
Ca  33.548660  29.117867  31.594481
Ca  32.948418  30.308573  35.575565
Ca  36.877201  26.759651  34.786572
Ca  36.594719  31.075396  34.394630
Ca  40.087540  28.521574  31.269913
Ca  39.612946  29.919807  36.557156
Ca  45.538643  26.060770  32.652119
Ca  43.055908  29.884645  34.870907
S  26.763830  27.484676  35.958359
S  27.106913  33.886749  34.568607
S  30.517838  30.049458  32.644211
S  30.081772  31.449713  34.221802
S  33.695297  32.420353  32.730392
S  36.850193  29.025347  31.796890
S  36.129799  29.241505  36.852360
S  40.442612  27.246189  34.395382
S  40.185669  31.394348  33.429096
S  43.500401  28.468309  31.586597
S  45.048691  28.462337  37.430889
24

generated by VMD

Ca  24.914974  29.079889  31.922279
Ca  26.651634  30.567709  35.526268
Ca  30.200949  28.172113  35.323719
Ca  30.383617  33.246128  33.484055
Ca  33.437649  29.665834  31.435230
Ca  33.171120  30.415325  35.549366
Ca  36.702549  26.828224  34.356510
Ca  36.896736  31.501286  34.581272
Ca  39.969162  28.717506  31.485039
Ca  39.718307  29.816175  36.362621
Ca  45.523441  25.744783  32.907478
Ca  42.877060  29.662184  34.769753
S  26.922981  27.382725  36.289249
S  27.010303  33.791710  34.421539
S  30.460899  30.096825  32.630970
S  30.099531  31.374830  36.280193
S  33.390354  27.473738  33.852116
S  33.907780  33.004696  33.190479
S  36.874222  29.481199  31.925749
S  36.304062  29.395096  36.815254
S  40.309517  26.936859  34.403797
S  40.387413  31.353317  33.518208
S  43.521507  28.239872  31.636480
S  44.798046  28.443382  37.363079
24

generated by VMD

Ca  24.780039  29.478054  31.941469
Ca  26.775635  30.752514  35.724102
Ca  30.155708  27.861423  34.972351
Ca  30.342823  33.298931  33.650330
Ca  33.268456  29.450840  31.405529
Ca  33.247829  30.275307  35.72516
Ca  36.727104  26.941565  34.523502
Ca  36.627117  31.411270  34.493855
| Element | X Coordination | Y Coordination | Z Coordination |
|---------|----------------|----------------|----------------|
| Ca      | 40.188206      | 28.752384      | 31.331566      |
| Ca      | 39.835548      | 30.106102      | 36.492214      |
| Ca      | 45.701660      | 25.409498      | 32.957470      |
| Ca      | 42.965603      | 29.907404      | 34.845100      |
| S       | 26.672749      | 27.653612      | 36.161156      |
| S       | 27.266026      | 33.776447      | 34.473125      |
| S       | 30.210295      | 29.940248      | 32.489056      |
| S       | 30.248241      | 31.269997      | 36.214775      |
| S       | 33.343613      | 27.450901      | 33.921417      |
| S       | 33.662018      | 32.522224      | 32.943718      |
| S       | 36.712311      | 29.420963      | 31.923557      |
| S       | 36.372635      | 29.274092      | 36.841320      |
| S       | 40.382576      | 27.165993      | 34.352264      |
| S       | 40.219082      | 31.552254      | 33.483925      |
| S       | 43.676853      | 28.255976      | 31.936571      |
| S       | 45.051815      | 28.463390      | 37.226578      |

24 generated by VMD
| Element | X Coordination | Y Coordination | Z Coordination |
|---------|----------------|----------------|----------------|
| Ca      | 25.152578      | 29.525618      | 32.128571      |
| Ca      | 26.564297      | 30.459694      | 35.791473      |
| Ca      | 30.186825      | 27.945337      | 34.971748      |
| Ca      | 30.291483      | 33.248962      | 33.368683      |
| Ca      | 33.395042      | 29.364616      | 31.425888      |
| Ca      | 33.010773      | 30.548134      | 35.334316      |
| Ca      | 36.802322      | 26.852596      | 34.677170      |
| Ca      | 36.867172      | 31.671001      | 34.689213      |
| Ca      | 40.157768      | 28.956036      | 31.389687      |
| Ca      | 39.972702      | 30.206997      | 36.845531      |
| Ca      | 45.608639      | 25.364786      | 32.531700      |
| Ca      | 43.062408      | 29.664265      | 34.813110      |
| S       | 26.896742      | 27.310648      | 36.455574      |
| S       | 26.835556      | 33.811596      | 34.380432      |
| S       | 30.448378      | 29.940514      | 32.345154      |
| S       | 30.010567      | 31.305851      | 36.096535      |
| S       | 33.449036      | 27.651169      | 33.881653      |
| S       | 33.609138      | 32.823086      | 32.813850      |
| S       | 36.742130      | 29.527439      | 32.119720      |
| S       | 36.438210      | 29.362328      | 36.926975      |
| S       | 40.307316      | 27.263622      | 34.574726      |
| S       | 40.244495      | 31.400841      | 33.740742      |
| S       | 43.549721      | 28.103758      | 31.376196      |
| S       | 44.830643      | 28.082541      | 37.352032      |

24 generated by VMD
| Element | X Coordination | Y Coordination | Z Coordination |
|---------|----------------|----------------|----------------|
| Ca      | 25.245157      | 29.710077      | 31.915993      |
| Ca      | 26.748383      | 30.496729      | 35.852783      |
|   |    |    |    |
|---|---|---|---|
| Ca | 30.207874 | 28.348434 | 35.496162 |
| Ca | 30.40524 | 33.033882 | 33.428196 |
| Ca | 33.553486 | 29.508390 | 31.321075 |
| Ca | 33.166828 | 30.265354 | 35.438065 |
| Ca | 36.562294 | 26.947744 | 34.44687 |
| Ca | 36.794075 | 31.390762 | 34.357910 |
| Ca | 39.549519 | 29.868210 | 36.266193 |
| Ca | 45.663086 | 26.151884 | 33.08749 |
| Ca | 42.827225 | 29.652637 | 34.958447 |
| S  | 26.801815 | 27.200226 | 36.192261 |
| S  | 27.327402 | 33.801682 | 34.698814 |
| S  | 30.628748 | 29.968794 | 32.517269 |
| S  | 30.308289 | 31.498501 | 36.373367 |
| S  | 33.144211 | 27.537336 | 33.848705 |
| S  | 33.810570 | 32.734573 | 32.894852 |
| S  | 36.715893 | 29.230690 | 31.879339 |
| S  | 36.142120 | 29.201216 | 36.658890 |
| S  | 40.195160 | 27.010153 | 34.388790 |
| S  | 40.250412 | 31.348946 | 33.561791 |
| S  | 43.485489 | 28.273966 | 31.563627 |
| S  | 44.838146 | 28.511784 | 37.460896 |

24
generated by VMD

|   |    |    |    |
|---|---|---|---|
| Ca | 25.062189 | 29.724611 | 31.897938 |
| Ca | 26.626610 | 30.437763 | 35.773045 |
| Ca | 30.157747 | 28.219702 | 35.107281 |
| Ca | 30.258224 | 33.189908 | 33.405289 |
| Ca | 33.554920 | 29.312838 | 31.417253 |
| Ca | 33.135246 | 30.314634 | 35.528988 |
| Ca | 36.645100 | 26.962538 | 34.483063 |
| Ca | 36.787151 | 31.405712 | 34.513138 |
| Ca | 40.154472 | 28.963261 | 31.661489 |
| Ca | 39.814724 | 29.99035 | 36.595680 |
| Ca | 45.686256 | 25.403811 | 32.870979 |
| Ca | 42.853210 | 29.926163 | 34.670532 |
| S  | 26.893776 | 27.454088 | 36.250931 |
| S  | 27.059101 | 33.765442 | 34.577755 |
| S  | 30.597385 | 29.958574 | 32.460930 |
| S  | 30.131252 | 31.411629 | 36.213303 |
| S  | 33.403477 | 27.428326 | 33.960724 |
| S  | 33.649147 | 32.610214 | 32.996696 |
| S  | 36.842739 | 29.314709 | 31.879515 |
| S  | 36.350582 | 29.362413 | 36.852001 |
| S  | 40.225845 | 27.014673 | 34.467697 |
| S  | 40.271744 | 31.522360 | 33.585201 |
|    |    |    |    |
|----|----|----|----|
| S  | 43.327335 | 28.165268 | 31.714058 |
| S  | 44.945675 | 28.524748 | 37.147297 |

24 generated by VMD

|    |    |    |    |
|----|----|----|----|
| Ca | 25.218157 | 29.898989 | 31.846415 |
| Ca | 26.496834 | 30.514593 | 35.702610 |
| Ca | 30.062119 | 28.003941 | 34.977722 |
| Ca | 30.281837 | 33.295708 | 33.618938 |
| Ca | 33.378216 | 29.210705 | 31.577150 |
| Ca | 33.072899 | 30.361750 | 35.337193 |
| Ca | 36.981392 | 26.858650 | 34.659359 |
| Ca | 36.882118 | 31.625130 | 34.452522 |
| Ca | 39.975151 | 29.001165 | 31.524111 |
| Ca | 39.770107 | 30.091423 | 36.597233 |
| Ca | 45.236862 | 25.887112 | 32.947777 |
| Ca | 42.940086 | 29.627375 | 34.941082 |
| S  | 26.814770 | 27.325058 | 36.308517 |
| S  | 27.130281 | 33.957954 | 34.670944 |
| S  | 30.372616 | 29.944550 | 32.556557 |
| S  | 30.050018 | 31.332073 | 36.240131 |
| S  | 33.555862 | 27.211323 | 34.038513 |
| S  | 33.552429 | 32.549301 | 32.499573 |
| S  | 36.817657 | 29.285530 | 32.042187 |
| S  | 36.269539 | 29.459948 | 36.729492 |
| S  | 40.425259 | 27.124821 | 34.423222 |
| S  | 40.505352 | 31.389292 | 33.634521 |
| S  | 43.420002 | 28.168482 | 31.651308 |
| S  | 45.224289 | 28.266556 | 37.053566 |

24 generated by VMD

|    |    |    |    |
|----|----|----|----|
| Ca | 25.090815 | 30.034101 | 31.908482 |
| Ca | 26.486231 | 30.554867 | 35.727970 |
| Ca | 29.825035 | 28.303410 | 35.112347 |
| Ca | 30.317783 | 33.026245 | 33.632702 |
| Ca | 33.662395 | 29.343405 | 31.198435 |
| Ca | 33.017021 | 30.190073 | 35.534157 |
| Ca | 36.622089 | 26.738913 | 34.896168 |
| Ca | 36.680290 | 31.457272 | 34.456783 |
| Ca | 40.115871 | 28.565681 | 31.569807 |
| Ca | 39.712746 | 30.222260 | 36.624004 |
| Ca | 45.438000 | 25.694815 | 32.598404 |
| Ca | 42.899502 | 29.806973 | 34.859718 |
| S  | 26.608870 | 27.424837 | 35.952766 |
| S  | 27.148806 | 33.833473 | 34.569088 |
| S  | 30.544537 | 29.958298 | 32.385155 |
| S  | 30.142319 | 31.235712 | 36.365021 |
|       |        |        |        |
|-------|--------|--------|--------|
| S     | 33.489670 | 27.442255 | 34.049603 |
| S     | 33.937805 | 32.502850 | 32.769005 |
| S     | 36.709339 | 28.994505 | 32.095810 |
| S     | 36.364162 | 29.353933 | 36.960545 |
| S     | 40.374866 | 27.254433 | 34.749153 |
| S     | 40.300228 | 31.402004 | 33.492523 |
| S     | 43.525467 | 28.449659 | 31.563086 |
| S     | 45.420097 | 28.601458 | 36.959957 |
| 24    | generated by VMD |
| Ca    | 25.121765 | 29.993483 | 31.955523 |
| Ca    | 26.702139 | 30.448845 | 35.889221 |
| Ca    | 30.227413 | 28.103146 | 34.967243 |
| Ca    | 30.252989 | 33.021420 | 33.525887 |
| Ca    | 33.483494 | 29.320663 | 31.422972 |
| Ca    | 33.101669 | 30.571568 | 35.460007 |
| Ca    | 36.810955 | 27.040867 | 34.587044 |
| Ca    | 36.717060 | 31.235491 | 34.323322 |
| Ca    | 40.182091 | 29.045040 | 31.533661 |
| Ca    | 39.740108 | 30.219864 | 36.584621 |
| Ca    | 45.354393 | 25.397152 | 32.958561 |
| Ca    | 42.862858 | 29.853630 | 34.709076 |
| S     | 26.886436 | 27.359842 | 36.054520 |
| S     | 27.145454 | 33.670681 | 34.629581 |
| S     | 30.368195 | 29.875029 | 32.363560 |
| S     | 30.105947 | 31.272827 | 36.295235 |
| S     | 33.522232 | 27.534641 | 34.082012 |
| S     | 33.807655 | 32.634022 | 32.747467 |
| S     | 36.663353 | 29.151747 | 31.809387 |
| S     | 36.255936 | 29.336452 | 36.939690 |
| S     | 40.272682 | 27.264315 | 34.677643 |
| S     | 40.344769 | 31.662733 | 33.783009 |
| S     | 43.255417 | 27.940481 | 31.744270 |
| S     | 45.248848 | 28.437410 | 36.987152 |
| 24    | generated by VMD |
| Ca    | 24.937506 | 29.727594 | 32.098686 |
| Ca    | 26.623394 | 30.163284 | 36.077770 |
| Ca    | 30.233498 | 28.340763 | 35.091011 |
| Ca    | 30.233269 | 33.261993 | 33.455532 |
| Ca    | 33.565216 | 29.403755 | 31.246035 |
| Ca    | 33.201550 | 30.452751 | 35.355919 |
| Ca    | 36.939335 | 27.090652 | 34.586666 |
| Ca    | 36.833855 | 31.461563 | 34.343014 |
| Ca    | 40.039616 | 28.896671 | 31.680674 |
| Ca    | 39.704494 | 29.917635 | 36.361664 |
Ca  45.336205  25.251461  32.954067
Ca  42.899605  29.962654  34.940792
S   26.824739  27.068493  34.673157
S   30.454506  30.179958  32.344120
S   30.098146  31.405098  36.357384
S   33.569483  27.625742  33.962955
S   33.820145  32.725380  32.652725
S   36.746540  29.263798  31.842884
S   40.525459  32.650366  34.625023
S   40.376335  31.599890  33.435764
S   43.357502  28.993027  31.927057
S   44.737907  28.431379  37.400135

24 generated by VMD
Ca  24.814217  29.831083  31.927698
Ca  26.634487  30.329807  35.641369
Ca  30.217583  28.078461  34.947384
Ca  30.250050  33.274647  33.697979
Ca  33.484863  29.373348  31.239962
Ca  33.111443  30.394892  35.634277
Ca  36.956406  26.982805  34.870491
Ca  36.493458  31.149080  34.141190
Ca  40.072590  28.685638  31.345179
Ca  39.932129  30.438145  36.542976
Ca  45.575897  25.391026  33.069912
Ca  43.000500  29.941647  34.678375
S   26.608299  27.182274  35.737709
S   27.004055  33.709949  34.966450
S   30.612886  30.230986  32.435474
S   30.052860  31.390425  36.363998
S   33.494144  27.681128  34.003567
S   33.765156  32.804291  32.919750
S   36.690483  28.949966  31.841106
S   36.414612  29.523739  36.904469
S   40.402187  27.257975  34.768936
S   40.310635  31.429943  33.585331
S   43.349360  27.874430  31.717392
S   45.191021  28.485708  37.049728

24 generated by VMD
Ca  25.350870  29.532053  31.887962
Ca  26.630100  30.152716  35.685719
Ca  30.133015  28.425770  35.153381
Ca  30.146889  33.272095  33.524193
|   |   |   |
|---|---|---|
| Ca | 33.778210 | 29.657076 | 31.611824 |
| Ca | 32.967686 | 30.448133 | 35.755577 |
| Ca | 36.525433 | 26.947412 | 34.721889 |
| Ca | 36.428963 | 31.601379 | 34.347054 |
| Ca | 40.317833 | 28.706442 | 31.544653 |
| Ca | 39.658752 | 30.285057 | 36.181805 |
| Ca | 45.411320 | 24.994801 | 32.830769 |
| Ca | 43.127869 | 29.837252 | 34.645187 |
| S  | 27.015862 | 26.924065 | 35.889812 |
| S  | 27.008457 | 33.523884 | 34.813160 |
| S  | 30.611410 | 30.228514 | 32.495567 |
| S  | 29.908176 | 31.455580 | 36.258846 |
| S  | 33.436066 | 27.919565 | 34.106354 |
| S  | 33.667030 | 32.862221 | 32.960236 |
| S  | 36.839775 | 29.135262 | 32.079777 |
| S  | 36.256916 | 29.559443 | 36.888542 |
| S  | 40.245861 | 27.162483 | 34.535686 |
| S  | 40.466961 | 31.548912 | 33.400501 |
| S  | 43.635719 | 27.837622 | 31.629145 |
| S  | 44.864746 | 28.383648 | 37.084793 |

24

generated by VMD

|   |   |   |
|---|---|---|
| Ca | 25.130947 | 29.665367 | 31.897713 |
| Ca | 26.319191 | 30.108807 | 35.755104 |
| Ca | 30.175909 | 28.486811 | 34.962669 |
| Ca | 29.835024 | 33.219345 | 33.753407 |
| Ca | 33.510330 | 29.328283 | 31.683655 |
| Ca | 33.177494 | 30.542891 | 35.724827 |
| Ca | 36.875900 | 27.360535 | 34.757416 |
| Ca | 36.717434 | 31.534882 | 34.245949 |
| Ca | 40.404266 | 28.927916 | 31.427715 |
| Ca | 39.906265 | 30.174477 | 36.174961 |
| Ca | 45.270050 | 24.814121 | 33.213669 |
| Ca | 43.405190 | 29.790817 | 34.378128 |
| S  | 26.863571 | 27.040844 | 35.563217 |
| S  | 26.479794 | 33.555542 | 34.845406 |
| S  | 30.396130 | 30.306786 | 32.363884 |
| S  | 29.917385 | 31.367369 | 36.486526 |
| S  | 33.433662 | 27.653959 | 34.298027 |
| S  | 33.512573 | 32.667873 | 32.975559 |
| S  | 36.846325 | 29.378403 | 31.915791 |
| S  | 36.384537 | 29.728584 | 36.853271 |
| S  | 40.383636 | 27.279812 | 34.545818 |
| S  | 40.769596 | 31.591393 | 33.353657 |
| S  | 43.627949 | 27.602186 | 31.786423 |
| S  | 45.090740 | 28.264420 | 37.067936 |
| 24 | generated by VMD |
|----|------------------|
| Ca | 25.030849 29.486895 31.872362 |
| Ca | 26.712561 30.184328 35.734131 |
| Ca | 30.281240 28.437641 35.085514 |
| Ca | 30.263878 33.387211 33.574249 |
| Ca | 33.194622 30.391605 35.732082 |
| Ca | 36.794365 27.251436 34.580845 |
| Ca | 36.757442 31.363850 34.220348 |
| Ca | 40.149296 28.705809 31.370275 |
| Ca | 39.844685 30.521967 36.474945 |
| Ca | 45.183899 24.991840 33.278206 |
| Ca | 42.914219 29.775707 34.485516 |
| S  | 26.818441 26.806820 35.374260 |
| S  | 26.925383 33.646004 34.935249 |
| S  | 30.458435 30.149672 32.557945 |
| S  | 30.006514 31.305735 36.446625 |
| S  | 33.494968 27.769180 34.205227 |
| S  | 33.763374 32.957026 33.062126 |
| S  | 36.777588 29.252378 31.795822 |
| S  | 36.423626 29.512701 36.795486 |
| S  | 40.270615 27.263676 34.620914 |
| S  | 40.425655 31.551998 33.377136 |
| S  | 43.325916 27.581293 31.647343 |
| S  | 45.087185 28.568071 37.151012 |

24

generated by VMD

| Ca | 24.748405 29.395000 31.614574 |
| Ca | 26.635345 29.935295 35.597466 |
| Ca | 30.218987 28.571686 34.998585 |
| Ca | 30.201183 33.342396 33.671516 |
| Ca | 33.579445 29.579710 31.884592 |
| Ca | 33.098492 30.695162 35.902973 |
| Ca | 36.673801 27.156704 34.900768 |
| Ca | 36.834679 31.478415 34.109661 |
| Ca | 40.071098 28.607960 31.285192 |
| Ca | 39.844540 30.261003 36.235249 |
| Ca | 45.668827 24.909418 33.246986 |
| Ca | 43.163361 29.750444 34.560749 |
| S  | 26.938534 26.871643 35.074505 |
| S  | 26.803635 33.441833 35.142872 |
| S  | 30.472322 30.386686 32.483875 |
| S  | 29.826830 31.325270 36.639210 |
| S  | 33.463055 27.904301 34.469627 |
| S  | 33.702888 32.993874 32.937828 |
| S     | 36.778362  | 29.108313  | 32.035500  |
|------|------------|------------|------------|
| S     | 36.390591  | 29.807077  | 36.781136  |
| S     | 40.331444  | 27.283476  | 34.531471  |
| S     | 40.557522  | 31.595991  | 33.245571  |
| S     | 43.297935  | 27.498421  | 31.601343  |
| S     | 45.127731  | 28.491289  | 37.079544  |

24

generated by VMD

| Ca   | 25.104183  | 29.738859  | 31.890928  |
|------|------------|------------|------------|
| Ca   | 26.700144  | 30.276260  | 35.858166  |
| Ca   | 29.945305  | 28.384939  | 35.048725  |
| Ca   | 30.426905  | 33.119091  | 33.622963  |
| Ca   | 33.664734  | 29.572639  | 31.556519  |
| Ca   | 33.107662  | 30.451618  | 35.484886  |
| Ca   | 35.566696  | 26.994513  | 34.698277  |
| Ca   | 36.703777  | 31.551285  | 34.422085  |
| Ca   | 40.298210  | 28.545576  | 31.377518  |
| Ca   | 40.008476  | 30.309896  | 36.462608  |
| Ca   | 45.396206  | 24.911072  | 33.312145  |
| Ca   | 42.994038  | 30.052319  | 34.523838  |
| S    | 26.731590  | 26.977327  | 35.423683  |
| S    | 26.889421  | 33.510681  | 34.958942  |
| S    | 30.601568  | 30.145670  | 32.384022  |
| S    | 30.040665  | 31.316393  | 36.532841  |
| S    | 33.157932  | 27.552622  | 34.151875  |
| S    | 33.804325  | 32.838909  | 32.954990  |
| S    | 36.859123  | 29.267282  | 32.014320  |
| S    | 36.318104  | 29.501554  | 36.871639  |
| S    | 40.166264  | 27.334831  | 34.650425  |
| S    | 40.298058  | 31.594959  | 33.421116  |
| S    | 43.407722  | 27.573069  | 31.500443  |
| S    | 45.242790  | 28.870037  | 36.907772  |

24

generated by VMD

| Ca   | 25.206173  | 29.876522  | 31.787928  |
|------|------------|------------|------------|
| Ca   | 26.590715  | 30.048866  | 35.745327  |
| Ca   | 30.016748  | 28.501314  | 35.180187  |
| Ca   | 30.160286  | 33.273033  | 33.488937  |
| Ca   | 33.654575  | 29.555992  | 31.607185  |
| Ca   | 33.190346  | 30.446238  | 35.924149  |
| Ca   | 36.699585  | 27.128277  | 34.734932  |
| Ca   | 36.854229  | 31.399128  | 34.302170  |
| Ca   | 40.230347  | 28.390505  | 31.229137  |
| Ca   | 39.720783  | 30.211407  | 36.294170  |
| Ca   | 45.259453  | 24.955538  | 33.319328  |
| Ca   | 43.076752  | 30.091181  | 34.427402  |
|   | S  | S  | S  |
|---|----|----|----|
|   | 26.930529 | 26.957821 | 35.414280 |
|   | 26.885483 | 33.502274 | 35.057323 |
|   | 30.566528 | 30.101974 | 32.565105 |
|   | 29.934519 | 31.402905 | 36.319195 |
|   | 33.548775 | 27.644407 | 34.20179 |
|   | 33.649666 | 32.788548 | 33.038490 |
|   | 36.816559 | 29.181097 | 32.051281 |
|   | 36.371555 | 29.671844 | 36.936951 |
|   | 33.912297 | 27.341999 | 34.570019 |
|   | 40.514069 | 31.500538 | 33.209747 |
|   | 43.461502 | 27.795563 | 31.513977 |
|   | 44.760441 | 28.624413 | 37.111256 |
| 24 | generated by VMD |
| Ca | 25.086149 | 30.204308 | 31.777201 |
| Ca | 26.465742 | 30.141672 | 35.624096 |
| Ca | 30.102606 | 28.144861 | 34.922703 |
| Ca | 30.244015 | 33.445057 | 33.889985 |
| Ca | 33.371353 | 29.172005 | 31.450703 |
| Ca | 33.275349 | 30.336567 | 35.486179 |
| Ca | 36.859024 | 27.153494 | 34.818619 |
| Ca | 36.874069 | 31.627319 | 33.983803 |
| Ca | 40.050976 | 28.571108 | 31.408560 |
| Ca | 39.879250 | 30.625900 | 36.141132 |
| Ca | 45.254433 | 25.027006 | 33.482040 |
| Ca | 43.077477 | 29.858536 | 34.536415 |
| S  | 26.870140 | 26.927311 | 35.442513 |
| S  | 26.887003 | 33.593185 | 35.172932 |
| S  | 30.479805 | 30.234602 | 32.500225 |
| S  | 30.02693 | 30.935337 | 36.624180 |
| S  | 33.477188 | 27.408274 | 34.210865 |
| S  | 33.730865 | 32.657127 | 33.089439 |
| S  | 36.722485 | 29.142588 | 31.895706 |
| S  | 36.488686 | 30.076328 | 36.884529 |
| S  | 40.436123 | 27.414074 | 34.629692 |
| S  | 40.512676 | 31.530104 | 33.153008 |
| S  | 43.348354 | 27.607077 | 31.674395 |
| S  | 44.914036 | 28.557558 | 37.232841 |
| 24 | generated by VMD |
| Ca | 24.971092 | 29.911747 | 31.864613 |
| Ca | 26.507561 | 30.286539 | 35.565651 |
| Ca | 29.967754 | 28.403723 | 34.782352 |
| Ca | 30.400257 | 33.112843 | 33.604301 |
| Ca | 33.650494 | 29.468678 | 31.983980 |
| Ca | 33.104050 | 30.474119 | 35.969429 |
|    |      |      |      |
|----|------|------|------|
| Ca | 36.639923 | 26.934315 | 34.971146 |
| Ca | 36.755192 | 31.764105 | 34.281 |
| Ca | 40.364437 | 28.546770 | 31.585165 |
| Ca | 39.868416 | 30.320972 | 36.087547 |
| Ca | 45.193539 | 25.217606 | 32.929237 |
| Ca | 42.886642 | 29.878241 | 34.345116 |
| S  | 26.638632 | 26.944483 | 35.287369 |
| S  | 27.126245 | 33.522430 | 34.650970 |
| S  | 30.485636 | 30.143251 | 32.341412 |
| S  | 29.759375 | 31.250519 | 36.415707 |
| S  | 33.346790 | 27.457111 | 34.499775 |
| S  | 33.810368 | 32.683208 | 33.255821 |
| S  | 36.932823 | 29.193914 | 32.298985 |
| S  | 36.601101 | 29.681301 | 37.123898 |
| S  | 40.362713 | 27.164064 | 36.82087 |
| S  | 40.447159 | 31.523396 | 33.230389 |
| S  | 43.607296 | 27.842932 | 31.315390 |
| S  | 45.006371 | 28.665094 | 36.959259 |

24 generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 25.260468 | 29.673775 | 31.955637 |
| Ca | 26.586988 | 30.223227 | 35.661377 |
| Ca | 30.159931 | 28.363483 | 35.020096 |
| Ca | 30.168474 | 33.553371 | 33.810097 |
| Ca | 33.650394 | 29.710571 | 31.794544 |
| Ca | 33.241108 | 30.525764 | 35.877365 |
| Ca | 36.646610 | 26.849436 | 34.712826 |
| Ca | 36.687805 | 31.697525 | 34.169884 |
| Ca | 40.035149 | 28.203442 | 31.360048 |
| Ca | 39.813873 | 30.591436 | 35.937874 |
| Ca | 45.548336 | 25.453426 | 33.395489 |
| Ca | 42.977367 | 29.789940 | 34.508095 |
| S  | 26.944252 | 26.891403 | 35.277191 |
| S  | 26.954447 | 33.443813 | 34.919842 |
| S  | 30.646841 | 30.262026 | 32.525173 |
| S  | 30.004820 | 31.264427 | 36.487171 |
| S  | 33.502914 | 27.749475 | 34.181370 |
| S  | 33.677204 | 32.999439 | 33.283272 |
| S  | 36.779659 | 29.109806 | 31.920809 |
| S  | 36.532623 | 29.570820 | 36.686966 |
| S  | 40.283161 | 27.284248 | 34.678955 |
| S  | 40.303829 | 31.256521 | 32.941875 |
| S  | 43.465313 | 27.721842 | 31.636747 |
| S  | 44.562309 | 28.402218 | 37.288025 |

24 generated by VMD
| Element | Value1  | Value2  | Value3  |
|---------|---------|---------|---------|
| Ca      | 25.351707 | 29.969692 | 31.661514 |
| Ca      | 26.446266 | 30.154560 | 35.708256 |
| Ca      | 30.063807 | 28.052462 | 35.002174 |
| Ca      | 30.268089 | 33.244732 | 33.710197 |
| Ca      | 33.417324 | 29.697453 | 31.798403 |
| Ca      | 33.003487 | 30.315115 | 35.655689 |
| Ca      | 36.858673 | 26.926052 | 34.693577 |
| Ca      | 36.982635 | 31.833368 | 34.411655 |
| Ca      | 40.064697 | 28.425821 | 31.331171 |
| Ca      | 39.895954 | 30.515989 | 36.053696 |
| Ca      | 45.379372 | 25.197741 | 33.571987 |
| Ca      | 43.009487 | 29.777040 | 34.355190 |
| S       | 26.755569 | 26.916063 | 35.571281 |
| S       | 26.932388 | 33.757324 | 34.930145 |
| S       | 30.551788 | 30.234095 | 32.574821 |
| S       | 29.927532 | 31.116217 | 36.531277 |
| S       | 33.426582 | 27.596066 | 34.082508 |
| S       | 33.661034 | 32.694431 | 33.125328 |
| S       | 36.846828 | 29.367514 | 32.029026 |
| S       | 36.514061 | 29.594172 | 36.763023 |
| S       | 40.278801 | 27.365993 | 34.677765 |
| S       | 40.428280 | 31.404413 | 33.073025 |
| S       | 43.306095 | 27.481014 | 31.587061 |
| S       | 45.063465 | 28.754063 | 37.131886 |

24

generated by VMD

| Element | Value1  | Value2  | Value3  |
|---------|---------|---------|---------|
| Ca      | 25.030817 | 29.925344 | 31.917686 |
| Ca      | 26.625925 | 30.226156 | 35.641933 |
| Ca      | 30.196827 | 28.449293 | 34.833897 |
| Ca      | 30.282990 | 33.156063 | 33.726906 |
| Ca      | 33.779980 | 29.745056 | 31.704977 |
| Ca      | 33.295120 | 30.446590 | 35.880192 |
| Ca      | 36.789291 | 26.903921 | 34.932880 |
| Ca      | 36.711788 | 31.363241 | 34.247478 |
| Ca      | 40.019608 | 28.110626 | 31.444597 |
| Ca      | 39.704967 | 30.584345 | 36.208538 |
| Ca      | 45.140541 | 25.278793 | 33.310101 |
| Ca      | 42.809937 | 29.984425 | 34.479313 |
| S       | 27.043686 | 26.735350 | 35.223400 |
| S       | 27.096361 | 33.566261 | 35.126099 |
| S       | 30.611731 | 30.360630 | 32.211246 |
| S       | 29.973406 | 31.190273 | 36.477715 |
| S       | 33.518700 | 27.896873 | 34.173840 |
| S       | 33.743931 | 32.892620 | 33.223530 |
| S       | 36.695957 | 28.940769 | 31.829050 |
| S       | 36.538780 | 29.590191 | 36.875553 |
| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| S    | 40.181118  | 27.255026  | 34.904945  |
| S    | 40.109909  | 31.157871  | 33.005016  |
| S    | 43.495525  | 27.810112  | 31.610973  |
| S    | 45.037045  | 28.821552  | 37.040905  |

24 generated by VMD

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Ca   | 25.100105  | 30.366476  | 32.028389  |
| Ca   | 26.218939  | 30.495399  | 36.077007  |
| Ca   | 30.278463  | 27.928465  | 34.765366  |
| Ca   | 30.139515  | 33.180691  | 33.840733  |
| Ca   | 33.569340  | 29.493273  | 31.443003  |
| Ca   | 33.238140  | 30.406034  | 35.487495  |
| Ca   | 36.874714  | 26.884398  | 35.032425  |
| Ca   | 36.664001  | 31.200022  | 34.034393  |
| Ca   | 40.250069  | 28.418922  | 31.528944  |
| Ca   | 39.551785  | 30.629005  | 36.281143  |
| Ca   | 45.433994  | 25.486959  | 33.216900  |
| Ca   | 42.986420  | 29.818138  | 34.625477  |
| S    | 26.843441  | 27.051380  | 35.419697  |
| S    | 26.764181  | 33.882481  | 35.208439  |
| S    | 30.703167  | 30.173550  | 32.372536  |
| S    | 29.836847  | 30.916134  | 36.266552  |
| S    | 33.660950  | 27.566442  | 34.059547  |
| S    | 33.681545  | 32.887684  | 32.951820  |
| S    | 36.821999  | 28.730207  | 31.774340  |
| S    | 36.280712  | 29.868099  | 36.886940  |
| S    | 40.520012  | 27.264402  | 34.890388  |
| S    | 40.359562  | 31.383673  | 33.180847  |
| S    | 43.569347  | 27.711237  | 31.570341  |
| S    | 45.086689  | 28.648376  | 37.087948  |

24 generated by VMD

| Atom | X          | Y          | Z          |
|------|------------|------------|------------|
| Ca   | 24.719357  | 30.186825  | 32.193996  |
| Ca   | 26.363632  | 30.218395  | 35.909946  |
| Ca   | 30.190102  | 28.203545  | 34.904167  |
| Ca   | 30.265188  | 33.250317  | 33.567467  |
| Ca   | 33.509201  | 29.758469  | 31.628096  |
| Ca   | 33.258858  | 30.401136  | 35.531754  |
| Ca   | 36.764130  | 26.949781  | 34.661560  |
| Ca   | 36.672741  | 31.103756  | 34.125618  |
| Ca   | 40.386055  | 28.455587  | 31.620745  |
| Ca   | 39.797894  | 30.422283  | 36.395695  |
| Ca   | 45.504414  | 25.350836  | 33.462734  |
| Ca   | 43.010654  | 30.035532  | 34.517727  |
| S    | 26.905731  | 26.984310  | 35.492317  |
| S    | 27.044657  | 33.685463  | 35.047180  |
S  30.507816  30.226954  32.371021
S  29.974957  31.094454  36.444001
S  33.451538  27.642696  33.915676
S  33.725651  32.790337  32.780441
S  36.748627  28.980806  31.835855
S  36.373547  29.523714  36.784012
S  40.349678  27.271343  31.835855
S  40.376877  31.376757  33.279919
S  43.461647  27.755911  31.508904
S  45.071011  28.722191  37.136627

24 generated by VMD
Ca  25.112564  30.119446  31.974014
Ca  26.245047  30.413982  35.854435
Ca  30.181406  28.158379  35.056602
Ca  30.176497  33.195541  33.636860
Ca  33.789288  29.800961  31.717461
Ca  33.128849  30.531307  35.534370
Ca  36.797295  26.820545  34.769947
Ca  36.760731  31.160297  34.135757
Ca  40.339031  28.458162  31.539457
Ca  39.507805  30.277346  36.490784
Ca  45.634632  25.246845  33.356537
Ca  42.807148  30.120165  34.413010
S  26.925272  27.052702  35.628300
S  26.820984  33.823944  34.939026
S  30.600281  30.122478  32.493095
S  29.980742  31.027399  36.533588
S  33.501694  27.709278  34.025394
S  33.813534  32.881424  32.810360
S  36.835636  28.833090  31.863708
S  36.232746  29.411123  36.712086
S  40.331406  27.142141  34.741203
S  40.204144  31.489271  33.359280
S  43.661442  27.762287  31.537483
S  45.045700  28.833284  36.907967

24 generated by VMD
Ca  24.830225  29.997553  31.779346
Ca  26.466873  30.548822  35.898823
Ca  30.086903  28.238938  35.053612
Ca  30.232544  33.168945  33.696163
Ca  33.652790  29.763786  31.590696
Ca  33.252052  30.361935  35.646557
Ca  36.687008  26.744226  34.894020
Ca  36.693371  31.072697  34.268913
| Ca   | 40.301609 | 28.489862 | 31.322292 |
| Ca   | 39.816544 | 30.055223 | 36.329643 |
| Ca   | 45.589642 | 25.469910 | 33.440838 |
| Ca   | 42.937931 | 30.079691 | 34.479950 |
| S    | 26.813686 | 27.179403 | 35.609905 |
| S    | 27.113392 | 33.840775 | 34.718449 |
| S    | 30.561052 | 30.176311 | 32.379868 |
| S    | 29.935619 | 31.131531 | 36.512520 |
| S    | 33.364857 | 27.503979 | 33.965641 |
| S    | 33.659878 | 32.899761 | 33.038799 |
| S    | 36.663303 | 28.808084 | 32.012135 |
| S    | 36.320568 | 29.347240 | 36.916740 |
| S    | 40.328751 | 27.073938 | 34.650848 |
| S    | 40.196579 | 31.405386 | 33.308250 |
| S    | 43.654270 | 27.962250 | 31.623285 |
| S    | 45.274433 | 29.071692 | 36.893406 |

24 generated by VMD

| Ca   | 25.139370 | 30.257002 | 31.857861 |
| Ca   | 26.332073 | 30.776985 | 35.809486 |
| Ca   | 30.311617 | 27.840178 | 34.744190 |
| Ca   | 30.077421 | 33.123131 | 33.884270 |
| Ca   | 33.581703 | 29.799973 | 31.943123 |
| Ca   | 33.256973 | 30.413185 | 35.453842 |
| Ca   | 36.764072 | 26.709253 | 34.680489 |
| Ca   | 36.797947 | 31.025059 | 34.097187 |
| Ca   | 40.099995 | 28.395773 | 31.644958 |
| Ca   | 39.840305 | 30.188644 | 36.444641 |
| Ca   | 45.640377 | 25.649157 | 33.405552 |
| Ca   | 42.800873 | 29.980356 | 34.350006 |
| S    | 26.761326 | 27.316681 | 35.595673 |
| S    | 26.903410 | 33.919064 | 34.885033 |
| S    | 30.600376 | 30.096645 | 32.518013 |
| S    | 30.067173 | 30.842104 | 36.399338 |
| S    | 33.500935 | 27.494703 | 34.120708 |
| S    | 33.753712 | 32.857662 | 33.049080 |
| S    | 36.598053 | 28.821453 | 31.739359 |
| S    | 36.428440 | 29.290911 | 36.668968 |
| S    | 40.330544 | 27.241421 | 34.794502 |
| S    | 40.263378 | 31.353096 | 33.154148 |
| S    | 43.383530 | 27.797468 | 31.625343 |
| S    | 45.200184 | 29.201517 | 37.164948 |

24 generated by VMD

| Ca   | 25.287592 | 30.362642 | 31.762054 |
| Ca   | 26.273510 | 30.316887 | 35.822376 |
|     |     |     |     |
|-----|-----|-----|-----|
| Ca  | 29.988956 | 28.144003 | 35.025948 |
| Ca  | 30.417089 | 33.166424 | 33.893013 |
| Ca  | 33.700356 | 29.909172 | 31.772625 |
| Ca  | 33.183243 | 30.253698 | 35.663849 |
| Ca  | 36.700409 | 26.777777 | 34.785362 |
| Ca  | 36.88504 | 30.969460 | 33.932083 |
| Ca  | 40.021950 | 28.367689 | 31.518921 |
| Ca  | 39.866947 | 30.268145 | 36.183830 |
| Ca  | 45.460098 | 25.504776 | 33.764778 |
| Ca  | 43.023876 | 30.114374 | 34.374931 |
| S   | 26.573200 | 26.997955 | 35.66420 |
| S   | 26.995159 | 33.736702 | 34.628170 |
| S   | 30.642918 | 30.260130 | 32.494938 |
| S   | 29.854240 | 30.970839 | 36.644772 |
| S   | 33.317966 | 27.614891 | 34.095097 |
| S   | 33.761101 | 32.892540 | 33.280910 |
| S   | 36.620209 | 28.817793 | 31.723503 |
| S   | 36.386417 | 29.389042 | 36.756973 |
| S   | 40.286613 | 27.252033 | 34.705074 |
| S   | 40.412354 | 31.362904 | 32.972191 |
| S   | 43.520306 | 27.765415 | 31.728220 |
| S   | 45.250854 | 29.176155 | 36.834690 |

24

generated by VMD

|     |     |     |     |
|-----|-----|-----|-----|
| Ca  | 25.257324 | 30.039862 | 31.693277 |
| Ca  | 26.435925 | 30.568491 | 35.679470 |
| Ca  | 30.407263 | 27.887428 | 34.882408 |
| Ca  | 30.171427 | 33.308842 | 34.091442 |
| Ca  | 33.570564 | 30.008093 | 31.850584 |
| Ca  | 33.076160 | 30.350481 | 35.604351 |
| Ca  | 36.794331 | 26.791651 | 34.726437 |
| Ca  | 36.873081 | 31.143208 | 34.082603 |
| Ca  | 40.094643 | 28.200285 | 31.360615 |
| Ca  | 39.709484 | 30.213455 | 36.372890 |
| Ca  | 45.591469 | 25.459230 | 33.625736 |
| Ca  | 42.662975 | 30.020107 | 34.516022 |
| S   | 26.978052 | 27.144016 | 35.609097 |
| S   | 26.921738 | 34.008602 | 34.898926 |
| S   | 30.556791 | 30.328171 | 32.611549 |
| S   | 29.931690 | 30.880539 | 36.527084 |
| S   | 33.514931 | 27.627460 | 33.905289 |
| S   | 33.669529 | 32.970375 | 33.150597 |
| S   | 36.662693 | 28.714794 | 31.846746 |
| S   | 36.293476 | 29.297319 | 36.708549 |
| S   | 40.341743 | 27.169796 | 34.761192 |
| S   | 40.240852 | 31.200974 | 32.894672 |
|   | 43.496723 | 27.671303 | 31.756426 |
|---|-----------|-----------|-----------|
| S | 45.181095 | 29.386955 | 36.874779 |

24

generated by VMD

| Ca | 24.745905 | 30.218988 | 31.749653 |
|----|-----------|-----------|-----------|
| Ca | 26.145994 | 30.533112 | 35.628868 |
| Ca | 29.936563 | 27.983870 | 35.144489 |
| Ca | 30.159786 | 33.218468 | 33.926094 |
| Ca | 33.677731 | 29.808838 | 31.699482 |
| Ca | 33.145084 | 30.207777 | 35.816170 |
| Ca | 36.813652 | 26.787851 | 34.813137 |
| Ca | 36.812668 | 31.425602 | 34.196106 |
| Ca | 40.137806 | 28.458839 | 31.435928 |
| Ca | 39.748749 | 29.876863 | 36.014271 |
| Ca | 45.747299 | 25.460096 | 33.516056 |
| Ca | 42.923084 | 29.935272 | 34.389851 |

| S  | 26.547421 | 27.230209 | 35.606277 |
|----|-----------|-----------|-----------|
| S  | 26.869473 | 33.873650 | 34.483181 |
| S  | 30.720440 | 30.182756 | 32.552765 |
| S  | 29.749798 | 30.987034 | 36.471123 |
| S  | 33.535278 | 27.636417 | 34.127033 |
| S  | 33.716282 | 32.792404 | 33.300743 |
| S  | 36.754040 | 28.857838 | 31.928732 |
| S  | 36.475719 | 29.408035 | 36.901123 |
| S  | 40.541981 | 27.100769 | 34.694946 |
| S  | 40.367641 | 31.414276 | 33.093239 |
| S  | 43.685844 | 27.809929 | 31.650381 |
| S  | 45.475689 | 29.182514 | 36.891060 |

24

generated by VMD

| Ca | 24.846710 | 29.944906 | 32.002106 |
|----|-----------|-----------|-----------|
| Ca | 26.307140 | 30.637575 | 35.794567 |
| Ca | 30.040565 | 27.852940 | 34.767681 |
| Ca | 30.257042 | 33.303722 | 33.796562 |
| Ca | 33.710941 | 30.071932 | 31.954800 |
| Ca | 33.030289 | 30.277344 | 35.597443 |
| Ca | 36.860039 | 26.605278 | 34.643684 |
| Ca | 36.919453 | 31.462646 | 34.307781 |
| Ca | 39.931847 | 28.191357 | 31.822058 |
| Ca | 39.923882 | 30.375645 | 36.211967 |
| Ca | 45.513615 | 25.714540 | 33.506447 |
| Ca | 43.019920 | 29.814470 | 34.293350 |
| S  | 26.572905 | 27.186150 | 35.427265 |
| S  | 26.899866 | 33.857132 | 34.812592 |
| S  | 30.660749 | 30.216496 | 32.366776 |
| S  | 29.896780 | 30.772293 | 36.273827 |
| S    | 33.504917 | 27.544313 | 34.000145 |
|------|-----------|-----------|-----------|
| S    | 33.712681 | 32.963604 | 33.451584 |
| S    | 36.677490 | 29.050428 | 31.896276 |
| S    | 36.425835 | 29.365082 | 36.660603 |
| S    | 40.318291 | 27.096973 | 34.855137 |
| S    | 40.541393 | 31.362843 | 32.956142 |
| S    | 43.433804 | 27.506424 | 31.782709 |
| S    | 45.427868 | 29.217304 | 36.849159 |

24

generated by VMD

| Ca   | 25.045151 | 30.156523 | 31.850716 |
|------|-----------|-----------|-----------|
| Ca   | 26.396404 | 30.645302 | 35.855896 |
| Ca   | 30.186710 | 27.938351 | 34.728718 |
| Ca   | 30.372803 | 33.181595 | 33.937931 |
| Ca   | 33.770550 | 29.837494 | 31.838896 |
| Ca   | 33.077412 | 30.232859 | 35.534981 |
| Ca   | 36.915695 | 26.859791 | 34.748196 |
| Ca   | 36.646870 | 31.495260 | 34.450596 |
| Ca   | 39.975964 | 28.235817 | 31.405310 |
| Ca   | 39.666142 | 30.101461 | 36.037567 |
| Ca   | 45.268951 | 25.499418 | 33.440708 |
| Ca   | 43.000755 | 29.851334 | 34.591686 |
| S    | 26.959118 | 27.153719 | 35.773487 |
| S    | 26.894011 | 33.809132 | 34.611923 |
| S    | 30.790289 | 30.165205 | 32.429405 |
| S    | 29.867489 | 30.978613 | 36.495338 |
| S    | 33.599361 | 27.477285 | 34.113136 |
| S    | 33.658905 | 32.754776 | 32.969482 |
| S    | 36.808617 | 29.106857 | 31.962738 |
| S    | 36.366062 | 29.379877 | 36.960697 |
| S    | 40.294003 | 27.271795 | 34.617897 |
| S    | 40.230515 | 31.319048 | 33.008785 |
| S    | 43.520508 | 27.891378 | 31.558372 |
| S    | 45.121628 | 29.048515 | 37.108269 |

24

generated by VMD

| Ca   | 25.020576 | 30.276423 | 31.702526 |
|------|-----------|-----------|-----------|
| Ca   | 26.367870 | 30.438313 | 35.808071 |
| Ca   | 30.160450 | 27.915865 | 34.831776 |
| Ca   | 30.394018 | 32.947449 | 34.042908 |
| Ca   | 33.805195 | 29.882935 | 32.003738 |
| Ca   | 33.160126 | 30.388927 | 35.616867 |
| Ca   | 36.847401 | 27.011534 | 34.952969 |
| Ca   | 36.854931 | 31.303545 | 34.187702 |
| Ca   | 40.039574 | 28.293564 | 31.364132 |
| Ca   | 39.701782 | 30.671185 | 36.141598 |
| Element | X Coord  | Y Coord  | Z Coord  |
|---------|----------|----------|----------|
| Ca      | 45.204506| 25.245199| 33.403332|
| Ca      | 42.924431| 29.774841| 34.528069|
| S       | 26.884056| 27.209764| 35.378975|
| S       | 26.801069| 33.642262| 34.639172|
| S       | 30.688787| 30.057232| 32.386242|
| S       | 29.853960| 30.876463| 36.540192|
| S       | 33.530964| 27.592934| 34.229496|
| S       | 33.821732| 32.946877| 33.212860|
| S       | 36.730000| 28.914587| 31.965405|
| S       | 36.254440| 29.541218| 36.973442|
| S       | 40.238140| 27.370739| 34.865143|
| S       | 40.377708| 31.357008| 32.856918|
| S       | 43.446495| 27.761688| 31.652906|
| S       | 45.325764| 28.970863| 36.746273|

24 generated by VMD

| Element | X Coord  | Y Coord  | Z Coord  |
|---------|----------|----------|----------|
| Ca      | 25.026442| 30.009441| 32.093914|
| Ca      | 26.438110| 30.357105| 36.059041|
| Ca      | 30.140566| 28.128410| 34.631790|
| Ca      | 30.401814| 32.870186| 34.142818|
| Ca      | 33.840008| 29.802950| 31.837271|
| Ca      | 33.142021| 30.671476| 35.510921|
| Ca      | 36.770882| 26.848759| 34.622894|
| Ca      | 36.826305| 31.700146| 33.901066|
| Ca      | 40.168682| 28.354935| 31.331842|
| Ca      | 39.568916| 30.525002| 35.967648|
| Ca      | 45.210426| 25.077106| 33.631508|
| Ca      | 42.821632| 29.828659| 34.486687|
| S       | 26.996534| 27.123257| 35.343414|
| S       | 26.944487| 33.703232| 35.067051|
| S       | 30.682102| 30.319698| 32.235023|
| S       | 29.842989| 30.768473| 36.665051|
| S       | 33.554012| 27.568117| 34.098927|
| S       | 33.675411| 32.804543| 33.044289|
| S       | 36.795193| 28.944635| 31.828608|
| S       | 36.352795| 29.618555| 36.755779|
| S       | 40.221088| 27.293978| 34.806141|
| S       | 40.275856| 31.494905| 32.813492|
| S       | 43.691174| 27.714268| 31.896053|
| S       | 45.046501| 28.863586| 37.267586|

24 generated by VMD

| Element | X Coord  | Y Coord  | Z Coord  |
|---------|----------|----------|----------|
| Ca      | 25.230780| 30.320913| 31.824772|
| Ca      | 26.301874| 30.573351| 35.792774|
| Ca      | 30.413456| 27.839352| 34.730236|
| Ca      | 30.215750| 33.196774| 34.093945|
| Element | Ca       | S        |
|---------|----------|----------|
|         | 33.763332| 39.637413|
|         | 32.934460| 30.545673|
|         | 36.961670| 36.911144|
|         | 40.136486| 26.211718|
|         | 39.637413| 26.733311|
|         | 45.436779| 30.620018|
|         | 42.969833| 29.818737|
|         | 45.157841| 33.686886|
|         | 25.155380| 33.642948|
|         | 26.211718| 36.770920|
|         | 30.158970| 36.337276|
|         | 30.154976| 40.419033|
|         | 33.702461| 40.119694|
|         | 33.028996| 45.157841|
|         | 36.911144| 26.784742|
|         | 36.772774| 30.415897|
|         | 40.291878| 30.154976|
|         | 39.734447| 30.782896|
|         | 45.411526| 25.155380|
|         | 42.815956| 30.119200|
|         | 26.784742| 30.201000|
|         | 26.728962| 30.481503|
|         | 30.158970| 28.249580|
|         | 26.307367| 28.249580|
|         | 30.158970| 33.297550|
|         | 30.119200| 33.297550|
|         | 30.158970| 33.297550|
|         | 30.119200| 33.297550|
|         | 30.158970| 33.297550|
|         | 30.119200| 33.297550|
|         | 30.158970| 33.297550|
|         | 30.119200| 33.297550|

24 generated by VMD
|   | Ca      | S       |
|---|---------|---------|
| 1 | 25.185692 | 30.652853 |
| 2 | 26.330748 | 30.357597 |
| 3 | 30.201961 | 27.931467 |
| 4 | 30.457389 | 33.127483 |
| 5 | 33.753811 | 29.759565 |
| 6 | 33.157379 | 30.488901 |
| 7 | 36.707947 | 26.807114 |
| 8 | 36.701675 | 31.206562 |
| 9 | 39.786156 | 30.340977 |
|10 | 42.855927 | 30.069128 |
|11 | 26.847799 | 27.044428 |
|12 | 27.094038 | 33.679543 |
|13 | 30.629284 | 29.987450 |
|14 | 29.982477 | 31.040045 |
|15 | 33.496635 | 27.607288 |
|16 | 33.867462 | 32.848827 |
|17 | 36.803890 | 28.381888 |
|18 | 36.268459 | 29.274809 |
|19 | 40.358948 | 27.246357 |
|20 | 40.094959 | 31.266933 |
|21 | 43.465710 | 27.776363 |
|22 | 45.302643 | 29.384233 |

|   | Ca      | S       |
|---|---------|---------|
| 1 | 25.378460 | 30.240807 |
| 2 | 26.332840 | 30.237169 |
| 3 | 30.181675 | 28.028627 |
| 4 | 30.436317 | 32.973248 |
| 5 | 33.658497 | 29.965168 |
| 6 | 33.220299 | 30.671873 |
| 7 | 36.750034 | 26.923042 |
| 8 | 36.875801 | 31.367249 |
| 9 | 40.154797 | 28.376198 |
|10 | 39.912132 | 30.508118 |
|11 | 44.989159 | 25.226471 |
|12 | 42.879414 | 29.908401 |
|13 | 26.712784 | 26.854080 |
|14 | 26.883759 | 33.503918 |
|15 | 30.572828 | 30.118269 |
|16 | 29.892506 | 31.056515 |
|17 | 33.452747 | 27.728420 |
|18 | 33.849838 | 32.965141 |

generated by VMD
|   | S        | 28.914312 | 31.959793 |
|---|----------|----------|-----------|
|   | S        | 29.622137 | 36.815224 |
|   | S        | 27.344053 | 34.666595 |
|   | S        | 31.414177 | 33.005695 |
|   | S        | 27.492430 | 31.599379 |
|   | S        | 28.951599 | 36.911690 |

24 generated by VMD
| Ca       | 25.067310 | 30.211245 | 31.602310 |
| Ca       | 26.436541 | 30.301512 | 35.446716 |
| Ca       | 30.267426 | 28.183798 | 34.853249 |
| Ca       | 30.296339 | 33.249371 | 33.872681 |
| Ca       | 33.508606 | 29.706316 | 31.929436 |
| Ca       | 33.194202 | 30.492630 | 35.954929 |
| Ca       | 36.828419 | 26.896984 | 35.043968 |
| Ca       | 36.661111 | 31.156067 | 34.320011 |
| Ca       | 39.997532 | 28.260965 | 31.497892 |
| Ca       | 39.952751 | 30.595409 | 36.094574 |
| Ca       | 45.194473 | 25.231396 | 33.480400 |
| Ca       | 42.998253 | 29.993879 | 34.188183 |
| S        | 27.127542 | 26.817810 | 35.166084 |
| S        | 26.850796 | 33.666744 | 34.800865 |
| S        | 30.497282 | 30.267653 | 32.369278 |
| S        | 29.960049 | 31.102732 | 36.374580 |
| S        | 33.489769 | 27.716022 | 34.360153 |
| S        | 33.786297 | 32.896790 | 33.350368 |
| S        | 36.513748 | 28.958513 | 32.069363 |
| S        | 36.478764 | 29.530567 | 37.035683 |
| S        | 40.318413 | 27.202599 | 34.878529 |
| S        | 40.193161 | 31.379532 | 33.050392 |
| S        | 43.330063 | 27.611576 | 31.541782 |
| S        | 45.480087 | 28.961250 | 36.749279 |

24 generated by VMD
| Ca       | 25.069754 | 30.211245 | 31.602310 |
| Ca       | 26.421459 | 30.312984 | 35.856815 |
| Ca       | 29.997145 | 28.369484 | 35.128918 |
| Ca       | 30.142904 | 33.458767 | 33.699643 |
| Ca       | 33.507015 | 29.665525 | 31.778467 |
| Ca       | 33.162830 | 30.546158 | 35.624943 |
| Ca       | 36.967560 | 26.941715 | 34.765007 |
| Ca       | 36.661072 | 31.019880 | 34.148983 |
| Ca       | 40.336765 | 28.430702 | 31.397541 |
| Ca       | 39.730206 | 30.586403 | 35.975834 |
| Ca       | 45.430916 | 25.126488 | 33.473995 |
| Ca       | 42.885098 | 30.002630 | 34.427711 |
|   | 26.961956 | 26.845631 | 35.205734 |
|---|-----------|-----------|-----------|
| 8 | 26.880898 | 33.635750 | 34.913551 |
| 8 | 30.529058 | 30.400520 | 32.497063 |
| 8 | 29.903572 | 31.237251 | 36.556465 |
| 8 | 33.523315 | 27.704100 | 34.112198 |
| 8 | 33.702419 | 32.903782 | 33.195274 |
| 8 | 36.749836 | 28.904495 | 31.743488 |
| 8 | 36.425858 | 29.379087 | 36.796547 |
| 8 | 40.437359 | 27.270462 | 34.846737 |
| 8 | 40.247116 | 31.427647 | 33.021141 |
| 8 | 43.439110 | 27.649284 | 31.653889 |
| 8 | 45.320629 | 28.715433 | 37.239975 |

24

generated by VMD

|   | 24.949799 | 29.985374 | 31.715046 |
|---|-----------|-----------|-----------|
| Ca| 26.236002 | 30.230520 | 35.609249 |
| Ca| 30.419416 | 28.146091 | 35.066601 |
| Ca| 30.203974 | 33.251144 | 33.873898 |
| Ca| 33.653873 | 30.023575 | 31.791548 |
| Ca| 33.150970 | 30.579828 | 35.834942 |
| Ca| 36.869141 | 26.985031 | 34.738579 |
| Ca| 36.580032 | 31.130163 | 34.125706 |
| Ca| 40.073681 | 28.125105 | 31.419567 |
| Ca| 39.696220 | 30.636709 | 36.088200 |
| Ca| 45.467262 | 25.208359 | 33.578003 |
| Ca| 43.039455 | 29.864796 | 34.448177 |

24

generated by VMD

|   | 27.055807 | 26.992887 | 35.208565 |
|---|-----------|-----------|-----------|
| Ca| 26.677734 | 33.695572 | 34.980114 |
| Ca| 30.562984 | 30.337034 | 35.62340 |
| Ca| 29.769434 | 31.066040 | 36.522354 |
| Ca| 33.620064 | 27.883755 | 34.107151 |
| Ca| 33.731781 | 33.103180 | 33.075314 |
| Ca| 36.596859 | 28.768377 | 31.885551 |
| Ca| 36.316261 | 29.459175 | 36.982105 |
| Ca| 40.423447 | 27.240891 | 34.930904 |
| Ca| 40.219837 | 31.272022 | 33.080826 |
| Ca| 43.550373 | 27.585958 | 31.563334 |
| Ca| 45.568489 | 28.819843 | 36.842686 |
|   | Ca   | S    |
|---|------|------|
|   | 36.926971 | 26.85398 |
|   | 36.592808 | 26.91204 |
|   | 40.181591 | 28.27716 |
|   | 39.644596 | 30.49124 |
|   | 45.603718 | 25.47404 |
|   | 42.876041 | 29.85634 |
|   | 26.859795 | 27.04706 |
|   | 26.832113 | 33.66544 |
|   | 30.666655 | 30.24898 |
|   | 29.901724 | 31.08196 |
|   | 33.605175 | 27.76363 |
|   | 33.732250 | 32.92186 |
|   | 36.776838 | 28.87538 |
|   | 36.309101 | 29.42471 |
|   | 40.353897 | 27.31311 |
|   | 40.229736 | 31.34750 |
|   | 43.362045 | 27.44109 |
|   | 45.246147 | 28.97382 |

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generated by VMD
| Element | x-coordinate | y-coordinate | z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 24.964611    | 29.985090    | 31.837925    |
| Ca      | 26.337633    | 30.150978    | 35.773609    |
| Ca      | 30.219555    | 28.229456    | 34.873535    |
| Ca      | 29.981493    | 33.193398    | 34.045639    |
| Ca      | 33.729397    | 30.098188    | 31.696011    |
| Ca      | 33.090031    | 30.614492    | 35.852562    |
| Ca      | 36.908657    | 27.024641    | 34.806572    |
| Ca      | 36.767281    | 31.321726    | 34.059147    |
| Ca      | 40.168613    | 27.956469    | 31.522377    |
| Ca      | 39.835796    | 30.296186    | 36.043827    |
| Ca      | 45.513866    | 24.987679    | 33.775688    |
| Ca      | 43.175163    | 29.924835    | 34.239437    |
| S       | 26.845844    | 26.814079    | 34.948589    |
| S       | 26.561354    | 33.597229    | 35.053677    |
| S       | 30.532585    | 30.552040    | 32.511524    |
| S       | 29.685711    | 30.866323    | 36.676163    |
| S       | 33.585258    | 28.071867    | 34.054657    |
| S       | 33.674683    | 33.111801    | 33.318195    |
| S       | 36.780693    | 29.172693    | 31.755589    |
| S       | 36.356911    | 29.576059    | 36.728619    |
| S       | 40.360569    | 27.152317    | 34.906235    |
| S       | 40.405251    | 31.217108    | 32.897179    |
| S       | 43.350723    | 27.102943    | 31.855350    |
| S       | 45.602264    | 29.373804    | 36.798603    |

24 generated by VMD

| Element | x-coordinate | y-coordinate | z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.142443    | 30.460505    | 31.340002    |
| Ca      | 26.241220    | 30.418182    | 35.705997    |
| Ca      | 30.364302    | 27.974634    | 34.796207    |
| Ca      | 30.206741    | 33.097446    | 34.317791    |
| Ca      | 33.709461    | 29.600718    | 31.474968    |
| Ca      | 33.086922    | 30.450970    | 35.823677    |
| Ca      | 36.799828    | 27.061829    | 34.797821    |
| Ca      | 36.570072    | 31.223495    | 34.123287    |
| Ca      | 40.032276    | 28.120333    | 31.505320    |
| Ca      | 39.825260    | 30.723122    | 36.137054    |
| Ca      | 45.617146    | 25.361586    | 33.659866    |
| Ca      | 42.879639    | 29.848272    | 34.299522    |
| S       | 26.789825    | 27.018566    | 35.498631    |
| S       | 26.582768    | 33.921764    | 34.919868    |
| S       | 30.687922    | 30.136578    | 32.662121    |
| S       | 29.740658    | 30.726522    | 36.675858    |
| S       | 33.676216    | 27.837732    | 33.988907    |
| S       | 33.589630    | 32.827187    | 33.323372    |
| S       | 36.823284    | 28.985296    | 31.847731    |
| S       | 36.525974    | 29.525133    | 36.802021    |
|   | 40.370857  | 27.281502  | 34.943947 |
|---|------------|------------|-----------|
| S | 40.297382  | 31.265114  | 32.862946 |
| S | 43.309814  | 27.304850  | 31.784449 |
| S | 45.304272  | 29.220074  | 36.739357 |
| 24 generated by VMD |
| Ca | 25.291386  | 30.264776  | 31.829348 |
| Ca | 26.256929  | 30.507757  | 35.773976 |
| Ca | 30.361202  | 27.919273  | 35.021198 |
| Ca | 29.970722  | 33.361710  | 34.027828 |
| Ca | 33.601746  | 30.007738  | 31.421894 |
| Ca | 32.213551  | 30.294729  | 35.832394 |
| Ca | 36.975948  | 29.07635   | 34.614513 |
| Ca | 36.552059  | 31.100042  | 34.199966 |
| Ca | 40.021523  | 27.999340  | 31.271994 |
| Ca | 39.68428   | 30.384766  | 35.996677 |
| Ca | 45.698650  | 25.424883  | 33.873791 |
| Ca | 42.885220  | 29.725695  | 34.300358 |
| S | 27.017763  | 27.203798  | 35.524612 |
| S | 26.690348  | 33.802700  | 34.798553 |
| S | 30.703045  | 30.191858  | 32.620483 |
| S | 29.713831  | 31.091114  | 36.531033 |
| S | 33.771496  | 27.834547  | 33.876690 |
| S | 33.656151  | 32.895748  | 33.480061 |
| S | 36.860062  | 29.079037  | 31.600655 |
| S | 36.335915  | 29.033611  | 36.839916 |
| S | 40.259670  | 27.101429  | 34.710861 |
| S | 40.116184  | 31.310625  | 33.009174 |
| S | 43.448769  | 27.372150  | 31.957335 |
| S | 45.345261  | 29.576479  | 36.917648 |
| 24 generated by VMD |
| Ca | 25.133179  | 30.412470  | 32.056717 |
| Ca | 26.092266  | 30.407013  | 35.853184 |
| Ca | 30.204378  | 28.166157  | 35.098217 |
| Ca | 30.091192  | 33.318825  | 33.955032 |
| Ca | 33.542870  | 29.697422  | 31.279135 |
| Ca | 33.214645  | 30.449697  | 35.631493 |
| Ca | 36.995609  | 26.993267  | 34.628586 |
| Ca | 36.541565  | 30.938728  | 33.943516 |
| Ca | 40.185669  | 27.957424  | 31.227320 |
| Ca | 39.631569  | 30.371885  | 36.251621 |
| Ca | 45.834854  | 25.691917  | 33.741184 |
| Ca | 42.859261  | 29.800287  | 34.556461 |
| S | 26.750881  | 26.987764  | 35.384155 |
| S | 26.924990  | 33.726845  | 35.262268 |
S  30.455515  30.335159  32.635429
S  29.827087  31.007792  36.563824
S  33.601082  27.926636  33.888622
S  33.746628  32.902657  32.911148
S  36.789223  28.957117  31.630747
S  36.380371  29.255507  36.679420
S  40.551975  27.093765  34.815987
S  40.238731  31.073936  33.007408
S  43.659344  27.630676  31.785017
S  45.181007  29.288473  37.244247

24
generated by VMD

Ca  24.846251  30.246862  32.162212
Ca  26.386614  30.384176  35.926262
Ca  30.359194  28.057142  34.800137
Ca  30.114643  33.406868  34.027054
Ca  33.536102  29.767553  31.383657
Ca  33.160038  30.467028  35.612614
Ca  36.944473  27.000498  34.61541
Ca  36.724003  31.115396  33.993980
Ca  40.195175  28.233421  31.400051
Ca  39.798347  30.449917  36.265827
Ca  45.522869  25.463165  33.759640
Ca  42.849995  29.837887  34.503769
S  27.088604  26.928202  35.356144
S  26.746561  33.646729  35.094028
S  30.568296  30.323162  32.448505
S  29.877886  30.935074  36.562077
S  33.649227  27.894749  33.867504
S  33.638702  32.832367  33.023514
S  36.779846  29.165722  31.540909
S  36.321064  29.427963  36.652542
S  40.255005  27.174612  34.856812
S  40.319706  31.254490  33.130829
S  43.424141  27.224863  31.857094
S  45.327103  29.153559  37.162289

24
generated by VMD

Ca  25.071421  30.021564  32.004189
Ca  26.462641  30.512396  35.877304
Ca  30.153603  28.121042  34.950783
Ca  30.063553  33.123940  34.206722
Ca  33.556076  29.732075  31.133406
Ca  33.349380  30.346354  35.624352
Ca  36.929516  27.211254  34.540737
Ca  36.842247  31.162107  34.044136
|   | Ca   |   | S   |   |
|---|------|---|-----|---|
|   | 40.181297 | 28.337315 | 31.311346 |
|   | 26.846373 | 26.891691 | 35.531197 |
|   | 26.674868 | 33.819843 | 34.803825 |
|   | 30.549107 | 30.251873 | 32.614990 |
|   | 29.874210 | 30.857620 | 36.712860 |
|   | 33.588455 | 27.699516 | 33.830029 |
|   | 33.661491 | 32.798378 | 33.224934 |
|   | 36.720016 | 29.257641 | 31.587229 |
|   | 36.475182 | 29.554775 | 36.727577 |
|   | 40.127857 | 27.429390 | 34.739895 |
|   | 40.409924 | 31.411879 | 33.022503 |
|   | 43.410152 | 27.361067 | 31.734169 |
|   | 45.086731 | 28.821495 | 37.452526 |

24 generated by VMD

|   | Ca   |   | S   |   |
|---|------|---|-----|---|
|   | 24.951128 | 29.875664 | 32.278343 |
|   | 26.617615 | 30.431963 | 36.005238 |
|   | 30.296442 | 28.167322 | 34.902164 |
|   | 30.018076 | 33.286972 | 33.911163 |
|   | 33.685806 | 29.777172 | 31.039391 |
|   | 33.350681 | 30.397009 | 35.237572 |
|   | 36.944656 | 26.999189 | 34.431499 |
|   | 36.711422 | 31.142490 | 34.157700 |
|   | 39.946671 | 28.311090 | 31.39300 |
|   | 39.645172 | 30.568470 | 36.250751 |
|   | 45.210495 | 25.299238 | 33.689381 |
|   | 42.902222 | 29.907591 | 34.529728 |
|   | 27.082653 | 27.015781 | 35.722668 |
|   | 26.856678 | 33.730648 | 35.090504 |
|   | 30.661772 | 30.281614 | 32.503998 |
|   | 30.100660 | 30.897299 | 36.547592 |
|   | 33.714676 | 27.711325 | 33.575806 |
|   | 33.743301 | 32.912148 | 33.126167 |
|   | 36.967777 | 29.223021 | 31.408802 |
|   | 36.396870 | 29.380894 | 36.689976 |
|   | 40.227127 | 27.390436 | 34.963848 |
|   | 40.037201 | 31.540865 | 33.196884 |
|   | 43.414108 | 27.386410 | 31.881920 |
|   | 44.950684 | 28.756783 | 37.490360 |

24 generated by VMD

|   | Ca   |   | S   |   |
|---|------|---|-----|---|
|   | 24.657682 | 30.097778 | 32.432430 |
|   | 26.469948 | 30.278072 | 35.900700 |
|   |   |   |   |
|---|---|---|---|
| Ca | 30.177759 | 28.260611 | 34.782478 |
| Ca | 30.285603 | 33.221603 | 33.664742 |
| Ca | 33.487518 | 29.577742 | 31.109861 |
| Ca | 30.543955 | 35.399822 |
| Ca | 36.840504 | 26.987917 | 34.489998 |
| Ca | 36.802048 | 33.221603 | 33.664742 |
| Ca | 33.408039 | 30.543955 | 35.399822 |
| Ca | 36.840504 | 26.987917 | 34.489998 |
| Ca | 36.802048 | 33.221603 | 33.664742 |
| Ca | 33.408039 | 30.543955 | 35.399822 |
| S  | 27.034655 | 26.799406 | 35.487480 |
| S  | 26.775562 | 33.422272 | 34.906181 |
| S  | 30.470760 | 30.313164 | 32.399715 |
| S  | 29.877180 | 31.083365 | 36.466357 |
| S  | 33.583069 | 27.743025 | 33.740585 |
| S  | 33.894886 | 32.937950 | 33.048019 |
| S  | 36.690243 | 29.348314 | 31.638718 |
| S  | 36.640430 | 29.526859 | 36.791370 |
| S  | 40.292305 | 27.433226 | 34.889286 |
| S  | 40.339069 | 31.279556 | 33.862926 |
| S  | 43.132965 | 27.435036 | 31.772953 |
| S  | 45.507267 | 28.913700 | 36.992298 |

24

generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 25.057674 | 29.947357 | 32.155190 |
| Ca | 26.283754 | 30.347218 | 36.005611 |
| Ca | 30.197737 | 28.228149 | 34.842037 |
| Ca | 30.104872 | 33.324982 | 33.758732 |
| Ca | 33.765621 | 29.860256 | 31.425644 |
| Ca | 33.152309 | 30.425127 | 35.741531 |
| Ca | 36.813068 | 27.040676 | 34.643581 |
| Ca | 36.537880 | 31.329510 | 34.266903 |
| Ca | 40.180817 | 28.313677 | 31.328682 |
| Ca | 39.830684 | 30.532461 | 36.130070 |
| Ca | 45.452667 | 25.311684 | 33.758732 |
| Ca | 42.935539 | 29.673700 | 34.520164 |
| S  | 26.920048 | 27.036568 | 35.513138 |
| S  | 26.787489 | 33.681400 | 34.815994 |
| S  | 30.558023 | 30.180212 | 32.379780 |
| S  | 29.989723 | 30.941828 | 36.400013 |
| S  | 33.516487 | 27.604238 | 33.953470 |
| S  | 33.687866 | 32.929817 | 33.252094 |
| S  | 36.805294 | 29.099142 | 31.902836 |
| S  | 36.468746 | 29.550905 | 36.788982 |
| S  | 40.359436 | 27.236670 | 34.698978 |
| S  | 40.303028 | 31.494902 | 33.015888 |
|   | 43.559692 | 27.572762 | 31.732340 |
|---|-----------|-----------|-----------|
| S | 45.157459 | 28.728058 | 37.219059 |

24
generated by VMD

|   | 25.130007 | 30.095610 | 32.051060 |
|---|-----------|-----------|-----------|
| Ca| 26.351526 | 30.232004 | 35.981197 |
|   | 30.494411 | 27.703201 | 35.033184 |
|   | 30.011616 | 33.053162 | 33.774124 |
|   | 33.618652 | 29.892105 | 31.340897 |
|   | 33.100914 | 30.630022 | 35.439587 |
|   | 37.220219 | 26.923534 | 34.232845 |
| Ca| 36.687691 | 31.350237 | 33.922741 |
|   | 40.064777 | 28.670017 | 31.673851 |
|   | 39.767014 | 30.656343 | 36.787521 |
| Ca| 45.155220 | 25.016928 | 33.581997 |
|   | 42.772362 | 29.713863 | 34.491707 |
| S | 27.181454 | 27.122313 | 35.716454 |
|   | 26.995428 | 33.615871 | 35.062077 |
| S | 30.424637 | 30.159298 | 32.509361 |
S  | 29.920353 | 30.990480 | 36.357567 |
S  | 33.740833 | 27.975269 | 33.720917 |
S  | 33.527939 | 32.980766 | 32.990726 |
S  | 36.745838 | 29.167978 | 31.458452 |
S  | 36.596684 | 29.577663 | 36.526112 |
S  | 40.211663 | 27.442320 | 35.158989 |
S  | 40.391644 | 31.431612 | 33.378319 |
S  | 43.234970 | 27.231688 | 31.955896 |
S  | 45.088573 | 28.759014 | 36.885181 |

24
generated by VMD

|   | 25.247370 | 29.684734 | 32.116150 |
|---|-----------|-----------|-----------|
| Ca| 26.728521 | 30.335291 | 36.040016 |
|   | 30.364229 | 27.978508 | 34.769264 |
|   | 30.296066 | 33.063889 | 33.768002 |
|   | 33.617306 | 29.953875 | 31.112280 |
|   | 33.272095 | 30.550192 | 35.446884 |
|   | 36.634514 | 26.545446 | 34.597668 |
|   | 36.919643 | 31.499271 | 34.300594 |
|   | 39.966026 | 28.524841 | 31.366476 |
|   | 39.786263 | 30.767670 | 36.534813 |
|   | 44.988670 | 25.162878 | 33.680908 |
|   | 42.668671 | 29.885113 | 34.686863 |
| S | 27.140686 | 26.964619 | 35.752522 |
| S | 27.117287 | 33.527264 | 35.057667 |
| S | 30.528080 | 30.254425 | 32.360977 |
S  | 30.181341 | 30.981667 | 36.416828 |
S  33.551945  27.894997  33.613415
S  33.765713  33.027214  33.039818
S  36.444195  29.529451  36.681126
S  40.042877  27.470251  34.839558
S  40.436672  31.445877  33.074112
S  43.124001  27.432859  31.847733
S  45.002388  28.739798  37.039993

24
generated by VMD
Ca  25.565342  29.421558  31.917032
Ca  26.404675  30.693841  36.060005
Ca  30.249321  30.035196  34.952812
Ca  30.155577  33.045490  33.893335
Ca  33.658531  30.129257  31.334305
Ca  33.144367  30.402636  35.631882
Ca  36.805248  26.946217  34.392040
Ca  36.690182  31.175518  34.232666
Ca  40.150623  28.384306  31.304096
Ca  39.710350  30.169975  36.500107
Ca  45.641109  25.338795  33.789131
Ca  42.685452  29.827055  34.391235
S  27.075773  27.075020  35.781883
S  26.733849  33.829041  34.831192
S  30.549271  30.259941  32.468296
S  29.978481  31.068024  36.528149
S  33.555729  28.055969  33.754448
S  33.730003  33.107822  33.288074
S  36.769154  29.126402  31.686398
S  36.371567  29.310274  36.731323
S  40.102524  27.195511  34.783554
S  40.307240  31.390965  33.061413
S  43.405178  27.460672  31.806875
S  44.994354  28.941967  36.905468

24
generated by VMD
Ca  25.496178  29.766020  31.519300
Ca  26.532593  30.326626  36.069763
Ca  30.219622  27.954121  34.923733
Ca  30.086761  33.352474  33.581699
Ca  33.580143  29.925131  31.314495
Ca  33.226929  30.356224  35.392117
Ca  36.843868  26.882702  34.576080
Ca  36.798363  31.687775  34.474483
Ca  39.971260  28.451183  31.589987
Ca  39.749821  30.686287  36.502930
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 45.268047 | 25.040979 | 33.340614 |
| Ca      | 42.779652 | 29.497890 | 34.638538 |
| S       | 27.096405 | 26.997053 | 36.254307 |
| S       | 26.820705 | 33.590305 | 34.839649 |
| S       | 30.482111 | 30.197792 | 32.372639 |
| S       | 30.126198 | 30.934219 | 36.309139 |
| S       | 33.587624 | 27.717913 | 33.691734 |
| S       | 33.629215 | 33.104687 | 33.208519 |
| S       | 36.791130 | 29.429518 | 36.704865 |
| S       | 40.061863 | 27.263781 | 34.898273 |
| S       | 40.435040 | 31.387043 | 33.372520 |
| S       | 43.175911 | 27.449265 | 31.714317 |
| S       | 45.287815 | 28.908165 | 36.770767 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.352428 | 29.801630 | 31.833540 |
| Ca      | 26.403170 | 30.656446 | 35.959080 |
| Ca      | 30.221096 | 28.056046 | 35.153965 |
| Ca      | 30.109051 | 33.063358 | 33.685757 |
| Ca      | 33.544468 | 29.509338 | 31.550560 |
| Ca      | 33.127975 | 30.337097 | 35.362213 |
| Ca      | 36.691193 | 26.789717 | 34.433201 |
| Ca      | 37.008709 | 31.658060 | 34.594624 |
| Ca      | 40.141850 | 28.646015 | 31.376707 |
| Ca      | 39.847126 | 30.458889 | 36.702164 |
| Ca      | 45.594997 | 25.401552 | 33.148331 |
| Ca      | 42.785660 | 29.782381 | 34.486542 |
| S       | 26.691652 | 27.302198 | 35.995502 |
| S       | 26.752094 | 33.815323 | 34.529701 |
| S       | 30.503904 | 30.048473 | 32.548683 |
| S       | 29.962263 | 31.091946 | 36.479595 |
| S       | 33.458450 | 27.417347 | 33.886711 |
| S       | 33.624985 | 32.683987 | 32.945412 |
| S       | 36.908894 | 29.234976 | 31.997478 |
| S       | 36.461758 | 29.536331 | 36.728828 |
| S       | 40.261246 | 27.361113 | 34.523956 |
| S       | 40.351383 | 31.632475 | 33.342445 |
| S       | 43.626659 | 27.744802 | 31.596058 |
| S       | 45.002754 | 28.361950 | 37.169704 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.263575 | 30.022907 | 31.929220 |
| Ca      | 26.369062 | 30.678019 | 35.865589 |
| Ca      | 30.048512 | 27.979671 | 35.023975 |
| Ca      | 30.186487 | 32.952602 | 33.574379 |
|   |    |    |    |
|---|---|---|---|
| Ca | 33.689781 | 29.653597 | 31.573927 |
| Ca | 33.117371 | 30.260817 | 35.516693 |
| Ca | 36.655468 | 26.870173 | 34.527050 |
| Ca | 36.764217 | 31.584536 | 34.336330 |
| Ca | 40.213097 | 28.643816 | 31.270452 |
| Ca | 39.807629 | 30.285559 | 36.654964 |
| Ca | 45.705032 | 25.494518 | 33.318436 |
| Ca | 42.845337 | 29.841387 | 34.615891 |
| S  | 26.729893 | 27.372078 | 35.927750 |
| S  | 26.795891 | 33.841599 | 34.803417 |
| S  | 30.505829 | 29.865131 | 32.437447 |
| S  | 29.890932 | 31.125629 | 36.325489 |
| S  | 33.487885 | 27.412737 | 33.943119 |
| S  | 33.669025 | 32.776772 | 33.020752 |
| S  | 36.849941 | 29.214550 | 32.069210 |
| S  | 36.438519 | 29.434860 | 36.724373 |
| S  | 40.084305 | 27.184097 | 34.624897 |
| S  | 40.413246 | 31.532082 | 33.361805 |
| S  | 43.478226 | 27.659056 | 31.798428 |
| S  | 45.424572 | 28.705181 | 36.787109 |

24

*generated by VMD*

|   |    |    |    |
|---|---|---|---|
| Ca | 25.307034 | 30.059851 | 32.152897 |
| Ca | 26.603069 | 30.745060 | 36.105286 |
| Ca | 30.182663 | 27.992153 | 34.976868 |
| Ca | 30.383480 | 32.984333 | 33.629845 |
| Ca | 33.493057 | 29.439240 | 31.163637 |
| Ca | 33.223114 | 30.407818 | 35.432457 |
| Ca | 36.736809 | 26.650898 | 34.508556 |
| Ca | 36.807598 | 31.12972 | 34.213573 |
| Ca | 40.074265 | 28.675804 | 31.520117 |
| Ca | 39.741844 | 30.485271 | 36.718086 |
| Ca | 45.414467 | 25.616497 | 33.434772 |
| Ca | 42.616886 | 30.041426 | 34.639439 |
| S  | 26.900051 | 27.358622 | 35.802895 |
| S  | 27.067245 | 33.826481 | 34.918777 |
| S  | 30.510109 | 30.007456 | 32.430695 |
| S  | 30.266356 | 31.006054 | 36.430843 |
| S  | 33.543427 | 27.551840 | 33.730507 |
| S  | 33.764759 | 32.744175 | 32.880379 |
| S  | 36.626476 | 29.019941 | 31.710844 |
| S  | 36.428730 | 29.216494 | 36.652611 |
| S  | 40.157944 | 27.282064 | 34.770470 |
| S  | 40.223694 | 31.513388 | 33.243443 |
| S  | 43.360863 | 27.928200 | 31.774710 |
| S  | 45.000000 | 28.725334 | 37.188908 |
|   |   |   |
|---|---|---|
| Ca | 25.161432 | 30.042278 | 31.827271 |
| Ca | 26.509575 | 30.538996 | 35.905190 |
| Ca | 30.115963 | 28.137428 | 35.181763 |
| Ca | 30.245968 | 33.128040 | 33.746464 |
| Ca | 33.451839 | 29.375368 | 31.321310 |
| Ca | 33.337021 | 30.237030 | 35.490196 |
| Ca | 36.822865 | 27.121540 | 34.519619 |
| Ca | 36.881855 | 31.399113 | 34.241623 |
| Ca | 40.054279 | 28.780870 | 31.397696 |
| Ca | 39.881783 | 30.573288 | 36.737453 |
| Ca | 45.280598 | 25.414471 | 33.284538 |
| Ca | 42.810848 | 29.933031 | 34.608543 |
| S  | 26.467749 | 27.305565 | 36.026077 |
| S  | 26.908054 | 33.761265 | 34.671574 |
| S  | 30.535704 | 29.683430 | 32.447979 |
| S  | 30.243149 | 30.922834 | 36.424664 |
| S  | 33.563908 | 27.339005 | 33.855228 |
| S  | 33.920013 | 32.897392 | 33.105175 |
| S  | 36.688953 | 29.204109 | 31.769979 |
| S  | 36.520325 | 29.537863 | 36.681656 |
| S  | 40.324181 | 27.328651 | 34.578125 |
| S  | 40.257347 | 31.452631 | 33.245312 |
| S  | 43.544346 | 27.818594 | 31.741060 |
| S  | 44.906227 | 28.458645 | 37.222191 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 25.389526 | 30.177988 | 31.873978 |
| Ca | 26.251360 | 30.557449 | 36.032372 |
| Ca | 30.117195 | 28.081663 | 35.300480 |
| Ca | 30.261099 | 32.986530 | 33.885052 |
| Ca | 33.652966 | 29.661423 | 31.443569 |
| Ca | 33.114681 | 30.261522 | 35.673901 |
| Ca | 36.860649 | 26.783236 | 34.515366 |
| Ca | 36.675888 | 31.160545 | 34.171009 |
| Ca | 40.355865 | 28.581560 | 31.225971 |
| Ca | 39.651642 | 30.397160 | 36.335518 |
| Ca | 45.529289 | 25.251307 | 33.594864 |
| Ca | 42.791512 | 29.987696 | 34.403545 |
| S  | 26.736294 | 27.270269 | 35.808113 |
| S  | 26.809860 | 33.895626 | 34.584576 |
| S  | 30.659781 | 30.015255 | 32.648415 |
| S  | 29.969170 | 31.114010 | 36.628307 |
| S  | 33.488964 | 27.534178 | 33.997299 |
| S  | 33.831020 | 32.791271 | 32.995659 |
| S    | 36.82095 | 29.053898 | 31.682083 |
| S    | 36.348278 | 29.337801 | 36.785713 |
| S    | 40.255394 | 27.266081 | 34.430855 |
| S    | 40.151913 | 31.358753 | 33.078205 |
| S    | 43.879875 | 27.955902 | 31.762112 |
| S    | 44.769489 | 28.910280 | 37.173779 |

24 generated by VMD

| Ca   | 25.204256 | 30.300367 | 32.091072 |
| Ca   | 26.369822 | 30.806280 | 35.998840 |
| Ca   | 30.369616 | 28.039009 | 34.980339 |
| Ca   | 30.134029 | 33.106319 | 33.743919 |
| Ca   | 33.710548 | 29.386442 | 31.237179 |
| Ca   | 33.082417 | 30.171492 | 35.737133 |
| Ca   | 37.001617 | 26.787180 | 34.710251 |
| Ca   | 36.443471 | 30.716745 | 34.258999 |
| Ca   | 40.238583 | 28.588781 | 31.311747 |
| Ca   | 39.535000 | 30.504581 | 36.390327 |
| Ca   | 45.471863 | 25.517426 | 33.323410 |
| Ca   | 42.712177 | 29.937256 | 34.484512 |

| S    | 26.998987 | 27.490953 | 35.907692 |
| S    | 26.818663 | 33.868038 | 34.613003 |
| S    | 30.628592 | 29.979317 | 32.432026 |
| S    | 30.022111 | 31.209641 | 36.463985 |
| S    | 33.746380 | 27.683523 | 33.879494 |
| S    | 33.695145 | 32.626999 | 32.985649 |
| S    | 36.876209 | 28.936197 | 31.715105 |
| S    | 36.212734 | 29.137619 | 36.954605 |
| S    | 40.362785 | 27.356455 | 34.441860 |
| S    | 40.092915 | 31.479021 | 33.448626 |
| S    | 43.683132 | 27.948740 | 31.704840 |
| S    | 45.021877 | 28.813023 | 37.219868 |

24 generated by VMD

| Ca   | 25.212503 | 30.296499 | 32.096382 |
| Ca   | 26.551313 | 30.801115 | 36.145264 |
| Ca   | 30.150492 | 28.012627 | 35.222717 |
| Ca   | 30.243589 | 32.941498 | 33.868248 |
| Ca   | 33.567200 | 29.366095 | 31.116755 |
| Ca   | 33.278603 | 30.202347 | 35.280003 |
| Ca   | 36.610649 | 26.669111 | 34.486942 |
| Ca   | 36.895279 | 30.874376 | 33.920471 |
| Ca   | 40.198212 | 28.832624 | 31.289068 |
| Ca   | 39.356472 | 30.286156 | 36.794487 |
| Ca   | 45.965569 | 25.739510 | 33.580101 |
| Ca   | 42.693901 | 30.041132 | 34.743931 |
S  26.706453  27.436602  35.939823
S  27.066624  33.973114  35.066059
S  30.543549  30.025883  32.528740
S  30.231812  31.117321  36.618225
S  33.286278  27.469217  33.623016
S  33.768768  32.564419  32.687065
S  36.761162  28.726248  31.494986
S  36.209484  29.305056  36.551830
S  40.039417  27.288519  34.475533
S  40.368862  31.411880  33.269203
S  43.690964  28.726248  31.494986
S  45.036709  29.014799  37.322323

24

generated by VMD

Ca  25.069214  30.186907  31.894047
Ca  26.415512  30.758881  36.048622
Ca  30.124262  27.914597  35.528336
Ca  30.252865  32.945553  33.857697
Ca  33.596428  29.465767  31.099499
Ca  33.090591  30.50100  35.405815
Ca  36.621620  26.782225  34.086849
Ca  36.837612  31.069658  33.947765
Ca  40.323860  28.983814  31.398127
Ca  39.911346  30.332729  36.750462
Ca  45.346909  25.316236  33.738289
Ca  42.940193  29.897549  34.534618
S  26.665932  27.380501  36.035587
S  27.070423  34.060066  34.849266
S  30.431826  29.999771  32.601486
S  29.929945  31.076828  36.673134
S  33.216419  27.435902  33.730240
S  33.639336  29.465767  32.736103
S  36.752888  29.019136  31.565004
S  36.445297  29.256886  36.516323
S  40.111172  27.444975  34.386330
S  40.520573  31.650307  33.363342
S  43.780666  28.786396  31.846930
S  45.338955  29.050533  37.436832

24

generated by VMD

Ca  25.122198  30.256353  31.966391
Ca  26.397526  30.638809  35.839912
Ca  30.273396  27.935589  34.997253
Ca  30.075626  32.726521  33.906944
Ca  33.679047  29.774189  31.040937
Ca  33.239990  30.183020  35.529114
Ca       36.658653       27.068222       34.527313
Ca       36.750641       31.230598       34.110287
Ca       40.176582       28.621527       31.284346
Ca       39.825462       30.614120       36.369003
Ca       45.074062       25.028847       33.876175
Ca       42.811886       30.009066       34.513111
S        26.918318       27.213873       35.963806
S        26.900002       33.982677       35.095154
S        30.513481       29.825434       32.443779
S        29.992176       30.751911       36.598347
S        33.602085       27.740702       33.708157
S        33.584232       32.701157       32.918007
S        36.814651       29.147943       31.809975
S        36.430759       29.529892       36.651070
S        40.118988       27.499836       34.802853
S        40.477123       31.486752       33.063400
S        43.585026       27.737867       31.864731
S        45.411957       28.686510       37.150673

24

generated by VMD

Ca       24.855686       30.200047       32.559250
Ca       26.341742       30.746361       36.238770
Ca       30.204720       27.770309       35.015354
Ca       30.307436       33.251053       33.542484
Ca       33.741734       29.603928       30.927580
Ca       33.227131       30.105824       35.220360
Ca       36.615700       26.778711       34.399071
Ca       36.782085       30.871271       33.928963
Ca       40.252647       28.742846       31.613939
Ca       39.613007       30.218515       36.530907
Ca       45.116135       25.608328       33.642719
Ca       42.614471       30.107880       34.906994
S        26.998524       27.351099       35.963505
S        27.204382       34.022110       35.023247
S        30.675611       30.127451       32.496296
S        29.902225       30.966782       36.415661
S        33.509449       27.515194       33.535538
S        33.910336       32.551613       32.890343
S        36.823757       28.831511       31.548384
S        36.382225       29.166399       36.549622
S        40.176125       27.207420       34.711720
S        40.386520       31.475641       33.264610
S        43.647007       28.097700       31.844809
S        45.145203       29.073418       37.260612

24

generated by VMD
|   | Ca       | 30.409454 | 32.145214 |
|---|----------|----------|----------|
| Ca| 25.227274| 30.582430| 35.988350|
| Ca| 30.179203| 27.698275| 35.132305|
| Ca| 30.384327| 33.147526| 33.690220|
| Ca| 33.658882| 29.722574| 31.260201|
| Ca| 33.168907| 30.156935| 35.405457|
| Ca| 36.541973| 26.678082| 34.570885|
| Ca| 36.627895| 30.842396| 33.825111|
| Ca| 40.172619| 28.708893| 31.666155|
| Ca| 39.663860| 30.428606| 36.369713|
| Ca| 45.426186| 25.493597| 33.606510|
| Ca| 43.002380| 30.292097| 34.500160|
| S | 26.745068| 27.245541| 35.666725|
| S | 27.327389| 34.102100| 35.186462|
| S | 30.646524| 30.100695| 32.633625|
| S | 29.894333| 31.003370| 36.471424|
| S | 33.360233| 27.489933| 33.739498|
| S | 33.742542| 32.688511| 32.822308|
| S | 36.675392| 28.546860| 31.764271|
| S | 36.285866| 29.314354| 36.686007|
| S | 40.157486| 27.247797| 34.754387|
| S | 40.233109| 31.461302| 33.160450|
| S | 43.773277| 27.921188| 31.864088|
| S | 45.168087| 29.108887| 37.120609|

24 generated by VMD

|   | Ca       | 30.401814 | 32.138031 |
|---|----------|----------|----------|
| Ca| 25.490292| 30.626959| 35.975773|
| Ca| 30.252331| 27.783979| 35.157204|
| Ca| 30.235363| 33.066341| 33.828144|
| Ca| 33.623215| 29.826097| 31.435871|
| Ca| 32.972050| 30.363047| 35.337460|
| Ca| 36.933327| 26.900194| 34.776203|
| Ca| 36.715557| 30.953045| 33.955124|
| Ca| 40.187202| 28.610416| 31.588785|
| Ca| 39.635662| 30.363234| 36.423294|
| Ca| 45.404984| 25.404858| 33.549274|
| Ca| 42.816319| 30.075985| 34.472500|
| S | 26.740929| 27.287567| 35.522430|
| S | 27.062847| 33.815720| 35.295120|
| S | 30.610296| 30.092424| 32.500610|
| S | 29.935371| 30.909655| 36.410145|
| S | 33.611301| 27.587139| 33.858433|
| S | 33.706108| 32.858253| 32.641388|
| S | 36.729393| 28.589792| 31.747925|
| S | 36.153149| 29.495657| 36.638466|
|      |        |        |        |
|------|--------|--------|--------|
| S    | 40.289738 | 27.232244 | 34.730301 |
| S    | 40.225182 | 31.358236 | 33.165100 |
| S    | 43.649471 | 27.794912 | 31.797640 |
| S    | 45.333591 | 28.993832 | 37.085476 |

generated by VMD

|      |        |        |        |
|------|--------|--------|--------|
| Ca   | 24.985901 | 30.421844 | 31.849577 |
| Ca   | 26.419373 | 30.429430 | 36.054825 |
| Ca   | 30.273352 | 28.031523 | 35.049858 |
| Ca   | 30.217535 | 33.307594 | 33.607864 |
| Ca   | 33.532665 | 29.374016 | 31.395996 |
| Ca   | 33.127010 | 30.287558 | 35.409229 |
| Ca   | 36.712925 | 26.874746 | 34.876408 |
| Ca   | 36.724834 | 31.316650 | 34.349720 |
| Ca   | 40.112217 | 28.540611 | 31.834396 |
| Ca   | 39.828304 | 30.325336 | 36.704536 |
| Ca   | 45.622379 | 25.336544 | 33.241150 |
| Ca   | 42.867523 | 30.001591 | 34.409336 |
| S    | 26.536030 | 27.175512 | 35.362083 |
| S    | 27.202850 | 33.728374 | 34.828785 |
| S    | 30.479404 | 30.036379 | 32.412209 |
| S    | 29.942621 | 31.050259 | 36.424328 |
| S    | 33.572662 | 27.481783 | 33.865955 |
| S    | 33.812145 | 32.642258 | 32.974972 |
| S    | 36.606991 | 29.057289 | 31.973341 |
| S    | 36.292511 | 29.578531 | 36.964249 |
| S    | 40.317753 | 27.047575 | 34.848095 |
| S    | 40.282436 | 31.342575 | 33.435589 |
| S    | 43.470303 | 27.742634 | 31.575998 |
| S    | 45.494167 | 29.260832 | 36.582218 |

generated by VMD

|      |        |        |        |
|------|--------|--------|--------|
| Ca   | 25.165354 | 30.513357 | 32.062012 |
| Ca   | 26.263012 | 30.466347 | 36.064640 |
| Ca   | 30.339401 | 27.712328 | 34.754551 |
| Ca   | 30.333969 | 33.207867 | 33.845509 |
| Ca   | 33.468563 | 29.309612 | 31.346777 |
| Ca   | 33.225788 | 30.460869 | 35.332687 |
| Ca   | 36.848595 | 26.969601 | 34.976234 |
| Ca   | 36.705090 | 31.112249 | 33.987812 |
| Ca   | 40.177559 | 28.757559 | 31.715343 |
| Ca   | 39.782169 | 30.500013 | 36.733326 |
| Ca   | 45.627129 | 25.288576 | 33.206242 |
| Ca   | 42.825069 | 29.900583 | 34.467926 |
| S    | 26.637373 | 27.241064 | 35.592136 |
| S    | 27.005138 | 33.874283 | 35.123634 |
|  |  |  |  |
|---|---|---|---|
| S | 30.453594 | 30.058874 | 32.534389 |
| S | 29.829834 | 30.879005 | 36.231518 |
| S | 33.643066 | 27.454601 | 33.850037 |
| S | 33.616295 | 32.736572 | 32.521561 |
| S | 36.656868 | 28.862993 | 31.873940 |
| S | 36.457069 | 29.642616 | 36.748077 |
| S | 40.262791 | 27.362991 | 34.996517 |
| S | 40.226639 | 31.575521 | 33.362679 |
| S | 43.474403 | 27.804228 | 31.718102 |
| S | 45.409046 | 28.699677 | 36.985069 |

24 generated by VMD

| Ca | 25.075245 | 30.271236 | 32.194096 |
| Ca | 26.444321 | 30.662886 | 35.952396 |
| Ca | 30.211784 | 27.617064 | 34.993362 |
| Ca | 30.418976 | 33.070641 | 33.669136 |
| Ca | 33.543911 | 29.517687 | 31.395283 |
| Ca | 33.077263 | 30.286335 | 35.339687 |
| Ca | 36.462639 | 26.945721 | 34.796772 |
| Ca | 36.995049 | 31.232649 | 34.103737 |
| Ca | 40.217098 | 28.650169 | 31.409302 |
| Ca | 39.719196 | 30.359978 | 36.628941 |
| Ca | 45.401337 | 25.535860 | 33.319527 |
| Ca | 42.716324 | 29.817348 | 34.738003 |
| S | 26.845539 | 27.151814 | 35.666862 |
| S | 27.325893 | 33.924900 | 35.026958 |
| S | 30.598185 | 30.020708 | 32.494640 |
| S | 30.034042 | 30.949781 | 36.381584 |
| S | 33.361755 | 27.342712 | 33.732052 |
| S | 33.882629 | 32.691624 | 32.796673 |
| S | 36.685219 | 29.027466 | 31.845140 |
| S | 36.273540 | 29.556679 | 36.746574 |
| S | 40.135460 | 27.353447 | 34.670563 |
| S | 40.400200 | 31.531347 | 33.353218 |
| S | 43.451336 | 27.794353 | 31.764420 |
| S | 45.156952 | 29.079008 | 37.011730 |

24 generated by VMD

| Ca | 24.846853 | 30.324232 | 31.957565 |
| Ca | 26.312477 | 30.525043 | 35.682751 |
| Ca | 30.285164 | 27.947237 | 34.825073 |
| Ca | 30.308210 | 33.171856 | 33.618683 |
| Ca | 33.697262 | 29.654184 | 31.568371 |
| Ca | 33.135937 | 30.425501 | 35.454403 |
| Ca | 36.735050 | 26.875061 | 35.271145 |
| Ca | 36.820992 | 31.155123 | 34.212208 |
|   |       |       |       |
|---|-------|-------|-------|
| Ca| 40.150162 | 28.584463 | 31.770720 |
| Ca| 39.860523 | 30.568022 | 36.491440 |
| Ca| 45.507481 | 25.368656 | 33.024410 |
| Ca| 42.975929 | 29.971437 | 34.557148 |
| S | 26.758366 | 27.053385 | 35.434822 |
| S | 26.872555 | 33.885944 | 34.847832 |
| S | 30.431919 | 30.082167 | 32.506287 |
| S | 29.909201 | 30.801746 | 36.402988 |
| S | 33.587578 | 27.592552 | 33.902355 |
| S | 33.687683 | 32.748726 | 32.960018 |
| S | 36.659416 | 28.824203 | 32.115009 |
| S | 36.456436 | 29.634758 | 36.913883 |
| S | 40.210724 | 27.185667 | 34.900440 |
| S | 40.427025 | 31.410322 | 33.339333 |
| S | 43.294094 | 27.791538 | 31.646423 |
| S | 45.502895 | 28.809563 | 36.627441 |

24

generated by VMD

|   |       |       |       |
|---|-------|-------|-------|
| Ca| 24.897240 | 30.160454 | 32.230228 |
| Ca| 26.515244 | 30.754793 | 35.778019 |
| Ca| 30.090553 | 27.522980 | 34.857399 |
| Ca| 30.260578 | 33.057117 | 33.938557 |
| Ca| 33.772194 | 29.764610 | 31.404081 |
| Ca| 33.016983 | 30.406939 | 35.518902 |
| Ca| 36.564545 | 27.065960 | 34.910191 |
| Ca| 36.759602 | 31.267889 | 34.000244 |
| Ca| 40.316555 | 28.508627 | 31.635885 |
| Ca| 39.798748 | 30.712488 | 36.427917 |
| Ca| 45.365417 | 25.320019 | 33.260876 |
| Ca| 42.991718 | 29.872963 | 34.581001 |
| S | 26.626411 | 27.137001 | 35.696003 |
| S | 27.002773 | 33.896664 | 34.811089 |
| S | 30.636078 | 29.892345 | 32.534264 |
| S | 29.936129 | 30.660885 | 36.382874 |
| S | 33.423325 | 27.561483 | 33.953056 |
| S | 33.712498 | 32.746445 | 32.851231 |
| S | 36.917870 | 29.002542 | 31.831013 |
| S | 36.299789 | 29.819513 | 36.855026 |
| S | 40.084301 | 27.335745 | 34.858887 |
| S | 40.575142 | 31.498749 | 33.126713 |
| S | 43.739281 | 28.044918 | 31.615479 |
| S | 45.130959 | 28.380280 | 36.971703 |

24

generated by VMD

|   |       |       |       |
|---|-------|-------|-------|
| Ca| 24.780720 | 30.334282 | 32.314503 |
| Ca| 26.274460 | 30.423107 | 35.922890 |
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| Ca      | 30.244780 | 27.880001 | 34.813423 |
| Ca      | 30.187069 | 30.405706 | 35.388481 |
| Ca      | 36.648842 | 27.086922 | 34.958874 |
| Ca      | 36.727798 | 31.481182 | 34.427860 |
| Ca      | 40.054508 | 28.447849 | 31.682659 |
| Ca      | 39.860790 | 30.399160 | 36.455765 |
| Ca      | 45.554539 | 25.331009 | 33.145390 |
| Ca      | 42.963715 | 29.838385 | 34.603123 |
| S       | 26.733084 | 27.037632 | 35.524910 |
| S       | 27.300949 | 33.567532 | 34.603382 |
| S       | 30.557726 | 30.060362 | 32.447357 |
| S       | 29.965317 | 30.927063 | 36.259220 |
| S       | 33.503922 | 27.392920 | 33.908623 |
| S       | 33.630219 | 32.783062 | 32.930420 |
| S       | 36.842827 | 29.226229 | 32.072720 |
| S       | 36.207417 | 29.808548 | 36.858425 |
| S       | 40.301559 | 27.160393 | 34.727818 |
| S       | 40.399517 | 31.397541 | 33.374737 |
| S       | 43.446487 | 27.916510 | 31.618502 |
| S       | 45.524277 | 28.627022 | 36.881931 |

24

generated by VMD

| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| Ca      | 24.726418 | 30.349813 | 32.047077 |
| Ca      | 26.082039 | 30.622791 | 35.920395 |
| Ca      | 30.216183 | 27.856173 | 35.143684 |
| Ca      | 30.162653 | 32.863983 | 33.559753 |
| Ca      | 33.592663 | 29.649370 | 31.157730 |
| Ca      | 33.292870 | 30.337061 | 35.742523 |
| Ca      | 36.879620 | 27.308323 | 35.119656 |
| Ca      | 36.878685 | 31.533972 | 34.313587 |
| Ca      | 40.136749 | 28.536322 | 31.654327 |
| Ca      | 39.919365 | 30.034733 | 36.430622 |
| Ca      | 45.566181 | 25.501209 | 32.914036 |
| Ca      | 43.115574 | 29.688074 | 34.661465 |
| S       | 26.569534 | 27.135115 | 35.592140 |
| S       | 26.919954 | 33.541832 | 34.546272 |
| S       | 30.559893 | 29.751953 | 32.490128 |
| S       | 29.822937 | 30.905956 | 36.260426 |
| S       | 33.656292 | 27.665157 | 33.980385 |
| S       | 33.793499 | 32.862961 | 32.802467 |
| S       | 36.724026 | 29.156813 | 31.959106 |
| S       | 36.418720 | 29.963198 | 37.120674 |
| S       | 40.323933 | 27.398314 | 34.680779 |
| S       | 40.505733 | 31.537628 | 33.463165 |
|     | 43.438343 | 27.852867 | 31.443672 |
|-----|-----------|-----------|-----------|
| S   | 45.132080 | 28.337852 | 37.026539 |

24 generated by VMD

|     | 24.762463 | 30.231153 | 32.178211 |
|-----|-----------|-----------|-----------|
| Ca  | 26.323343 | 30.381464 | 36.444550 |
|     | 30.126604 | 27.891764 | 35.018673 |
|     | 30.224928 | 32.848198 | 33.345726 |
|     | 33.799316 | 29.831860 | 31.302912 |
|     | 33.073715 | 30.279575 | 35.364143 |
|     | 36.847260 | 27.140842 | 34.788109 |
|     | 36.652393 | 31.614267 | 34.137539 |
|     | 40.166424 | 28.389112 | 31.586178 |
|     | 39.786087 | 30.219757 | 36.502300 |
|     | 45.607513 | 25.281654 | 33.189053 |
|     | 43.090641 | 29.802881 | 34.689342 |
|     | 26.611250 | 27.102594 | 35.787231 |
|     | 27.052216 | 33.533401 | 34.895546 |
|     | 30.576405 | 29.965000 | 32.294659 |
|     | 29.891104 | 31.054817 | 36.311848 |
|     | 33.687458 | 27.648335 | 33.686954 |
|     | 33.628796 | 33.085495 | 32.838730 |
|     | 36.922062 | 29.234211 | 31.905565 |
|     | 36.294502 | 29.842840 | 36.703247 |
|     | 40.331867 | 27.440512 | 34.813549 |
|     | 40.378124 | 31.376749 | 33.341393 |
|     | 43.506657 | 27.860609 | 31.714600 |
|     | 45.092842 | 28.334375 | 37.190716 |

24 generated by VMD

|     | 25.173424 | 29.508429 | 32.006451 |
|-----|-----------|-----------|-----------|
| Ca  | 26.249361 | 30.528868 | 36.066875 |
|     | 30.280289 | 27.908455 | 35.172913 |
|     | 30.077509 | 33.251583 | 33.569706 |
|     | 34.070946 | 29.930180 | 31.513517 |
|     | 33.003525 | 30.598846 | 35.570923 |
|     | 36.751602 | 27.123798 | 34.887966 |
|     | 36.564526 | 31.427624 | 34.384399 |
|     | 40.332783 | 28.593542 | 31.172915 |
|     | 39.728058 | 30.482672 | 36.424961 |
|     | 45.661160 | 25.239811 | 32.975124 |
|     | 42.872761 | 29.578163 | 34.539158 |
| S   | 27.074800 | 27.112255 | 35.737782 |
|     | 26.828150 | 33.495796 | 34.571133 |
|     | 30.683315 | 30.200827 | 32.598442 |
|     | 29.833811 | 31.251600 | 36.382019 |
|   |   |   |   |
|---|---|---|---|
| S | 33.587139 | 27.834332 | 33.920368 |
| S | 33.570499 | 32.953270 | 32.987499 |
| S | 36.964115 | 29.187479 | 32.062721 |
| S | 36.093311 | 29.680548 | 36.844612 |
| S | 40.340061 | 27.235527 | 34.527016 |
| S | 40.325233 | 31.314938 | 33.345242 |
| S | 43.569786 | 27.808418 | 31.563505 |
| S | 44.797722 | 28.144407 | 37.205418 |

24

generated by VMD

| Ca | 25.255875 | 30.122902 | 32.134022 |
| Ca | 26.400227 | 30.432318 | 36.046146 |
| Ca | 30.344944 | 27.876314 | 35.130188 |
| Ca | 30.290146 | 32.955811 | 33.482288 |
| Ca | 33.726093 | 29.766451 | 31.499445 |
| Ca | 33.030022 | 30.604719 | 35.487560 |
| Ca | 36.637455 | 27.083313 | 34.923679 |
| Ca | 36.666168 | 31.260138 | 34.149536 |
| Ca | 40.169434 | 28.583080 | 31.697254 |
| Ca | 39.651245 | 30.250219 | 36.398109 |
| Ca | 45.486427 | 25.404057 | 32.986122 |
| Ca | 42.823528 | 29.660860 | 34.516644 |
| S | 26.922958 | 27.052563 | 35.615082 |
| S | 27.080544 | 33.633148 | 34.882389 |
| S | 30.542612 | 29.990562 | 32.256737 |
| S | 29.921354 | 30.973270 | 36.287231 |
| S | 33.632618 | 27.799099 | 33.926407 |
| S | 33.745350 | 33.017040 | 32.792820 |
| S | 36.825249 | 29.026079 | 32.032730 |
| S | 36.289558 | 29.775177 | 36.932129 |
| S | 40.120079 | 27.130270 | 34.682835 |
| S | 40.424561 | 31.485849 | 33.508640 |
| S | 43.381599 | 27.890116 | 31.525314 |
| S | 45.065918 | 28.618071 | 37.147457 |

24

generated by VMD

| Ca | 24.781935 | 30.144859 | 32.170925 |
| Ca | 26.280991 | 30.541977 | 35.928158 |
| Ca | 30.171228 | 27.954773 | 34.935669 |
| Ca | 29.948393 | 32.935062 | 33.677586 |
| Ca | 33.814259 | 29.342813 | 31.338570 |
| Ca | 33.098885 | 30.599785 | 35.447948 |
| Ca | 36.853252 | 27.159346 | 34.955894 |
| Ca | 36.839581 | 31.389055 | 34.316593 |
| Ca | 40.300983 | 28.726860 | 31.836964 |
| Ca | 39.756016 | 30.334259 | 36.359383 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 45.298714 | 25.226517 | 32.963596 |
| Ca      | 42.913841 | 29.827431 | 34.566338 |
| S       | 26.700226 | 27.152008 | 35.805000 |
| S       | 26.714344 | 33.606789 | 34.534508 |
| S       | 30.765806 | 30.045473 | 32.341309 |
| S       | 29.917397 | 30.973244 | 36.340321 |
| S       | 33.701714 | 27.681952 | 34.021271 |
| S       | 33.767704 | 32.872955 | 32.853355 |
| S       | 36.896637 | 29.179354 | 31.992937 |
| S       | 36.400459 | 29.712500 | 36.889641 |
| S       | 40.259048 | 27.148844 | 34.674820 |
| S       | 40.543404 | 31.677435 | 33.666573 |
| S       | 43.484459 | 27.861019 | 31.518698 |
| S       | 45.224613 | 28.297096 | 36.894615 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 24.922840 | 30.007843 | 32.173573 |
| Ca      | 26.365843 | 30.586000 | 35.850037 |
| Ca      | 30.251963 | 27.992981 | 35.031200 |
| Ca      | 30.136330 | 33.091385 | 33.485683 |
| Ca      | 33.895657 | 29.668888 | 31.510914 |
| Ca      | 33.282055 | 30.553391 | 35.465374 |
| Ca      | 36.808887 | 27.160992 | 34.878330 |
| Ca      | 36.744534 | 31.252148 | 34.329838 |
| Ca      | 39.939568 | 28.681200 | 31.726545 |
| Ca      | 39.745613 | 30.188936 | 36.753902 |
| Ca      | 45.381390 | 25.150862 | 32.803146 |
| Ca      | 42.648048 | 29.846607 | 34.623234 |
| S       | 27.015095 | 27.194271 | 35.699295 |
| S       | 26.835594 | 33.556240 | 34.565273 |
| S       | 30.719828 | 29.935778 | 32.418442 |
| S       | 29.940113 | 31.154652 | 36.311092 |
| S       | 33.870525 | 27.633574 | 33.884212 |
| S       | 33.582088 | 32.823959 | 32.959667 |
| S       | 36.901371 | 29.148525 | 31.910004 |
| S       | 36.375645 | 29.458353 | 36.872803 |
| S       | 40.282642 | 27.208387 | 34.846165 |
| S       | 40.404377 | 31.658739 | 33.403831 |
| S       | 43.325817 | 27.889978 | 31.608097 |
| S       | 45.058022 | 28.547703 | 36.920094 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.264223 | 30.182281 | 31.909435 |
| Ca      | 26.398205 | 30.671955 | 35.836201 |
| Ca      | 30.385254 | 27.574356 | 34.927681 |
| Ca      | 30.238424 | 33.202480 | 33.684628 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 33.505608    | 29.571407    | 31.591354    |
| Ca      | 33.096550    | 30.414616    | 35.537243    |
| Ca      | 37.082321    | 26.996914    | 34.654121    |
| Ca      | 36.728527    | 31.149889    | 34.149765    |
| Ca      | 39.820370    | 28.660305    | 32.052757    |
| Ca      | 39.851162    | 30.598085    | 36.647652    |
| Ca      | 45.084343    | 25.175293    | 32.795998    |
| Ca      | 42.819206    | 29.944162    | 34.652981    |
| S       | 26.832678    | 27.192554    | 35.613354    |
| S       | 26.846100    | 33.769005    | 34.737831    |
| S       | 30.600933    | 29.958960    | 32.600567    |
| S       | 30.021057    | 30.970535    | 36.116348    |
| S       | 33.656307    | 27.593893    | 34.110222    |
| S       | 33.681541    | 32.833462    | 32.817940    |
| S       | 36.558226    | 29.066166    | 31.815210    |
| S       | 36.55408     | 29.467949    | 36.676861    |
| S       | 40.367447    | 27.339872    | 35.204788    |
| S       | 40.566700    | 31.609745    | 33.377220    |
| S       | 43.143448    | 27.905041    | 31.678956    |
| S       | 45.319870    | 28.542503    | 36.841988    |

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generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.090916    | 30.119289    | 31.871824    |
| Ca      | 26.460644    | 30.407019    | 35.883717    |
| Ca      | 30.248716    | 28.076126    | 35.043736    |
| Ca      | 30.053596    | 33.263500    | 33.576878    |
| Ca      | 33.677273    | 29.297447    | 31.574356    |
| Ca      | 33.100914    | 30.536789    | 35.555550    |
| Ca      | 36.737968    | 27.024607    | 35.015663    |
| Ca      | 36.909119    | 31.242573    | 34.273743    |
| Ca      | 40.140606    | 28.711910    | 31.805292    |
| Ca      | 39.797287    | 30.746010    | 36.629406    |
| Ca      | 45.252972    | 25.240597    | 32.779041    |
| Ca      | 42.626770    | 29.599699    | 34.461090    |
| S       | 27.022810    | 26.959448    | 35.378693    |
| S       | 26.961081    | 33.567921    | 34.649834    |
| S       | 30.702414    | 29.995726    | 32.450684    |
| S       | 29.971722    | 31.328506    | 36.342548    |
| S       | 33.502377    | 27.696827    | 34.252411    |
| S       | 33.628998    | 32.675304    | 32.926754    |
| S       | 36.877235    | 29.040775    | 32.102612    |
| S       | 36.301620    | 29.626484    | 36.963142    |
| S       | 40.089649    | 27.204117    | 34.687485    |
| S       | 40.498493    | 31.662357    | 33.410564    |
| S       | 43.449398    | 27.972841    | 31.678179    |
| S       | 45.331356    | 28.395529    | 36.717449    |
| Element | X    | Y    | Z    |
|---------|------|------|------|
| Ca      | 25.074549 | 29.681129 | 32.058990 |
| Ca      | 26.452984 | 30.357361 | 35.735222 |
| Ca      | 30.374031 | 28.128077 | 34.952152 |
| Ca      | 30.031485 | 33.158089 | 33.668251 |
| Ca      | 33.714661 | 29.817760 | 31.738167 |
| Ca      | 33.213596 | 30.483379 | 35.573528 |
| Ca      | 36.748112 | 27.074589 | 34.673580 |
| Ca      | 36.780258 | 31.528633 | 34.231499 |
| Ca      | 40.081223 | 28.648514 | 31.694933 |
| Ca      | 39.899773 | 30.461906 | 36.719303 |
| Ca      | 45.242401 | 25.111298 | 32.767006 |
| Ca      | 42.767735 | 29.494907 | 34.730061 |
| S       | 27.076866 | 26.967615 | 35.614914 |
| S       | 26.666645 | 33.575691 | 34.556435 |
| S       | 30.486729 | 30.175007 | 32.435097 |
| S       | 30.051271 | 31.209156 | 36.332806 |
| S       | 33.587635 | 27.716240 | 34.134281 |
| S       | 33.579758 | 32.917362 | 32.860832 |
| S       | 36.860058 | 29.246792 | 31.875278 |
| S       | 36.288685 | 29.687477 | 36.767258 |
| S       | 40.101105 | 27.308809 | 35.009636 |
| S       | 40.609955 | 31.523788 | 33.468979 |
| S       | 43.330940 | 27.778028 | 31.666756 |
| S       | 45.413437 | 28.339809 | 36.765800 |

Generated by VMD
|    |      |      |      |
|----|------|------|------|
| S  | 36.874001 | 29.083971 | 31.947292 |
| S  | 36.353382 | 29.664448 | 36.891380 |
| S  | 40.141415 | 27.535385 | 34.969578 |
| S  | 40.574165 | 31.767097 | 33.90278 |
| S  | 43.410908 | 27.835136 | 31.665634 |
| S  | 45.012268 | 28.124723 | 36.775856 |

24 generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 25.105528 | 29.869295 | 32.162609 |
| Ca | 26.326965 | 30.114792 | 36.222591 |
| Ca | 30.207441 | 28.338409 | 35.138199 |
| Ca | 29.948151 | 33.007019 | 33.461666 |
| Ca | 33.662289 | 29.862827 | 31.330656 |
| Ca | 33.245159 | 30.732670 | 35.481152 |
| Ca | 36.808323 | 27.136511 | 34.744591 |
| Ca | 36.953133 | 31.623270 | 34.004726 |
| Ca | 40.131157 | 28.650621 | 31.628437 |
| Ca | 39.874683 | 30.454035 | 36.571632 |
| Ca | 45.297825 | 25.032484 | 33.013798 |
| Ca | 42.892727 | 29.623783 | 34.794579 |
| S  | 26.978882 | 26.644398 | 35.762699 |
| S  | 26.593355 | 33.327450 | 34.793472 |
| S  | 30.498877 | 30.166496 | 32.361839 |
| S  | 29.885065 | 31.258495 | 36.473980 |
| S  | 33.560505 | 28.101185 | 33.969658 |
| S  | 33.615074 | 32.922546 | 32.644184 |
| S  | 36.807537 | 29.277449 | 31.778959 |
| S  | 36.440868 | 29.729965 | 36.585716 |
| S  | 40.269619 | 27.273186 | 34.658085 |
| S  | 40.827198 | 31.502560 | 33.457920 |
| S  | 43.532951 | 27.739082 | 31.776093 |
| S  | 44.970604 | 28.002893 | 37.213444 |

24 generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 25.084217 | 29.957644 | 32.053108 |
| Ca | 26.366917 | 30.224007 | 36.061321 |
| Ca | 30.281715 | 28.264198 | 34.830692 |
| Ca | 30.160748 | 32.918247 | 33.470993 |
| Ca | 33.611927 | 29.627865 | 31.484369 |
| Ca | 33.163910 | 30.722832 | 35.590939 |
| Ca | 36.917336 | 27.083540 | 34.882832 |
| Ca | 36.813961 | 31.546158 | 34.261562 |
| Ca | 39.953297 | 28.599152 | 31.957546 |
| Ca | 40.033131 | 30.578775 | 36.861256 |
| Ca | 45.368210 | 25.196962 | 32.586803 |
| Ca | 42.928959 | 29.647358 | 34.642159 |
|  |  |  |  |
|---|---|---|---|
| S | 27.105213 | 26.816063 | 35.437672 |
| S | 26.846537 | 33.525074 | 34.678383 |
| S | 30.405939 | 30.054335 | 32.216175 |
| S | 29.831047 | 31.232407 | 36.320690 |
| S | 33.510426 | 27.881683 | 34.021324 |
| S | 33.573643 | 32.934761 | 32.769234 |
| S | 36.712528 | 29.218895 | 32.057728 |
| S | 36.368855 | 29.743412 | 36.846123 |
| S | 40.274101 | 27.296303 | 35.101360 |
| S | 40.509178 | 31.497944 | 33.428795 |
| S | 43.136131 | 27.763628 | 31.646610 |
| S | 45.475891 | 28.060135 | 36.823009 |

24
generated by VMD

| Ca  | 24.932835 | 30.028786 | 32.233089 |
| Ca  | 26.437864 | 30.276512 | 35.937046 |
| Ca  | 30.501757 | 27.954586 | 34.851780 |
| Ca  | 30.358015 | 32.956730 | 33.618320 |
| Ca  | 33.573441 | 29.573860 | 31.512129 |
| Ca  | 33.234470 | 30.668835 | 35.338272 |
| Ca  | 36.945560 | 27.153225 | 34.293846 |
| Ca  | 36.983215 | 31.432917 | 34.020439 |
| Ca  | 39.925026 | 28.753002 | 31.764214 |
| Ca  | 39.684090 | 30.609091 | 36.556385 |
| Ca  | 45.073269 | 25.227070 | 33.294563 |
| Ca  | 42.748730 | 29.834057 | 34.686646 |
| S   | 26.917189 | 26.906641 | 35.756363 |
| S   | 27.026466 | 33.758678 | 34.847397 |
| S   | 30.508848 | 30.002892 | 32.366951 |
| S   | 30.018148 | 30.967764 | 36.436832 |
| S   | 33.449902 | 27.579239 | 33.953907 |
| S   | 33.705406 | 32.891968 | 33.031319 |
| S   | 36.754421 | 29.339039 | 31.691904 |
| S   | 36.383202 | 29.605150 | 36.502796 |
| S   | 40.134304 | 27.380737 | 35.026749 |
| S   | 40.511959 | 31.623777 | 33.124653 |
| S   | 43.172134 | 27.686537 | 32.002838 |
| S   | 45.453621 | 28.180302 | 37.182251 |

24
generated by VMD

| Ca  | 24.843960 | 30.060389 | 32.376446 |
| Ca  | 26.281694 | 30.133326 | 36.049942 |
| Ca  | 30.141502 | 28.164627 | 35.220856 |
| Ca  | 30.297880 | 32.978336 | 33.365402 |
| Ca  | 33.308575 | 29.519001 | 31.563086 |
| Ca  | 33.215607 | 30.516733 | 35.186981 |
Ca  36.884510  27.237038  34.491596
Ca  37.113972  31.695789  34.136181
Ca  39.991131  29.023548  31.889866
Ca  40.075443  30.682440  36.811069
Ca  45.369030  25.108875  32.906075
Ca  43.037022  29.696058  34.898750
S   26.914225  26.904760  35.674355
S   26.932480  33.561398  34.709801
S   30.363672  29.886969  32.352802
S   29.895493  31.083750  36.338909
S   33.487770  27.563599  33.883701
S   33.580887  32.739964  32.505192
S   36.704311  29.550686  31.830210
S   36.397198  29.744253  36.596264
S   40.272125  27.410719  34.901966
S   40.849304  31.583153  33.463608
S   43.281631  27.740778  31.772587
S   45.194439  27.805204  37.105049

24
generated by VMD
Ca  25.034924  29.982973  32.374866
Ca  26.466604  30.125801  36.100193
Ca  30.105961  27.997116  34.930164
Ca  30.358559  33.001244  33.482307
Ca  33.533852  29.532749  31.340286
Ca  33.248394  30.883381  35.417652
Ca  36.711143  27.349461  34.549026
Ca  37.200680  31.591764  34.032917
Ca  40.017063  28.871180  31.822483
Ca  39.843166  30.773975  36.855473
Ca  45.295708  24.747532  32.946384
Ca  42.756714  29.591248  34.816006
S   26.914574  26.494545  35.594501
S   27.102205  33.482231  34.850925
S   30.317812  30.026302  32.358501
S   30.013788  30.995377  36.434948
S   33.329338  27.798210  34.031689
S   33.679501  32.836441  32.504387
S   36.843300  29.365074  31.719978
S   36.459084  29.933506  36.754951
S   40.076630  27.398645  34.970852
S   40.817650  31.703676  33.430782
S   43.387913  27.821619  31.610308
S   44.919327  28.087378  37.101147

24
generated by VMD
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 24.997908    | 30.162704    | 31.871885    |
| Ca      | 26.554802    | 30.360458    | 35.914413    |
| Ca      | 30.294325    | 27.973427    | 35.048561    |
| Ca      | 30.204622    | 32.891773    | 33.819729    |
| Ca      | 33.512291    | 29.602766    | 31.304564    |
| Ca      | 33.175213    | 30.654203    | 35.451248    |
| Ca      | 36.771244    | 27.031775    | 34.509884    |
| Ca      | 36.988075    | 31.324553    | 34.012451    |
| Ca      | 39.995205    | 28.718372    | 31.662504    |
| Ca      | 39.844521    | 30.829564    | 36.544621    |
| Ca      | 45.495361    | 25.168451    | 33.096622    |
| Ca      | 42.894745    | 29.848822    | 34.672314    |
| S       | 26.945831    | 26.929945    | 35.752468    |
| S       | 26.849539    | 33.623714    | 34.924957    |
| S       | 30.556108    | 30.097359    | 32.525951    |
| S       | 30.086231    | 30.925501    | 36.456661    |
| S       | 33.485928    | 27.792542    | 34.007160    |
| S       | 33.636211    | 32.766342    | 32.737743    |
| S       | 36.661423    | 29.073034    | 31.765890    |
| S       | 36.463676    | 29.752357    | 36.729771    |
| S       | 40.186108    | 27.461411    | 34.825287    |
| S       | 40.467976    | 31.467690    | 33.220650    |
| S       | 43.371265    | 27.682449    | 31.982862    |
| S       | 44.995308    | 28.152145    | 37.192444    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 24.977314    | 29.929243    | 32.022606    |
| Ca      | 26.187595    | 30.238888    | 35.795525    |
| Ca      | 30.100170    | 28.220264    | 35.028397    |
| Ca      | 30.041864    | 33.057610    | 33.721527    |
| Ca      | 33.562393    | 29.616566    | 31.371456    |
| Ca      | 33.280872    | 30.445690    | 35.322418    |
| Ca      | 36.845951    | 27.285622    | 34.610573    |
| Ca      | 37.180542    | 31.387861    | 34.072521    |
| Ca      | 40.123142    | 28.747147    | 31.793829    |
| Ca      | 40.116100    | 30.733936    | 36.707264    |
| Ca      | 45.397308    | 24.950100    | 33.029388    |
| Ca      | 43.012245    | 29.694172    | 34.591347    |
| S       | 26.931389    | 26.821280    | 35.833843    |
| S       | 26.762453    | 33.635696    | 34.916899    |
| S       | 30.416813    | 30.050447    | 32.406845    |
| S       | 29.662191    | 31.012976    | 36.476131    |
| S       | 33.366833    | 27.630684    | 34.042587    |
| S       | 33.516006    | 32.950558    | 32.753044    |
| S       | 36.830475    | 29.231722    | 31.730680    |
| S       | 36.388699    | 29.900707    | 36.665794    |
|   |   |   |
|---|---|---|
| S | 40.391132 | 27.585192 | 35.041222 |
| S | 40.785797 | 31.722380 | 33.232491 |
| S | 43.433598 | 27.679903 | 31.801146 |
| S | 45.123013 | 27.862774 | 37.038380 |

24 generated by VMD

| Ca | 25.217178 | 30.143536 | 31.792627 |
| Ca | 26.244047 | 30.422903 | 36.075012 |
| Ca | 30.216259 | 28.052029 | 34.865673 |
| Ca | 29.946856 | 33.203812 | 33.735382 |
| Ca | 33.643856 | 29.258896 | 31.469618 |
| Ca | 33.383244 | 30.392639 | 35.425968 |
| Ca | 36.842575 | 27.066046 | 34.768974 |
| Ca | 36.953579 | 31.486267 | 34.007801 |
| Ca | 40.106857 | 28.983196 | 31.783087 |
| Ca | 39.826809 | 30.808159 | 36.731205 |
| Ca | 45.407364 | 25.036407 | 32.961128 |
| Ca | 42.891083 | 29.766014 | 34.490078 |
| S | 26.915092 | 27.073364 | 35.703419 |
| S | 26.746490 | 33.658302 | 34.923817 |
| S | 30.675484 | 30.044920 | 32.373085 |
| S | 29.939415 | 31.031969 | 36.464802 |
| S | 33.612946 | 27.533478 | 34.027878 |
| S | 33.511971 | 32.678097 | 32.77325 |
| S | 36.765556 | 28.980749 | 31.977940 |
| S | 36.593052 | 29.749317 | 36.609386 |
| S | 40.479946 | 27.546314 | 35.063423 |
| S | 40.503334 | 31.721279 | 33.306320 |
| S | 43.183689 | 27.672419 | 31.679092 |
| S | 44.827309 | 28.081238 | 37.017551 |

24 generated by VMD

| Ca | 25.133152 | 30.201778 | 32.074356 |
| Ca | 26.257824 | 30.277779 | 35.785427 |
| Ca | 30.063292 | 28.214396 | 35.090267 |
| Ca | 30.207897 | 33.001690 | 33.714294 |
| Ca | 33.717533 | 29.177521 | 31.367805 |
| Ca | 33.148865 | 30.429377 | 35.463032 |
| Ca | 36.886532 | 27.356668 | 34.709156 |
| Ca | 36.769680 | 31.812559 | 34.416431 |
| Ca | 40.001434 | 28.613712 | 31.632145 |
| Ca | 39.911808 | 30.835161 | 36.421787 |
| Ca | 45.522514 | 24.947258 | 32.868954 |
| Ca | 42.921799 | 29.817926 | 34.705997 |
| S | 26.878382 | 27.028265 | 35.629959 |
| S | 27.046431 | 33.494446 | 34.707275 |
| S    | 30.534943 | 29.873274 | 32.386841 |
|------|-----------|-----------|-----------|
| S    | 29.837244 | 30.944996 | 36.637569 |
| S    | 33.633492 | 27.657059 | 34.021107 |
| S    | 33.653275 | 32.613266 | 32.699463 |
| S    | 33.633492 | 27.657059 | 34.021107 |
| S    | 33.653275 | 32.613266 | 32.699463 |
| S    | 36.410854 | 29.841558 | 36.766754 |
| S    | 40.307610 | 27.500023 | 34.983349 |
| S    | 40.450645 | 31.683310 | 33.406250 |
| S    | 43.248920 | 27.704189 | 31.536507 |
| S    | 44.886612 | 27.947208 | 37.045033 |

24

generated by VMD

| Ca   | 25.648087 | 30.89317  | 31.254147 |
|------|-----------|-----------|-----------|
| Ca   | 26.258577 | 30.274208 | 35.846878 |
| Ca   | 30.203041 | 27.999031 | 35.251892 |
| Ca   | 30.276806 | 33.050774 | 33.840954 |
| Ca   | 33.526714 | 29.321129 | 31.498919 |
| Ca   | 33.214211 | 30.260984 | 35.741348 |
| Ca   | 36.816357 | 27.299835 | 34.828796 |
| Ca   | 36.820602 | 31.457047 | 34.167076 |
| Ca   | 40.054657 | 28.597738 | 31.655235 |
| Ca   | 39.719963 | 30.873922 | 36.406189 |
| Ca   | 35.229527 | 25.088516 | 32.924377 |
| Ca   | 42.920628 | 29.862867 | 34.532871 |
| S    | 26.918974 | 26.745525 | 35.987370 |
| S    | 26.988171 | 33.672337 | 34.739559 |
| S    | 30.442295 | 29.894890 | 32.543064 |
| S    | 29.778233 | 30.930180 | 36.590008 |
| S    | 33.568336 | 27.576401 | 34.173935 |
| S    | 33.639767 | 32.543362 | 32.636966 |
| S    | 36.824856 | 29.224033 | 31.820778 |
| S    | 36.418934 | 29.824591 | 36.791561 |
| S    | 40.336491 | 27.569725 | 35.029083 |
| S    | 40.465076 | 31.517487 | 33.134007 |
| S    | 43.321938 | 27.731003 | 31.637058 |
| S    | 45.041718 | 28.266533 | 36.998764 |

24

generated by VMD

| Ca   | 25.397833 | 30.307467 | 32.111134 |
|------|-----------|-----------|-----------|
| Ca   | 26.241907 | 30.355314 | 36.009109 |
| Ca   | 30.148510 | 27.945124 | 35.220642 |
| Ca   | 30.160568 | 33.230598 | 33.439213 |
| Ca   | 33.528442 | 29.467533 | 31.503319 |
| Ca   | 33.225468 | 30.454805 | 35.574253 |
| Ca   | 36.904278 | 27.231890 | 34.978634 |
| Ca   | 36.709911 | 31.366756 | 34.147728 |
| Element | X1  | Y1  | Z1  |
|---------|-----|-----|-----|
| Ca      | 40.149036 | 28.532482 | 31.735380 |
| Ca      | 39.706676 | 30.501377 | 36.498035 |
| Ca      | 45.753819 | 25.341187 | 32.814693 |
| Ca      | 42.829605 | 29.995337 | 34.689095 |
| S       | 26.880976 | 26.887135 | 35.400681 |
| S       | 26.862003 | 33.543983 | 34.684643 |
| S       | 30.650772 | 30.111942 | 32.492172 |
| S       | 29.790327 | 31.160452 | 36.321548 |
| S       | 33.623089 | 27.667788 | 34.189487 |
| S       | 33.668350 | 32.804943 | 32.717873 |
| S       | 36.768013 | 29.115629 | 31.991770 |
| S       | 36.304974 | 29.807137 | 36.874088 |
| S       | 40.414085 | 27.223850 | 34.898911 |
| S       | 40.471565 | 31.572847 | 33.39773 |
| S       | 43.318970 | 27.768364 | 31.534918 |
| S       | 44.924744 | 27.997458 | 36.804626 |

24 generated by VMD

| Element | X2  | Y2  | Z2  |
|---------|-----|-----|-----|
| Ca      | 25.302923 | 30.476343 | 31.961554 |
| Ca      | 26.483921 | 30.230648 | 36.002487 |
| Ca      | 29.964951 | 28.082748 | 35.153961 |
| Ca      | 30.338428 | 32.961845 | 33.826103 |
| Ca      | 33.610897 | 29.404348 | 31.304451 |
| Ca      | 33.137547 | 30.498924 | 35.296242 |
| Ca      | 36.688488 | 27.159100 | 34.861053 |
| Ca      | 36.786217 | 31.802185 | 34.020508 |
| Ca      | 39.924866 | 28.576035 | 31.708891 |
| Ca      | 39.840549 | 30.574406 | 36.479504 |
| Ca      | 45.943871 | 25.270576 | 33.175533 |
| Ca      | 42.835972 | 29.980499 | 34.584362 |
| S       | 26.588186 | 26.930872 | 35.462627 |
| S       | 27.222897 | 33.481125 | 34.934212 |
| S       | 30.581585 | 30.073374 | 32.461891 |
| S       | 29.864626 | 30.809885 | 36.679565 |
| S       | 33.535175 | 27.654339 | 34.135281 |
| S       | 33.676407 | 32.757427 | 32.543350 |
| S       | 36.653229 | 29.112427 | 31.922482 |
| S       | 36.339077 | 29.849379 | 36.711285 |
| S       | 40.180954 | 27.312113 | 34.940231 |
| S       | 40.416264 | 31.379612 | 33.11050 |
| S       | 43.466320 | 27.773735 | 31.743593 |
| S       | 45.050636 | 28.239407 | 37.010517 |

24 generated by VMD

| Element | X3  | Y3  | Z3  |
|---------|-----|-----|-----|
| Ca      | 25.401180 | 29.994980 | 32.035301 |
| Ca      | 26.027754 | 30.335190 | 35.735920 |
Ca  30.051950  28.114037  35.206303
Ca  30.423605  33.181507  33.846397
Ca  33.543648  29.211740  31.462692
Ca  33.149513  30.535149  35.419346
Ca  36.877373  27.282478  34.799686
Ca  36.850773  31.259804  33.924038
Ca  39.976185  28.831352  31.713761
Ca  39.791203  30.826416  36.359940
Ca  45.533373  25.218945  33.061314
Ca  42.976373  29.857962  34.628109
S   26.732538  26.853651  35.346878
S   27.155504  33.654167  35.010113
S   30.487244  30.224920  32.598923
S   29.928003  30.905380  36.615616
S   33.601589  27.681322  34.241940
S   33.704750  32.672733  32.637733
S   36.774719  29.112408  31.647654
S   36.400211  29.835268  34.827126
S   40.572186  31.638086  33.216854
S   43.226345  27.748074  31.833006
S   44.972424  27.975060  37.102722

generated by VMD
Ca  25.491995  30.229420  32.029583
Ca  26.224045  30.406004  35.844654
Ca  30.385347  28.033310  35.143177
Ca  30.034168  33.129032  33.620331
Ca  33.629597  29.472696  31.417276
Ca  33.239666  30.498425  35.553131
Ca  36.771572  27.182619  34.693394
Ca  36.810524  31.454468  34.125576
Ca  40.067730  28.502110  31.748705
Ca  39.749855  30.790024  36.551121
Ca  45.852226  25.141520  33.094025
Ca  42.775570  29.876814  34.341709
S   26.993807  26.908075  35.407707
S   26.861126  33.651730  35.042416
S   30.577267  30.027411  32.522709
S   29.691261  31.016598  36.574615
S   33.625301  27.764116  34.010242
S   33.620777  32.719101  32.836426
S   36.831821  29.136518  31.818571
S   36.415516  29.765854  36.827705
S   40.184875  27.364929  34.989292
S   40.473259  31.479204  33.157745

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generated by VMD

S  43.377346  27.644480  31.700609
S  44.749283  28.196932  36.979973

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Ca  25.376417  30.401518  32.066841
Ca  26.199434  30.358654  35.890648
Ca  30.161663  28.201677  35.003975
Ca  30.172319  33.063679  33.589146
Ca  33.627655  29.544083  31.342466
Ca  33.216389  30.627378  35.562328
Ca  36.835613  27.230776  34.936028
Ca  36.677860  30.987167  33.955845
Ca  40.107677  28.664642  31.637402
Ca  39.674923  30.676308  36.412651
Ca  46.156334  25.449928  33.136501
Ca  42.685112  29.826366  34.650856
S  26.792469  26.934984  35.537155
S  27.119961  33.594028  35.054657
S  30.470514  29.99022  32.377098
S  29.862825  31.094482  36.582039
S  33.571751  27.804050  34.063866
S  33.648815  32.756878  32.822376
S  36.706753  28.829590  31.704533
S  36.379150  29.644243  36.941875
S  40.314137  27.182455  34.926426
S  40.268028  31.380249  33.188000
S  43.467392  27.821556  31.659801
S  44.940712  28.317673  36.988125

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generated by VMD

Ca  25.259878  30.414309  31.860359
Ca  26.444260  30.624796  35.849907
Ca  30.262299  27.925268  35.228165
Ca  30.255095  32.732674  33.743755
Ca  33.515423  29.423998  31.138432
Ca  33.239902  30.549364  35.515213
Ca  36.920231  26.976099  34.713913
Ca  36.866840  31.069502  34.063053
Ca  40.002499  28.589584  31.765081
Ca  39.633488  30.931076  36.627800
Ca  46.099609  25.785679  32.961670
Ca  42.777252  29.959297  34.611786
S  26.610607  27.186970  35.499352
S  27.194317  33.881519  34.992256
S  30.405773  29.794828  32.491951
S  29.932058  31.035084  36.533165
| S         | E1        | E2        | E3        |
|----------|-----------|-----------|-----------|
| S 33.406002 | 27.670383 | 34.014423 |
| S 33.825130 | 32.632019 | 32.904438 |
| S 36.573101 | 28.813908 | 31.802919 |
| S 36.474426 | 29.502068 | 36.694111 |
| S 40.198421 | 27.487370 | 35.002037 |
| S 40.356857 | 31.360291 | 33.220909 |
| S 43.263069 | 27.834473 | 31.755024 |
| S 44.917408 | 28.210831 | 37.040962 |

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generated by VMD

| Ca       | E1        | E2        | E3        |
|----------|-----------|-----------|-----------|
| Ca 25.396795 | 30.352528 | 32.045532 |
| Ca 26.124697 | 30.742832 | 35.695194 |
| Ca 30.165371 | 27.955077 | 35.258183 |
| Ca 30.310373 | 32.862270 | 33.683475 |
| Ca 33.361057 | 29.519617 | 31.394180 |
| Ca 33.218643 | 30.132881 | 35.469921 |
| Ca 36.898438 | 26.925247 | 34.483200 |
| Ca 36.810711 | 31.362644 | 33.973461 |
| Ca 39.951969 | 28.756128 | 31.846434 |
| Ca 39.975922 | 30.818171 | 36.444584 |
| Ca 45.661579 | 25.526049 | 33.130413 |
| Ca 42.795982 | 29.882904 | 34.613304 |
| S 26.704802 | 27.148626 | 35.583393 |
| S 27.252745 | 33.915070 | 35.104694 |
| S 30.410770 | 29.822912 | 32.460300 |
| S 30.096239 | 31.054068 | 36.546253 |
| S 33.483074 | 27.298285 | 33.858257 |
| S 33.716301 | 32.531433 | 32.849346 |
| S 36.643349 | 29.176416 | 31.820786 |
| S 36.519413 | 29.679319 | 36.632298 |
| S 40.170807 | 27.271105 | 34.874146 |
| S 40.473053 | 31.509489 | 33.179981 |
| S 43.346863 | 27.802559 | 31.850250 |
| S 44.944923 | 28.505371 | 37.233124 |

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generated by VMD

| Ca       | E1        | E2        | E3        |
|----------|-----------|-----------|-----------|
| Ca 25.351377 | 30.433403 | 31.970606 |
| Ca 26.326227 | 30.388569 | 35.811916 |
| Ca 30.020023 | 28.248268 | 35.130692 |
| Ca 30.207125 | 33.210419 | 33.354202 |
| Ca 33.577827 | 29.400919 | 31.337656 |
| Ca 32.992855 | 30.606071 | 35.515438 |
| Ca 36.900787 | 26.686655 | 34.807274 |
| Ca 36.781139 | 30.962681 | 34.039494 |
| Ca 40.055298 | 28.602417 | 31.645752 |
| Ca 39.620640 | 30.513771 | 36.667297 |
Ca  46.123055  26.103785  32.631378
Ca  42.720661  29.840372  34.706627
S  26.836792  27.128162  36.034615
S  27.138945  33.714928  34.895157
S  30.537748  30.092682  32.266232
S  29.707012  31.290760  36.386642
S  33.405491  27.604546  33.993523
S  33.786945  32.579037  32.962646
S  36.677803  28.657831  31.907524
S  36.403027  29.382795  36.784599
S  40.278252  27.255678  34.982464
S  40.386589  31.448011  33.380997
S  43.448914  28.034296  31.658909
S  45.149464  28.205355  37.159153
24 generated by VMD
Ca  25.377739  30.495134  31.968330
Ca  26.263973  30.322582  35.910526
Ca  30.033642  28.196405  35.152546
Ca  30.337364  32.958637  33.463837
Ca  33.442261  29.338266  31.399069
Ca  33.074799  30.477804  35.621033
Ca  36.630665  27.013506  34.659313
Ca  36.84852  31.067394  33.991940
Ca  40.062450  28.717737  31.854134
Ca  39.664413  30.468513  36.556705
Ca  46.190182  25.895700  32.847984
Ca  42.747578  29.822233  34.613232
S  26.928772  26.986647  35.897610
S  27.296112  33.801319  34.908043
S  30.501492  30.011112  32.442368
S  29.727072  31.054180  36.462425
S  33.469349  27.766008  34.084694
S  33.860077  32.516880  32.621689
S  36.706661  28.982010  31.698019
S  36.338547  29.580505  36.806004
S  40.244030  27.325851  34.877636
S  40.438305  31.541832  33.297855
S  43.384975  27.910200  31.652861
S  44.868580  28.140894  37.242847
24 generated by VMD
Ca  25.325661  30.622509  31.754414
Ca  26.362490  30.617020  35.774521
Ca  29.938721  28.248798  35.115997
Ca  30.223639  33.039188  33.562939
|  | Ca       | 25.165731 | 30.737652 | 32.046043 |
|  | Ca       | 26.268280 | 30.726330 | 35.931862 |
|  | Ca       | 29.642506 | 28.397938 | 35.157295 |
|  | Ca       | 30.333687 | 32.980900 | 33.464546 |
|  | Ca       | 33.435154 | 29.091639 | 31.406366 |
|  | Ca       | 33.194984 | 30.164457 | 35.424107 |
|  | Ca       | 36.917461 | 26.791710 | 34.695354 |
|  | Ca       | 36.848217 | 30.825096 | 33.928104 |
|  | Ca       | 40.258369 | 28.596727 | 31.691406 |
|  | Ca       | 39.642242 | 30.560066 | 36.598984 |
|  | Ca       | 46.419907 | 26.216413 | 32.758312 |
|  | Ca       | 42.731110 | 30.115477 | 34.846943 |
|  | S        | 26.254925 | 27.457367 | 35.821262 |
|  | S        | 27.268631 | 33.883266 | 35.002296 |
|  | S        | 30.407946 | 29.782433 | 32.462902 |
|  | S        | 29.931940 | 31.278271 | 36.472404 |
|  | S        | 33.487309 | 27.236595 | 34.133598 |
|  | S        | 33.696793 | 32.319252 | 32.747181 |
|  | S        | 36.702663 | 28.414820 | 31.613535 |
|  | S        | 36.467327 | 29.274805 | 36.720043 |
|  | S        | 40.520031 | 27.348072 | 34.842785 |
|  | S        | 40.336742 | 31.560797 | 33.321808 |
|  | S        | 43.701977 | 28.412966 | 31.665867 |
|  | S        | 44.817284 | 28.218376 | 37.277706 |
| Element | X-coordinate 1 | Y-coordinate 1 | Z-coordinate 1 | X-coordinate 2 | Y-coordinate 2 | Z-coordinate 2 |
|---------|----------------|----------------|----------------|----------------|----------------|----------------|
| Ca      | 25.533587      | 30.607910      | 31.856747      | 26.198208      | 30.780293      | 35.802944      |
| Ca      | 30.141186      | 28.308001      | 35.134743      | 30.445969      | 33.074802      | 33.673958      |
| Ca      | 33.377911      | 28.965425      | 31.708954      | 33.197121      | 30.780293      | 35.448261      |
| Ca      | 36.748425      | 26.504812      | 34.772545      | 36.818825      | 30.889177      | 34.063297      |
| Ca      | 39.962582      | 28.663595      | 36.636553      | 39.702396      | 30.605076      | 36.545052      |
| Ca      | 46.295876      | 26.561596      | 32.603363      | 42.652931      | 29.931303      | 34.814762      |
| S       | 26.584599      | 27.283836      | 35.667973      | 27.027876      | 34.036892      | 34.741871      |
| S       | 30.535517      | 29.929630      | 32.541454      | 29.876499      | 31.179634      | 36.514294      |
| S       | 33.539303      | 27.317709      | 34.230129      | 33.539303      | 27.317709      | 34.230129      |
| S       | 33.807728      | 32.445267      | 32.837170      | 36.734722      | 28.574413      | 31.945116      |
| S       | 36.509666      | 29.217213      | 36.755116      | 36.509666      | 29.217213      | 36.755116      |
| S       | 40.311428      | 27.283564      | 34.759987      | 40.311428      | 27.283564      | 34.759987      |
| S       | 40.245171      | 31.386717      | 33.039238      | 40.245171      | 31.386717      | 33.039238      |
| S       | 43.429317      | 28.170715      | 31.728462      | 43.429317      | 28.170715      | 31.728462      |
| S       | 44.757141      | 28.279396      | 37.208698      | 44.757141      | 28.279396      | 37.208698      |
|   |   |   |
|---|---|---|
| S | 36.664307 | 28.488754 | 31.997120 |
| S | 36.460262 | 29.499281 | 36.759682 |
| S | 40.269691 | 27.348179 | 34.923615 |
| S | 40.530308 | 31.394972 | 33.189468 |
| S | 43.624237 | 28.176435 | 31.605150 |
| S | 45.080532 | 27.956434 | 37.023827 |

24 generated by VMD

| Ca | 25.257189 | 30.050985 | 31.641071 |
| Ca | 26.334494 | 30.870426 | 35.637081 |
| Ca | 30.040632 | 27.931467 | 35.368248 |
| Ca | 33.606339 | 29.616423 | 31.753788 |
| Ca | 32.220543 | 30.269506 | 35.606682 |
| Ca | 36.678288 | 26.942245 | 34.884060 |
| Ca | 36.622238 | 31.040783 | 34.051743 |
| Ca | 40.154518 | 28.647234 | 31.453318 |
| Ca | 43.667568 | 30.468855 | 36.383873 |
| Ca | 46.313530 | 26.123665 | 32.654163 |
| Ca | 42.766655 | 29.919767 | 34.723213 |
| S | 26.442492 | 27.298218 | 35.555248 |
| S | 27.228794 | 33.960541 | 34.462288 |
| S | 30.626671 | 29.925064 | 32.742371 |
| S | 29.854540 | 31.008926 | 36.630131 |
| S | 33.446308 | 27.336637 | 34.310440 |
| S | 33.669762 | 32.770702 | 32.929047 |
| S | 36.628906 | 28.708033 | 31.954865 |
| S | 36.424881 | 29.525888 | 36.795715 |
| S | 40.275860 | 27.278883 | 34.838234 |
| S | 40.272896 | 31.373758 | 32.978809 |
| S | 43.586082 | 28.089579 | 31.681646 |
| S | 44.952568 | 28.097910 | 37.135948 |

24 generated by VMD

| Ca | 25.327425 | 30.621809 | 31.851698 |
| Ca | 26.210855 | 30.450104 | 36.001423 |
| Ca | 29.998764 | 28.212584 | 35.206234 |
| Ca | 30.240232 | 33.218357 | 33.827564 |
| Ca | 33.706120 | 29.521917 | 31.434828 |
| Ca | 33.178654 | 30.298033 | 35.312592 |
| Ca | 36.690449 | 26.618773 | 34.839493 |
| Ca | 36.818386 | 31.127169 | 33.712139 |
| Ca | 40.162914 | 28.586632 | 31.637476 |
| Ca | 39.863365 | 30.692287 | 36.560810 |
| Ca | 46.382828 | 26.128506 | 33.012424 |
| Ca | 42.776440 | 29.992794 | 34.796852 |
|   |   |   |   |
|---|---|---|---|
| S | 26.652794 | 27.200603 | 35.768303 |
| S | 26.859196 | 33.834610 | 34.860085 |
| S | 30.552643 | 30.050432 | 32.588047 |
| S | 29.739182 | 30.952160 | 36.660633 |
| S | 33.395676 | 27.421442 | 33.991261 |
| S | 33.656998 | 32.593231 | 32.617310 |
| S | 36.731678 | 28.449263 | 31.953598 |
| S | 36.434238 | 29.707190 | 36.565029 |
| S | 40.295345 | 27.327698 | 35.012405 |
| S | 40.379044 | 31.326803 | 33.066158 |
| S | 43.469002 | 28.054968 | 31.692957 |
| S | 44.911629 | 28.004036 | 37.061386 |

24

generated by VMD

| Ca | 24.935371 | 30.354189 | 31.831469 |
| Ca | 26.486471 | 30.413954 | 35.738583 |
| Ca | 30.021713 | 28.177879 | 35.232135 |
| Ca | 30.324730 | 30.059944 | 33.899021 |
| Ca | 33.837677 | 29.935339 | 31.331726 |
| Ca | 33.180855 | 30.600628 | 35.311668 |
| Ca | 36.767845 | 26.759190 | 34.981876 |
| Ca | 36.770355 | 30.870243 | 33.839973 |
| Ca | 40.149391 | 28.584463 | 31.676279 |
| Ca | 39.673325 | 30.695560 | 36.442623 |
| Ca | 46.104034 | 25.897219 | 32.803429 |
| Ca | 42.774677 | 30.010355 | 34.758617 |

24

generated by VMD

| Ca | 25.037025 | 29.909935 | 31.969484 |
| Ca | 26.250929 | 30.358578 | 35.907352 |
| Ca | 29.986391 | 28.190691 | 35.372467 |
| Ca | 29.973484 | 32.950394 | 33.472183 |
| Ca | 33.445343 | 29.829227 | 31.337208 |
| Ca | 33.009155 | 30.650188 | 35.374561 |
|   |   |   |
|---|---|---|
|Ca | 37.056458 | 27.330601 | 35.046841 |
|Ca | 36.709847 | 31.525772 | 33.971573 |
|Ca | 40.323204 | 30.589549 | 36.345318 |
|Ca | 46.315548 | 25.642288 | 32.578407 |
|Ca | 43.060165 | 29.366427 | 34.748123 |
|S  | 26.773594 | 27.039103 | 35.877880 |
|S  | 26.714884 | 33.699494 | 34.605850 |
|S  | 30.510876 | 29.895214 | 32.545525 |
|S  | 29.714106 | 31.272242 | 36.526619 |
|S  | 33.565517 | 27.672609 | 34.009243 |
|S  | 33.654339 | 32.816605 | 32.736137 |
|S  | 36.799416 | 28.867292 | 32.052780 |
|S  | 36.290108 | 29.892488 | 36.770031 |
|S  | 40.455372 | 27.236086 | 34.890644 |
|S  | 40.731365 | 31.453972 | 33.610985 |
|S  | 43.615677 | 28.286867 | 31.559061 |
|S  | 44.606976 | 27.190393 | 37.100563 |

24 generated by VMD

|   |   |   |
|---|---|---|
|Ca | 25.163231 | 29.958309 | 31.935661 |
|Ca | 26.315964 | 30.728012 | 35.661083 |
|Ca | 30.041464 | 27.875286 | 35.335159 |
|Ca | 30.196329 | 32.982170 | 33.851883 |
|Ca | 33.757538 | 30.277586 | 31.483013 |
|Ca | 33.091255 | 30.359573 | 35.400772 |
|Ca | 36.762707 | 26.868202 | 34.999832 |
|Ca | 36.851933 | 31.162243 | 33.927269 |
|Ca | 40.374886 | 28.404177 | 31.907047 |
|Ca | 39.786293 | 30.604563 | 36.597931 |
|Ca | 46.254562 | 26.065256 | 32.476498 |
|Ca | 42.744511 | 29.834465 | 34.580219 |
|S  | 26.722567 | 27.152065 | 35.957859 |
|S  | 27.172756 | 33.830574 | 34.147331 |
|S  | 30.481062 | 29.898647 | 32.465107 |
|S  | 29.921637 | 30.898384 | 36.568737 |
|S  | 33.413555 | 27.593260 | 33.998356 |
|S  | 33.702274 | 33.025536 | 32.986877 |
|S  | 36.772850 | 28.589838 | 32.208252 |
|S  | 36.205814 | 29.632868 | 36.823784 |
|S  | 40.112022 | 27.282707 | 35.217781 |
|S  | 40.459862 | 31.418417 | 33.224045 |
|S  | 43.532455 | 28.238274 | 31.499783 |
|S  | 44.596489 | 27.711000 | 36.776367 |

24 generated by VMD
| Ca    | 25.031748 | 29.934032 | 32.287201 |
| Ca    | 26.382889 | 30.592445 | 35.944492 |
| Ca    | 30.230211 | 28.084896 | 35.109180 |
| Ca    | 30.125847 | 33.197708 | 33.766541 |
| Ca    | 33.586067 | 29.943092 | 31.484253 |
| Ca    | 33.220291 | 30.489896 | 35.109180 |
| Ca    | 36.831093 | 26.727898 | 34.904156 |
| Ca    | 36.934414 | 30.709394 | 33.766914 |
| Ca    | 40.163048 | 28.694483 | 31.468227 |
| Ca    | 39.619106 | 30.789991 | 36.397984 |
| Ca    | 46.240063 | 26.289444 | 32.939739 |
| Ca    | 42.758480 | 29.677454 | 34.976582 |
| S     | 26.733980 | 27.044106 | 35.933674 |
| S     | 26.905600 | 33.956013 | 34.563576 |
| S     | 30.583401 | 30.201063 | 32.484024 |
| S     | 29.979910 | 31.082041 | 36.528847 |
| S     | 33.539066 | 27.592245 | 33.827633 |
| S     | 33.875576 | 32.910294 | 32.821583 |
| S     | 36.703167 | 28.267315 | 31.887693 |
| S     | 36.363220 | 29.492716 | 36.637154 |
| S     | 40.276398 | 27.303709 | 34.698002 |
| S     | 40.439777 | 31.454458 | 33.095600 |
| S     | 43.441605 | 28.262465 | 31.838184 |
| S     | 44.468994 | 27.694317 | 37.341522 |

24 generated by VMD

| Ca    | 25.469534 | 30.010633 | 32.052994 |
| Ca    | 26.372667 | 30.707481 | 35.966358 |
| Ca    | 30.267107 | 27.947451 | 35.203304 |
| Ca    | 30.167789 | 33.391243 | 33.817322 |
| Ca    | 33.451698 | 29.954487 | 31.462072 |
| Ca    | 33.188602 | 30.186335 | 35.430538 |
| Ca    | 36.710583 | 26.739330 | 34.716606 |
| Ca    | 36.711922 | 30.868382 | 33.679882 |
| Ca    | 40.175533 | 28.858578 | 31.669125 |
| Ca    | 39.763824 | 30.757748 | 36.573067 |
| Ca    | 46.084126 | 25.751965 | 32.776665 |
| Ca    | 42.861134 | 29.782225 | 34.792072 |
| S     | 26.508568 | 27.260386 | 36.147408 |
| S     | 26.801390 | 33.821079 | 34.347519 |
| S     | 30.516722 | 30.067459 | 32.544903 |
| S     | 29.896673 | 30.909399 | 36.507313 |
| S     | 33.578342 | 27.406275 | 33.868347 |
| S     | 33.698227 | 32.887859 | 32.926121 |
| S     | 36.659824 | 28.469475 | 31.706482 |
| S     | 36.390999 | 29.631868 | 36.627796 |
| S      | 40.220585 | 27.359787 | 34.692726 |
|--------|-----------|-----------|-----------|
| S      | 40.576260 | 31.428070 | 33.405563 |
| S      | 43.493164 | 28.134085 | 31.839216 |
| S      | 44.868572 | 28.059834 | 37.277390 |

24

generated by VMD

| Ca     | 24.888588 | 30.101137 | 32.273914 |
|--------|-----------|-----------|-----------|
| Ca     | 26.057297 | 30.695885 | 35.774963 |
| Ca     | 29.966400 | 28.175617 | 35.137909 |
| Ca     | 30.342510 | 32.864918 | 33.485058 |
| Ca     | 33.667477 | 29.712254 | 31.590307 |
| Ca     | 33.276291 | 30.435459 | 35.355022 |
| Ca     | 36.681664 | 26.914417 | 34.758930 |
| Ca     | 36.857616 | 30.894955 | 34.197437 |
| Ca     | 40.332077 | 28.594189 | 31.539988 |
| Ca     | 39.577309 | 30.555418 | 36.706177 |
| Ca     | 46.257679 | 26.161705 | 32.878780 |
| Ca     | 42.651394 | 29.796844 | 34.778557 |
| S      | 26.660419 | 27.309124 | 35.830242 |
| S      | 27.218386 | 33.765823 | 34.818691 |
| S      | 30.503445 | 29.943632 | 32.412003 |
| S      | 29.675104 | 31.111113 | 36.391113 |
| S      | 33.581203 | 27.664547 | 34.098083 |
| S      | 33.867123 | 32.717518 | 32.738682 |
| S      | 36.808838 | 28.658411 | 31.814325 |
| S      | 36.334106 | 29.512842 | 36.863213 |
| S      | 40.237656 | 27.166037 | 34.777653 |
| S      | 40.398724 | 31.414658 | 33.153561 |
| S      | 43.729595 | 28.251062 | 31.560867 |
| S      | 44.862881 | 27.973827 | 37.095219 |

24

generated by VMD

| Ca     | 25.201193 | 29.910109 | 32.195972 |
|--------|-----------|-----------|-----------|
| Ca     | 26.367943 | 30.725906 | 36.049545 |
| Ca     | 30.221973 | 28.167297 | 35.403633 |
| Ca     | 30.183130 | 33.120838 | 33.638381 |
| Ca     | 33.610386 | 29.961010 | 31.164520 |
| Ca     | 33.133041 | 30.545822 | 35.518909 |
| Ca     | 36.968410 | 26.560606 | 34.596283 |
| Ca     | 36.695538 | 30.683136 | 33.695107 |
| Ca     | 39.968830 | 28.790981 | 31.607929 |
| Ca     | 39.700729 | 30.813501 | 36.647667 |
| Ca     | 46.243587 | 26.061945 | 32.971909 |
| Ca     | 42.695015 | 29.820612 | 34.928333 |
| S      | 26.845318 | 27.328737 | 36.064392 |
| S      | 26.918171 | 33.772385 | 34.545929 |
|   |     |     |     |
|---|-----|-----|-----|
| S | 30.592390 | 30.107687 | 32.577606 |
| S | 29.800890 | 31.058352 | 36.429352 |
| S | 33.596409 | 27.719875 | 33.82079 |
| S | 33.768150 | 32.897892 | 32.922398 |
| S | 36.715027 | 28.348324 | 31.497917 |
| S | 36.347702 | 29.288290 | 36.491676 |
| S | 40.330868 | 31.11284 | 34.880276 |
| S | 40.432384 | 31.411388 | 33.256279 |
| S | 43.490986 | 28.257391 | 31.766603 |
| S | 44.605816 | 27.828037 | 37.362526 |

24 generated by VMD

| Ca       |     |     |     |
|----------|-----|-----|-----|
| Ca       | 25.356827 | 29.810890 | 31.867336 |
| Ca       | 26.471159 | 30.855585 | 35.903866 |
| Ca       | 30.405384 | 28.111835 | 35.231941 |
| Ca       | 30.039839 | 32.943439 | 33.758816 |
| Ca       | 33.353539 | 29.843208 | 31.322510 |
| Ca       | 33.173756 | 30.620161 | 35.462177 |
| Ca       | 37.012047 | 26.675613 | 34.861328 |
| Ca       | 36.723717 | 30.926317 | 34.102154 |
| Ca       | 39.946411 | 28.702810 | 31.889025 |
| Ca       | 39.726627 | 30.296103 | 36.728935 |
| Ca       | 46.256081 | 26.024891 | 32.698997 |
| Ca       | 42.801929 | 30.047077 | 34.581741 |
| S       | 26.845200 | 27.383709 | 35.934242 |
| S       | 26.646730 | 33.960911 | 34.281315 |
| S       | 30.560347 | 29.910908 | 32.538662 |
| S       | 30.105938 | 31.124126 | 36.49332 |
| S       | 33.704624 | 27.742216 | 33.917831 |
| S       | 33.797993 | 32.897957 | 33.085133 |
| S       | 36.601128 | 28.569571 | 31.614273 |
| S       | 36.328026 | 29.290829 | 36.770897 |
| S       | 40.281807 | 27.139986 | 34.996651 |
| S       | 40.289894 | 31.451849 | 33.271538 |
| S       | 43.393341 | 28.225189 | 31.724049 |
| S       | 44.611568 | 27.836231 | 36.987896 |

24 generated by VMD

| Ca       |     |     |     |
|----------|-----|-----|-----|
| Ca       | 25.605593 | 29.772970 | 31.698769 |
| Ca       | 26.337219 | 30.640808 | 35.798317 |
| Ca       | 30.265131 | 28.000702 | 35.214588 |
| Ca       | 30.092508 | 32.966022 | 33.475990 |
| Ca       | 33.561668 | 30.020996 | 31.420292 |
| Ca       | 33.021027 | 30.526535 | 35.523106 |
| Ca       | 36.973698 | 27.048214 | 35.067265 |
| Ca       | 36.685940 | 31.324308 | 34.004017 |
|   |       |       |       |
|---|-------|-------|-------|
| Ca| 40.034401 | 28.763182 | 31.839668 |
| Ca| 39.971199 | 30.392355 | 36.868900 |
| Ca| 45.968853 | 25.790876 | 32.139854 |
| Ca| 42.942047 | 29.704523 | 34.736649 |
| S | 26.867096 | 27.215921 | 35.847916 |
| S | 26.772346 | 33.809376 | 34.393177 |
| S | 30.569582 | 29.937466 | 32.578815 |
| S | 29.850201 | 31.118198 | 36.385796 |
| S | 33.621098 | 27.570990 | 34.100483 |
| S | 33.490398 | 32.933815 | 33.057396 |
| S | 36.522236 | 28.662291 | 32.052326 |
| S | 36.479160 | 29.836189 | 36.760105 |
| S | 40.322113 | 27.279640 | 35.088364 |
| S | 40.302860 | 31.529030 | 33.502758 |
| S | 43.254833 | 27.942911 | 31.612347 |
| S | 44.922688 | 27.604040 | 36.863869 |
|   | generated by VMD |       |       |
| Ca| 25.583473 | 29.233238 | 32.095669 |
| Ca| 26.048014 | 30.733839 | 35.551445 |
| Ca| 30.352144 | 28.089882 | 35.534241 |
| Ca| 30.341764 | 33.116051 | 33.643387 |
| Ca| 33.428371 | 30.032000 | 31.466391 |
| Ca| 33.259453 | 30.468267 | 35.251968 |
| Ca| 37.047760 | 27.022131 | 34.968105 |
| Ca| 36.884548 | 31.027990 | 34.164711 |
| Ca| 39.926537 | 28.903976 | 31.648878 |
| Ca| 39.711914 | 30.398199 | 37.022518 |
| Ca| 45.930855 | 25.718266 | 32.095486 |
| Ca| 42.885120 | 29.861506 | 34.841522 |
| S | 26.780617 | 27.328077 | 36.032894 |
| S | 27.050047 | 33.821873 | 33.924400 |
| S | 30.574162 | 29.997654 | 32.671669 |
| S | 29.859087 | 31.205795 | 36.484650 |
| S | 33.534496 | 27.480976 | 34.034142 |
| S | 33.787727 | 32.894730 | 32.927467 |
| S | 36.546040 | 28.809763 | 31.796438 |
| S | 36.385323 | 29.539896 | 36.820290 |
| S | 40.376518 | 27.448280 | 34.873276 |
| S | 40.252071 | 31.604048 | 33.641296 |
| S | 43.412018 | 28.296719 | 31.537046 |
| S | 44.475807 | 27.358219 | 37.002819 |
|   | generated by VMD |       |       |
| Ca| 25.538731 | 29.594837 | 31.777897 |
| Ca| 26.024366 | 30.697117 | 35.747402 |
| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 30.279032 | 28.077047 | 35.376472 |
| Ca      | 30.331184 | 33.111710 | 33.891136 |
| Ca      | 33.547523 | 29.975050 | 31.427444 |
| Ca      | 33.175327 | 30.432581 | 35.434616 |
| Ca      | 36.820675 | 27.041822 | 34.937405 |
| Ca      | 36.820332 | 31.208618 | 33.991119 |
| Ca      | 40.307484 | 28.486053 | 31.712187 |
| Ca      | 39.763500 | 30.469910 | 36.604759 |
| Ca      | 45.737545 | 25.819153 | 32.324001 |
| Ca      | 42.847309 | 29.822584 | 34.724300 |
| S       | 27.052580 | 27.136694 | 35.931328 |
| S       | 26.915955 | 33.861553 | 34.401669 |
| S       | 30.530254 | 30.141520 | 32.653915 |
| S       | 29.830351 | 31.024271 | 36.704132 |
| S       | 33.416893 | 27.567148 | 34.080715 |
| S       | 33.726177 | 32.844818 | 32.689610 |
| S       | 36.807545 | 28.745916 | 31.880009 |
| S       | 36.209820 | 29.618988 | 36.727585 |
| S       | 40.192722 | 27.378342 | 35.069115 |
| S       | 40.466396 | 31.340197 | 33.300259 |
| S       | 43.644421 | 28.310127 | 31.503475 |
| S       | 44.447811 | 27.685368 | 37.140217 |

24 generated by VMD

| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 25.357464 | 29.917858 | 31.973537 |
| Ca      | 26.147125 | 30.631790 | 35.797501 |
| Ca      | 30.327694 | 27.807089 | 35.354340 |
| Ca      | 30.222090 | 33.218281 | 33.498547 |
| Ca      | 33.497314 | 29.965195 | 31.517036 |
| Ca      | 33.137936 | 30.343542 | 35.517338 |
| Ca      | 36.956234 | 26.879459 | 35.036942 |
| Ca      | 36.835014 | 31.181313 | 33.836502 |
| Ca      | 40.151386 | 28.675919 | 31.924620 |
| Ca      | 39.823734 | 30.297998 | 36.615765 |
| Ca      | 45.971230 | 25.919106 | 32.373264 |
| Ca      | 43.095211 | 29.933998 | 34.672176 |
| S       | 26.824234 | 27.302374 | 35.712383 |
| S       | 26.768801 | 33.887943 | 34.385628 |
| S       | 30.501740 | 30.151020 | 32.648415 |
| S       | 29.861643 | 31.082653 | 36.527065 |
| S       | 33.400639 | 27.382215 | 34.144245 |
| S       | 33.649670 | 32.939178 | 32.833157 |
| S       | 36.597839 | 28.543127 | 31.921715 |
| S       | 36.388954 | 29.611145 | 36.695652 |
| S       | 40.229599 | 27.239725 | 34.906509 |
| S       | 40.394318 | 31.474077 | 33.386822 |
|   |        |        |        |
|---|--------|--------|--------|
| S | 43.540443 | 28.213789 | 31.598341 |
| S | 44.753494 | 27.792585 | 37.153130 |

24

generated by VMD

|   |        |        |        |
|---|--------|--------|--------|
| Ca | 25.459278 | 29.817200 | 31.845112 |
| Ca | 26.143888 | 30.653622 | 35.511757 |
| Ca | 30.304665 | 28.116669 | 35.367123 |
| Ca | 30.234152 | 33.152607 | 33.632362 |
| Ca | 33.603580 | 29.526163 | 31.551752 |
| Ca | 33.208694 | 30.675283 | 35.632854 |
| Ca | 36.800400 | 27.176302 | 35.153816 |
| Ca | 36.908367 | 30.951090 | 34.129845 |
| Ca | 40.168846 | 28.744699 | 31.706226 |
| Ca | 39.806408 | 30.284611 | 36.747177 |
| Ca | 45.985920 | 25.895967 | 32.082947 |
| Ca | 42.729412 | 29.848825 | 34.659718 |
| S  | 26.545660 | 27.142719 | 35.641464 |
| S  | 26.802313 | 33.836533 | 34.416553 |
| S  | 30.616880 | 29.974714 | 32.630630 |
| S  | 29.615913 | 31.032635 | 36.525124 |
| S  | 33.704426 | 27.806816 | 34.355850 |
| S  | 33.811573 | 32.744892 | 32.798599 |
| S  | 36.790901 | 28.661835 | 31.993660 |
| S  | 36.307598 | 29.655588 | 37.065182 |
| S  | 40.257996 | 27.289286 | 34.775948 |
| S  | 40.414680 | 31.577490 | 33.308670 |
| S  | 43.480801 | 28.089468 | 31.429626 |
| S  | 44.731510 | 27.736395 | 37.068748 |

24

generated by VMD

|   |        |        |        |
|---|--------|--------|--------|
| Ca | 25.624832 | 30.002562 | 31.769354 |
| Ca | 26.458685 | 30.696808 | 35.760818 |
| Ca | 30.229158 | 27.847677 | 35.419922 |
| Ca | 30.137432 | 33.052475 | 33.445202 |
| Ca | 33.515194 | 29.833616 | 31.393316 |
| Ca | 33.091343 | 30.397932 | 35.577801 |
| Ca | 36.763752 | 27.075684 | 34.850765 |
| Ca | 36.715378 | 31.100698 | 33.991871 |
| Ca | 40.289917 | 28.639009 | 31.926622 |
| Ca | 39.936131 | 30.249752 | 36.912113 |
| Ca | 46.127396 | 25.923721 | 32.018135 |
| Ca | 42.672970 | 29.843237 | 34.736340 |
| S  | 26.591888 | 27.358612 | 36.118195 |
| S  | 27.056969 | 33.881290 | 34.520931 |
| S  | 30.495407 | 29.911097 | 32.559460 |
| S  | 29.832214 | 30.915310 | 36.484001 |
|   |    |    |    |
|---|----|----|----|
| S | 33.479355 | 27.569330 | 34.007248 |
| S | 33.687611 | 32.866169 | 32.654 |
| S | 36.747852 | 28.523434 | 31.817131 |
| S | 36.216557 | 29.842964 | 36.867535 |
| S | 40.284565 | 27.318033 | 35.010284 |
| S | 40.164703 | 31.544163 | 33.456547 |
| S | 43.604733 | 28.271015 | 31.564741 |
| S | 44.709835 | 27.726782 | 37.167408 |

24

generated by VMD

| Ca | 25.356129 | 29.954842 | 32.072075 |
| Ca | 26.514526 | 30.836397 | 35.994068 |
| Ca | 30.630648 | 27.931070 | 35.322853 |
| Ca | 30.391714 | 32.868965 | 33.526443 |
| Ca | 33.418175 | 29.805706 | 30.988293 |
| Ca | 33.244663 | 30.506161 | 35.346561 |
| Ca | 36.755993 | 26.805265 | 34.904335 |
| Ca | 36.763729 | 31.009981 | 33.853134 |
| Ca | 40.110569 | 28.611826 | 31.815546 |
| Ca | 39.754833 | 30.315886 | 36.864033 |
| Ca | 46.060551 | 26.323158 | 32.365601 |
| Ca | 42.521671 | 29.760111 | 34.819412 |
| S | 27.005371 | 27.248743 | 35.935814 |
| S | 27.046984 | 34.038307 | 34.823704 |
| S | 30.502689 | 29.840645 | 32.576515 |
| S | 29.939833 | 31.023207 | 36.488468 |
| S | 33.459427 | 27.600319 | 33.861691 |
| S | 33.877918 | 32.733891 | 32.609692 |
| S | 36.561489 | 28.537960 | 31.641899 |
| S | 36.361034 | 29.703852 | 36.610550 |
| S | 40.073730 | 27.295994 | 35.067440 |
| S | 40.307068 | 31.456263 | 33.423805 |
| S | 43.517799 | 28.487686 | 31.648464 |
| S | 44.257305 | 27.695192 | 37.470318 |

24

generated by VMD

| Ca | 25.170172 | 30.115414 | 32.143200 |
| Ca | 26.334538 | 30.663473 | 36.096748 |
| Ca | 29.946791 | 28.214256 | 35.404430 |
| Ca | 30.158035 | 32.911987 | 33.438305 |
| Ca | 33.655003 | 29.791536 | 31.163868 |
| Ca | 33.243587 | 30.460590 | 35.290424 |
| Ca | 36.795071 | 26.792399 | 34.967487 |
| Ca | 36.728611 | 31.149538 | 33.776440 |
| Ca | 40.199791 | 28.592365 | 31.726660 |
| Ca | 39.862671 | 30.193699 | 36.855549 |
|   |   |   |   |
|---|---|---|---|
|Ca | 45.915249 | 26.083807 | 32.598305 |
|Ca | 42.978439 | 29.863735 | 34.656792 |
|S  | 26.913939 | 27.147358 | 35.793106 |
|S  | 27.007170 | 33.716038 | 34.703968 |
|S  | 30.523552 | 29.885517 | 32.594574 |
|S  | 29.901417 | 31.152073 | 36.604046 |
|S  | 33.409325 | 27.614363 | 33.888020 |
|S  | 33.816246 | 32.899117 | 32.633965 |
|S  | 36.738510 | 28.609711 | 31.810904 |
|S  | 36.414848 | 29.580709 | 36.552170 |
|S  | 40.260704 | 27.314150 | 34.849770 |
|S  | 40.353031 | 31.482628 | 33.327030 |
|S  | 43.601570 | 28.379286 | 31.565224 |
|S  | 44.505650 | 27.800781 | 37.589676 |
|24 | Generated by VMD |

|   |   |   |   |
|---|---|---|---|
|Ca | 25.523193 | 30.351118 | 31.837475 |
|Ca | 26.410431 | 30.657526 | 36.294712 |
|Ca | 30.346113 | 28.085835 | 35.316910 |
|Ca | 30.164867 | 32.845097 | 33.722038 |
|Ca | 33.490707 | 29.893803 | 30.967329 |
|Ca | 33.190632 | 30.538168 | 35.116310 |
|Ca | 36.960720 | 26.850416 | 34.803574 |
|Ca | 36.640396 | 31.137226 | 33.443439 |
|Ca | 40.034164 | 28.487398 | 31.833506 |
|Ca | 39.781319 | 29.817274 | 36.924847 |
|Ca | 46.387714 | 26.277325 | 32.723671 |
|Ca | 42.930965 | 29.800528 | 34.878468 |
|S  | 27.144381 | 27.178766 | 36.005348 |
|S  | 26.863522 | 33.805069 | 34.860050 |
|S  | 30.378963 | 30.008887 | 32.678333 |
|S  | 29.774660 | 31.085562 | 36.663166 |
|S  | 33.415455 | 27.629105 | 33.823219 |
|S  | 33.454971 | 32.869915 | 32.345909 |
|S  | 36.607914 | 28.578161 | 31.696245 |
|S  | 36.527775 | 29.890448 | 36.451939 |
|S  | 40.174221 | 27.159912 | 34.944874 |
|S  | 40.157066 | 31.343781 | 33.522018 |
|S  | 43.472549 | 28.226803 | 31.841866 |
|S  | 44.601116 | 27.881290 | 37.335495 |

24 generated by VMD
| Element | Value 1     | Value 2     | Value 3     |
|---------|------------|------------|------------|
| Ca      | 33.50679   | 29.853153  | 30.778187  |
| Ca      | 33.134060  | 30.537069  | 35.479279  |
| Ca      | 36.726730  | 27.055307  | 34.866150  |
| Ca      | 36.563515  | 31.009382  | 33.985363  |
| Ca      | 40.106468  | 28.608952  | 31.788092  |
| Ca      | 39.691338  | 29.863539  | 37.019318  |
| Ca      | 46.403481  | 26.312466  | 32.235653  |
| Ca      | 42.945202  | 29.751534  | 34.710197  |
| S       | 26.661499  | 27.266184  | 35.966164  |
| S       | 26.843979  | 33.672951  | 34.470894  |
| S       | 30.706501  | 29.959799  | 32.714306  |
| S       | 30.015322  | 31.193583  | 36.762650  |
| S       | 33.218884  | 27.617247  | 33.857067  |
| S       | 33.627476  | 32.727047  | 32.523224  |
| S       | 36.653313  | 28.415081  | 31.647593  |
| S       | 36.229340  | 29.687195  | 36.752602  |
| S       | 40.232635  | 27.116177  | 35.024471  |
| S       | 40.168289  | 31.388374  | 33.636688  |
| S       | 43.605690  | 28.205238  | 31.707277  |
| S       | 44.985775  | 28.080585  | 37.112686  |

24 generated by VMD

| Element | Value 1     | Value 2     | Value 3     |
|---------|------------|------------|------------|
| Ca      | 25.831177  | 30.342962  | 31.502035  |
| Ca      | 26.175554  | 30.839048  | 36.267715  |
| Ca      | 30.143139  | 27.943607  | 35.440308  |
| Ca      | 30.167721  | 33.026241  | 33.682541  |
| Ca      | 33.755535  | 29.734201  | 31.428738  |
| Ca      | 33.073021  | 30.216856  | 35.338139  |
| Ca      | 36.709629  | 26.615602  | 35.089611  |
| Ca      | 36.802414  | 31.049273  | 33.722809  |
| Ca      | 40.156193  | 28.393158  | 31.796160  |
| Ca      | 39.698891  | 30.051588  | 36.762447  |
| Ca      | 46.042751  | 25.947422  | 32.182144  |
| Ca      | 43.173309  | 30.387278  | 34.699276  |
| S       | 26.722454  | 27.378725  | 36.024059  |
| S       | 26.816448  | 33.870037  | 34.590546  |
| S       | 30.553822  | 30.050467  | 32.625881  |
| S       | 29.825958  | 31.140387  | 36.588066  |
| S       | 33.223824  | 27.427872  | 33.892071  |
| S       | 33.662582  | 32.861858  | 32.608910  |
| S       | 36.888020  | 28.260134  | 31.914932  |
| S       | 36.248192  | 29.688915  | 36.541836  |
| S       | 40.146751  | 27.209862  | 35.093185  |
| S       | 40.077919  | 31.257055  | 33.488178  |
| S       | 43.754017  | 28.559349  | 31.545422  |
| S       | 44.784588  | 28.139492  | 37.205715  |
| Element | Z1   | Z2   | Z3   |
|---------|------|------|------|
| Ca      | 25.247997 | 30.478725 | 31.660416 |
| Ca      | 26.500324 | 30.549927 | 36.046753 |
| Ca      | 30.034241 | 28.233232 | 35.174633 |
| Ca      | 30.113298 | 33.065384 | 33.621529 |
| Ca      | 33.575924 | 29.761826 | 31.303953 |
| Ca      | 33.270958 | 30.206661 | 35.323303 |
| Ca      | 36.657547 | 27.029343 | 35.090496 |
| Ca      | 36.731030 | 30.982498 | 33.789669 |
| Ca      | 40.229542 | 28.379078 | 31.811670 |
| Ca      | 39.902424 | 29.954113 | 36.828503 |
| Ca      | 46.289513 | 26.141661 | 32.362366 |
| Ca      | 42.803993 | 30.122154 | 34.763927 |
| S       | 26.684160 | 27.341318 | 35.702568 |
| S       | 26.907257 | 33.648392 | 34.755856 |
| S       | 30.461229 | 30.069206 | 32.532459 |
| S       | 30.079288 | 31.168856 | 36.506798 |
| S       | 33.349575 | 27.305361 | 34.024044 |
| S       | 33.652042 | 28.719685 | 32.852154 |
| S       | 36.711254 | 28.334625 | 31.984226 |
| S       | 36.375359 | 29.801414 | 36.787594 |
| S       | 40.122364 | 27.230103 | 35.144821 |
| S       | 40.338596 | 31.329687 | 33.300514 |
| S       | 43.458363 | 28.188417 | 31.567738 |
| S       | 44.937641 | 28.349754 | 37.094765 |

24 generated by VMD

| Element | Z1   | Z2   | Z3   |
|---------|------|------|------|
| Ca      | 25.825594 | 30.463505 | 31.365934 |
| Ca      | 26.514267 | 30.244184 | 36.000191 |
| Ca      | 30.235273 | 28.172140 | 35.064503 |
| Ca      | 30.092676 | 33.158882 | 33.762054 |
| Ca      | 33.496170 | 29.843426 | 31.494164 |
| Ca      | 33.296120 | 30.406061 | 35.348469 |
| Ca      | 36.638672 | 27.124817 | 35.060543 |
| Ca      | 36.823669 | 31.167767 | 33.638786 |
| Ca      | 39.853115 | 28.681084 | 32.041119 |
| Ca      | 39.960537 | 30.075478 | 37.036537 |
| Ca      | 45.893997 | 25.930805 | 32.338081 |
| Ca      | 42.948360 | 29.817646 | 34.350780 |
| S       | 27.041340 | 26.910032 | 36.177898 |
| S       | 26.702312 | 33.630280 | 34.522030 |
| S       | 30.480919 | 30.034483 | 32.545914 |
| S       | 29.897289 | 31.124632 | 36.691196 |
| S       | 33.326519 | 27.542606 | 33.844818 |
| S       | 33.563141 | 32.834057 | 32.787960 |
|    | 36.715652 | 28.731253 | 31.781273 |
|----|-----------|------------|------------|
| S  | 36.505466 | 29.973543  | 36.678936  |
| S  | 40.291138 | 27.201029  | 35.190025  |
| S  | 40.362053 | 31.423216  | 33.467560  |
| S  | 43.235050 | 27.741198  | 31.724611  |
| S  | 44.734512 | 28.159264  | 37.117332  |

24 generated by VMD

| Ca | 25.505762 | 30.196945 | 31.468323 |
|----|-----------|------------|------------|
| Ca | 26.297840 | 30.479862  | 35.971157  |
| Ca | 30.015484 | 28.170517  | 35.061565  |
| Ca | 30.127077 | 33.160091  | 33.894085  |
| Ca | 33.015484 | 29.971634  | 31.387386  |
| Ca | 33.110729 | 30.566320  | 35.363918  |
| Ca | 36.666790 | 26.970554  | 30.015018  |
| Ca | 36.730556 | 30.903952  | 33.668297  |
| Ca | 40.315937 | 28.521816  | 31.789112  |
| Ca | 39.966179 | 29.899210  | 36.694916  |
| Ca | 46.268005 | 25.880146  | 32.707664  |
| Ca | 43.012337 | 29.896376  | 34.685143  |

| S  | 26.701630 | 27.141171  | 36.147190  |
|----|-----------|------------|------------|
| S  | 26.661943 | 33.738094  | 34.773266  |
| S  | 30.468325 | 30.247536  | 32.514851  |
| S  | 29.743206 | 31.037838  | 36.610340  |
| S  | 33.348007 | 27.577190  | 33.968964  |
| S  | 33.684170 | 32.890255  | 32.797325  |
| S  | 36.720879 | 28.351952  | 32.853170  |
| S  | 36.372242 | 29.847683  | 36.770012  |
| S  | 40.011406 | 27.194159  | 34.846478  |
| S  | 40.233864 | 31.220217  | 33.342064  |
| S  | 43.642857 | 28.082542  | 31.704689  |
| S  | 45.256985 | 28.439810  | 36.995831  |

24 generated by VMD

| Ca | 25.620705 | 30.441294  | 31.281734  |
|----|-----------|------------|------------|
| Ca | 26.432552 | 30.471050  | 35.889427  |
| Ca | 29.986940 | 28.248978  | 35.312691  |
| Ca | 30.475712 | 33.044659  | 33.811020  |
| Ca | 33.577812 | 29.744713  | 31.476873  |
| Ca | 33.313766 | 30.475426  | 35.363445  |
| Ca | 36.730400 | 26.805542  | 35.015152  |
| Ca | 36.851097 | 30.844202  | 33.672398  |
| Ca | 39.909679 | 28.285227  | 31.671326  |
| Ca | 39.822495 | 30.110298  | 36.850758  |
| Ca | 45.773201 | 26.238716  | 32.329266  |
| Ca | 42.854458 | 30.069427  | 34.780048  |
|     | S        | Ca       | S        | Ca       |
|-----|----------|----------|----------|----------|
| 24  | 26.829573| 25.862217| 27.115067| 30.258698|
|     | 27.012383| 25.982590| 33.615334| 30.545559|
|     | 30.463074| 30.089165| 31.094227| 28.214022|
|     | 30.378208| 30.291821| 34.719761| 33.473629|
|     | 33.863461| 33.622948| 32.830002| 29.761530|
|     | 36.599499| 33.173252| 31.80716| 30.206354|
|     | 36.341606| 36.757683| 36.148468| 36.000591|
|     | 40.153473| 36.694397| 33.768688| 28.508081|
|     | 40.213341| 40.243786| 31.836267| 30.218311|
|     | 43.338737| 46.106781| 32.254929| 26.210676|
|     | 44.972065| 42.918045| 34.647797| 29.946854|
|     | 44.972065| 26.895355| 35.984871| 26.988459|
|     | 46.106781| 26.852943| 34.862595| 33.917118|
|     | 44.849686| 30.536148| 32.530521| 30.235620|
|     | 43.487221| 29.850929| 36.387760| 31.231190|
|     | 40.159517| 33.256649| 34.121109| 27.348104|
|     | 33.596172| 33.706287| 32.688400| 32.689713|
|     | 33.152888| 36.645912| 32.101612| 28.243551|
|     | 36.344738| 28.819817| 36.688324| 29.819817|
|     | 40.315971| 40.105915| 35.216541| 27.114084|
|     | 43.487221| 43.487221| 31.585880| 28.409014|
|     | 44.849686| 44.849686| 37.077301| 28.017664|

generated by VMD
|   |   |   |
|---|---|---|
| Ca | 36.764179 | 26.935291 | 34.969826 |
| Ca | 36.767277 | 31.323439 | 33.572189 |
| Ca | 39.747921 | 29.864687 | 36.868351 |
| Ca | 45.969261 | 25.975805 | 32.372169 |
| Ca | 42.786503 | 29.853914 | 34.672035 |
| S  | 27.089842 | 27.243078 | 36.318684 |
| S  | 26.884441 | 33.807564 | 34.683495 |
| S  | 30.307368 | 29.895819 | 32.573456 |
| S  | 29.953779 | 31.044764 | 36.549637 |
| S  | 33.447464 | 27.360889 | 34.055443 |
| S  | 33.402893 | 32.738346 | 32.634399 |
| S  | 36.674934 | 28.686487 | 31.910635 |
| S  | 36.421280 | 29.751675 | 36.469395 |
| S  | 40.504795 | 27.050934 | 34.966007 |
| S  | 40.244427 | 31.488373 | 33.483261 |
| S  | 43.422550 | 28.186338 | 31.728323 |
| S  | 44.831619 | 28.134127 | 37.212227 |

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generated by VMD

|   |   |   |
|---|---|---|
| Ca | 25.673260 | 30.559828 | 31.242620 |
| Ca | 26.264969 | 30.740635 | 36.183907 |
| Ca | 30.190437 | 28.059259 | 35.323158 |
| Ca | 30.189219 | 33.192345 | 33.469360 |
| Ca | 33.290199 | 29.824482 | 31.508877 |
| Ca | 33.203674 | 30.204107 | 35.326672 |
| Ca | 36.832546 | 26.846581 | 34.912876 |
| Ca | 36.655426 | 30.988861 | 33.668976 |
| Ca | 40.170986 | 28.694668 | 31.741098 |
| Ca | 39.906994 | 29.979582 | 37.007950 |
| Ca | 46.078136 | 26.264709 | 32.307938 |
| Ca | 42.701077 | 29.904530 | 34.758373 |
| S  | 26.974907 | 27.195284 | 36.212116 |
| S  | 26.978073 | 33.781242 | 34.664669 |
| S  | 30.378010 | 29.899336 | 32.521057 |
| S  | 29.898613 | 31.152134 | 36.396729 |
| S  | 33.417404 | 27.266142 | 34.342930 |
| S  | 33.705189 | 32.832447 | 32.712925 |
| S  | 36.531239 | 28.366756 | 31.872091 |
| S  | 36.458675 | 29.683359 | 36.594276 |
| S  | 40.386917 | 27.212133 | 35.005451 |
| S  | 40.130493 | 31.346031 | 33.423115 |
| S  | 43.567322 | 28.230404 | 31.496572 |
| S  | 44.850189 | 28.166584 | 37.336941 |

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generated by VMD
| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 25.880112 | 30.151340 | 31.471046 |
| Ca      | 26.266973 | 30.734642 | 36.330490 |
| Ca      | 30.008381 | 28.096380 | 35.186951 |
| Ca      | 30.190617 | 33.108658 | 33.366978 |
| Ca      | 33.453560 | 29.719088 | 31.571083 |
| Ca      | 33.068340 | 30.427788 | 35.369698 |
| Ca      | 36.820301 | 27.027742 | 34.865879 |
| Ca      | 36.730991 | 31.224331 | 33.881214 |
| Ca      | 40.194889 | 28.652325 | 31.768736 |
| Ca      | 40.025940 | 29.880026 | 36.854450 |
| Ca      | 46.256603 | 26.010218 | 32.381573 |
| Ca      | 42.950680 | 29.856365 | 34.629723 |
| S       | 26.509771 | 27.283171 | 35.859524 |
| S       | 26.950397 | 33.655510 | 34.830647 |
| S       | 30.415358 | 29.985725 | 32.480068 |
| S       | 29.717897 | 31.191462 | 36.410622 |
| S       | 33.341076 | 27.412397 | 34.265331 |
| S       | 33.597954 | 32.763023 | 32.800350 |
| S       | 36.570988 | 28.500466 | 31.777300 |
| S       | 36.400951 | 29.826944 | 36.672359 |
| S       | 40.348583 | 27.174786 | 35.038784 |
| S       | 40.195385 | 31.406445 | 33.546669 |
| S       | 43.531971 | 28.159487 | 31.636070 |
| S       | 45.006126 | 28.143507 | 37.035133 |

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generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 25.634830 | 30.297926 | 31.565008 |
| Ca      | 26.252424 | 30.522036 | 36.168655 |
| Ca      | 30.000368 | 28.380615 | 35.344315 |
| Ca      | 30.217661 | 33.021179 | 33.143986 |
| Ca      | 33.514843 | 29.544516 | 31.286648 |
| Ca      | 33.173645 | 30.550951 | 35.393299 |
| Ca      | 36.958195 | 27.052378 | 35.001740 |
| Ca      | 36.762508 | 31.112261 | 33.962124 |
| Ca      | 39.911812 | 28.754555 | 31.865463 |
| Ca      | 39.906990 | 30.024769 | 37.010426 |
| Ca      | 46.094860 | 26.184166 | 31.899786 |
| Ca      | 43.020382 | 29.843716 | 34.839638 |
| S       | 26.718609 | 27.180971 | 35.916512 |
| S       | 27.104700 | 33.453899 | 34.638565 |
| S       | 30.467438 | 29.967308 | 32.430138 |
| S       | 29.888123 | 31.271784 | 36.465466 |
| S       | 33.271481 | 27.375954 | 34.241482 |
| S       | 33.911186 | 32.808323 | 32.698574 |
| S       | 36.553787 | 28.487526 | 31.895054 |
| S       | 36.411205 | 29.660490 | 36.743179 |
|   |          |          |          |
|---|----------|----------|----------|
| S | 40.343643| 27.236645| 35.036705|
| S | 40.154083| 31.588509| 33.576080|
| S | 43.195007| 28.179138| 31.851397|
| S | 44.966080| 27.891800| 37.056438|

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generated by VMD

| Ca  |          |          |          |
|-----|----------|----------|----------|
| Ca  | 25.222996| 30.425108| 31.404676|
| Ca  | 26.004791| 30.585722| 36.346069|
| Ca  | 30.045654| 28.092543| 35.291279|
| Ca  | 30.231014| 33.151978| 35.519814|
| Ca  | 33.610439| 29.761316| 31.349350|
| Ca  | 33.202194| 30.259087| 35.174988|
| Ca  | 36.990631| 26.873144| 34.897438|
| Ca  | 36.702988| 31.474480| 33.402794|
| Ca  | 40.059502| 28.494755| 31.957792|
| Ca  | 40.013512| 30.047171| 36.943497|
| Ca  | 46.245865| 26.068771| 32.529346|
| Ca  | 42.960503| 29.919178| 34.681347|
| S   | 26.673862| 27.075150| 35.969868|
| S   | 26.964769| 33.775890| 35.074787|
| S   | 30.407114| 30.032919| 32.521736|
| S   | 29.998970| 31.088461| 36.526176|
| S   | 33.442959| 27.346014| 33.985092|
| S   | 33.570576| 32.771912| 32.480232|
| S   | 36.677845| 28.529406| 31.913059|
| S   | 36.521629| 29.824886| 36.384861|
| S   | 40.249020| 27.215702| 35.079880|
| S   | 40.175972| 31.402567| 33.584353|
| S   | 43.522919| 28.134804| 31.739031|
| S   | 44.938183| 28.040438| 37.272774|

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generated by VMD

| Ca  |          |          |          |
|-----|----------|----------|----------|
| Ca  | 25.412668| 30.227863| 31.666561|
| Ca  | 26.151497| 30.525717| 36.000885|
| Ca  | 30.190920| 28.212282| 35.033756|
| Ca  | 30.222572| 33.369106| 33.703026|
| Ca  | 33.553196| 29.861586| 31.584225|
| Ca  | 33.288528| 30.374079| 35.405037|
| Ca  | 36.701748| 26.691717| 34.922150|
| Ca  | 36.730515| 30.841213| 33.513897|
| Ca  | 39.992855| 28.629133| 31.897797|
| Ca  | 39.973465| 29.935583| 36.897564|
| Ca  | 46.345398| 26.294853| 32.552532|
| Ca  | 42.796276| 29.976482| 34.611805|
| S   | 26.775723| 27.221134| 36.059036|
| S   | 26.798702| 33.848312| 34.803272|
|    | 30.573404 | 30.315979 | 32.405525 |
|----|-----------|-----------|-----------|
| S  | 29.896784 | 30.869265 | 36.417133 |
| S  | 33.590117 | 30.572292 | 34.070393 |
| S  | 33.660469 | 32.827866 | 32.713882 |
| S  | 36.562973 | 28.220169 | 31.849545 |
| S  | 36.557236 | 29.715792 | 36.560101 |
| S  | 40.290572 | 27.129683 | 35.054314 |
| S  | 40.168537 | 31.413471 | 33.490295 |
| S  | 43.523441 | 28.010475 | 36.560101 |
| S  | 44.848358 | 28.308954 | 37.183472 |

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generated by VMD

| Ca   | 25.277040 | 30.029205 | 31.667467 |
|------|-----------|-----------|-----------|
| Ca   | 25.943548 | 30.704855 | 35.950985 |
| Ca   | 30.000544 | 28.276716 | 34.997562 |
| Ca   | 30.376583 | 33.205936 | 33.688007 |
| Ca   | 33.460003 | 29.856485 | 31.689878 |
| Ca   | 33.046890 | 30.384722 | 35.403151 |
| Ca   | 36.956779 | 26.784227 | 34.704620 |
| Ca   | 36.665557 | 30.877478 | 33.831409 |
| Ca   | 40.148102 | 28.516287 | 31.885834 |
| Ca   | 40.111271 | 29.958115 | 36.622807 |
| Ca   | 46.074188 | 26.174522 | 32.817604 |
| Ca   | 42.985332 | 30.157644 | 34.540104 |
| S    | 26.709650 | 27.253454 | 35.907810 |
| S    | 27.123446 | 33.798035 | 34.900135 |
| S    | 30.404797 | 30.134691 | 32.403385 |
| S    | 29.750671 | 31.083437 | 36.438496 |
| S    | 33.426903 | 27.551605 | 34.070511 |
| S    | 33.742233 | 32.870773 | 32.909382 |
| S    | 36.578350 | 28.466410 | 31.759581 |
| S    | 36.460732 | 29.564568 | 36.619740 |
| S    | 40.562263 | 27.093861 | 34.914425 |
| S    | 40.062489 | 31.277573 | 33.514446 |
| S    | 43.497322 | 27.930508 | 31.603613 |
| S    | 45.068287 | 28.440310 | 37.187641 |

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generated by VMD

| Ca   | 25.214558 | 30.190720 | 31.901119 |
|------|-----------|-----------|-----------|
| Ca   | 26.360188 | 30.723963 | 35.875664 |
| Ca   | 29.844286 | 28.123468 | 35.276402 |
| Ca   | 30.450279 | 33.095257 | 33.745800 |
| Ca   | 33.625439 | 29.592941 | 31.410427 |
| Ca   | 33.158226 | 30.322422 | 35.337456 |
| Ca   | 36.887196 | 27.120132 | 34.811615 |
| Ca   | 36.701736 | 30.982782 | 33.859093 |
Ca  40.164417  28.674353  31.657295
Ca  39.990360  29.904272  36.931015
Ca  45.846905  26.115864  32.897385
Ca  42.996666  30.128061  34.550831
S   26.419071  27.198811  35.808907
S   27.107405  33.918938  34.681438
S   30.588495  29.994802  32.508720
S   29.793486  30.969690  36.571701
S   33.410519  27.397659  34.050785
S   33.858521  32.668800  32.681259
S   36.571426  28.599895  31.730717
S   36.450447  29.614365  36.725945
S   40.426777  27.381351  34.876137
S   40.121246  31.255745  33.561783
S   43.521545  28.106619  31.574310
S   44.922783  28.310516  37.005001

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generated by VMD
Ca  25.704832  30.543854  31.796465
Ca  26.323912  30.578291  35.875378
Ca  29.830978  27.783337  35.370514
Ca  30.458376  33.140606  33.707169
Ca  33.305733  30.031366  31.292915
Ca  33.065819  30.154400  35.433987
Ca  37.112869  27.233299  34.742634
Ca  36.671486  30.819407  33.764648
Ca  39.934914  28.435274  31.642380
Ca  39.923023  30.080139  36.588497
Ca  45.771515  25.766960  33.116386
Ca  43.014511  30.400690  34.428291
S   26.415428  27.152847  35.729965
S   27.154608  33.865753  34.852741
S   30.587482  30.154400  32.734970
S   29.828440  30.770609  36.625626
S   33.512253  27.427366  33.870247
S   33.924145  32.793373  32.922916
S   36.472744  28.463650  31.469456
S   36.340702  29.701077  36.754730
S   40.566383  27.391356  34.900398
S   40.039043  31.283916  33.272099
S   43.327057  27.730623  31.840977
S   45.147636  28.728149  37.297318

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generated by VMD
Ca  25.337980  30.240744  31.646662
Ca  26.397221  30.609589  35.702805
| Element | X Coordinate | Y Coordinate | Z Coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 30.068844    | 27.952972    | 35.529572    |
| Ca      | 30.139812    | 30.397595    | 35.514111    |
| Ca      | 33.412788    | 29.857841    | 31.482008    |
| Ca      | 33.022121    | 33.11198     | 33.757454    |
| Ca      | 37.197083    | 26.940502    | 34.568878    |
| Ca      | 36.693916    | 31.328915    | 34.014748    |
| Ca      | 40.250175    | 28.748962    | 31.630112    |
| Ca      | 39.883591    | 30.209755    | 36.564396    |
| Ca      | 45.599934    | 25.294914    | 33.131756    |
| Ca      | 42.969650    | 30.053341    | 34.317455    |
| S       | 26.621943    | 27.300957    | 35.840702    |
| S       | 26.914324    | 33.821125    | 34.481991    |
| S       | 30.434006    | 30.023819    | 32.768555    |
| S       | 29.853703    | 31.015211    | 36.633194    |
| S       | 33.506374    | 27.345301    | 34.063694    |
| S       | 33.621315    | 32.702496    | 33.036037    |
| S       | 36.657116    | 28.780941    | 31.784927    |
| S       | 36.476315    | 29.521263    | 36.599804    |
| S       | 40.496895    | 27.363592    | 34.676033    |
| S       | 40.136005    | 31.418079    | 33.387691    |
| S       | 43.692970    | 27.871132    | 31.670120    |
| S       | 45.049759    | 28.568996    | 37.228001    |

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generated by VMD

| Element | X Coordinate | Y Coordinate | Z Coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.438473    | 30.234369    | 31.521997    |
| Ca      | 26.461388    | 30.620867    | 35.819443    |
| Ca      | 30.025261    | 27.860008    | 35.361141    |
| Ca      | 30.113457    | 32.997467    | 33.887939    |
| Ca      | 33.401936    | 29.839424    | 31.480116    |
| Ca      | 33.144772    | 30.287271    | 35.373779    |
| Ca      | 36.902084    | 27.143017    | 34.820999    |
| Ca      | 36.688080    | 31.157927    | 33.692444    |
| Ca      | 40.160770    | 28.870464    | 31.764351    |
| Ca      | 40.162895    | 30.156776    | 36.724529    |
| Ca      | 45.297440    | 25.259071    | 33.078468    |
| Ca      | 43.230991    | 30.023643    | 34.340931    |
| S       | 26.557266    | 27.184544    | 35.628635    |
| S       | 26.742456    | 33.857430    | 34.668968    |
| S       | 30.472998    | 30.050671    | 32.741898    |
| S       | 29.930853    | 30.792330    | 36.745720    |
| S       | 33.462963    | 27.487162    | 34.036251    |
| S       | 33.454285    | 32.826256    | 32.842667    |
| S       | 36.624744    | 28.764774    | 31.863913    |
| S       | 36.600922    | 29.868034    | 36.671951    |
| S       | 40.606808    | 27.280560    | 34.873577    |
| S       | 40.356239    | 31.556225    | 33.271919    |
|   | X        | Y        | Z        |
|---|----------|----------|----------|
| S | 43.44522 | 27.75429 | 31.57629 |
| S | 45.15126 | 28.51877 | 37.24282 |
| Ca| 25.46950 | 30.19881 | 31.86239 |
| Ca| 26.31833 | 30.80185 | 35.82294 |
| Ca| 30.32726 | 27.81673 | 35.30593 |
| Ca| 30.25356 | 33.03607 | 34.08871 |
| Ca| 33.54266 | 29.80506 | 31.18039 |
| Ca| 33.04190 | 30.13328 | 35.44500 |
| Ca| 37.20367 | 27.03656 | 34.71911 |
| Ca| 36.55617 | 31.02376 | 33.89899 |
| Ca| 40.25286 | 28.65441 | 31.58816 |
| Ca| 39.95697 | 30.62606 | 36.86576 |
| Ca| 45.05011 | 25.08654 | 32.97284 |
| Ca| 42.98379 | 30.10181 | 34.38543 |
| S | 26.82228 | 27.47754 | 35.63132 |
| S | 26.66604 | 33.76057 | 34.45867 |
| S | 30.5974 | 30.13221 | 32.63568 |
| S | 29.93476 | 30.91934 | 36.58268 |
| S | 33.72558 | 27.30468 | 34.03426 |
| S | 33.53775 | 32.78835 | 32.92440 |
| S | 36.74730 | 28.61540 | 31.75882 |
| S | 36.40518 | 29.58721 | 36.73241 |
| S | 40.54526 | 27.56736 | 35.03344 |
| S | 40.06896 | 31.55420 | 33.39197 |
| S | 43.32188 | 27.90068 | 31.69547 |
| S | 45.09548 | 28.46268 | 37.01675 |

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generated by VMD

|   | X        | Y        | Z        |
|---|----------|----------|----------|
| Ca| 25.50997 | 30.25561 | 31.57445 |
| Ca| 26.28717 | 30.77761 | 35.59297 |
| Ca| 29.81868 | 27.81682 | 35.44950 |
| Ca| 30.00761 | 32.93418 | 33.94943 |
| Ca| 33.56967 | 29.94752 | 31.58295 |
| Ca| 33.04563 | 30.02036 | 35.56482 |
| Ca| 36.83115 | 26.91201 | 34.78910 |
| Ca| 36.69224 | 31.25734 | 33.83856 |
| Ca| 40.11727 | 28.49103 | 31.73910 |
| Ca| 40.43548 | 30.50913 | 36.77182 |
| Ca| 45.59325 | 25.38026 | 32.85485 |
| Ca| 43.01709 | 30.14198 | 34.25127 |
| S | 26.35904 | 27.47253 | 35.60098 |
| S | 26.53754 | 33.88395 | 34.33812 |
| S | 30.52873 | 30.02227 | 32.76627 |
| S | 29.80348 | 30.89325 | 36.56241 |
|   |   |   |   |
|---|---|---|---|
| S | 33.235023 | 27.282726 | 34.023346 |
| S | 33.607880 | 32.830265 | 33.336143 |
| S | 36.669357 | 28.641230 | 31.973866 |
| S | 36.676521 | 29.854982 | 36.738239 |
| S | 40.563530 | 27.191757 | 34.870129 |
| S | 40.341473 | 31.445629 | 33.279476 |
| S | 43.677254 | 27.900248 | 31.582392 |
| S | 45.508907 | 28.528477 | 37.000446 |

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generated by VMD

| Ca | 25.303873 | 30.157486 | 31.770905 |
| Ca | 26.164007 | 30.749058 | 35.720329 |
| Ca | 29.750059 | 28.026325 | 35.498775 |
| Ca | 30.201868 | 32.825806 | 33.864307 |
| Ca | 33.718121 | 30.123413 | 31.463091 |
| Ca | 33.295822 | 30.235907 | 35.380909 |
| Ca | 37.085320 | 26.760878 | 34.851791 |
| Ca | 36.776588 | 30.994648 | 33.527233 |
| Ca | 40.107327 | 28.541538 | 31.764162 |
| Ca | 40.312199 | 30.511137 | 36.978153 |
| Ca | 45.213295 | 25.443947 | 32.783859 |
| Ca | 43.040863 | 30.190460 | 34.372047 |
| S  | 26.122850 | 27.201847 | 35.508869 |
| S  | 26.947475 | 34.051926 | 34.396317 |
| S  | 30.591522 | 29.873035 | 32.730499 |
| S  | 29.725334 | 30.869671 | 36.780331 |
| S  | 33.484074 | 27.413263 | 34.000767 |
| S  | 33.560120 | 32.829433 | 33.109943 |
| S  | 36.743912 | 28.394360 | 31.913044 |
| S  | 36.701447 | 29.662340 | 36.562057 |
| S  | 40.511539 | 27.360561 | 35.080639 |
| S  | 40.298241 | 31.602819 | 33.270771 |
| S  | 43.049463 | 28.242691 | 31.512964 |
| S  | 45.283421 | 28.328882 | 37.188957 |

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generated by VMD

| Ca | 25.550987 | 30.286140 | 31.657736 |
| Ca | 26.262426 | 30.598797 | 35.871101 |
| Ca | 30.018869 | 28.016914 | 35.552639 |
| Ca | 30.226877 | 33.009628 | 33.907631 |
| Ca | 33.766045 | 29.575651 | 31.644974 |
| Ca | 33.255890 | 30.258575 | 35.266441 |
| Ca | 36.989254 | 26.999149 | 35.039154 |
| Ca | 36.750523 | 31.210020 | 33.584167 |
| Ca | 40.102417 | 28.748861 | 31.722761 |
| Ca | 40.184410 | 30.539207 | 36.925243 |
|   | Ca     |   | S     |   | S     |   |
|---|--------|---|--------|---|--------|---|
|   | 45.200829 |   | 25.480959 |   | 32.575130 |
|   | 43.023495 |   | 30.026329 |   | 34.710865 |
|   | 26.446869 |   | 27.113449 |   | 35.273991 |
|   | 26.779018 |   | 33.847992 |   | 34.370087 |
|   | 30.482702 |   | 30.061874 |   | 32.663288 |
|   | 29.880224 |   | 31.002647 |   | 36.596191 |
|   | 33.559925 |   | 27.369843 |   | 34.181049 |
|   | 33.617229 |   | 32.734825 |   | 32.676266 |
|   | 36.703831 |   | 28.455635 |   | 31.992104 |
|   | 36.500340 |   | 29.835974 |   | 36.676605 |
|   | 40.380184 |   | 27.497423 |   | 35.215446 |
|   | 40.243004 |   | 31.525719 |   | 33.316521 |
|   | 43.497147 |   | 28.131535 |   | 31.467497 |
|   | 45.011360 |   | 28.064230 |   | 37.143719 |

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generated by VMD

|   | Ca     |   | S     |   | S     |   |
|---|--------|---|--------|---|--------|---|
|   | 25.29407 |   | 30.072166 |   | 31.727238 |
|   | 26.143408 |   | 30.877079 |   | 35.463886 |
|   | 29.997574 |   | 27.815622 |   | 35.250736 |
|   | 30.052820 |   | 32.960468 |   | 33.858986 |
|   | 33.507332 |   | 29.818626 |   | 31.757352 |
|   | 33.191315 |   | 30.249920 |   | 35.632427 |
|   | 37.039692 |   | 27.132652 |   | 35.169170 |
|   | 36.636665 |   | 31.137207 |   | 34.054234 |
|   | 40.253361 |   | 28.726952 |   | 31.860184 |
|   | 40.282787 |   | 30.313761 |   | 36.756413 |
|   | 45.215256 |   | 25.477047 |   | 32.259266 |
|   | 43.464199 |   | 29.962465 |   | 34.386215 |
|   | 26.500645 |   | 27.209236 |   | 35.448509 |
|   | 26.768768 |   | 34.131607 |   | 33.958778 |
|   | 30.444569 |   | 29.975323 |   | 32.558319 |
|   | 29.663965 |   | 30.820465 |   | 36.562260 |
|   | 33.557285 |   | 27.341206 |   | 34.460278 |
|   | 33.595936 |   | 32.711613 |   | 33.120949 |
|   | 36.705132 |   | 28.517582 |   | 32.223080 |
|   | 36.629288 |   | 29.926609 |   | 36.928928 |
|   | 40.463104 |   | 27.291092 |   | 34.902050 |
|   | 40.360687 |   | 31.596975 |   | 33.439693 |
|   | 43.463097 |   | 28.247990 |   | 31.361439 |
|   | 45.247604 |   | 28.077751 |   | 36.890110 |

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generated by VMD

|   | Ca     |   | S     |   | S     |   |
|---|--------|---|--------|---|--------|---|
|   | 25.247351 |   | 30.113052 |   | 31.610056 |
|   | 26.420567 |   | 30.740442 |   | 35.616413 |
|   | 29.837664 |   | 27.984089 |   | 35.580456 |
|   | 30.127718 |   | 32.879295 |   | 33.791122 |
| Element | x1     | y1     | z1     | x2     | y2     | z2     |
|---------|--------|--------|--------|--------|--------|--------|
| Ca      | 33.646790 | 29.718082 | 31.786003 | Ca      | 32.997234 | 30.306034 | 35.616657 |
| Ca      | 37.223534 | 26.827986 | 35.157314 | Ca      | 36.705986 | 31.245804 | 33.824299 |
| Ca      | 40.290337 | 28.851160 | 31.866772 | Ca      | 40.221260 | 30.600500 | 36.620426 |
| Ca      | 45.253262 | 25.270046 | 32.259502 | Ca      | 43.123993 | 29.984810 | 34.374493 |
| S       | 26.328342 | 27.187874 | 35.423397 | S       | 26.678873 | 33.950119 | 34.230133 |
| S       | 30.565035 | 29.864250 | 32.668022 | S       | 29.880945 | 31.024494 | 36.666634 |
| S       | 33.469887 | 27.501076 | 34.276901 | S       | 33.613457 | 32.664967 | 32.918808 |
| S       | 36.871712 | 28.670521 | 32.088352 | S       | 36.514191 | 29.727848 | 36.692142 |
| S       | 40.558548 | 27.513941 | 34.949650 | S       | 40.318928 | 31.619242 | 33.453033 |
| S       | 43.610405 | 28.201710 | 31.512583 | S       | 44.927902 | 27.944048 | 37.047424 |

24 generated by VMD

| Element | x1     | y1     | z1     | x2     | y2     | z2     |
|---------|--------|--------|--------|--------|--------|--------|
| Ca      | 25.374144 | 30.003731 | 31.530239 | Ca      | 26.102573 | 30.700462 | 35.797127 |
| Ca      | 30.026657 | 27.920675 | 35.333168 | Ca      | 30.202570 | 33.093487 | 33.754154 |
| Ca      | 33.537189 | 30.090349 | 31.622377 | Ca      | 33.164417 | 30.305479 | 35.382938 |
| Ca      | 36.962250 | 27.030670 | 35.037628 | Ca      | 36.824554 | 30.976063 | 33.930599 |
| Ca      | 40.028126 | 28.792707 | 31.811420 | Ca      | 40.123367 | 30.246063 | 36.815361 |
| Ca      | 45.775032 | 25.484200 | 32.452080 | Ca      | 43.042740 | 29.882458 | 34.408421 |
| S       | 26.624687 | 27.154968 | 35.731735 | S       | 26.576395 | 33.849636 | 34.259941 |
| S       | 30.649584 | 30.109116 | 32.631287 | S       | 29.921644 | 31.040489 | 36.415054 |
| S       | 33.522446 | 27.266159 | 34.407242 | S       | 33.708099 | 32.922482 | 33.091141 |
| S       | 36.658669 | 28.490257 | 31.960361 | S       | 36.566437 | 29.754768 | 36.810940 |
| S       | 40.250492 | 27.480331 | 35.058315 | S       | 40.199585 | 31.612751 | 33.346737 |
| S       | 43.580105 | 28.052193 | 31.624592 | S       | 45.012157 | 28.131889 | 36.817841 |
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.463745  | 30.089083  | 31.443375  |
| Ca      | 26.018847  | 30.549417  | 35.592255  |
| Ca      | 30.083576  | 27.940969  | 35.612900  |
| Ca      | 30.042397  | 33.156013  | 33.712814  |
| Ca      | 33.710526  | 29.840561  | 31.796379  |
| Ca      | 32.992107  | 30.330111  | 35.767822  |
| Ca      | 37.085815  | 31.032286  | 35.082836  |
| Ca      | 40.339890  | 33.156013  | 33.712814  |
| Ca      | 45.256813  | 30.355061  | 37.032455  |
| Ca      | 43.042336  | 29.931837  | 34.293602  |
| S       | 26.576504  | 27.225548  | 35.32539   |
| S       | 26.569468  | 33.715759  | 34.330162  |
| S       | 30.635515  | 30.089813  | 32.732529  |
| S       | 29.626291  | 31.129765  | 36.591461  |
| S       | 33.584770  | 27.527849  | 34.443069  |
| S       | 33.645897  | 32.910076  | 33.127346  |
| S       | 36.845287  | 28.456541  | 32.034050  |
| S       | 36.586746  | 29.916338  | 36.722828  |
| S       | 40.538673  | 27.369240  | 34.983887  |
| S       | 40.305237  | 31.524376  | 33.279945  |
| S       | 43.487083  | 27.879833  | 31.283224  |
| S       | 45.046719  | 28.293655  | 36.746735  |

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generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.522358  | 29.792391  | 31.422466  |
| Ca      | 26.167496  | 30.559639  | 35.813232  |
| Ca      | 30.234449  | 27.944927  | 35.672394  |
| Ca      | 29.991592  | 32.937019  | 33.694241  |
| Ca      | 33.637520  | 30.058865  | 31.661921  |
| Ca      | 33.269512  | 30.300600  | 35.443165  |
| Ca      | 37.055111  | 27.103069  | 34.884441  |
| Ca      | 36.706116  | 31.255049  | 34.021797  |
| Ca      | 40.302895  | 28.993736  | 31.735594  |
| Ca      | 40.284752  | 30.665192  | 36.997128  |
| Ca      | 44.856110  | 24.769838  | 32.596840  |
| Ca      | 43.177380  | 29.776596  | 34.387058  |
| S       | 26.490206  | 27.155857  | 35.606674  |
| S       | 26.564354  | 33.820328  | 34.254208  |
| S       | 30.695732  | 29.884741  | 32.878277  |
| S       | 29.716066  | 31.089161  | 36.498032  |
| S       | 33.692673  | 27.490555  | 34.138374  |
| S       | 33.351456  | 32.923576  | 33.042461  |
|    |     |     |     |
|----|-----|-----|-----|
| S  | 36.896881 | 28.742344 | 31.970871 |
| S  | 36.656898 | 29.857985 | 36.736504 |
| S  | 40.423676 | 27.608963 | 34.900425 |
| S  | 40.343200 | 31.817884 | 33.408958 |
| S  | 43.475864 | 27.821270 | 31.448265 |
| S  | 44.916458 | 28.021809 | 36.817444 |

24 generated by VMD

|    |     |     |     |
|----|-----|-----|-----|
| Ca | 25.735586 | 29.853905 | 31.531605 |
| Ca | 26.301500 | 30.379993 | 35.421368 |
| Ca | 30.339102 | 28.075546 | 35.659740 |
| Ca | 30.228447 | 33.046120 | 33.847111 |
| Ca | 33.619408 | 29.986519 | 31.654819 |
| Ca | 33.074730 | 30.452446 | 35.669849 |
| Ca | 37.186382 | 27.118475 | 34.948685 |
| Ca | 36.509098 | 31.043297 | 33.767323 |
| Ca | 40.123936 | 28.751883 | 31.789989 |
| Ca | 40.161278 | 30.638891 | 37.112511 |
| Ca | 44.923786 | 25.052181 | 32.531979 |
| Ca | 42.965096 | 29.843548 | 34.387955 |
| S  | 26.747372 | 27.027325 | 35.347744 |
| S  | 26.609657 | 33.653824 | 34.308228 |
| S  | 30.617647 | 30.037859 | 32.924385 |
| S  | 29.782507 | 31.142399 | 36.689724 |
| S  | 33.696827 | 27.751425 | 34.193619 |
| S  | 33.511761 | 33.046227 | 33.036121 |
| S  | 36.745975 | 28.561811 | 31.885149 |
| S  | 36.596062 | 29.921589 | 36.705360 |
| S  | 45.497391 | 27.531845 | 35.224415 |
| S  | 40.436932 | 31.627935 | 33.310356 |
| S  | 43.237816 | 27.824932 | 31.283144 |
| S  | 44.785606 | 28.021437 | 36.766975 |

24 generated by VMD

|    |     |     |     |
|----|-----|-----|-----|
| Ca | 25.659559 | 30.139503 | 31.656738 |
| Ca | 26.192297 | 30.591984 | 35.713135 |
| Ca | 30.238836 | 27.819157 | 35.330666 |
| Ca | 30.353863 | 32.980934 | 33.753746 |
| Ca | 33.801079 | 29.744427 | 31.722681 |
| Ca | 33.249405 | 30.301673 | 35.758877 |
| Ca | 37.074474 | 27.084654 | 35.312145 |
| Ca | 36.582031 | 31.319830 | 33.854950 |
| Ca | 40.097702 | 28.914095 | 32.145451 |
| Ca | 40.050648 | 30.863413 | 36.824703 |
| Ca | 44.939087 | 25.121511 | 32.355652 |
| Ca | 42.959114 | 29.844221 | 34.331280 |
|   |          |          |          |
|---|----------|----------|----------|
| S | 26.353817 | 27.167692 | 35.161289 |
| S | 26.893614 | 33.703545 | 34.280964 |
| S | 30.729485 | 29.941780 | 32.666321 |
| S | 29.793505 | 31.046431 | 36.445549 |
| S | 33.759346 | 27.361397 | 34.295612 |
| S | 33.662460 | 32.842270 | 32.880207 |
| S | 36.778664 | 28.502794 | 32.186924 |
| S | 36.673183 | 30.016420 | 36.897682 |
| S | 40.405594 | 27.542252 | 35.192764 |
| S | 40.286316 | 31.767038 | 33.482201 |
| S | 42.986092 | 28.028000 | 31.229927 |
| S | 44.913719 | 28.016397 | 36.551270 |

24 generated by VMD

| Ca |          |          |          |
|----|----------|----------|----------|
| Ca | 25.377171 | 30.223917 | 31.778559 |
| Ca | 26.276527 | 30.612883 | 35.809948 |
| Ca | 29.936071 | 27.953373 | 35.538555 |
| Ca | 30.211172 | 32.938492 | 33.502518 |
| Ca | 33.419624 | 29.708036 | 31.420351 |
| Ca | 33.250946 | 30.044952 | 35.405529 |
| Ca | 37.067162 | 27.299978 | 35.159069 |
| Ca | 36.946388 | 31.247473 | 34.125904 |
| Ca | 40.237808 | 28.980190 | 32.125446 |
| Ca | 40.049210 | 30.485239 | 36.860981 |
| Ca | 45.136169 | 25.072472 | 32.231331 |
| Ca | 43.159405 | 29.732870 | 34.375027 |
| S  | 26.232443 | 27.108541 | 35.358521 |
| S  | 26.764576 | 33.662853 | 34.353687 |
| S  | 30.509027 | 29.833891 | 32.735355 |
| S  | 29.867151 | 31.108688 | 36.406597 |
| S  | 33.527771 | 27.228855 | 34.148235 |
| S  | 33.752377 | 32.769997 | 32.715805 |
| S  | 36.807041 | 28.723057 | 32.048416 |
| S  | 36.454105 | 29.984657 | 36.926216 |
| S  | 40.425789 | 27.541481 | 35.203094 |
| S  | 40.667938 | 31.828642 | 33.769325 |
| S  | 43.242977 | 28.081852 | 31.489191 |
| S  | 45.115055 | 28.218998 | 36.542976 |

24 generated by VMD

| Ca |          |          |          |
|----|----------|----------|----------|
| Ca | 25.655046 | 29.974403 | 31.644098 |
| Ca | 26.068157 | 30.761940 | 35.853451 |
| Ca | 30.077314 | 27.884256 | 35.840302 |
| Ca | 30.269020 | 33.005161 | 33.384167 |
| Ca | 33.365681 | 29.656322 | 31.603189 |
| Ca | 33.036541 | 30.338875 | 35.498108 |
| Ca  | 37.270615 | 27.196205 | 34.912935 |
| Ca  | 36.661697 | 31.120892 | 34.110432 |
| Ca  | 40.154980 | 28.99990 | 32.063164 |
| Ca  | 39.919846 | 30.108723 | 37.034744 |
| Ca  | 45.308685 | 25.122547 | 32.384773 |
| Ca  | 43.149818 | 29.842176 | 34.139935 |
| S   | 26.612040 | 27.321377 | 35.444981 |
| S   | 26.587997 | 33.779652 | 34.250450 |
| S   | 30.545954 | 29.993685 | 32.784149 |
| S   | 29.684420 | 31.159689 | 36.427952 |
| S   | 33.751152 | 27.519966 | 34.349628 |
| S   | 33.773628 | 32.653233 | 32.865406 |
| S   | 36.760933 | 28.789326 | 31.724319 |
| S   | 36.423752 | 29.657812 | 36.849140 |
| S   | 40.669136 | 27.538971 | 35.056377 |
| S   | 40.297272 | 31.717707 | 33.807671 |
| S   | 43.558163 | 28.141788 | 31.263878 |
| S   | 44.831985 | 28.106712 | 36.731106 |

24 generated by VMD

| Ca  | 25.733631 | 29.992332 | 31.573383 |
| Ca  | 26.158760 | 30.590471 | 36.002949 |
| Ca  | 30.062166 | 27.870070 | 35.599773 |
| Ca  | 30.092703 | 33.084507 | 33.494545 |
| Ca  | 33.624241 | 29.998966 | 31.463114 |
| Ca  | 32.987900 | 30.282526 | 35.462673 |
| Ca  | 37.142044 | 27.409809 | 35.010021 |
| Ca  | 36.668526 | 31.307522 | 33.935558 |
| Ca  | 40.294205 | 28.961771 | 31.966829 |
| Ca  | 39.821800 | 30.270241 | 36.967712 |
| Ca  | 45.132545 | 24.720455 | 32.682102 |
| Ca  | 43.122231 | 29.856060 | 34.253632 |
| S   | 26.571146 | 27.131132 | 35.763462 |
| S   | 26.749327 | 33.516331 | 34.583763 |
| S   | 30.590600 | 30.036797 | 32.654613 |
| S   | 29.840631 | 30.963167 | 36.548416 |
| S   | 33.720997 | 27.508968 | 34.030785 |
| S   | 33.691830 | 32.882381 | 32.743156 |
| S   | 36.893936 | 28.841320 | 31.743238 |
| S   | 36.227261 | 29.928200 | 36.832253 |
| S   | 40.482502 | 27.498642 | 35.055733 |
| S   | 40.216584 | 31.660561 | 33.573589 |
| S   | 43.667191 | 27.851982 | 31.352509 |
| S   | 44.932743 | 28.227173 | 36.736866 |

24 generated by VMD
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.647785    | 30.231163    | 31.491024    |
| Ca      | 26.445860    | 30.487530    | 35.904999    |
| Ca      | 29.988096    | 27.973175    | 35.524864    |
| Ca      | 30.208408    | 33.198151    | 33.564751    |
| Ca      | 33.519794    | 29.575714    | 31.691692    |
| Ca      | 33.306541    | 30.480385    | 35.511318    |
| Ca      | 37.207375    | 27.158627    | 35.132942    |
| Ca      | 36.753925    | 31.163509    | 34.074291    |
| Ca      | 40.093563    | 29.014233    | 32.098679    |
| Ca      | 39.981358    | 30.063053    | 36.928852    |
| Ca      | 44.885445    | 24.851839    | 32.294788    |
| Ca      | 43.102867    | 29.987455    | 34.057217    |
| S       | 26.571997    | 27.120771    | 35.188763    |
| S       | 26.778425    | 33.718636    | 34.465431    |
| S       | 30.582663    | 29.948566    | 32.613380    |
| S       | 29.867378    | 31.113382    | 36.457996    |
| S       | 33.592861    | 27.402542    | 34.387356    |
| S       | 33.744339    | 32.565140    | 32.826565    |
| S       | 36.745266    | 28.527769    | 31.970243    |
| S       | 36.415081    | 29.860809    | 36.907932    |
| S       | 40.479740    | 27.526367    | 34.958458    |
| S       | 40.104885    | 31.759808    | 33.855400    |
| S       | 43.456551    | 27.972565    | 31.332085    |
| S       | 44.953674    | 28.690186    | 36.791672    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.293753    | 30.139114    | 31.659645    |
| Ca      | 26.384487    | 30.559158    | 35.868393    |
| Ca      | 30.105413    | 27.942753    | 35.409912    |
| Ca      | 30.265636    | 32.914856    | 33.525852    |
| Ca      | 33.572124    | 29.631365    | 31.586563    |
| Ca      | 33.050369    | 30.602633    | 35.401333    |
| Ca      | 37.127769    | 27.242952    | 35.006767    |
| Ca      | 36.657597    | 31.134104    | 33.821796    |
| Ca      | 40.268429    | 29.103563    | 32.140636    |
| Ca      | 39.915649    | 30.093830    | 37.049675    |
| Ca      | 44.873318    | 24.753998    | 32.345715    |
| Ca      | 43.066536    | 29.908680    | 34.391499    |
| S       | 26.507477    | 27.144714    | 35.593601    |
| S       | 26.936060    | 33.739899    | 34.642662    |
| S       | 30.520737    | 29.827284    | 32.556805    |
| S       | 29.861557    | 30.941654    | 36.501522    |
| S       | 33.676685    | 27.690521    | 34.321026    |
| S       | 33.620468    | 32.690800    | 32.633141    |
| S       | 36.866730    | 28.817730    | 31.624872    |
| S       | 36.371113    | 29.851622    | 36.764469    |
S        40.411083       27.360626       34.977386
S        40.235062       31.663845       33.984108
S        43.691559       28.072329       31.449350
S        45.154301       28.563349       36.774017

24

generated by VMD
Ca       25.368608       30.325893       31.752304
Ca       26.267307       30.478355       35.962524
Ca       30.031435       28.006405       35.361404
Ca       30.308334       33.154537       33.370590
Ca       33.611332       29.573338       31.507761
Ca       33.107986       30.212193       35.424210
Ca       37.018421       27.255873       34.953793
Ca       36.648369       31.039833       33.759682
Ca       40.056248       28.936855       32.304199
Ca       39.864914       30.226767       37.203064
Ca       45.075302       24.926966       32.302021
Ca       43.029648       29.917561       34.301220
S        26.649622       27.105944       35.288635
S        27.144333       33.588234       34.759434
S        30.611847       30.031033       32.620266
S        29.817245       31.067593       36.452438
S        33.568169       27.407953       34.113258
S        33.781693       32.860474       32.673801
S        36.829769       28.522123       31.784708
S        36.384869       29.899044       36.793949
S        40.496960       27.519436       35.469440
S        40.007706       31.650915       33.931999
S        43.453941       27.978697       31.385078
S        45.299828       28.705378       36.554893

24

generated by VMD
Ca       25.204103       30.520006       31.881889
Ca       26.277603       30.525312       35.863949
Ca       30.146709       27.840380       35.639824
Ca       30.433964       33.045654       33.549492
Ca       33.534061       29.721210       31.371223
Ca       33.045750       30.331633       35.236912
Ca       37.151886       27.137562       34.998901
Ca       36.728081       31.078276       33.575928
Ca       40.023579       28.987654       32.425434
Ca       39.888771       29.942955       36.950493
Ca       45.313473       24.926476       32.391003
Ca       43.090683       30.081051       34.405197
S        26.472391       27.101410       35.436226
S        26.781523       33.736206       34.625198
S    30.523361       30.000389       32.732723
S    29.891331       31.097227       36.599461
S    33.548820       27.366051       33.985401
S    33.815464       32.641075       32.483589
S    36.880733       28.431484       31.899366
S    36.348370       29.877647       36.528313
S    40.420883       27.357836       35.205429
S    40.163277       31.736380       33.985035
S    43.579189       28.247917       31.597322
S    45.169876       28.659586       36.662373

24 generated by VMD
Ca   25.670107       30.158770       31.520115
Ca   26.304703       30.561319       35.841461
Ca   30.042887       27.693344       35.522820
Ca   30.44361       33.026119       33.507511
Ca   33.574169       29.727734       31.400454
Ca   33.080914       30.329533       35.342159
Ca   36.943398       27.301657       35.366920
Ca   36.76577       31.053024       33.726994
Ca   40.146381       29.009478       32.305458
Ca   39.930241       30.130030       37.103951
Ca   44.943413       24.926937       32.057381
Ca   43.244961       29.831417       34.206017
S    26.212193       27.177999       35.384216
S    26.825640       33.642788       34.533710
S    30.471210       29.826239       32.794216
S    29.751150       31.177666       36.420250
S    33.609356       27.489010       34.194073
S    33.758076       32.870888       32.884148
S    36.776497       28.538380       32.010914
S    36.351505       30.046541       36.811420
S    40.528069       27.576511       35.215855
S    40.265755       31.754080       33.994198
S    43.446526       28.085190       31.314535
S    45.346985       28.456728       36.572052

24 generated by VMD
Ca   25.203350       30.373589       31.708359
Ca   26.233105       30.686367       35.901096
Ca   29.984636       27.824219       35.559669
Ca   30.260162       33.044964       33.286911
Ca   33.674099       29.790840       31.460581
Ca   32.964714       30.252724       35.293774
Ca   37.252377       27.156008       35.369797
Ca   36.651871       30.860380       33.906345
Ca       40.183384       28.989855       32.073013
Ca       40.151012       30.071533       37.032803
Ca       44.685108       25.129337       32.155674
Ca       43.083267       29.960701       34.175316
S        26.410839       27.224018       35.354717
S        26.956589       33.783005       34.730740
S        30.542482       29.766378       32.541561
S        29.685431       31.045429       36.212765
S        33.719879       27.422375       34.284649
S        33.855972       32.790279       32.787422
S        36.894630       28.418987       32.022820
S        36.503330       29.913313       37.004486
S        40.593357       27.428749       35.146244
S        40.099567       31.561356       33.885635
S        43.684151       27.428749       31.728929
S        45.160568       28.592243       36.846493

24
generated by VMD
Ca       25.288956       30.297176       31.591537
Ca       26.313608       30.694838       35.628384
Ca       30.291374       27.764980       35.718906
Ca       30.176081       32.788864       33.421684
Ca       33.669720       29.754749       31.479279
Ca       33.078220       30.336033       35.447975
Ca       37.112537       27.137300       35.117332
Ca       36.862873       31.081451       33.936523
Ca       40.060760       28.966099       32.269199
Ca       40.017899       30.383997       37.201828
Ca       44.531120       25.068508       32.259968
Ca       42.957764       29.794258       34.246933
S        26.605997       27.161570       35.461014
S        26.960396       33.769733       34.448227
S        30.564203       29.803490       32.721931
S        29.718781       30.991436       36.443501
S        33.588402       27.457693       34.178265
S        33.796967       32.883362       32.867302
S        36.845959       28.507931       31.796041
S        36.394756       29.910088       36.792294
S        40.527241       27.591515       35.267654
S        40.292484       31.708532       33.904076
S        43.473000       28.160267       31.122047
S        45.304779       28.377522       36.708874

24
generated by VMD
Ca       25.773819       30.170841       31.486794
Ca       26.039993       30.692066       35.645115
| Element | Value1  | Value2  | Value3   |
|---------|---------|---------|----------|
| Ca      | 29.828049 | 27.743555 | 35.739677 |
| Ca      | 30.223406 | 33.022705 | 33.536110 |
| Ca      | 33.585423 | 30.010729 | 31.802399 |
| Ca      | 32.983837 | 30.327129 | 35.544102 |
| Ca      | 37.106228 | 27.195862 | 35.282692 |
| Ca      | 36.658035 | 31.009769 | 33.953285 |
| Ca      | 40.222008 | 28.905602 | 32.106274 |
| Ca      | 40.001652 | 30.110077 | 36.732086 |
| Ca      | 45.113834 | 25.195095 | 32.398876 |
| Ca      | 43.112694 | 29.606693 | 34.195763 |
| S       | 26.299511 | 27.218199 | 35.370819 |
| S       | 26.800301 | 33.723244 | 34.490635 |
| S       | 30.495344 | 29.933743 | 32.800957 |
| S       | 29.624172 | 31.039370 | 36.505341 |
| S       | 33.661793 | 27.428509 | 34.338097 |
| S       | 33.801807 | 32.934402 | 32.619129 |
| S       | 36.843925 | 28.491346 | 32.032890 |
| S       | 36.346375 | 29.895252 | 36.892223 |
| S       | 40.559177 | 27.336905 | 35.026909 |
| S       | 40.322723 | 31.691317 | 33.721230 |
| S       | 43.617989 | 28.186039 | 31.123131 |
| S       | 45.411705 | 28.522980 | 36.686230 |

24 generated by VMD

| Element | Value1  | Value2  | Value3   |
|---------|---------|---------|----------|
| Ca      | 25.756462 | 30.024048 | 31.624365 |
| Ca      | 26.138060 | 30.765348 | 35.641914 |
| Ca      | 30.012625 | 27.866182 | 35.595417 |
| Ca      | 30.318480 | 32.974701 | 33.433861 |
| Ca      | 33.467838 | 29.664770 | 31.280226 |
| Ca      | 33.044777 | 30.336166 | 35.611618 |
| Ca      | 37.212399 | 27.062279 | 35.266716 |
| Ca      | 36.623417 | 30.946365 | 34.056316 |
| Ca      | 40.011906 | 29.080708 | 32.302929 |
| Ca      | 40.226402 | 30.281952 | 37.076828 |
| Ca      | 44.903820 | 25.053387 | 32.158310 |
| Ca      | 43.064613 | 29.918840 | 34.334805 |
| S       | 26.464317 | 27.182470 | 35.524082 |
| S       | 26.923761 | 33.918262 | 34.357700 |
| S       | 30.581921 | 29.831263 | 32.751072 |
| S       | 29.587898 | 31.144016 | 36.44450 |
| S       | 33.590481 | 27.615168 | 34.001625 |
| S       | 33.720673 | 32.716469 | 32.839466 |
| S       | 36.777000 | 28.569017 | 31.803465 |
| S       | 36.426594 | 29.634598 | 36.929111 |
| S       | 40.517536 | 27.474907 | 35.276642 |
| S       | 40.233845 | 31.878233 | 34.070766 |
S  43.343357  28.050423  31.289158
S  45.485653  28.401821  36.359833

24

generated by VMD
Ca  25.686794  30.076807  31.588531
Ca  25.997818  30.715370  35.679405
Ca  30.101063  27.866116  35.404163
Ca  30.168215  33.062073  33.477577
Ca  33.746624  29.876616  31.472445
Ca  33.061859  30.304590  35.437397
Ca  37.119526  27.095383  35.383522
Ca  36.538689  31.047800  33.929749
Ca  39.942410  28.952644  32.205288
Ca  39.921856  30.145529  36.936069
Ca  45.321690  25.209967  32.102505
Ca  43.014008  29.781866  34.105228
S  26.336874  27.155678  35.392334
S  26.910946  33.909920  34.748806
S  30.781471  29.935049  32.594456
S  29.784672  31.095556  36.301880
S  33.635868  27.320518  34.226288
S  33.760254  32.874725  33.028233
S  36.718040  28.378685  31.984959
S  36.529575  29.981602  36.947346
S  40.483887  27.281359  35.089882
S  40.147614  31.662489  33.872940
S  43.397961  28.009336  31.364265
S  45.326191  28.651756  36.757458

24

generated by VMD
Ca  25.673279  30.202759  31.555964
Ca  26.075705  30.791265  35.970215
Ca  29.798288  27.843882  35.422955
Ca  30.310677  33.098259  33.568501
Ca  33.627552  29.586893  31.693596
Ca  33.035835  30.362141  35.557888
Ca  36.981945  27.011850  35.306854
Ca  36.728146  30.925766  34.134178
Ca  40.249378  28.958031  31.971251
Ca  39.950809  30.003733  36.799641
Ca  45.611477  25.325249  32.183090
Ca  43.132568  29.780857  34.167393
S  26.210623  27.361736  35.452805
S  26.956192  33.780067  34.450603
S  30.615864  29.859138  32.637196
S  29.740044  31.195364  36.292637
|   |        |        |        |
|---|--------|--------|--------|
| S | 33.492962 | 27.352007 | 34.400791 |
| S | 33.632545 | 32.743736 | 32.656883 |
| S | 36.778706 | 28.592419 | 32.106304 |
| S | 36.281826 | 29.608406 | 36.962151 |
| S | 40.334465 | 27.388186 | 34.872765 |
| S | 40.230991 | 31.689806 | 33.738472 |
| S | 43.780148 | 28.256388 | 31.481543 |
| S | 45.203815 | 28.673439 | 36.646969 |

24 generated by VMD

| Ca |        |        |        |
|----|--------|--------|--------|
| Ca | 25.866024 | 30.061356 | 31.322758 |
| Ca | 26.255941 | 30.764030 | 35.940590 |
| Ca | 30.196087 | 27.766384 | 35.495365 |
| Ca | 30.271933 | 33.099903 | 33.711174 |
| Ca | 33.549679 | 29.970308 | 31.560738 |
| Ca | 33.141281 | 30.428200 | 35.634533 |
| Ca | 36.979248 | 26.948002 | 35.226959 |
| Ca | 36.513210 | 30.800278 | 33.944347 |
| Ca | 40.051525 | 28.822464 | 31.819565 |
| Ca | 39.887249 | 30.085762 | 36.859184 |
| Ca | 45.384487 | 25.181164 | 32.629581 |
| Ca | 43.112846 | 29.885941 | 33.946098 |
| S | 26.421801 | 27.195360 | 35.441055 |
| S | 26.826370 | 33.926422 | 34.253197 |
| S | 30.659004 | 29.921314 | 32.800724 |
| S | 29.716076 | 31.175900 | 36.583370 |
| S | 33.482944 | 27.613861 | 34.172565 |
| S | 33.776951 | 32.821911 | 33.223598 |
| S | 36.722668 | 28.303555 | 31.941027 |
| S | 36.372463 | 29.615486 | 36.994102 |
| S | 40.348740 | 27.440758 | 34.863228 |
| S | 40.089951 | 31.596085 | 33.599644 |
| S | 43.741013 | 28.105354 | 31.387707 |
| S | 45.066444 | 28.861637 | 36.679626 |

24 generated by VMD

| Ca |        |        |        |
|----|--------|--------|--------|
| Ca | 25.631296 | 30.106707 | 31.407372 |
| Ca | 26.131336 | 31.029373 | 35.748684 |
| Ca | 29.989662 | 27.712624 | 35.646675 |
| Ca | 30.362675 | 32.781654 | 33.494728 |
| Ca | 33.494652 | 29.909521 | 31.689064 |
| Ca | 33.158642 | 30.146076 | 35.427906 |
| Ca | 37.117447 | 26.999901 | 35.133568 |
| Ca | 36.740665 | 31.210672 | 34.094711 |
| Ca | 40.054642 | 29.109373 | 32.127388 |
| Ca | 39.927494 | 29.898249 | 36.866856 |
|      |       |       |       |
|------|-------|-------|-------|
| Ca   | 45.232929 | 25.198032 | 32.230457 |
| Ca   | 43.039116  | 29.814760  | 34.230663  |
| S    | 26.323198  | 27.561504  | 35.609280  |
| S    | 26.934275  | 33.873962  | 34.073612  |
| S    | 30.496485  | 29.537926  | 32.689877  |
| S    | 29.670528  | 30.904659  | 36.427177  |
| S    | 33.642418  | 27.259594  | 34.440315  |
| S    | 33.634438  | 32.776546  | 33.101963  |
| S    | 36.761429  | 28.791527  | 32.084549  |
| S    | 36.441475  | 29.874712  | 36.949478  |
| S    | 40.514183  | 27.396042  | 34.877316  |
| S    | 40.378792  | 31.765985  | 33.768059  |
| S    | 43.533791  | 28.200024  | 31.155508  |
| S    | 45.222218  | 28.532021  | 36.755535  |

24 generated by VMD

|      |       |       |       |
|------|-------|-------|-------|
| Ca   | 25.676380 | 30.251976 | 31.428904 |
| Ca   | 26.130589  | 30.736431  | 35.665962  |
| Ca   | 29.854218  | 27.976004  | 35.964874  |
| Ca   | 30.029234  | 32.817947  | 33.470509  |
| Ca   | 33.638325  | 29.810167  | 31.391109  |
| Ca   | 32.956688  | 30.295982  | 35.534168  |
| Ca   | 36.944347  | 27.253679  | 35.300781  |
| Ca   | 36.673458  | 31.051188  | 34.257637  |
| Ca   | 40.118420  | 29.066931  | 31.964174  |
| Ca   | 39.975376  | 29.813881  | 36.664555  |
| Ca   | 45.658401  | 25.187321  | 32.288677  |
| Ca   | 43.187134  | 29.721033  | 34.129303  |
| S    | 26.339073  | 27.328083  | 35.561993  |
| S    | 26.682367  | 33.809349  | 34.144951  |
| S    | 30.502438  | 29.838009  | 32.889568  |
| S    | 29.621023  | 31.165846  | 36.527847  |
| S    | 33.437763  | 27.541447  | 34.308037  |
| S    | 33.661098  | 32.636948  | 32.949417  |
| S    | 36.772972  | 28.580975  | 31.926594  |
| S    | 36.392670  | 29.860649  | 37.112564  |
| S    | 40.541649  | 27.236578  | 34.701649  |
| S    | 40.368546  | 31.703644  | 33.889538  |
| S    | 44.027672  | 28.141100  | 31.248106  |
| S    | 45.244091  | 28.565639  | 36.709946  |

24 generated by VMD

|      |       |       |       |
|------|-------|-------|-------|
| Ca   | 25.826262 | 30.245644 | 31.469246 |
| Ca   | 26.361897  | 30.546846  | 35.940891  |
| Ca   | 30.004230  | 27.851254  | 35.534370  |
| Ca   | 30.245832  | 32.911060  | 33.723522  |
| Element | X-Cor | Y-Cor | Z-Cor |
|---------|-------|-------|-------|
| Ca      | 33.551624 | 29.871305 | 31.592978 |
| Ca      | 32.998062 | 30.142443 | 35.510155 |
| Ca      | 37.096111 | 27.397280 | 35.027599 |
| Ca      | 36.637417 | 31.202446 | 33.885071 |
| Ca      | 40.143185 | 28.866841 | 31.923359 |
| Ca      | 39.790783 | 30.302992 | 36.748482 |
| Ca      | 45.327946 | 24.968681 | 32.620865 |
| Ca      | 43.175762 | 29.615913 | 34.123730 |
| S       | 26.337109 | 27.139832 | 35.027599 |
| S       | 26.873692 | 33.692677 | 35.458912 |
| S       | 30.561760 | 29.917341 | 32.832161 |
| S       | 29.801407 | 30.930096 | 36.679146 |
| S       | 33.592571 | 27.493675 | 34.144768 |
| S       | 33.589649 | 32.834583 | 32.862053 |
| S       | 36.786457 | 28.638128 | 31.753645 |
| S       | 36.286316 | 30.184694 | 36.709141 |
| S       | 40.477890 | 27.618439 | 35.009605 |
| S       | 40.379341 | 31.716074 | 33.566826 |
| S       | 43.726528 | 27.815792 | 31.404091 |
| S       | 44.862106 | 28.467350 | 36.929436 |

24 generated by VMD

| Element | X-Cor | Y-Cor | Z-Cor |
|---------|-------|-------|-------|
| Ca      | 25.406824 | 30.076305 | 31.428421 |
| Ca      | 26.166489 | 30.780224 | 35.698425 |
| Ca      | 30.005775 | 27.862370 | 35.596291 |
| Ca      | 30.334816 | 32.723919 | 33.872810 |
| Ca      | 33.592117 | 29.852646 | 31.407646 |
| Ca      | 33.208580 | 30.249798 | 35.571201 |
| Ca      | 37.102341 | 27.193970 | 35.285263 |
| Ca      | 36.757534 | 31.024509 | 33.744896 |
| Ca      | 40.201340 | 28.958534 | 31.912926 |
| Ca      | 40.033089 | 30.078548 | 36.956467 |
| Ca      | 45.001980 | 25.108839 | 32.350517 |
| Ca      | 43.206673 | 29.800898 | 34.228996 |
| S       | 26.042698 | 27.269791 | 35.231987 |
| S       | 26.850500 | 33.845474 | 34.429184 |
| S       | 30.504736 | 29.821484 | 32.825920 |
| S       | 29.775723 | 31.012650 | 36.727829 |
| S       | 33.450089 | 27.517651 | 34.236778 |
| S       | 33.658241 | 32.872707 | 32.838459 |
| S       | 36.740334 | 28.407587 | 31.882492 |
| S       | 36.629639 | 30.074486 | 36.753769 |
| S       | 40.484852 | 27.346428 | 34.973961 |
| S       | 40.362785 | 31.617323 | 33.781830 |
| S       | 43.505322 | 28.196972 | 31.383419 |
| S       | 45.411503 | 28.698341 | 36.911114 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.299650 | 30.486961 | 31.458364 |
| Ca      | 25.977571 | 30.624165 | 35.823303 |
| Ca      | 30.044184 | 27.852238 | 35.659348 |
| Ca      | 33.563828 | 29.566658 | 31.913692 |
| Ca      | 33.246815 | 30.490446 | 35.509361 |
| Ca      | 36.986168 | 27.278559 | 35.334160 |
| Ca      | 36.732018 | 31.219948 | 33.828495 |
| Ca      | 40.330959 | 29.217520 | 31.841366 |
| Ca      | 39.890999 | 29.953485 | 36.914921 |
| Ca      | 45.533054 | 25.009140 | 32.503780 |
| Ca      | 43.226120 | 29.628178 | 34.114017 |
| S       | 25.874252 | 27.278160 | 35.180893 |
| S       | 26.799700 | 33.782921 | 34.467815 |
| S       | 30.429485 | 29.539961 | 32.818184 |
| S       | 29.708296 | 31.025894 | 36.441193 |
| S       | 33.728146 | 27.536758 | 34.580582 |
| S       | 33.407505 | 32.686569 | 32.766052 |
| S       | 36.899220 | 28.679337 | 31.917322 |
| S       | 36.298965 | 30.106693 | 36.802734 |
| S       | 40.397606 | 27.488701 | 34.639534 |
| S       | 40.486408 | 31.864239 | 33.732738 |
| S       | 43.764977 | 27.922810 | 31.443022 |
| S       | 45.218662 | 28.410137 | 36.725403 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.121586 | 30.582956 | 31.692608 |
| Ca      | 26.210005 | 30.678198 | 35.751575 |
| Ca      | 30.402527 | 27.770182 | 35.910789 |
| Ca      | 30.256039 | 32.800304 | 33.454384 |
| Ca      | 33.318542 | 29.513647 | 31.567226 |
| Ca      | 33.332245 | 30.422998 | 35.218040 |
| Ca      | 37.081997 | 27.184422 | 34.979248 |
| Ca      | 36.735435 | 31.205387 | 33.867607 |
| Ca      | 40.015526 | 29.182503 | 31.988262 |
| Ca      | 39.910854 | 30.090870 | 36.924873 |
| Ca      | 45.323540 | 25.156748 | 32.662514 |
| Ca      | 43.082657 | 29.629942 | 34.223724 |
| S       | 25.770306 | 27.379696 | 35.060287 |
| S       | 27.011108 | 33.823174 | 34.717133 |
| S       | 30.462149 | 29.473186 | 32.972832 |
| S       | 29.861485 | 31.062141 | 36.490562 |
| S       | 33.689381 | 27.278519 | 34.495037 |
| S       | 33.674789 | 32.519653 | 32.604885 |
|   | X    | Y    | Z    |
|---|------|------|------|
| S | 36.759159 | 28.723867 | 31.571331 |
| S | 36.399143  | 28.723867 | 31.571331 |
| S | 40.396217  | 27.464773 | 34.792305 |
| S | 40.425716  | 31.746418 | 33.967289 |
| S | 43.776417  | 28.169495 | 31.594326 |
| S | 45.417000  | 28.712437 | 36.839588 |
| Ca| 25.119886  | 30.723452 | 31.768373 |
| Ca| 26.149406  | 30.770626 | 35.898266 |
| Ca| 30.361877  | 27.486153 | 35.530865 |
| Ca| 30.216324  | 33.007187 | 33.633728 |
| Ca| 33.402744  | 29.502037 | 31.494455 |
| Ca| 33.215881  | 30.169146 | 35.236355 |
| Ca| 36.923351  | 27.196804 | 35.259773 |
| Ca| 36.723061  | 31.372614 | 33.605576 |
| Ca| 40.061188  | 28.963284 | 31.886898 |
| Ca| 40.084450  | 29.966127 | 36.756996 |
| Ca| 45.537457  | 25.452765 | 32.704357 |
| Ca| 43.246353  | 29.687943 | 34.299915 |
| S | 25.983244  | 27.279903 | 35.043171 |
| S | 27.015177  | 34.073746 | 34.945549 |
| S | 30.473351  | 29.582485 | 32.850811 |
| S | 29.790442  | 30.755817 | 36.457146 |
| S | 33.627960  | 27.104389 | 34.361359 |
| S | 33.548176  | 32.665508 | 32.496197 |
| S | 36.554443  | 28.638565 | 31.932219 |
| S | 36.441502  | 30.155861 | 36.639507 |
| S | 40.492458  | 27.528534 | 34.796471 |
| S | 40.432018  | 31.740860 | 33.738419 |
| S | 43.733215  | 27.990931 | 31.659380 |
| S | 45.299934  | 28.576687 | 37.034870 |

24 generated by VMD

|   | X    | Y    | Z    |
|---|------|------|------|
| Ca| 24.887877  | 30.586937 | 31.922314 |
| Ca| 26.345337  | 30.670616 | 35.783104 |
| Ca| 30.454454  | 27.665083 | 35.512432 |
| Ca| 30.034792  | 32.862877 | 33.748970 |
| Ca| 33.405125  | 29.622356 | 31.244905 |
| Ca| 33.179855  | 30.322521 | 35.296822 |
| Ca| 37.055790  | 27.367872 | 35.302078 |
| Ca| 36.829681  | 31.186310 | 33.781200 |
| Ca| 40.150127  | 28.775536 | 31.859516 |
| Ca| 39.960297  | 30.222301 | 36.777214 |
| Ca| 45.754711  | 25.291615 | 32.540604 |
| Ca| 43.259506  | 29.634430 | 34.363792 |
| S     | 25.699730 | 27.214930 | 34.750591 |
|-------|-----------|-----------|-----------|
| S     | 26.802788 | 33.859200 | 36.581207 |
| S     | 30.433798 | 29.892982 | 32.764118 |
| S     | 29.915768 | 30.857094 | 35.077     |
| S     | 33.601177 | 27.287949 | 34.349953 |
| S     | 33.581326 | 32.812202 | 32.476162 |
| S     | 36.620129 | 28.459097 | 31.947849 |
| S     | 36.331249 | 30.034153 | 36.732052 |
| S     | 40.457275 | 27.628901 | 35.042831 |
| S     | 40.528004 | 31.608841 | 33.456169 |
| S     | 43.780731 | 27.910126 | 31.682640 |
| S     | 45.364357 | 28.617432 | 37.036835 |

24

generated by VMD

| Ca    | 24.867161 | 30.532986 | 31.923378 |
|-------|-----------|-----------|-----------|
| Ca    | 26.398310 | 30.558353 | 35.784138 |
| Ca    | 30.508898 | 27.817329 | 35.805027 |
| Ca    | 30.196154 | 32.797409 | 33.616467 |
| Ca    | 33.542694 | 29.379675 | 31.297600 |
| Ca    | 33.257832 | 30.455875 | 35.166313 |
| Ca    | 37.250778 | 27.166950 | 35.016911 |
| Ca    | 36.935978 | 31.281357 | 33.901924 |
| Ca    | 40.163155 | 29.059772 | 31.906822 |
| Ca    | 39.965176 | 30.234598 | 36.990788 |
| Ca    | 45.208641 | 25.095034 | 32.527172 |
| Ca    | 43.189636 | 29.764263 | 34.306751 |
| S     | 25.644661 | 27.235167 | 34.920074 |
| S     | 26.901733 | 33.765343 | 34.744549 |
| S     | 30.417519 | 29.702782 | 32.900105 |
| S     | 29.957954 | 31.010750 | 36.661770 |
| S     | 33.673439 | 27.489147 | 34.210384 |
| S     | 33.611866 | 32.558182 | 32.434040 |
| S     | 36.736694 | 28.599161 | 31.794561 |
| S     | 36.417873 | 29.933361 | 36.778652 |
| S     | 40.380684 | 27.521526 | 34.993755 |
| S     | 40.472752 | 31.842005 | 33.809097 |
| S     | 43.654015 | 28.030243 | 31.593624 |
| S     | 45.080353 | 28.560188 | 36.946777 |

24

generated by VMD

| Ca    | 25.232342 | 30.579323 | 31.865604 |
|-------|-----------|-----------|-----------|
| Ca    | 26.231678 | 30.759151 | 36.036148 |
| Ca    | 30.316021 | 27.959690 | 35.607246 |
| Ca    | 30.137104 | 32.716949 | 33.735970 |
| Ca    | 33.572956 | 29.486223 | 31.328972 |
| Ca    | 33.135986 | 30.347885 | 35.292110 |
| Ca   | 36.892853 | 26.972246 | 35.040268 |
|------|-----------|-----------|-----------|
| Ca   | 36.880211 | 31.268717 | 33.675732 |
| Ca   | 40.168327 | 29.121473 | 31.758434 |
| Ca   | 40.251469 | 30.119486 | 36.915073 |
| Ca   | 45.501263 | 25.469849 | 32.787346 |
| Ca   | 43.166077 | 29.431133 | 34.277272 |
| S    | 25.822365 | 27.283554 | 35.211899 |
| S    | 26.842484 | 33.799992 | 34.724007 |
| S    | 30.419701 | 29.752748 | 32.771847 |
| S    | 29.782345 | 31.021225 | 36.805820 |
| S    | 33.344894 | 27.460320 | 34.071442 |
| S    | 33.393829 | 32.454517 | 32.457577 |
| S    | 36.966228 | 28.607430 | 31.741608 |
| S    | 36.571655 | 29.839027 | 36.594925 |
| S    | 40.302235 | 27.302549 | 34.744499 |
| S    | 40.497528 | 31.748821 | 33.561180 |
| S    | 43.685364 | 28.137047 | 31.704468 |
| S    | 45.319103 | 28.752111 | 37.170761 |

generated by VMD

| Ca   | 25.306681 | 30.608936 | 31.795170 |
|------|-----------|-----------|-----------|
| Ca   | 26.240416 | 30.681236 | 35.759857 |
| Ca   | 30.545612 | 27.707569 | 35.654743 |
| Ca   | 30.193110 | 32.982597 | 33.694481 |
| Ca   | 33.306313 | 29.445076 | 31.580505 |
| Ca   | 33.224281 | 30.272427 | 35.440395 |
| Ca   | 36.794319 | 27.088200 | 35.111687 |
| Ca   | 36.710789 | 31.116795 | 33.821064 |
| Ca   | 40.089317 | 29.156731 | 31.800600 |
| Ca   | 40.248215 | 30.168270 | 36.808960 |
| Ca   | 45.532330 | 25.419281 | 32.715160 |
| Ca   | 43.103001 | 29.596088 | 34.260456 |
| S    | 26.031195 | 27.217628 | 35.131107 |
| S    | 26.843349 | 34.008968 | 34.525486 |
| S    | 30.487728 | 29.754280 | 32.895702 |
| S    | 29.785143 | 30.865200 | 36.385319 |
| S    | 33.641392 | 27.303446 | 34.421638 |
| S    | 33.759850 | 32.543995 | 32.684631 |
| S    | 36.704861 | 28.573460 | 31.830387 |
| S    | 36.652458 | 30.025909 | 36.770954 |
| S    | 40.102123 | 27.452747 | 34.746136 |
| S    | 40.216660 | 31.722973 | 33.671379 |
| S    | 43.746857 | 28.096928 | 31.567940 |
| S    | 45.167866 | 28.582710 | 36.957451 |

generated by VMD
|   | Ca   | S     |   |
|---|------|-------|---|
|   | 25.452721 | 30.566847 | 31.577799 |
|   | 26.182837 | 30.470558 | 35.965828 |
|   | 30.119680 | 27.845758 | 35.623131 |
|   | 30.282469 | 33.252808 | 33.693611 |
|   | 33.597126 | 29.697962 | 31.555359 |
|   | 33.117519 | 30.312340 | 35.328423 |
|   | 36.957687 | 26.957722 | 35.104927 |
|   | 36.701271 | 31.027372 | 33.739456 |
|   | 39.954304 | 28.813133 | 31.942867 |
|   | 40.094997 | 30.365177 | 36.592026 |
|   | 45.584457 | 25.763561 | 32.796680 |
|   | 43.080650 | 29.563112 | 34.166847 |
|   | 26.497738 | 27.088535 | 35.395332 |
|   | 26.782675 | 33.840187 | 34.719753 |
|   | 30.528530 | 29.927078 | 32.798519 |
|   | 29.818968 | 30.957367 | 36.377895 |
|   | 33.525734 | 27.441921 | 34.173481 |
|   | 33.816719 | 32.820274 | 32.729591 |
|   | 36.683739 | 28.409199 | 31.835835 |
|   | 36.535549 | 29.867828 | 36.708565 |
|   | 40.284657 | 27.295233 | 35.022121 |
|   | 40.207802 | 31.506485 | 33.529694 |
|   | 43.521923 | 28.146389 | 31.561934 |
|   | 45.104160 | 28.454578 | 37.091099 |

24 generated by VMD

|   | Ca   | S     |   |
|---|------|-------|---|
|   | 25.244064 | 30.364277 | 31.745548 |
|   | 26.165791 | 30.599571 | 35.820671 |
|   | 30.174702 | 27.883291 | 35.626003 |
|   | 30.16833 | 33.061859 | 33.750023 |
|   | 33.648613 | 29.555683 | 31.620518 |
|   | 33.038986 | 30.342405 | 35.562351 |
|   | 36.842484 | 27.014133 | 35.043682 |
|   | 36.814865 | 30.992664 | 33.854084 |
|   | 40.193623 | 28.895430 | 31.818104 |
|   | 40.085449 | 30.111660 | 36.695728 |
|   | 45.710415 | 25.670868 | 32.546825 |
|   | 43.086227 | 29.604107 | 34.297745 |
|   | 26.009047 | 27.282448 | 35.344975 |
|   | 26.724440 | 33.856750 | 34.546566 |
|   | 30.655783 | 29.986309 | 32.751701 |
|   | 29.691639 | 30.975529 | 36.367897 |
|   | 33.525173 | 27.362690 | 34.354675 |
|   | 33.746525 | 32.772236 | 32.782154 |
|   | 36.739037 | 28.555710 | 31.868519 |
|   | 36.529335 | 29.929640 | 36.753899 |
|  |  |  |
|---|---|---|
| S | 40.297756 | 27.237816 | 34.781441 |
| S | 40.534084 | 31.626610 | 33.444489 |
| S | 43.709122 | 28.147896 | 31.516356 |
| S | 45.105930 | 28.561790 | 37.136826 |

24 generated by VMD

| Ca | 25.361343 | 30.350475 | 31.716555 |
| Ca | 26.130678 | 30.615875 | 36.023041 |
| Ca | 30.063894 | 27.980247 | 35.517593 |
| Ca | 30.235329 | 33.006691 | 33.634094 |
| Ca | 33.698597 | 29.657131 | 31.348497 |
| Ca | 33.077263 | 30.362663 | 35.408981 |
| Ca | 36.807667 | 27.010914 | 35.206551 |
| Ca | 36.683517 | 30.923622 | 33.888702 |
| Ca | 40.003357 | 28.667099 | 32.000050 |
| Ca | 40.296284 | 30.311895 | 36.806801 |
| Ca | 45.603241 | 25.723616 | 32.252769 |
| Ca | 43.065025 | 29.637878 | 34.477966 |
| S | 26.181484 | 27.227505 | 35.237934 |
| S | 26.840504 | 33.781837 | 34.519981 |
| S | 30.694742 | 29.991377 | 32.625923 |
| S | 29.679255 | 31.054348 | 36.578499 |
| S | 33.368305 | 27.489449 | 34.197941 |
| S | 33.750992 | 32.801895 | 32.740131 |
| S | 36.765568 | 28.297792 | 31.961723 |
| S | 36.589611 | 29.816793 | 36.807728 |
| S | 40.368340 | 27.243801 | 34.987373 |
| S | 40.340675 | 31.644733 | 33.550694 |
| S | 43.472042 | 28.295494 | 31.553665 |
| S | 45.356224 | 28.498230 | 36.987499 |

24 generated by VMD

| Ca | 25.463081 | 30.414038 | 31.879885 |
| Ca | 26.235590 | 30.785847 | 35.837711 |
| Ca | 30.087839 | 27.674351 | 35.582054 |
| Ca | 30.503284 | 32.844261 | 33.922958 |
| Ca | 33.720394 | 29.702198 | 31.470675 |
| Ca | 33.119823 | 30.213814 | 35.510216 |
| Ca | 36.807869 | 27.093382 | 34.950874 |
| Ca | 36.708012 | 31.176207 | 33.563816 |
| Ca | 40.177937 | 28.839371 | 32.051712 |
| Ca | 39.982483 | 30.292461 | 36.712006 |
| Ca | 45.641781 | 25.652252 | 32.301670 |
| Ca | 42.967445 | 29.681206 | 34.402924 |
| S | 26.166716 | 27.262596 | 35.423016 |
| S | 26.962568 | 33.859135 | 34.459759 |
| S   | 30.680454 | 29.841911 | 32.780186 |
| S   | 29.870653 | 30.871544 | 36.506592 |
| S   | 33.428730 | 27.399950 | 34.158218 |
| S   | 33.748112 | 32.740261 | 32.541134 |
| S   | 36.780800 | 28.457558 | 31.739609 |
| S   | 36.388401 | 29.920788 | 34.386761 |
| S   | 40.239201 | 27.262026 | 34.99672 |
| S   | 40.237263 | 31.784845 | 33.552803 |
| S   | 43.584023 | 28.207718 | 31.683907 |
| S   | 44.931477 | 28.413719 | 37.260201 |

24 generated by VMD

| Ca  | 25.057112 | 30.556696 | 31.650471 |
| Ca  | 26.273483 | 30.938919 | 35.833530 |
| Ca  | 30.117821 | 27.756958 | 35.354397 |
| Ca  | 30.335625 | 32.813316 | 33.526527 |
| Ca  | 33.643539 | 29.527409 | 31.565845 |
| Ca  | 32.906563 | 30.508877 | 35.499672 |
| Ca  | 36.904499 | 26.826159 | 35.081429 |
| Ca  | 36.645390 | 30.853453 | 33.855923 |
| Ca  | 40.163712 | 28.934593 | 32.186344 |
| Ca  | 40.005817 | 30.042049 | 36.961121 |
| Ca  | 45.901455 | 25.901871 | 32.301361 |
| Ca  | 42.957680 | 29.770319 | 34.339592 |
| S   | 26.254099 | 27.426407 | 35.617859 |
| S   | 26.941460 | 34.073990 | 34.570602 |
| S   | 30.560795 | 29.769354 | 32.616207 |
| S   | 29.716690 | 31.037764 | 36.409607 |
| S   | 33.568920 | 27.283511 | 34.386761 |
| S   | 33.673576 | 32.584335 | 32.807144 |
| S   | 36.874931 | 28.398325 | 31.788429 |
| S   | 36.509991 | 29.673283 | 36.642296 |
| S   | 40.406826 | 27.163452 | 34.908821 |
| S   | 40.073208 | 31.731350 | 33.742970 |
| S   | 43.757141 | 28.285475 | 31.523041 |
| S   | 45.183605 | 28.538488 | 36.860764 |

24 generated by VMD

| Ca  | 25.317007 | 30.308010 | 31.719427 |
| Ca  | 26.312067 | 30.846893 | 35.957928 |
| Ca  | 29.941141 | 27.943268 | 35.531639 |
| Ca  | 30.241619 | 32.693214 | 33.817066 |
| Ca  | 33.586552 | 29.723904 | 31.388069 |
| Ca  | 33.186245 | 29.994764 | 35.257267 |
| Ca  | 36.864273 | 27.062210 | 34.792664 |
| Ca  | 36.726181 | 31.049103 | 33.720444 |
|     | X        | Y        | Z        |
|-----|----------|----------|----------|
| Ca  | 40.013672| 28.849419| 31.887611|
| Ca  | 40.100471| 30.199539| 36.879417|
| Ca  | 45.864010| 25.647730| 32.590755|
| Ca  | 42.941818| 29.700600| 34.370296|
| S   | 26.239491| 27.521263| 35.649979|
| S   | 27.081211| 33.999680| 34.607273|
| S   | 30.581757| 29.728054| 32.689152|
| S   | 29.997051| 30.978035| 36.665264|
| S   | 33.465977| 27.315231| 33.801525|
| S   | 33.513798| 32.657887| 32.787849|
| S   | 36.734016| 28.548466| 31.707726|
| S   | 36.666012| 29.762299| 36.612736|
| S   | 40.208660| 27.296696| 34.815338|
| S   | 40.267685| 31.706646| 33.685619|
| S   | 43.574135| 28.150898| 31.807919|
| S   | 45.008991| 28.707582| 37.287701|

24
generated by VMD

|     | X        | Y        | Z        |
|-----|----------|----------|----------|
| Ca  | 25.447870| 30.401672| 31.514160|
| Ca  | 26.448751| 30.864820| 35.890869|
| Ca  | 29.968185| 27.993763| 35.793133|
| Ca  | 30.076885| 32.703369| 33.548210|
| Ca  | 33.713276| 29.653906| 31.505268|
| Ca  | 33.117893| 30.484482| 35.533276|
| Ca  | 37.031960| 26.864302| 35.042324|
| Ca  | 36.661900| 30.842930| 33.786301|
| Ca  | 40.320213| 28.974865| 31.906876|
| Ca  | 39.957813| 30.063831| 36.832718|
| Ca  | 45.871124| 25.650385| 32.539333|
| Ca  | 42.762074| 29.665573| 34.304161|
| S   | 26.306450| 27.413774| 35.598675|
| S   | 26.930367| 33.762905| 34.645195|
| S   | 30.534428| 29.662199| 32.815845|
| S   | 29.727583| 31.270767| 36.464912|
| S   | 33.586216| 27.541626| 34.185856|
| S   | 33.643883| 32.639359| 32.797855|
| S   | 36.950348| 28.573284| 31.619999|
| S   | 36.393661| 29.686565| 36.718563|
| S   | 40.327850| 27.160852| 34.728100|
| S   | 40.144524| 31.739948| 33.671795|
| S   | 43.665848| 28.252357| 31.682278|
| S   | 44.844818| 28.523897| 36.905014|

24
generated by VMD

|     | X        | Y        | Z        |
|-----|----------|----------|----------|
| Ca  | 25.438360| 30.403042| 31.564470|
| Ca  | 26.316757| 31.000496| 35.863205|
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 30.240467 | 27.842690 | 35.755875 |
| Ca      | 30.096325 | 32.679798 | 33.476906 |
| Ca      | 33.646076 | 29.705750 | 31.625109 |
| Ca      | 33.027378 | 30.319143 | 35.463181 |
| Ca      | 36.965313 | 27.040844 | 35.089275 |
| Ca      | 36.439989 | 30.907732 | 33.834824 |
| Ca      | 40.253689 | 29.021568 | 32.137714 |
| Ca      | 39.803467 | 30.016010 | 36.838337 |
| Ca      | 46.224392 | 25.640049 | 32.227798 |
| Ca      | 42.937416 | 29.711319 | 34.231888 |
| S       | 25.837719 | 27.543045 | 35.407139 |
| S       | 26.897358 | 34.069199 | 34.591320 |
| S       | 30.590830 | 29.505398 | 32.677876 |
| S       | 29.784252 | 31.106422 | 36.595917 |
| S       | 33.665970 | 27.319151 | 34.295143 |
| S       | 33.546200 | 32.643837 | 32.808784 |
| S       | 36.990852 | 28.563560 | 31.768841 |
| S       | 36.281471 | 29.802662 | 36.772881 |
| S       | 40.421494 | 27.293159 | 34.841045 |
| S       | 40.076294 | 31.660265 | 33.755661 |
| S       | 43.818111 | 28.171293 | 31.574827 |
| S       | 45.137012 | 28.424953 | 36.832695 |

24

generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.281889 | 30.321642 | 31.680429 |
| Ca      | 26.478361 | 30.451191 | 35.913696 |
| Ca      | 30.169443 | 28.308090 | 35.795868 |
| Ca      | 30.157730 | 32.934250 | 33.500538 |
| Ca      | 33.666809 | 29.699297 | 31.364319 |
| Ca      | 33.112617 | 30.531195 | 35.434723 |
| Ca      | 36.917007 | 26.978775 | 35.130426 |
| Ca      | 36.444920 | 30.960222 | 33.730240 |
| Ca      | 40.205166 | 28.911116 | 32.167015 |
| Ca      | 39.860153 | 29.970379 | 36.962868 |
| Ca      | 46.167847 | 25.574635 | 32.334518 |
| Ca      | 42.901443 | 29.724827 | 34.443813 |
| S       | 26.093437 | 27.175079 | 35.458443 |
| S       | 26.913799 | 33.748909 | 34.664589 |
| S       | 30.617897 | 29.851871 | 32.659889 |
| S       | 29.846548 | 31.205353 | 36.545048 |
| S       | 33.500793 | 27.661274 | 34.091656 |
| S       | 33.662422 | 32.764786 | 32.653622 |
| S       | 36.930492 | 28.505741 | 31.756580 |
| S       | 36.322178 | 29.848072 | 36.742142 |
| S       | 40.232510 | 27.074162 | 34.949314 |
| S       | 40.046799 | 31.504364 | 33.840782 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.478477    | 30.156010    | 31.464237    |
| Ca      | 26.094284    | 30.647266    | 35.651127    |
| Ca      | 30.049351    | 28.173660    | 35.885258    |
| Ca      | 30.101986    | 33.005840    | 33.300224    |
| Ca      | 33.720047    | 29.765074    | 31.728924    |
| Ca      | 33.060635    | 30.540163    | 35.546921    |
| Ca      | 36.789654    | 26.951302    | 35.310295    |
| Ca      | 36.732529    | 31.022400    | 33.801506    |
| Ca      | 40.282070    | 28.994064    | 32.035011    |
| Ca      | 39.886040    | 29.832056    | 37.022285    |
| Ca      | 46.487511    | 25.682129    | 31.909178    |
| Ca      | 42.922150    | 29.565384    | 34.161892    |
| S       | 25.882015    | 27.172451    | 35.563896    |
| S       | 26.835617    | 33.825718    | 34.612556    |
| S       | 30.623318    | 29.699993    | 32.850216    |
| S       | 29.614281    | 31.241543    | 36.306011    |
| S       | 33.375408    | 27.526295    | 34.298233    |
| S       | 33.636539    | 32.845131    | 32.940128    |
| S       | 36.971947    | 28.560555    | 32.057480    |
| S       | 36.439678    | 29.906780    | 36.789612    |
| S       | 40.363678    | 27.078545    | 34.535088    |
| S       | 40.359737    | 31.578362    | 33.805740    |
| S       | 43.803802    | 28.107910    | 31.564894    |
| S       | 44.923157    | 28.512768    | 36.889996    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.392452    | 30.287584    | 31.454872    |
| Ca      | 26.102989    | 30.857422    | 35.603642    |
| Ca      | 29.777424    | 28.002340    | 35.731419    |
| Ca      | 30.058510    | 32.972614    | 33.373894    |
| Ca      | 33.553982    | 29.791103    | 31.688805    |
| Ca      | 33.089203    | 30.326160    | 35.575920    |
| Ca      | 37.270149    | 26.851654    | 35.064846    |
| Ca      | 36.863670    | 30.928663    | 34.032246    |
| Ca      | 39.978828    | 28.915310    | 32.098877    |
| Ca      | 40.083359    | 30.137274    | 36.888863    |
| Ca      | 45.996037    | 25.595572    | 32.197369    |
| Ca      | 43.216370    | 29.832691    | 34.165089    |
| S       | 25.932034    | 27.479881    | 35.361877    |
| S       | 26.808611    | 33.798317    | 34.464767    |
| S       | 30.593491    | 29.808544    | 32.761162    |
| S       | 29.709957    | 31.207424    | 36.412903    |
S       33.257187       27.255339       34.276432
S       33.775204       32.672836       33.060280
S       36.669407       28.338844       31.939634
S       36.617920       29.532417       36.994591
S       40.545853       27.329353       34.880943
S       40.202549       31.747227       33.838669
S       43.609215       27.981297       31.387495
S       45.329494       28.741524       36.776169
24
generated by VMD
Ca       25.491274       29.881832       31.380981
Ca       26.182919       30.740433       35.693844
Ca       30.039618       28.368759       35.659397
Ca       30.211750       33.011551       33.375721
Ca       33.625423       29.839718       31.575890
Ca       32.977272       30.374537       35.528976
Ca       37.293007       27.002720       35.349239
Ca       36.655178       30.791225       33.965820
Ca       39.992500       28.979565       32.336773
Ca       39.925781       29.805676       37.069538
Ca       45.544300       25.453054       31.766844
Ca       43.158405       30.005867       34.151115
S       26.213701       27.244324       35.634277
S       26.846287       33.926525       34.250038
S       30.543564       29.835436       32.752907
S       29.732882       31.331467       36.422844
S       33.714348       27.499657       34.145519
S       33.771126       32.749054       32.816269
S       36.810471       28.505878       31.958851
S       36.375237       29.501926       37.013351
S       40.602825       27.206535       35.044964
S       40.034561       31.644318       34.114193
S       43.507389       28.321737       31.571323
S       45.184120       28.369530       36.452045
24
generated by VMD
Ca       25.768394       29.891666       31.158203
Ca       26.228886       30.698296       35.578636
Ca       29.847176       28.062084       35.618000
Ca       30.214668       33.263699       33.410656
Ca       33.537693       30.019859       31.787174
Ca       33.143356       30.285351       35.551529
Ca       37.054943       27.231632       35.321777
Ca       36.709469       30.966154       34.066502
Ca       39.873951       28.645592       32.245628
Ca       40.096771       30.059734       37.157280
| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 45.785969 | 25.628714 | 31.782093 |
| Ca      | 43.279568  | 29.785553  | 34.005562  |
| S       | 26.354372  | 27.268867  | 35.565334  |
| S       | 26.845825  | 33.704254  | 34.339455  |
| S       | 30.520363  | 29.917912  | 32.756424  |
| S       | 29.722040  | 31.066780  | 36.378273  |
| S       | 33.530743  | 27.381233  | 34.295597  |
| S       | 33.791233  | 32.801743  | 32.974087  |
| S       | 36.638458  | 28.430445  | 32.083076  |
| S       | 36.342331  | 29.897116  | 36.976753  |
| S       | 40.405769  | 27.413132  | 35.213356  |
| S       | 40.201668  | 31.637648  | 33.834839  |
| S       | 43.348682  | 28.177271  | 31.326616  |
| S       | 45.191563  | 28.156713  | 36.603870  |

24 generated by VMD

| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 25.645372 | 29.886557 | 31.259951 |
| Ca      | 26.019804 | 30.647234 | 35.488541 |
| Ca      | 29.982826 | 28.096596 | 35.577579 |
| Ca      | 30.225435 | 33.088795 | 33.473621 |
| Ca      | 33.493633 | 29.771912 | 31.861141 |
| Ca      | 33.090275 | 30.266491 | 35.661781 |
| Ca      | 37.087696 | 27.349781 | 35.395275 |
| Ca      | 36.710087 | 31.132015 | 34.192841 |
| Ca      | 39.987461 | 29.041111 | 31.976318 |
| Ca      | 39.895885 | 29.763588 | 37.231033 |
| Ca      | 45.806263 | 25.669151 | 31.882885 |
| Ca      | 43.240643 | 29.615143 | 34.017570 |
| S       | 26.160315 | 27.327862 | 35.432346 |
| S       | 26.798964 | 33.703899 | 34.217167 |
| S       | 30.589336 | 29.925007 | 32.759357 |
| S       | 29.607645 | 31.206871 | 36.413574 |
| S       | 33.661575 | 27.484213 | 34.576561 |
| S       | 33.781345 | 32.737991 | 32.851311 |
| S       | 36.685856 | 28.536564 | 32.193726 |
| S       | 36.325703 | 30.042038 | 37.095707 |
| S       | 40.486393 | 27.342743 | 34.862591 |
| S       | 40.365086 | 31.558933 | 33.851582 |
| S       | 43.482449 | 27.986807 | 31.333324 |
| S       | 45.303829 | 28.210140 | 36.424866 |

24 generated by VMD

| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 25.563637 | 29.786671 | 31.486929 |
| Ca      | 26.055540 | 30.835958 | 35.710297 |
| Ca      | 29.913139 | 28.123585 | 35.779179 |
| Ca      | 30.448158 | 33.069527 | 33.266510 |
| Ca     | 33.614502 | 30.018549 | 31.669580 |
|--------|-----------|-----------|-----------|
| Ca     | 33.112610 | 30.346481 | 35.536224 |
| Ca     | 36.888412 | 27.145100 | 35.087955 |
| Ca     | 36.544014 | 30.896557 | 33.839516 |
| Ca     | 40.080093 | 28.879564 | 32.243855 |
| Ca     | 39.759350 | 29.424381 | 37.145027 |
| Ca     | 45.827412 | 25.770323 | 31.729467 |
| Ca     | 42.987469 | 29.760834 | 34.404274 |
| S      | 26.397593 | 27.275734 | 35.751873 |
| S      | 27.062252 | 33.860825 | 34.178108 |
| S      | 30.604498 | 29.746376 | 32.674244 |
| S      | 29.864101 | 31.276215 | 36.375538 |
| S      | 33.636004 | 27.540306 | 34.162903 |
| S      | 33.725006 | 32.841698 | 33.006607 |
| S      | 36.846283 | 28.513668 | 31.872093 |
| S      | 36.385235 | 29.729195 | 36.894531 |
| S      | 40.220051 | 27.208944 | 35.025658 |
| S      | 40.009674 | 31.442749 | 34.261780 |
| S      | 43.604816 | 28.365383 | 31.387320 |
| S      | 45.283428 | 28.532791 | 36.541298 |

24 generated by VMD

| Ca     | 25.540186 | 29.955019 | 31.580036 |
|--------|-----------|-----------|-----------|
| Ca     | 26.245163 | 30.708954 | 35.745815 |
| Ca     | 30.038866 | 28.075829 | 35.723995 |
| Ca     | 30.315332 | 33.065479 | 33.453522 |
| Ca     | 33.663200 | 29.919498 | 31.598309 |
| Ca     | 32.992695 | 30.376570 | 35.563702 |
| Ca     | 37.002659 | 27.295658 | 35.288177 |
| Ca     | 36.582245 | 30.862633 | 33.871670 |
| Ca     | 40.102787 | 29.035290 | 32.014549 |
| Ca     | 39.873203 | 29.870457 | 36.986023 |
| Ca     | 45.564850 | 25.676706 | 32.024895 |
| Ca     | 43.136883 | 29.712082 | 34.231880 |
| S      | 26.328247 | 27.159008 | 35.700134 |
| S      | 26.872715 | 33.672649 | 34.310799 |
| S      | 30.654413 | 29.834824 | 32.669258 |
| S      | 29.817734 | 31.231033 | 36.338303 |
| S      | 33.499832 | 27.513004 | 34.373337 |
| S      | 33.835438 | 32.817272 | 32.812634 |
| S      | 36.786625 | 28.408237 | 31.820408 |
| S      | 36.316021 | 29.884369 | 36.790855 |
| S      | 40.529804 | 27.489243 | 34.970993 |
| S      | 40.184303 | 31.585938 | 33.921280 |
| S      | 43.656994 | 28.306679 | 31.463453 |
| S      | 44.893734 | 27.934994 | 36.776653 |
| Element | X          | Y          | Z          |
|---------|-----------|------------|------------|
| Ca      | 25.356981 | 29.786861  | 31.801327  |
| Ca      | 26.182634 | 30.619064  | 35.764317  |
| Ca      | 30.075584 | 28.284042  | 35.688519  |
| Ca      | 30.387987 | 33.006981  | 33.270153  |
| Ca      | 33.700413 | 29.487991  | 31.473255  |
| Ca      | 33.282818 | 30.517920  | 35.354492  |
| Ca      | 36.990608 | 27.169994  | 35.181725  |
| Ca      | 36.891720 | 31.143135  | 34.111679  |
| Ca      | 40.228531 | 29.055202  | 32.274502  |
| Ca      | 39.779896 | 29.277832  | 37.305042  |
| Ca      | 45.660656 | 26.239052  | 31.179989  |
| Ca      | 43.036713 | 29.595333  | 34.627590  |
| S       | 26.156841 | 27.402351  | 36.072544  |
| S       | 26.805168 | 33.817581  | 33.841202  |
| S       | 30.576475 | 29.770191  | 32.674488  |
| S       | 29.774555 | 31.525982  | 36.207554  |
| S       | 33.575104 | 27.416485  | 34.413258  |
| S       | 33.789799 | 32.641750  | 32.512974  |
| S       | 36.896564 | 28.674660  | 31.791235  |
| S       | 36.315029 | 29.771606  | 36.970772  |
| S       | 40.298954 | 27.023132  | 34.984913  |
| S       | 40.217918 | 31.437166  | 34.499176  |
| S       | 43.583851 | 28.929909  | 31.371651  |
| S       | 44.869125 | 27.792957  | 36.658279  |
S  36.853901  28.842875  32.112663
S  36.485256  30.135986  37.107620
S  40.164345  27.220436  35.083015
S  40.372639  31.556932  34.431435
S  43.489445  28.545904  31.317335
S  45.188747  27.365763  36.472275

generated by VMD
Ca  25.135878  29.469074  31.744404
Ca  26.321903  30.675205  35.484909
Ca  29.999819  28.161938  35.687428
Ca  30.112507  33.190941  33.324043
Ca  33.572094  29.674988  31.532084
Ca  33.222435  30.548754  35.309395
Ca  36.710503  27.321804  35.126968
Ca  36.868229  31.204529  33.813610
Ca  40.210796  29.130676  32.426552
Ca  39.618866  29.325621  37.229336
Ca  46.051395  26.251230  31.545723
Ca  43.128990  29.323769  34.384758
S  26.530746  27.306023  35.984663
S  26.682581  33.877373  34.412465
S  30.660069  29.794098  32.611691
S  29.826088  31.387295  36.143669
S  33.461769  27.491543  34.294838
S  33.725834  32.670261  32.587101
S  36.887489  28.771910  31.854897
S  36.402168  30.169540  36.960808
S  40.166794  27.009470  34.984367
S  40.414272  31.438038  34.486828
S  43.595047  28.645226  31.306450
S  45.127594  27.552059  36.792122

generated by VMD
Ca  25.538580  29.684889  31.859062
Ca  26.007387  30.702326  35.653229
Ca  29.966124  28.158260  35.555473
Ca  30.057068  33.181751  33.432522
Ca  33.651707  30.103090  31.612087
Ca  33.106853  30.418852  35.423271
Ca  37.110867  27.112961  34.837730
Ca  36.675106  30.869799  33.673935
Ca  39.957130  28.701061  32.196495
Ca  40.093330  29.640144  37.045052
Ca  46.038792  26.229942  31.993908
Ca  43.018375  29.563770  34.443832
| S     | 26.525963 | 27.127985 | 35.875267 |
| S     | 26.514593 | 34.001427 | 34.373871 |
| S     | 30.574038 | 30.071379 | 32.675686 |
| S     | 29.738789 | 31.269999 | 36.327240 |
| S     | 33.693535 | 27.713306 | 33.997936 |
| S     | 33.736629 | 32.909622 | 32.849747 |
| S     | 36.776878 | 28.477972 | 31.694885 |
| S     | 36.545654 | 29.756956 | 36.812111 |
| S     | 40.271770 | 27.079739 | 35.134621 |
| S     | 40.199677 | 31.359224 | 34.114502 |
| S     | 43.381126 | 28.259951 | 31.513618 |
| S     | 45.253975 | 27.996979 | 36.934566 |

24 generated by VMD

| Ca    | 25.248329 | 29.611015 | 31.820917 |
| Ca    | 26.211031 | 30.919445 | 35.976311 |
| Ca    | 30.077755 | 28.205070 | 35.705463 |
| Ca    | 30.124315 | 32.986313 | 33.425198 |
| Ca    | 33.473694 | 29.992039 | 31.193203 |
| Ca    | 33.106895 | 30.247240 | 35.264370 |
| Ca    | 36.781040 | 27.037197 | 34.726410 |
| Ca    | 36.729103 | 31.089041 | 34.007011 |
| Ca    | 40.229000 | 28.940563 | 32.223778 |
| Ca    | 39.926544 | 29.325727 | 36.813160 |
| Ca    | 46.144367 | 26.107254 | 31.968506 |
| Ca    | 43.236294 | 29.657585 | 34.470402 |
| S     | 26.562124 | 27.419312 | 36.102440 |
| S     | 26.670275 | 33.893604 | 34.144653 |
| S     | 30.467258 | 29.842445 | 32.594349 |
| S     | 29.830820 | 31.343822 | 36.344345 |
| S     | 33.340248 | 27.539444 | 33.810318 |
| S     | 33.661396 | 32.782265 | 32.891945 |
| S     | 36.816578 | 28.810352 | 31.921349 |
| S     | 36.367786 | 29.667393 | 36.834347 |
| S     | 40.281635 | 27.025520 | 34.888809 |
| S     | 40.333080 | 31.514641 | 34.157654 |
| S     | 43.613716 | 28.295404 | 31.686462 |
| S     | 45.200619 | 28.138721 | 37.059235 |

24 generated by VMD

| Ca    | 25.233236 | 29.639584 | 31.700161 |
| Ca    | 26.014977 | 30.881332 | 35.607170 |
| Ca    | 29.809750 | 27.991310 | 36.008968 |
| Ca    | 30.182758 | 32.893345 | 33.294800 |
| Ca    | 33.486557 | 29.539875 | 31.266975 |
| Ca    | 33.294205 | 30.444164 | 35.458740 |
| Element | X Coordinates | Y Coordinates | Z Coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 36.654915     | 27.119373     | 34.894699     |
| Ca      | 36.948429     | 31.080006     | 34.214102     |
| Ca      | 40.208969     | 29.254601     | 32.097042     |
| Ca      | 39.871399     | 29.489820     | 36.942787     |
| Ca      | 46.323914     | 26.306484     | 31.604046     |
| Ca      | 43.276428     | 29.451725     | 34.575283     |
| S       | 26.354612     | 27.416409     | 35.996696     |
| S       | 26.736710     | 33.969410     | 33.979080     |
| S       | 30.486679     | 29.762491     | 32.809898     |
| S       | 29.598457     | 31.412621     | 36.382706     |
| S       | 33.497181     | 27.636040     | 34.041901     |
| S       | 33.889343     | 32.570190     | 32.680862     |
| S       | 36.826744     | 28.827940     | 32.071053     |
| S       | 36.418015     | 29.830753     | 37.131149     |
| S       | 40.095810     | 27.141150     | 34.665318     |
| S       | 40.525593     | 31.566095     | 34.167931     |
| S       | 43.546124     | 28.407019     | 31.551609     |
| S       | 45.153126     | 27.759701     | 36.887749     |

24 generated by VMD

| Element | X Coordinates | Y Coordinates | Z Coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 25.558208     | 29.632198     | 31.768871     |
| Ca      | 26.160034     | 30.641483     | 35.729328     |
| Ca      | 30.139725     | 28.188852     | 35.710342     |
| Ca      | 30.191084     | 32.999184     | 33.311039     |
| Ca      | 33.510292     | 29.559631     | 31.607758     |
| Ca      | 33.105152     | 30.634003     | 35.505653     |
| Ca      | 36.609009     | 27.167158     | 34.926407     |
| Ca      | 36.626720     | 31.048944     | 34.061775     |
| Ca      | 40.180199     | 29.260635     | 32.054432     |
| Ca      | 39.903526     | 29.575842     | 36.566906     |
| Ca      | 46.152153     | 26.046371     | 31.889473     |
| Ca      | 43.118248     | 29.407135     | 34.554241     |
| S       | 26.637917     | 27.333191     | 36.149357     |
| S       | 26.636948     | 33.786793     | 33.989761     |
| S       | 30.586829     | 29.865070     | 32.717777     |
| S       | 29.773071     | 31.34610      | 36.396603     |
| S       | 33.548691     | 27.728970     | 34.183323     |
| S       | 33.792046     | 32.744328     | 32.713093     |
| S       | 36.893375     | 28.680027     | 31.882061     |
| S       | 36.476799     | 29.939907     | 36.980278     |
| S       | 40.081532     | 26.901316     | 34.613464     |
| S       | 40.380966     | 31.741005     | 34.147404     |
| S       | 43.591694     | 28.596935     | 31.559387     |
| S       | 44.771080     | 27.567760     | 37.012005     |

24 generated by VMD
|   |   |   |
|---|---|---|
| Ca | 25.133139 | 29.591930 | 31.948940 |
| Ca | 26.102659 | 30.637657 | 35.574562 |
| Ca | 30.249138 | 28.022354 | 35.831841 |
| Ca | 30.082489 | 33.146347 | 33.074379 |
| Ca | 33.533531 | 29.905350 | 31.632355 |
| Ca | 33.145519 | 30.492821 | 35.520020 |
| Ca | 37.119728 | 27.012285 | 35.121422 |
| Ca | 36.587914 | 30.743982 | 33.996657 |
| Ca | 40.091339 | 28.994846 | 32.018288 |
| Ca | 39.876991 | 29.510296 | 36.790916 |
| Ca | 45.837059 | 26.140400 | 31.709034 |
| Ca | 43.183811 | 29.470726 | 34.577461 |
| S  | 36.690315 | 27.417503 | 36.091652 |
| S  | 26.698647 | 33.925819 | 34.182339 |
| S  | 30.653818 | 29.796062 | 32.725044 |
| S  | 29.710476 | 31.444725 | 36.129829 |
| S  | 33.881252 | 27.876362 | 34.209396 |
| S  | 33.708309 | 32.943359 | 32.669044 |
| S  | 36.963890 | 28.557693 | 31.576420 |
| S  | 36.500690 | 29.673023 | 36.910927 |
| S  | 40.486923 | 27.092995 | 34.844658 |
| S  | 40.282871 | 31.700951 | 34.149704 |
| S  | 43.445904 | 28.799377 | 31.519011 |
| S  | 44.467525 | 27.494576 | 37.223797 |

24

generated by VMD
S  40.346790  27.084164  34.703442
S  40.123863  31.567066  33.921150
S  43.654732  28.437464  31.731455
S  45.109997  27.906418  36.996780

24
generated by VMD
Ca  25.326351  29.995007  31.904551
Ca  26.369642  30.755894  35.653282
Ca  29.923937  28.124050  35.685165
Ca  30.205580  32.919037  33.442539
Ca  33.645477  29.423859  31.362314
Ca  33.162453  30.544048  35.606556
Ca  36.755051  26.899120  35.046776
Ca  36.434181  30.670748  33.826096
Ca  40.348061  29.110882  31.976879
Ca  39.688618  29.992111  36.714031
Ca  45.848358  26.020161  32.059692
Ca  42.967361  29.505516  34.496315
S  26.569260  27.233627  35.824173
S  26.978729  34.071365  34.353996
S  30.606140  29.882915  32.859062
S  29.803303  31.211960  36.470978
S  33.656963  27.781878  34.148346
S  33.800503  32.670776  32.613483
S  37.004051  28.472874  31.698704
S  36.331379  29.797806  36.921764
S  40.248585  27.159536  34.759811
S  39.994816  31.595203  33.839663
S  43.828964  28.708557  31.659245
S  44.936119  27.844418  37.107944

24
generated by VMD
Ca  25.380222  30.004826  31.730322
Ca  26.431322  30.611614  35.563267
Ca  30.168148  28.239616  35.829811
Ca  30.332596  33.000755  33.214554
Ca  33.638382  29.453926  31.544197
Ca  33.194180  30.586889  35.631645
Ca  36.774319  26.988398  35.151688
Ca  36.637184  30.800791  33.966515
Ca  40.038139  29.079430  32.030266
Ca  39.802376  29.611198  36.692856
Ca  45.627316  26.255844  31.973186
Ca  43.034977  29.632771  34.468685
S  26.449837  27.316177  35.769276
S  27.011202  33.789455  34.221184
|   | X       | Y       | Z       |
|---|---------|---------|---------|
| S | 30.601316 | 29.894573 | 32.776497 |
| S | 29.836832 | 31.362219 | 36.401260 |
| S | 33.620041 | 27.704241 | 34.232063 |
| S | 33.933777 | 32.552017 | 32.815941 |
| S | 36.789734 | 28.388172 | 31.752956 |
| S | 36.437866 | 29.653238 | 36.974636 |
| S | 40.210754 | 27.078478 | 34.687340 |
| S | 40.139416 | 31.721264 | 33.968044 |
| S | 43.398609 | 28.675516 | 31.546299 |
| S | 44.939751 | 27.990023 | 37.088184 |

24 generated by VMD

| Ca   | X       | Y       | Z       |
|------|---------|---------|---------|
| Ca   | 25.436047 | 29.942226 | 31.949371 |
| Ca   | 26.490599 | 30.529535 | 35.668659 |
| Ca   | 30.292400 | 28.205315 | 35.666180 |
| Ca   | 30.326458 | 32.878239 | 33.558319 |
| Ca   | 33.658539 | 29.672516 | 31.294874 |
| Ca   | 33.058601 | 30.777508 | 35.768635 |
| Ca   | 36.907795 | 27.129490 | 34.771637 |
| Ca   | 36.710854 | 30.975189 | 33.761292 |
| Ca   | 39.765282 | 28.926437 | 32.124023 |
| Ca   | 39.707943 | 30.031059 | 36.622475 |
| Ca   | 45.541836 | 25.684759 | 32.524498 |
| Ca   | 42.809750 | 29.612871 | 34.489059 |
| Ca   | 25.452766 | 29.814384 | 31.795666 |
| Ca   | 26.531200 | 30.532204 | 35.841034 |
| Ca   | 30.119787 | 28.179875 | 35.727585 |
| Ca   | 30.134127 | 33.159359 | 33.363483 |
| Ca   | 33.516747 | 29.791559 | 31.412624 |
| Ca   | 33.175636 | 30.609547 | 35.492176 |
| Ca   | 37.015362 | 26.770752 | 34.770893 |
| Ca   | 36.549435 | 30.840071 | 33.910686 |

755
| Element | Value1      | Value2      | Value3      |
|---------|-------------|-------------|-------------|
| Ca      | 40.049858   | 28.808950   | 31.962334   |
| Ca      | 39.822395   | 30.173016   | 36.814854   |
| Ca      | 45.445091   | 25.607267   | 32.256958   |
| Ca      | 42.870842   | 29.776844   | 34.663548   |
| S       | 26.655293   | 27.199898   | 35.950035   |
| S       | 26.739431   | 33.660927   | 34.255291   |
| S       | 30.540783   | 30.083050   | 32.745800   |
| S       | 29.919449   | 31.339691   | 36.423702   |
| S       | 33.537025   | 27.892553   | 34.036591   |
| S       | 33.887024   | 32.922161   | 32.820549   |
| S       | 36.698483   | 28.460432   | 31.690094   |
| S       | 36.591251   | 29.380386   | 36.595642   |
| S       | 40.301178   | 27.220303   | 34.985207   |
| S       | 40.146183   | 31.600033   | 33.748146   |
| S       | 43.724613   | 28.600971   | 31.779064   |
| S       | 45.009949   | 27.967180   | 36.988823   |
| S       | 26.419210   | 30.701557   | 35.991489   |

24 generated by VMD
| Element | Value1      | Value2      | Value3      |
|---------|-------------|-------------|-------------|
| Ca      | 25.482235   | 30.155579   | 31.629261   |
| Ca      | 26.367928   | 30.773876   | 35.774452   |
| Ca      | 30.159929   | 28.005737   | 35.819214   |
| Ca      | 30.233250   | 32.848705   | 33.506283   |
| Ca      | 33.514782   | 29.654469   | 31.538921   |
| Ca      | 33.220551   | 30.370647   | 35.592037   |
| Ca      | 36.841541   | 27.157692   | 34.999863   |
| Ca      | 36.532772   | 30.885082   | 33.727009   |
| Ca      | 40.003647   | 28.853239   | 31.932621   |
| Ca      | 39.930241   | 30.069923   | 36.374664   |
| Ca      | 45.485481   | 26.013828   | 32.458004   |
| Ca      | 43.056923   | 29.706686   | 34.609261   |
| S       | 26.718933   | 27.439816   | 35.687164   |
| S       | 26.940090   | 33.835529   | 34.486481   |
| S       | 30.627033   | 29.732040   | 32.867634   |
| S       | 29.938633   | 31.222979   | 36.365715   |
| S       | 33.599731   | 27.577929   | 34.075111   |
| S       | 33.636883   | 32.666523   | 32.859810   |
| S       | 36.790005   | 28.338760   | 31.727501   |
| S       | 36.471748   | 29.775961   | 36.707275   |
| S       | 40.216244   | 26.934994   | 34.722763   |
| S       | 40.276237   | 31.745495   | 33.743767   |
| S       | 43.580643   | 28.658867   | 31.615894   |
| S       | 44.808460   | 27.967075   | 37.209972   |

24 generated by VMD
| Element | Value1      | Value2      | Value3      |
|---------|-------------|-------------|-------------|
| Ca      | 25.426851   | 29.718086   | 31.616024   |
| Ca      | 26.419210   | 30.701557   | 35.991489   |
| Element | Ca       | 30.287294 | 28.094473 | 35.750862 |
|----------|----------|-----------|-----------|-----------|
|          | 29.969013| 33.067623 | 33.375626 |
|          | 33.651295| 29.911760 | 31.485806 |
|          | 33.097294| 30.525822 | 35.616409 |
|          | 36.635361| 26.869820 | 34.843147 |
|          | 36.771736| 30.939285 | 33.808544 |
|          | 40.138630| 29.026268 | 31.866169 |
|          | 40.041916| 29.980558 | 36.549862 |
|          | 45.574635| 25.700989 | 32.521553 |
|          | 42.847046| 29.687477 | 34.538513 |
|          | 26.713428| 27.418438 | 35.771549 |
|          | 26.634113| 33.746109 | 34.582623 |
|          | 30.732277| 29.848093 | 32.779408 |
|          | 29.766817| 31.244759 | 36.358597 |
|          | 33.526184| 27.601837 | 34.122143 |
|          | 33.715214| 32.792198 | 32.748981 |
|          | 36.824432| 28.568933 | 31.831263 |
|          | 36.477055| 29.760902 | 36.723228 |
|          | 40.187962| 27.026810 | 34.589020 |
|          | 40.426193| 31.809252 | 33.740334 |
|          | 43.715832| 28.330181 | 31.791025 |
|          | 44.854107| 28.020222 | 37.028511 |

24

generated by VMD

| Element | Ca       | 25.359867 | 29.993317 | 32.060402 |
|----------|----------|-----------|-----------|-----------|
|          | 26.468557| 30.691620 | 35.914238 |
|          | 30.467552| 27.805031 | 35.699795 |
|          | 30.304146| 32.899651 | 33.554310 |
|          | 33.692154| 29.981857 | 31.397987 |
|          | 33.244499| 30.549500 | 35.537945 |
|          | 36.650982| 26.860210 | 34.860302 |
|          | 36.704926| 31.159775 | 33.421371 |
|          | 40.079174| 28.945936 | 31.921503 |
|          | 39.827084| 30.061356 | 36.952072 |
|          | 45.549744| 25.648968 | 32.640503 |
|          | 42.954472| 29.692810 | 34.619835 |
|          | 26.787598| 27.231815 | 35.727650 |
|          | 26.736279| 33.833961 | 34.408516 |
|          | 30.682980| 29.835009 | 32.789585 |
|          | 29.935459| 31.005772 | 36.509247 |
|          | 33.493469| 27.577204 | 34.118210 |
|          | 33.662212| 32.920498 | 32.544983 |
|          | 36.758610| 28.518261 | 31.744316 |
|          | 36.562714| 29.834183 | 36.343109 |
|          | 40.204781| 27.274111 | 34.744289 |
|          | 40.115967| 31.795132 | 33.605305 |
| Element | X1          | Y1          | Z1          |
|---------|-------------|-------------|-------------|
| S       | 43.630402   | 28.507410   | 31.740814   |
| S       | 44.560211   | 27.768024   | 37.174454   |

generated by VMD

| Element | X2          | Y2          | Z2          |
|---------|-------------|-------------|-------------|
| Ca      | 25.236832   | 29.753147   | 31.740215   |
| Ca      | 26.160345   | 30.633949   | 35.782928   |
| Ca      | 30.279564   | 27.950661   | 35.679779   |
| Ca      | 30.361059   | 32.885162   | 33.523781   |
| Ca      | 33.599659   | 30.029274   | 31.435488   |
| Ca      | 33.095985   | 30.589886   | 35.533428   |

generated by VMD

| Element | X3          | Y3          | Z3          |
|---------|-------------|-------------|-------------|
| Ca      | 36.817719   | 27.083612   | 34.979809   |
| Ca      | 36.718624   | 31.058918   | 33.815617   |
| Ca      | 40.103760   | 29.099129   | 32.089199   |
| Ca      | 40.056416   | 30.077892   | 36.787907   |
| Ca      | 45.387779   | 25.721579   | 32.468018   |
| Ca      | 43.011089   | 29.481693   | 34.403221   |
| S       | 26.874638   | 27.214630   | 35.761665   |
| S       | 26.969526   | 33.703842   | 34.199425   |
| S       | 30.564220   | 29.797012   | 32.679207   |
| S       | 29.606382   | 31.155344   | 36.463150   |
| S       | 33.382557   | 27.701626   | 34.184540   |
| S       | 33.718483   | 32.930714   | 32.937969   |
| S       | 36.788376   | 28.678280   | 31.828911   |
| S       | 36.579933   | 29.794653   | 36.659538   |
| S       | 40.215405   | 27.100958   | 34.690994   |
| S       | 40.406834   | 31.860882   | 33.765308   |
| S       | 43.417946   | 28.173214   | 31.518005   |
| S       | 45.080765   | 27.915379   | 37.102577   |

generated by VMD

| Element | X4          | Y4          | Z4          |
|---------|-------------|-------------|-------------|
| Ca      | 25.368624   | 29.760141   | 31.973686   |
| Ca      | 26.612986   | 30.506889   | 35.931549   |
| Ca      | 30.352922   | 27.990156   | 35.639553   |
| Ca      | 30.351988   | 33.218700   | 33.469913   |
| Ca      | 33.575275   | 29.875601   | 31.567060   |
| Ca      | 33.349220   | 30.465351   | 35.501972   |
| Ca      | 36.632137   | 26.903976   | 34.553165   |
| Ca      | 36.718227   | 31.010059   | 33.682541   |
| Ca      | 40.072067   | 28.908165   | 31.793476   |
| Ca      | 39.617950   | 30.245918   | 36.956295   |
| Ca      | 45.529404   | 25.483717   | 32.728916   |
| Ca      | 42.748623   | 29.645782   | 34.513107   |
| S       | 26.916004   | 27.115223   | 35.906487   |
| S       | 26.879463   | 33.721321   | 34.536484   |
| S       | 30.672770   | 30.080128   | 32.775036   |
| S       | 30.041759   | 31.151157   | 36.435009   |
|    |      X   |      Y   |      Z   |
|----|---------|---------|---------|
| S  | 33.496822 | 27.686792 | 33.901154 |
| S  | 33.763203 | 32.860455 | 31.443953 |
| S  | 36.805855 | 28.647217 | 36.507755 |
| S  | 40.17147  | 27.133112 | 34.750561 |
| S  | 40.162186 | 31.706837 | 33.706905 |
| S  | 43.595707 | 28.397961 | 31.842199 |
| S  | 44.646595 | 28.159580 | 37.262539 |

24

generated by VMD

|    |      X   |      Y   |      Z   |
|----|---------|---------|---------|
| Ca | 25.322803 | 30.028618 | 31.736549 |
| Ca | 26.527353 | 30.717789 | 36.061424 |
| Ca | 30.232298 | 29.68386  | 35.687981 |
| Ca | 30.027868 | 33.093994 | 33.320812 |
| Ca | 33.456768 | 29.837273 | 31.297741 |
| Ca | 33.082554 | 30.374462 | 35.316082 |
| Ca | 37.046787 | 27.066536 | 35.008465 |
| Ca | 36.611759 | 30.885262 | 33.812580 |
| Ca | 40.072876 | 28.909794 | 32.079681 |
| Ca | 39.731869 | 30.058254 | 36.719143 |
| Ca | 45.527485 | 25.626518 | 32.264702 |
| Ca | 42.952560 | 29.709406 | 34.688393 |
| S  | 26.614834 | 27.455017 | 35.811703 |
| S  | 26.846180 | 33.733002 | 34.492790 |
| S  | 30.702564 | 29.913034 | 32.577240 |
| S  | 30.083664 | 31.060116 | 36.452110 |
| S  | 33.521793 | 27.471928 | 34.136902 |
| S  | 33.717209 | 32.824787 | 32.704029 |
| S  | 36.754337 | 28.608543 | 31.715298 |
| S  | 36.365055 | 29.639696 | 36.637821 |
| S  | 40.327957 | 27.149088 | 34.804119 |
| S  | 40.180511 | 31.666958 | 33.800541 |
| S  | 43.578491 | 28.479637 | 31.776825 |
| S  | 45.148327 | 28.113247 | 37.127716 |

24

generated by VMD

|    |      X   |      Y   |      Z   |
|----|---------|---------|---------|
| Ca | 25.261681 | 29.780476 | 31.571323 |
| Ca | 26.392132 | 30.777620 | 35.808254 |
| Ca | 30.154318 | 28.009571 | 35.781845 |
| Ca | 30.228954 | 32.945747 | 33.704967 |
| Ca | 33.638405 | 30.069790 | 31.512733 |
| Ca | 33.042603 | 30.582468 | 35.490559 |
| Ca | 37.048358 | 26.829884 | 34.760406 |
| Ca | 36.603516 | 30.817335 | 33.819855 |
| Ca | 40.134907 | 28.766621 | 31.933598 |
| Ca | 39.858685 | 30.183437 | 36.656208 |
| Ca  | 45.699005 | 25.890497 | 32.382957 |
| Ca  | 42.883804 | 29.572639 | 34.669250 |
| S   | 26.688671 | 27.450615 | 35.993828 |
| S   | 26.926018 | 33.738735 | 34.243668 |
| S   | 30.615751 | 29.979822 | 32.764160 |
| S   | 29.925632 | 31.145115 | 36.633121 |
| S   | 33.539036 | 27.671610 | 34.136333 |
| S   | 33.732403 | 32.884686 | 32.785011 |
| S   | 36.792885 | 28.547943 | 31.644333 |
| S   | 36.429550 | 29.437706 | 36.603638 |
| S   | 40.423756 | 27.064068 | 34.550709 |
| S   | 40.221096 | 31.573208 | 33.552464 |
| S   | 43.610054 | 28.470749 | 31.597530 |
| S   | 44.582413 | 28.201080 | 37.433830 |

24 generated by VMD

| Ca  | 25.311975 | 29.612263 | 31.864559 |
| Ca  | 26.383755 | 30.712357 | 36.022381 |
| Ca  | 30.256569 | 27.967319 | 35.752167 |
| Ca  | 30.124538 | 33.003227 | 33.257130 |
| Ca  | 33.516121 | 30.103260 | 31.339771 |
| Ca  | 33.029076 | 30.545517 | 35.390629 |
| Ca  | 37.013161 | 27.139793 | 34.965759 |
| Ca  | 36.525150 | 31.109985 | 33.894333 |
| Ca  | 40.023552 | 28.989040 | 31.944586 |
| Ca  | 39.805588 | 30.021219 | 36.753185 |
| Ca  | 45.599510 | 25.620544 | 32.426079 |
| Ca  | 42.949440 | 29.572792 | 34.502903 |
| S   | 26.634138 | 27.361382 | 35.914822 |
| S   | 26.773806 | 33.487968 | 34.299606 |
| S   | 30.777222 | 29.829075 | 32.694706 |
| S   | 29.949717 | 31.161806 | 36.413815 |
| S   | 33.717606 | 27.674789 | 34.159809 |
| S   | 33.866745 | 33.022701 | 32.747681 |
| S   | 36.809715 | 28.895386 | 31.538548 |
| S   | 36.366215 | 29.727880 | 36.688248 |
| S   | 40.260197 | 26.975552 | 34.804974 |
| S   | 40.340611 | 31.847612 | 33.896507 |
| S   | 43.543732 | 28.332930 | 31.588955 |
| S   | 44.855759 | 27.676983 | 37.169571 |

24 generated by VMD

| Ca  | 25.529434 | 29.910454 | 31.578659 |
| Ca  | 26.381636 | 30.709091 | 35.855198 |
| Ca  | 30.155676 | 28.117832 | 35.758430 |
| Ca  | 30.064198 | 33.105728 | 33.509663 |
| Element | X  | Y  | Z  |
|---------|----|----|----|
| Ca      | 33.547035 | 29.775831 | 31.571362 |
| Ca      | 33.209793 | 30.331104 | 35.556339 |
| Ca      | 36.844288 | 26.868961 | 34.851173 |
| Ca      | 36.764324 | 30.986811 | 33.770969 |
| Ca      | 40.052258 | 28.900467 | 31.910030 |
| Ca      | 39.925461 | 30.271540 | 36.862595 |
| Ca      | 45.550621 | 25.796520 | 32.403992 |
| Ca      | 42.918060 | 29.529860 | 34.406120 |
| S       | 26.407049 | 27.350388 | 35.874001 |
| S       | 26.758463 | 33.799076 | 34.316273 |
| S       | 30.521671 | 29.839653 | 32.721867 |
| S       | 29.870846 | 31.155338 | 36.585392 |
| S       | 33.596119 | 27.471745 | 34.269402 |
| S       | 33.664055 | 32.900440 | 32.793098 |
| S       | 36.821732 | 28.577465 | 31.584232 |
| S       | 36.620567 | 29.688210 | 36.498184 |
| S       | 40.391476 | 27.039806 | 34.786053 |
| S       | 40.370747 | 31.715302 | 33.728168 |
| S       | 43.653728 | 28.552265 | 31.553263 |
| S       | 44.814667 | 27.997522 | 37.288933 |

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generated by VMD

| Element | X  | Y  | Z  |
|---------|----|----|----|
| Ca      | 25.479362 | 29.864899 | 31.756248 |
| Ca      | 26.637844 | 30.701286 | 35.946320 |
| Ca      | 30.257227 | 27.984541 | 35.663582 |
| Ca      | 30.211311 | 32.851013 | 33.480103 |
| Ca      | 33.443695 | 30.011944 | 31.391285 |
| Ca      | 33.176727 | 30.522820 | 35.364277 |
| Ca      | 37.084297 | 27.020924 | 35.027695 |
| Ca      | 36.811996 | 31.046253 | 33.733986 |
| Ca      | 39.903191 | 28.937908 | 32.050949 |
| Ca      | 39.833172 | 30.257812 | 36.757133 |
| Ca      | 45.590973 | 25.845175 | 32.052990 |
| Ca      | 43.119526 | 29.545845 | 34.618629 |
| S       | 26.472004 | 27.307537 | 35.778999 |
| S       | 26.934551 | 33.740784 | 34.462513 |
| S       | 30.458851 | 29.751501 | 32.626637 |
| S       | 30.056175 | 31.037029 | 36.439014 |
| S       | 33.537037 | 27.636230 | 34.074532 |
| S       | 33.693211 | 32.897911 | 32.680950 |
| S       | 36.576611 | 28.505947 | 31.774017 |
| S       | 36.442608 | 29.864189 | 36.524292 |
| S       | 40.310318 | 26.966797 | 35.127434 |
| S       | 40.353775 | 31.719782 | 33.694542 |
| S       | 43.489315 | 28.609894 | 31.696968 |
| S       | 44.560059 | 27.763420 | 37.307579 |
|    |    |    |    |
|----|----|----|----|
| Ca | 25.596815 | 29.515991 | 31.742367 |
| Ca | 26.155411 | 30.891167 | 35.963974 |
| Ca | 30.241934 | 28.094131 | 35.708290 |
| Ca | 30.238222 | 35.963974 | 33.454822 |
| Ca | 33.487736 | 29.915710 | 31.311682 |
| Ca | 33.106735 | 30.469711 | 35.484486 |
| Ca | 37.085236 | 26.859793 | 34.902882 |
| Ca | 36.633698 | 30.965199 | 33.945782 |
| Ca | 40.052399 | 28.904293 | 31.894468 |
| Ca | 39.958694 | 29.843109 | 36.715630 |
| Ca | 45.609909 | 25.926857 | 32.138901 |
| Ca | 42.986912 | 29.550869 | 34.548645 |
| S  | 26.729416 | 27.425385 | 35.993389 |
| S  | 26.924307 | 33.679653 | 34.264362 |
| S  | 30.564404 | 29.980591 | 32.657906 |
| S  | 29.828930 | 31.283552 | 36.473896 |
| S  | 33.551472 | 27.712875 | 33.950821 |
| S  | 33.658916 | 32.905899 | 32.962017 |
| S  | 36.705273 | 28.687969 | 31.655123 |
| S  | 36.521091 | 29.461967 | 36.700050 |
| S  | 40.247196 | 26.982914 | 34.813019 |
| S  | 40.321953 | 31.574116 | 33.790489 |
| S  | 43.467087 | 28.556129 | 31.674023 |
| S  | 44.760185 | 28.112017 | 37.393028 |

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|    |    |    |    |
|----|----|----|----|
| Ca | 25.563961 | 29.802227 | 31.758770 |
| Ca | 26.458862 | 30.691124 | 35.933811 |
| Ca | 30.320589 | 28.047503 | 35.94063 |
| Ca | 30.451675 | 32.834187 | 33.508034 |
| Ca | 33.592598 | 29.855412 | 31.380329 |
| Ca | 33.257984 | 30.426666 | 35.453167 |
| Ca | 36.881310 | 27.068977 | 34.633945 |
| Ca | 37.000000 | 31.214390 | 33.779102 |
| Ca | 40.082397 | 28.982960 | 31.953981 |
| Ca | 39.873245 | 30.268684 | 36.860279 |
| Ca | 45.644733 | 26.025982 | 32.207588 |
| Ca | 42.993816 | 29.299557 | 34.530144 |
| S  | 26.230106 | 27.378174 | 35.842426 |
| S  | 26.765242 | 33.548283 | 34.171410 |
| S  | 30.574202 | 29.842709 | 32.834126 |
| S  | 29.863525 | 31.224060 | 36.665359 |
| S  | 33.478111 | 27.524303 | 34.066135 |
| S  | 33.804771 | 32.770905 | 32.923592 |
S  
36.692966  28.551476  31.479597
S  
36.596802  29.801086  36.518204
S  
40.055073  27.222660  34.815716
S  
40.361553  31.694839  33.718769
S  
43.529087  28.436005  31.695669
S  
44.361271  27.879230  37.361366

24

generated by VMD

Ca  
25.471218  30.014965  31.918682
Ca  
26.436646  30.935707  35.883976
Ca  
29.962067  27.961569  35.804462
Ca  
30.367254  32.667141  33.389618
Ca  
33.511223  29.923361  31.310019
Ca  
33.217121  30.133419  35.385376
Ca  
36.981842  26.953758  34.629059
Ca  
36.872425  31.131516  34.080914
Ca  
39.961044  29.015621  31.988338
Ca  
39.708733  30.345148  36.893024
Ca  
45.477386  25.557945  32.582310
Ca  
42.787624  29.727976  34.531639

S  
26.464367  27.529819  35.779114
S  
27.161827  33.767136  34.268715
S  
30.602011  29.601963  32.776714
S  
30.052786  31.070194  36.404034
S  
33.532093  27.350079  33.991783
S  
33.755424  32.741165  33.012939
S  
36.710129  28.746517  31.433086
S  
36.536785  29.549702  36.678421
S  
40.233299  27.223522  34.888733
S  
40.206886  31.701904  33.593132
S  
43.417274  28.454218  31.721897
S  
45.066424  28.287014  37.084705

24

generated by VMD

Ca  
25.446743  29.880283  31.704479
Ca  
26.442314  30.751446  35.873123
Ca  
29.972433  27.952438  35.752956
Ca  
29.893351  33.034050  33.599815
Ca  
33.349022  29.748951  31.655169
Ca  
33.213951  30.357002  35.437851
Ca  
36.621666  26.825062  34.498817
Ca  
36.873009  31.540522  33.685169
Ca  
40.335411  29.045181  31.854420
Ca  
39.949635  30.396820  36.527813
Ca  
45.909546  25.460745  32.523369
Ca  
43.030357  29.485626  34.610893
|    |          |          |          |
|----|----------|----------|----------|
| S  | 26.438854| 27.213352| 36.171608|
| S  | 26.809486| 33.779251| 34.373047|
| S  | 30.289186| 29.800192| 32.753914|
| S  | 29.894283| 31.010258| 36.569088|
| S  | 33.326817| 27.468334| 34.120632|
| S  | 33.582977| 32.755440| 32.852421|
| S  | 36.804028| 28.842270| 31.599003|
| S  | 36.602833| 29.763021| 36.341610|
| S  | 40.036415| 27.364740| 34.643551|
| S  | 40.880814| 31.815086| 33.490566|
| S  | 43.992508| 28.359688| 31.833805|
| S  | 44.738232| 27.741631| 37.557663|

24

generated by VMD

|    |          |          |          |
|----|----------|----------|----------|
| Ca | 25.247669| 29.780895| 31.653923|
| Ca | 26.286308| 30.724125| 35.566921|
| Ca | 30.186850| 28.013357| 35.704437|
| Ca | 30.176291| 32.925072| 33.544640|
| Ca | 33.412380| 29.718693| 31.707581|
| Ca | 33.241596| 30.485256| 35.570053|
| Ca | 36.947041| 26.893406| 34.720028|
| Ca | 36.971214| 31.380840| 33.885582|
| Ca | 40.079048| 28.910700| 31.927189|
| Ca | 40.022278| 30.339985| 36.828732|
| Ca | 45.768074| 25.734772| 32.180149|
| Ca | 42.988686| 29.572592| 34.533306|
| S  | 26.583225| 27.271759| 35.866158|
| S  | 26.742203| 33.725616| 34.123329|
| S  | 30.454512| 29.771320| 32.796352|
| S  | 29.801640| 31.181007| 36.459732|
| S  | 33.482876| 27.631153| 34.189304|
| S  | 33.721878| 32.851452| 32.976109|
| S  | 36.719326| 28.778309| 31.876087|
| S  | 36.661186| 29.742100| 36.689571|
| S  | 40.181496| 27.374096| 34.813290|
| S  | 40.467480| 31.568193| 33.574345|
| S  | 43.493671| 28.419117| 31.552994|
| S  | 44.797001| 27.597635| 37.290848|

24

generated by VMD

|    |          |          |          |
|----|----------|----------|----------|
| Ca | 25.381401| 29.748119| 31.697052|
| Ca | 26.344322| 30.295504| 35.772964|
| Ca | 30.143518| 28.126141| 35.827641|
| Ca | 30.346794| 32.949505| 33.646645|
| Ca | 33.532192| 30.066299| 31.551426|
| Ca | 33.041878| 30.442305| 35.339355|
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Ca      | 36.818737  | 27.196609  | 35.067242  |
| Ca      | 36.675621  | 31.240532  | 33.682968  |
| Ca      | 40.318100  | 28.865211  | 31.879461  |
| Ca      | 40.115753  | 30.520557  | 36.638515  |
| Ca      | 45.603210  | 25.621763  | 32.371006  |
| Ca      | 42.967091  | 29.362431  | 34.584488  |
| S       | 26.626141  | 27.064037  | 35.714607  |
| S       | 27.007465  | 33.624943  | 34.469326  |
| S       | 30.624941  | 29.931307  | 32.781677  |
| S       | 29.843815  | 31.188251  | 36.560329  |
| S       | 33.321678  | 27.565155  | 34.199997  |
| S       | 33.837887  | 32.954960  | 32.837421  |
| S       | 36.715374  | 28.606312  | 31.641806  |
| S       | 36.536232  | 30.020714  | 36.587139  |
| S       | 40.049568  | 27.351093  | 34.704933  |
| S       | 40.465607  | 31.623646  | 33.426140  |
| S       | 43.553146  | 28.400124  | 31.734356  |
| S       | 44.563450  | 27.625904  | 37.314262  |

24 generated by VMD

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Ca      | 25.610535  | 30.091639  | 31.552986  |
| Ca      | 26.398651  | 30.283535  | 35.772533  |
| Ca      | 29.880846  | 28.283646  | 35.997223  |
| Ca      | 30.258556  | 33.077385  | 33.420094  |
| Ca      | 33.508492  | 29.635933  | 31.596083  |
| Ca      | 33.284878  | 30.511250  | 35.540703  |
| Ca      | 37.078011  | 27.195099  | 34.822300  |
| Ca      | 36.781307  | 31.017374  | 33.725491  |
| Ca      | 40.098652  | 28.818468  | 31.781731  |
| Ca      | 39.973339  | 30.306248  | 36.749752  |
| Ca      | 45.570591  | 25.832039  | 32.238129  |
| Ca      | 42.818878  | 29.514744  | 34.506943  |
| S       | 26.432644  | 27.027668  | 35.532372  |
| S       | 26.827906  | 33.752136  | 34.469536  |
| S       | 30.666904  | 29.776541  | 32.876705  |
| S       | 29.912107  | 31.357632  | 36.635067  |
| S       | 33.728573  | 27.729139  | 34.369495  |
| S       | 33.713531  | 32.707211  | 32.905029  |
| S       | 36.685162  | 28.410069  | 31.646626  |
| S       | 36.775284  | 29.832542  | 36.658852  |
| S       | 40.278500  | 27.308767  | 34.842236  |
| S       | 40.303337  | 31.716413  | 33.430840  |
| S       | 43.682163  | 28.443371  | 31.624340  |
| S       | 44.165012  | 27.762581  | 37.335648  |

24 generated by VMD
|   | Ca       | 25.303946 | 30.048189 | 31.781723 |
|---|----------|-----------|-----------|-----------|
|   | Ca       | 26.530024 | 30.339298 | 35.923435 |
|   | Ca       | 30.260439 | 28.282393 | 35.595936 |
|   | Ca       | 30.052977 | 33.055580 | 33.406734 |
|   | Ca       | 33.546597 | 29.770443 | 31.674835 |
|   | Ca       | 33.276863 | 30.739113 | 35.389374 |
|   | Ca       | 37.002293 | 27.072929 | 34.990852 |
|   | Ca       | 36.750610 | 31.127598 | 33.455391 |
|   | Ca       | 40.049622 | 28.754654 | 32.177368 |
|   | Ca       | 39.808342 | 30.321888 | 36.685829 |
|   | Ca       | 46.011517 | 25.657085 | 32.184765 |
|   | Ca       | 42.948818 | 29.621727 | 34.511230 |
|   | S        | 26.688120 | 26.852150 | 35.99655  |
|   | S        | 26.752127 | 33.623894 | 34.666317 |
|   | S        | 30.475800 | 29.859802 | 32.646236 |
|   | S        | 29.971342 | 31.289078 | 36.569221 |
|   | S        | 33.718269 | 27.869158 | 34.253899 |
|   | S        | 33.649498 | 32.898399 | 32.631351 |
|   | S        | 36.874290 | 28.304379 | 31.796303 |
|   | S        | 36.431255 | 30.002649 | 36.518646 |
|   | S        | 40.202221 | 27.263689 | 35.089558 |
|   | S        | 40.359638 | 31.743910 | 33.619377 |
|   | S        | 43.616550 | 28.588337 | 31.726635 |
|   | S        | 44.152763 | 27.305042 | 37.135963 |

24

generated by VMD

| Ca       | 25.436089 | 29.890551 | 31.837799 |
|----------|-----------|-----------|-----------|
| Ca       | 26.509052 | 30.372835 | 35.946022 |
| Ca       | 30.301691 | 27.969265 | 35.658207 |
| Ca       | 30.367331 | 32.804985 | 33.105648 |
| Ca       | 33.524529 | 29.928802 | 31.527073 |
| Ca       | 33.281712 | 30.550678 | 35.417778 |
| Ca       | 36.790886 | 27.173130 | 35.045551 |
| Ca       | 36.797443 | 31.317053 | 33.894203 |
| Ca       | 40.169701 | 29.008568 | 32.007088 |
| Ca       | 39.877552 | 30.610497 | 36.706665 |
| Ca       | 45.392956 | 25.303892 | 31.969666 |
| Ca       | 42.878250 | 29.474930 | 34.596390 |
| S        | 26.642235 | 27.017262 | 35.755211 |
| S        | 26.930912 | 33.461357 | 34.629192 |
| S        | 30.632484 | 29.744644 | 32.669273 |
| S        | 29.946087 | 31.227955 | 36.397461 |
| S        | 33.477711 | 27.633057 | 34.245934 |
| S        | 33.779549 | 32.948586 | 32.557903 |
| S        | 36.723877 | 28.803852 | 31.806725 |
| S        | 36.461796 | 29.974537 | 36.789146 |
|   | X     | Y     | Z     |
|---|-------|-------|-------|
| S | 40.253265 | 27.489758 | 34.944336 |
| S | 40.599716 | 31.847900 | 33.598511 |
| S | 43.537567 | 28.390352 | 31.636545 |
| S | 44.121483 | 27.447014 | 37.288391 |

24 generated by VMD

| Ca | X     | Y     | Z     |
|----|-------|-------|-------|
| Ca | 25.302483 | 29.964237 | 31.979816 |
| Ca | 26.151354 | 30.564774 | 35.855576 |
| Ca | 30.040924 | 28.344437 | 35.409714 |
| Ca | 30.223972 | 33.044945 | 33.500381 |
| Ca | 33.463989 | 29.305088 | 31.407227 |
| Ca | 33.326839 | 30.684109 | 35.364712 |
| Ca | 37.068699 | 27.094103 | 34.969368 |
| Ca | 36.852768 | 30.978340 | 33.743755 |
| Ca | 40.210114 | 29.058640 | 31.946877 |
| Ca | 39.769558 | 30.681549 | 36.874424 |
| Ca | 45.347103 | 25.370636 | 32.207302 |
| Ca | 42.983936 | 29.782005 | 34.702076 |
| S  | 26.679451 | 27.086971 | 35.851810 |
| S  | 26.874392 | 33.533375 | 34.762123 |
| S  | 30.474710 | 29.836193 | 32.492004 |
| S  | 30.136641 | 31.266714 | 36.496391 |
| S  | 33.710350 | 27.709179 | 34.156017 |
| S  | 33.682167 | 32.467438 | 32.633450 |
| S  | 36.966560 | 28.540352 | 31.618799 |
| S  | 36.517838 | 29.853498 | 36.671841 |
| S  | 40.354618 | 27.541302 | 34.880035 |
| S  | 40.024538 | 31.705547 | 33.600792 |
| S  | 43.755596 | 28.609291 | 31.666803 |
| S  | 44.115219 | 27.368685 | 37.239464 |

24 generated by VMD

| Ca | X     | Y     | Z     |
|----|-------|-------|-------|
| Ca | 25.790253 | 29.605331 | 31.770935 |
| Ca | 26.532278 | 30.519321 | 35.958443 |
| Ca | 30.166067 | 28.262264 | 35.476387 |
| Ca | 30.027063 | 32.978127 | 33.554974 |
| Ca | 33.382751 | 29.553572 | 31.530140 |
| Ca | 33.167046 | 30.589020 | 35.487419 |
| Ca | 36.827721 | 27.180765 | 34.785938 |
| Ca | 36.797016 | 31.311796 | 33.933990 |
| Ca | 40.198601 | 28.970512 | 31.715099 |
| Ca | 39.921246 | 30.365841 | 36.753567 |
| Ca | 45.725159 | 25.701942 | 32.494793 |
| Ca | 42.930500 | 29.455318 | 34.620987 |
| S  | 26.896160 | 27.118349 | 35.830528 |
| S  | 26.653397 | 33.748482 | 34.581757 |
|   | 30.270760 | 29.940170 | 32.616013 |
|---|-----------|-----------|-----------|
| S | 29.995749 | 31.421061 | 36.420822 |
| S | 33.498837 | 27.722496 | 34.219875 |
| S | 33.623150 | 32.801956 | 32.742126 |
| S | 36.700340 | 28.632698 | 31.706884 |
| S | 36.532890 | 29.876781 | 36.734833 |
| S | 40.299450 | 27.276869 | 34.598385 |
| S | 40.399498 | 31.584049 | 33.546974 |
| S | 43.688473 | 28.408268 | 31.697741 |
| S | 44.409462 | 27.366379 | 37.252125 |

24 generated by VMD

| Ca | 25.338058 | 29.976234 | 31.789970 |
|---|-----------|-----------|-----------|
| Ca | 26.559902 | 30.661858 | 36.009510 |
| Ca | 30.315548 | 28.097622 | 35.621243 |
| Ca | 30.082500 | 33.092598 | 33.605972 |
| Ca | 33.364002 | 29.442652 | 31.328154 |
| Ca | 33.348721 | 30.425468 | 35.392162 |
| Ca | 36.821980 | 27.212593 | 34.661995 |
| Ca | 36.858929 | 31.215796 | 33.745632 |
| Ca | 40.233021 | 29.007536 | 31.733582 |
| Ca | 39.794285 | 30.541811 | 36.885464 |
| Ca | 45.679317 | 25.511063 | 32.601639 |
| Ca | 42.688431 | 29.468761 | 34.720425 |
| S | 26.868149 | 27.089073 | 36.100929 |
| S | 26.643303 | 33.756897 | 34.458862 |
| S | 30.533838 | 29.948029 | 32.770214 |
| S | 30.108469 | 31.260710 | 36.564533 |
| S | 33.476715 | 27.464935 | 34.046936 |
| S | 33.671951 | 32.653938 | 32.658146 |
| S | 36.709309 | 28.473988 | 31.465431 |
| S | 36.588631 | 29.763260 | 36.617435 |
| S | 40.188549 | 27.483692 | 34.623684 |
| S | 40.384674 | 31.617043 | 33.402218 |
| S | 43.965351 | 28.754616 | 31.676050 |
| S | 44.210354 | 27.471172 | 37.550533 |

24 generated by VMD

| Ca | 25.036892 | 30.133163 | 32.020809 |
|---|-----------|-----------|-----------|
| Ca | 26.580173 | 30.549757 | 36.069946 |
| Ca | 30.234274 | 28.036697 | 35.659813 |
| Ca | 30.231565 | 32.795231 | 33.407532 |
| Ca | 33.350258 | 29.434326 | 30.978718 |
| Ca | 33.443367 | 30.360132 | 35.303871 |
| Ca | 36.807549 | 26.907269 | 34.618114 |
| Ca | 37.010242 | 31.291161 | 33.914993 |
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 40.245926  | 29.020340  | 31.818621  |
| Ca      | 39.809719  | 30.508999  | 36.597378  |
| Ca      | 45.394665  | 25.900925  | 32.808666  |
| Ca      | 43.076508  | 29.344458  | 34.685764  |
| S       | 26.786114  | 27.072088  | 35.943779  |
| S       | 26.680645  | 33.884499  | 34.919857  |
| S       | 30.387106  | 29.891739  | 32.577560  |
| S       | 30.184982  | 31.388988  | 36.530899  |
| S       | 33.367607  | 27.638903  | 33.849159  |
| S       | 33.830605  | 32.556412  | 32.513596  |
| S       | 36.756454  | 28.598042  | 31.647758  |
| S       | 36.717255  | 29.671566  | 36.481281  |
| S       | 40.135727  | 27.258690  | 34.733589  |
| S       | 40.453651  | 31.728230  | 33.471684  |
| S       | 43.678493  | 28.626299  | 31.643688  |
| S       | 44.234112  | 27.793442  | 37.833549  |

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generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.338669  | 29.73524   | 31.988731  |
| Ca      | 26.647686  | 30.659639  | 36.045265  |
| Ca      | 30.296244  | 27.956264  | 35.741974  |
| Ca      | 30.432859  | 33.021019  | 33.543140  |
| Ca      | 33.270672  | 29.933651  | 31.400528  |
| Ca      | 33.365574  | 30.436392  | 35.175613  |
| Ca      | 36.978230  | 26.848536  | 34.421883  |
| Ca      | 36.817242  | 31.215466  | 33.358437  |
| Ca      | 39.967117  | 29.020184  | 31.933464  |
| Ca      | 39.611366  | 30.400688  | 36.868053  |
| Ca      | 45.470966  | 25.504753  | 32.798130  |
| Ca      | 42.714577  | 29.757027  | 34.914158  |
| S       | 27.018221  | 27.153656  | 36.296753  |
| S       | 27.044949  | 33.829376  | 34.544872  |
| S       | 30.354599  | 29.928185  | 32.711040  |
| S       | 30.253775  | 31.157639  | 36.434505  |
| S       | 33.457386  | 27.371624  | 33.904449  |
| S       | 33.796356  | 32.711971  | 32.711769  |
| S       | 36.701363  | 28.746880  | 31.100311  |
| S       | 36.637642  | 29.516441  | 36.184864  |
| S       | 40.126366  | 27.442017  | 34.900902  |
| S       | 40.328239  | 31.720078  | 33.594391  |
| S       | 43.661953  | 28.759539  | 31.936249  |
| S       | 44.141804  | 27.566788  | 37.521164  |

24

generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.363159  | 29.980673  | 31.762144  |
| Ca      | 26.332088  | 30.846584  | 35.869545  |
| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 30.282076 | 27.950569 | 35.938114 |
| Ca      | 30.084980 | 33.022606 | 33.453732 |
| Ca      | 33.302238 | 30.206669 | 35.411594 |
| Ca      | 36.881077 | 27.011387 | 34.470394 |
| Ca      | 36.868862 | 31.067953 | 33.635639 |
| Ca      | 40.073803 | 29.104918 | 31.859552 |
| Ca      | 39.847073 | 30.277557 | 36.699024 |
| Ca      | 45.695962 | 25.886753 | 32.505043 |
| Ca      | 43.058891 | 29.506641 | 34.711720 |
| S       | 26.614088 | 33.975220 | 34.469379 |
| S       | 30.607313 | 29.650368 | 32.951462 |
| S       | 29.951336 | 31.245352 | 36.369576 |
| S       | 33.597847 | 27.420908 | 34.171654 |
| S       | 33.461826 | 32.617516 | 32.557095 |
| S       | 36.730804 | 28.771107 | 31.308453 |
| S       | 36.583275 | 29.618740 | 36.396400 |
| S       | 40.274433 | 27.320400 | 34.665283 |
| S       | 40.454239 | 31.702400 | 33.601677 |
| S       | 43.900917 | 28.842957 | 31.808151 |
| S       | 44.208885 | 27.461845 | 37.647575 |

24 generated by VMD

| Element | X2 | Y2 | Z2 |
|---------|----|----|----|
| Ca      | 25.418346 | 29.866741 | 31.876034 |
| Ca      | 26.299232 | 30.913197 | 35.750675 |
| Ca      | 30.276211 | 27.808010 | 35.641342 |
| Ca      | 30.241476 | 32.839397 | 33.847416 |
| Ca      | 33.355476 | 29.720974 | 31.543919 |
| Ca      | 33.330025 | 30.392933 | 35.342628 |
| Ca      | 36.759533 | 26.978474 | 34.696148 |
| Ca      | 36.978855 | 31.368839 | 33.724731 |
| Ca      | 40.174667 | 28.958279 | 31.893377 |
| Ca      | 39.873215 | 30.341042 | 36.830944 |
| Ca      | 45.652149 | 26.132374 | 32.504242 |
| Ca      | 42.905235 | 29.287008 | 34.517838 |
| S       | 26.637428 | 27.316383 | 36.071911 |
| S       | 26.933784 | 34.028400 | 33.835178 |
| S       | 30.436192 | 29.681543 | 32.735435 |
| S       | 29.978529 | 31.027435 | 36.639229 |
| S       | 33.436100 | 27.367826 | 34.326603 |
| S       | 33.622009 | 32.655792 | 32.902145 |
| S       | 36.721951 | 28.802553 | 31.678810 |
| S       | 36.637550 | 29.747072 | 36.514481 |
| S       | 40.169167 | 27.135883 | 34.454559 |
| S       | 40.547089 | 31.795670 | 33.724876 |
S  43.621941  28.633041  31.348974
S  44.427765  27.592533  37.629143

24 generated by VMD
Ca  25.408829  29.893406  31.923523
Ca  26.435444  30.757370  35.956360
Ca  30.174137  27.993622  35.755783
Ca  30.142277  33.045467  33.660229
Ca  33.237980  29.628162  31.375134
Ca  33.164371  30.411957  35.162586
Ca  36.947853  26.858498  34.768356
Ca  36.802372  31.091061  33.499676
Ca  40.173157  28.961039  31.665703
Ca  39.928757  30.203487  36.925838
Ca  45.889191  26.393753  32.864315
Ca  43.173958  29.241077  34.612316
S  26.751993  27.295847  35.999451
S  26.779669  34.007210  34.526257
S  30.457720  29.841854  32.627831
S  29.995131  31.183752  36.605751
S  33.392117  27.382750  33.967850
S  33.613895  32.799664  32.712231
S  36.682335  28.626770  31.540802
S  36.758808  29.739090  36.510357
S  40.265614  27.315609  34.536476
S  40.534767  31.582687  33.788124
S  43.616741  28.441732  31.489201
S  44.106819  27.695572  37.556534

24 generated by VMD
Ca  25.700285  29.776928  32.034485
Ca  26.678513  30.642052  36.063965
Ca  30.003235  28.086746  35.700981
Ca  30.259613  33.040817  33.733021
Ca  33.287804  29.803318  31.305717
Ca  33.298016  30.387188  35.223137
Ca  36.945946  27.173012  34.571045
Ca  36.742432  31.018394  33.744816
Ca  39.949802  28.906897  31.722029
Ca  39.846283  30.206106  36.799942
Ca  46.046883  26.261875  32.690159
Ca  43.086525  29.416399  34.623459
S  26.581854  27.290653  36.032570
S  26.833046  33.719513  34.435326
S  30.494030  30.015682  32.752605
S  30.202026  31.224916  36.403595
|    | 33.339336 | 27.495806 | 33.951550 |
|----|-----------|-----------|-----------|
| S  | 33.884247 | 32.811874 | 32.723557 |
| S  | 36.571083 | 28.530396 | 31.405668 |
| S  | 36.543823 | 29.622650 | 36.537148 |
| S  | 40.292866 | 27.062469 | 34.642059 |
| S  | 40.376667 | 31.605368 | 33.502308 |
| S  | 43.512737 | 28.490124 | 31.542694 |
| S  | 43.956749 | 27.802219 | 37.888863 |

24 generated by VMD

|    | 25.455591 | 30.028412 | 32.246075 |
|----|-----------|-----------|-----------|
| Ca | 26.613842 | 30.526451 | 36.270012 |
| Ca | 30.235479 | 27.939890 | 35.695587 |
| Ca | 30.451742 | 32.858459 | 33.606667 |
| Ca | 33.336624 | 29.939690 | 31.121014 |
| Ca | 33.174576 | 30.419844 | 35.153847 |
| Ca | 36.832436 | 27.291033 | 34.578465 |
| Ca | 37.102722 | 31.074707 | 33.742432 |
| Ca | 40.003113 | 28.800482 | 31.632532 |
| Ca | 39.714394 | 30.163925 | 36.527817 |
| Ca | 45.685287 | 26.300024 | 33.282330 |
| Ca | 43.136696 | 29.499678 | 34.630295 |
| S  | 26.647436 | 27.087559 | 35.882328 |
| S  | 27.039484 | 33.627853 | 34.743973 |
| S  | 30.437622 | 29.936615 | 32.580936 |
| S  | 30.106394 | 31.054281 | 36.498543 |
| S  | 33.354553 | 27.538200 | 33.837566 |
| S  | 34.060162 | 32.863243 | 32.668205 |
| S  | 36.526031 | 28.740818 | 31.426353 |
| S  | 36.499828 | 29.802166 | 36.428116 |
| S  | 40.083206 | 27.299892 | 34.752880 |
| S  | 40.428295 | 31.434044 | 33.368294 |
| S  | 43.532352 | 28.329132 | 31.520121 |
| S  | 43.976078 | 27.835018 | 37.836285 |

24 generated by VMD

|    | 25.421612 | 29.791960 | 32.057972 |
|----|-----------|-----------|-----------|
| Ca | 26.458656 | 30.783157 | 36.114693 |
| Ca | 30.144894 | 28.007763 | 35.641850 |
| Ca | 30.332947 | 32.959717 | 33.510735 |
| Ca | 33.472229 | 29.864691 | 31.292912 |
| Ca | 33.240234 | 30.349268 | 35.212105 |
| Ca | 36.856995 | 27.035957 | 34.694641 |
| Ca | 36.566799 | 30.924583 | 33.628571 |
| Ca | 40.273556 | 28.941837 | 31.783119 |
| Ca | 39.594131 | 29.932022 | 36.662628 |
|   |   |   |   |
|---|---|---|---|
| Ca | 45.682537 | 26.210808 | 32.742458 |
| Ca | 43.083805 | 29.462948 | 34.636143 |
| S  | 26.788448 | 27.164810 | 36.282787 |
| S  | 27.077427 | 33.885876 | 34.436226 |
| S  | 30.597082 | 30.015957 | 32.794308 |
| S  | 29.982029 | 31.205118 | 36.500618 |
| S  | 33.398380 | 27.510828 | 33.972389 |
| S  | 33.895302 | 32.962234 | 32.552311 |
| S  | 36.730000 | 28.544571 | 31.520115 |
| S  | 36.346218 | 29.499237 | 36.498230 |
| S  | 40.275826 | 27.256813 | 34.491341 |
| S  | 40.229763 | 31.700993 | 33.581619 |
| S  | 43.749817 | 28.669762 | 31.575493 |
| S  | 44.235115 | 27.710514 | 37.847397 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 25.360209 | 29.921070 | 32.312065 |
| Ca | 26.658060 | 30.684925 | 36.233998 |
| Ca | 30.398550 | 28.085136 | 35.739975 |
| Ca | 30.278038 | 33.092751 | 33.524944 |
| Ca | 33.503407 | 29.760748 | 31.082619 |
| Ca | 33.281319 | 30.382637 | 35.191242 |
| Ca | 36.735462 | 26.960760 | 34.499660 |
| Ca | 36.705582 | 30.821768 | 33.372673 |
| Ca | 40.040905 | 28.926292 | 31.852324 |
| Ca | 39.532646 | 30.020390 | 36.613384 |
| Ca | 45.815914 | 26.257404 | 33.071842 |
| Ca | 42.952862 | 29.646114 | 34.654266 |
| S  | 26.988438 | 27.103836 | 36.251820 |
| S  | 26.910183 | 33.786846 | 34.984642 |
| S  | 30.610266 | 30.040951 | 32.663364 |
| S  | 30.144199 | 31.356419 | 36.352402 |
| S  | 33.477200 | 27.643917 | 33.670784 |
| S  | 33.857906 | 32.776360 | 32.379204 |
| S  | 36.609196 | 28.539162 | 31.085766 |
| S  | 36.521164 | 29.421001 | 36.226036 |
| S  | 40.198708 | 27.161659 | 34.777126 |
| S  | 40.224346 | 31.670216 | 33.605679 |
| S  | 43.692039 | 28.704178 | 31.853867 |
| S  | 43.937347 | 27.626827 | 38.031651 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 25.440073 | 29.434263 | 32.023323 |
| Ca | 26.492601 | 30.942196 | 36.112694 |
| Ca | 30.479269 | 28.015804 | 35.855137 |
| Ca | 30.030771 | 33.109474 | 33.518505 |
| Element | Ca     | Ca     | Ca     | Ca     | Ca     | Ca     | Ca     |
|---------|--------|--------|--------|--------|--------|--------|--------|
|        | 33.406506 | 29.877106 | 31.050522 | 33.324829 | 30.604883 | 35.441 | 685 |
|        | Ca     | 36.775734 | 26.968962 | 33.471893 | 40.181690 | 28.845505 | 31.633274 |
|        |        | 39.418530 | 29.870350 | 36.610687 | 46.115479 | 26.653904 | 33.027012 |
|        |        | 42.897400 | 29.350975 | 34.679470 | 42.897400 | 29.350975 | 34.679470 |
|        | S     | 26.993546 | 27.351582 | 36.276978 | 26.871227 | 34.013813 | 34.799717 |
|        |        | 30.618290 | 30.097075 | 32.848927 | 29.971119 | 31.189137 | 36.603439 |
|        |        | 33.553833 | 27.833935 | 33.687252 | 33.856258 | 32.787460 | 32.696991 |
|        |        | 36.680103 | 28.525602 | 31.114204 | 36.407581 | 29.310066 | 36.263626 |
|        |        | 40.105804 | 27.020401 | 34.507431 | 40.010584 | 27.020401 | 34.507431 |
|        |        | 40.037983 | 31.432526 | 33.595596 | 43.747322 | 28.610615 | 31.666222 |
|        |        | 44.057404 | 27.716854 | 38.148777 | 44.057404 | 27.716854 | 38.148777 |

24 generated by VMD

| Element | Ca     | Ca     | Ca     | Ca     | Ca     | Ca     | Ca     |
|---------|--------|--------|--------|--------|--------|--------|--------|
|        | 25.338163 | 29.536663 | 32.353783 | 26.573452 | 30.635735 | 36.114384 |
|        | Ca     | 30.432083 | 28.067083 | 35.756447 | 30.069578 | 33.009735 | 33.584007 |
|        |        | 33.321732 | 30.034784 | 30.921658 | 33.130138 | 30.599203 | 35.108257 |
|        |        | 36.987606 | 27.280632 | 34.283302 | 36.680103 | 28.525602 | 31.114204 |
|        |        | 36.646385 | 31.209488 | 33.553600 | 40.285427 | 29.033947 | 31.726311 |
|        |        | 39.720806 | 29.800518 | 36.615570 | 40.010584 | 27.020401 | 34.507431 |
|        |        | 46.008270 | 26.200651 | 33.542812 | 43.127407 | 29.110638 | 34.696762 |
|        |        | 44.057404 | 27.716854 | 38.148777 | 44.057404 | 27.716854 | 38.148777 |

---

| Element | S     | S     | S     | S     | S     | S     | S     |
|---------|--------|--------|--------|--------|--------|--------|--------|
|        | 26.993546 | 27.351582 | 36.276978 | 26.871227 | 34.013813 | 34.799717 |
|        | S     | 30.618290 | 30.097075 | 32.848927 | 29.971119 | 31.189137 | 36.603439 |
|        |        | 33.553833 | 27.833935 | 33.687252 | 33.856258 | 32.787460 | 32.696991 |
|        |        | 36.680103 | 28.525602 | 31.114204 | 36.407581 | 29.310066 | 36.263626 |
|        |        | 40.105804 | 27.020401 | 34.507431 | 40.010584 | 27.020401 | 34.507431 |
|        |        | 40.037983 | 31.432526 | 33.595596 | 43.747322 | 28.610615 | 31.666222 |
|        |        | 44.057404 | 27.716854 | 38.148777 | 44.057404 | 27.716854 | 38.148777 |

24 generated by VMD

| Element | S     | S     | S     | S     | S     | S     | S     |
|---------|--------|--------|--------|--------|--------|--------|--------|
|        | 27.010082 | 27.098171 | 36.360619 | 26.565273 | 33.831852 | 34.907185 |
|        | S     | 30.356556 | 30.016956 | 32.746185 | 30.117241 | 31.221760 | 36.521042 |
|        |        | 33.396072 | 27.822191 | 33.492119 | 33.573467 | 33.098862 | 32.588680 |
|        |        | 36.794781 | 28.901691 | 31.140770 | 36.371330 | 29.509861 | 36.312935 |
|        |        | 40.246574 | 27.141844 | 34.491940 | 40.365181 | 31.443481 | 33.616013 |
|        |        | 43.792404 | 28.094131 | 31.723698 | 44.203842 | 27.691563 | 37.872616 |
|  |  |  |  |
|---|---|---|---|
| Ca | 25.337595 | 29.820892 | 32.135464 |
| Ca | 26.472612 | 30.871662 | 36.137684 |
| Ca | 30.235477 | 28.030437 | 35.636620 |
| Ca | 29.925058 | 33.116013 | 33.461834 |
| Ca | 33.274811 | 29.882641 | 31.443745 |
| Ca | 33.341682 | 30.244179 | 35.217937 |
| Ca | 36.653923 | 26.851929 | 34.399326 |
| Ca | 36.716488 | 31.171700 | 33.720428 |
| Ca | 40.390163 | 29.121881 | 31.668703 |
| Ca | 39.873554 | 30.095718 | 36.522823 |
| Ca | 46.100803 | 26.064800 | 33.022633 |
| Ca | 43.329781 | 29.158148 | 34.716591 |
| S  | 26.722349 | 27.371447 | 36.371258 |
| S  | 26.542509 | 33.751259 | 34.508438 |
| S  | 30.406898 | 29.831696 | 32.721401 |
| S  | 30.053707 | 31.353275 | 36.449615 |
| S  | 33.305981 | 27.393089 | 33.668076 |
| S  | 33.443069 | 32.914635 | 32.637650 |
| S  | 36.806580 | 28.836420 | 31.597916 |
| S  | 36.532673 | 29.502426 | 36.372948 |
| S  | 40.292847 | 27.152550 | 34.487835 |
| S  | 40.347847 | 31.642437 | 33.593853 |
| S  | 43.926819 | 28.426685 | 31.723160 |
| S  | 44.400688 | 27.785435 | 37.814789 |
S        36.773491       28.758907       31.601995
S        36.388924       29.601158       36.520138
S        40.275906       26.966303       34.525589
S        40.426220       31.655716       36.520138
S        43.614841       28.214672       31.688969
S        44.492802       27.885332       37.338135

24

generated by VMD

Ca       25.361605       29.662615       32.283562
Ca       26.708761       30.472748       36.125519
Ca       30.526152       28.331680       35.859543
Ca       30.043802       33.273788       33.303322
Ca       33.575840       29.996754       31.356853
Ca       33.412254       30.619564       35.085632
Ca       36.709335       26.710976       34.347342
Ca       36.725090       30.882309       33.569016
Ca       40.062641       28.837021       31.760239
Ca       39.392532       29.879009       36.693451
Ca       45.920013       26.340347       32.991730
Ca       42.666203       29.488176       34.819183
S        27.123629       27.099871       36.162956
S        26.861752       33.853298       34.788898
S        30.521061       29.975239       32.686886
S        30.091314       31.470699       36.281666
S        33.472897       27.743858       33.711044
S        33.804150       32.963646       32.765976
S        36.830994       28.535849       31.352974
S        36.349464       29.393183       36.240265
S        40.098179       27.005396       34.610256
S        40.105148       31.469646       33.684113
S        43.679466       28.563480       31.917797
S        44.391655       27.822290       37.631639

24

generated by VMD

Ca       25.050171       29.925163       32.177067
Ca       26.490980       30.605476       36.252857
Ca       30.373444       28.234724       35.683640
Ca       30.238420       32.898018       33.564903
Ca       33.411407       29.720497       31.340948
Ca       33.323921       30.612297       35.167435
Ca       36.761253       27.221491       34.452492
Ca       36.767811       31.071810       33.749626
Ca       40.192520       29.115673       31.666603
Ca       39.765881       29.521381       36.587753
Ca       45.842651       26.568047       33.220787
Ca       43.221619       29.369686       34.646683
| S   | 26.798733  | 27.161121  | 36.244152  |
| S   | 26.749901  | 33.753674  | 34.419781  |
| S   | 30.362467  | 29.739475  | 32.556480  |
| S   | 30.094084  | 31.371380  | 36.600266  |
| S   | 33.449841  | 27.767036  | 33.853436  |
| S   | 33.820541  | 32.680904  | 32.586300  |
| S   | 36.738926  | 28.822144  | 31.289707  |
| S   | 36.339382  | 29.554123  | 36.436653  |
| S   | 40.096882  | 26.974716  | 34.250881  |
| S   | 40.535633  | 31.591026  | 33.683071  |
| S   | 43.664524  | 28.380281  | 31.611134  |
| S   | 44.342945  | 27.731253  | 37.988064  |

24

generated by VMD

| Ca  | 25.536335 | 29.503965 | 32.065567 |
| Ca  | 26.551899 | 30.770420 | 35.866840 |
| Ca  | 30.366716 | 28.069759 | 35.782925 |
| Ca  | 30.339748 | 33.133873 | 33.664013 |
| Ca  | 33.395485 | 30.031910 | 31.459553 |
| Ca  | 33.361729 | 30.552574 | 35.374226 |
| Ca  | 36.639721 | 26.966259 | 34.461784 |
| Ca  | 36.812832 | 30.983332 | 33.666241 |
| Ca  | 39.993984 | 28.757038 | 31.689404 |
| Ca  | 39.691784 | 29.725422 | 36.682003 |
| Ca  | 45.984325 | 26.722425 | 33.037842 |
| Ca  | 42.691082 | 29.241745 | 34.258926 |
| Ca  | 26.974413 | 27.177116 | 35.979202 |
| Ca  | 26.757565 | 33.869991 | 34.392654 |
| Ca  | 30.575439 | 29.956686 | 32.795727 |
| Ca  | 30.011087 | 31.363483 | 36.487740 |
| Ca  | 33.281765 | 27.677483 | 34.035492 |
| Ca  | 33.768990 | 32.995564 | 32.958378 |
| Ca  | 36.643909 | 28.736198 | 31.289347 |
| Ca  | 36.507908 | 29.464523 | 36.422485 |
| Ca  | 40.074909 | 26.914055 | 34.362957 |
| Ca  | 40.124722 | 31.524155 | 33.559654 |
| Ca  | 43.573166 | 28.424339 | 31.95327 |
| Ca  | 44.684330 | 27.829132 | 38.342339 |

24

generated by VMD

| Ca  | 25.436756 | 29.702177 | 32.126053 |
| Ca  | 26.421925 | 30.743328 | 35.877033 |
| Ca  | 30.478228 | 28.035112 | 35.833649 |
| Ca  | 30.226761 | 32.974552 | 33.359089 |
| Ca  | 33.506371 | 29.972540 | 31.286684 |
| Ca  | 33.337223 | 30.500965 | 35.351059 |
|    |    |    |                  |
| Ca | 36.748219 | 27.036573 | 34.499454 |
| Ca | 36.927723 | 30.886517 | 33.735649 |
| Ca | 40.074837 | 29.044088 | 31.391245 |
| Ca | 39.670227 | 29.811653 | 36.713154 |
| Ca | 45.697712 | 26.794865 | 33.052025 |
| Ca | 42.603535 | 29.337400 | 34.532539 |
| S  | 26.964146 | 27.359554 | 36.299431 |
| S  | 26.928896 | 33.876747 | 34.601807 |
| S  | 30.628658 | 29.840252 | 32.683308 |
| S  | 29.906103 | 31.264738 | 36.527496 |
| S  | 33.543133 | 27.670212 | 33.932198 |
| S  | 33.712059 | 32.08193 | 32.665535 |
| S  | 36.770367 | 28.659254 | 31.447578 |
| S  | 36.557388 | 29.565586 | 36.433140 |
| S  | 40.081001 | 26.962553 | 34.400311 |
| S  | 40.360928 | 31.480405 | 33.495445 |
| S  | 43.467216 | 28.618004 | 31.558428 |
| S  | 44.384514 | 27.489777 | 38.228455 |

24

|    |    |    |                  |
| Ca | 25.299038 | 29.909336 | 31.996447 |
| Ca | 26.227190 | 30.952465 | 36.040329 |
| Ca | 30.287806 | 28.074898 | 35.753456 |
| Ca | 30.191221 | 33.132236 | 33.277248 |
| Ca | 33.663765 | 29.794178 | 31.522635 |
| Ca | 33.319496 | 30.357025 | 35.542576 |
| Ca | 36.718327 | 26.913231 | 34.715904 |
| Ca | 36.655346 | 30.979984 | 33.659863 |
| Ca | 40.269985 | 28.877373 | 31.462334 |
| Ca | 39.861294 | 29.60281 | 36.792961 |
| Ca | 45.905846 | 27.232960 | 32.883457 |
| Ca | 42.860825 | 29.337379 | 34.265957 |
| S  | 26.312580 | 27.381676 | 35.961060 |
| S  | 26.790926 | 33.858284 | 34.318787 |
| S  | 30.609234 | 29.825542 | 32.869968 |
| S  | 29.771872 | 31.387550 | 36.447121 |
| S  | 33.374817 | 27.586960 | 34.010609 |
| S  | 33.668510 | 32.722080 | 33.009357 |
| S  | 36.816536 | 28.456028 | 31.616211 |
| S  | 36.539536 | 29.611057 | 36.585129 |
| S  | 40.337921 | 26.912453 | 34.345848 |
| S  | 40.332066 | 31.213024 | 33.550732 |
| S  | 43.748756 | 28.630163 | 31.187656 |
| S  | 44.870991 | 27.639219 | 38.215080 |

24

generated by VMD
| Ca  | 25.529808 | 29.852070 | 32.010433 |
|-----|----------|----------|-----------|
| Ca  | 26.558872 | 30.929031 | 36.320129 |
| Ca  | 30.341158 | 27.964951 | 35.906487 |
| Ca  | 30.340658 | 32.987343 | 33.508942 |
| Ca  | 33.585529 | 29.840355 | 31.203995 |
| Ca  | 33.137154 | 30.442993 | 35.455269 |
| Ca  | 36.735397 | 26.994444 | 34.365257 |
| Ca  | 36.726948 | 30.960011 | 33.606407 |
| Ca  | 40.136261 | 28.846275 | 31.616817 |
| Ca  | 39.628090 | 29.882673 | 36.586594 |
| Ca  | 45.66681  | 26.729725 | 33.254967 |
| Ca  | 42.734329 | 29.414825 | 34.266712 |
| S   | 26.826403 | 27.166962 | 36.112434 |
| S   | 26.915678 | 33.867607 | 34.464207 |
| S   | 30.687624 | 29.924314 | 32.845367 |
| S   | 30.032017 | 31.300787 | 36.570595 |
| S   | 33.486378 | 27.641813 | 33.790428 |
| S   | 33.778030 | 32.822086 | 32.613770 |
| S   | 36.834827 | 28.632027 | 31.352131 |
| S   | 36.332336 | 29.344692 | 36.407722 |
| S   | 40.109032 | 26.974724 | 34.384869 |
| S   | 40.157597 | 31.632420 | 33.598316 |
| S   | 43.12057  | 28.522526 | 31.428953 |
| S   | 44.641087 | 27.715933 | 38.359894 |

24 generated by VMD

| Ca  | 25.146610 | 30.105373 | 32.140278 |
|-----|----------|----------|-----------|
| Ca  | 26.583221 | 30.693821 | 36.126465 |
| Ca  | 30.296698 | 28.247234 | 35.788708 |
| Ca  | 30.167936 | 32.890236 | 33.602470 |
| Ca  | 33.567039 | 29.635096 | 31.258556 |
| Ca  | 33.142433 | 30.503727 | 35.343475 |
| Ca  | 36.807419 | 27.172695 | 34.674843 |
| Ca  | 36.679070 | 30.877123 | 33.549969 |
| Ca  | 40.230350 | 29.046616 | 31.678329 |
| Ca  | 39.743050 | 29.711613 | 36.479919 |
| Ca  | 45.807281 | 26.713013 | 33.184029 |
| Ca  | 42.837242 | 29.423073 | 34.413395 |
| S   | 26.704193 | 27.146509 | 35.946682 |
| S   | 26.886093 | 33.807602 | 34.708115 |
| S   | 30.467882 | 29.899124 | 32.653450 |
| S   | 30.076790 | 31.378181 | 36.522476 |
| S   | 33.476460 | 27.620243 | 34.063427 |
| S   | 33.557709 | 32.642681 | 32.398052 |
| S   | 36.897285 | 28.578651 | 31.315153 |
| S   | 36.444103 | 29.652119 | 36.500729 |
S  40.188042  26.947563  34.220436
S  40.427517  31.639252  33.642948
S  43.711807  28.497519  31.608139
S  44.587551  27.562332  38.210598
24

generated by VMD
Ca  24.903990  30.266258  31.685711
Ca  26.441269  30.796808  35.910862
Ca  30.366467  28.285559  35.848221
Ca  30.427954  32.728989  33.565048
Ca  33.483791  29.525303  31.256136
Ca  33.269299  30.632553  35.216656
Ca  36.804371  27.008434  34.920109
Ca  36.729912  30.871775  33.624252
Ca  40.089287  29.113987  31.618938
Ca  40.105350  29.599428  36.590874
Ca  45.935509  27.175903  33.152058
Ca  42.861610  29.539413  32.205082
S  26.781963  27.227394  36.082142
S  27.189827  33.817028  34.586685
S  30.445503  29.708136  32.823162
S  29.991819  31.302347  36.773727
S  33.388264  27.534058  34.141930
S  33.526836  32.574669  32.390099
S  36.789013  28.390804  31.436495
S  36.531700  29.730616  36.585739
S  40.315327  27.011141  34.262318
S  40.313431  31.750529  33.748283
S  43.532372  28.676161  31.176991
S  44.208992  27.324081  38.414276
24

generated by VMD
Ca  25.161848  30.493828  31.826052
Ca  26.454561  30.641909  36.141041
Ca  30.302483  28.116447  35.782204
Ca  30.448685  32.835102  33.431072
Ca  33.376629  29.814377  31.176853
Ca  33.299141  30.530668  35.387203
Ca  36.908287  26.939001  34.741905
Ca  36.534557  30.692774  33.439819
Ca  39.943359  28.844595  31.748100
Ca  39.763161  29.816978  36.930550
Ca  46.142509  27.093302  32.965836
Ca  42.703499  29.333706  34.449341
S  26.729809  27.215902  36.221424
S  27.076670  33.836388  34.613144
| S   | 30.515978 | 29.732002 | 32.672062 |
|-----|-----------|-----------|-----------|
| S   | 30.089857 | 31.271114 | 36.513123 |
| S   | 33.524979 | 27.717663 | 33.867294 |
| S   | 33.791016 | 32.823032 | 32.488773 |
| S   | 36.619514 | 28.292673 | 31.334969 |
| S   | 36.423744 | 29.590570 | 36.358234 |
| S   | 40.382710 | 26.850140 | 34.469712 |
| S   | 40.076981 | 31.522537 | 33.868839 |
| S   | 43.407459 | 28.527615 | 31.364794 |
| S   | 44.756474 | 27.859118 | 38.239082 |

24
generated by VMD

| Ca  | 25.402222 | 30.456932 | 32.029388 |
|-----|-----------|-----------|-----------|
| Ca  | 26.289639 | 31.073460 | 36.096458 |
| Ca  | 30.258530 | 27.961061 | 35.523132 |
| Ca  | 30.382689 | 32.909359 | 33.625744 |
| Ca  | 33.403381 | 29.427462 | 31.445683 |
| Ca  | 33.266464 | 30.358353 | 35.342777 |
| Ca  | 36.737968 | 26.629147 | 34.422352 |
| Ca  | 36.731319 | 30.726868 | 33.540241 |
| Ca  | 40.042938 | 28.958282 | 31.395388 |
| Ca  | 39.646660 | 29.806053 | 36.580723 |
| Ca  | 45.874699 | 27.397495 | 33.679310 |
| Ca  | 42.712601 | 29.429873 | 34.107330 |
| S   | 26.532656 | 27.497046 | 36.010311 |
| S   | 27.418972 | 34.096611 | 34.801571 |
| S   | 30.454964 | 29.633562 | 32.754589 |
| S   | 29.946131 | 31.211599 | 36.555725 |
| S   | 33.343842 | 27.372856 | 34.228897 |
| S   | 33.829887 | 32.427383 | 32.699303 |
| S   | 36.667755 | 28.439438 | 31.230852 |
| S   | 36.457813 | 29.272264 | 36.340328 |
| S   | 40.301041 | 27.018734 | 34.241314 |
| S   | 40.360615 | 31.582920 | 33.604233 |
| S   | 43.635033 | 28.540472 | 31.264214 |
| S   | 44.736042 | 28.164186 | 38.510742 |

24
generated by VMD

| Ca  | 25.071880 | 30.360962 | 32.350937 |
|-----|-----------|-----------|-----------|
| Ca  | 26.590733 | 30.864857 | 35.971199 |
| Ca  | 30.273151 | 27.966955 | 35.447525 |
| Ca  | 30.530451 | 32.882790 | 33.499348 |
| Ca  | 33.401386 | 29.802261 | 31.358343 |
| Ca  | 33.322735 | 30.494083 | 35.157330 |
| Ca  | 36.794754 | 26.641899 | 34.437756 |
| Ca  | 36.774712 | 30.745770 | 33.419960 |
| Element | Ca   | S    | 24 generated by VMD |
|---------|------|------|---------------------|
| Ca      | 40.004524 | 29.139181 | 31.411776 |
| Ca      | 39.638672 | 29.760422 | 36.476074 |
| Ca      | 45.786285 | 27.365419 | 33.512562 |
| Ca      | 42.790073 | 29.396694 | 34.241456 |
| S       | 26.797422 | 27.321894 | 36.446251 |
| S       | 27.378546 | 33.875175 | 34.793343 |
| S       | 32.554798 | 30.443119 | 29.798525 |
| S       | 34.273613 | 30.152626 | 31.041758 |
| S       | 35.05026 | 33.452499 | 27.359653 |
| S       | 32.544128 | 33.942844 | 32.759018 |
| S       | 31.143137 | 36.716835 | 28.492517 |
| S       | 36.273613 | 40.162590 | 27.105778 |
| S       | 34.302322 | 40.176250 | 31.573982 |
| S       | 33.776535 | 43.437912 | 28.295799 |
| S       | 34.35946 | 44.277790 | 28.028156 |

24 generated by VMD

| Element | Ca   | S    | 24 generated by VMD |
|---------|------|------|---------------------|
| Ca      | 25.122446 | 30.232992 | 32.330288 |
| Ca      | 26.508293 | 30.647160 | 36.149384 |
| Ca      | 30.053112 | 28.337763 | 35.518787 |
| Ca      | 30.380398 | 32.987366 | 33.331047 |
| Ca      | 33.576111 | 29.721603 | 31.327002 |
| Ca      | 33.151348 | 30.377596 | 35.231239 |
| Ca      | 36.835125 | 26.678818 | 34.546818 |
| Ca      | 36.698914 | 30.994331 | 35.500275 |
| Ca      | 40.120998 | 29.103462 | 31.685425 |
| Ca      | 39.863674 | 28.842333 | 36.855251 |
| Ca      | 46.069725 | 27.151764 | 33.234928 |
| Ca      | 42.687489 | 29.292309 | 34.272205 |
| S       | 26.850183 | 27.159639 | 35.959564 |
| S       | 27.210964 | 33.809921 | 34.933197 |
| S       | 30.531162 | 29.917187 | 32.593117 |
| S       | 29.956215 | 31.406740 | 36.395256 |
| S       | 33.234852 | 27.354378 | 34.180344 |
| S       | 33.526508 | 32.811775 | 32.375298 |
| S       | 36.912621 | 28.556114 | 31.428490 |
| S       | 36.645855 | 29.375599 | 36.342510 |
| S       | 40.244446 | 26.956198 | 34.343254 |
| S       | 40.196259 | 31.646957 | 33.685394 |
| S       | 43.492321 | 28.189000 | 31.277424 |
| S       | 44.564911 | 27.840462 | 38.534264 |
|   | Ca       | 30.007824 | 28.292244 | 35.627174 |
|---|----------|-----------|-----------|-----------|
| Ca | 30.246765| 32.962543 | 33.605652 |
| Ca | 33.525745| 29.611668 | 31.435770 |
| Ca | 33.142761| 30.354391 | 35.408615 |
| Ca | 36.823269| 26.804493 | 34.041534 |
| Ca | 36.899427| 30.921169 | 33.669716 |
| Ca | 40.111263| 29.121729 | 31.399734 |
| Ca | 39.969006| 29.703403 | 36.404430 |
| Ca | 46.000000| 27.153156 | 33.797195 |
| S  | 26.728104| 34.062622 | 36.198601 |
| Ca | 37.111746| 27.177984 | 36.198601 |
| Ca | 30.452980| 29.852600 | 32.761040 |
| S  | 29.830484| 31.293163 | 36.644341 |
| S  | 33.410774| 27.278971 | 34.003822 |
| S  | 33.669308| 32.568325 | 32.806545 |
| S  | 36.725742| 28.750881 | 31.386496 |
| S  | 36.631504| 29.447552 | 36.312439 |
| S  | 40.337265| 26.982563 | 34.052788 |
| S  | 40.391930| 31.494621 | 33.422485 |
| S  | 43.541958| 28.028730 | 31.316395 |
| S  | 44.588051| 28.149166 | 38.869415 |

generated by VMD

|   | Ca       | 25.246944 | 30.293596 | 32.363068 |
|---|----------|-----------|-----------|-----------|
| Ca | 26.610569| 30.763725 | 36.088169 |
| Ca | 30.335133| 28.087015 | 35.260113 |
| Ca | 30.345163| 33.004028 | 33.547066 |
| Ca | 33.385315| 29.706247 | 31.328520 |
| Ca | 33.283966| 30.331766 | 35.259323 |
| Ca | 36.711742| 26.722826 | 34.230545 |
| Ca | 36.759834| 31.016571 | 33.474838 |
| Ca | 39.886036| 29.015556 | 31.551218 |
| Ca | 39.738049| 29.724178 | 36.679199 |
| Ca | 45.948414| 27.275070 | 33.539421 |
| Ca | 42.789833| 29.177580 | 34.278450 |
| S  | 26.673363| 27.352242 | 36.082695 |
| S  | 27.024286| 33.967121 | 34.899918 |
| S  | 30.451122| 29.890263 | 32.647339 |
| S  | 30.133797| 31.120941 | 36.532597 |
| S  | 33.481449| 27.471132 | 34.003151 |
| S  | 33.627575| 32.644505 | 32.751152 |
| S  | 36.637421| 28.543509 | 31.369556 |
| S  | 36.671906| 29.432459 | 36.257011 |
| S  | 40.171413| 26.842215 | 34.247768 |
| S  | 40.467773| 31.501659 | 33.519051 |
| X   | Y   | Z   |
|-----|-----|-----|
| 43.585911 | 28.117641 | 31.324301 |
| 44.466858 | 28.389568 | 38.796215 |

24 generated by VMD

| Ca   | X     | Y     | Z     |
|------|-------|-------|-------|
| 24.850203 | 30.350782 | 32.629250 |
| 26.799141 | 30.583303 | 36.209991 |
| 30.208614 | 28.068802 | 35.376999 |
| 30.144077 | 32.989689 | 33.571640 |
| 33.353081 | 29.802885 | 31.196514 |
| 33.327221 | 30.355087 | 35.151669 |
| 36.824471 | 26.877071 | 34.244686 |
| 36.876221 | 30.927629 | 33.252861 |
| 40.180218 | 28.956226 | 31.524046 |
| 39.625210 | 29.879148 | 36.730461 |
| 45.868008 | 26.948608 | 33.667786 |
| 42.811783 | 29.287540 | 34.360188 |
| 26.885891 | 27.220619 | 35.847427 |
| 27.219343 | 33.892555 | 35.255253 |
| 30.463449 | 29.952492 | 32.563843 |
| 30.288336 | 31.209114 | 36.569347 |
| 33.549736 | 27.514774 | 33.681637 |
| 33.530163 | 32.765068 | 32.651470 |
| 36.721428 | 28.352474 | 31.068356 |
| 36.537720 | 29.560547 | 36.062305 |
| 40.249546 | 26.876774 | 34.469662 |
| 40.397297 | 31.563662 | 33.627853 |
| 43.561737 | 28.004684 | 31.422874 |
| 44.161003 | 28.451843 | 38.894569 |

24 generated by VMD

| Ca   | X     | Y     | Z     |
|------|-------|-------|-------|
| 25.388176 | 30.648554 | 32.065998 |
| 26.716841 | 30.610538 | 36.333954 |
| 30.354544 | 28.247984 | 35.486061 |
| 30.355387 | 33.041824 | 33.522282 |
| 33.149860 | 29.579910 | 31.389912 |
| 33.321590 | 30.409502 | 34.972637 |
| 36.659435 | 26.469816 | 34.500946 |
| 36.719620 | 30.867470 | 33.405334 |
| 40.145164 | 28.859741 | 31.329784 |
| 39.743263 | 29.761433 | 36.698959 |
| 46.096779 | 27.178986 | 33.782490 |
| 42.657623 | 29.402378 | 34.231949 |
| 26.944305 | 27.285221 | 35.954082 |
| 27.107639 | 33.831680 | 35.409454 |
| 30.304497 | 29.952522 | 32.493134 |
| 30.240662 | 31.278502 | 36.542862 |
| S  | 33.442940 | 27.414566 | 34.012108 |
| S  | 33.611465 | 32.658607 | 32.545528 |
| S  | 36.641216 | 28.402718 | 31.454777 |
| S  | 36.557404 | 29.399788 | 36.205620 |
| S  | 40.329056 | 26.862730 | 34.150394 |
| S  | 40.185345 | 31.568413 | 33.203575 |
| S  | 43.607220 | 28.177521 | 31.402962 |
| S  | 44.153854 | 28.481018 | 38.935913 |

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generated by VMD

| Ca | 25.171959 | 30.368244 | 32.103157 |
| Ca | 26.647154 | 30.725687 | 36.161972 |
| Ca | 30.165758 | 28.200089 | 35.650021 |
| Ca | 30.409735 | 32.976547 | 33.644676 |
| Ca | 33.438347 | 29.560329 | 31.407936 |
| Ca | 33.188145 | 30.414690 | 35.225735 |
| Ca | 36.605495 | 26.865227 | 34.212002 |
| Ca | 37.026970 | 30.775911 | 33.272598 |
| Ca | 40.329754 | 28.901546 | 31.171665 |
| Ca | 39.665855 | 29.908072 | 36.649879 |
| Ca | 46.071579 | 27.092142 | 33.793934 |
| Ca | 42.716396 | 29.157860 | 34.336208 |
| S  | 26.615158 | 27.281300 | 35.941772 |
| S  | 27.068817 | 33.791534 | 35.258171 |
| S  | 30.491980 | 29.913000 | 32.727432 |
| S  | 30.060511 | 31.275896 | 36.673424 |
| S  | 33.232967 | 27.403025 | 34.264587 |
| S  | 33.602425 | 32.668648 | 32.567650 |
| S  | 36.905365 | 28.515795 | 31.027781 |
| S  | 36.503265 | 29.437098 | 36.112801 |
| S  | 40.092869 | 27.002457 | 34.114231 |
| S  | 40.409977 | 31.425220 | 33.458145 |
| S  | 43.658104 | 28.305149 | 31.455204 |
| S  | 44.355335 | 28.425966 | 38.799759 |

24

generated by VMD

| Ca | 25.119465 | 30.309803 | 31.922680 |
| Ca | 26.505035 | 30.694532 | 35.927429 |
| Ca | 30.294991 | 28.358339 | 35.622868 |
| Ca | 30.312447 | 33.047775 | 33.496532 |
| Ca | 33.424767 | 29.155596 | 31.581768 |
| Ca | 33.463581 | 30.478508 | 35.412235 |
| Ca | 36.633663 | 26.764362 | 34.195019 |
| Ca | 36.905602 | 30.942146 | 33.451694 |
| Ca | 40.017986 | 29.346125 | 31.431755 |
| Ca | 39.967815 | 29.816311 | 36.524216 |
|    |    |    |    |
|----|----|----|----|
| Ca | 45.872166 | 26.957203 | 33.623055 |
| Ca | 42.866760 | 29.421143 | 34.229733 |
| S  | 26.108315 | 27.313351 | 35.993122 |
| S  | 27.015421 | 33.901886 | 34.969280 |
| S  | 30.443340 | 29.760500 | 32.822533 |
| S  | 30.200478 | 31.290560 | 36.577045 |
| S  | 33.413681 | 27.363890 | 34.228527 |
| S  | 33.554737 | 32.346146 | 32.584042 |
| S  | 36.747559 | 28.477493 | 31.496696 |
| S  | 36.776104 | 29.469006 | 36.301208 |
| S  | 40.240059 | 27.108145 | 34.050976 |
| S  | 40.435669 | 31.797691 | 33.632568 |
| S  | 43.691948 | 28.289701 | 31.387794 |
| S  | 44.422302 | 27.981220 | 38.567947 |
|    |    |    |    |
|    |    |    |    |
| Ca | 24.906731 | 30.475903 | 32.051498 |
| Ca | 26.711514 | 30.588419 | 36.144791 |
| Ca | 30.248146 | 28.154581 | 35.511978 |
| Ca | 30.196510 | 33.068474 | 33.674938 |
| Ca | 33.388683 | 29.247751 | 31.433907 |
| Ca | 33.441929 | 30.253233 | 35.043636 |
| Ca | 36.795486 | 26.835936 | 34.164017 |
| Ca | 36.954002 | 31.468340 | 33.673260 |
| Ca | 40.021454 | 29.259981 | 31.538715 |
| Ca | 40.043491 | 29.847681 | 36.790348 |
| Ca | 45.755535 | 27.005518 | 33.450424 |
| Ca | 42.704632 | 29.292137 | 34.343575 |
| S  | 26.576017 | 27.268177 | 36.035461 |
| S  | 26.891693 | 33.799408 | 34.855530 |
| S  | 30.361017 | 29.929384 | 32.614899 |
| S  | 30.423874 | 31.231506 | 36.507950 |
| S  | 33.322205 | 27.176731 | 33.893826 |
| S  | 33.512890 | 32.503025 | 32.462929 |
| S  | 36.628838 | 28.670475 | 31.510605 |
| S  | 36.710472 | 29.538719 | 36.226562 |
| S  | 40.054535 | 27.060131 | 34.422863 |
| S  | 40.683968 | 31.628447 | 33.519512 |
| S  | 43.296734 | 27.980362 | 31.421749 |
| S  | 44.803585 | 28.107058 | 38.737713 |

24 generated by VMD

|    |    |    |    |
|----|----|----|----|
| Ca | 25.055328 | 30.252445 | 32.077438 |
| Ca | 26.550739 | 30.505304 | 35.987530 |
| Ca | 30.266888 | 28.202671 | 35.387920 |
| Ca | 30.290667 | 32.979431 | 33.443031 |
| Element | X Coordination | Y Coordination | Z Coordination |
|---------|----------------|----------------|----------------|
| Ca      | 33.277897      | 29.221127      | 31.572243      |
| Ca      | 33.628338      | 30.608000      | 35.096786      |
| Ca      | 36.710442      | 26.992165      | 34.491184      |
| Ca      | 36.963531      | 31.694424      | 33.728642      |
| Ca      | 39.868195      | 29.353598      | 31.507929      |
| Ca      | 39.918922      | 29.470600      | 37.059490      |
| Ca      | 45.949265      | 26.890720      | 33.139366      |
| Ca      | 42.669029      | 29.262796      | 34.305706      |
| S       | 26.599670      | 27.259232      | 35.922089      |
| S       | 26.992407      | 33.742844      | 34.925858      |
| S       | 30.330847      | 29.723192      | 32.484360      |
| S       | 30.428986      | 31.106451      | 36.380581      |
| S       | 33.421486      | 27.411303      | 34.145302      |
| S       | 33.730946      | 32.661705      | 32.402279      |
| S       | 36.572601      | 28.796003      | 31.636887      |
| S       | 36.709309      | 29.625816      | 36.370522      |
| S       | 40.089413      | 27.065498      | 34.350861      |
| S       | 40.448708      | 31.599346      | 33.780136      |
| S       | 43.203514      | 27.941612      | 31.460995      |
| S       | 44.756813      | 28.025080      | 38.373672      |

Generated by VMD

| Element | X Coordination | Y Coordination | Z Coordination |
|---------|----------------|----------------|----------------|
| Ca      | 25.285566      | 30.713860      | 32.309887      |
| Ca      | 26.881241      | 30.507240      | 36.319122      |
| Ca      | 30.119934      | 28.320839      | 35.114685      |
| Ca      | 30.101479      | 33.137283      | 33.415375      |
| Ca      | 33.304127      | 28.978331      | 30.990829      |
| Ca      | 33.367367      | 30.412622      | 34.998722      |
| Ca      | 36.453320      | 26.816940      | 34.243134      |
| Ca      | 36.780041      | 31.259809      | 33.749359      |
| Ca      | 39.984547      | 29.284437      | 31.837524      |
| Ca      | 39.844147      | 29.743055      | 36.941605      |
| Ca      | 45.791763      | 27.155308      | 33.498100      |
| Ca      | 42.604008      | 29.455116      | 34.334045      |
| S       | 26.877258      | 27.301529      | 36.273727      |
| S       | 27.193041      | 33.796272      | 35.248680      |
| S       | 30.381224      | 29.747749      | 32.377983      |
| S       | 30.411915      | 31.217773      | 36.380432      |
| S       | 33.249722      | 27.214859      | 33.782883      |
| S       | 33.606983      | 32.333790      | 32.178017      |
| S       | 36.801605      | 28.547293      | 31.543468      |
| S       | 36.678276      | 29.580965      | 36.307308      |
| S       | 39.979050      | 27.041214      | 34.431442      |
| S       | 40.458633      | 31.753313      | 33.853283      |
| S       | 43.268173      | 28.060316      | 31.481590      |
| S       | 45.010406      | 28.011501      | 38.419571      |

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|    |        |        |        |
|----|--------|--------|--------|
| Ca | 25.079741 | 30.479334 | 32.332710 |
| Ca | 26.904011 | 30.615053 | 36.166199 |
| Ca | 30.301716 | 28.171846 | 35.259579 |
| Ca | 30.150389 | 33.024567 | 33.224518 |
| Ca | 33.146683 | 29.243614 | 31.366085 |
| Ca | 33.533161 | 30.640626 | 35.092316 |
| Ca | 36.921417 | 26.717491 | 34.306931 |
| Ca | 36.793396 | 31.423460 | 33.274414 |
| Ca | 39.907581 | 29.197008 | 31.763378 |
| Ca | 39.842262 | 29.568857 | 36.880627 |
| Ca | 45.926872 | 27.345119 | 33.731262 |
| Ca | 42.790451 | 29.345139 | 34.385735 |
| S  | 26.529718 | 27.202106 | 36.169754 |
| S  | 27.117844 | 33.784332 | 35.216679 |
| S  | 30.303997 | 29.855284 | 32.628777 |
| S  | 30.317625 | 31.383514 | 36.254650 |
| S  | 33.508259 | 27.413004 | 33.935951 |
| S  | 33.475674 | 32.480423 | 32.314766 |
| S  | 36.646481 | 28.368980 | 31.596405 |
| S  | 36.711872 | 29.531948 | 36.160507 |
| S  | 40.132385 | 26.973391 | 34.329407 |
| S  | 40.270691 | 31.657934 | 33.723587 |
| S  | 43.434185 | 28.525461 | 31.478104 |
| S  | 44.687496 | 27.439474 | 38.438354 |

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|    |        |        |        |
|----|--------|--------|--------|
| Ca | 24.915836 | 30.598940 | 32.446182 |
| Ca | 27.205999 | 30.651087 | 35.878765 |
| Ca | 30.473976 | 28.219193 | 35.239426 |
| Ca | 30.126245 | 32.964043 | 33.381851 |
| Ca | 33.175797 | 29.132143 | 31.123341 |
| Ca | 33.566898 | 30.403225 | 35.121319 |
| Ca | 36.844833 | 26.496778 | 34.141144 |
| Ca | 36.877426 | 31.535568 | 33.455257 |
| Ca | 39.771866 | 29.107704 | 31.815514 |
| Ca | 39.707348 | 29.286993 | 36.920502 |
| Ca | 45.644089 | 27.554321 | 33.747139 |
| Ca | 42.801647 | 29.477901 | 34.460953 |
| S  | 26.530937 | 27.176517 | 36.302963 |
| S  | 27.433592 | 34.040955 | 35.295193 |
| S  | 30.389977 | 29.736551 | 32.457783 |
| S  | 30.505402 | 31.280704 | 36.309799 |
| S  | 33.456665 | 27.380653 | 33.864826 |
| S  | 33.386337 | 32.413536 | 32.238205 |
|    |          |          |          |
|----|----------|----------|----------|
| S  | 36.632301| 28.600452| 31.482235|
| S  | 36.679680| 29.326920| 36.059063|
| S  | 40.035339| 26.907148| 34.352974|
| S  | 40.449215| 31.810032| 33.912491|
| S  | 43.117588| 28.218710| 31.565132|
| S  | 44.704933| 28.071335| 38.458660|
| 24 | generated by VMD |
| Ca | 24.931702| 30.574463| 32.482925|
| Ca | 26.832684| 30.823458| 36.116096|
| Ca | 30.226978| 28.197153| 35.473358|
| Ca | 30.212456| 29.045033| 33.215179|
| Ca | 33.151894| 28.982227| 31.192713|
| Ca | 33.380775| 30.301748| 35.116650|
| Ca | 36.735153| 27.032709| 34.116802|
| Ca | 37.075962| 31.360764| 33.864391|
| Ca | 40.136200| 29.370249| 31.471359|
| Ca | 39.929241| 29.887348| 36.629681|
| Ca | 45.838779| 27.346897| 33.514988|
| Ca | 42.833611| 29.433462| 34.607841|
| S  | 26.592972| 27.116215| 36.264336|
| S  | 26.897121| 33.855824| 34.883217|
| S  | 30.187534| 29.565714| 32.556068|
| S  | 30.344376| 31.393665| 36.208233|
| S  | 33.372444| 27.348228| 33.996208|
| S  | 33.515854| 32.308762| 32.351707|
| S  | 36.707901| 28.771837| 31.573177|
| S  | 36.771652| 29.490402| 36.394684|
| S  | 39.998268| 27.135880| 34.204102|
| S  | 40.735550| 31.666773| 33.700073|
| S  | 43.355057| 28.289013| 31.648350|
| S  | 44.669682| 27.227106| 38.448570|
| 24 | generated by VMD |
| Ca | 25.016842| 30.737219| 32.649578|
| Ca | 26.883707| 30.383724| 36.083572|
| Ca | 30.075796| 28.214396| 35.441456|
| Ca | 30.455984| 33.023689| 33.403084|
| Ca | 33.215103| 28.889748| 30.815697|
| Ca | 33.502052| 30.236063| 35.027020|
| Ca | 36.431904| 27.312061| 34.360443|
| Ca | 37.051399| 31.707542| 33.641243|
| Ca | 40.068321| 29.086336| 31.637653|
| Ca | 39.800087| 29.777580| 36.712109|
| Ca | 45.774422| 27.215498| 33.470772|
| Ca | 42.821518| 29.427973| 34.568687|
|     |     |     |     |
|-----|-----|-----|-----|
| S   | 26.587828 | 26.874727 | 36.384159 |
| S   | 27.344877 | 33.777946 | 35.202507 |
| S   | 30.516874 | 29.724779 | 32.423233 |
| S   | 30.278748 | 31.195692 | 36.324024 |
| S   | 33.117050 | 27.177040 | 33.660465 |
| S   | 33.585155 | 32.257935 | 32.028000 |
| S   | 36.564854 | 28.906040 | 31.551468 |
| S   | 36.622421 | 30.089397 | 36.300270 |
| S   | 39.809677 | 27.019047 | 34.360847 |
| S   | 40.614159 | 31.649895 | 33.806240 |
| S   | 43.548382 | 28.447145 | 31.619831 |
| S   | 44.746643 | 27.259880 | 38.558304 |

generated by VMD

|     |     |     |     |
|-----|-----|-----|-----|
| Ca  | 24.686327 | 30.788973 | 32.656780 |
| Ca  | 26.897629 | 30.575151 | 36.022232 |
| Ca  | 30.188688 | 28.332623 | 35.238441 |
| Ca  | 30.151478 | 32.904491 | 33.182396 |
| Ca  | 33.298267 | 28.946783 | 31.233337 |
| Ca  | 33.499313 | 30.446344 | 34.988041 |
| Ca  | 36.928894 | 26.741465 | 34.248493 |
| Ca  | 37.212524 | 31.586962 | 33.799896 |
| Ca  | 39.920849 | 29.113766 | 31.675585 |
| Ca  | 39.863289 | 29.549145 | 36.946213 |
| Ca  | 45.585613 | 27.088514 | 33.471275 |
| Ca  | 42.768547 | 29.621355 | 34.533772 |
| S   | 26.673462 | 27.118181 | 36.211029 |
| S   | 27.263470 | 33.853325 | 35.091057 |
| S   | 30.204334 | 29.574905 | 32.469322 |
| S   | 30.389698 | 31.380802 | 36.201660 |
| S   | 33.460228 | 27.114483 | 33.898430 |
| S   | 33.324768 | 32.338799 | 32.029427 |
| S   | 36.654030 | 28.828320 | 31.809513 |
| S   | 36.665802 | 29.516289 | 36.119072 |
| S   | 40.115990 | 27.076309 | 34.546703 |
| S   | 40.572002 | 31.808964 | 33.617371 |
| S   | 43.303802 | 28.688051 | 31.533503 |
| S   | 44.804893 | 27.397387 | 38.507130 |

generated by VMD
Ca       36.697823       26.942783       34.201
Ca       37.024494       31.534204       33.784554
Ca       40.093964       29.173691       31.420000
Ca       39.939369       29.567238       36.689728
Ca       45.832489       27.328091       33.484364
Ca       43.008709       29.621046       34.808224

S        26.463795       27.216948       36.397083
S        27.152142       33.897720       35.017178
S        30.146458       29.463873       32.458630
S        30.393494       31.334513       36.285549
S        33.310501       27.266266       34.016090
S        33.525753       32.176689       32.086727
S        36.695030       28.688004       31.593502
S        36.730915       29.686007       36.310539
S        40.087353       27.128185       34.166206
S        40.655239       31.553137       33.758156
S        43.605473       28.626728       31.523849
S        44.511116       27.426285       38.501293

24 generated by VMD

Ca       24.778778       30.388521       32.351555
Ca       26.907585       30.705885       35.869461
Ca       30.025146       28.259811       35.448524
Ca       30.203074       33.004608       33.168823
Ca       32.998405       29.102386       31.213825
Ca       33.488529       30.341524       35.109867
Ca       36.724640       26.939556       34.451588
Ca       37.119850       31.379505       34.039597
Ca       39.870129       29.015495       31.725214
Ca       40.059853       29.703306       36.854122
Ca       45.813656       27.404829       33.168915
Ca       43.000156       29.341000       34.461758

S        26.606178       27.064968       36.015736
S        27.273588       34.015495       34.876492
S        30.037951       29.733425       32.599148
S        30.321604       31.319740       36.247654
S        33.211430       27.236662       33.796566
S        33.540161       32.347630       32.301258
S        36.350845       28.985962       31.724964
S        36.695717       29.511385       36.463814
S        40.098824       26.996111       34.444939
S        40.704277       31.479500       33.806080
S        43.381649       28.506153       31.424652
S        45.221828       27.607965       38.466110

24 generated by VMD
| Ca       | 24.690748 | 30.523113 | 32.348377 |
| Ca       | 26.838581 | 30.586473 | 35.984169 |
| Ca       | 30.105988 | 28.315290 | 35.344067 |
| Ca       | 30.155254 | 32.988323 | 33.393303 |
| Ca       | 33.080101 | 29.106052 | 31.402218 |
| Ca       | 33.604427 | 30.550972 | 35.156128 |
| Ca       | 36.825932 | 27.073889 | 34.41318  |
| Ca       | 36.919968 | 31.746206 | 33.760643 |
| Ca       | 40.073250 | 29.115097 | 31.776924 |
| Ca       | 40.032192 | 29.453382 | 36.734299 |
| Ca       | 45.919147 | 27.138119 | 33.726700 |
| Ca       | 43.100933 | 29.413317 | 34.167473 |
| S        | 26.669701 | 26.968111 | 35.908398 |
| S        | 26.978189 | 33.767776 | 34.998749 |
| S        | 30.171101 | 29.670782 | 32.403751 |
| S        | 30.362812 | 31.239954 | 36.392258 |
| S        | 33.270660 | 27.302559 | 33.948788 |
| S        | 33.478874 | 32.565453 | 32.362274 |
| S        | 36.541447 | 28.879221 | 31.644119 |
| S        | 36.639034 | 29.663919 | 36.334003 |
| S        | 40.083771 | 27.195520 | 34.377007 |
| S        | 40.535690 | 31.576740 | 33.856186 |
| S        | 43.529430 | 28.005297 | 31.275301 |
| S        | 44.826633 | 27.545898 | 38.321220 |

24

generated by VMD

| Ca       | 24.535259 | 30.459042 | 32.361053 |
| Ca       | 26.655960 | 30.536900 | 35.976830 |
| Ca       | 30.063507 | 28.525537 | 35.298779 |
| Ca       | 30.351933 | 32.825661 | 33.394592 |
| Ca       | 33.345169 | 29.171993 | 31.150322 |
| Ca       | 33.446976 | 30.310076 | 35.330650 |
| Ca       | 36.557896 | 26.879894 | 34.646389 |
| Ca       | 36.983868 | 31.372023 | 33.665459 |
| Ca       | 39.862949 | 29.111397 | 31.528339 |
| Ca       | 40.174049 | 29.276333 | 36.678890 |
| Ca       | 45.769577 | 27.370884 | 33.486893 |
| Ca       | 42.888668 | 29.566545 | 34.598690 |
| S        | 26.687202 | 27.198746 | 35.960876 |
| S        | 27.007515 | 33.840488 | 34.818760 |
| S        | 30.219706 | 29.765272 | 32.528938 |
| S        | 30.202169 | 31.484238 | 36.486790 |
| S        | 33.374153 | 27.429237 | 33.999950 |
| S        | 33.570377 | 32.466766 | 32.332386 |
| S        | 36.702168 | 28.456184 | 31.807991 |
| S        | 36.623993 | 29.675646 | 36.386581 |
|   |   |   |   |
|---|---|---|---|
| S | 40.006821 | 26.988029 | 34.214268 |
| S | 40.650581 | 31.451244 | 33.618511 |
| S | 43.588520 | 28.662098 | 31.359753 |
| S | 45.164864 | 27.567177 | 38.398994 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 24.790033 | 30.687698 | 32.472256 |
| Ca | 26.677906 | 30.775597 | 36.140991 |
| Ca | 30.026907 | 28.388054 | 35.321152 |
| Ca | 30.343269 | 32.568790 | 33.259136 |
| Ca | 33.269897 | 28.744711 | 30.783026 |
| Ca | 33.404572 | 30.431196 | 35.053833 |
| Ca | 36.748138 | 26.967674 | 34.323978 |
| Ca | 37.039795 | 31.569355 | 33.937847 |
| Ca | 39.981014 | 29.424047 | 31.816626 |
| Ca | 39.862770 | 29.412680 | 36.847397 |
| Ca | 45.785595 | 27.502575 | 33.649269 |
| Ca | 42.805607 | 29.551498 | 34.444740 |
| S | 26.559952 | 27.290251 | 36.485241 |
| S | 27.303772 | 33.902138 | 34.994019 |
| S | 30.329708 | 29.609005 | 32.361053 |
| S | 30.390591 | 31.347965 | 36.357803 |
| S | 33.323685 | 27.254438 | 33.880085 |
| S | 33.598167 | 31.960815 | 31.960091 |
| S | 36.675743 | 28.671303 | 31.667023 |
| S | 36.726562 | 29.624096 | 36.483177 |
| S | 40.059494 | 27.160044 | 34.317158 |
| S | 40.451275 | 31.764683 | 33.931141 |
| S | 43.643780 | 28.680134 | 31.467842 |
| S | 44.635735 | 27.102657 | 38.075859 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 24.805088 | 30.648394 | 32.260509 |
| Ca | 26.929323 | 30.675922 | 36.065090 |
| Ca | 30.008818 | 28.077156 | 35.479477 |
| Ca | 30.284595 | 32.747368 | 33.299576 |
| Ca | 33.233723 | 28.810673 | 31.086790 |
| Ca | 33.534100 | 30.535254 | 35.225327 |
| Ca | 36.519501 | 27.136377 | 34.209549 |
| Ca | 37.034103 | 31.520367 | 33.738342 |
| Ca | 40.043571 | 29.423054 | 31.590837 |
| Ca | 39.869255 | 30.001282 | 37.029453 |
| Ca | 45.832230 | 27.248730 | 33.616528 |
| Ca | 42.836849 | 29.333031 | 34.506378 |
| S | 26.741934 | 27.085060 | 36.434063 |
| S | 27.303694 | 33.816143 | 34.848476 |
|  |  |  |  |
|---|---|---|---|
| S  | 30.350901 | 29.626566 | 32.507774 |
| S  | 30.246914 | 31.396591 | 36.450073 |
| S  | 33.307026 | 27.282322 | 34.010719 |
| S  | 33.361451 | 32.137421 | 32.084515 |
| S  | 36.738708 | 28.926048 | 31.586340 |
| S  | 36.668011 | 29.638767 | 36.390999 |
| S  | 40.065845 | 27.040251 | 34.087158 |
| S  | 40.498856 | 31.669743 | 34.065978 |
| S  | 43.514057 | 28.443867 | 33.852783 |
| S  | 44.505295 | 27.171061 | 38.320427 |

24

|  |  |  |  |
|---|---|---|---|
| S  | 26.683056 | 27.117542 | 36.399918 |
| S  | 27.341438 | 33.814400 | 35.008030 |
| S  | 30.291481 | 29.870783 | 32.619095 |
| S  | 30.246912 | 31.346149 | 36.276093 |
| S  | 33.373379 | 27.496685 | 33.992943 |
| S  | 33.672493 | 32.332062 | 32.232567 |
| S  | 36.536770 | 28.681875 | 31.595037 |
| S  | 36.586929 | 29.647919 | 36.253239 |
| S  | 40.104240 | 27.102322 | 34.386448 |
| S  | 40.716118 | 31.674520 | 33.758324 |
| S  | 43.460712 | 28.633703 | 31.428961 |
| S  | 44.601135 | 26.718622 | 38.177601 |

24

|  |  |  |  |
|---|---|---|---|
| Ca | 25.048187 | 30.480629 | 32.479652 |
| Ca | 26.821774 | 30.415264 | 36.066925 |
| Ca | 30.140949 | 28.234404 | 35.703793 |
| Ca | 30.253614 | 32.933254 | 33.073090 |
| Ca | 33.274376 | 29.160158 | 31.062674 |
| Ca | 33.345829 | 30.577232 | 34.964127 |
| Ca | 36.569069 | 26.961424 | 34.100647 |
| Ca | 37.024242 | 31.617296 | 33.654568 |
| Element | X-position | Y-position | Z-position |
|---------|------------|------------|------------|
| Ca      | 39.902393  | 29.415201  | 31.735949  |
| Ca      | 39.967686  | 29.595072  | 36.745399  |
| Ca      | 45.929176  | 27.517807  | 33.829170  |
| Ca      | 42.777790  | 29.415657  | 36.547630  |
| S       | 26.885794  | 26.771957  | 36.490687  |
| S       | 27.286341  | 33.909042  | 34.904488  |
| S       | 30.302633  | 29.721306  | 32.589531  |
| S       | 30.191551  | 31.421602  | 36.170219  |
| S       | 32.294243  | 27.382002  | 33.897217  |
| S       | 33.633514  | 32.406303  | 32.140617  |
| S       | 36.517761  | 29.736217  | 36.266972  |
| S       | 39.922848  | 27.051947  | 34.369316  |
| S       | 40.618713  | 31.739275  | 33.806259  |
| S       | 43.542805  | 28.538280  | 31.664415  |
| S       | 44.587353  | 26.603916  | 38.062424  |

24  
generated by VMD

| Element | X-position | Y-position | Z-position |
|---------|------------|------------|------------|
| Ca      | 24.182957  | 30.379774  | 32.367767  |
| Ca      | 26.789589  | 30.492580  | 35.886547  |
| Ca      | 29.753853  | 28.248148  | 35.475899  |
| Ca      | 30.092234  | 32.901974  | 33.063717  |
| Ca      | 33.420181  | 29.343992  | 31.303993  |
| Ca      | 33.344170  | 30.521927  | 35.047630  |
| Ca      | 36.676071  | 26.939327  | 34.490906  |
| Ca      | 37.144142  | 31.607517  | 34.031048  |
| Ca      | 40.163548  | 29.200783  | 32.013889  |
| Ca      | 40.099796  | 29.552485  | 36.816422  |
| Ca      | 46.066628  | 27.318560  | 33.074371  |
| Ca      | 43.080044  | 29.298613  | 34.362930  |
| S       | 26.429407  | 27.026176  | 36.456741  |
| S       | 27.001356  | 33.603271  | 34.564606  |
| S       | 30.279446  | 29.785759  | 32.419331  |
| S       | 30.025372  | 31.431025  | 36.149307  |
| S       | 33.100769  | 27.282631  | 33.971115  |
| S       | 33.603058  | 32.653927  | 32.288986  |
| S       | 36.802849  | 29.029253  | 31.896170  |
| S       | 36.736931  | 29.643435  | 36.459637  |
| S       | 40.193966  | 27.139399  | 34.490639  |
| S       | 40.720081  | 31.740646  | 33.959797  |
| S       | 43.541183  | 28.255472  | 31.381130  |
| S       | 45.186230  | 26.990759  | 38.049904  |

24  
generated by VMD

| Element | X-position | Y-position | Z-position |
|---------|------------|------------|------------|
| Ca      | 24.524261  | 30.531910  | 32.185928  |
| Ca      | 26.705526  | 30.668072  | 35.852314  |
|     |      |      |     |
|-----|------|------|-----|
| Ca  | 29.693054 | 28.275658 | 35.596832 |
| Ca  | 30.224119 | 32.643860 | 32.984024 |
| Ca  | 33.253700 | 28.881201 | 31.317284 |
| Ca  | 33.351959 | 30.629299 | 35.391701 |
| Ca  | 36.518295 | 26.960640 | 34.643333 |
| Ca  | 37.252239 | 31.634256 | 34.066292 |
| Ca  | 40.068489 | 29.447918 | 31.702841 |
| Ca  | 40.147167 | 29.756807 | 36.628960 |
| Ca  | 46.076775 | 27.192598 | 32.963242 |
| Ca  | 43.041542 | 29.263678 | 34.405338 |
| S   | 26.419445 | 27.011444 | 36.214596 |
| S   | 27.159325 | 33.824852 | 34.634834 |
| S   | 26.08004  | 29.584934 | 32.586330 |
| S   | 30.045509 | 31.342747 | 36.223946 |
| S   | 33.243267 | 27.316326 | 34.220497 |
| S   | 33.692184 | 32.124466 | 32.245041 |
| S   | 36.739662 | 28.940664 | 31.965843 |
| S   | 36.657974 | 29.879320 | 36.666397 |
| S   | 40.114555 | 27.096767 | 34.127453 |
| S   | 40.886513 | 31.744335 | 33.862389 |
| S   | 43.707539 | 28.680336 | 31.422520 |
| S   | 44.702721 | 26.959309 | 38.122749 |

24

generated by VMD

|     |      |      |     |
|-----|------|------|-----|
| Ca  | 24.520632 | 30.229540 | 32.318100 |
| Ca  | 26.696558 | 30.581617 | 36.001087 |
| Ca  | 29.826691 | 28.194866 | 35.566418 |
| Ca  | 30.314430 | 32.783768 | 33.022930 |
| Ca  | 33.118946 | 29.148985 | 31.398478 |
| Ca  | 33.396065 | 30.829428 | 35.300808 |
| Ca  | 36.533154 | 27.072115 | 34.501205 |
| Ca  | 37.076405 | 31.547993 | 33.834923 |
| Ca  | 40.173904 | 29.124788 | 31.658827 |
| Ca  | 40.059616 | 29.546873 | 36.750664 |
| Ca  | 45.979797 | 27.355587 | 33.035011 |
| Ca  | 43.231598 | 29.476748 | 34.644508 |
| S   | 26.509212 | 26.929909 | 35.989933 |
| S   | 27.010506 | 33.796696 | 34.616241 |
| S   | 30.151028 | 29.701723 | 32.560535 |
| S   | 30.056528 | 31.423298 | 36.181866 |
| S   | 33.186272 | 27.611668 | 34.232269 |
| S   | 33.805004 | 32.522301 | 32.416401 |
| S   | 36.702190 | 28.832111 | 31.841160 |
| S   | 36.619663 | 29.732536 | 36.527954 |
| S   | 40.129318 | 26.942036 | 34.445431 |
| S   | 40.679508 | 31.506226 | 33.744514 |
|   | X   | Y   | Z   |
|---|-----|-----|-----|
| S | 43.598312 | 28.658638 | 31.516201 |
| S | 45.058601 | 26.841938 | 37.925213 |

24 generated by VMD

|   | X   | Y   | Z   |
|---|-----|-----|-----|
| Ca | 24.454298 | 30.462955 | 32.211044 |
| Ca | 26.589813 | 30.546066 | 35.681446 |
| Ca | 29.805813 | 28.148279 | 35.354828 |
| Ca | 30.187368 | 32.701267 | 33.090923 |
| Ca | 33.320621 | 29.126305 | 31.320679 |
| Ca | 33.379391 | 30.696114 | 35.342129 |
| Ca | 36.565182 | 26.967625 | 34.560059 |
| Ca | 36.914642 | 31.494560 | 33.855942 |
| Ca | 39.992447 | 29.134132 | 32.070713 |
| Ca | 40.335583 | 29.900667 | 36.896652 |
| Ca | 46.026127 | 27.477261 | 33.052586 |
| Ca | 43.021233 | 29.469803 | 34.339546 |
| S  | 26.380455 | 27.033602 | 36.270393 |
| S  | 27.359648 | 33.783653 | 34.687122 |
| S  | 30.303509 | 29.639473 | 32.436634 |
| S  | 30.028996 | 31.332157 | 36.263447 |
| S  | 33.242474 | 27.635349 | 34.247704 |
| S  | 33.638756 | 32.419876 | 32.228130 |
| S  | 36.698139 | 28.750523 | 31.884245 |
| S  | 36.743546 | 29.686888 | 36.661743 |
| S  | 40.113731 | 27.132816 | 34.531982 |
| S  | 40.639748 | 31.664337 | 33.868843 |
| S  | 43.563328 | 28.553444 | 31.474030 |
| S  | 45.129025 | 26.634266 | 37.699867 |

24 generated by VMD

|   | X   | Y   | Z   |
|---|-----|-----|-----|
| Ca | 24.766575 | 30.294899 | 32.340221 |
| Ca | 26.735249 | 30.446449 | 35.993629 |
| Ca | 29.931122 | 28.290634 | 35.417469 |
| Ca | 30.350739 | 32.825321 | 33.022800 |
| Ca | 33.291641 | 28.976444 | 31.411470 |
| Ca | 33.331821 | 30.757151 | 35.255730 |
| Ca | 36.660412 | 27.062353 | 34.505966 |
| Ca | 37.017426 | 31.655695 | 33.932442 |
| Ca | 40.042412 | 29.342361 | 31.865097 |
| Ca | 40.082897 | 29.984333 | 36.654747 |
| Ca | 45.657291 | 27.244705 | 33.243572 |
| Ca | 43.082882 | 29.347269 | 34.369591 |
| S  | 26.634726 | 26.959240 | 36.078125 |
| S  | 27.267864 | 33.680851 | 34.697903 |
| S  | 30.373085 | 29.630323 | 32.445816 |
| S  | 30.093319 | 31.350138 | 36.282597 |
S    33.240959  27.463322  34.377605
S    33.670303  32.387650  32.279335
S    36.691242  29.058537  31.871580
S    36.741364  29.704044  36.594715
S    40.119015  27.098991  34.212395
S    40.583000  31.740801  33.726154
S    43.565147  28.449457  31.522070
S    44.503456  26.640394  37.929646
24 generated by VMD
Ca   24.703245  30.434767  32.359436
Ca   26.623909  30.450438  35.919312
Ca   30.070679  28.473791  35.261658
Ca   30.079748  32.839226  33.128078
Ca   33.378620  28.841898  31.401896
Ca   33.206715  30.836418  35.186928
Ca   36.663746  27.019831  34.628086
Ca   36.861710  31.635639  33.706764
Ca   40.093998  29.348669  31.792023
Ca   40.172005  29.527784  36.865757
Ca   45.874268  27.233965  32.955055
Ca   43.033649  29.349451  34.456024
S    26.701149  26.944258  36.273468
S    27.225746  33.732353  34.748386
S    30.248001  29.750130  32.315361
S    30.007143  31.439871  36.325138
S    33.205166  27.601709  34.252094
S    33.659756  32.316177  32.342674
S    36.763695  28.682920  31.838520
S    36.572750  29.728237  36.531319
S    40.213509  27.103477  34.264717
S    40.688419  31.543320  33.809662
S    43.530731  28.678291  31.451588
S    44.855530  26.878815  38.207745
24 generated by VMD
Ca   24.441446  30.276218  32.469513
Ca   26.638762  30.443304  35.992702
Ca   30.054329  28.278458  35.698071
Ca   30.023449  32.905228  33.275272
Ca   33.345879  29.277416  31.110725
Ca   33.378357  30.580128  35.220139
Ca   36.618900  27.067829  34.111111
Ca   36.981400  31.728809  33.638088
Ca   40.155560  29.173615  31.763988
Ca   40.115883  29.768484  36.668587
| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 45.829529 | 27.265469 | 33.778111 |
| Ca      | 42.882576 | 29.335936 | 34.302349 |
| S       | 27.121113 | 26.932718 | 36.215336 |
| S       | 27.056883 | 33.772564 | 34.847210 |
| S       | 30.338436 | 29.797052 | 32.529469 |
| S       | 29.996391 | 31.373240 | 36.246792 |
| S       | 33.374790 | 27.620966 | 34.035946 |
| S       | 33.499405 | 32.505993 | 32.331238 |
| S       | 36.753292 | 28.878098 | 31.627949 |
| S       | 40.061062 | 27.012363 | 34.395069 |
| S       | 40.697475 | 31.614128 | 33.635788 |
| S       | 43.644135 | 28.427046 | 31.511223 |
| S       | 44.733303 | 26.636160 | 38.311417 |

24 generated by VMD

| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 24.366898 | 30.223713 | 32.772724 |
| Ca      | 26.788734 | 30.225960 | 35.910175 |
| Ca      | 30.203915 | 28.098219 | 35.250881 |
| Ca      | 30.200226 | 32.904900 | 33.243061 |
| Ca      | 33.533638 | 29.512226 | 31.171940 |
| Ca      | 33.489986 | 30.548828 | 35.058830 |
| Ca      | 36.562618 | 27.295702 | 34.145458 |
| Ca      | 37.142735 | 31.779154 | 33.742779 |
| Ca      | 40.164581 | 29.164680 | 31.846684 |
| Ca      | 39.875065 | 30.046783 | 36.652748 |
| Ca      | 45.734795 | 26.780178 | 33.690994 |
| Ca      | 42.864864 | 29.184006 | 34.401855 |
| S       | 27.071945 | 26.618849 | 36.549641 |
| S       | 27.114311 | 33.563957 | 34.838802 |
| S       | 30.398119 | 29.804920 | 32.464668 |
| S       | 30.182592 | 31.205639 | 36.326294 |
| S       | 33.185173 | 27.563820 | 34.023315 |
| S       | 33.720135 | 32.694000 | 32.345299 |
| S       | 36.889809 | 29.195847 | 31.608902 |
| S       | 36.547905 | 30.260586 | 36.239773 |
| S       | 40.066669 | 27.090427 | 34.401794 |
| S       | 40.752090 | 31.665535 | 33.700867 |
| S       | 43.639538 | 28.279720 | 31.232143 |
| S       | 43.937519 | 26.683758 | 38.411121 |

24 generated by VMD

| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 24.381100 | 30.114178 | 32.530323 |
| Ca      | 26.281536 | 29.903822 | 35.839722 |
| Ca      | 30.338131 | 28.456196 | 35.107750 |
| Ca      | 29.966274 | 33.188545 | 33.116978 |
|   | Ca       | S        |
|---|----------|----------|
| 1 | 33.317745 | 32.461159 |
| 2 | 33.497044 | 35.427483 |
| 3 | 36.624897 | 34.382851 |
| 4 | 37.148388 | 33.801319 |
| 5 | 40.218895 | 31.673468 |
| 6 | 40.093658 | 36.546814 |
| 7 | 45.927845 | 33.956932 |
| 8 | 42.985092 | 34.255375 |
| 9 | 27.307827 | 36.529114 |
|10 | 26.751200 | 34.818024 |
|11 | 30.256622 | 32.384262 |
|12 | 30.144669 | 36.411217 |
|13 | 33.317699 | 34.064030 |
|14 | 33.565842 | 32.628223 |
|15 | 36.818401 | 31.455969 |
|16 | 36.623596 | 36.464859 |
|17 | 39.908379 | 34.317387 |
|18 | 40.827652 | 33.719769 |
|19 | 43.738979 | 31.272221 |
|20 | 44.392479 | 38.147541 |

24 generated by VMD

|   | Ca       | S        |
|---|----------|----------|
| 1 | 24.678736 | 32.461159 |
| 2 | 26.464449 | 35.943142 |
| 3 | 30.229834 | 35.132973 |
| 4 | 29.946810 | 32.960564 |
| 5 | 33.233925 | 31.373203 |
| 6 | 33.526581 | 35.430061 |
| 7 | 36.665489 | 34.541729 |
| 8 | 37.226055 | 33.929634 |
| 9 | 40.109814 | 31.932137 |
|10 | 40.184593 | 36.762730 |
|11 | 45.839020 | 33.174389 |
|12 | 42.974983 | 34.217903 |
|13 | 27.312460 | 36.209457 |
|14 | 26.916037 | 34.668980 |
|15 | 30.048128 | 32.263733 |
|16 | 29.903925 | 36.211037 |
|17 | 33.238701 | 34.137871 |
|18 | 33.340229 | 32.578762 |
|19 | 36.689518 | 31.698622 |
|20 | 36.606773 | 36.513039 |
|21 | 39.976559 | 34.629581 |
|22 | 40.798874 | 33.870811 |
|23 | 43.606876 | 31.359137 |
|24 | 44.915497 | 38.030083 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 24.565554 | 29.997326 | 32.681015 |
| Ca      | 26.449961  | 30.261923  | 36.264778  |
| Ca      | 30.305511  | 28.459930  | 35.302364  |
| Ca      | 30.087303  | 32.784000  | 33.397583  |
| Ca      | 33.488602  | 29.577803  | 30.836182  |
| Ca      | 33.257130  | 30.637638  | 34.973251  |
| Ca      | 36.749512  | 27.128838  | 34.256760  |
| Ca      | 37.079754  | 31.713068  | 33.638268  |
| Ca      | 40.041271  | 29.271885  | 31.938358  |
| Ca      | 39.964970  | 29.903666  | 36.580894  |
| Ca      | 45.515877  | 26.619646  | 33.521690  |
| Ca      | 43.131802  | 29.254211  | 34.443764  |
| S       | 27.344498  | 27.023666  | 36.401711  |
| S       | 26.999798  | 33.525196  | 34.889503  |
| S       | 30.285572  | 29.712173  | 32.346680  |
| S       | 29.940479  | 31.389845  | 36.499001  |
| S       | 33.414791  | 27.666912  | 33.653667  |
| S       | 33.720669  | 32.757107  | 32.381184  |
S  36.817078  28.769850  31.508827
S  36.435818  29.849262  36.244522
S  40.086662  27.254990  34.493866
S  40.642467  31.803349  33.763363
S  43.598522  28.256462  31.596922
S  44.510220  26.772614  38.416573

24

generated by VMD
Ca  24.689713  30.099033  32.443081
Ca  26.093184  30.224779  36.141129
Ca  30.319559  28.449408  35.210022
Ca  30.016800  32.840576  33.338730
Ca  33.506680  29.675571  31.148024
Ca  33.106499  30.656740  35.293617
Ca  36.746140  27.234135  34.423820
Ca  36.960060  31.725590  33.632984
Ca  40.319851  29.150818  31.817926
Ca  40.098740  30.110874  36.629868
Ca  45.801579  26.811134  33.609322
Ca  43.230484  29.140652  34.361462
S  27.191074  26.923109  36.330681
S  26.874414  33.699356  35.130451
S  30.220671  29.839025  32.376278
S  29.711296  31.202063  36.384956
S  33.384533  27.712034  33.888763
S  33.313324  32.674145  32.372940
S  36.918720  28.744087  31.456165
S  36.572548  30.054764  36.237007
S  40.060375  27.198397  34.510536
S  40.879452  31.604858  33.727436
S  43.753551  27.950092  31.439690
S  44.664631  26.670212  38.125793

24

generated by VMD
Ca  24.355537  30.474539  32.411560
Ca  26.433651  30.333912  35.868156
Ca  30.265413  28.234890  35.264740
Ca  30.164322  32.983685  33.146282
Ca  33.436741  29.317513  31.355797
Ca  33.367744  30.466747  35.127758
Ca  36.779343  26.940464  34.550694
Ca  36.940865  31.622717  33.920170
Ca  40.098934  29.375618  31.894295
Ca  39.979355  30.033850  36.753113
Ca  45.506382  26.683418  33.206982
Ca  43.183746  29.535885  34.157665
| S    | 27.254719  | 27.010431  | 36.280251  |
|------|------------|------------|------------|
| S    | 27.118328  | 33.674583  | 34.736397  |
| S    | 30.340710  | 29.740582  | 32.190044  |
| S    | 29.942234  | 31.145290  | 36.268497  |
| S    | 33.415878  | 27.547009  | 34.037811  |
| S    | 33.719696  | 32.492035  | 32.437721  |
| S    | 36.839577  | 28.779078  | 31.974491  |
| S    | 36.417637  | 29.892023  | 36.543472  |
| S    | 40.056538  | 27.178604  | 34.592110  |
| S    | 40.586113  | 31.817478  | 33.896439  |
| S    | 43.323074  | 28.094332  | 31.400358  |
| S    | 44.907455  | 27.016754  | 38.015915  |

24

generated by VMD

| Ca   | 24.643002  | 30.677505  | 31.764744  |
|------|------------|------------|------------|
| Ca   | 26.198429  | 30.467484  | 35.504620  |
| Ca   | 30.128899  | 27.947365  | 35.481003  |
| Ca   | 30.331417  | 32.745827  | 33.319740  |
| Ca   | 33.396076  | 29.306326  | 31.310833  |
| Ca   | 33.435226  | 30.408062  | 35.148571  |
| Ca   | 36.732918  | 27.410282  | 34.543381  |
| Ca   | 36.842781  | 31.588291  | 33.695152  |
| Ca   | 40.176559  | 29.463715  | 32.017151  |
| Ca   | 40.105270  | 30.051392  | 36.694492  |
| Ca   | 45.927845  | 26.749119  | 33.053055  |
| Ca   | 43.059868  | 29.340343  | 34.179157  |
| Ca   | 26.786770  | 27.150547  | 36.904171  |
| Ca   | 27.384703  | 33.778614  | 34.812687  |
| Ca   | 30.467720  | 29.663692  | 32.645039  |
| Ca   | 29.644077  | 30.851234  | 36.523949  |
| Ca   | 33.401085  | 27.428404  | 34.079678  |
| Ca   | 33.521519  | 32.367374  | 32.277496  |
| Ca   | 36.762321  | 28.748104  | 31.680805  |
| Ca   | 36.429916  | 30.030228  | 36.597500  |
| Ca   | 40.068195  | 27.300873  | 34.487080  |
| Ca   | 40.661961  | 31.902657  | 33.927769  |
| Ca   | 43.670326  | 28.055563  | 31.320560  |
| Ca   | 44.657024  | 26.958372  | 38.062088  |

24

generated by VMD

| Ca   | 24.518854  | 30.612255  | 31.908218  |
|------|------------|------------|------------|
| Ca   | 26.429354  | 30.576412  | 35.685802  |
| Ca   | 30.330967  | 27.869301  | 35.136818  |
| Ca   | 30.158501  | 32.653656  | 33.387520  |
| Ca   | 33.261868  | 29.414307  | 31.446751  |
| Ca   | 33.546909  | 30.356482  | 35.379227  |
|   | Ca   | S     |
|---|------|-------|
|   | 36.733936 | 27.279575 | 34.640320 |
|   | 37.049183 | 31.706387 | 33.654453 |
|   | 39.928688 | 29.335760 | 31.825033 |
|   | 40.214165 | 29.920666 | 36.646706 |
|   | 45.654369 | 26.610577 | 33.386719 |
|   | 43.047009 | 29.475079 | 34.145004 |
|   | 27.006027 | 27.100605 | 36.439079 |
|   | 27.134262 | 33.840481 | 34.785423 |
|   | 30.219944 | 29.523132 | 32.391747 |
|   | 29.949110 | 30.982691 | 36.410175 |
|   | 33.488419 | 27.489689 | 33.970924 |
|   | 33.415428 | 32.549889 | 32.748661 |
|   | 36.612225 | 28.976896 | 31.751339 |
|   | 36.648708 | 29.986469 | 36.569088 |
|   | 40.057285 | 27.218214 | 34.392868 |
|   | 40.646606 | 31.744789 | 33.588505 |
|   | 43.442348 | 27.893379 | 31.550423 |
|   | 44.898479 | 27.274691 | 38.189968 |

24 generated by VMD

|   | Ca   | S     |
|---|------|-------|
|   | 24.524239 | 30.706669 | 32.113129 |
|   | 26.578087 | 30.644716 | 35.706825 |
|   | 30.181770 | 27.839310 | 35.228954 |
|   | 30.307339 | 32.850986 | 33.212299 |
|   | 33.140064 | 29.128006 | 31.308361 |
|   | 33.263512 | 30.289354 | 35.447788 |
|   | 36.849834 | 26.988539 | 34.547329 |
|   | 36.930798 | 31.524517 | 33.678196 |
|   | 40.019257 | 29.427059 | 32.002228 |
|   | 40.076988 | 29.709921 | 36.666878 |
|   | 45.508865 | 26.979652 | 33.212624 |
|   | 43.029144 | 29.494875 | 34.295837 |
|   | 26.842278 | 27.258945 | 36.547298 |
|   | 27.231125 | 33.912418 | 34.689156 |
|   | 30.224319 | 29.744333 | 32.539696 |
|   | 29.949932 | 30.971878 | 36.266403 |
|   | 33.442081 | 27.383339 | 33.991447 |
|   | 33.736145 | 32.482063 | 32.564190 |
|   | 36.822041 | 28.778799 | 31.723434 |
|   | 36.555351 | 29.710901 | 36.435001 |
|   | 40.205925 | 27.088573 | 34.251759 |
|   | 40.616512 | 31.808002 | 33.913940 |
|   | 43.341370 | 28.066969 | 31.427879 |
|   | 45.056747 | 27.601580 | 38.260059 |

24 generated by VMD
| Element | X1      | Y1      | Z1      |
|---------|---------|---------|---------|
| Ca      | 24.736069 | 30.441257 | 32.022514 |
| Ca      | 26.250177 | 30.642532 | 35.649780 |
| Ca      | 30.456718 | 28.214481 | 35.631775 |
| Ca      | 30.179031 | 32.802086 | 33.144547 |
| Ca      | 33.409737 | 29.103642 | 31.223785 |
| Ca      | 33.374405 | 30.440929 | 35.396191 |
| Ca      | 36.808849 | 26.843945 | 34.507439 |
| Ca      | 36.720901 | 31.657116 | 33.662971 |
| Ca      | 39.945930 | 29.448605 | 31.810562 |
| Ca      | 40.011780 | 29.820499 | 36.720657 |
| Ca      | 45.638329 | 27.034414 | 33.152550 |
| Ca      | 42.975235 | 29.512697 | 34.429756 |
| S       | 26.985865 | 27.324362 | 36.414566 |
| S       | 27.171309 | 33.900543 | 34.698845 |
| S       | 30.462336 | 29.638103 | 32.588932 |
| S       | 29.742422 | 31.292740 | 36.379013 |
| S       | 33.544888 | 27.301203 | 34.158997 |
| S       | 33.636024 | 32.403095 | 32.504601 |
| S       | 36.808064 | 28.590160 | 31.733429 |
| S       | 36.506378 | 29.664021 | 36.520714 |
| S       | 40.133968 | 27.203934 | 34.479580 |
| S       | 40.540825 | 31.806181 | 33.934181 |
| S       | 43.468189 | 28.384624 | 31.424667 |
| S       | 44.926460 | 26.920210 | 37.840649 |

24

generated by VMD

| Element | X1      | Y1      | Z1      |
|---------|---------|---------|---------|
| Ca      | 24.819376 | 30.402100 | 31.860664 |
| Ca      | 26.377323 | 30.724186 | 35.732433 |
| Ca      | 30.286438 | 27.903511 | 35.391434 |
| Ca      | 30.197628 | 32.979858 | 33.205936 |
| Ca      | 33.367386 | 28.925690 | 31.610884 |
| Ca      | 33.309532 | 30.388933 | 35.207443 |
| Ca      | 36.655014 | 27.080963 | 34.720081 |
| Ca      | 36.983891 | 31.519260 | 33.915421 |
| Ca      | 39.848190 | 29.628901 | 31.837734 |
| Ca      | 40.339405 | 29.856730 | 36.607109 |
| Ca      | 45.796547 | 27.043896 | 33.089645 |
| Ca      | 43.108444 | 29.525358 | 34.308876 |
| S       | 26.743212 | 27.420967 | 36.500198 |
| S       | 27.058197 | 33.805187 | 34.469543 |
| S       | 30.262709 | 29.578600 | 32.742023 |
| S       | 29.763069 | 31.174870 | 36.261414 |
| S       | 33.470222 | 27.309044 | 34.257847 |
| S       | 33.544445 | 32.442238 | 32.453224 |
| S       | 36.687698 | 28.695042 | 31.819630 |
| S       | 36.422848 | 29.870293 | 36.622681 |
S       40.242603  27.314793  34.315796
S       40.698479  31.844385  33.941322
S       43.589802  28.323357  31.291382
S       44.861458  26.633322  37.867943

24
generated by VMD
Ca    24.678188  30.050831  31.852261
Ca    26.748474  30.649019  35.746529
Ca    30.266254  27.975327  35.915863
Ca    30.312016  32.663830  33.172325
Ca    33.355175  29.589546  31.259724
Ca    33.392616  30.287870  35.116299
Ca    36.532776  27.076981  34.669514
Ca    37.118439  31.648561  33.827515
Ca    39.999672  29.409439  31.793432
Ca    40.124065  29.894106  36.873165
Ca    45.489662  26.733397  32.810848
Ca    43.033852  29.623882  34.524277
S     26.940262  27.233179  36.404110
S     27.196344  33.736435  34.469658
S     30.489470  29.608986  32.740417
S     30.033644  31.244570  36.455391
S     33.248055  27.271023  34.111641
S     33.522686  32.618229  32.310856
S     36.711021  28.757776  31.793419
S     36.440903  30.103493  36.518116
S     40.002956  27.252823  34.429237
S     40.777771  31.702850  33.874130
S     43.481834  28.611950  31.215126
S     44.537777  26.647285  38.146935

24
generated by VMD
Ca    24.480923  30.181946  32.046654
Ca    26.611542  30.550953  36.179485
Ca    30.273838  28.108715  35.463982
Ca    30.495108  32.894623  33.120216
Ca    33.250984  29.183254  31.223713
Ca    33.336712  30.440182  35.268162
Ca    36.767540  27.257763  34.710674
Ca    37.062073  31.833656  33.815540
Ca    40.076981  29.414993  31.748674
Ca    40.035610  29.746254  36.849262
Ca    45.761047  27.096479  33.003838
Ca    42.843803  29.384544  34.587749
S     26.789406  27.081568  36.250137
S     26.977341  33.720959  34.640129
|   |     |     |     |
|---|---|---|---|
| S | 30.416470 | 29.666508 | 32.460323 |
| S | 29.976677 | 31.227161 | 36.271011 |
| S | 33.500248 | 27.456791 | 34.152573 |
| S | 33.724171 | 32.332085 | 32.328835 |
| S | 36.781082 | 28.933893 | 31.756577 |
| S | 36.588558 | 30.115513 | 36.552345 |
| S | 40.026104 | 27.147421 | 34.202671 |
| S | 40.706589 | 31.655209 | 33.949459 |
| S | 43.277748 | 28.268158 | 31.369560 |
| S | 44.673374 | 26.692780 | 38.079170 |

24 generated by VMD

| Ca | 24.683596 | 30.500034 | 31.883404 |
| Ca | 26.571945 | 30.733381 | 35.895844 |
| Ca | 30.135059 | 28.113775 | 35.596737 |
| Ca | 30.155931 | 32.607117 | 33.155365 |
| Ca | 33.348263 | 29.243881 | 31.512432 |
| Ca | 33.128288 | 30.527802 | 35.22851 |
| Ca | 36.779335 | 26.812511 | 34.636959 |
| Ca | 36.953556 | 31.606966 | 33.925484 |
| Ca | 39.907379 | 29.382984 | 31.996910 |
| Ca | 40.111694 | 29.958389 | 36.801296 |
| Ca | 45.875614 | 27.174252 | 32.850212 |
| Ca | 43.097900 | 29.283770 | 34.444199 |
| S | 26.701668 | 27.440863 | 36.135750 |
| S | 27.071156 | 33.733776 | 34.521301 |
| S | 30.354849 | 29.465401 | 32.527084 |
| S | 30.039602 | 31.158459 | 36.346497 |
| S | 33.439537 | 27.483944 | 34.309952 |
| S | 33.562099 | 32.359726 | 32.264000 |
| S | 36.704773 | 28.705492 | 31.964407 |
| S | 36.579655 | 29.779375 | 36.586536 |
| S | 40.117085 | 27.202286 | 34.412903 |
| S | 40.790535 | 31.747953 | 33.885632 |
| S | 43.343613 | 28.442833 | 31.342384 |
| S | 44.980820 | 26.926418 | 37.812580 |

24 generated by VMD

| Ca | 24.657822 | 30.603897 | 32.383713 |
| Ca | 26.597788 | 30.723480 | 35.683971 |
| Ca | 30.226646 | 28.130714 | 35.574718 |
| Ca | 30.130196 | 32.740730 | 33.163643 |
| Ca | 33.329475 | 28.965017 | 31.447933 |
| Ca | 33.393738 | 30.427259 | 35.405418 |
| Ca | 36.681950 | 27.002150 | 34.418774 |
| Ca | 36.707340 | 31.801184 | 33.869625 |
Ca    40.079853  29.280994  31.983963
Ca    40.194332  29.859192  36.824791
Ca    45.985947  27.658257  33.301098
Ca    43.051548  29.644173  34.258308
S     26.766022  27.161114  36.017750
S     27.226578  33.991428  34.513618
S     30.333775  29.460474  32.583359
S     30.165808  31.182741  36.198036
S     34.00414  27.232698  34.191132
S     33.710491  32.267303  32.411255
S     36.643307  28.871803  31.939148
S     36.565727  29.787365  36.555779
S     39.945446  27.237858  34.367432
S     40.559566  31.710022  33.802616
S     43.389294  28.173676  31.504513
S     44.690857  26.477859  37.630085

24
generated by VMD
Ca    24.648560  30.572447  31.819080
Ca    26.367352  30.659182  35.823719
Ca    30.194794  28.056368  35.741871
Ca    30.259375  32.744999  33.169140
Ca    33.290398  29.070210  31.207912
Ca    33.407017  30.162020  35.073765
Ca    36.918861  27.173252  34.600777
Ca    37.000351  31.728691  33.807178
Ca    39.935085  29.468576  31.935047
Ca    39.963181  30.063095  37.012699
Ca    45.889771  27.166927  32.989738
Ca    43.145592  29.369659  34.341446
S     26.774391  27.315132  36.424980
S     27.137022  33.739090  34.611164
S     30.404503  29.517357  32.761963
S     29.926346  31.087622  36.305050
S     33.425434  27.155373  33.992229
S     33.622246  32.460011  32.325535
S     36.646030  28.960299  31.911886
S     36.530746  30.102856  36.411076
S     40.036690  27.401543  34.569294
S     40.684692  31.662642  33.981525
S     43.278793  28.160910  31.373360
S     44.946594  26.593164  37.840252

24
generated by VMD
Ca    24.887415  30.056824  31.978020
Ca    26.560543  30.778835  35.710747
| Element | X                  | Y                  | Z                  |
|---------|--------------------|--------------------|--------------------|
| Ca      | 30.261635          | 27.872852          | 35.280987          |
| Ca      | 30.212118          | 33.118233          | 32.969810          |
| Ca      | 33.311295          | 29.223791          | 31.731331          |
| Ca      | 33.822670          | 27.062323          | 34.825275          |
| Ca      | 36.831535          | 31.463921          | 34.076691          |
| Ca      | 39.97892           | 29.353994          | 31.758034          |
| Ca      | 40.082603          | 29.667896          | 36.834049          |
| Ca      | 45.794956          | 27.424889          | 32.799454          |
| Ca      | 43.177029          | 29.477886          | 34.376442          |
| S       | 26.932230          | 27.292227          | 36.421852          |
| S       | 26.931515          | 33.938004          | 34.319145          |
| S       | 30.282713          | 29.652813          | 32.491234          |
| S       | 29.979223          | 31.325935          | 36.199860          |
| S       | 33.523525          | 27.339514          | 34.325958          |
| S       | 33.634007          | 32.480469          | 32.698723          |
| S       | 36.665787          | 28.720417          | 31.984371          |
| S       | 36.564980          | 29.767670          | 36.868492          |
| S       | 40.091625          | 27.310904          | 34.340111          |
| S       | 40.674408          | 31.660381          | 33.821747          |
| S       | 43.333889          | 28.390198          | 31.239449          |
| S       | 44.567928          | 26.515083          | 37.711697          |

24

generated by VMD

| Element | X                  | Y                  | Z                  |
|---------|--------------------|--------------------|--------------------|
| Ca      | 24.802441          | 30.103495          | 31.775623          |
| Ca      | 26.204250          | 30.551491          | 35.688271          |
| Ca      | 30.274513          | 28.124628          | 36.031796          |
| Ca      | 30.309605          | 32.679028          | 33.129131          |
| Ca      | 33.411484          | 29.469799          | 31.218975          |
| Ca      | 33.241009          | 30.681374          | 35.491917          |
| Ca      | 36.779392          | 27.035831          | 34.575790          |
| Ca      | 37.059479          | 31.593575          | 33.767555          |
| Ca      | 40.059128          | 29.505161          | 31.897861          |
| Ca      | 40.163280          | 29.772877          | 36.690613          |
| Ca      | 45.782738          | 26.999458          | 33.026283          |
| Ca      | 43.054680          | 29.666206          | 34.294273          |
| S       | 26.725964          | 27.200600          | 36.360691          |
| S       | 27.006754          | 33.750027          | 34.458546          |
| S       | 30.329060          | 29.512539          | 32.703423          |
| S       | 29.850903          | 31.210436          | 36.413734          |
| S       | 33.283409          | 27.647102          | 34.331306          |
| S       | 33.627895          | 32.566170          | 32.448067          |
| S       | 36.695232          | 28.680359          | 31.788166          |
| S       | 36.572258          | 30.025381          | 36.537922          |
| S       | 40.187515          | 27.113535          | 34.245533          |
| S       | 40.754303          | 31.844893          | 33.884373          |
|      |       |       |       |
|------|-------|-------|-------|
| S    | 43.578186 | 28.318165 | 31.417654 |
| S    | 44.680443  | 26.339247  | 37.853218  |

24 generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 25.282480 | 30.332596 | 31.970942  |
| Ca  | 26.364832  | 30.954103  | 35.999245  |
| Ca  | 30.004078  | 27.910830  | 35.878326  |
| Ca  | 30.312904  | 32.672512  | 33.200912  |
| Ca  | 33.419701  | 29.230654  | 31.276024  |
| Ca  | 33.378036  | 30.281834  | 35.232933  |
| Ca  | 36.565304  | 26.958954  | 34.541912  |
| Ca  | 36.752319  | 31.698013  | 33.847565  |
| Ca  | 40.078358  | 29.451775  | 31.770050  |
| Ca  | 40.059078  | 29.737776  | 36.681820  |
| Ca  | 46.010296  | 27.439745  | 33.326321  |
| Ca  | 42.989281  | 29.519001  | 34.326004  |
| S   | 26.624760  | 27.442480  | 36.359753  |
| S   | 27.106340  | 33.910805  | 34.519127  |
| S   | 30.499737  | 29.532578  | 32.824974  |
| S   | 29.970066  | 31.133308  | 36.426674  |
| S   | 33.212250  | 27.228489  | 34.229908  |
| S   | 33.695538  | 32.425106  | 32.186478  |
| S   | 36.755165  | 28.805920  | 31.771503  |
| S   | 36.438148  | 29.783730  | 36.498238  |
| S   | 40.123035  | 27.133335  | 34.164078  |
| S   | 40.603840  | 31.698284  | 33.898518  |
| S   | 43.677635  | 28.384216  | 31.259399  |
| S   | 44.510666  | 26.725370  | 37.839985  |

24 generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 25.152325 | 30.134930 | 31.947304  |
| Ca  | 26.411390  | 30.763269  | 35.943779  |
| Ca  | 30.325140  | 28.150681  | 35.878044  |
| Ca  | 30.089497  | 33.012875  | 33.229820  |
| Ca  | 33.338058  | 29.140903  | 31.327976  |
| Ca  | 33.236713  | 30.417595  | 35.126995  |
| Ca  | 36.691460  | 27.044479  | 34.322311  |
| Ca  | 36.843323  | 31.508919  | 33.802689  |
| Ca  | 39.847347  | 29.508904  | 31.735636  |
| Ca  | 40.132061  | 29.715439  | 36.815105  |
| Ca  | 45.884876  | 27.401957  | 33.415642  |
| Ca  | 42.923859  | 29.338661  | 34.355797  |
| S   | 26.914738  | 27.308641  | 36.347778  |
| S   | 26.887251  | 33.816166  | 34.669788  |
| S   | 30.510036  | 29.748837  | 32.722088  |
| S   | 30.115822  | 31.397209  | 36.303062  |
|    | X Value | Y Value | Z Value  |
|----|---------|---------|----------|
| S  | 33.369026 | 27.311472 | 34.314449 |
| S  | 33.599327 | 32.287003 | 32.229301 |
| S  | 36.607216 | 28.877998 | 31.652393 |
| S  | 36.459129 | 29.764709 | 36.437717 |
| S  | 40.091171 | 27.073624 | 34.201435 |
| S  | 40.659073 | 31.574633 | 33.908703 |
| S  | 43.591476 | 28.453583 | 31.439129 |
| S  | 44.753719 | 26.638922 | 37.903786 |

24

Generated by VMD

| Ca  | X Value | Y Value | Z Value  |
|-----|---------|---------|----------|
| Ca  | 24.941219 | 30.216764 | 31.939346 |
| Ca  | 26.247414 | 31.058456 | 36.037609 |
| Ca  | 30.086664 | 27.924843 | 35.701607 |
| Ca  | 30.213886 | 32.643089 | 33.085625 |
| Ca  | 33.379047 | 29.242290 | 31.551542 |
| Ca  | 33.266392 | 30.296824 | 35.264774 |
| Ca  | 36.695068 | 27.235191 | 34.708584 |
| Ca  | 36.876335 | 31.478207 | 33.818867 |
| Ca  | 40.183651 | 29.450750 | 31.834248 |
| Ca  | 40.138206 | 29.676682 | 36.647469 |
| Ca  | 45.829117 | 27.563927 | 33.057693 |
| Ca  | 42.982224 | 29.459381 | 34.423321 |
| S  | 26.560059 | 27.631073 | 36.195843 |
| S  | 27.147135 | 33.972187 | 34.457508 |
| S  | 30.428564 | 29.408852 | 32.594719 |
| S  | 29.988895 | 31.083170 | 36.364155 |
| S  | 33.385185 | 27.198299 | 34.428112 |
| S  | 33.536125 | 32.331242 | 32.291931 |
| S  | 36.864449 | 28.679756 | 31.831036 |
| S  | 36.597496 | 29.863466 | 36.592083 |
| S  | 40.099819 | 27.147881 | 34.063549 |
| S  | 40.715904 | 31.747171 | 33.885063 |
| S  | 43.455734 | 28.650173 | 31.415752 |
| S  | 44.815311 | 26.431725 | 37.840267 |

24

Generated by VMD

| Ca  | X Value | Y Value | Z Value  |
|-----|---------|---------|----------|
| Ca  | 25.001619 | 30.230705 | 31.937031 |
| Ca  | 26.653208 | 30.878714 | 35.745644 |
| Ca  | 29.995037 | 28.083933 | 35.826405 |
| Ca  | 30.230314 | 32.761887 | 33.130676 |
| Ca  | 33.465210 | 29.105083 | 31.473171 |
| Ca  | 33.343662 | 30.176361 | 35.451782 |
| Ca  | 36.546734 | 26.928448 | 34.380951 |
| Ca  | 36.692497 | 31.489162 | 33.783585 |
| Ca  | 40.116245 | 29.313931 | 31.637611 |
| Ca  | 39.969185 | 29.845692 | 36.639580 |
|    | Ca       | 46.000027 | 27.426964 | 33.174881 |
|----|----------|-----------|-----------|-----------|
|    | Ca       | 42.968292 | 29.448254 | 34.344017 |
|    | S        | 26.717457 | 27.444323 | 36.057148 |
|    | S        | 27.313910 | 34.072556 | 34.573929 |
|    | S        | 30.544655 | 29.610134 | 32.843189 |
|    | S        | 29.975204 | 31.192583 | 36.589535 |
|    | S        | 33.238476 | 27.289654 | 34.376106 |
|    | S        | 33.659172 | 32.319054 | 32.308372 |
|    | S        | 36.815052 | 28.670746 | 31.755459 |
|    | S        | 36.436470 | 29.769085 | 36.694473 |
|    | S        | 39.980377 | 27.218021 | 34.328346 |
|    | S        | 40.497566 | 31.701298 | 33.774040 |
|    | S        | 43.602222 | 28.576435 | 31.266705 |
|    | S        | 44.671284 | 26.838388 | 37.938095 |

24 generated by VMD

|    | Ca       | 24.680662 | 30.140705 | 31.913109 |
|----|----------|-----------|-----------|-----------|
|    | Ca       | 26.602165 | 30.778738 | 35.675617 |
|    | Ca       | 30.465588 | 28.038439 | 35.833210 |
|    | Ca       | 30.049843 | 32.883965 | 33.268661 |
|    | Ca       | 33.362167 | 29.454004 | 31.599541 |
|    | Ca       | 33.310413 | 30.418711 | 35.238167 |
|    | Ca       | 36.673538 | 27.081116 | 34.401176 |
|    | Ca       | 37.157360 | 31.572021 | 33.669304 |
|    | Ca       | 40.157482 | 29.249554 | 31.614487 |
|    | Ca       | 40.408887 | 29.650053 | 36.631218 |
|    | Ca       | 45.774296 | 27.445959 | 33.427769 |
|    | Ca       | 42.866230 | 29.219172 | 34.497929 |
|    | S        | 26.932560 | 27.357273 | 36.356709 |
|    | S        | 26.860495 | 33.703178 | 34.470108 |
|    | S        | 30.389435 | 29.722729 | 32.828645 |
|    | S        | 30.035128 | 31.253878 | 36.577194 |
|    | S        | 33.370773 | 27.406662 | 34.357464 |
|    | S        | 33.430347 | 32.550499 | 32.298306 |
|    | S        | 36.713425 | 28.716236 | 31.586742 |
|    | S        | 36.604897 | 29.879873 | 36.410442 |
|    | S        | 40.078789 | 27.110256 | 34.196320 |
|    | S        | 40.728603 | 31.553368 | 33.756378 |
|    | S        | 43.576317 | 28.631702 | 31.430645 |
|    | S        | 44.567505 | 26.573362 | 37.991779 |

24 generated by VMD

|    | Ca       | 25.750929 | 29.865555 | 31.879652 |
|----|----------|-----------|-----------|-----------|
|    | Ca       | 26.243412 | 30.564522 | 35.934692 |
|    | Ca       | 30.247471 | 28.131767 | 35.599644 |
|    | Ca       | 30.294710 | 32.970978 | 33.121078 |
|   |   |   |
|---|---|---|
| Ca | 33.312046 | 29.159416 | 31.676487 |
| Ca | 33.371861 | 30.572140 | 35.397087 |
| Ca | 36.607018 | 26.756454 | 34.547012 |
| Ca | 37.096901 | 31.636057 | 33.884544 |
| Ca | 40.026783 | 29.466259 | 31.763357 |
| Ca | 40.213169 | 30.130875 | 36.727135 |
| Ca | 45.612389 | 27.282551 | 33.103127 |
| Ca | 42.926136 | 29.333641 | 34.230209 |
| S  | 26.609737 | 27.343189 | 36.103451 |
| S  | 27.056362 | 33.611740 | 34.576752 |
| S  | 30.387707 | 29.760435 | 32.618767 |
| S  | 29.871885 | 31.377209 | 36.360794 |
| S  | 33.343452 | 27.376099 | 34.526997 |
| S  | 33.671112 | 32.513321 | 32.559410 |
| S  | 36.809330 | 28.849728 | 32.032887 |
| S  | 36.534927 | 29.928001 | 36.463192 |
| S  | 39.977463 | 27.163967 | 34.338840 |
| S  | 40.820568 | 31.771599 | 33.692688 |
| S  | 43.302925 | 28.286333 | 31.138021 |
| S  | 44.345642 | 26.539532 | 37.754799 |

24
generated by VMD

|   |   |   |
|---|---|---|
| Ca | 25.103607 | 29.917000 | 32.179672 |
| Ca | 26.457369 | 30.713161 | 35.871368 |
| Ca | 30.346342 | 28.090969 | 35.515137 |
| Ca | 30.026127 | 32.825432 | 33.100922 |
| Ca | 33.166714 | 29.164467 | 31.655247 |
| Ca | 33.356853 | 30.680878 | 35.201103 |
| Ca | 36.591915 | 27.078674 | 34.583141 |
| Ca | 37.020123 | 31.420715 | 33.927860 |
| Ca | 40.115974 | 29.422649 | 31.759151 |
| Ca | 40.146030 | 29.834175 | 36.695358 |
| Ca | 45.741257 | 27.182055 | 33.096523 |
| Ca | 43.041538 | 29.299179 | 34.563953 |
| S  | 26.889208 | 27.431398 | 36.307972 |
| S  | 26.793085 | 33.759571 | 34.367664 |
| S  | 30.324863 | 29.649435 | 32.546093 |
| S  | 30.133472 | 31.313578 | 36.257271 |
| S  | 33.280392 | 27.406910 | 34.247208 |
| S  | 33.455853 | 32.635559 | 32.530029 |
| S  | 36.672619 | 28.816839 | 31.783037 |
| S  | 36.626720 | 29.819233 | 36.558617 |
| S  | 39.963329 | 27.256981 | 34.300163 |
| S  | 40.906307 | 31.672653 | 33.941978 |
| S  | 43.551395 | 28.601662 | 31.343542 |
| S  | 44.722755 | 26.397243 | 37.698990 |
Ca       25.062004       30.385469       31.992458
Ca       26.516125       30.878056       35.913467
Ca       29.836342       30.385469       31.992458
Ca       30.185541       32.667023       33.151581
Ca       33.396935       28.674709       31.528877
Ca       33.187973       30.543575       35.268181
Ca       36.406693       27.046150       34.631569
Ca       36.990715       31.703690       33.820797
Ca       40.020195       29.634920       31.780113
Ca       40.185757       29.987118       36.714737
Ca       45.696022       27.050293       32.864758
Ca       43.190563       29.567659       34.377594
S        26.585033       27.392113       35.899216
S        27.226162       33.936687       34.600708
S        30.447245       29.378300       32.726906
S        29.970598       31.183168       36.399632
S        33.270805       27.152416       34.371494
S        33.614944       32.163727       32.309254
S        36.747982       28.711189       31.896770
S        36.621174       30.053188       36.566505
S        40.020031       27.308559       34.361897
S        40.795612       31.805590       33.919739
S        43.598423       28.650854       31.349642
S        44.861053       26.535028       37.860138

Ca       25.332016       30.101677       32.073112
Ca       26.278690       30.642750       36.116051
Ca       30.313063       28.106359       35.475048
Ca       30.167528       32.988014       33.155846
Ca       33.299725       29.057638       31.279257
Ca       33.409645       30.555492       35.298706
Ca       36.850704       27.165981       34.687836
Ca       36.876827       31.705074       33.630211
Ca       39.931278       29.551994       31.785086
Ca       40.133629       30.023384       36.684216
Ca       45.555569       26.888956       33.143471
Ca       43.005718       29.457273       34.531349
S        27.077847       27.159615       36.311790
S        26.968353       33.733315       34.602669
S        30.430456       29.729492       32.623241
S        30.071316       31.181953       36.331627
S        33.550442       27.569798       34.072266
S        33.596565       32.298023       32.336464
S     36.632351  28.711391  31.792656
S     36.703579  29.902531  36.496048
S     40.092831  27.348103  34.377323
S     40.419159  31.864368  33.921669
S     43.365997  28.371628  31.393225
S     44.370548  26.276598  37.911541

24 generated by VMD
Ca    24.907696  30.102245  32.160465
Ca    26.360050  30.656040  36.182320
Ca    30.495045  27.995258  35.503830
Ca    29.940754  32.963932  33.128517
Ca    33.389713  29.344078  31.308006
Ca    33.258072  30.560001  35.302361
Ca    37.042522  26.962650  34.481964
Ca    36.619331  31.913589  33.519676
Ca    40.170536  29.594162  31.803509
Ca    40.002556  30.121317  36.525898
Ca    45.648483  26.678310  33.278191
Ca    43.219891  29.236765  34.491756
S     26.988390  27.163048  36.258743
S     26.923567  33.664387  34.770512
S     30.370510  29.780685  32.511475
S     29.877953  31.166048  36.405125
S     33.363155  27.636135  34.267567
S     33.399467  32.476028  32.252869
S     36.813778  28.889523  31.771633
S     36.514111  29.755098  36.308453
S     40.182957  27.234648  34.402649
S     40.888275  31.813984  33.801094
S     43.459129  28.194994  31.547148
S     44.597939  26.488392  38.046967

24 generated by VMD
Ca    24.703308  30.359144  32.194580
Ca    26.291323  30.489954  36.125034
Ca    30.396709  28.288803  35.350174
Ca    29.934059  32.911491  33.302963
Ca    33.294689  29.094059  31.263025
Ca    33.254597  30.809841  35.189571
Ca    36.745556  26.703220  34.569633
Ca    36.931896  31.586246  33.672554
Ca    39.998188  29.349754  31.854515
Ca    40.121391  30.193336  36.585075
Ca    46.165363  26.953671  33.669846
Ca    43.042625  29.252731  34.271053
|   |   |   |   |
|---|---|---|---|
| S | 27.069044 | 27.045286 | 36.042526 |
| S | 26.954910 | 33.633339 | 35.053040 |
| S | 30.340069 | 29.740555 | 32.499695 |
| S | 30.077141 | 31.260632 | 36.477482 |
| S | 33.510296 | 27.817162 | 34.095215 |
| S | 33.437717 | 32.450871 | 32.089340 |
| S | 36.705658 | 28.682384 | 31.765228 |
| S | 36.514584 | 29.844898 | 36.426918 |
| S | 40.059231 | 27.364092 | 34.490131 |
| S | 40.619320 | 31.905272 | 33.540352 |
| S | 43.624874 | 28.265949 | 31.500347 |
| S | 44.635223 | 26.388721 | 38.002438 |

24

generated by VMD

| Ca |   |   |   |
|----|---|---|---|
| Ca | 24.659592 | 30.086525 | 32.173260 |
| Ca | 26.548729 | 30.526642 | 35.893364 |
| Ca | 30.025467 | 28.026169 | 35.537186 |
| Ca | 29.972275 | 32.661018 | 33.107983 |
| Ca | 33.242722 | 29.193813 | 31.406971 |
| Ca | 33.432747 | 30.706192 | 35.279327 |
| Ca | 36.687176 | 26.855352 | 34.413643 |
| Ca | 37.019623 | 31.969151 | 33.810158 |
| Ca | 40.055382 | 29.463835 | 31.811501 |
| Ca | 40.205326 | 29.970589 | 36.693558 |
| Ca | 45.889786 | 27.004047 | 33.437023 |
| Ca | 42.999104 | 29.262260 | 34.411839 |
| S  | 26.741547 | 27.089718 | 36.216022 |
| S  | 27.245125 | 33.708817 | 35.010891 |
| S  | 30.268818 | 29.722401 | 32.477871 |
| S  | 30.244873 | 31.153965 | 36.183819 |
| S  | 33.311409 | 27.541405 | 34.153988 |
| S  | 33.558617 | 32.665932 | 32.170265 |
| S  | 36.723831 | 29.107899 | 31.742491 |
| S  | 36.742527 | 29.960451 | 36.428864 |
| S  | 40.064381 | 27.121826 | 34.372959 |
| S  | 40.819038 | 31.829346 | 33.826084 |
| S  | 44.420876 | 28.117868 | 31.441259 |
| S  | 44.554844 | 26.646149 | 38.030399 |

24

generated by VMD

| Ca |   |   |   |
|----|---|---|---|
| Ca | 24.609619 | 30.105534 | 32.360352 |
| Ca | 26.812389 | 30.302298 | 36.367424 |
| Ca | 30.419495 | 28.318457 | 35.505325 |
| Ca | 30.043055 | 32.747944 | 32.904636 |
| Ca | 33.466946 | 29.423496 | 31.311039 |
| Ca | 33.316845 | 30.910017 | 35.231792 |
|   |       |       |       |
|---|-------|-------|-------|
| Ca| 36.768036 | 27.031212 | 34.244633 |
| Ca| 36.727711 | 31.661152 | 33.512177 |
| Ca| 39.997353 | 29.449532 | 31.847240 |
| Ca| 39.972691 | 29.895638 | 36.941391 |
| Ca| 45.757122 | 26.840729 | 33.369846 |
| Ca| 43.065506 | 29.199753 | 34.528664 |
| S | 27.039537 | 26.879597 | 36.268467 |
| S | 27.114286 | 33.331512 | 34.786221 |
| S | 30.367771 | 29.698088 | 32.560722 |
| S | 30.005980 | 31.514368 | 36.289848 |
| S | 33.414505 | 27.862349 | 34.119579 |
| S | 33.499573 | 32.767288 | 32.145725 |
| S | 36.849884 | 28.833122 | 31.616020 |
| S | 36.532207 | 29.965229 | 36.208630 |
| S | 40.025051 | 27.254608 | 34.493885 |
| S | 40.627621 | 31.755260 | 33.898418 |
| S | 43.623322 | 28.373466 | 31.487774 |
| S | 44.377365 | 26.270721 | 38.030869 |

24

generated by VMD

|   |       |       |       |
|---|-------|-------|-------|
| Ca| 24.240448 | 29.935680 | 32.560398 |
| Ca| 26.644709 | 30.421438 | 36.142086 |
| Ca| 30.275654 | 28.061914 | 35.383217 |
| Ca| 30.127880 | 32.761929 | 32.901520 |
| Ca| 33.338646 | 29.356281 | 31.208870 |
| Ca| 33.552692 | 30.912165 | 35.343960 |
| Ca| 36.820946 | 27.135365 | 34.504803 |
| Ca| 36.957397 | 31.810028 | 33.592266 |
| Ca| 40.162132 | 29.490349 | 31.831928 |
| Ca| 40.061398 | 29.987234 | 36.424332 |
| Ca| 45.650024 | 26.977989 | 33.442921 |
| Ca| 43.061264 | 28.956533 | 34.549004 |
| S | 27.043018 | 27.053204 | 36.020111 |
| S | 27.057926 | 33.642517 | 34.996971 |
| S | 30.308205 | 29.783836 | 32.344234 |
| S | 30.240135 | 31.121620 | 36.369164 |
| S | 33.374294 | 27.740746 | 34.208420 |
| S | 33.635571 | 32.550232 | 32.353115 |
| S | 36.771461 | 28.910286 | 31.718166 |
| S | 36.675201 | 29.868071 | 36.329689 |
| S | 39.996948 | 27.175125 | 34.347782 |
| S | 40.755268 | 31.890991 | 33.714615 |
| S | 43.681515 | 28.357090 | 31.422810 |
| S | 44.001202 | 26.490738 | 38.320312 |

24

generated by VMD
| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 24.575605 | 29.996101 | 32.319996 |
| Ca      | 26.635159 | 30.456879 | 35.940178 |
| Ca      | 30.346844 | 32.525391 | 32.839588 |
| Ca      | 26.394260 | 29.49559  | 31.310417 |
| Ca      | 30.481453 | 30.799389 | 35.244267 |
| Ca      | 36.768867 | 27.386131 | 34.679085 |
| Ca      | 36.913124 | 31.754013 | 33.669647 |
| Ca      | 40.009369 | 29.313782 | 31.789783 |
| Ca      | 39.911903 | 29.676704 | 36.718555 |
| Ca      | 45.665802 | 27.070118 | 33.330910 |
| Ca      | 42.990448 | 29.173939 | 34.567600 |
| Ca      | 27.126698 | 27.133173 | 36.359158 |
| S       | 26.765697 | 33.541500 | 34.785721 |
| S       | 30.415363 | 29.471413 | 32.441372 |
| S       | 30.073006 | 31.232664 | 36.257114 |
| S       | 33.498997 | 27.844915 | 34.027237 |
| S       | 33.660606 | 32.775253 | 32.437767 |
| S       | 36.783321 | 29.188328 | 31.669323 |
| S       | 36.458401 | 29.970108 | 36.455826 |
| S       | 40.058144 | 27.157412 | 34.305996 |
| S       | 40.788898 | 31.538654 | 33.877834 |
| S       | 43.408913 | 28.316628 | 31.402622 |
| S       | 44.538864 | 26.295105 | 37.943573 |

24 generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 24.740238 | 29.984638 | 32.505402 |
| Ca      | 26.520842 | 30.394346 | 36.055351 |
| Ca      | 30.231535 | 28.249832 | 35.548794 |
| Ca      | 30.241232 | 32.829514 | 32.901245 |
| Ca      | 33.229694 | 29.381514 | 31.273148 |
| Ca      | 33.440125 | 30.463972 | 35.266132 |
| Ca      | 36.720264 | 27.105133 | 34.431110 |
| Ca      | 37.032368 | 31.693420 | 33.873016 |
| Ca      | 40.091526 | 29.210800 | 31.988377 |
| Ca      | 40.105755 | 29.929287 | 36.643921 |
| Ca      | 45.590580 | 26.895805 | 33.188560 |
| Ca      | 42.962704 | 29.362980 | 34.454880 |
| S       | 27.052963 | 27.114258 | 36.262573 |
| S       | 27.034002 | 33.549999 | 34.745926 |
| S       | 30.304081 | 29.624741 | 32.502476 |
| S       | 29.880283 | 31.365919 | 36.104633 |
| S       | 33.459991 | 27.684109 | 34.058041 |
| S       | 33.971317 | 32.703621 | 32.319241 |
| S       | 36.763756 | 28.949368 | 31.772972 |
| S       | 36.527412 | 29.811899 | 36.505234 |
S  39.956608  27.255543  34.565876
S  40.754120  31.865644  33.814293
S  43.597939  28.531956  31.285709
S  44.224579  26.433159  37.963814

24 generated by VMD
Ca  24.703243  30.139050  32.342579
Ca  26.417883  30.564547  36.240387
Ca  30.313738  28.351418  35.622349
Ca  29.916283  32.887070  32.777157
Ca  33.297722  29.199831  31.262367
Ca  33.394417  30.429640  35.162308
Ca  36.598549  26.840206  34.523331
Ca  37.198250  31.613424  33.716381
Ca  40.041054  29.300409  31.933544
Ca  40.077652  29.822935  36.802116
Ca  45.792397  27.159086  33.074955
Ca  43.116673  29.445883  34.748409
S  27.053997  27.225147  36.259872
S  27.071590  33.608215  35.022682
S  30.438868  29.713568  32.472672
S  29.888708  31.406254  35.950226
S  33.309059  27.425140  34.067181
S  33.776932  32.539661  32.086700
S  36.667229  28.742126  31.782822
S  36.627918  29.876068  36.341869
S  40.171909  27.346977  34.508709
S  40.719036  31.704124  34.050682
S  43.401855  28.650654  31.483700
S  44.438946  26.400003  37.797745

24 generated by VMD
Ca  24.802828  30.018076  32.164295
Ca  26.545429  30.671118  35.857864
Ca  30.290224  28.185551  35.444988
Ca  29.944445  32.879768  32.985611
Ca  33.363785  29.274193  31.241699
Ca  33.476887  30.580891  34.951973
Ca  36.795906  26.727539  34.493935
Ca  36.991512  31.946753  33.753784
Ca  39.915569  29.328440  32.110920
Ca  40.160919  29.670059  36.783886
Ca  45.686707  26.972279  33.220020
Ca  43.148754  29.582226  34.516148
S  27.000364  27.314444  36.609001
S  27.084927  33.633163  34.903290
|     |        |        |                  |
|-----|--------|--------|------------------|
| S   | 30.416334 | 29.532574 | 32.580490       |
| S   | 30.082785 | 31.311626 | 36.168411       |
| S   | 33.389656 | 27.425179 | 34.034485       |
| S   | 33.444607 | 32.641312 | 32.304733       |
| S   | 36.618530 | 28.840530 | 31.915588       |
| S   | 36.671589 | 29.844067 | 36.174149       |
| S   | 40.043217 | 27.054543 | 34.529362       |
| S   | 40.737549 | 31.912714 | 34.043686       |
| S   | 43.385090 | 28.626568 | 31.486172       |
| S   | 44.436230 | 26.417782 | 37.756157       |

24 generated by VMD

| Ca  |        |        |                  |
|-----|--------|--------|------------------|
| Ca  | 24.493618 | 30.039465 | 32.203728       |
| Ca  | 26.505993 | 30.449862 | 35.881123       |
| Ca  | 30.339352 | 28.193768 | 35.521996       |
| Ca  | 29.860825 | 33.003345 | 33.101181       |
| Ca  | 33.347160 | 29.710238 | 31.290495       |
| Ca  | 33.489769 | 30.686424 | 35.100510       |
| Ca  | 36.685436 | 26.948795 | 34.537560       |
| Ca  | 37.115570 | 31.616768 | 33.662704       |
| Ca  | 39.853283 | 29.102716 | 31.812929       |
| Ca  | 40.133057 | 29.844532 | 36.568531       |
| Ca  | 45.467628 | 26.788311 | 33.256790       |
| Ca  | 43.173840 | 29.367527 | 34.596874       |
| S   | 27.190987 | 27.021397 | 36.370663       |
| S   | 26.943829 | 33.590534 | 35.022793       |
| S   | 30.386887 | 29.878681 | 32.495895       |
| S   | 29.912266 | 31.242146 | 36.212788       |
| S   | 33.303928 | 27.522255 | 34.103642       |
| S   | 33.456375 | 32.739067 | 32.225296       |
| S   | 36.670593 | 28.652115 | 31.766685       |
| S   | 36.586246 | 29.893480 | 36.218197       |
| S   | 40.148228 | 27.093521 | 34.490093       |
| S   | 40.968262 | 31.686554 | 33.919670       |
| S   | 43.622925 | 28.563976 | 31.622704       |
| S   | 44.777840 | 26.755932 | 38.047913       |

24 generated by VMD

| Ca  |        |        |                  |
|-----|--------|--------|------------------|
| Ca  | 24.455223 | 30.105289 | 31.981287       |
| Ca  | 26.507940 | 30.731255 | 36.108593       |
| Ca  | 30.359810 | 28.162914 | 35.351063       |
| Ca  | 29.878544 | 33.220238 | 33.016449       |
| Ca  | 33.351658 | 29.484882 | 31.282150       |
| Ca  | 33.389233 | 30.531425 | 35.057854       |
| Ca  | 36.881836 | 26.532551 | 34.697632       |
| Ca  | 36.941460 | 31.711319 | 33.777134       |
| Ca   | 39.983421 | 28.980026 | 31.945734 |
| Ca   | 40.072693 | 29.821857 | 36.666512 |
| Ca   | 45.597794 | 26.892082 | 33.119614 |
| Ca   | 43.128910 | 29.507137 | 34.452374 |
| S    | 27.078568 | 27.150099 | 36.499714 |
| S    | 26.879055 | 33.783333 | 34.949448 |
| S    | 30.412392 | 29.791412 | 32.486774 |
| S    | 33.598866 | 27.497524 | 33.993988 |
| S    | 33.454060 | 32.712368 | 32.535789 |
| S    | 36.755787 | 28.728172 | 31.834106 |
| S    | 36.621403 | 29.567982 | 36.351147 |
| S    | 40.099823 | 27.050255 | 34.785744 |
| S    | 40.596130 | 31.711258 | 33.803692 |
| S    | 43.549114 | 28.650681 | 31.415108 |
| S    | 44.965725 | 26.866718 | 37.996658 |

24 generated by VMD

| Ca   | 24.980282 | 29.835369 | 32.097424 |
| Ca   | 26.760500 | 30.484880 | 36.141445 |
| Ca   | 30.525814 | 28.074829 | 35.597404 |
| Ca   | 29.930119 | 33.114792 | 33.210457 |
| Ca   | 33.340358 | 29.680702 | 31.116364 |
| Ca   | 33.427437 | 30.500174 | 35.035015 |
| Ca   | 36.639473 | 26.915154 | 34.560207 |
| Ca   | 37.027958 | 31.831623 | 33.545887 |
| Ca   | 39.902554 | 29.342018 | 32.122551 |
| Ca   | 39.998833 | 30.133163 | 36.920593 |
| Ca   | 45.380596 | 26.679653 | 33.129963 |
| Ca   | 43.070175 | 29.245113 | 34.424644 |
| S    | 27.105209 | 27.084927 | 36.241653 |
| S    | 26.808985 | 33.713875 | 35.083973 |
| S    | 30.513861 | 29.691624 | 32.525139 |
| S    | 30.343100 | 31.303219 | 36.139790 |
| S    | 33.343586 | 27.452019 | 33.926487 |
| S    | 33.580524 | 32.782833 | 32.370720 |
| S    | 36.742012 | 28.736778 | 31.580448 |
| S    | 36.512627 | 29.703213 | 36.211006 |
| S    | 39.952423 | 27.144102 | 34.717327 |
| S    | 40.626556 | 31.751682 | 33.822071 |
| S    | 43.316643 | 28.297070 | 31.389366 |
| S    | 44.514065 | 26.892548 | 38.120853 |

24 generated by VMD

| Ca   | 24.539368 | 30.295448 | 32.227558 |
| Ca   | 26.464565 | 30.582911 | 36.099487 |
| Element | X1    | Y1    | Z1    |
|---------|-------|-------|-------|
| Ca      | 30.333870 | 28.342123 | 35.517342 |
| Ca      | 29.843773 | 32.984505 | 33.180771 |
| Ca      | 33.295120 | 29.309406 | 31.031784 |
| Ca      | 33.353001 | 30.340090 | 35.059204 |
| Ca      | 36.746704 | 26.899307 | 34.477188 |
| Ca      | 36.935242 | 31.594151 | 33.745396 |
| Ca      | 40.169594 | 29.099712 | 31.983149 |
| Ca      | 40.124779 | 30.005457 | 36.652168 |
| Ca      | 45.748287 | 26.844021 | 33.260502 |
| Ca      | 43.133644 | 29.460199 | 34.547840 |
| S       | 27.023663 | 27.270964 | 36.336082 |
| S       | 26.840849 | 33.666183 | 34.951263 |
| S       | 30.309222 | 29.742393 | 32.593109 |
| S       | 30.041039 | 31.378098 | 36.293480 |
| S       | 33.262505 | 27.473003 | 33.935127 |
| S       | 33.532509 | 32.422909 | 32.343849 |
| S       | 36.841869 | 28.643234 | 31.549822 |
| S       | 36.569714 | 29.687607 | 36.292877 |
| S       | 39.995579 | 27.187307 | 34.686504 |
| S       | 40.786232 | 31.728310 | 33.738239 |
| S       | 43.811623 | 28.653889 | 31.506285 |
| S       | 44.739571 | 26.780228 | 38.021732 |

24 generated by VMD

| Element | X1    | Y1    | Z1    |
|---------|-------|-------|-------|
| Ca      | 24.764397 | 30.197989 | 32.050869 |
| Ca      | 26.572386 | 30.366518 | 35.914955 |
| Ca      | 30.278143 | 28.317493 | 35.580585 |
| Ca      | 29.961956 | 33.030422 | 33.097801 |
| Ca      | 33.343578 | 29.570427 | 31.075752 |
| Ca      | 33.470348 | 30.444611 | 35.121605 |
| Ca      | 36.831455 | 26.807867 | 34.560776 |
| Ca      | 37.083046 | 31.724388 | 33.685535 |
| Ca      | 40.024006 | 29.314945 | 32.019691 |
| Ca      | 40.048294 | 30.248951 | 36.664658 |
| Ca      | 45.387932 | 26.554070 | 33.243252 |
| Ca      | 43.131092 | 29.130230 | 34.482014 |
| S       | 26.982254 | 27.063797 | 36.444099 |
| S       | 26.844810 | 33.671829 | 35.004879 |
| S       | 30.403687 | 29.808475 | 32.590530 |
| S       | 29.986137 | 31.237900 | 36.295311 |
| S       | 33.365273 | 27.497021 | 34.005798 |
| S       | 33.541916 | 32.462448 | 32.392479 |
| S       | 36.727654 | 28.685369 | 31.664679 |
| S       | 36.512108 | 29.751785 | 36.171051 |
| S       | 39.986649 | 27.171494 | 34.586002 |
| S       | 40.756042 | 31.887421 | 33.797203 |
| S  | 43.443378 | 28.475418 | 31.484795 |
| S  | 44.987366 | 26.970497 | 38.096321 |

24 generated by VMD

| Ca | 25.014536 | 30.162018 | 32.223091 |
| Ca | 26.301466 | 30.605648 | 36.203953 |
| Ca | 30.298397 | 28.100025 | 35.636963 |
| Ca | 30.066553 | 32.939140 | 33.169647 |
| Ca | 33.467186 | 29.464159 | 31.075045 |
| Ca | 33.386330 | 30.242352 | 35.151134 |
| Ca | 36.660088 | 26.852821 | 34.33107  |
| Ca | 36.908573 | 31.508900 | 33.567104 |
| Ca | 40.229717 | 29.295811 | 31.771622 |
| Ca | 39.879921 | 30.136982 | 36.458290 |
| Ca | 45.485626 | 26.529406 | 33.399776 |
| Ca | 42.850380 | 29.364855 | 34.409698 |
| S  | 27.073187 | 27.281052 | 36.319519 |
| S  | 27.045860 | 33.744972 | 35.197803 |
| S  | 30.586052 | 29.747887 | 32.747334 |
| S  | 30.036541 | 31.178417 | 36.322876 |
| S  | 33.270157 | 27.367985 | 33.822487 |
| S  | 33.741093 | 32.692093 | 32.313099 |
| S  | 37.016563 | 28.622749 | 31.553242 |
| S  | 36.379395 | 29.799473 | 36.275333 |
| S  | 39.944901 | 27.139914 | 34.619926 |
| S  | 40.731316 | 31.880104 | 33.704044 |
| S  | 43.644844 | 28.462999 | 31.501106 |
| S  | 44.415184 | 27.271669 | 38.254417 |

24 generated by VMD

| Ca | 25.035944 | 29.857922 | 32.118591 |
| Ca | 26.477829 | 30.390911 | 36.007992 |
| Ca | 30.361820 | 27.961365 | 35.476837 |
| Ca | 30.000154 | 33.165005 | 33.033806 |
| Ca | 33.393589 | 29.489750 | 31.225233 |
| Ca | 33.391796 | 30.478401 | 35.085526 |
| Ca | 36.706005 | 27.278297 | 34.566261 |
| Ca | 37.169720 | 31.756355 | 33.664677 |
| Ca | 40.075928 | 29.483204 | 31.705738 |
| Ca | 39.940704 | 29.707323 | 36.579243 |
| Ca | 45.406895 | 26.497574 | 33.187798 |
| Ca | 43.044342 | 29.287056 | 34.504486 |
| S  | 26.932137 | 27.181316 | 36.445480 |
| S  | 26.898489 | 33.777489 | 34.942848 |
| S  | 30.604704 | 29.677242 | 32.640659 |
| S  | 29.965618 | 31.089642 | 36.204510 |
| S   | 33.415684 | 27.506241 | 34.129536 |
| S   | 33.505260 | 32.736187 | 32.513138 |
| S   | 36.802589 | 28.799343 | 31.736752 |
| S   | 36.479809 | 30.052118 | 36.363945 |
| S   | 40.034176 | 27.333313 | 34.424812 |
| S   | 40.815338 | 31.749435 | 33.914948 |
| S   | 43.292488 | 28.323902 | 31.417614 |
| S   | 44.682907 | 26.812056 | 38.140289 |

24 generated by VMD

| Ca  | 24.875221 | 29.967426 | 32.485401 |
| Ca  | 26.522009 | 30.532223 | 36.143425 |
| Ca  | 30.077684 | 28.109177 | 35.762821 |
| Ca  | 30.116699 | 33.234016 | 32.890812 |
| Ca  | 33.381882 | 29.472866 | 31.115309 |
| Ca  | 33.098679 | 30.517117 | 35.108582 |
| Ca  | 36.654598 | 26.939411 | 34.570244 |
| Ca  | 37.049343 | 31.450674 | 33.636337 |
| Ca  | 40.011047 | 29.228943 | 32.001614 |
| Ca  | 39.870262 | 29.571146 | 36.521904 |
| Ca  | 46.078220 | 27.168381 | 32.994713 |
| Ca  | 43.232040 | 29.318010 | 34.556660 |
| S   | 26.881409 | 27.149773 | 36.179832 |
| S   | 26.857384 | 33.729805 | 34.886440 |
| S   | 30.575638 | 29.934410 | 32.510101 |
| S   | 29.832367 | 31.426533 | 36.080666 |
| S   | 33.192471 | 27.423260 | 34.000301 |
| S   | 33.865776 | 32.790142 | 32.548248 |
| S   | 36.674938 | 28.647655 | 31.671497 |
| S   | 36.450226 | 29.597956 | 36.360077 |
| S   | 40.066315 | 27.069935 | 34.539757 |
| S   | 40.567276 | 31.675806 | 33.841339 |
| S   | 43.611496 | 28.489975 | 31.538477 |
| S   | 44.890987 | 26.946766 | 38.086143 |

24 generated by VMD

| Ca  | 24.984282 | 29.938251 | 32.042950 |
| Ca  | 26.288956 | 30.707726 | 36.057167 |
| Ca  | 30.090984 | 28.139610 | 35.82314 |
| Ca  | 30.295002 | 32.957478 | 32.884361 |
| Ca  | 33.330246 | 29.446150 | 31.370527 |
| Ca  | 33.344147 | 30.327444 | 35.332184 |
| Ca  | 36.751648 | 26.792444 | 34.605007 |
| Ca  | 36.791672 | 31.564047 | 34.047470 |
| Ca  | 39.928486 | 29.484581 | 31.970798 |
| Ca  | 39.925285 | 30.020975 | 36.460796 |
| Element | X  | Y  | Z  |
|---------|----|----|----|
| Ca      | 45.664318 | 26.989109 | 33.082840 |
| Ca      | 43.008804 | 29.299477 | 34.315784 |
| S       | 26.809460 | 27.288939 | 36.318756 |
| S       | 26.992619 | 33.780735 | 34.527428 |
| S       | 30.450684 | 29.595039 | 32.601761 |
| S       | 30.054674 | 31.266670 | 36.090244 |
| S       | 33.388493 | 27.476820 | 34.04859 |
| S       | 33.798504 | 32.730545 | 32.700214 |
| S       | 36.860817 | 28.764322 | 31.979469 |
| S       | 36.600277 | 29.518362 | 36.519081 |
| S       | 40.069599 | 27.195911 | 34.530022 |
| S       | 40.678295 | 31.992544 | 33.727875 |
| S       | 43.371319 | 28.322165 | 31.345383 |
| S       | 44.955383 | 26.792107 | 37.889416 |

24 generated by VMD

| Element | X  | Y  | Z  |
|---------|----|----|----|
| Ca      | 25.126396 | 29.971153 | 32.135014 |
| Ca      | 26.496250 | 30.551777 | 35.978073 |
| Ca      | 30.009644 | 28.022640 | 35.561787 |
| Ca      | 29.955688 | 33.089897 | 32.882103 |
| Ca      | 33.317390 | 29.458099 | 31.559219 |
| Ca      | 33.337025 | 30.457970 | 35.382992 |
| Ca      | 36.878660 | 27.104284 | 34.650208 |
| Ca      | 36.950027 | 31.453194 | 33.913315 |
| Ca      | 40.008987 | 29.377823 | 31.751537 |
| Ca      | 40.047611 | 29.723640 | 36.411568 |
| Ca      | 45.627228 | 26.842712 | 33.004478 |
| Ca      | 43.059647 | 29.453306 | 34.552269 |
| S       | 26.696022 | 27.202471 | 36.152447 |
| S       | 26.992382 | 33.919060 | 34.618179 |
| S       | 30.380667 | 29.777512 | 32.580429 |
| S       | 29.875317 | 31.277752 | 36.113834 |
| S       | 33.475861 | 27.478622 | 34.290104 |
| S       | 33.558136 | 32.556614 | 32.588463 |
| S       | 36.791843 | 28.694942 | 31.774055 |
| S       | 36.536705 | 29.719383 | 36.652363 |
| S       | 40.072735 | 27.232113 | 34.410263 |
| S       | 40.832191 | 31.807869 | 33.794380 |
| S       | 43.435154 | 28.402847 | 31.366713 |
| S       | 44.972145 | 26.815708 | 37.906952 |

24 generated by VMD

| Element | X  | Y  | Z  |
|---------|----|----|----|
| Ca      | 25.126591 | 29.979326 | 32.104675 |
| Ca      | 26.509871 | 30.688005 | 35.959293 |
| Ca      | 30.201416 | 28.316307 | 35.438652 |
| Ca      | 30.096325 | 32.777256 | 33.044327 |
|   |   |   |
|---|---|---|
| Ca | 33.240257 | 29.549732 | 31.493864 |
| Ca | 33.395584 | 30.393341 | 35.273632 |
| Ca | 36.722569 | 26.907566 | 34.327995 |
| Ca | 36.958027 | 31.443642 | 33.676048 |
| Ca | 39.874798 | 29.273903 | 31.786301 |
| Ca | 39.827000 | 29.460890 | 36.402313 |
| Ca | 45.741875 | 27.103954 | 33.378109 |
| Ca | 42.990967 | 29.479057 | 34.601360 |
| S  | 27.070271 | 27.417152 | 36.563187 |
| S  | 27.138336 | 33.831070 | 34.908813 |
| S  | 30.289686 | 29.558117 | 32.550621 |
| S  | 30.115566 | 31.407726 | 36.175144 |
| S  | 33.409245 | 27.412048 | 34.079117 |
| S  | 33.696239 | 32.639244 | 32.639526 |
| S  | 36.618927 | 28.641531 | 31.464508 |
| S  | 36.504745 | 29.613699 | 36.293427 |
| S  | 40.161503 | 27.090309 | 34.202072 |
| S  | 40.599453 | 31.843828 | 33.852539 |
| S  | 43.31259 | 28.529087 | 31.585228 |
| S  | 44.713318 | 27.034592 | 38.229958 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 25.235685 | 29.974773 | 32.163303 |
| Ca | 26.597214 | 30.790485 | 35.844364 |
| Ca | 30.295815 | 28.227619 | 35.685562 |
| Ca | 30.094021 | 32.862839 | 32.987934 |
| Ca | 33.345219 | 29.337412 | 31.402607 |
| Ca | 33.308819 | 30.509809 | 35.162006 |
| Ca | 36.636597 | 26.686054 | 34.457588 |
| Ca | 36.882675 | 31.380882 | 33.726734 |
| Ca | 39.845665 | 29.203865 | 31.659306 |
| Ca | 39.719727 | 29.635025 | 36.505939 |
| Ca | 45.884587 | 27.540730 | 33.92712 |
| Ca | 42.836403 | 29.421261 | 34.437561 |
| S  | 27.104824 | 27.502129 | 36.301212 |
| S  | 27.174900 | 33.893692 | 34.956753 |
| S  | 30.357649 | 29.690666 | 32.542843 |
| S  | 30.121544 | 31.400558 | 36.263027 |
| S  | 33.345467 | 27.455875 | 34.222576 |
| S  | 33.663742 | 32.594681 | 32.611771 |
| S  | 36.597282 | 28.549282 | 31.711712 |
| S  | 36.416302 | 29.513504 | 36.448807 |
| S  | 40.046265 | 27.154007 | 34.255978 |
| S  | 40.618362 | 31.477312 | 33.846996 |
| S  | 43.706810 | 28.707809 | 31.364700 |
| S  | 44.584526 | 26.881145 | 38.078693 |
|   |   |   |
|---|---|---|
| Ca | 25.315153 | 29.745152 | 32.317791 |
| Ca | 26.453201 | 30.799652 | 36.022251 |
| Ca | 30.414696 | 27.954048 | 35.703468 |
| Ca | 30.196924 | 33.024872 | 33.161827 |
| Ca | 33.299507 | 29.551544 | 31.222569 |
| Ca | 33.293159 | 30.581646 | 35.104088 |
| Ca | 36.751289 | 26.625393 | 34.317791 |
| Ca | 36.893082 | 31.491280 | 33.739296 |
| Ca | 39.866386 | 29.202085 | 31.822046 |
| Ca | 39.686272 | 29.676426 | 36.683151 |
| Ca | 45.507923 | 27.187153 | 33.195072 |
| Ca | 42.900566 | 29.458870 | 34.493355 |
| S  | 27.386944 | 27.465076 | 36.369404 |
| S  | 26.958813 | 33.816246 | 34.625103 |
| S  | 30.513596 | 29.749262 | 32.683853 |
| S  | 30.076870 | 31.390221 | 36.371788 |
| S  | 33.394264 | 27.603292 | 33.906700 |
| S  | 33.772900 | 32.720707 | 32.478180 |
| S  | 36.641548 | 28.577389 | 31.560463 |
| S  | 36.520187 | 29.571495 | 36.208744 |
| S  | 39.997364 | 26.981176 | 34.280891 |
| S  | 40.492710 | 31.584415 | 33.939632 |
| S  | 43.353455 | 28.736677 | 31.550529 |
| S  | 44.747139 | 26.897312 | 38.272606 |

24

generated by VMD

|   |   |   |
|---|---|---|
| Ca | 25.302227 | 30.011612 | 32.114468 |
| Ca | 26.408255 | 30.740301 | 36.058929 |
| Ca | 30.194139 | 28.153130 | 35.655708 |
| Ca | 30.147720 | 33.075401 | 33.059494 |
| Ca | 33.412136 | 29.288322 | 31.366089 |
| Ca | 33.247765 | 30.537556 | 35.187553 |
| Ca | 36.713005 | 26.643196 | 34.432281 |
| Ca | 36.885506 | 31.153252 | 33.921448 |
| Ca | 40.066750 | 29.291981 | 31.725714 |
| Ca | 39.821342 | 29.973722 | 36.555649 |
| Ca | 45.529537 | 27.200630 | 33.206543 |
| Ca | 42.922161 | 29.439310 | 34.523342 |
| S  | 27.157761 | 27.410559 | 36.343025 |
| S  | 26.785139 | 33.910892 | 34.752388 |
| S  | 30.402662 | 29.699535 | 32.636189 |
| S  | 29.952446 | 31.522640 | 36.193020 |
| S  | 33.395912 | 27.436914 | 34.083897 |
| S  | 33.764420 | 32.620426 | 32.513016 |
S  36.766663  28.414684  31.586040
S  36.417854  29.436350  36.460793
S  40.097713  27.250568  34.424088
S  40.571156  31.680798  33.811466
S  43.404408  28.693588  31.399071
S  45.067249  26.806000  38.020451

24 generated by VMD
Ca  25.277237  29.353424  32.107903
Ca  26.602848  30.433855  35.936447
Ca  30.278191  28.322227  35.764755
Ca  30.146030  32.998474  33.056889
Ca  33.262924  29.709160  31.457170
Ca  33.411797  30.746132  35.476788
Ca  36.849018  26.927856  34.333656
Ca  36.889023  31.585941  33.654076
Ca  39.806328  29.317167  31.769760
Ca  39.840759  29.600590  36.642975
Ca  45.280769  26.577480  33.032135
Ca  42.948090  29.402954  34.727795
S  27.296583  27.188938  36.094402
S  26.794054  33.696152  34.725021
S  30.433460  29.748472  32.505451
S  29.955914  31.611069  36.315357
S  33.450676  27.776064  34.197990
S  33.879040  32.838295  32.625740
S  36.554592  28.677267  31.483013
S  36.644840  29.664513  36.373688
S  40.074032  27.077156  34.306892
S  40.578278  31.738487  33.843990
S  43.385738  28.528439  31.571796
S  44.793694  26.871304  38.026985

24 generated by VMD
Ca  25.113651  29.729729  32.301910
Ca  26.679962  30.651674  36.193325
Ca  30.151505  28.025789  35.88764
Ca  30.032196  32.854763  32.950867
Ca  33.554478  29.445669  31.314180
Ca  33.421005  30.511784  35.209373
Ca  36.575367  27.042870  34.511551
Ca  36.950104  31.641159  33.785744
Ca  40.046925  29.439514  31.892643
Ca  39.658920  29.946995  36.342705
Ca  45.270943  26.794895  33.104347
Ca  42.966034  29.318764  34.698662
| S     | 27.308041 | 27.382793 | 36.377739 |
|-------|-----------|-----------|-----------|
| S     | 26.880455 | 33.582596 | 34.709728 |
| S     | 30.644104 | 29.804008 | 32.641533 |
| S     | 30.027885 | 31.379139 | 36.311352 |
| S     | 33.350254 | 27.450382 | 33.977303 |
| S     | 33.853500 | 32.712601 | 32.397408 |
| S     | 36.868244 | 28.762802 | 31.476572 |
| S     | 36.412636 | 29.745384 | 36.400505 |
| S     | 39.891499 | 27.193005 | 34.321625 |
| S     | 40.715252 | 31.732803 | 33.929787 |
| S     | 43.408096 | 28.643970 | 31.493977 |
| S     | 44.652779 | 26.598242 | 38.099129 |

24 generated by VMD

| Ca    | 25.522007 | 29.692131 | 32.026859 |
|-------|-----------|-----------|-----------|
| Ca    | 26.559177 | 30.794085 | 35.982010 |
| Ca    | 30.289841 | 28.186161 | 35.760052 |
| Ca    | 30.023470 | 33.143337 | 33.035919 |
| Ca    | 33.501873 | 29.438940 | 31.414122 |
| Ca    | 33.343670 | 30.468992 | 35.296528 |
| Ca    | 36.707474 | 26.900253 | 34.441162 |
| Ca    | 36.765808 | 31.479412 | 33.913982 |
| Ca    | 39.986092 | 29.479256 | 31.689665 |
| Ca    | 40.004143 | 29.595043 | 36.726562 |
| Ca    | 45.504894 | 26.950764 | 33.090351 |
| Ca    | 42.828918 | 29.295807 | 34.283371 |
| S     | 27.327602 | 27.297321 | 36.367004 |
| S     | 26.707968 | 33.868988 | 34.541885 |
| S     | 30.582531 | 29.706932 | 32.629452 |
| S     | 29.957867 | 31.470844 | 36.249878 |
| S     | 33.456612 | 27.520580 | 34.113880 |
| S     | 33.729576 | 32.598022 | 32.604435 |
| S     | 36.818741 | 28.629866 | 31.771061 |
| S     | 36.560989 | 29.601837 | 36.574715 |
| S     | 39.972977 | 27.146717 | 34.288445 |
| S     | 40.309448 | 31.681557 | 33.946110 |
| S     | 43.450722 | 28.532909 | 31.200863 |
| S     | 44.521561 | 26.911661 | 38.082355 |

24 generated by VMD

| Ca    | 25.464937 | 29.493549 | 32.144859 |
|-------|-----------|-----------|-----------|
| Ca    | 26.627209 | 30.793488 | 36.176159 |
| Ca    | 30.315529 | 28.131939 | 35.872227 |
| Ca    | 30.136845 | 32.935120 | 33.073257 |
| Ca    | 33.458862 | 29.695686 | 31.375681 |
| Ca    | 33.156948 | 30.148247 | 35.291225 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 36.718674 | 27.018623 | 34.226673 |
| Ca      | 36.925434 | 31.871014 | 33.592 |
| Ca      | 39.967297 | 29.496883 | 31.723125 |
| Ca      | 39.533531 | 29.687698 | 36.128944 |
| Ca      | 45.593964 | 26.726379 | 33.425426 |
| Ca      | 42.869572 | 29.275936 | 33.386986 |
| S       | 27.281292 | 27.538719 | 34.488682 |
| S       | 26.898415 | 33.758659 | 34.646130 |
| S       | 30.581923 | 29.746830 | 32.768044 |
| S       | 29.966850 | 31.326811 | 36.345978 |
| S       | 33.316647 | 27.327194 | 33.983646 |
| S       | 33.728554 | 32.767998 | 32.901451 |
| S       | 36.762848 | 28.770817 | 31.283672 |
| S       | 36.378132 | 29.553051 | 36.183197 |
| S       | 39.973640 | 27.200428 | 34.045303 |
| S       | 40.784840 | 31.752562 | 33.931824 |
| S       | 43.551933 | 28.395302 | 31.476368 |
| S       | 44.440002 | 26.978455 | 38.559696 |

24

generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.474358 | 30.126305 | 31.835876 |
| Ca      | 26.697342 | 30.744881 | 35.825531 |
| Ca      | 30.368473 | 27.948736 | 35.690903 |
| Ca      | 30.302193 | 33.060890 | 33.254723 |
| Ca      | 33.400322 | 29.130062 | 31.516546 |
| Ca      | 33.348118 | 30.383318 | 35.535545 |
| Ca      | 36.717644 | 26.940639 | 34.503204 |
| Ca      | 36.878143 | 31.631487 | 33.515991 |
| Ca      | 39.841328 | 29.361971 | 31.957428 |
| Ca      | 39.969185 | 29.727760 | 36.400501 |
| Ca      | 45.348545 | 26.963591 | 33.296318 |
| Ca      | 42.800453 | 29.433262 | 34.143490 |
| S       | 27.239599 | 27.234413 | 36.197426 |
| S       | 27.070019 | 33.801033 | 34.785332 |
| S       | 30.483952 | 29.794340 | 32.740096 |
| S       | 30.053368 | 31.075829 | 36.399994 |
| S       | 33.483475 | 27.448631 | 34.284180 |
| S       | 33.849319 | 32.509972 | 32.690552 |
| S       | 36.689533 | 28.593313 | 31.468304 |
| S       | 36.693668 | 29.773949 | 36.126251 |
| S       | 39.853981 | 27.246231 | 34.352837 |
| S       | 40.548958 | 31.908596 | 33.840103 |
| S       | 43.140663 | 28.406090 | 31.281284 |
| S       | 44.181301 | 27.146118 | 38.380276 |

24

generated by VMD
|     | X       | Y       | Z       |
|-----|---------|---------|---------|
| S   | 40.165485 | 27.087307 | 34.257812 |
| S   | 40.540245 | 31.837193 | 33.681080 |
| S   | 43.411350 | 28.460102 | 31.583633 |
| S   | 44.388123 | 27.310883 | 38.399384 |

24 generated by VMD

| Ca  | X       | Y       | Z       |
|-----|---------|---------|---------|
| Ca  | 25.245462 | 30.385330 | 32.216629 |
| Ca  | 26.583630 | 30.602192 | 36.093571 |
| Ca  | 30.374811 | 27.871834 | 35.811203 |
| Ca  | 30.339890 | 32.887794 | 33.349136 |
| Ca  | 33.229198 | 29.647167 | 31.263519 |
| Ca  | 33.196499 | 30.318558 | 35.177689 |
| Ca  | 36.737507 | 26.823977 | 34.281395 |
| Ca  | 37.048599 | 31.492498 | 33.480484 |
| Ca  | 39.843266 | 29.209427 | 31.727596 |
| Ca  | 39.573669 | 29.942997 | 36.385017 |
| Ca  | 45.319546 | 26.784145 | 33.672165 |
| Ca  | 42.979610 | 29.548222 | 34.456135 |
| S   | 27.062181 | 27.141666 | 36.051880 |
| S   | 27.392105 | 33.715073 | 35.107956 |
| S   | 30.457508 | 29.698587 | 32.722439 |
| S   | 30.215328 | 31.265106 | 36.438923 |
| S   | 33.301720 | 27.322201 | 34.026108 |
| S   | 33.820583 | 32.717236 | 32.374660 |
| S   | 36.557930 | 28.674210 | 31.210972 |
| S   | 36.570591 | 29.522045 | 35.890369 |
| S   | 40.012684 | 27.269154 | 34.423721 |
| S   | 40.574749 | 31.713459 | 33.759590 |
| S   | 43.355331 | 28.176458 | 31.562180 |
| S   | 44.641403 | 27.662079 | 38.547371 |

24 generated by VMD

| Ca  | X       | Y       | Z       |
|-----|---------|---------|---------|
| Ca  | 26.487015 | 30.939850 | 35.911228 |
| Ca  | 30.238663 | 27.904427 | 35.935410 |
| Ca  | 30.135622 | 32.683079 | 33.307518 |
| Ca  | 33.324718 | 29.394386 | 31.359461 |
| Ca  | 33.379066 | 30.277496 | 35.169426 |
| Ca  | 36.774979 | 26.772217 | 34.273220 |
| Ca  | 37.117439 | 31.526562 | 33.778694 |
| Ca  | 39.845406 | 29.127655 | 31.535847 |
| Ca  | 39.875675 | 30.073576 | 36.415432 |
| Ca  | 45.387951 | 27.077587 | 33.579407 |
| Ca  | 42.834877 | 29.748325 | 34.524208 |
| S   | 26.759373 | 27.465469 | 36.069969 |
| S   | 27.199493 | 33.971542 | 34.965393 |
|     |       |       |       |
|-----|-------|-------|-------|
| S   | 30.463007 | 29.489643 | 32.829975 |
| S   | 30.018776 | 31.103977 | 36.362751 |
| S   | 33.371891 | 27.216387 | 34.195732 |
| S   | 33.687191 | 32.454121 | 32.443062 |
| S   | 36.703232 | 28.485451 | 31.420712 |
| S   | 36.659836 | 29.440857 | 36.130863 |
| S   | 40.080166 | 27.254911 | 34.354286 |
| S   | 40.755646 | 31.909218 | 33.358414 |
| S   | 43.452290 | 28.543314 | 31.473417 |
| S   | 44.821846 | 27.080944 | 38.575184 |

24 generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 25.056252 | 30.234699 | 31.935467 |
| Ca  | 26.484522 | 30.579704 | 35.761951 |
| Ca  | 30.253128 | 28.098598 | 35.769424 |
| Ca  | 30.394400 | 32.796246 | 33.373825 |
| Ca  | 33.452469 | 29.514248 | 31.572531 |
| Ca  | 33.305603 | 30.359253 | 35.368202 |
| Ca  | 36.635544 | 26.847466 | 34.421062 |
| Ca  | 37.040405 | 31.448460 | 33.764084 |
| Ca  | 39.789574 | 29.415428 | 31.717339 |
| Ca  | 40.015404 | 30.082714 | 36.367531 |
| Ca  | 45.438042 | 27.015915 | 33.497604 |
| Ca  | 42.903275 | 29.415184 | 34.254963 |
| S   | 26.990797 | 27.196938 | 36.092735 |
| S   | 27.132301 | 33.706059 | 34.641811 |
| S   | 30.437885 | 29.685057 | 32.697128 |
| S   | 30.115288 | 31.135387 | 36.459282 |
| S   | 33.257320 | 27.465958 | 34.314812 |
| S   | 33.704227 | 32.671276 | 32.555275 |
| S   | 36.747505 | 28.600687 | 31.701487 |
| S   | 36.731495 | 29.795700 | 36.383442 |
| S   | 39.919449 | 27.127739 | 34.243843 |
| S   | 40.780964 | 31.706280 | 33.502068 |
| S   | 43.342686 | 28.315910 | 31.222090 |
| S   | 44.505379 | 27.176512 | 38.412716 |

24 generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 24.875191 | 30.137646 | 32.269428 |
| Ca  | 26.344894 | 30.648842 | 35.816200 |
| Ca  | 30.160370 | 27.692329 | 35.782082 |
| Ca  | 30.211901 | 32.834423 | 33.330000 |
| Ca  | 33.402397 | 29.330492 | 31.325153 |
| Ca  | 33.376842 | 30.464931 | 35.246052 |
| Ca  | 36.629295 | 27.097485 | 34.787663 |
| Ca  | 37.122231 | 31.688335 | 33.664734 |
| Element | X1  | Y1  | Z1  | X2  | Y2  | Z2  |
|---------|-----|-----|-----|-----|-----|-----|
| Ca      | 40.071640 | 29.413963 | 31.697033 | 39.918831 | 30.053381 | 36.202110 |
| Ca      | 45.366474 | 26.497822 | 33.225685 | 43.154297 | 29.634743 | 34.353645 |
| S       | 26.828712 | 27.028854 | 35.958389 | 26.980072 | 33.875660 | 34.780422 |
| S       | 30.482351 | 29.775181 | 32.855328 | 30.482351 | 29.634743 | 34.353645 |
| S       | 33.394039 | 27.480768 | 34.055050 | 33.806984 | 32.617695 | 32.445953 |
| S       | 36.858406 | 28.829754 | 31.593956 | 36.566525 | 29.872486 | 36.379555 |
| S       | 40.051315 | 27.206608 | 34.345779 | 40.820740 | 31.804981 | 33.612225 |
| S       | 43.496506 | 28.359417 | 31.483980 | 43.496506 | 28.359417 | 31.483980 |
| S       | 44.621792 | 26.883802 | 38.403534 | 44.621792 | 26.883802 | 38.403534 |

24

generated by VMD

| Ca | 24.856709 | 30.274754 | 31.967806 |
| Ca | 26.496357 | 30.473814 | 36.114826 |
| Ca | 30.416687 | 28.019810 | 35.881153 |
| Ca | 29.962940 | 32.912926 | 33.173462 |
| Ca | 33.241714 | 29.367788 | 31.243252 |
| Ca | 33.485313 | 30.485912 | 35.159252 |
| Ca | 36.768967 | 26.924568 | 34.375160 |
| Ca | 37.060753 | 31.731636 | 33.719875 |
| Ca | 39.974121 | 29.481195 | 31.662874 |
| Ca | 39.680954 | 30.063862 | 36.399433 |
| Ca | 45.626007 | 26.165916 | 33.314636 |
| Ca | 43.226524 | 29.410677 | 34.595078 |
| S  | 27.024097 | 27.073286 | 36.227364 |
| S  | 27.051617 | 33.820305 | 34.974987 |
| S  | 30.353025 | 29.575747 | 32.878571 |
| S  | 30.043095 | 31.266529 | 36.436394 |
| S  | 33.365360 | 27.405273 | 34.052471 |
| S  | 33.585354 | 32.540146 | 32.316906 |
| S  | 36.796223 | 28.841436 | 31.421066 |
| S  | 36.620205 | 29.713879 | 36.125801 |
| S  | 40.053822 | 27.412132 | 34.344799 |
| S  | 40.918304 | 31.910473 | 33.702126 |
| S  | 43.720333 | 28.291847 | 31.605515 |
| S  | 44.105358 | 27.227440 | 38.337845 |

24

generated by VMD

| Ca | 24.731312 | 30.118141 | 32.077179 |
| Ca | 26.462309 | 30.626797 | 35.804146 |
|   | Ca   | S    |
|---|------|------|
| 1 | 30.528519 | 27.915051 | 35.735237 |
| 2 | 29.981340 | 32.973389 | 33.192169 |
| 3 | 33.116806 | 29.527790 | 31.592451 |
| 4 | 33.240238 | 30.581581 | 35.157448 |
| 5 | 36.859673 | 27.068054 | 34.454552 |
| 6 | 37.320381 | 29.384258 | 31.758408 |
| 7 | 34.322533 | 30.581581 | 35.157448 |
| 8 | 36.859673 | 27.068054 | 34.454552 |
| 9 | 37.320381 | 29.384258 | 31.758408 |
| 10 | 34.322533 | 30.581581 | 35.157448 |
| 11 | 36.859673 | 27.068054 | 34.454552 |
| 12 | 37.320381 | 29.384258 | 31.758408 |

24 generated by VMD

|   | Ca   | S    |
|---|------|------|
| 1 | 25.010120 | 30.410316 | 31.901934 |
| 2 | 26.590044 | 30.651649 | 35.746170 |
| 3 | 30.511475 | 28.090561 | 35.910618 |
| 4 | 30.264824 | 32.555679 | 33.316044 |
| 5 | 33.305122 | 29.392056 | 31.225046 |
| 6 | 33.217686 | 30.278999 | 35.290077 |
| 7 | 36.719780 | 26.807726 | 34.465099 |
| 8 | 33.051224 | 29.392056 | 31.225046 |
| 9 | 33.217686 | 30.278999 | 35.290077 |
| 10 | 36.719780 | 26.807726 | 34.465099 |
| 11 | 33.051224 | 29.392056 | 31.225046 |
| 12 | 33.217686 | 30.278999 | 35.290077 |
| 13 | 36.719780 | 26.807726 | 34.465099 |
| 14 | 33.051224 | 29.392056 | 31.225046 |
| 15 | 33.217686 | 30.278999 | 35.290077 |
| 16 | 36.719780 | 26.807726 | 34.465099 |
| 17 | 33.051224 | 29.392056 | 31.225046 |
| 18 | 33.217686 | 30.278999 | 35.290077 |
| 19 | 36.719780 | 26.807726 | 34.465099 |
| 20 | 33.051224 | 29.392056 | 31.225046 |
| 21 | 33.217686 | 30.278999 | 35.290077 |
| 22 | 36.719780 | 26.807726 | 34.465099 |
| 23 | 33.051224 | 29.392056 | 31.225046 |
| 24 | 33.217686 | 30.278999 | 35.290077 |
S   43.706715   28.238256   31.379080
S   44.297813   27.695152   38.294445

24 generated by VMD

Ca  25.162615   30.610203   31.807281
Ca  26.299149   30.904655   35.770844
Ca  30.603508   27.724714   35.889240
Ca  30.220530   32.657917   33.464920
Ca  33.322960   29.415020   31.289507
Ca  33.288586   30.345806   35.163799
Ca  36.845375   26.729702   34.379528
Ca  36.882904   31.381786   33.694706
Ca  39.826599   29.147512   31.815252
Ca  39.597679   29.816357   36.420273
Ca  45.939301   26.982145   33.505272
Ca  42.782234   29.413221   34.126907
S   27.141346   27.511225   36.310081
S   27.229759   34.058254   34.857528
S   30.409826   29.617722   32.991798
S   29.992960   31.187553   36.498684
S   33.481003   27.298292   34.065880
S   33.594688   32.620361   32.374832
S   36.690595   28.522049   31.463421
S   36.492058   29.377586   36.218708
S   40.168663   27.183840   34.216209
S   40.378143   31.912590   33.931694
S   43.506683   28.267191   31.117142
S   44.568287   27.705685   38.659054

24 generated by VMD

Ca  25.163721   30.472340   31.993530
Ca  26.306177   30.827076   35.987232
Ca  30.445435   27.776772   35.830341
Ca  30.419109   32.670925   33.771786
Ca  33.357441   29.214653   31.276747
Ca  33.348450   30.269022   35.302578
Ca  36.919266   26.854286   34.062557
Ca  37.134628   31.419601   33.490227
Ca  39.900982   29.610107   31.732763
Ca  39.553833   30.074051   36.273453
Ca  45.536736   26.464100   33.944080
Ca  42.905720   29.620548   34.353451
S   27.151349   27.449251   36.159801
S   26.983967   33.950279   34.777584
S   30.517578   29.720257   32.984318
S   29.940056   31.084553   36.762360
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| S       | 33.420856 | 27.246407 | 34.285149 |
| S       | 33.645687 | 32.498436 | 32.249115 |
| S       | 36.602333 | 28.628874 | 31.017994 |
| S       | 36.642208 | 29.541023 | 35.972656 |
| S       | 40.063938 | 27.330898 | 34.108665 |
| S       | 40.664845 | 32.014473 | 33.742508 |
| S       | 43.533340 | 28.082394 | 31.364422 |
| S       | 44.276325 | 27.571093 | 38.587368 |

24 generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 25.283291 | 30.637199 | 31.917616 |
| Ca      | 26.645805 | 30.606701 | 35.910664 |
| Ca      | 30.420937 | 27.852135 | 35.455475 |
| Ca      | 30.500626 | 32.675789 | 33.865253 |
| Ca      | 33.393524 | 29.521145 | 31.305233 |
| Ca      | 33.302238 | 30.262627 | 35.329773 |
| Ca      | 36.895359 | 26.773701 | 34.613396 |
| Ca      | 37.061455 | 31.386417 | 33.426605 |
| Ca      | 39.778351 | 29.082008 | 31.454330 |
| Ca      | 39.759598 | 30.192591 | 36.313831 |
| Ca      | 45.499943 | 26.963526 | 33.897003 |
| Ca      | 42.691669 | 29.608044 | 34.182755 |
| S       | 26.959511 | 27.319275 | 35.958412 |
| S       | 27.336874 | 33.903091 | 35.284821 |
| S       | 30.502899 | 29.794346 | 32.775730 |
| S       | 30.084137 | 30.880997 | 36.610771 |
| S       | 33.449326 | 27.227261 | 34.152481 |
| S       | 33.782791 | 32.701336 | 32.346134 |
| S       | 36.554878 | 28.348110 | 31.406067 |
| S       | 36.602604 | 29.752602 | 36.119797 |
| S       | 40.019928 | 27.352459 | 34.422619 |
| S       | 40.494030 | 31.776546 | 33.199833 |
| S       | 43.386230 | 28.053223 | 31.414825 |
| S       | 44.027927 | 27.720234 | 38.667328 |

24 generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 25.464748 | 30.517662 | 31.672344 |
| Ca      | 26.381760 | 30.813725 | 35.759712 |
| Ca      | 30.530136 | 27.917776 | 35.787643 |
| Ca      | 30.212893 | 33.082401 | 33.665691 |
| Ca      | 33.343567 | 29.376225 | 31.395981 |
| Ca      | 33.362835 | 30.207258 | 35.391907 |
| Ca      | 36.936451 | 26.406315 | 34.762039 |
| Ca      | 36.856709 | 31.158424 | 33.783765 |
| Ca      | 39.910721 | 29.223906 | 31.329632 |
| Ca      | 39.802807 | 30.204006 | 36.232544 |
|   |   |   |   |
|---|---|---|---|
| Ca | 45.494881 | 26.702005 | 33.409626 |
| Ca | 42.89091   | 29.804144 | 34.036198 |
| S  | 27.032887  | 27.521366 | 35.871346 |
| S  | 26.829037  | 33.977264 | 35.115585 |
| S  | 30.433439  | 29.820089 | 32.983734 |
| S  | 30.017166  | 31.129383 | 36.586216 |
| S  | 33.426746  | 27.214432 | 34.270462 |
| S  | 33.648907  | 32.594254 | 32.529617 |
| S  | 36.732628  | 28.217144 | 31.557751 |
| S  | 36.643265  | 29.363136 | 36.335106 |
| S  | 40.247871  | 27.356142 | 34.273701 |
| S  | 40.632858  | 31.732885 | 33.089867 |
| S  | 43.617722  | 28.167185 | 31.246449 |
| S  | 43.983791  | 27.884266 | 38.940254 |

24 generated by VMD

| Ca | 25.495468 | 30.468351 | 31.482986 |
| Ca | 26.398634 | 30.652834 | 35.531872 |
| Ca | 30.281757 | 27.993990 | 35.685745 |
| Ca | 30.063393 | 32.527847 | 33.679993 |
| Ca | 33.442970 | 29.304535 | 31.628330 |
| Ca | 33.262772 | 30.643337 | 35.665756 |
| Ca | 36.652096 | 27.164186 | 34.572666 |
| Ca | 37.069649 | 31.539040 | 33.801762 |
| Ca | 40.018402 | 29.431084 | 31.511669 |
| Ca | 39.955612 | 30.148289 | 36.295609 |
| Ca | 45.592384 | 26.430969 | 33.676971 |
| Ca | 42.939304 | 29.274982 | 34.021923 |
| S  | 27.116158 | 27.285997 | 35.956184 |
| S  | 26.926125 | 33.947418 | 35.147919 |
| S  | 30.456924 | 29.495165 | 32.816620 |
| S  | 29.877323 | 31.034225 | 36.526104 |
| S  | 33.463867 | 27.522118 | 34.489600 |
| S  | 33.227310 | 32.388184 | 32.518028 |
| S  | 36.783218 | 28.587206 | 31.550749 |
| S  | 36.705589 | 29.988350 | 36.452435 |
| S  | 39.979248 | 27.268772 | 34.187687 |
| S  | 40.740616 | 31.829916 | 33.459473 |
| S  | 43.586918 | 28.005171 | 31.092640 |
| S  | 44.398144 | 27.459429 | 38.277550 |

24 generated by VMD

| Ca | 25.709963 | 30.491951 | 31.619474 |
| Ca | 26.110214 | 30.827442 | 35.691444 |
| Ca | 30.209213 | 27.869175 | 35.830627 |
| Ca | 30.168634 | 32.460926 | 33.872265 |
| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 33.343483 | 29.021755 | 31.241940 |
| Ca      | 33.274872 | 30.360920 | 35.529381 |
| Ca      | 36.745872 | 27.007853 | 34.518478 |
| Ca      | 37.040398 | 31.690710 | 33.701653 |
| Ca      | 40.275787 | 29.296108 | 31.201595 |
| Ca      | 39.997978 | 30.306129 | 36.231628 |
| Ca      | 45.233181 | 26.103405 | 33.294327 |
| Ca      | 43.130634 | 29.533512 | 34.256477 |
| S       | 26.694744 | 27.433126 | 35.906746 |
| S       | 26.925501 | 34.069920 | 34.885201 |
| S       | 30.409534 | 29.509123 | 32.963615 |
| S       | 29.652437 | 31.005196 | 36.741451 |
| S       | 33.359047 | 27.440836 | 34.337517 |
| S       | 33.536327 | 32.288433 | 32.693909 |
| S       | 36.762283 | 28.729820 | 31.562601 |
| S       | 36.595928 | 29.802822 | 36.578014 |
| S       | 40.130104 | 27.501232 | 34.288532 |
| S       | 40.781787 | 31.867691 | 33.359131 |
| S       | 43.789024 | 28.085560 | 31.241949 |
| S       | 44.551575 | 27.687759 | 38.482773 |

24 generated by VMD

| Element | X2   | Y2   | Z2   |
|---------|------|------|------|
| Ca      | 25.543715 | 30.197336 | 31.462782 |
| Ca      | 26.148338 | 30.767103 | 35.609787 |
| Ca      | 30.390779 | 28.053860 | 35.900303 |
| Ca      | 30.182751 | 32.802647 | 33.758282 |
| Ca      | 33.277359 | 29.315182 | 31.473061 |
| Ca      | 33.586720 | 30.169415 | 35.609570 |
| Ca      | 36.721420 | 27.154865 | 34.317112 |
| Ca      | 36.848251 | 31.583828 | 33.915672 |
| Ca      | 40.089874 | 29.345230 | 31.445496 |
| Ca      | 40.004360 | 29.947495 | 36.244350 |
| Ca      | 45.487911 | 26.405605 | 33.361190 |
| Ca      | 42.907082 | 29.441216 | 34.182156 |
| S       | 26.948074 | 27.431746 | 36.029636 |
| S       | 26.868481 | 34.047600 | 34.655590 |
| S       | 30.449673 | 29.511883 | 32.954449 |
| S       | 29.622341 | 31.242023 | 36.763004 |
| S       | 33.387154 | 27.371555 | 34.385071 |
| S       | 33.466942 | 32.440960 | 32.706573 |
| S       | 36.814674 | 28.661404 | 31.537704 |
| S       | 36.614105 | 29.737942 | 36.463013 |
| S       | 40.016796 | 27.240124 | 34.028595 |
| S       | 40.633732 | 31.811277 | 33.478691 |
| S       | 43.695747 | 28.036633 | 31.394773 |
| S       | 44.727638 | 27.674456 | 38.353737 |
| Atom | X | Y | Z |
|------|---|---|---|
| Ca   | 25.485645 | 30.091702 | 31.358332 |
| Ca   | 26.114183 | 30.612759 | 35.511585 |
| Ca   | 30.281321 | 28.041693 | 36.012138 |
| Ca   | 30.178864 | 32.852192 | 33.852554 |
| Ca   | 33.414955 | 29.759315 | 31.517757 |
| Ca   | 33.311310 | 30.314116 | 35.249229 |
| Ca   | 36.655418 | 27.093914 | 34.601490 |
| Ca   | 37.355732 | 31.580032 | 33.990547 |
| Ca   | 40.213806 | 29.132786 | 31.375675 |
| Ca   | 40.126595 | 30.123074 | 35.970760 |
| Ca   | 45.250538 | 26.009464 | 33.434681 |
| Ca   | 43.199909 | 29.605305 | 34.036022 |
| S    | 26.875488 | 27.254982 | 36.044632 |
| S    | 26.768456 | 33.883064 | 34.782772 |
| S    | 30.396812 | 29.791199 | 33.031677 |
| S    | 29.449811 | 31.018360 | 36.709644 |
| S    | 33.190998 | 27.365543 | 34.243763 |
| S    | 33.501568 | 32.619194 | 32.881386 |
| S    | 36.784031 | 28.832266 | 31.734598 |
| S    | 36.505028 | 29.709795 | 36.646877 |
| S    | 40.093037 | 27.125717 | 34.163471 |
| S    | 40.819996 | 31.611885 | 33.139282 |
| S    | 43.737808 | 27.983263 | 31.342859 |
| S    | 44.727448 | 27.979816 | 38.390229 |

24

generated by VMD

| Atom | X | Y | Z |
|------|---|---|---|
| Ca   | 25.326248 | 30.491888 | 31.600067 |
| Ca   | 26.177067 | 30.654903 | 35.689529 |
| Ca   | 30.387493 | 27.853157 | 35.767464 |
| Ca   | 30.090466 | 32.798973 | 33.755215 |
| Ca   | 33.390659 | 29.602100 | 31.542179 |
| Ca   | 33.248482 | 30.243015 | 35.489338 |
| Ca   | 36.689651 | 26.924831 | 34.446472 |
| Ca   | 37.239101 | 31.566618 | 33.840286 |
| Ca   | 40.231480 | 29.060490 | 31.301884 |
| Ca   | 39.962406 | 30.195862 | 36.047962 |
| Ca   | 45.566521 | 26.434931 | 33.586079 |
| Ca   | 43.125198 | 29.535927 | 34.165367 |
| S    | 26.881344 | 27.312019 | 36.164028 |
| S    | 26.819042 | 33.877033 | 34.826019 |
| S    | 30.487661 | 29.756342 | 32.994499 |
| S    | 29.650534 | 31.070721 | 36.663155 |
| S    | 33.313793 | 27.281610 | 34.223404 |
| S    | 33.606194 | 32.631378 | 32.756359 |
| Element | X  | Y  | Z  |
|---------|----|----|----|
| S       | 26.01105 | 27.332087 | 36.218849 |
| S       | 26.568029 | 33.87718 | 34.374077 |
| S       | 30.501755 | 29.852930 | 33.013561 |
| S       | 29.981462 | 31.168280 | 36.744003 |
| S       | 33.373623 | 27.328585 | 34.143555 |
| S       | 33.583286 | 32.736572 | 32.881809 |
| S       | 36.745335 | 28.890388 | 31.611504 |
| S       | 36.625175 | 29.662851 | 36.391438 |
| S       | 40.098125 | 27.506744 | 34.060406 |
| S       | 40.671459 | 31.679640 | 33.207859 |
| S       | 43.486572 | 27.753656 | 31.253437 |
| S       | 44.493671 | 27.447947 | 38.498196 |

24 generated by VMD

| Element | X  | Y  | Z  |
|---------|----|----|----|
| Ca      | 25.995298 | 29.768272 | 31.845695 |
| Ca      | 26.392353 | 30.621807 | 35.981476 |
| Ca      | 30.470970 | 28.171486 | 35.897518 |
| Ca      | 30.284019 | 32.906773 | 33.90692 |
| Ca      | 33.253475 | 29.814495 | 31.323895 |
| Ca      | 33.302246 | 30.533419 | 35.361000 |
| Ca      | 36.665600 | 26.869415 | 34.011429 |
| Ca      | 36.738422 | 31.288239 | 33.437546 |
| Ca      | 40.095093 | 29.221722 | 31.282204 |
| Ca      | 39.840485 | 30.232403 | 36.172264 |
| Ca      | 45.345993 | 26.443569 | 34.144367 |
| Ca      | 43.100487 | 29.475307 | 34.098270 |
| S       | 27.167664 | 27.196112 | 36.071785 |
| S       | 26.856592 | 33.794991 | 34.897945 |
| S       | 30.396236 | 29.923058 | 33.046879 |
| S       | 29.890163 | 31.152971 | 36.835243 |
| S       | 33.305775 | 27.584660 | 33.928730 |
| S       | 33.624706 | 32.697041 | 32.788254 |
| S       | 36.514877 | 28.659809 | 31.316622 |
| S       | 36.580193 | 29.596460 | 36.113262 |
| S       | 40.015629 | 27.355583 | 34.073223 |
| S       | 40.787056 | 31.646452 | 33.177269 |
| S       | 43.694603 | 27.866955 | 31.456497 |
| S       | 44.115891 | 27.570442 | 38.778538 |

24 generated by VMD

| Element | X  | Y  | Z  |
|---------|----|----|----|
| Ca      | 25.792456 | 29.974007 | 31.580669 |
| Ca      | 26.724613 | 30.383659 | 36.183105 |
| Ca      | 30.277359 | 28.025364 | 35.652527 |
| Ca      | 30.448332 | 32.922268 | 33.700760 |
| Ca      | 33.341942 | 29.875637 | 31.307907 |
| Ca      | 33.319145 | 30.374559 | 35.187725 |
|   |     |     |     |
|---|-----|-----|-----|
| Ca | 36.641594 | 26.903196 | 34.257431 |
| Ca | 36.820183 | 26.903196 | 34.257431 |
| Ca | 39.796101 | 29.181961 | 31.667542 |
| Ca | 40.002716 | 30.503910 | 36.598675 |
| Ca | 44.969666 | 26.174263 | 33.523647 |
| Ca | 42.795258 | 29.566366 | 34.206688 |
| S  | 27.041916 | 27.041748 | 35.810806 |
| S  | 27.332766 | 27.041916 | 35.810806 |
| S  | 30.397697 | 29.888687 | 32.845329 |
| S  | 30.081432 | 31.182034 | 36.707783 |
| S  | 33.259514 | 27.455074 | 33.984646 |
| S  | 33.743717 | 32.792000 | 32.521461 |
| S  | 36.600849 | 28.590294 | 31.288248 |
| S  | 36.530396 | 29.747007 | 36.250412 |
| S  | 39.798473 | 27.396469 | 34.709976 |
| S  | 40.587860 | 31.739136 | 33.166729 |
| S  | 43.125652 | 27.867828 | 31.553474 |
| S  | 45.004211 | 27.765471 | 38.556248 |

24

generated by VMD

|   |     |     |     |
|---|-----|-----|-----|
| Ca | 25.488457 | 29.842081 | 31.769176 |
| Ca | 26.594004 | 30.533201 | 36.175053 |
| Ca | 30.411266 | 28.071486 | 35.649471 |
| Ca | 30.198483 | 32.977966 | 33.623604 |
| Ca | 33.399052 | 29.815006 | 31.442417 |
| Ca | 33.329887 | 30.351357 | 35.552296 |
| Ca | 36.665222 | 27.006432 | 34.303997 |
| Ca | 37.002953 | 31.552807 | 33.846905 |
| Ca | 40.031746 | 29.157833 | 31.685055 |
| Ca | 39.938957 | 30.334225 | 36.198002 |
| Ca | 45.300194 | 26.468884 | 33.651260 |
| Ca | 42.920753 | 29.360729 | 34.059052 |
| S  | 27.117487 | 27.328583 | 35.811188 |
| S  | 26.663300 | 33.652466 | 34.544586 |
| S  | 30.434315 | 29.886282 | 32.847042 |
| S  | 29.958069 | 31.289680 | 36.671913 |
| S  | 33.285072 | 27.569839 | 34.006920 |
| S  | 33.507339 | 32.828220 | 32.908348 |
| S  | 36.606533 | 28.665977 | 31.407621 |
| S  | 36.630669 | 29.603519 | 36.408039 |
| S  | 39.956833 | 27.191074 | 34.306427 |
| S  | 40.685989 | 31.707060 | 33.396378 |
| S  | 43.520279 | 27.856997 | 31.286377 |
| S  | 44.787003 | 27.565674 | 38.479618 |

24

generated by VMD
| Ca  | 25.393839 | 29.669977 | 31.618946 |
| Ca  | 26.446405 | 30.776428 | 36.008911 |
| Ca  | 30.263451 | 28.181517 | 35.850796 |
| Ca  | 30.283514 | 32.863144 | 33.678467 |
| Ca  | 33.482845 | 29.714493 | 31.425259 |
| Ca  | 33.198719 | 30.383432 | 35.530834 |
| Ca  | 36.730442 | 26.880581 | 34.173702 |
| Ca  | 37.015221 | 31.398191 | 33.874737 |
| Ca  | 40.082382 | 29.237396 | 31.548519 |
| Ca  | 39.875114 | 30.328272 | 36.322533 |
| Ca  | 45.510307 | 26.399359 | 33.552650 |
| Ca  | 42.875626 | 29.448795 | 34.147923 |
| S   | 26.938175 | 27.315908 | 35.769745 |
| S   | 26.938892 | 33.760490 | 34.660255 |
| S   | 30.570316 | 29.789429 | 32.802509 |
| S   | 29.943626 | 31.233515 | 36.871490 |
| S   | 33.366402 | 27.535835 | 34.086990 |
| S   | 33.568645 | 32.677353 | 32.790092 |
| S   | 36.684723 | 28.705269 | 31.626791 |
| S   | 36.605179 | 29.523024 | 36.325069 |
| S   | 39.948212 | 27.281153 | 34.366016 |
| S   | 40.655174 | 31.815268 | 33.308590 |
| S   | 43.349045 | 27.898098 | 31.376183 |
| S   | 44.707695 | 27.574471 | 38.313686 |

24 generated by VMD

| Ca  | 25.364513 | 29.363733 | 31.536064 |
| Ca  | 26.659832 | 30.697311 | 35.709972 |
| Ca  | 30.466949 | 28.092020 | 35.904099 |
| Ca  | 30.218533 | 32.937149 | 33.825039 |
| Ca  | 33.341473 | 29.882328 | 31.592060 |
| Ca  | 33.272274 | 30.541809 | 35.430607 |
| Ca  | 36.695953 | 27.093718 | 34.322193 |
| Ca  | 36.946880 | 31.444118 | 33.939754 |
| Ca  | 39.996254 | 29.169828 | 31.376295 |
| Ca  | 39.910244 | 30.167324 | 36.492825 |
| Ca  | 45.395145 | 26.682972 | 33.438679 |
| Ca  | 42.949368 | 29.257648 | 34.091438 |
| S   | 27.196980 | 27.287178 | 35.818916 |
| S   | 26.955875 | 33.858456 | 34.353195 |
| S   | 30.419350 | 29.871840 | 32.925869 |
| S   | 29.970943 | 31.223059 | 36.715622 |
| S   | 33.312794 | 27.402174 | 34.235321 |
| S   | 33.583267 | 32.860901 | 32.984993 |
| S   | 36.534203 | 28.755611 | 31.542614 |
| S   | 36.635166 | 29.670950 | 36.429115 |
|       |          |          |          |
|-------|----------|----------|----------|
| Ca    | 25.628796| 29.733261| 31.580961|
| Ca    | 26.233858| 30.702446| 35.600788|
| Ca    | 30.036919| 28.397770| 35.863144|
| Ca    | 30.234978| 32.922401| 33.747917|
| Ca    | 33.358768| 29.591721| 31.505596|
| Ca    | 33.254639| 30.361835| 35.601036|
| Ca    | 36.641911| 26.960608| 34.526260|
| Ca    | 36.843899| 31.277740| 34.024361|
| Ca    | 39.826569| 29.262890| 31.507060|
| Ca    | 40.118015| 30.019461| 36.246746|
| Ca    | 45.725510| 26.680502| 33.465412|
| Ca    | 43.092525| 29.618599| 34.071626|
| S     | 26.947289| 27.442013| 36.005745|
| S     | 26.700493| 33.760925| 34.472561|
| S     | 30.544552| 29.824114| 32.828316|
| S     | 29.807041| 31.344046| 36.684643|
| S     | 33.383408| 27.463978| 34.245171|
| S     | 33.775322| 32.651875| 32.992256|
| S     | 36.654110| 28.390825| 31.517612|
| S     | 36.592297| 29.577106| 36.492607|
| S     | 40.097004| 27.326977| 34.175797|
| S     | 40.603958| 31.708643| 33.339331|
| S     | 43.453865| 28.124302| 31.282328|
| S     | 44.878098| 27.247395| 38.250706|

24

generated by VMD

|       |          |          |          |
|-------|----------|----------|----------|
| Ca    | 25.411400| 30.038115| 32.036327|
| Ca    | 26.377743| 30.670557| 35.891861|
| Ca    | 29.983158| 28.219563| 35.886528|
| Ca    | 30.339455| 33.111462| 33.341293|
| Ca    | 33.429207| 29.605377| 31.533369|
| Ca    | 33.188911| 30.201277| 35.459751|
| Ca    | 36.613510| 26.965092| 34.644253|
| Ca    | 36.765114| 31.059200| 33.930691|
| Ca    | 40.156319| 29.163479| 31.565039|
| Ca    | 39.915833| 30.019672| 36.276112|
| Ca    | 45.849808| 27.205887| 33.351357|
| Ca    | 42.941460| 29.475288| 34.108719|
| S     | 26.957787| 27.284548| 35.689331|
| S     | 27.164726| 33.823940| 34.728306|
|   |   |   |   |
|---|---|---|---|
| S | 30.505251 | 29.822647 | 32.893055 |
| S | 29.994019 | 31.304386 | 36.453568 |
| S | 33.273338 | 27.389103 | 34.128418 |
| S | 33.819180 | 32.574104 | 32.743019 |
| S | 36.628490 | 28.495394 | 31.440449 |
| S | 36.557137 | 29.639572 | 36.570747 |
| S | 40.046822 | 27.127579 | 34.245197 |
| S | 40.431416 | 31.671513 | 33.418423 |
| S | 43.546806 | 28.098419 | 31.355167 |
| S | 44.534279 | 27.411182 | 38.339676 |

24 generated by VMD

| Ca |   |   |   |
|----|---|---|---|
| Ca | 24.966953 | 30.115265 | 32.175842 |
| Ca | 26.523403 | 30.733952 | 35.857876 |
| Ca | 29.934381 | 28.214123 | 35.800682 |
| Ca | 30.093029 | 32.965679 | 33.396103 |
| Ca | 33.392891 | 29.691095 | 31.370869 |
| Ca | 33.319336 | 30.364532 | 35.237389 |
| Ca | 36.597202 | 26.795307 | 34.363537 |
| Ca | 36.879433 | 31.102476 | 33.621830 |
| Ca | 40.241077 | 29.194365 | 31.474230 |
| Ca | 39.862640 | 29.767292 | 36.642189 |
| Ca | 45.897507 | 27.156555 | 33.521492 |
| Ca | 42.962379 | 29.459810 | 34.279633 |
| S | 26.896099 | 27.365192 | 35.895634 |
| S | 26.981867 | 33.944984 | 34.844986 |
| S | 30.406626 | 29.879684 | 32.868206 |
| S | 30.136082 | 31.183216 | 36.596729 |
| S | 33.284630 | 27.359449 | 34.102879 |
| S | 33.563812 | 32.659401 | 32.585350 |
| S | 36.658306 | 28.520885 | 31.471981 |
| S | 36.551983 | 29.504139 | 36.278683 |
| S | 40.093330 | 27.165056 | 34.157845 |
| S | 40.517166 | 31.471863 | 33.495598 |
| S | 43.768421 | 28.130463 | 31.505901 |
| S | 44.905315 | 27.464652 | 38.485306 |

24 generated by VMD
|    |      |      |      |
|---|------|------|------|
| Ca | 39.944038 | 29.327030 | 31.615595 |
| Ca | 39.927814 | 30.076458 | 36.532280 |
| Ca | 45.540016 | 26.995363 | 33.649040 |
| Ca | 43.046638 | 29.591452 | 34.219128 |
| S  | 27.010658 | 27.409332 | 36.030388 |
| S  | 27.107355 | 33.885254 | 34.637234 |
| S  | 30.515139 | 29.688606 | 32.80557 |
| S  | 30.060230 | 31.260433 | 36.485741 |
| S  | 33.413506 | 27.265968 | 33.961742 |
| S  | 33.699093 | 32.562798 | 32.701130 |
| S  | 36.604378 | 28.491261 | 31.458427 |
| S  | 36.534576 | 29.554321 | 36.306076 |
| S  | 40.075382 | 27.169647 | 34.202888 |
| S  | 40.502327 | 31.850510 | 33.442970 |
| S  | 43.588577 | 28.089867 | 31.407160 |
| S  | 44.721725 | 27.448513 | 38.518707 |
|    |      |      |      |
| 24 | generated by VMD |
| Ca | 24.901142 | 30.250736 | 32.412117 |
| Ca | 26.553753 | 30.783619 | 36.018188 |
| Ca | 30.234922 | 28.125010 | 35.539173 |
| Ca | 30.411222 | 32.784271 | 33.501308 |
| Ca | 33.438347 | 29.563597 | 31.228617 |
| Ca | 33.247574 | 30.198717 | 35.272816 |
| Ca | 36.742203 | 26.984188 | 34.545528 |
| Ca | 36.793480 | 31.096825 | 33.610924 |
| Ca | 40.123302 | 29.077240 | 31.676826 |
| Ca | 39.711311 | 30.104616 | 36.356251 |
| Ca | 45.805862 | 27.369898 | 33.703049 |
| Ca | 42.717892 | 29.583809 | 34.406044 |
| S  | 26.998878 | 27.348459 | 35.774418 |
| S  | 27.363085 | 33.863495 | 34.902370 |
| S  | 30.363953 | 29.775942 | 32.583622 |
| S  | 30.195726 | 31.163609 | 36.597500 |
| S  | 33.247917 | 27.369148 | 34.006855 |
| S  | 33.605530 | 32.654907 | 32.601677 |
| S  | 36.647457 | 28.415482 | 31.416258 |
| S  | 36.517479 | 29.598745 | 36.409069 |
| S  | 39.974976 | 27.247150 | 34.238209 |
| S  | 40.562981 | 31.702747 | 33.333279 |
| S  | 43.591934 | 28.121216 | 31.484196 |
| S  | 44.682983 | 27.207979 | 38.412357 |
|    |      |      |      |
| 24 | generated by VMD |
| Ca | 25.011354 | 29.902206 | 32.196548 |
| Ca | 26.486870 | 30.579540 | 35.898857 |
| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 30.325113| 28.017101| 35.674137|
| Ca      | 30.209122| 30.570986| 35.415817|
| Ca      | 36.782928| 27.119953| 34.576244|
| Ca      | 36.792469| 31.107756| 33.557281|
| Ca      | 40.194408| 29.081684| 31.414410|
| Ca      | 39.784363| 30.174322| 36.431107|
| Ca      | 45.473946| 26.768269| 33.703053|
| Ca      | 42.779648| 29.324244| 34.199425|
| S       | 27.061451| 27.247414| 35.686993|
| S       | 27.053707| 33.850727| 34.987633|
| S       | 30.549782| 29.899796| 32.795773|
| S       | 29.998043| 31.104069| 36.512203|
| S       | 33.372700| 27.504240| 34.015083|
| S       | 33.598297| 32.707989| 32.739735|
| S       | 36.632290| 28.601524| 31.423292|
| S       | 36.539543| 29.789116| 36.389858|
| S       | 40.043903| 27.179241| 34.277531|
| S       | 40.555531| 31.564507| 33.336338|
| S       | 43.730026| 28.059292| 31.480846|
| S       | 44.748966| 27.444771| 38.472572|

Generated by VMD
S  43.636158  28.031021  31.473671
S  44.857826  27.602655  38.287331

24
generated by VMD

Ca  24.945007  30.299423  32.072464
Ca  26.461754  30.829313  35.956440
Ca  30.072567  27.916893  35.856598
Ca  30.448631  32.775265  33.613312
Ca  33.480301  29.555622  31.421375
Ca  33.365658  30.209427  35.299068
Ca  36.772087  27.038677  34.602242
Ca  37.013870  31.028999  33.600685
Ca  39.797501  29.155394  31.622461
Ca  39.947250  30.239441  36.391277
Ca  45.760365  27.098827  33.576035
Ca  42.994011  29.566971  34.147747
S  26.704224  27.279226  35.520370
S  27.270992  34.100861  34.825008
S  30.578552  29.727230  32.772987
S  29.881788  31.037407  36.561436
S  33.380775  27.280739  34.057632
S  33.750877  32.537327  32.69169
S  36.578861  28.229267  31.469429
S  36.524727  29.700554  36.402569
S  40.027969  27.256176  34.509148
S  40.613152  31.857445  33.357292
S  43.461048  28.239828  31.362823
S  44.601898  27.431089  38.333111

24
generated by VMD

Ca  25.114601  30.239397  31.966436
Ca  26.472488  30.593813  35.910351
Ca  30.220451  27.942762  35.956482
Ca  30.393799  32.807835  33.676437
Ca  33.481869  29.720207  31.227257
Ca  33.177605  30.517303  35.399391
Ca  36.807434  26.941422  34.678993
Ca  36.721649  30.973579  33.323761
Ca  40.153664  28.967066  31.598282
Ca  39.780289  30.269825  36.406773
Ca  45.678112  26.799721  33.533188
Ca  42.863144  29.623922  34.155354
S  26.827988  27.237175  35.455818
S  27.323116  33.902039  35.140987
S  30.555202  29.819420  32.888882
S  29.835005  31.147308  36.566891
S  33.352390  27.422459  34.081871
S  33.707054  32.729481  32.643059
S  36.673546  28.394547  31.455921
S  36.550663  29.861423  36.436539
S  40.164719  27.198246  34.406509
S  40.487717  31.586681  33.381798
S  43.600365  28.128078  31.365805
S  44.491058  27.567739  38.373787
24

generated by VMD

Ca  25.237217  30.232349  31.702239
Ca  26.501913  30.748516  35.874786
Ca  30.466644  29.892626  35.801754
Ca  30.130207  33.066105  33.595505
Ca  33.452007  29.487347  31.707756
Ca  33.318142  30.349255  35.352509
Ca  36.792183  26.829336  34.547581
Ca  36.809639  31.329142  33.607307
Ca  40.060913  29.135777  31.561146
Ca  39.742275  30.134468  36.347954
Ca  45.572094  26.468712  33.406189
Ca  42.911030  29.781467  34.179195
S  26.883278  27.398956  35.642155
S  26.838554  33.865429  34.528633
S  30.593956  29.903866  32.863121
S  29.998934  31.107368  36.566608
S  33.413200  27.217159  34.371445
S  33.623985  32.664974  32.627743
S  36.745010  28.303993  31.648527
S  36.505569  29.635830  36.390491
S  40.155025  31.200176  34.275883
S  40.188027  31.795719  33.390823
S  43.599167  28.332130  31.172373
S  44.695049  27.414043  38.177406

24

generated by VMD

Ca  24.931149  30.319260  31.921221
Ca  26.457535  30.892292  35.930107
Ca  30.203590  27.817669  35.861401
Ca  30.211601  32.877594  33.436378
Ca  33.325993  29.584496  31.675703
Ca  33.286713  30.072416  35.379974
Ca  36.887802  26.835991  34.541641
Ca  36.881248  31.121159  33.671421
Ca  40.041031  29.276321  31.491964
Ca  40.020844  30.368195  36.354053
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 45.708740 | 26.838947 | 33.572052 |
| Ca      | 43.071728 | 29.813831 | 34.021412 |
| S       | 26.748199 | 27.479439 | 35.776382 |
| S       | 26.865368 | 33.977379 | 34.481312 |
| S       | 30.487579 | 29.603539 | 32.843536 |
| S       | 30.023979 | 31.220821 | 36.542938 |
| S       | 33.412907 | 27.143568 | 34.132111 |
| S       | 33.759132 | 32.641026 | 32.929428 |
| S       | 36.683205 | 28.439735 | 31.602905 |
| S       | 36.585281 | 29.577366 | 36.510479 |
| S       | 40.129482 | 27.379448 | 34.280960 |
| S       | 40.601883 | 31.828724 | 33.400284 |
| S       | 43.653057 | 28.105219 | 31.434944 |
| S       | 44.455860 | 27.176956 | 38.238007 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.017567 | 29.961166 | 32.115494 |
| Ca      | 26.480370 | 30.987928 | 35.943283 |
| Ca      | 30.214128 | 28.104601 | 35.488701 |
| Ca      | 30.232973 | 32.792606 | 33.558659 |
| Ca      | 33.403065 | 29.706944 | 31.505312 |
| Ca      | 33.297844 | 30.181496 | 35.347076 |
| Ca      | 36.622093 | 26.778702 | 34.496769 |
| Ca      | 36.845730 | 31.170876 | 33.699600 |
| Ca      | 40.101349 | 29.299379 | 31.505981 |
| Ca      | 40.075474 | 30.061985 | 36.520073 |
| Ca      | 45.833740 | 26.763205 | 33.572155 |
| Ca      | 42.716251 | 29.618750 | 34.036476 |
| S       | 26.771198 | 27.366886 | 36.098991 |
| S       | 26.918108 | 33.976608 | 34.401184 |
| S       | 30.393183 | 29.687452 | 32.648994 |
| S       | 29.976088 | 31.095615 | 36.637707 |
| S       | 33.342911 | 27.404627 | 34.059807 |
| S       | 33.680599 | 32.722965 | 32.857994 |
| S       | 36.802635 | 28.577856 | 31.676682 |
| S       | 36.699394 | 29.490959 | 36.494267 |
| S       | 40.082836 | 27.366024 | 34.209400 |
| S       | 40.491882 | 31.863211 | 33.358532 |
| S       | 43.778080 | 28.167717 | 31.514696 |
| S       | 44.656380 | 27.243843 | 38.282776 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.148260 | 30.038069 | 31.974087 |
| Ca      | 26.457130 | 31.119932 | 35.784679 |
| Ca      | 30.209122 | 27.996166 | 35.738132 |
| Ca      | 30.214649 | 32.858654 | 33.653267 |
| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 33.490372 | 29.547260 | 31.488020 |
| Ca      | 33.271084 | 30.336803 | 35.608833 |
| Ca      | 36.698776 | 26.566132 | 34.357147 |
| Ca      | 36.842613 | 31.083694 | 33.839275 |
| Ca      | 39.973053 | 29.160419 | 31.536287 |
| Ca      | 39.941013 | 29.866995 | 36.461208 |
| Ca      | 45.825649 | 27.193058 | 33.491882 |
| Ca      | 42.969215 | 29.748932 | 34.085274 |
| S       | 26.857084 | 27.517616 | 35.868454 |
| S       | 26.905806 | 34.091198 | 34.362400 |
| S       | 30.437122 | 29.841072 | 32.776497 |
| S       | 29.932104 | 31.193474 | 36.689304 |
| S       | 33.312962 | 27.358513 | 34.058128 |
| S       | 33.752491 | 32.516960 | 32.928085 |
| S       | 36.637077 | 28.340645 | 31.406927 |
| S       | 36.596233 | 29.445045 | 36.559391 |
| S       | 40.100780 | 27.068882 | 34.140541 |
| S       | 40.460018 | 31.620361 | 33.432224 |
| S       | 43.517155 | 28.237104 | 31.474506 |
| S       | 44.884075 | 27.644409 | 38.316174 |

24

generated by VMD

| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 25.184746 | 29.842909 | 31.958359 |
| Ca      | 26.274349 | 31.084423 | 35.907986 |
| Ca      | 29.842840 | 28.088520 | 35.704540 |
| Ca      | 30.371010 | 32.744370 | 33.492500 |
| Ca      | 33.436161 | 29.795681 | 31.586586 |
| Ca      | 33.135426 | 30.112829 | 35.366085 |
| Ca      | 36.513420 | 26.898851 | 34.318417 |
| Ca      | 36.779404 | 31.396893 | 33.816208 |
| Ca      | 40.353161 | 29.271427 | 31.383797 |
| Ca      | 40.111496 | 29.855762 | 36.575794 |
| Ca      | 46.031460 | 27.032532 | 33.499134 |
| Ca      | 43.043785 | 29.341070 | 34.162560 |
| S       | 26.640909 | 27.578518 | 36.249176 |
| S       | 26.946838 | 33.840260 | 34.150288 |
| S       | 30.471558 | 29.624159 | 32.783371 |
| S       | 29.756798 | 31.121054 | 36.554375 |
| S       | 33.175034 | 27.202778 | 34.073189 |
| S       | 33.742466 | 32.676380 | 33.170914 |
| S       | 36.745300 | 28.844818 | 31.701496 |
| S       | 36.513775 | 29.670633 | 36.604424 |
| S       | 40.081856 | 27.263466 | 34.082455 |
| S       | 40.549629 | 31.656334 | 33.518517 |
| S       | 43.716084 | 28.022528 | 31.256451 |
| S       | 45.016396 | 27.425163 | 38.114105 |
|   | Ca    | S     |
|---|-------|-------|
| 24 | 24.981352 | 30.054514 | 31.962748 |
| 24 | 26.364559 | 30.929714 | 35.850258 |
| 24 | 30.145027 | 28.144464 | 35.734085 |
| 24 | 30.383133 | 32.994122 | 33.497776 |
| 24 | 33.439152 | 29.669456 | 31.427153 |
| 24 | 33.089645 | 30.253275 | 35.626652 |
| 24 | 36.727585 | 26.624033 | 34.95846 |
| 24 | 36.702763 | 30.840706 | 33.686501 |
| 24 | 40.151695 | 28.912010 | 31.286644 |
| 24 | 39.821316 | 29.954638 | 36.580463 |
| 24 | 45.917904 | 27.338058 | 33.438797 |
| 24 | 42.896595 | 29.604456 | 34.207180 |
| 24 | 26.742769 | 27.532150 | 35.727470 |
| 24 | 27.070057 | 34.071926 | 34.568390 |
| 24 | 30.430958 | 29.868647 | 32.783005 |
| 24 | 29.905434 | 31.246437 | 36.541286 |
| 24 | 33.199135 | 27.437288 | 34.230858 |
| 24 | 33.796253 | 32.604225 | 32.981441 |
| 24 | 36.737106 | 28.307955 | 31.474884 |
| 24 | 36.532066 | 29.362209 | 36.564735 |
| 24 | 40.138046 | 27.126987 | 34.307858 |
| 24 | 40.342743 | 31.413895 | 33.491180 |
| 24 | 43.693684 | 28.311588 | 31.325397 |
| 24 | 45.224926 | 27.788641 | 38.240128 |

24 generated by VMD
| S | 36.624588 | 28.382681 | 31.529209 |
| S | 36.372551 | 29.288162 | 36.338566 |
| S | 40.035347 | 27.093395 | 34.292816 |
| S | 40.240936 | 31.392647 | 33.453434 |
| S | 43.509995 | 28.042871 | 31.372213 |
| S | 44.977176 | 27.809898 | 38.520233 |

24 generated by VMD

| Ca | 25.171883 | 29.812662 | 31.947081 |
| Ca | 26.529774 | 30.802874 | 35.720940 |
| Ca | 30.061382 | 28.206333 | 35.799698 |
| Ca | 30.394608 | 32.823570 | 33.669083 |
| Ca | 33.395695 | 29.779091 | 31.503719 |
| Ca | 33.261005 | 30.322891 | 35.508545 |
| Ca | 36.565571 | 26.846176 | 34.312752 |
| Ca | 36.786148 | 31.172920 | 33.655025 |
| Ca | 40.002220 | 29.104485 | 31.766750 |
| Ca | 39.942940 | 29.916758 | 36.418774 |
| Ca | 45.678410 | 27.245502 | 33.487091 |
| Ca | 42.828636 | 29.630901 | 34.165802 |
| S | 26.776100 | 27.407684 | 35.859924 |
| S | 27.093916 | 33.899281 | 34.322388 |
| S | 30.523962 | 29.793903 | 32.810059 |
| S | 30.061609 | 31.244658 | 36.659073 |
| S | 33.349960 | 27.451519 | 34.228649 |
| S | 33.780914 | 32.699471 | 32.944847 |
| S | 36.556225 | 28.587057 | 31.574375 |
| S | 36.631444 | 29.403276 | 36.319092 |
| S | 39.933113 | 27.110376 | 34.294075 |
| S | 40.445435 | 31.685293 | 33.529160 |
| S | 43.592796 | 28.082535 | 31.458397 |
| S | 45.067509 | 27.362249 | 38.075325 |

24 generated by VMD

| Ca | 25.122875 | 30.014420 | 32.204922 |
| Ca | 26.481697 | 30.866360 | 35.913883 |
| Ca | 30.288776 | 27.772121 | 35.807922 |
| Ca | 30.266182 | 32.952011 | 33.454426 |
| Ca | 33.342922 | 29.821056 | 31.102909 |
| Ca | 33.241573 | 30.234503 | 35.405479 |
| Ca | 36.797325 | 26.738634 | 34.474464 |
| Ca | 36.706894 | 30.995840 | 33.746479 |
| Ca | 39.935760 | 29.174658 | 31.689438 |
| Ca | 39.605934 | 30.260332 | 36.498074 |
| Ca | 45.854042 | 26.766825 | 33.343689 |
| Ca | 42.989925 | 29.762417 | 34.164501 |
S  27.049046  27.341961  35.697090
S  27.167629  34.078362  34.468761
S  30.576626  29.736809  32.669815
S  29.851105  31.257801  36.534485
S  33.438160  27.423182  34.071537
S  33.700817  34.071537
S  36.548820  28.503656  31.634552
S  36.352646  29.578098  36.611313
S  40.087143  27.237099  34.624443
S  40.282551  31.641884  33.585587
S  43.518128  28.116390  34.599490
S  45.255280  27.261292  38.023289

24 generated by VMD
Ca  25.012505  30.010311  32.033741
Ca  26.379805  30.916935  35.871342
Ca  30.252563  28.079248  35.863628
Ca  30.068249  32.887127  33.553921
Ca  33.420841  29.826305  31.309143
Ca  33.291336  30.359863  35.365540
Ca  36.674480  26.713757  34.164885
Ca  36.740658  31.131098  33.729923
Ca  40.214733  29.077736  31.392118
Ca  39.881538  29.789293  36.576721
Ca  45.857712  26.994410  33.692730
Ca  42.749573  29.540981  34.141365
S  26.884655  27.407200  35.987770
S  26.945654  33.991924  34.572830
S  30.528267  29.765411  32.828480
S  29.798544  31.278492  36.611998
S  33.382759  27.556332  33.984097
S  33.648994  32.752823  32.734016
S  36.697514  28.516792  31.621609
S  36.509567  29.411896  36.454010
S  40.082508  26.959505  34.034519
S  40.423042  31.493641  33.326698
S  43.808918  28.317419  31.485092
S  45.179497  27.612900  38.393623

24 generated by VMD
Ca  24.879755  30.081320  32.325069
Ca  26.335358  30.790262  35.918369
Ca  30.220182  28.115185  35.862831
Ca  30.247824  32.981380  33.654510
Ca  33.527054  29.721212  31.240757
Ca  33.135620  30.300470  35.479916
| Column 1 | Column 2 | Column 3 | Column 4 |
|----------|----------|----------|----------|
| Ca       | 36.803768| 26.899641| 34.552528|
| Ca       | 36.662888| 30.987019| 33.591278|
| Ca       | 40.168591| 29.037498| 31.640341|
| Ca       | 39.995144| 29.989613| 36.253448|
| Ca       | 45.710297| 26.728687| 33.433380|
| Ca       | 43.142269| 29.719669| 34.268425|
| S        | 26.954647| 27.239117| 35.611557|
| S        | 26.849873| 34.013702| 34.583889|
| S        | 30.582384| 29.862965| 32.841541|
| S        | 29.985884| 31.247635| 36.532570|
| S        | 33.388184| 27.485111| 33.923943|
| S        | 33.643684| 32.655663| 32.801094|
| S        | 36.719353| 28.524408| 31.578667|
| S        | 36.506916| 29.550108| 36.307510|
| S        | 40.283253| 27.035622| 34.343716|
| S        | 40.294727| 31.691313| 33.424343|
| S        | 43.720051| 28.193409| 31.445415|
| S        | 44.676140| 27.540384| 38.415565|

24

generated by VMD

| Column 1 | Column 2 | Column 3 | Column 4 |
|----------|----------|----------|----------|
| Ca       | 24.851254| 30.020456| 32.180698|
| Ca       | 26.435757| 30.619202| 35.925694|
| Ca       | 30.330448| 28.219000| 35.757931|
| Ca       | 30.317224| 32.844383| 33.453030|
| Ca       | 33.420109| 29.922470| 31.472603|
| Ca       | 33.138730| 30.454796| 35.482708|
| Ca       | 36.872643| 26.764011| 34.479733|
| Ca       | 36.766460| 31.124714| 33.678261|
| Ca       | 40.155869| 29.019093| 31.607075|
| Ca       | 39.763542| 30.039498| 36.290852|
| Ca       | 45.693764| 26.528408| 33.445400|
| Ca       | 42.941441| 29.782618| 34.250046|
| S        | 26.976469| 27.119862| 35.623260|
| S        | 27.092339| 33.892418| 34.736977|
| S        | 30.439705| 29.845268| 32.767227|
| S        | 29.908176| 31.445480| 36.527576|
| S        | 33.503159| 27.509350| 34.034485|
| S        | 33.518356| 32.846199| 32.743744|
| S        | 36.629990| 28.612347| 31.528128|
| S        | 36.359055| 29.512501| 36.383438|
| S        | 40.298988| 27.040714| 34.356537|
| S        | 40.444828| 31.673977| 33.378651|
| S        | 43.685272| 28.069681| 31.602119|
| S        | 45.009338| 27.484192| 38.324585|

24

generated by VMD
|   |          |          |          |
|---|----------|----------|----------|
| Ca | 25.383305 | 29.954908 | 32.273232 |
| Ca | 26.437458 | 30.815571 | 35.985622 |
| Ca | 30.288841 | 28.079208 | 35.804958 |
| Ca | 30.287640 | 32.857986 | 33.324390 |
| Ca | 33.465504 | 29.942823 | 31.298676 |
| Ca | 33.240314 | 30.338316 | 35.289612 |
| Ca | 36.826092 | 26.892992 | 34.491108 |
| Ca | 36.811844 | 30.971485 | 33.575222 |
| Ca | 39.972897 | 29.162327 | 31.424210 |
| Ca | 39.679459 | 29.942381 | 36.499111 |
| Ca | 45.546635 | 26.865210 | 33.593658 |
| Ca | 42.955658 | 29.677650 | 34.317604 |
| S  | 26.981602 | 27.151024 | 36.035778 |
| S  | 27.201916 | 34.009106 | 34.644138 |
| S  | 30.497307 | 29.805321 | 32.764256 |
| S  | 29.847752 | 31.327908 | 36.406066 |
| S  | 33.510086 | 27.525646 | 34.026745 |
| S  | 33.618332 | 32.829300 | 32.804111 |
| S  | 36.529411 | 28.406908 | 31.281425 |
| S  | 36.468880 | 29.413076 | 36.399952 |
| S  | 40.122917 | 27.148832 | 34.302124 |
| S  | 40.318611 | 31.582977 | 33.610611 |
| S  | 43.420456 | 28.386364 | 31.487219 |
| S  | 45.021069 | 27.304066 | 38.390610 |

24

generated by VMD

|   |          |          |          |
|---|----------|----------|----------|
| Ca | 24.961361 | 29.846962 | 32.328957 |
| Ca | 26.410009 | 30.753664 | 35.947155 |
| Ca | 30.356859 | 28.195662 | 35.966820 |
| Ca | 30.335056 | 32.997536 | 33.374924 |
| Ca | 33.485825 | 29.846369 | 31.300758 |
| Ca | 33.254524 | 30.184277 | 35.297298 |
| Ca | 36.711380 | 26.981531 | 34.623405 |
| Ca | 36.739231 | 30.963772 | 33.769352 |
| Ca | 40.045067 | 29.303904 | 31.363501 |
| Ca | 39.803638 | 29.919228 | 36.387390 |
| Ca | 45.435379 | 26.559252 | 33.419289 |
| Ca | 42.866463 | 29.712843 | 34.375782 |
| S  | 27.083542 | 27.389309 | 35.908413 |
| S  | 27.015778 | 33.801453 | 34.552433 |
| S  | 30.668463 | 29.840248 | 32.747631 |
| S  | 29.901821 | 31.242546 | 36.347309 |
| S  | 33.458431 | 27.433834 | 33.976185 |
| S  | 33.825577 | 32.718025 | 32.688660 |
| S  | 36.665806 | 28.551800 | 31.502258 |
| S  | 36.479126 | 29.586273 | 36.560738 |
| Atom | X  | Y  | Z  |
|------|----|----|----|
| S    | 40.193535 | 27.165901 | 34.023479 |
| S    | 40.292732 | 31.598881 | 33.529377 |
| S    | 43.583916 | 28.431637 | 31.585270 |
| S    | 44.860428 | 27.366550 | 38.454308 |

24

generated by VMD

| Atom | X  | Y  | Z  |
|------|----|----|----|
| Ca   | 25.207304 | 30.111485 | 32.130577 |
| Ca   | 26.478874 | 30.993969 | 36.028576 |
| Ca   | 30.345770 | 28.084963 | 35.744419 |
| Ca   | 30.105932 | 32.974831 | 33.376690 |
| Ca   | 33.346386 | 29.717428 | 31.172050 |
| Ca   | 33.036907 | 30.181652 | 35.176834 |
| Ca   | 36.918438 | 26.765377 | 34.575001 |
| Ca   | 36.645180 | 31.039177 | 33.840420 |
| Ca   | 39.988388 | 29.139894 | 31.735800 |
| Ca   | 39.969074 | 29.767569 | 36.444740 |
| Ca   | 45.539921 | 27.199741 | 33.474560 |
| Ca   | 42.971889 | 29.865915 | 34.270557 |
| S    | 26.964861 | 27.487431 | 35.950859 |
| S    | 26.963764 | 34.180172 | 34.734692 |
| S    | 30.523661 | 29.786928 | 32.647423 |
| S    | 30.038700 | 31.153667 | 36.449467 |
| S    | 33.378284 | 27.278496 | 33.997036 |
| S    | 33.580959 | 32.581112 | 32.688251 |
| S    | 36.706184 | 28.318930 | 31.607925 |
| S    | 36.475014 | 29.458191 | 36.434444 |
| S    | 40.246094 | 26.910521 | 34.312565 |
| S    | 40.474106 | 31.672548 | 33.566292 |
| S    | 43.490818 | 28.311270 | 31.445133 |
| S    | 45.037327 | 27.410105 | 38.226360 |

24

generated by VMD

| Atom | X  | Y  | Z  |
|------|----|----|----|
| Ca   | 24.847040 | 30.048178 | 32.478424 |
| Ca   | 26.422108 | 30.924055 | 36.098877 |
| Ca   | 30.302410 | 27.911741 | 35.605858 |
| Ca   | 30.194798 | 32.883553 | 33.341110 |
| Ca   | 33.190758 | 29.521755 | 31.088715 |
| Ca   | 33.100132 | 30.325558 | 35.009243 |
| Ca   | 36.861866 | 26.855270 | 34.311962 |
| Ca   | 36.774548 | 31.393250 | 33.682941 |
| Ca   | 39.998337 | 29.292305 | 31.815794 |
| Ca   | 40.089798 | 30.006193 | 36.497807 |
| Ca   | 45.343487 | 26.661802 | 33.486401 |
| Ca   | 43.083904 | 29.936113 | 34.508514 |
| S    | 27.106606 | 27.325668 | 36.114754 |
| S    | 27.203159 | 34.063713 | 34.804661 |
| Column 1 | Column 2 | Column 3 |
|---------|---------|---------|
| 30.333580 | 29.789436 | 32.595135 |
| 29.828548 | 31.102551 | 36.429264 |
| 33.397488 | 27.248985 | 33.877022 |
| 33.635880 | 32.569767 | 32.500095 |
| 36.721130 | 28.522877 | 31.624018 |
| 36.604481 | 29.653494 | 36.329483 |
| 40.258160 | 27.161005 | 34.187584 |
| 40.657902 | 31.711082 | 33.537971 |
| 43.632610 | 28.509775 | 31.624846 |
| 44.845085 | 26.973333 | 38.480274 |

24 generated by VMD

| Column 1 | Column 2 | Column 3 |
|---------|---------|---------|
| 24.918806 | 30.098997 | 32.416111 |
| 26.569584 | 31.105980 | 36.059742 |
| 30.258427 | 27.903563 | 35.643070 |
| 30.242800 | 32.930107 | 33.543587 |
| 33.325954 | 29.533720 | 31.351013 |
| 33.296722 | 30.122112 | 35.309811 |
| 36.825523 | 26.588493 | 34.265472 |
| 36.677357 | 31.240540 | 33.510490 |
| 40.132160 | 29.373852 | 31.538685 |
| 39.800949 | 30.016127 | 36.689114 |
| 45.571148 | 26.901621 | 33.473969 |
| 42.880913 | 29.793291 | 34.438316 |
| 27.155659 | 27.571085 | 36.238525 |
| 27.065680 | 33.993031 | 34.127678 |
| 30.389526 | 29.842642 | 32.734802 |
| 29.987532 | 31.146091 | 36.448578 |
| 33.246376 | 27.227598 | 33.976082 |
| 33.629429 | 32.497883 | 32.820942 |
| 36.813133 | 28.548187 | 31.569988 |
| 36.625515 | 29.320124 | 36.172104 |
| 40.207569 | 27.228745 | 34.175186 |
| 40.515976 | 31.722523 | 33.638050 |
| 43.615749 | 28.425413 | 31.483082 |
| 44.681469 | 27.259701 | 38.406303 |

24 generated by VMD

| Column 1 | Column 2 | Column 3 |
|---------|---------|---------|
| 25.127550 | 30.024769 | 32.344883 |
| 26.688129 | 30.888435 | 35.943954 |
| 30.426258 | 28.004322 | 35.572803 |
| 30.253363 | 32.738003 | 33.428474 |
| 33.453110 | 29.362982 | 31.285570 |
| 33.401424 | 30.231363 | 35.153824 |
| 36.698261 | 26.792999 | 34.295940 |
| 36.803459 | 31.184816 | 33.865997 |
Ca 39.924145 29.521172 31.593128
Ca 39.791252 30.166351 34.53655
Ca 45.106491 26.512480 33.362030
Ca 42.747707 29.773991 34.453655
S 27.353947 27.608932 36.278015
S 27.170471 33.908260 34.657360
S 30.473848 26.512480 33.362030
S 40.029343 27.336422 34.396156
S 30.190826 31.212341 36.319649
S 33.443947 27.317505 33.925781
S 33.777832 32.454742 32.537426
S 36.662891 28.450214 31.520493
S 36.531551 29.451342 36.409771
S 40.029343 27.336422 34.396156
S 40.396172 31.873432 37.13692
S 43.336777 28.558935 31.497995
S 44.645153 27.263622 38.312191

24

generated by VMD
Ca 24.849213 29.934845 32.291920
Ca 26.446981 30.760172 36.068024
Ca 30.215002 28.141964 35.812523
Ca 30.209568 29.763535 33.295776
Ca 33.429469 29.599422 31.313530
Ca 33.257637 30.271105 35.274895
Ca 36.786171 26.855312 33.968513
Ca 36.861305 31.298950 33.894089
Ca 40.300583 29.380211 31.421095
Ca 39.799606 30.015095 36.565086
Ca 45.274609 26.178871 33.737293
Ca 43.022758 29.891306 34.240726
S 27.070610 27.376160 36.330921
S 26.983139 34.010070 34.655384
S 30.563446 29.618929 32.680057
S 30.038286 31.352940 36.461430
S 33.391376 27.292593 33.819462
S 33.656834 32.598694 32.602856
S 36.885704 28.785980 31.449327
S 36.433105 29.351784 36.334242
S 40.115616 27.389320 34.220402
S 40.509922 31.875656 33.676254
S 43.679062 28.312368 31.508249
S 44.658401 27.335503 38.400887

24

generated by VMD
Ca 25.171543 29.426720 32.247528
Ca 26.710712 30.867348 36.119827
| Ca   | 30.265642 | 28.027611 | 35.579372 |
|------|-----------|-----------|-----------|
| Ca   | 30.179359 | 32.928635 | 33.299744 |
| Ca   | 33.341240 | 29.744579 | 31.022966 |
| Ca   | 33.417137 | 30.084618 | 35.058277 |
| Ca   | 36.700077 | 26.928637 | 34.213318 |
| Ca   | 36.758175 | 32.928635 | 33.299744 |
| Ca   | 40.005341 | 29.391909 | 31.871664 |
| Ca   | 39.828297 | 30.145584 | 36.638329 |
| Ca   | 45.143517 | 26.301178 | 33.349262 |
| Ca   | 43.018867 | 29.766272 | 34.620892 |
| S    | 27.193478 | 27.576702 | 36.491066 |
| S    | 27.033958 | 33.944946 | 34.714401 |
| S    | 30.450463 | 29.882963 | 32.569080 |
| S    | 30.263489 | 31.213154 | 36.395264 |
| S    | 33.334915 | 27.259665 | 33.737373 |
| S    | 33.652416 | 32.653210 | 32.607174 |
| S    | 36.642731 | 28.663025 | 31.436901 |
| S    | 36.531803 | 29.563400 | 36.424671 |
| S    | 40.071621 | 27.279251 | 34.383739 |
| S    | 40.499733 | 31.773296 | 33.774124 |
| S    | 43.546516 | 28.624815 | 31.549339 |
| S    | 44.669338 | 26.998995 | 38.205891 |

24 generated by VMD

| Ca   | 24.947281 | 29.723555 | 31.840908 |
|------|-----------|-----------|-----------|
| Ca   | 26.208324 | 30.767269 | 35.818047 |
| Ca   | 30.009682 | 28.024803 | 35.675747 |
| Ca   | 30.179041 | 32.950836 | 33.288223 |
| Ca   | 33.536453 | 29.566341 | 31.543541 |
| Ca   | 33.238331 | 30.300617 | 35.359840 |
| Ca   | 36.498875 | 26.983166 | 34.435467 |
| Ca   | 36.976669 | 31.171181 | 33.848602 |
| Ca   | 40.290131 | 29.396965 | 31.561771 |
| Ca   | 40.069405 | 29.952690 | 36.519478 |
| Ca   | 45.380409 | 26.559338 | 33.274963 |
| Ca   | 43.012611 | 29.631428 | 34.185181 |
| S    | 26.851112 | 27.500139 | 36.494587 |
| S    | 26.961882 | 33.813374 | 34.512180 |
| S    | 30.614229 | 29.722385 | 32.756165 |
| S    | 29.727608 | 31.231007 | 36.465866 |
| S    | 33.351074 | 27.433622 | 34.072441 |
| S    | 33.632305 | 32.621643 | 32.728966 |
| S    | 36.918644 | 28.670940 | 31.601675 |
| S    | 36.568195 | 29.894894 | 36.649818 |
| S    | 40.115738 | 27.303385 | 34.205490 |
| S    | 40.692673 | 31.790434 | 33.644657 |
|    |    |    |    |
|----|----|----|----|
| S  | 43.742821 | 28.521338 | 31.405727 |
| S  | 44.910370 | 26.860010 | 38.141388 |

24 generated by VMD

|    |    |    |    |
|----|----|----|----|
| Ca | 25.455978 | 29.875910 | 32.169334 |
| Ca | 26.400024 | 31.223125 | 36.020061 |
| Ca | 30.241390 | 27.902124 | 35.724274 |
| Ca | 30.304913 | 32.835106 | 33.334957 |
| Ca | 33.503441 | 29.545338 | 31.135696 |
| Ca | 33.130562 | 30.167675 | 35.332184 |
| Ca | 36.646042 | 26.685837 | 34.151039 |
| Ca | 36.884171 | 31.028280 | 33.804947 |
| Ca | 40.122532 | 29.389832 | 31.614780 |
| Ca | 39.953392 | 29.907511 | 36.666969 |
| Ca | 45.436546 | 26.972233 | 33.346687 |
| Ca | 42.746655 | 29.677090 | 34.377144 |
| S  | 27.147224 | 27.884869 | 36.732002 |
| S  | 27.055450 | 34.054165 | 34.493458 |
| S  | 30.487846 | 29.604113 | 32.859245 |
| S  | 29.967508 | 31.242283 | 36.456810 |
| S  | 33.412468 | 27.178173 | 33.735470 |
| S  | 33.516304 | 32.392643 | 32.605747 |
| S  | 36.897747 | 28.506594 | 31.387489 |
| S  | 36.383308 | 29.307215 | 36.289021 |
| S  | 39.991337 | 27.216747 | 34.166744 |
| S  | 40.546761 | 31.803944 | 33.687050 |
| S  | 43.633408 | 28.792048 | 31.409174 |
| S  | 44.568913 | 27.198582 | 38.530334 |

24 generated by VMD

|    |    |    |    |
|----|----|----|----|
| Ca | 25.016142 | 29.851997 | 32.361851 |
| Ca | 26.388580 | 31.066813 | 35.901260 |
| Ca | 30.081615 | 28.057205 | 35.684475 |
| Ca | 30.209564 | 32.726482 | 33.562893 |
| Ca | 33.465065 | 29.673532 | 31.310570 |
| Ca | 33.076340 | 30.178871 | 35.245560 |
| Ca | 36.768852 | 26.867622 | 34.375351 |
| Ca | 36.704849 | 31.120888 | 33.697716 |
| Ca | 40.158001 | 29.482262 | 31.589260 |
| Ca | 40.004299 | 29.900139 | 36.329510 |
| Ca | 45.486961 | 26.690659 | 33.323952 |
| Ca | 43.084164 | 29.760525 | 34.388386 |
| S  | 26.757828 | 27.627995 | 36.313652 |
| S  | 26.907413 | 33.994377 | 34.330551 |
| S  | 30.472267 | 29.606979 | 32.721321 |
| S  | 29.920326 | 31.139816 | 36.501228 |
S  33.497093  27.339771  34.068779
S  33.561161  32.590244  32.589027
S  36.891273  28.837654  31.461864
S  36.530609  29.571074  36.410416
S  40.234085  27.033186  34.125519
S  40.675930  31.628563  33.812550
S  43.651051  28.510448  31.429581
S  44.890411  27.134331  38.495480
24

generated by VMD

Ca  25.195110  29.718060  32.225479
Ca  26.584301  30.935169  35.846729
Ca  30.389881  28.137579  35.800037
Ca  30.239365  32.945835  33.260536
Ca  33.231743  29.578846  31.164818
Ca  33.431381  30.360596  34.940048
Ca  36.625835  26.799547  34.391552
Ca  36.900959  31.178556  33.902405
Ca  39.850540  29.380177  31.802627
Ca  39.675468  29.463839  36.646961
Ca  45.917213  27.345165  33.109158
Ca  42.926361  29.518764  34.503506
S  27.287003  27.702824  36.586201
S  26.742107  34.008373  34.311920
S  30.531219  29.759415  32.776058
S  30.271576  31.328857  36.440098
S  33.353001  27.329771  33.892681
S  33.622040  32.653358  32.305309
S  36.644615  28.561651  31.768995
S  36.270435  29.406666  36.441711
S  40.167946  26.970953  34.267570
S  40.389595  31.628046  34.072140
S  43.410896  28.841951  31.482086
S  44.775295  26.837418  38.092388
24

generated by VMD

Ca  25.025845  29.731989  32.380070
Ca  26.430084  31.268602  36.102562
Ca  30.112869  27.809898  35.527359
Ca  30.124790  32.959724  33.269955
Ca  33.400528  29.519989  31.516893
Ca  33.200199  30.123220  35.295929
Ca  36.635361  26.828695  34.393131
Ca  36.629505  31.269028  33.764500
Ca  40.017414  29.522533  31.810923
Ca  39.693417  29.793304  36.495510
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 45.874577    | 27.219143    | 33.442009    |
| Ca      | 43.029411    | 29.529409    | 34.213898    |
| S       | 27.052971    | 27.716408    | 36.460686    |
| S       | 30.370403    | 29.715601    | 32.704166    |
| S       | 30.041172    | 31.214317    | 36.26515     |
| S       | 33.22711     | 27.160614    | 34.028725    |
| S       | 33.591824    | 32.481495    | 32.500767    |
| S       | 36.860485    | 28.689030    | 31.459406    |
| S       | 36.392990    | 29.497936    | 36.378868    |
| S       | 40.173645    | 27.217512    | 34.132946    |
| S       | 40.510101    | 31.809376    | 34.073074    |
| S       | 43.853485    | 28.636772    | 31.416494    |
| S       | 45.102303    | 26.588675    | 38.061203    |

24 generated by VMD

| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 24.841949    | 29.617920    | 32.339489    |
| Ca      | 26.420937    | 30.997046    | 35.941223    |
| Ca      | 30.460531    | 28.000881    | 35.890949    |
| Ca      | 29.979733    | 33.039616    | 33.174362    |
| Ca      | 33.325905    | 29.540184    | 31.461304    |
| Ca      | 33.329994    | 30.313799    | 35.130264    |
| Ca      | 36.772072    | 26.871571    | 34.396378    |
| Ca      | 36.836544    | 31.247709    | 33.785439    |
| Ca      | 39.983410    | 29.529034    | 31.582890    |
| Ca      | 39.868855    | 29.753035    | 36.745419    |
| Ca      | 45.930656    | 27.097643    | 33.215881    |
| Ca      | 42.928242    | 29.469112    | 34.545387    |
| S       | 26.998852    | 27.481901    | 36.366329    |
| S       | 26.907368    | 34.033520    | 34.364220    |
| S       | 30.459236    | 29.745327    | 32.745571    |
| S       | 29.907978    | 31.410393    | 36.170650    |
| S       | 33.479523    | 27.304375    | 33.958252    |
| S       | 33.604588    | 32.657772    | 32.445538    |
| S       | 36.807274    | 28.691116    | 31.694523    |
| S       | 36.480663    | 29.569950    | 36.334385    |
| S       | 40.157623    | 27.149775    | 34.106674    |
| S       | 40.523750    | 31.775806    | 34.032722    |
| S       | 43.610760    | 28.549131    | 31.515097    |
| S       | 44.817505    | 26.544800    | 38.087814    |

24 generated by VMD

| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.143917    | 29.488895    | 32.089523    |
| Ca      | 26.371258    | 31.035311    | 35.796722    |
| Ca      | 30.079693    | 28.036417    | 35.791637    |
| Ca      | 30.273407    | 32.795933    | 33.182190    |
|   |   |   |   |
|---|---|---|---|
| Ca | 33.327087 | 29.571363 | 31.398222 |
| Ca | 33.386635 | 30.244698 | 35.362400 |
| Ca | 36.975578 | 31.510775 | 34.059246 |
| Ca | 39.004827 | 29.576637 | 31.882053 |
| Ca | 39.854984 | 29.701092 | 36.526104 |
| Ca | 45.599800 | 27.164627 | 33.270058 |
| Ca | 42.892765 | 29.490551 | 34.295628 |
| S  | 27.031265 | 27.680424 | 36.504990 |
| S  | 27.173098 | 33.963753 | 34.204494 |
| S  | 30.343784 | 29.558632 | 32.709290 |
| S  | 29.823753 | 31.287479 | 36.169529 |
| S  | 33.259075 | 27.417940 | 34.079758 |
| S  | 33.645252 | 32.660732 | 32.848839 |
| S  | 36.642635 | 28.924160 | 31.651745 |
| S  | 36.604294 | 29.388250 | 36.450546 |
| S  | 40.053562 | 27.143938 | 34.029156 |
| S  | 40.766766 | 31.837929 | 33.965668 |
| S  | 43.448391 | 28.336660 | 31.404558 |
| S  | 45.232121 | 26.868721 | 38.127274 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 25.018591 | 29.949060 | 32.033768 |
| Ca | 26.358570 | 30.900360 | 35.870899 |
| Ca | 29.983631 | 28.384525 | 35.711796 |
| Ca | 30.178003 | 32.834595 | 33.210014 |
| Ca | 33.272362 | 29.224798 | 31.524734 |
| Ca | 33.188774 | 30.098429 | 35.373352 |
| Ca | 36.512302 | 26.819073 | 34.406837 |
| Ca | 36.915161 | 31.339655 | 33.929111 |
| Ca | 40.150066 | 29.447847 | 31.658195 |
| Ca | 40.272606 | 29.748043 | 36.628487 |
| Ca | 45.869804 | 27.137249 | 33.427753 |
| Ca | 43.009239 | 29.732979 | 34.149773 |
| S  | 26.677616 | 27.608759 | 36.055206 |
| S  | 26.831795 | 34.008774 | 34.357967 |
| S  | 30.314255 | 29.621025 | 32.828560 |
| S  | 29.830263 | 31.506058 | 36.566986 |
| S  | 33.084824 | 27.157318 | 34.127392 |
| S  | 33.605381 | 32.353895 | 32.568092 |
| S  | 36.849785 | 28.723225 | 31.873245 |
| S  | 36.601967 | 29.513611 | 36.555523 |
| S  | 40.231522 | 27.219757 | 34.092300 |
| S  | 40.608093 | 31.802277 | 33.738411 |
| S  | 43.765499 | 28.450130 | 31.361034 |
| S  | 45.303799 | 26.805447 | 37.981266 |
| 24 | generated by VMD |
|----|------------------|
| Ca | 25.435696       |
| Ca | 26.513615       |
| Ca | 30.246824       |
| Ca | 30.436913       |
| Ca | 33.290306       |
| Ca | 33.228855       |
| Ca | 36.607826       |
| Ca | 36.889103       |
| Ca | 39.767975       |
| Ca | 39.857338       |
| Ca | 45.882423       |
| Ca | 42.931393       |
| S  | 27.008631       |
| S  | 27.210327       |
| S  | 30.472008       |
| S  | 29.909698       |
| S  | 33.220028       |
| S  | 33.712593       |
| S  | 36.573227       |
| S  | 36.220547       |
| S  | 40.133640       |
| S  | 40.470959       |
| S  | 43.383121       |
| S  | 45.030823       |
| Ca | 25.295326       |
| Ca | 26.384022       |
| Ca | 30.140373       |
| Ca | 30.419533       |
| Ca | 33.253822       |
| Ca | 33.165943       |
| Ca | 36.734085       |
| Ca | 36.815884       |
| Ca | 39.843449       |
| Ca | 39.882397       |
| Ca | 45.895832       |
| Ca | 42.918442       |
| S  | 26.803137       |
| S  | 27.240517       |
| S  | 30.421543       |
| S  | 29.884830       |
| S  | 33.147079       |
| S  | 33.759651       |

| 24 | generated by VMD |
|----|------------------|
| Ca | 26.513615       |
| Ca | 30.246824       |
| Ca | 30.436913       |
| Ca | 33.290306       |
| Ca | 33.228855       |
| Ca | 36.607826       |
| Ca | 36.889103       |
| Ca | 39.767975       |
| Ca | 39.857338       |
| Ca | 45.882423       |
| Ca | 42.931393       |
| S  | 27.008631       |
| S  | 27.210327       |
| S  | 30.472008       |
| S  | 29.909698       |
| S  | 33.220028       |
| S  | 33.712593       |
| S  | 36.573227       |
| S  | 36.220547       |
| S  | 40.133640       |
| S  | 40.470959       |
| S  | 43.383121       |
| S  | 45.030823       |

866
S  36.530899  28.400858  31.826893
S  36.482796  29.320427  36.480171
S  40.190121  27.082481  34.320328
S  40.462154  31.672146  33.768173
S  43.554024  28.560352  31.294518
S  45.208050  27.227955  37.726994

24 generated by VMD

Ca  25.138889  30.222965  31.933218
Ca  26.268814  31.011990  35.802071
Ca  30.120770  28.041346  35.760735
Ca  30.287527  32.777012  33.393330
Ca  33.355972  29.318012  31.255192
Ca  33.086029  30.333429  35.337582
Ca  36.641479  26.792404  34.551453
Ca  36.893147  31.155071  33.917233
Ca  39.893425  29.063026  31.908728
Ca  39.786682  29.880716  36.570114
Ca  45.924664  27.601768  32.949753
Ca  43.094078  29.748436  34.362770
S  26.801758  27.729435  36.215611
S  26.933342  34.162724  34.449364
S  30.459974  29.682451  32.634880
S  29.875305  31.274479  36.390537
S  33.236851  27.328838  34.243782
S  33.690556  32.358299  32.462357
S  36.680328  28.321665  31.729567
S  36.263153  29.427330  36.513004
S  40.371601  26.965744  34.329849
S  40.517956  31.584431  33.989845
S  43.485176  28.710781  31.378771
S  45.626312  26.899067  37.951084

24 generated by VMD

Ca  24.997477  29.881149  31.868683
Ca  26.354134  30.886185  35.693493
Ca  30.280598  27.946589  35.708427
Ca  30.152822  32.890011  33.343456
Ca  33.553139  29.614353  31.730984
Ca  33.277046  30.195446  35.518719
Ca  36.649139  26.701595  34.703396
Ca  36.828411  31.210176  33.703838
Ca  40.028416  29.344282  31.606556
Ca  39.956062  29.973021  36.789387
Ca  45.656807  27.312244  33.144249
Ca  42.877796  29.541910  34.150330
S  26.825932  27.534739  36.188465
S  27.023897  34.061195  34.085270
S  30.600014  29.780048  32.809467
S  29.766769  31.302048  36.306541
S  33.275852  27.304945  34.226292
S  33.544041  32.630093  32.781780
S  36.846596  28.567736  31.870865
S  36.581707  29.724255  36.510334
S  40.050404  27.086315  34.345707
S  40.504768  31.705128  33.832634
S  43.393669  28.484756  31.344154
S  45.408363  26.713207  37.767715

24

24

generated by VMD

Ca  25.298689  29.898808  32.016277
Ca  26.458553  31.383005  35.891006
Ca  30.223814  27.934387  35.900963
Ca  30.149797  32.652210  33.238949
Ca  33.576427  29.334717  31.321522
Ca  33.224358  30.108011  35.404907
Ca  36.556221  26.863081  34.637375
Ca  36.699486  31.192198  33.947720
Ca  39.904106  29.404045  31.905485
Ca  39.730827  29.576498  36.534084
Ca  45.923462  27.387999  32.829754
Ca  42.982502  29.659203  34.484997
S  26.819195  27.832901  36.193024
S  27.070404  34.298325  34.234684
S  30.512613  29.467550  32.800117
S  29.928902  31.403542  36.373322
S  33.313988  27.102144  34.204903
S  33.556305  32.328651  32.406826
S  36.869530  28.544495  31.526711
S  36.273338  29.491402  36.584972
S  40.134087  27.115690  34.052956
S  40.404991  31.723824  34.264397
S  43.485477  28.839336  31.458803
S  45.336739  26.849365  37.816986

24

generated by VMD

Ca  25.232096  29.913074  31.839745
Ca  26.440203  31.126320  35.783321
Ca  30.022270  28.102978  35.834629
Ca  30.258602  32.640835  33.463730
Ca  33.366287  29.015078  31.508717
Ca  33.306137  30.331837  35.402302
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 36.405979 | 27.128849 | 34.454006 |
| Ca      | 37.027416 | 31.388710 | 34.083000 |
| Ca      | 40.157162 | 29.635763 | 31.741791 |
| Ca      | 39.951294 | 29.633911 | 36.454807 |
| Ca      | 45.689537 | 26.912231 | 33.101093 |
| Ca      | 43.236160 | 29.702398 | 34.397179 |
| S       | 26.628204 | 27.648428 | 36.303345 |
| S       | 27.138519 | 34.041279 | 34.041409 |
| S       | 30.250816 | 29.510281 | 32.752728 |
| S       | 29.881268 | 31.251572 | 36.526126 |
| S       | 33.213924 | 27.325453 | 34.341480 |
| S       | 33.545162 | 32.120483 | 32.562656 |
| S       | 36.656872 | 28.657804 | 31.653545 |
| S       | 36.443153 | 29.643661 | 36.614956 |
| S       | 40.079315 | 27.272652 | 34.092411 |
| S       | 40.676273 | 31.822277 | 33.962925 |
| S       | 43.712978 | 28.800909 | 31.196087 |
| S       | 45.114288 | 26.764603 | 37.919209 |

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Generated by VMD
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.207163  | 29.877575  | 31.936132  |
| Ca      | 26.334509  | 31.109365  | 35.879795  |
| Ca      | 30.082085  | 28.026543  | 35.828327  |
| Ca      | 30.103333  | 32.993343  | 33.074188  |
| Ca      | 33.383686  | 29.202641  | 31.506588  |
| Ca      | 33.212795  | 31.109365  | 35.879795  |
| Ca      | 36.717419  | 26.937046  | 34.499874  |
| Ca      | 36.831913  | 31.237192  | 33.969013  |
| Ca      | 40.139130  | 29.501223  | 31.882267  |
| Ca      | 39.962906  | 29.704163  | 36.777557  |
| Ca      | 45.830040  | 27.187853  | 33.100288  |
| Ca      | 43.034958  | 29.569433  | 34.300739  |
| S       | 26.774092  | 27.651699  | 36.098057  |
| S       | 26.909874  | 34.128746  | 34.383907  |
| S       | 30.470392  | 29.591337  | 32.968018  |
| S       | 29.772999  | 31.393816  | 36.171314  |
| S       | 33.315483  | 27.257530  | 34.323929  |
| S       | 33.456230  | 32.292957  | 32.539600  |
| S       | 36.826042  | 28.619488  | 31.612516  |
| S       | 36.589436  | 29.605230  | 36.619980  |
| S       | 40.121895  | 27.164740  | 34.120857  |
| S       | 40.577656  | 31.715097  | 33.977814  |
| S       | 43.508453  | 28.676373  | 31.245277  |
| S       | 45.271404  | 26.728668  | 37.803238  |

generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.252089  | 29.653938  | 32.148613  |
| Ca      | 26.252701  | 31.195843  | 35.986774  |
| Ca      | 30.159575  | 27.889847  | 35.763855  |
| Ca      | 30.120651  | 32.764809  | 33.338936  |
| Ca      | 33.458248  | 29.192356  | 31.309830  |
| Ca      | 33.339916  | 30.258711  | 35.279579  |
| Ca      | 36.609169  | 26.972570  | 34.244843  |
| Ca      | 36.797424  | 31.391832  | 33.868042  |
| Ca      | 40.225952  | 29.586658  | 31.469166  |
| Ca      | 39.896786  | 29.769306  | 36.748932  |
| Ca      | 45.574604  | 27.181753  | 33.409317  |
| Ca      | 42.850845  | 29.539314  | 34.493671  |
| S       | 26.904633  | 27.715439  | 36.518230  |
| S       | 26.988483  | 34.280334  | 34.372223  |
| S       | 30.459053  | 29.536764  | 32.781067  |
| S       | 29.888847  | 31.173370  | 36.372517  |
| S       | 33.373894  | 27.249104  | 34.103058  |
| S       | 33.839466  | 32.430973  | 32.351238  |
| S       | 36.876129  | 28.797264  | 31.447048  |
| S       | 36.494816  | 29.512400  | 36.493683  |
S  40.011234  27.325209  34.160660
S  40.496643  31.779394  34.019753
S  43.537712  28.644991  31.415644
S  45.025009  26.549191  37.934059

24
generated by VMD
Ca  25.196299  29.519855  32.354607
Ca  26.595295  31.171497  35.925884
Ca  30.269917  28.088264  35.858425
Ca  30.229683  32.435764  33.240700
Ca  33.368759  29.462875  31.217865
Ca  33.214386  30.510019  35.386745
Ca  36.552345  26.952560  34.076134
Ca  36.743134  31.308254  33.769165
Ca  40.154999  29.662127  31.619440
Ca  39.639435  29.643232  36.497684
Ca  45.871925  27.149181  33.498833
Ca  42.793594  29.442610  34.518311
S  27.149143  27.769608  36.583565
S  27.250883  34.200012  34.456673
S  30.499325  29.471470  32.690742
S  30.024817  31.210045  36.503735
S  33.298710  27.348248  33.924362
S  33.568329  32.498802  32.447803
S  36.649879  28.807056  31.345957
S  36.358196  29.481529  36.268021
S  39.970146  27.119152  33.978401
S  40.445499  31.839775  33.991886
S  43.779633  28.732643  31.650890
S  44.809555  26.567732  38.224831

24
generated by VMD
Ca  25.033207  29.050308  32.168777
Ca  26.553473  30.971731  35.858883
Ca  30.208942  28.114773  35.758778
Ca  30.334211  32.805012  33.401569
Ca  33.605148  29.810844  31.371164
Ca  33.254932  30.440529  35.315952
Ca  36.495388  27.021366  33.960117
Ca  36.946850  31.365971  33.732338
Ca  40.154766  29.546450  31.557173
Ca  39.782696  29.667257  36.541454
Ca  45.802258  27.200134  33.464985
Ca  42.800083  29.413120  34.373375
S  27.247133  27.497292  36.774269
S  26.918133  33.904476  34.493031
|     | 30.486172 | 29.722860 | 32.665466 |
|-----|-----------|-----------|-----------|
| S   | 29.955841 | 31.436195 | 36.454811 |
| S   | 33.190849 | 27.567009 | 34.041222 |
| S   | 33.821899 | 32.723438 | 32.596462 |
| S   | 36.799816 | 28.836235 | 31.403194 |
| S   | 36.379997 | 29.452715 | 36.285118 |
| S   | 39.969872 | 27.279484 | 34.057751 |
| S   | 40.579609 | 31.830193 | 33.838001 |
| S   | 43.647129 | 28.324692 | 31.524780 |
| S   | 44.465469 | 26.409254 | 38.392078 |

generated by VMD

|     | 25.270596 | 29.527964 | 32.336056 |
|-----|-----------|-----------|-----------|
| Ca  | 25.038353 | 29.741371 | 32.325386 |
| Ca  | 26.261215 | 31.067841 | 36.051331 |
| Ca  | 30.223892 | 27.896980 | 35.638382 |
| Ca  | 30.227032 | 32.927773 | 33.067589 |
| Ca  | 33.312862 | 29.455675 | 31.345583 |
| Ca  | 33.174145 | 30.324348 | 35.353123 |
| Ca  | 36.769783 | 26.870058 | 34.166618 |
| Ca  | 36.780754 | 31.355759 | 33.802086 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 40.085258 | 29.610653 | 31.481819 |
| Ca      | 39.770565 | 29.846451 | 36.564682 |
| Ca      | 45.752392 | 26.979925 | 33.178616 |
| Ca      | 42.928715 | 29.512094 | 34.612949 |
| S       | 27.181063 | 27.488144 | 36.473862 |
| S       | 27.056946 | 33.977188 | 34.533424 |
| S       | 30.540833 | 29.775309 | 32.652031 |
| S       | 29.866732 | 31.310083 | 36.277485 |
| S       | 33.375763 | 27.427950 | 34.064064 |
| S       | 33.733578 | 32.419315 | 32.524456 |
| S       | 36.649117 | 28.823866 | 31.611729 |
| S       | 36.417210 | 29.558315 | 36.381199 |
| S       | 40.138351 | 27.097553 | 34.104683 |
| S       | 40.525974 | 31.629398 | 33.856030 |
| S       | 43.620903 | 28.469639 | 31.613560 |
| S       | 45.002422 | 26.825726 | 38.349995 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.003471 | 29.767662 | 32.613586 |
| Ca      | 26.474695 | 30.960917 | 36.095211 |
| Ca      | 30.254705 | 28.132740 | 35.742546 |
| Ca      | 30.156231 | 32.833706 | 32.992477 |
| Ca      | 33.446480 | 29.539482 | 31.444981 |
| Ca      | 33.363705 | 30.322191 | 35.306541 |
| Ca      | 36.517166 | 26.877741 | 34.176220 |
| Ca      | 36.825699 | 31.238457 | 33.893986 |
| Ca      | 40.021473 | 29.452017 | 31.582268 |
| Ca      | 39.813786 | 29.860090 | 36.414715 |
| Ca      | 45.694782 | 27.066124 | 33.492081 |
| Ca      | 43.083229 | 29.596548 | 34.455482 |
| S       | 27.043030 | 27.403582 | 36.341564 |
| S       | 27.167978 | 33.914066 | 34.304249 |
| S       | 30.413429 | 29.548513 | 32.655575 |
| S       | 29.984228 | 31.279882 | 36.287991 |
| S       | 33.244362 | 27.384396 | 34.037495 |
| S       | 33.659134 | 32.611809 | 32.715454 |
| S       | 36.694653 | 28.818405 | 31.406635 |
| S       | 36.500229 | 29.515987 | 36.323681 |
| S       | 40.019051 | 27.251659 | 33.999184 |
| S       | 40.754166 | 31.828411 | 33.828266 |
| S       | 43.686333 | 28.575462 | 31.644735 |
| S       | 44.611954 | 26.611605 | 38.275826 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.085434 | 30.005302 | 32.533161 |
| Ca      | 26.473885 | 30.996025 | 36.168243 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 30.075184 | 27.956837 | 35.662933 |
| Ca      | 30.560566 | 32.921684 | 33.193169 |
| Ca      | 33.184669 | 29.282063 | 31.354286 |
| Ca      | 33.186672 | 30.222006 | 35.137058 |
| Ca      | 36.508362 | 26.796513 | 33.935886 |
| Ca      | 36.838226 | 31.233286 | 33.846638 |
| Ca      | 40.317696 | 29.612661 | 31.296082 |
| Ca      | 39.849266 | 29.935610 | 36.447762 |
| Ca      | 45.697891 | 26.989925 | 33.819969 |
| Ca      | 42.770782 | 29.746336 | 34.452560 |
| S       | 26.886253 | 27.537199 | 36.589439 |
| S       | 27.510582 | 33.851208 | 34.494110 |
| S       | 30.238724 | 29.622646 | 32.668449 |
| S       | 30.257580 | 31.221169 | 36.360142 |
| S       | 33.221146 | 27.324886 | 34.063160 |
| S       | 33.745018 | 32.416420 | 32.443394 |
| S       | 36.709488 | 28.836458 | 31.369111 |
| S       | 36.388027 | 29.117521 | 36.335445 |
| S       | 40.014587 | 27.272366 | 33.935738 |
| S       | 40.625835 | 31.905542 | 33.741947 |
| S       | 43.690777 | 28.477417 | 31.715168 |
| S       | 44.597248 | 27.110260 | 38.472023 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 24.708752 | 30.010130 | 32.390579 |
| Ca      | 26.337305 | 30.868319 | 35.870770 |
| Ca      | 29.992313 | 27.990484 | 35.776218 |
| Ca      | 30.345110 | 33.034389 | 33.174545 |
| Ca      | 33.498329 | 29.287350 | 31.395504 |
| Ca      | 33.136070 | 30.532553 | 35.350246 |
| Ca      | 36.491615 | 27.043377 | 34.453884 |
| Ca      | 36.883080 | 31.193981 | 33.992886 |
| Ca      | 40.203430 | 29.427921 | 31.421896 |
| Ca      | 40.018158 | 29.665833 | 36.548878 |
| Ca      | 45.634590 | 27.128929 | 33.506317 |
| Ca      | 42.796448 | 29.542618 | 34.225430 |
| S       | 26.966347 | 27.522724 | 36.282158 |
| S       | 27.110886 | 33.774887 | 34.501896 |
| S       | 30.621542 | 29.703257 | 32.687077 |
| S       | 29.909126 | 31.285421 | 36.316799 |
| S       | 33.185341 | 27.151054 | 34.163738 |
| S       | 33.777821 | 32.457718 | 32.461990 |
| S       | 36.869240 | 28.529228 | 31.630112 |
| S       | 36.491692 | 29.663877 | 36.583427 |
| S       | 40.098476 | 27.194517 | 34.067593 |
| S       | 40.603638 | 31.808800 | 33.638542 |
|   | X   | Y   | Z   |
|---|-----|-----|-----|
| S | 44.025352 | 28.796034 | 31.275988 |
| S | 44.729244 | 26.777987 | 38.314247 |

24 generated by VMD

|   | X   | Y   | Z   |
|---|-----|-----|-----|
| Ca | 24.866503 | 29.737402 | 32.424355 |
| Ca | 26.443455 | 31.156918 | 35.955841 |
| Ca | 30.234844 | 28.252535 | 35.936649 |
| Ca | 30.411598 | 32.800667 | 33.444492 |
| Ca | 33.469269 | 29.352680 | 31.163525 |
| Ca | 33.200142 | 30.252035 | 35.237785 |
| Ca | 36.538719 | 26.742720 | 34.196281 |
| Ca | 36.799248 | 31.128754 | 33.725403 |
| Ca | 40.160648 | 29.572292 | 31.620926 |
| Ca | 39.796722 | 29.748367 | 36.690269 |
| Ca | 45.676537 | 27.212593 | 33.590777 |
| Ca | 42.763546 | 29.636683 | 34.487198 |
| S  | 27.048702 | 27.691025 | 36.379078 |
| S  | 27.160084 | 34.042625 | 34.309193 |
| S  | 30.603373 | 29.590206 | 32.780262 |
| S  | 29.889278 | 31.328493 | 36.484364 |
| S  | 33.278107 | 27.130318 | 33.892166 |
| S  | 33.752224 | 32.489838 | 32.389244 |
| S  | 36.899357 | 28.731750 | 31.382233 |
| S  | 36.293022 | 29.294823 | 36.331726 |
| S  | 39.988140 | 27.175798 | 34.159817 |
| S  | 40.412224 | 31.652100 | 33.917419 |
| S  | 43.713348 | 28.746244 | 31.495781 |
| S  | 45.034828 | 26.924538 | 38.267570 |

24 generated by VMD

|   | X   | Y   | Z   |
|---|-----|-----|-----|
| Ca | 25.139648 | 29.939743 | 32.199993 |
| Ca | 26.635735 | 31.082993 | 35.985287 |
| Ca | 30.255230 | 27.918427 | 35.842812 |
| Ca | 30.463013 | 32.695080 | 33.219376 |
| Ca | 33.414719 | 29.434042 | 31.504551 |
| Ca | 33.158440 | 30.315798 | 35.274811 |
| Ca | 36.643761 | 26.863861 | 34.462364 |
| Ca | 36.971420 | 31.073622 | 33.747444 |
| Ca | 40.012512 | 29.624781 | 31.545944 |
| Ca | 39.744896 | 30.168743 | 36.696583 |
| Ca | 45.423912 | 26.965939 | 33.213020 |
| Ca | 42.947281 | 29.705338 | 34.554901 |
| S  | 27.076767 | 27.584042 | 36.239670 |
| S  | 27.125956 | 33.900787 | 34.388283 |
| S  | 30.448826 | 29.528980 | 32.760719 |
| S  | 30.029686 | 31.248352 | 36.361145 |
|   |   |   |
|---|---|---|
| S | 33.207119 | 27.256506 | 34.098442 |
| S | 33.862175 | 32.381042 | 32.504124 |
| S | 36.686375 | 28.550774 | 31.562326 |
| S | 36.456120 | 29.620022 | 36.318012 |
| S | 40.094368 | 27.372084 | 34.160336 |
| S | 40.541504 | 31.785503 | 33.721481 |
| S | 43.434425 | 28.745747 | 31.570112 |
| S | 44.660049 | 26.629210 | 38.098976 |

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generated by VMD

| Ca | 24.988150 | 29.470650 | 32.480186 |
| Ca | 26.492233 | 31.386044 | 36.202332 |
| Ca | 30.180141 | 28.000683 | 35.614220 |
| Ca | 30.076717 | 33.003063 | 33.109142 |
| Ca | 33.307297 | 29.414753 | 31.307240 |
| Ca | 33.256401 | 30.005705 | 35.207817 |
| Ca | 36.608437 | 26.756042 | 34.090462 |
| Ca | 36.898033 | 31.126564 | 34.032410 |
| Ca | 40.217850 | 29.526009 | 31.425213 |
| Ca | 40.010250 | 29.802425 | 36.785103 |
| Ca | 45.560356 | 27.164816 | 33.349514 |
| Ca | 42.928200 | 29.746367 | 34.682358 |
| S | 27.272032 | 27.880798 | 36.634655 |
| S | 26.884768 | 34.133859 | 34.284943 |
| S | 30.531265 | 29.645737 | 32.644157 |
| S | 30.029816 | 31.266212 | 36.236111 |
| S | 33.280071 | 27.076717 | 33.886761 |
| S | 33.656868 | 32.464386 | 32.516216 |
| S | 36.708614 | 28.838493 | 31.449768 |
| S | 36.446163 | 29.225216 | 36.321411 |
| S | 40.168518 | 27.326195 | 34.127808 |
| S | 40.639458 | 31.754356 | 33.843975 |
| S | 43.569069 | 28.730862 | 31.563656 |
| S | 44.723156 | 26.638988 | 38.236168 |

24

generated by VMD

| Ca | 24.984406 | 29.740627 | 32.494522 |
| Ca | 26.515345 | 30.720217 | 35.927555 |
| Ca | 30.345528 | 28.167810 | 35.802612 |
| Ca | 30.319006 | 33.124954 | 33.216251 |
| Ca | 33.327530 | 29.242081 | 31.319874 |
| Ca | 33.174446 | 30.520081 | 35.245232 |
| Ca | 36.585045 | 26.639086 | 34.124435 |
| Ca | 36.713814 | 31.494793 | 33.762287 |
| Ca | 39.937138 | 29.664679 | 31.784601 |
| Ca | 39.838787 | 29.663269 | 36.585941 |
|  | Ca        |  | S        |  |  |  |
|---|---|---|---|---|---|---|
|   | 45.659489 | 27.324207 | 33.576935 |   |   |   |
|   | 42.892483 | 29.451366 | 34.544098 |   |   |   |
|   | 27.314682 | 27.367603 | 36.345753 |   |   |   |
|   | 27.027729 | 33.921715 | 34.552391 |   |   |   |
|   | 30.570990 | 29.781834 | 32.708710 |   |   |   |
|   | 29.995316 | 31.530426 | 36.322670 |   |   |   |
|   | 33.277405 | 27.385773 | 34.107300 |   |   |   |
|   | 33.817333 | 32.413311 | 32.362465 |   |   |   |
|   | 36.689480 | 28.680340 | 31.473286 |   |   |   |
|   | 36.467873 | 29.422596 | 36.290119 |   |   |   |
|   | 40.007961 | 27.201780 | 34.006279 |   |   |   |
|   | 40.787285 | 31.710306 | 33.895058 |   |   |   |
|   | 43.616001 | 28.508675 | 31.318096 |   |   |   |
|   | 44.568851 | 26.713902 | 38.264202 |   |   |   |

24 generated by VMD

|   | Ca        |  | S        |  |  |  |
|---|---|---|---|---|---|---|
|   | 24.827972 | 30.007751 | 32.139526 |   |   |   |
|   | 26.379431 | 31.117287 | 35.816891 |   |   |   |
|   | 30.393887 | 27.984985 | 35.842674 |   |   |   |
|   | 30.192005 | 32.690308 | 33.367432 |   |   |   |
|   | 33.401157 | 29.543633 | 31.322025 |   |   |   |
|   | 33.262508 | 30.183332 | 35.288540 |   |   |   |
|   | 36.677750 | 26.897415 | 34.186180 |   |   |   |
|   | 36.892773 | 31.261137 | 33.965038 |   |   |   |
|   | 40.075962 | 29.428366 | 31.624142 |   |   |   |
|   | 39.719849 | 29.770191 | 36.492336 |   |   |   |
|   | 45.705338 | 27.165251 | 33.236473 |   |   |   |
|   | 43.036282 | 29.639027 | 34.625801 |   |   |   |
|   | 27.280378 | 27.724674 | 36.704247 |   |   |   |
|   | 26.775215 | 34.010986 | 34.020638 |   |   |   |
|   | 30.498180 | 29.640793 | 32.742382 |   |   |   |
|   | 29.935112 | 31.276516 | 36.402184 |   |   |   |
|   | 33.256233 | 27.188044 | 33.965057 |   |   |   |
|   | 33.808987 | 32.537407 | 32.768700 |   |   |   |
|   | 36.692093 | 28.630775 | 31.435160 |   |   |   |
|   | 36.401058 | 29.327213 | 36.384514 |   |   |   |
|   | 40.007183 | 27.098301 | 34.287186 |   |   |   |
|   | 40.726597 | 31.668835 | 33.896515 |   |   |   |
|   | 43.521030 | 28.588566 | 31.388912 |   |   |   |
|   | 44.966805 | 27.010614 | 38.128204 |   |   |   |

24 generated by VMD

|   | Ca        |  | S        |  |  |  |
|---|---|---|---|---|---|---|
|   | 25.116371 | 29.871391 | 32.041718 |   |   |   |
|   | 26.325974 | 31.158506 | 35.585537 |   |   |   |
|   | 30.254669 | 27.989727 | 35.830940 |   |   |   |
|   | 30.174099 | 32.867638 | 33.389797 |   |   |   |
| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 33.486717 | 29.647251 | 31.417780 |
| Ca      | 33.124077 | 30.465309 | 35.477    |
| Ca      | 36.846149 | 26.862738 | 34.753532 |
| Ca      | 36.629036 | 30.745592 | 33.987465 |
| Ca      | 39.997192 | 29.481846 | 31.760296 |
| Ca      | 39.904427 | 29.637115 | 36.532391 |
| Ca      | 45.813614 | 27.297232 | 33.04142  |
| Ca      | 42.717182 | 29.524218 | 34.236542 |
| S       | 27.121777 | 27.656254 | 36.309490 |
| S       | 26.880901 | 34.023285 | 33.843159 |
| S       | 30.645336 | 29.772764 | 32.783756 |
| S       | 29.874130 | 31.110876 | 36.339355 |
| S       | 33.446499 | 27.495193 | 34.286457 |
| S       | 33.719753 | 32.697323 | 32.833263 |
| S       | 36.539989 | 28.402161 | 31.452332 |
| S       | 36.452480 | 29.385078 | 36.739445 |
| S       | 40.179176 | 27.084782 | 34.101284 |
| S       | 40.462269 | 31.654280 | 33.919361 |
| S       | 43.442860 | 28.540657 | 31.316936 |
| S       | 45.279312 | 27.020191 | 37.952255 |

24

*generated by VMD*
| Element | x1 | y1 | z1 |
|---------|----|----|----|
| Ca      | 24.687725 | 29.883663 | 32.249985 |
| Ca      | 26.178207 | 30.831383 | 35.665730 |
| Ca      | 30.184383 | 28.225559 | 35.727848 |
| Ca      | 30.241501 | 32.881248 | 33.404667 |
| Ca      | 33.618797 | 29.861801 | 31.538521 |
| Ca      | 33.295059 | 30.375362 | 35.383949 |
| Ca      | 36.665928 | 27.062777 | 34.579369 |
| Ca      | 36.671665 | 31.022446 | 33.807442 |
| Ca      | 40.027626 | 28.977230 | 31.585014 |
| Ca      | 40.050552 | 29.841160 | 36.423141 |
| Ca      | 45.956764 | 27.449598 | 33.535980 |
| Ca      | 42.788826 | 29.635399 | 34.212685 |
| S       | 27.196724 | 27.390343 | 36.208679 |
| S       | 26.825171 | 33.978992 | 34.190987 |
| S       | 30.614500 | 29.851536 | 32.756569 |
| S       | 29.781200 | 31.255075 | 36.438282 |
| S       | 33.345505 | 27.409626 | 34.002117 |
| S       | 33.730892 | 32.786648 | 32.966923 |
| S       | 36.665009 | 28.641041 | 31.478355 |
| S       | 36.685165 | 29.394035 | 36.623291 |
| S       | 40.098595 | 26.847942 | 34.202736 |
| S       | 40.419273 | 31.492041 | 33.487228 |
| S       | 43.721081 | 28.429100 | 31.435272 |
| S       | 44.983803 | 26.867374 | 38.125973 |

| Element | x2 | y2 | z2 |
|---------|----|----|----|
| Ca      | 24.822414 | 29.957146 | 32.131031 |
| Ca      | 26.325657 | 30.869854 | 35.711861 |
| Ca      | 30.204998 | 28.129139 | 35.906761 |
| Ca      | 30.245567 | 32.859039 | 33.436718 |
| Ca      | 33.377377 | 29.673607 | 31.306845 |
| Ca      | 33.283134 | 30.113804 | 35.463535 |
| Ca      | 36.530113 | 26.916149 | 34.078213 |
| Ca      | 36.819160 | 30.993431 | 33.841816 |
| Ca      | 40.206875 | 29.314110 | 31.565054 |
| Ca      | 39.991508 | 29.858480 | 36.370033 |
| Ca      | 45.902767 | 27.294943 | 33.704628 |
| Ca      | 42.938931 | 29.508497 | 34.269741 |
| S       | 27.005634 | 27.558674 | 36.461285 |
| S       | 26.861500 | 33.979324 | 34.314434 |
| S       | 30.499632 | 29.786940 | 32.775528 |
| S       | 29.950809 | 31.322567 | 36.439705 |
| S       | 33.123360 | 27.353981 | 34.043694 |
| S       | 33.689133 | 32.605579 | 32.669669 |
| Element | First Coordinate | Second Coordinate | Third Coordinate |
|---------|------------------|-------------------|------------------|
| S       | 36.711777        | 28.651796         | 31.583197        |
| S       | 36.439743        | 29.406073         | 36.537899        |
| S       | 40.003429        | 27.202385         | 34.153320        |
| S       | 40.593475        | 31.592745         | 33.543049        |
| S       | 44.710247        | 28.478802         | 31.43067         |
| S       | 45.196655        | 26.964254         | 38.312397        |

24 generated by VMD

| Element | First Coordinate | Second Coordinate | Third Coordinate |
|---------|------------------|-------------------|------------------|
| Ca      | 25.052622        | 29.763395         | 31.979204        |
| Ca      | 26.331177        | 30.852718         | 35.995174        |
| Ca      | 30.099682        | 28.073875         | 35.447750        |
| Ca      | 30.205788        | 33.018303         | 33.324661        |
| Ca      | 33.412659        | 30.141811         | 31.307442        |
| Ca      | 33.195019        | 30.448586         | 35.321751        |
| Ca      | 36.790779        | 26.722502         | 34.555569        |
| Ca      | 36.756775        | 31.166950         | 33.920750        |
| Ca      | 40.021805        | 28.888535         | 31.499199        |
| Ca      | 39.917622        | 29.596706         | 36.437927        |
| Ca      | 46.079487        | 27.423798         | 33.732704        |
| Ca      | 42.662296        | 29.446453         | 34.001488        |
| S       | 27.144848        | 27.352253         | 36.410439        |
| S       | 27.067020        | 34.006111         | 34.473755        |
| S       | 30.534325        | 29.857159         | 32.614838        |
| S       | 29.936039        | 31.158964         | 36.481888        |
| S       | 33.370338        | 27.512968         | 34.037422        |
| S       | 33.545486        | 33.008278         | 33.013218        |
| S       | 36.578747        | 28.701622         | 31.638702        |
| S       | 36.451401        | 29.346680         | 36.517124        |
| S       | 40.202408        | 26.922421         | 34.127399        |
| S       | 40.374969        | 31.471779         | 33.561005        |
| S       | 43.722351        | 28.094448         | 31.177631        |
| S       | 44.980282        | 27.415043         | 38.453709        |

24 generated by VMD

| Element | First Coordinate | Second Coordinate | Third Coordinate |
|---------|------------------|-------------------|------------------|
| Ca      | 25.154312        | 29.980568         | 31.892071        |
| Ca      | 26.229263        | 30.899872         | 35.741890        |
| Ca      | 30.033363        | 28.050274         | 35.836048        |
| Ca      | 30.380974        | 32.750763         | 33.219040        |
| Ca      | 33.434422        | 29.836567         | 31.672457        |
| Ca      | 33.128250        | 30.383762         | 35.564838        |
| Ca      | 36.767532        | 26.895618         | 34.432632        |
| Ca      | 36.754921        | 30.893524         | 34.119320        |
| Ca      | 40.023724        | 29.065849         | 31.485674        |
| Ca      | 39.951256        | 29.838600         | 36.440979        |
| Ca      | 46.082718        | 27.446522         | 33.751762        |
| Ca      | 42.818939        | 29.657475         | 34.130424        |
|   |      |      |      |
|---|------|------|------|
| S | 26.999695 | 27.593681 | 36.379791 |
| S | 27.018444 | 34.038429 | 34.077469 |
| S | 30.443790 | 29.639442 | 32.792736 |
| S | 29.856609 | 31.362293 | 36.486610 |
| S | 33.425442 | 27.400501 | 34.186417 |
| S | 33.574173 | 32.749195 | 33.122833 |
| S | 36.622437 | 28.851112 | 31.579847 |
| S | 36.615070 | 29.153393 | 36.697495 |
| S | 40.216434 | 26.952089 | 33.834110 |
| S | 40.445347 | 31.499060 | 33.435005 |
| S | 43.898926 | 28.210545 | 31.095270 |
| S | 44.557869 | 27.242279 | 38.055908 |

24

generated by VMD

| Ca   |      |      |      |
|------|------|------|------|
| Ca   | 24.925632 | 29.671621 | 31.965847 |
| Ca   | 26.459740 | 30.991850 | 35.859119 |
| Ca   | 30.251810 | 28.117147 | 35.723377 |
| Ca   | 30.437550 | 32.870255 | 33.315777 |
| Ca   | 33.317116 | 29.877726 | 31.463295 |
| Ca   | 33.229160 | 30.484447 | 35.280003 |
| Ca   | 36.647163 | 26.922089 | 34.478600 |
| Ca   | 36.717712 | 31.021080 | 33.832401 |
| Ca   | 40.123089 | 29.275658 | 31.524105 |
| Ca   | 39.751175 | 29.537992 | 36.689671 |
| Ca   | 46.116276 | 27.790283 | 33.748894 |
| Ca   | 42.634609 | 29.385273 | 34.238598 |
| S    | 27.079891 | 27.602554 | 36.627853 |
| S    | 27.140491 | 33.875740 | 34.300781 |
| S    | 30.470901 | 29.781216 | 32.838997 |
| S    | 29.992373 | 31.211178 | 36.372417 |
| S    | 33.399349 | 27.462311 | 34.003281 |
| S    | 33.692341 | 32.706932 | 32.871540 |
| S    | 36.628296 | 28.731659 | 31.256643 |
| S    | 36.494114 | 29.344639 | 36.521469 |
| S    | 40.136082 | 27.035645 | 34.008583 |
| S    | 40.348873 | 31.534977 | 33.725327 |
| S    | 43.735058 | 28.224628 | 31.167315 |
| S    | 44.705124 | 26.934460 | 38.216751 |

24

generated by VMD

| Ca   |      |      |      |
|------|------|------|------|
| Ca   | 24.944790 | 29.960379 | 31.963926 |
| Ca   | 26.072258 | 30.930626 | 35.728291 |
| Ca   | 30.084156 | 28.067894 | 35.930538 |
| Ca   | 30.243244 | 32.755737 | 33.296688 |
| Ca   | 33.420662 | 29.729782 | 31.574360 |
| Ca   | 33.182213 | 30.320511 | 35.394958 |
| Element | X Coord   | Y Coord   | Z Coord   |
|---------|-----------|-----------|-----------|
| Ca      | 36.758450 | 27.238003 | 34.545670 |
| Ca      | 36.819569 | 31.132175 | 33.933578 |
| Ca      | 40.079071 | 29.406551 | 31.428604 |
| Ca      | 39.924736 | 29.513618 | 36.459232 |
| Ca      | 46.006943 | 27.282906 | 33.521584 |
| Ca      | 42.880558 | 29.466232 | 34.156296 |
| S       | 26.939583 | 27.520403 | 36.353218 |
| S       | 26.935717 | 33.925657 | 34.134033 |
| S       | 30.478201 | 29.505253 | 32.866035 |
| S       | 29.668125 | 31.260494 | 36.379074 |
| S       | 33.482674 | 27.363266 | 34.171021 |
| S       | 33.736980 | 32.686363 | 32.846718 |
| S       | 36.723473 | 28.942184 | 31.615448 |
| S       | 36.510651 | 29.613722 | 36.695005 |
| S       | 40.173588 | 27.154314 | 33.873726 |
| S       | 40.498917 | 31.595966 | 33.725029 |
| S       | 43.756058 | 28.136141 | 31.378395 |
| S       | 45.113323 | 26.882355 | 38.054825 |

24 generated by VMD

| Element | X Coord   | Y Coord   | Z Coord   |
|---------|-----------|-----------|-----------|
| Ca      | 25.235905 | 29.570126 | 32.033340 |
| Ca      | 26.214806 | 30.817955 | 35.911518 |
| Ca      | 30.113342 | 28.149624 | 35.795792 |
| Ca      | 30.234100 | 32.984226 | 33.88992 |
| Ca      | 33.334831 | 29.638268 | 31.611294 |
| Ca      | 33.162792 | 30.422550 | 35.604020 |
| Ca      | 36.429123 | 27.189669 | 34.301140 |
| Ca      | 36.967228 | 31.229298 | 33.908482 |
| Ca      | 40.144958 | 29.484344 | 31.627695 |
| Ca      | 39.815231 | 29.910133 | 36.278488 |
| Ca      | 46.081890 | 27.409164 | 33.493107 |
| Ca      | 42.957180 | 29.253241 | 34.149422 |
| S       | 26.818600 | 27.311274 | 36.234024 |
| S       | 27.057213 | 33.697922 | 34.247944 |
| S       | 30.522171 | 29.790506 | 32.835945 |
| S       | 29.964306 | 31.342371 | 36.361919 |
| S       | 33.237392 | 27.411785 | 34.260021 |
| S       | 33.705849 | 32.787685 | 32.711700 |
| S       | 36.728600 | 28.795927 | 31.559200 |
| S       | 36.425812 | 29.641308 | 36.542377 |
| S       | 39.882690 | 27.207630 | 34.058525 |
| S       | 40.803200 | 31.670559 | 33.745377 |
| S       | 43.777512 | 28.043148 | 31.399651 |
| S       | 44.819248 | 26.632679 | 38.014248 |

24 generated by VMD
|   | Ca   |   |   |
|---|------|---|---|
|   | 25.098152 | 29.740200 | 32.015308 |
|   | 26.185616 | 30.911095 | 35.966515 |
|   | 30.432861 | 28.043560 | 35.587795 |
|   | 30.165569 | 33.021282 | 33.316921 |
|   | 33.318024 | 29.775364 | 31.485947 |
|   | 33.130058 | 30.419937 | 35.415157 |
|   | 37.123936 | 27.048756 | 34.338573 |
|   | 36.97369 | 31.147697 | 33.917305 |
|   | 39.839622 | 29.218273 | 31.791348 |
|   | 40.009468 | 30.016148 | 36.743450 |
|   | 45.980350 | 27.428806 | 33.456310 |
|   | 42.982006 | 29.306162 | 34.254669 |
|   | 27.183222 | 27.422560 | 36.468113 |
|   | 26.726948 | 33.922211 | 34.252960 |
|   | 30.489632 | 29.820679 | 32.666607 |
|   | 29.717228 | 31.222664 | 36.314510 |
|   | 33.607029 | 27.613575 | 33.985195 |
|   | 33.481495 | 32.886417 | 32.909218 |
|   | 36.577080 | 28.684900 | 31.356966 |
|   | 36.541088 | 29.413912 | 36.411423 |
|   | 40.225414 | 27.091888 | 34.496925 |
|   | 40.413879 | 31.681398 | 33.592113 |
|   | 43.659878 | 27.991549 | 31.416153 |
|   | 44.847996 | 26.562374 | 37.871239 |

24 generated by VMD

|   | Ca   |   |   |
|---|------|---|---|
|   | 25.225878 | 29.671949 | 32.114220 |
|   | 26.155365 | 30.752602 | 35.553879 |
|   | 30.088131 | 28.308083 | 35.934811 |
|   | 30.230747 | 32.743530 | 33.516895 |
|   | 33.483768 | 29.402529 | 31.268059 |
|   | 33.198235 | 30.461758 | 35.425259 |
|   | 36.626038 | 26.828836 | 34.137150 |
|   | 36.822426 | 31.232372 | 33.940163 |
|   | 39.990959 | 29.452724 | 31.707924 |
|   | 40.113083 | 29.612915 | 36.414833 |
|   | 45.954140 | 27.506437 | 33.441364 |
|   | 42.979359 | 29.578026 | 34.391247 |
|   | 27.022964 | 27.649460 | 36.634789 |
|   | 26.801418 | 33.941002 | 33.980522 |
|   | 30.542763 | 29.785141 | 32.837387 |
|   | 29.651226 | 31.469347 | 36.529659 |
|   | 33.183594 | 27.474403 | 34.127697 |
|   | 33.764977 | 32.680130 | 32.819599 |
|   | 36.728634 | 28.731310 | 31.534451 |
|   | 36.584621 | 29.413597 | 36.530712 |
S  40.070099  27.008484  34.000751
S  40.672089  31.712967  33.872204
S  43.595787  28.302944  31.306564
S  44.947540  26.670855  38.010609

24 generated by VMD
Ca  25.379744  29.181635  31.809311
Ca  26.180607  30.545164  35.485863
Ca  30.265312  28.087103  36.068321
Ca  30.176825  32.968739  33.354050
Ca  33.369354  29.868361  31.466351
Ca  33.225327  30.609941  35.458744
Ca  36.506264  27.261585  34.458931
Ca  36.897224  31.450611  33.686142
Ca  39.994556  29.397491  31.482128
Ca  40.108574  29.680912  36.491074
Ca  45.769772  27.307602  33.383522
Ca  42.928936  29.224745  34.404774
S  27.210728  27.414356  36.571129
S  26.941647  33.713257  34.192078
S  30.540480  29.796772  33.020462
S  29.587763  31.376759  36.450722
S  33.265434  27.667053  34.185356
S  33.680946  32.835289  32.935467
S  36.626846  29.081356  31.536913
S  36.665062  29.944464  36.521004
S  39.991226  26.964523  33.908485
S  40.809677  31.489531  33.654930
S  43.556171  28.304768  31.474157
S  44.755444  26.219439  38.030827

24 generated by VMD
Ca  25.366444  29.776104  31.705984
Ca  26.322601  30.929600  35.575672
Ca  30.088654  28.164194  36.019409
Ca  30.318474  32.833385  33.690277
Ca  33.357273  29.833103  31.496407
Ca  33.399010  30.237854  35.573967
Ca  36.388046  26.922428  34.422745
Ca  36.891068  31.034027  33.689621
Ca  39.913151  29.251953  31.477127
Ca  39.805145  29.677691  36.447601
Ca  46.040504  27.746201  33.973621
Ca  42.840450  29.546427  34.120327
S  27.080482  27.674034  36.491562
S  26.916893  33.955933  34.002354
S  30.502758  29.825832  32.886257
S  29.759609  31.182766  36.673332
S  33.140343  27.278755  34.250740
S  33.802017  32.69243  33.143295
S  36.61585  28.534611  31.382906
S  36.668381  29.494152  36.326111
S  39.894451  27.042564  33.893417
S  40.529438  31.606083  33.535221
S  43.871986  28.228706  31.437750
S  44.920189  26.945705  37.814972

24 generated by VMD
Ca  25.402798  29.507471  32.163757
Ca  26.320698  30.930531  35.647449
Ca  30.230202  28.056274  35.900024
Ca  30.254890  32.926704  33.370682
Ca  33.417053  30.025093  31.256844
Ca  33.158951  30.389378  35.463657
Ca  36.654171  27.106270  34.469204
Ca  36.805656  31.143387  33.718674
Ca  40.090237  29.217010  31.523422
Ca  39.823151  29.477654  36.731293
Ca  46.509243  27.831238  33.331734
Ca  42.877056  29.184711  34.396553
S  27.107561  27.602835  36.443291
S  26.707851  34.006966  34.220928
S  30.420700  29.702888  32.816948
S  29.847393  31.287632  36.465893
S  33.445305  27.549824  33.971527
S  33.559177  32.834854  33.056328
S  36.710453  28.868460  31.295013
S  36.564350  29.567760  36.434216
S  39.913151  26.893059  34.098476
S  40.409966  31.389545  33.820229
S  43.432415  27.956945  31.420135
S  44.771584  26.934944  38.014400

24 generated by VMD
Ca  25.611464  29.513184  31.840588
Ca  26.158787  30.963772  35.672794
Ca  30.016144  28.214836  35.931313
Ca  30.111893  32.891293  33.481163
Ca  33.385059  29.733204  31.327562
Ca  33.076263  30.272068  35.596329
Ca  36.634415  26.861174  34.292561
Ca  36.423725  31.173170  33.990112
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 40.200275 | 29.28889 | 31.624712 |
| Ca      | 39.880241 | 29.817089 | 36.700367 |
| Ca      | 47.301853 | 27.769369 | 33.338253 |
| Ca      | 42.908413 | 29.390854 | 34.199833 |
| S       | 26.910400 | 27.693920 | 36.305340 |
| S       | 26.647205 | 34.128136 | 34.296165 |
| S       | 30.461510 | 29.879070 | 32.818859 |
| S       | 29.729248 | 31.455690 | 36.533661 |
| S       | 33.167286 | 27.501068 | 34.079678 |
| S       | 33.574944 | 32.770638 | 32.819027 |
| S       | 36.662323 | 28.733198 | 31.651802 |
| S       | 36.482998 | 29.330822 | 36.566540 |
| S       | 40.011341 | 27.060520 | 34.117218 |
| S       | 40.491951 | 31.622587 | 33.845402 |
| S       | 43.456490 | 27.501047 | 31.288176 |
| S       | 45.129707 | 26.835773 | 37.713135 |

24 generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 25.326748 | 29.249027 | 31.976704 |
| Ca      | 26.190239 | 30.958878 | 35.553970 |
| Ca      | 29.965094 | 28.094597 | 36.025661 |
| Ca      | 30.160885 | 32.837227 | 33.528202 |
| Ca      | 33.590412 | 30.074118 | 31.644329 |
| Ca      | 33.066406 | 30.549129 | 35.614643 |
| Ca      | 36.495579 | 26.992823 | 34.349270 |
| Ca      | 36.910744 | 31.041515 | 34.058353 |
| Ca      | 40.106358 | 29.116615 | 31.537926 |
| Ca      | 39.861004 | 29.430550 | 36.360626 |
| Ca      | 46.937698 | 27.977678 | 33.310162 |
| Ca      | 43.008907 | 29.181776 | 34.093357 |
| S       | 26.820442 | 27.676300 | 36.311970 |
| S       | 26.855364 | 34.080360 | 33.979053 |
| S       | 30.561527 | 29.862137 | 32.929989 |
| S       | 29.586309 | 31.289185 | 36.517788 |
| S       | 33.103207 | 27.509186 | 34.167747 |
| S       | 33.703617 | 32.867897 | 33.118187 |
| S       | 36.717678 | 28.803448 | 31.474674 |
| S       | 36.347828 | 29.528770 | 36.636482 |
| S       | 39.953819 | 26.892368 | 33.926109 |
| S       | 40.605919 | 31.454689 | 33.615009 |
| S       | 43.846691 | 27.985394 | 31.343548 |
| S       | 44.711479 | 26.937689 | 37.956898 |

24 generated by VMD

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| Ca      | 25.478519 | 29.634939 | 32.128574 |
| Ca      | 26.198362 | 30.971161 | 35.934258 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 30.045002    | 28.062637    | 35.649162    |
| Ca      | 30.080597    | 32.966499    | 33.479637    |
| Ca      | 33.397934    | 30.173183    | 31.450375    |
| Ca      | 32.979351    | 30.481010    | 35.339272    |
| Ca      | 36.549377    | 26.893509    | 34.35973     |
| Ca      | 36.767746    | 31.005083    | 33.659241    |
| Ca      | 40.086300    | 28.898870    | 31.511822    |
| Ca      | 39.868969    | 29.361917    | 36.474453    |
| Ca      | 47.029949    | 28.393509    | 33.66874     |
| Ca      | 42.935745    | 29.048544    | 34.217365    |
| S       | 26.942986    | 27.639643    | 36.475334    |
| S       | 26.804115    | 33.971046    | 34.419441    |
| S       | 30.419165    | 29.982603    | 32.786690    |
| S       | 29.651852    | 31.295273    | 36.514034    |
| S       | 33.227116    | 27.569910    | 33.915466    |
| S       | 33.609554    | 32.973862    | 32.871887    |
| S       | 36.633804    | 28.584000    | 31.500961    |
| S       | 36.408802    | 29.449322    | 36.449515    |
| S       | 40.082813    | 26.717291    | 34.158066    |
| S       | 40.312355    | 31.290646    | 33.490456    |
| S       | 43.894737    | 28.041927    | 31.514128    |
| S       | 45.028702    | 26.980511    | 38.071598    |

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generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.551079    | 29.486952    | 32.007885    |
| Ca      | 26.248840    | 30.912884    | 35.733967    |
| Ca      | 30.214127    | 28.298746    | 35.998848    |
| Ca      | 30.082993    | 32.962215    | 33.649792    |
| Ca      | 33.377323    | 30.003544    | 31.276768    |
| Ca      | 33.239666    | 30.671537    | 35.484680    |
| Ca      | 36.588799    | 26.879753    | 34.310013    |
| Ca      | 36.624786    | 30.768673    | 33.763206    |
| Ca      | 39.808041    | 28.966284    | 31.320446    |
| Ca      | 39.734104    | 29.311131    | 36.344345    |
| Ca      | 46.846161    | 28.414635    | 33.867111    |
| Ca      | 42.772057    | 29.105501    | 34.283905    |
| S       | 27.215532    | 27.552860    | 36.435234    |
| S       | 26.704597    | 33.929604    | 34.212173    |
| S       | 30.562183    | 29.990196    | 32.958599    |
| S       | 29.776184    | 31.404961    | 36.709702    |
| S       | 33.413586    | 27.821886    | 34.005085    |
| S       | 33.700737    | 32.994553    | 32.878372    |
| S       | 36.524551    | 28.509995    | 31.136246    |
| S       | 36.338570    | 29.399429    | 36.517124    |
| S       | 39.896633    | 26.704065    | 33.792431    |
| S       | 40.431122    | 31.288876    | 33.584267    |
S  43.799023  28.116768  31.496212
S  44.983116  26.896328  38.264286

24 generated by VMD
Ca  25.520170  29.508366  31.899277
Ca  26.232494  31.133179  35.669540
Ca  30.082808  27.996052  35.863853
Ca  30.145271  33.029938  33.688511
Ca  33.217781  29.916031  31.522991
Ca  33.070705  30.346207  35.378551
Ca  36.511604  26.859802  34.189484
Ca  36.905014  30.928761  33.815029
Ca  39.957474  28.957018  31.690720
Ca  39.951645  29.584095  36.669098
Ca  47.128479  28.653112  33.493587
Ca  42.870224  29.123817  34.253857
S  26.952843  27.750551  36.524391
S  26.911619  34.080368  34.120979
S  30.377052  29.781094  32.754913
S  29.768047  31.381775  36.486984
S  33.093422  27.509060  34.077408
S  33.677883  32.737484  33.022652
S  36.543457  28.730133  31.338726
S  36.555573  29.390018  36.448872
S  40.023575  26.715294  34.189312
S  40.640125  31.365028  33.658127
S  43.457359  28.085850  31.259241
S  44.839355  26.828384  38.014629

24 generated by VMD
Ca  25.326984  29.864798  31.726421
Ca  26.304913  31.101740  35.744514
Ca  30.355484  28.045589  36.029728
Ca  30.297974  32.765533  33.516296
Ca  33.323669  29.484245  31.309704
Ca  33.360744  30.191111  35.329369
Ca  36.626862  27.136684  34.634869
Ca  36.842148  31.085396  33.803345
Ca  40.101101  29.267157  31.500858
Ca  39.767384  29.475378  36.405338
Ca  46.764057  28.335562  33.794495
Ca  42.730415  29.243708  34.250748
S  26.911076  27.773977  36.483185
S  26.761238  34.100956  34.282627
S  30.422085  29.676981  32.988617
S  29.688091  31.248281  36.624954
|  | X       | Y       | Z       |
|---|---------|---------|---------|
| S | 33.326351 | 27.407856 | 34.035664 |
| S | 33.702709 | 32.595112 | 32.862091 |
| S | 36.584034 | 28.849083 | 31.363844 |
| S | 36.382622 | 29.585136 | 36.553982 |
| S | 39.916130 | 26.875092 | 33.884285 |
| S | 40.627655 | 31.475529 | 33.553238 |
| S | 43.504608 | 28.175035 | 31.396982 |
| S | 44.806472 | 26.631516 | 37.955521 |

24

generated by VMD

|  | X       | Y       | Z       |
|---|---------|---------|---------|
| Ca | 25.469639 | 30.123978 | 31.797283 |
| Ca | 26.343670 | 31.220131 | 35.782867 |
| Ca | 30.028223 | 28.140610 | 36.047436 |
| Ca | 29.965240 | 32.908649 | 33.655659 |
| Ca | 33.201637 | 29.431454 | 31.291245 |
| Ca | 33.270115 | 30.153084 | 35.485157 |
| Ca | 36.548607 | 27.013187 | 34.295708 |
| Ca | 36.551514 | 30.826324 | 33.694305 |
| Ca | 40.265598 | 29.175934 | 31.500942 |
| Ca | 39.749943 | 29.409655 | 36.323788 |
| Ca | 46.939575 | 28.872023 | 33.656052 |
| Ca | 42.937737 | 29.142794 | 34.235771 |
| S | 26.893805 | 27.924429 | 36.805294 |
| S | 26.626549 | 34.233566 | 34.250576 |
| S | 30.423729 | 29.659733 | 33.037155 |
| S | 29.718523 | 31.419924 | 36.479168 |
| S | 33.245064 | 27.201498 | 33.817978 |
| S | 33.709743 | 32.425213 | 32.910534 |
| S | 36.801659 | 28.757217 | 31.134657 |
| S | 36.277397 | 29.326374 | 36.429871 |
| S | 40.143417 | 26.758507 | 33.896408 |
| S | 40.452782 | 31.373524 | 33.720490 |
| S | 43.816490 | 28.071222 | 31.358521 |
| S | 45.078671 | 26.822388 | 38.422951 |

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generated by VMD

|  | X       | Y       | Z       |
|---|---------|---------|---------|
| Ca | 25.094854 | 29.818748 | 32.038826 |
| Ca | 26.251251 | 31.293034 | 35.591095 |
| Ca | 30.015076 | 27.967833 | 35.815723 |
| Ca | 29.907593 | 32.851471 | 33.385059 |
| Ca | 33.324543 | 29.476803 | 31.378445 |
| Ca | 33.182243 | 30.125078 | 35.505371 |
| Ca | 36.384968 | 27.012915 | 34.408089 |
| Ca | 36.889778 | 30.998751 | 33.929630 |
| Ca | 40.389484 | 29.504665 | 31.401726 |
| Ca | 39.979950 | 29.659958 | 36.470585 |
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 47.166451     | 28.109756     | 33.413986     |
| Ca      | 42.909252     | 29.213139     | 34.334835     |
| S       | 26.980934     | 28.172190     | 36.835888     |
| S       | 26.702011     | 34.208744     | 34.223148     |
| S       | 30.377663     | 29.459465     | 32.797836     |
| S       | 29.744106     | 31.351463     | 36.412663     |
| S       | 33.157372     | 27.065193     | 34.054394     |
| S       | 33.500313     | 32.440033     | 32.761898     |
| S       | 36.831760     | 28.802231     | 31.318226     |
| S       | 36.229019     | 29.375292     | 36.691612     |
| S       | 40.073929     | 27.105122     | 33.877850     |
| S       | 40.641342     | 31.598507     | 33.964062     |
| S       | 43.780220     | 28.227732     | 31.326664     |
| S       | 44.919773     | 26.553282     | 38.093079     |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 25.276987     | 29.744387     | 32.040382     |
| Ca      | 26.407028     | 31.250359     | 35.793167     |
| Ca      | 30.120014     | 28.181128     | 35.980564     |
| Ca      | 30.104490     | 32.989479     | 33.497204     |
| Ca      | 33.335735     | 29.577087     | 31.513411     |
| Ca      | 33.124687     | 30.268267     | 35.424339     |
| Ca      | 36.484043     | 26.844707     | 34.221512     |
| Ca      | 36.751015     | 30.815716     | 33.851326     |
| Ca      | 40.183582     | 29.307823     | 31.312002     |
| Ca      | 39.778336     | 29.266447     | 36.203323     |
| Ca      | 46.977585     | 28.534832     | 33.954811     |
| Ca      | 42.881329     | 29.365877     | 34.255615     |
| S       | 27.071856     | 28.070522     | 36.804401     |
| S       | 26.674603     | 33.971027     | 33.934090     |
| S       | 30.459381     | 29.762806     | 32.834114     |
| S       | 29.823811     | 31.370562     | 36.550545     |
| S       | 33.082962     | 27.353027     | 34.220970     |
| S       | 33.697289     | 32.601360     | 32.925453     |
| S       | 36.589115     | 28.738552     | 31.149261     |
| S       | 36.258835     | 29.152906     | 36.377258     |
| S       | 40.121841     | 26.822889     | 33.627918     |
| S       | 40.403595     | 31.371521     | 33.972469     |
| S       | 43.894928     | 28.312431     | 31.392632     |
| S       | 44.930901     | 26.717701     | 38.193935     |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 25.375463     | 29.678350     | 31.872740     |
| Ca      | 26.481789     | 31.152403     | 35.685940     |
| Ca      | 30.233223     | 28.158440     | 36.113060     |
| Ca      | 30.105469     | 32.895626     | 33.717323     |
| Element | Ca       | 29.538788 | 31.407625 |
|---------|---------|-----------|-----------|
| Ca      | 33.378334 | 30.181011 | 35.553349 |
| Ca      | 36.288296 | 27.169003 | 34.360390 |
| Ca      | 36.837933 | 31.222031 | 33.907009 |
| Ca      | 40.332680 | 29.190624 | 31.305016 |
| Ca      | 39.796520 | 29.514790 | 36.070137 |
| Ca      | 46.542072 | 28.274338 | 33.881126 |
| S       | 27.123178 | 27.830889 | 36.753338 |
| S       | 26.710337 | 33.904030 | 34.007378 |
| S       | 30.555738 | 29.733824 | 32.892864 |
| S       | 29.963409 | 31.320007 | 36.579414 |
| S       | 33.148621 | 27.147190 | 33.928303 |
| S       | 33.600395 | 32.552414 | 32.893757 |
| S       | 36.713173 | 28.898924 | 31.285385 |
| S       | 36.381695 | 29.576895 | 36.500824 |
| S       | 39.800175 | 26.985022 | 33.741024 |
| S       | 40.683521 | 31.464130 | 33.701405 |
| S       | 43.708923 | 28.342497 | 31.350555 |
| S       | 44.694870 | 26.466988 | 38.267284 |

24 generated by VMD

| Element | Ca       | 29.532013 | 32.202072 |
|---------|---------|-----------|-----------|
| Ca      | 25.240961 | 31.398918 | 35.826241 |
| Ca      | 26.283508 | 27.782001 | 35.674103 |
| Ca      | 30.075745 | 32.921600 | 33.78311 |
| Ca      | 33.385120 | 29.281950 | 31.298717 |
| Ca      | 33.121483 | 30.147629 | 35.514023 |
| Ca      | 36.486610 | 27.119440 | 34.451084 |
| Ca      | 36.845139 | 31.158581 | 34.04793 |
| Ca      | 40.432823 | 29.449131 | 31.347065 |
| Ca      | 39.836651 | 29.319929 | 36.287552 |
| Ca      | 46.835354 | 28.584888 | 33.749695 |
| Ca      | 42.880192 | 29.273277 | 34.285744 |
| S       | 27.142200 | 31.398918 | 35.826241 |
| S       | 26.737116 | 34.280754 | 33.894409 |
| S       | 30.532505 | 29.747337 | 32.860989 |
| S       | 29.865025 | 31.139269 | 36.374592 |
| S       | 33.171379 | 27.129179 | 34.204903 |
| S       | 33.638512 | 32.484875 | 32.709255 |
| S       | 36.919586 | 29.037405 | 31.520464 |
| S       | 36.03707 | 29.408688 | 36.613018 |
| S       | 39.817806 | 27.003437 | 33.712349 |
| S       | 40.624966 | 31.467377 | 33.846558 |
| S       | 43.621540 | 28.518728 | 31.306599 |
| S       | 44.554596 | 26.072788 | 37.992924 |
24

|   | generated by VMD |
|---|-----------------|
| Ca | 25.100328       | 29.964046 | 32.057537 |
| Ca | 26.273502       | 31.313412 | 35.759689 |
| Ca | 29.965561       | 27.950563 | 35.780979 |
| Ca | 30.193737       | 32.956192 | 33.554092 |
| Ca | 33.274376       | 29.423616 | 31.178526 |
| Ca | 33.259087       | 29.973835 | 35.488171 |
| Ca | 36.485630       | 27.223389 | 34.334148 |
| Ca | 36.938225       | 31.000523 | 33.735378 |
| Ca | 40.489880       | 29.253292 | 31.313311 |
| Ca | 39.730515       | 29.469141 | 36.448574 |
| Ca | 46.810295       | 28.712929 | 33.763439 |
| Ca | 42.857513       | 29.232384 | 34.488285 |
| S  | 27.002327       | 28.098480 | 37.062202 |
| S  | 26.784634       | 34.121262 | 34.247704 |
| S  | 30.500702       | 29.762444 | 32.872074 |
| S  | 29.894434       | 31.116802 | 36.464386 |
| S  | 33.126614       | 26.974104 | 33.990143 |
| S  | 33.753559       | 32.462212 | 32.645084 |
| S  | 36.885784       | 28.649391 | 31.204529 |
| S  | 36.247131       | 29.411419 | 36.540230 |
| S  | 39.988861       | 26.959700 | 33.859413 |
| S  | 40.526062       | 31.312849 | 33.762733 |
| S  | 43.808949       | 28.429747 | 31.383427 |
| S  | 44.536201       | 26.619677 | 38.096695 |

24

|   | generated by VMD |
|---|-----------------|
| Ca | 24.913794       | 30.109200 | 31.801373 |
| Ca | 26.328598       | 31.434214 | 35.672501 |
| Ca | 30.197441       | 27.880951 | 36.232563 |
| Ca | 30.134666       | 32.792862 | 33.428699 |
| Ca | 33.305534       | 29.177513 | 31.597111 |
| Ca | 33.320004       | 30.280746 | 35.557518 |
| Ca | 36.661591       | 26.872982 | 34.571064 |
| Ca | 36.720890       | 30.979279 | 33.633766 |
| Ca | 40.156609       | 29.359499 | 31.407181 |
| Ca | 39.859322       | 29.462675 | 36.424931 |
| Ca | 47.051643       | 28.770355 | 33.607296 |
| Ca | 42.896626       | 29.068932 | 34.294502 |
| S  | 26.709389       | 27.909315 | 36.517883 |
| S  | 26.811672       | 34.154045 | 33.792770 |
| S  | 30.399158       | 29.675358 | 33.097954 |
| S  | 29.853397       | 31.322805 | 36.594646 |
| S  | 33.244904       | 27.214535 | 34.231590 |
| S  | 33.738770       | 32.399693 | 32.883053 |
|   | X-coordinates | Y-coordinates | Z-coordinates |
|---|---------------|---------------|---------------|
| S | 36.730068     | 28.752230     | 31.347504     |
| S | 36.433083     | 29.286880     | 36.574249     |
| S | 40.011414     | 26.889721     | 33.718193     |
| S | 40.510025     | 31.470478     | 33.642040     |
| S | 43.956390     | 28.626209     | 31.366142     |
| S | 44.488857     | 26.500904     | 38.036102     |

24 generated by VMD

|   | X-coordinates | Y-coordinates | Z-coordinates |
|---|---------------|---------------|---------------|
| Ca| 25.353453     | 30.032707     | 31.927021     |
| Ca| 26.226120     | 31.205017     | 35.917416     |
| Ca| 30.065691     | 27.989164     | 36.049782     |
| Ca| 30.389456     | 32.680069     | 33.265015     |
| Ca| 33.348793     | 29.600040     | 31.519730     |
| Ca| 33.015430     | 30.381098     | 35.594193     |
| Ca| 36.469860     | 27.103468     | 34.341110     |
| Ca| 36.792004     | 30.865635     | 33.622005     |
| Ca| 40.340439     | 29.193010     | 31.251354     |
| Ca| 39.698399     | 29.426104     | 36.44138      |
| Ca| 46.887646     | 28.781204     | 33.721611     |
| Ca| 42.740963     | 29.304525     | 34.457512     |
| S | 26.772053     | 27.857588     | 36.662392     |
| S | 27.233053     | 34.019306     | 34.322250     |
| S | 30.484055     | 29.540026     | 32.868359     |
| S | 29.851635     | 31.410395     | 36.488201     |
| S | 33.150852     | 27.304512     | 34.047024     |
| S | 33.687531     | 32.443165     | 32.830357     |
| S | 36.740925     | 28.591017     | 31.142681     |
| S | 36.283409     | 29.492640     | 36.363731     |
| S | 40.008205     | 26.973696     | 33.957855     |
| S | 40.299786     | 31.235325     | 33.701221     |
| S | 43.760143     | 28.499062     | 31.439922     |
| S | 44.834927     | 26.462666     | 38.095860     |

24 generated by VMD

|   | X-coordinates | Y-coordinates | Z-coordinates |
|---|---------------|---------------|---------------|
| Ca| 25.384495     | 30.002811     | 31.933445     |
| Ca| 26.190744     | 31.493525     | 36.070438     |
| Ca| 30.081350     | 27.914528     | 35.815292     |
| Ca| 30.223532     | 32.801685     | 33.063934     |
| Ca| 33.179443     | 29.228783     | 31.554932     |
| Ca| 33.008621     | 30.210754     | 35.310272     |
| Ca| 36.537884     | 26.781277     | 34.593708     |
| Ca| 36.885368     | 30.783735     | 34.067471     |
| Ca| 40.256561     | 29.331585     | 31.530800     |
| Ca| 39.686867     | 29.432545     | 36.457470     |
| Ca| 46.981651     | 29.202114     | 33.383644     |
| Ca| 42.913948     | 29.105587     | 34.460052     |
S  26.989456  28.168049  36.817455
S  27.205944  34.384819  34.016605
S  30.189339  29.538359  32.705685
S  29.764553  31.312994  36.206974
S  33.232998  27.093180  34.093285
S  33.570808  32.315510  32.770065
S  36.643246  28.717617  31.578003
S  35.980461  29.331202  36.647041
S  40.553326  26.824232  33.923901
S  40.511219  31.352976  34.030624
S  43.778847  28.724228  31.331392
S  45.183311  26.339334  37.668236

24 generated by VMD
Ca  25.438435  29.651552  32.016132
Ca  26.279003  31.006399  35.893555
Ca  30.025639  28.152723  36.042320
Ca  30.392000  32.867088  33.122932
Ca  33.523376  29.060019  31.132339
Ca  33.185364  30.574421  35.513046
Ca  36.394283  27.003159  34.589260
Ca  36.849274  31.124975  33.787781
Ca  40.247555  29.334072  31.482899
Ca  39.555275  29.582005  36.610062
Ca  46.634796  28.878311  33.349724
Ca  42.699284  29.122192  34.462044
S  26.837685  27.906069  36.617798
S  27.161938  33.793800  34.237831
S  30.632774  29.659672  32.853806
S  30.012312  31.571850  36.384956
S  33.088505  27.319563  34.455269
S  33.884243  32.460960  32.483913
S  36.845989  28.755697  31.400684
S  36.307217  29.485146  36.650085
S  39.842331  27.023491  33.842297
S  40.400230  31.430305  33.947506
S  43.579056  28.867722  31.332014
S  44.617340  25.760227  37.822468

24 generated by VMD
Ca  25.071190  29.872059  32.001984
Ca  26.632830  31.176369  35.951504
Ca  30.052700  28.047718  35.939453
Ca  30.393862  32.990791  33.215668
Ca  33.310928  29.293268  31.232210
Ca  33.102467  30.363409  35.357838
|   |         |         |         |
|---|---------|---------|---------|
| Ca| 36.473804 | 27.084606 | 34.422455 |
| Ca| 36.885078 | 30.976562 | 33.993599 |
| Ca| 40.162682 | 29.129234 | 31.469152 |
| Ca| 39.787395 | 29.376610 | 36.306335 |
| Ca| 46.798958 | 29.147293 | 33.603260 |
| Ca| 42.840950 | 29.153488 | 34.393604 |
| S | 26.851376 | 27.827930 | 36.796005 |
| S | 27.152273 | 34.067249 | 34.142151 |
| S | 30.362715 | 29.701223 | 32.822678 |
| S | 29.989326 | 31.367687 | 36.372654 |
| S | 33.130188 | 27.183372 | 34.216232 |
| S | 33.734695 | 32.349869 | 32.631687 |
| S | 36.657936 | 28.766201 | 31.381649 |
| S | 36.287201 | 29.389875 | 36.554588 |
| S | 39.982777 | 26.812346 | 33.781685 |
| S | 40.490372 | 31.298939 | 33.966045 |
| S | 43.775902 | 28.762056 | 31.311777 |
| S | 44.500759 | 26.253325 | 38.166470 |

24 generated by VMD

|   |         |         |         |
|---|---------|---------|---------|
| Ca| 25.118931 | 29.866215 | 32.269703 |
| Ca| 26.451416 | 31.255741 | 35.769371 |
| Ca| 29.899158 | 28.241062 | 35.980362 |
| Ca| 30.158039 | 32.731293 | 33.057472 |
| Ca| 33.316200 | 29.052383 | 31.241287 |
| Ca| 33.177994 | 30.484264 | 35.476662 |
| Ca| 36.372101 | 27.034557 | 34.276638 |
| Ca| 36.854923 | 30.984642 | 34.028030 |
| Ca| 40.330585 | 29.143578 | 31.446005 |
| Ca| 39.910248 | 29.197817 | 36.364220 |
| Ca| 46.905643 | 29.427170 | 33.635849 |
| Ca| 42.769577 | 29.012024 | 34.381897 |
| S | 26.706057 | 27.996271 | 36.624672 |
| S | 27.309879 | 34.083206 | 34.418198 |
| S | 30.419172 | 29.598816 | 32.836735 |
| S | 29.927116 | 31.525867 | 36.335163 |
| S | 33.095192 | 27.189413 | 34.195389 |
| S | 33.740726 | 32.206314 | 32.536205 |
| S | 36.789742 | 28.953007 | 31.332266 |
| S | 36.093948 | 29.273094 | 36.608669 |
| S | 39.906464 | 26.697819 | 33.697113 |
| S | 40.528770 | 31.353952 | 33.998066 |
| S | 43.782848 | 28.754320 | 31.374956 |
| S | 44.869263 | 26.328598 | 38.145767 |

24 generated by VMD
Ca       25.320660       30.108231       32.026291  
Ca       26.620440       31.341677       35.994583  
Ca       30.039492       27.942410       35.968246  
Ca       30.291307       32.598648       33.328056  
Ca       33.367058       29.113775       31.336664  
Ca       33.145584       30.228870       35.488453  
Ca       36.373070       26.975389       34.440475  
Ca       36.728691       31.040169       33.859047  
Ca       40.226696       29.307404       31.405968  
Ca       39.691513       29.556231       36.427032  
Ca       46.719330       28.824617       33.923988  
Ca       42.728909       29.339821       34.389828  
S        26.779373       27.982946       36.395977  
S        27.408566       34.205872       34.379807  
S        30.548660       29.414644       32.815964  
S        30.018959       31.280533       36.414986  
S        33.078030       27.207090       34.286865  
S        33.634392       32.124252       32.505344  
S        36.570339       28.888134       31.337124  
S        36.406364       29.403500       36.501770  
S        39.921848       27.127098       33.848824  
S        40.460926       31.446699       33.694981  
S        43.763275       28.625246       31.443483  
S        44.590385       26.308170       37.816948  

24 generated by VMD

Ca       25.147682       29.908905       32.075958  
Ca       26.182150       31.306229       36.122112  
Ca       30.018539       28.095201       35.800560  
Ca       30.031237       32.733768       33.271530  
Ca       33.455166       29.474873       31.290152  
Ca       33.138298       30.378082       35.316483  
Ca       36.521996       26.932760       34.245911  
Ca       36.855217       30.948826       33.772823  
Ca       40.360909       29.079361       31.371813  
Ca       39.769917       29.409529       36.433064  
Ca       46.748585       29.258110       33.672749  
Ca       42.876228       29.157146       34.632812  
S        26.945175       27.972368       36.971100  
S        26.963932       33.995762       34.419289  
S        30.478451       29.630629       32.697582  
S        29.733910       31.431013       36.378330  
S        33.101551       27.415234       34.083366  
S        33.604561       32.395069       32.550930  
S        36.812714       28.797361       31.336327  
S        36.339462       29.426140       36.411324
|  |  |  |  |
|---|---|---|---|
| S | 40.080627 | 26.772234 | 33.831253 |
| S | 40.610207 | 31.165401 | 33.706188 |
| S | 43.943722 | 28.602844 | 31.519306 |
| S | 44.713684 | 26.104572 | 38.119740 |

24

generated by VMD

| Ca | 24.943378 | 29.684872 | 32.285927 |
| Ca | 26.455963 | 31.224997 | 36.120750 |
| Ca | 30.232628 | 28.111435 | 35.802433 |
| Ca | 30.254190 | 33.075752 | 33.063557 |
| Ca | 33.295689 | 29.581036 | 31.291573 |
| Ca | 33.150372 | 30.645819 | 35.085106 |
| Ca | 36.626862 | 26.702484 | 34.484264 |
| Ca | 36.686222 | 30.665724 | 33.789768 |
| Ca | 40.086876 | 29.072531 | 31.599813 |
| Ca | 39.660454 | 28.974646 | 36.696526 |
| Ca | 46.779381 | 29.392700 | 33.626190 |
| Ca | 42.822353 | 29.447174 | 34.588181 |
| S  | 27.234200 | 27.976044 | 36.923439 |
| S  | 27.205135 | 33.882019 | 34.434055 |
| S  | 30.470114 | 29.838554 | 32.489651 |
| S  | 29.976109 | 31.503981 | 36.258793 |
| S  | 33.211201 | 27.429642 | 33.851299 |
| S  | 33.749748 | 32.754456 | 32.490524 |
| S  | 36.589806 | 28.496727 | 31.368340 |
| S  | 36.168396 | 29.052214 | 36.435070 |
| S  | 40.090065 | 26.682102 | 33.905807 |
| S  | 40.322487 | 31.177532 | 33.911362 |
| S  | 43.758202 | 28.705387 | 31.570873 |
| S  | 44.661663 | 26.313589 | 37.957394 |

24

generated by VMD

| Ca | 24.970654 | 29.894320 | 32.209892 |
| Ca | 26.171700 | 31.057823 | 35.744110 |
| Ca | 29.979256 | 28.133411 | 35.950630 |
| Ca | 30.271011 | 32.700130 | 33.243786 |
| Ca | 33.357464 | 29.655682 | 31.182497 |
| Ca | 33.035713 | 30.418943 | 35.216053 |
| Ca | 36.559139 | 26.779789 | 34.266830 |
| Ca | 36.881405 | 30.820677 | 33.874001 |
| Ca | 40.195328 | 29.306688 | 31.308645 |
| Ca | 39.607731 | 29.341219 | 36.548367 |
| Ca | 47.125874 | 28.822811 | 33.949692 |
| Ca | 42.900753 | 29.105452 | 34.402630 |
| S  | 27.146282 | 27.960911 | 37.175449 |
| S  | 27.084003 | 33.982498 | 34.343033 |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| S | 30.450638 | 29.717793 | 32.849304 |
| S | 29.885420 | 31.451370 | 36.403057 |
| S | 33.216545 | 27.512405 | 33.920818 |
| S | 33.727081 | 32.541595 | 32.603367 |
| S | 36.586029 | 28.825895 | 31.226120 |
| S | 36.243355 | 29.151262 | 36.354580 |
| S | 40.025497 | 26.830133 | 33.810635 |
| S | 40.557404 | 31.296062 | 33.835030 |
| S | 43.837570 | 28.518919 | 31.367870 |
| S | 44.618050 | 26.565596 | 38.244270 |

| Ca | 24.889729 | 30.044161 | 32.480705 |
| Ca | 26.394810 | 31.004211 | 36.174324 |
| Ca | 30.265121 | 28.073908 | 35.671066 |
| Ca | 30.481243 | 32.862797 | 33.266129 |
| Ca | 33.506924 | 29.456190 | 31.157940 |
| Ca | 33.134232 | 30.326729 | 35.267254 |
| Ca | 36.662746 | 27.012550 | 34.500328 |
| Ca | 36.631386 | 31.095278 | 33.797211 |
| Ca | 40.225796 | 29.062485 | 31.249949 |
| Ca | 39.774979 | 29.312410 | 36.396690 |
| Ca | 46.504402 | 29.080639 | 34.028690 |
| Ca | 42.708946 | 29.288267 | 34.334820 |
| S | 27.011574 | 27.716707 | 36.540577 |
| S | 27.194859 | 34.034416 | 34.511944 |
| S | 30.602264 | 29.767191 | 32.745461 |
| S | 29.846985 | 31.295691 | 36.491829 |
| S | 33.209431 | 27.514631 | 33.889759 |
| S | 33.790836 | 32.477936 | 32.391182 |
| S | 36.724008 | 28.700222 | 31.288939 |
| S | 36.187786 | 29.331802 | 36.468292 |
| S | 40.050365 | 26.829548 | 33.930969 |
| S | 40.319206 | 31.307623 | 33.760612 |
| S | 43.804073 | 28.337051 | 31.403347 |
| S | 44.506790 | 26.458950 | 38.282650 |

|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| S | 24.753565 | 30.166969 | 32.665581 |
| S | 26.329937 | 31.044762 | 36.106510 |
| S | 30.148706 | 28.335283 | 35.768684 |
| S | 30.359638 | 32.756790 | 33.065506 |
| S | 33.357231 | 29.231089 | 31.442236 |
| S | 33.229385 | 30.424843 | 35.231400 |
| S | 36.738506 | 26.731588 | 34.466919 |
| S | 36.811333 | 30.666677 | 33.769421 |
|  |  |  |  |
|---|---|---|---|
| Ca | 40.100315 | 29.291138 | 31.405142 |
| Ca | 39.697575 | 29.180220 | 36.398567 |
| Ca | 46.586372 | 29.368031 | 33.837112 |
| Ca | 39.697575 | 29.180220 | 36.398567 |
| Ca | 46.586372 | 29.368031 | 33.837112 |
| S  | 27.125973 | 27.817371 | 36.604397 |
| S  | 27.379204 | 34.044727 | 34.318020 |
| S  | 30.386055 | 29.696205 | 32.499447 |
| S  | 33.783016 | 32.435501 | 32.433716 |
| S  | 36.797832 | 28.569857 | 31.150606 |
| S  | 36.297958 | 29.059034 | 36.517365 |
| S  | 39.847562 | 26.750568 | 33.762047 |
| S  | 40.433594 | 31.410561 | 33.958668 |
| S  | 43.790207 | 28.729412 | 31.550098 |
| S  | 44.509571 | 26.428835 | 38.218174 |

24

generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 25.051281 | 29.907230 | 32.391762 |
| Ca | 26.554871 | 31.327755 | 36.098995 |
| Ca | 30.175482 | 27.904575 | 35.763237 |
| Ca | 30.347607 | 32.861889 | 33.447983 |
| Ca | 33.294834 | 29.514622 | 31.365196 |
| Ca | 33.191425 | 30.312130 | 35.111435 |
| Ca | 36.482006 | 26.646412 | 34.158386 |
| Ca | 36.741714 | 30.784605 | 33.726933 |
| Ca | 40.124107 | 29.271166 | 31.477495 |
| Ca | 39.578194 | 29.287621 | 36.485065 |
| Ca | 46.814804 | 29.098480 | 34.092697 |
| Ca | 42.731052 | 29.116238 | 34.393761 |
| S  | 27.161089 | 27.862843 | 36.967052 |
| S  | 27.112375 | 34.051884 | 34.249706 |
| S  | 30.396534 | 29.778008 | 32.774651 |
| S  | 30.049454 | 31.479855 | 36.496162 |
| S  | 33.203285 | 27.366573 | 33.780296 |
| S  | 33.823017 | 32.522858 | 32.344250 |
| S  | 36.733177 | 28.692001 | 31.119114 |
| S  | 36.245930 | 29.101921 | 36.358780 |
| S  | 39.912529 | 26.870266 | 33.895279 |
| S  | 40.441353 | 31.414249 | 33.805367 |
| S  | 43.847393 | 28.649536 | 31.498034 |
| S  | 44.420437 | 26.568718 | 38.229012 |

24

generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 25.058470 | 29.922630 | 32.514427 |
| Ca | 26.580534 | 31.199245 | 36.186729 |
|   |     |     |     |
|---|-----|-----|-----|
| Ca | 30.173578 | 27.983757 | 35.550545 |
| Ca | 30.458183 | 32.722687 | 33.61713 |
| Ca | 33.337860 | 29.496222 | 31.122490 |
| Ca | 33.163532 | 30.298500 | 35.13026 |
| Ca | 36.611748 | 27.065458 | 34.145046 |
| Ca | 36.807106 | 31.171757 | 33.935364 |
| Ca | 40.119583 | 29.301632 | 31.506622 |
| Ca | 39.646240 | 29.335632 | 36.61804 |
| Ca | 46.578896 | 28.736900 | 33.918636 |
| Ca | 42.594879 | 29.189072 | 34.346684 |
| S  | 27.242886 | 27.833439 | 36.890240 |
| S  | 27.311779 | 33.900574 | 34.382175 |
| S  | 30.434744 | 29.705666 | 32.563889 |
| S  | 29.972290 | 31.319843 | 36.449738 |
| S  | 33.299828 | 27.412321 | 33.889191 |
| S  | 33.759949 | 23.519508 | 32.332214 |
| S  | 36.718498 | 28.720768 | 31.190031 |
| S  | 36.130051 | 29.249969 | 36.425098 |
| S  | 39.949970 | 26.982485 | 33.852020 |
| S  | 40.304214 | 31.357082 | 33.890381 |
| S  | 43.721550 | 28.381351 | 31.499912 |
| S  | 44.457489 | 26.584929 | 38.285526 |

24

generated by VMD

|   |     |     |     |
|---|-----|-----|-----|
| Ca | 25.187691 | 30.028332 | 32.537895 |
| Ca | 26.397602 | 31.333897 | 36.247749 |
| Ca | 30.140144 | 28.096710 | 35.823002 |
| Ca | 30.334656 | 32.858227 | 33.307766 |
| Ca | 33.233055 | 29.337288 | 31.105177 |
| Ca | 33.036983 | 30.188808 | 35.101212 |
| Ca | 36.604134 | 26.859222 | 34.181583 |
| Ca | 36.680492 | 30.823292 | 34.03543 |
| Ca | 40.254097 | 29.185074 | 31.467896 |
| Ca | 39.723167 | 29.133184 | 36.319576 |
| Ca | 46.942795 | 28.969036 | 33.763729 |
| Ca | 42.825901 | 29.322929 | 34.284771 |
| S  | 27.071968 | 28.001183 | 36.787025 |
| S  | 27.000294 | 33.919701 | 34.033745 |
| S  | 30.288017 | 29.809349 | 32.658352 |
| S  | 29.916098 | 31.344690 | 36.522808 |
| S  | 33.202248 | 27.474394 | 33.842373 |
| S  | 33.883614 | 32.435955 | 32.489178 |
| S  | 36.815453 | 28.742571 | 31.396555 |
| S  | 36.280045 | 29.097490 | 36.525654 |
| S  | 40.059341 | 26.920864 | 33.858665 |
| S  | 40.320724 | 31.382792 | 33.930950 |
|   | X         | Y         | Z         |
|---|-----------|-----------|-----------|
| S | 43.782112 | 28.498367 | 31.438168 |
| S | 44.453300 | 26.628059 | 38.373379 |

24

generated by VMD

| Ca | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| Ca | 25.256643 | 29.948942 | 32.448296 |
| Ca | 26.257236 | 31.100855 | 36.214256 |
| Ca | 29.904381 | 28.297745 | 36.918930 |
| Ca | 30.351387 | 32.768230 | 33.146111 |
| Ca | 33.456696 | 29.466703 | 31.188416 |
| Ca | 33.206272 | 30.302599 | 35.120419 |
| Ca | 36.316715 | 26.995916 | 34.215279 |
| Ca | 36.737362 | 30.950409 | 33.595169 |
| Ca | 40.339294 | 29.227646 | 31.420813 |
| Ca | 39.728878 | 29.220325 | 36.480255 |
| Ca | 46.774300 | 29.227367 | 34.042534 |
| Ca | 42.754562 | 29.291685 | 34.514206 |
| S  | 26.975792 | 27.847889 | 36.832413 |
| S  | 27.068249 | 33.951488 | 34.456871 |
| S  | 30.493389 | 29.708797 | 32.858669 |
| S  | 29.800310 | 31.485981 | 36.384106 |
| S  | 33.070225 | 27.384716 | 33.969452 |
| S  | 33.695290 | 32.463074 | 32.429893 |
| S  | 36.879105 | 28.630871 | 31.089699 |
| S  | 36.398365 | 29.241266 | 36.341175 |
| S  | 40.019142 | 26.928707 | 33.897156 |
| S  | 40.357918 | 31.276464 | 33.915291 |
| S  | 43.967903 | 28.558443 | 31.682426 |
| S  | 44.624496 | 26.111576 | 37.868847 |

24

generated by VMD

| Ca | X         | Y         | Z         |
|----|-----------|-----------|-----------|
| Ca | 25.579660 | 29.964794 | 32.091461 |
| Ca | 26.609732 | 31.328053 | 36.121735 |
| Ca | 30.337490 | 27.940247 | 35.864067 |
| Ca | 30.235699 | 33.109715 | 33.113808 |
| Ca | 33.348854 | 29.640532 | 31.514370 |
| Ca | 33.337765 | 30.330322 | 35.432678 |
| Ca | 36.602386 | 26.547585 | 34.482025 |
| Ca | 36.684982 | 30.563927 | 33.679916 |
| Ca | 40.115936 | 29.120865 | 31.408886 |
| Ca | 39.539848 | 29.300789 | 36.367538 |
| Ca | 46.581886 | 29.574430 | 33.887390 |
| Ca | 42.733124 | 29.244980 | 34.541763 |
| S  | 27.115047 | 27.906616 | 36.564304 |
| S  | 27.061729 | 34.204903 | 34.188934 |
| S  | 30.417259 | 29.668537 | 32.972248 |
| S  | 30.044798 | 31.387272 | 36.321980 |
| S       | 33.297825 | 27.435459 | 34.239719 |
|---------|-----------|-----------|-----------|
| S       | 33.723637 | 32.640808 | 32.740883 |
| S       | 36.450912 | 28.440104 | 31.187229 |
| S       | 36.399590 | 28.993065 | 36.430321 |
| S       | 39.990719 | 26.718754 | 33.686935 |
| S       | 40.132996 | 31.156578 | 33.676079 |
| S       | 43.686714 | 28.565920 | 31.520672 |
| S       | 44.405418 | 26.607141 | 37.995811 |

24

generated by VMD

| Ca      | 25.145859 | 29.895279 | 32.488716 |
|---------|-----------|-----------|-----------|
| Ca      | 26.823168 | 31.43917 | 35.950451 |
| Ca      | 30.213272 | 28.037624 | 35.818035 |
| Ca      | 30.314087 | 32.788109 | 33.275860 |
| Ca      | 33.353703 | 29.370806 | 31.216240 |
| Ca      | 33.290230 | 30.264965 | 35.265446 |
| Ca      | 36.378143 | 26.754328 | 34.185013 |
| Ca      | 36.627270 | 30.898178 | 33.760921 |
| Ca      | 40.043327 | 29.464128 | 31.537437 |
| Ca      | 39.646347 | 29.189461 | 36.469158 |
| Ca      | 46.621357 | 29.325104 | 34.004139 |
| Ca      | 42.619732 | 29.220287 | 34.360954 |
| S       | 27.172583 | 27.990982 | 36.785553 |
| S       | 27.210327 | 34.240192 | 34.092751 |
| S       | 30.355907 | 29.522629 | 32.781586 |
| S       | 30.274952 | 31.301012 | 36.432365 |
| S       | 33.110195 | 27.246761 | 34.067204 |
| S       | 33.741074 | 32.389328 | 32.557114 |
| S       | 36.576813 | 28.674221 | 31.270937 |
| S       | 36.414661 | 29.042469 | 36.323822 |
| S       | 40.053959 | 26.846176 | 33.699104 |
| S       | 40.308926 | 31.474140 | 33.933754 |
| S       | 43.792572 | 28.644360 | 31.620552 |
| S       | 44.345459 | 26.375954 | 38.133553 |

24

generated by VMD

| Ca      | 25.180153 | 29.872250 | 32.470314 |
|---------|-----------|-----------|-----------|
| Ca      | 26.501152 | 31.608311 | 36.197552 |
| Ca      | 30.251640 | 27.954586 | 35.780727 |
| Ca      | 30.173697 | 32.693356 | 33.261749 |
| Ca      | 33.360298 | 29.528076 | 31.392147 |
| Ca      | 33.194023 | 30.316305 | 35.295822 |
| Ca      | 36.850654 | 26.800772 | 34.281948 |
| Ca      | 36.573761 | 30.739483 | 33.536354 |
| Ca      | 40.088829 | 29.382446 | 31.310556 |
| Ca      | 39.716808 | 29.084644 | 36.542088 |
| Element | X1  | Y1  | Z1  |
|---------|-----|-----|-----|
| Ca      | 46.883911 | 29.354332 | 33.908142 |
| Ca      | 42.888084 | 29.111851 | 34.075199 |
| S       | 27.090311  | 28.049118 | 36.808624 |
| S       | 26.930298  | 34.192566 | 34.075199 |
| S       | 30.416767  | 29.635893 | 32.845657 |
| S       | 29.950645  | 31.338272 | 36.318264 |
| S       | 33.174114  | 27.283623 | 33.963379 |
| S       | 33.601070  | 32.570518 | 32.604485 |
| S       | 36.710526  | 28.523659 | 31.179173 |
| S       | 36.311695  | 29.281319 | 36.326832 |
| S       | 40.124714  | 26.759560 | 33.656864 |
| S       | 40.316818  | 31.348297 | 33.951660 |
| S       | 43.893368  | 28.690590 | 31.584753 |
| S       | 44.520538  | 26.271549 | 38.207558 |

24 generated by VMD

| Element | X1  | Y1  | Z1  |
|---------|-----|-----|-----|
| Ca      | 25.362392 | 29.834229 | 32.113937 |
| Ca      | 26.513548 | 31.342779 | 35.865726 |
| Ca      | 29.962208 | 28.343822 | 35.946857 |
| Ca      | 30.188129 | 32.710648 | 33.249207 |
| Ca      | 33.431789 | 29.623783 | 31.411091 |
| Ca      | 33.234894 | 30.298428 | 35.496178 |
| Ca      | 36.529472 | 26.855995 | 34.02916 |
| Ca      | 36.755844 | 30.799545 | 33.891830 |
| Ca      | 40.152771 | 29.266644 | 31.482330 |
| Ca      | 39.620720 | 29.179464 | 36.381668 |
| Ca      | 46.632896 | 29.504803 | 33.700851 |
| Ca      | 42.818119 | 28.892540 | 34.243309 |
| S       | 26.958805 | 27.870323 | 36.834507 |
| S       | 26.924623 | 34.182522 | 33.939541 |
| S       | 30.397135 | 29.614302 | 32.798111 |
| S       | 29.913708 | 31.451397 | 36.483799 |
| S       | 33.228718 | 27.288307 | 34.081398 |
| S       | 33.848198 | 32.430340 | 32.786308 |
| S       | 36.708652 | 28.610146 | 31.297829 |
| S       | 36.197105 | 29.220402 | 36.663021 |
| S       | 40.087456 | 26.675808 | 33.675064 |
| S       | 40.399799 | 31.329437 | 33.867367 |
| S       | 43.881992 | 28.606308 | 31.341854 |
| S       | 44.684956 | 26.459476 | 38.076061 |

24 generated by VMD

| Element | X1  | Y1  | Z1  |
|---------|-----|-----|-----|
| Ca      | 25.186546 | 30.022030 | 32.343765 |
| Ca      | 26.340572 | 31.502213 | 36.100620 |
| Ca      | 30.064388 | 28.067734 | 35.688633 |
| Ca      | 30.431988 | 32.682701 | 33.135845 |
|   |   |   |   |
|---|---|---|---|
| Ca | 33.445660 | 29.461876 | 31.417599 |
| Ca | 33.209625 | 30.379471 | 35.454891 |
| Ca | 36.455322 | 26.522915 | 34.438793 |
| Ca | 36.804680 | 30.805449 | 33.648167 |
| Ca | 40.326920 | 29.257454 | 31.551155 |
| Ca | 39.796745 | 29.014473 | 36.363144 |
| Ca | 46.519767 | 29.675146 | 33.700687 |
| Ca | 42.769981 | 29.168205 | 34.326714 |
| S  | 27.128925 | 27.988449 | 36.797935 |
| S  | 26.750839 | 34.079567 | 33.924465 |
| S  | 30.448830 | 29.640934 | 32.676373 |
| S  | 30.078583 | 31.477406 | 36.521637 |
| S  | 33.093796 | 27.313295 | 34.157856 |
| S  | 33.828716 | 32.470043 | 32.614609 |
| S  | 36.674465 | 28.538857 | 31.386684 |
| S  | 36.302860 | 29.128683 | 36.549030 |
| S  | 40.119637 | 26.776299 | 33.698429 |
| S  | 40.370472 | 31.304722 | 34.017387 |
| S  | 43.697781 | 28.773380 | 31.340008 |
| S  | 44.588463 | 26.340136 | 38.176277 |

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generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 25.269730 | 29.420240 | 32.190670 |
| Ca | 26.356422 | 31.336065 | 36.058964 |
| Ca | 30.064365 | 28.131191 | 35.866646 |
| Ca | 30.282141 | 32.787979 | 33.136555 |
| Ca | 33.214077 | 29.683655 | 31.358807 |
| Ca | 33.241764 | 30.329571 | 35.262112 |
| Ca | 36.503059 | 26.796909 | 34.333565 |
| Ca | 36.724346 | 31.097160 | 33.833420 |
| Ca | 40.176201 | 29.337534 | 31.372805 |
| Ca | 39.707100 | 29.166517 | 36.415718 |
| Ca | 46.862110 | 28.984097 | 33.808643 |
| Ca | 42.840115 | 29.181768 | 34.476841 |
| S  | 27.218666 | 28.231075 | 37.267345 |
| S  | 26.842907 | 33.918118 | 34.095383 |
| S  | 30.319918 | 29.561337 | 32.725079 |
| S  | 29.872322 | 31.402573 | 36.358433 |
| S  | 33.155674 | 27.321770 | 33.785343 |
| S  | 33.791241 | 32.702042 | 32.828743 |
| S  | 36.683281 | 28.835999 | 31.253765 |
| S  | 36.255966 | 29.177794 | 36.364441 |
| S  | 39.980865 | 26.963520 | 33.576061 |
| S  | 40.605022 | 31.477444 | 33.996170 |
| S  | 44.024094 | 28.473553 | 31.517609 |
| S  | 44.442497 | 26.073486 | 38.147518 |
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.662064  | 29.767145  | 32.009159  |
| Ca      | 26.423956  | 31.174747  | 36.177662  |
| Ca      | 30.203632  | 28.013100  | 35.898891  |
| Ca      | 30.385071  | 32.757046  | 33.214405  |
| Ca      | 33.205109  | 29.593613  | 31.391579  |
| Ca      | 33.268330  | 30.292690  | 35.384239  |
| Ca      | 36.428631  | 27.082067  | 34.355312  |
| Ca      | 36.590858  | 30.810135  | 33.658428  |
| Ca      | 40.412373  | 29.234451  | 31.237450  |
| Ca      | 39.712872  | 29.318562  | 36.586426  |
| Ca      | 46.623425  | 29.094433  | 34.063942  |
| Ca      | 42.729568  | 29.295527  | 34.478809  |
| S       | 27.299717  | 28.086674  | 37.141369  |
| S       | 27.098759  | 33.895760  | 34.099800  |
| S       | 30.291496  | 29.735981  | 32.769245  |
| S       | 30.065145  | 31.314453  | 36.573681  |
| S       | 33.139519  | 27.389568  | 33.953964  |
| S       | 33.785072  | 32.504551  | 32.595028  |
| S       | 36.630981  | 28.740164  | 30.998823  |
| S       | 36.382130  | 29.381477  | 36.397751  |
| S       | 39.771248  | 26.907501  | 33.766899  |
| S       | 40.323097  | 31.318340  | 33.804237  |
| S       | 43.758881  | 28.667805  | 31.523714  |
| S       | 44.241978  | 26.015591  | 37.949875  |

24 generated by VMD
|     |  S       |  S       |  S       |  S       |  S       |  S       |  S       |  S       |  S       |  S       |
|-----|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
|     | 36.721031| 28.736195| 31.221384| 36.252361| 29.011166| 36.619377| 40.043419| 26.938622| 33.436928| 40.315365|
|     | 31.221384| 36.619377| 33.436928| 36.619377| 33.436928| 40.315365| 43.768833| 28.994400| 31.465206| 44.367424|
|     | 31.221384| 36.619377| 33.436928| 36.619377| 33.436928| 40.315365| 43.768833| 28.994400| 31.465206| 44.367424|
|     | 31.221384| 36.619377| 33.436928| 36.619377| 33.436928| 40.315365| 43.768833| 28.994400| 31.465206| 44.367424|
|     |          |          |          |          |          |          |          |          |          |          |
|     | 24 generated by VMD
|     | Ca       | 25.444124| 29.650299| 32.288242| 26.413603| 31.369734| 36.011463| 30.147253| 27.988728| 35.784035|
|     | Ca       | 26.413603| 31.369734| 36.011463| 30.147253| 27.988728| 35.784035| 30.246449| 32.839592| 33.360226|
|     | Ca       | 30.147253| 27.988728| 35.784035| 30.246449| 32.839592| 33.360226| 33.346790| 29.418900| 31.337013|
|     | Ca       | 33.346790| 29.418900| 31.337013| 33.346790| 29.418900| 31.337013| 33.285759| 30.177402| 35.314774|
|     | Ca       | 33.285759| 30.177402| 35.314774| 33.285759| 30.177402| 35.314774| 36.586910| 26.860992| 33.903782|
|     | Ca       | 36.586910| 26.860992| 33.903782| 36.583958| 31.160412| 33.852066| 40.074638| 29.241055| 31.768562|
|     | Ca       | 39.670128| 29.533070| 36.558067| 46.792545| 28.804901| 33.196171| 42.712139| 29.191502| 34.624538|
|     | Ca       | 42.712139| 29.191502| 34.624538| 27.441284| 28.363638| 37.150570| 26.683588| 34.033607| 33.772503|
|     | Ca       | 27.441284| 28.363638| 37.150570| 26.683588| 34.033607| 33.772503| 30.456951| 29.544949| 32.798584|
|     | Ca       | 30.456951| 29.544949| 32.798584| 30.456951| 29.544949| 32.798584| 30.153236| 31.309177| 36.402222|
|     | Ca       | 33.367329| 27.328484| 33.762760| 33.367329| 27.328484| 33.762760| 33.762550| 32.400566| 32.685196|
|     | Ca       | 33.762550| 32.400566| 32.685196| 33.770691| 28.883869| 31.313335| 36.274830| 29.062187| 36.400024|
|     | Ca       | 36.274830| 29.062187| 36.400024| 39.860043| 26.861885| 33.973625| 40.534203| 31.563671| 34.072052|
|     | Ca       | 40.534203| 31.563671| 34.072052| 43.452049| 28.539482| 31.579838| 44.372925| 26.263309| 38.121033|
|     | Ca       | 44.372925| 26.263309| 38.121033|          |          |          |          |          |          |
|     | 24 generated by VMD
|     | Ca       | 25.118542| 29.668144| 32.138214| 26.509953| 31.358273| 36.070053| 29.959837| 28.118553| 35.574669|
|     | Ca       | 29.959837| 28.118553| 35.574669| 30.394245| 32.736351| 33.299053| 33.368843| 29.732811| 31.398981|
|     | Ca       | 33.368843| 29.732811| 31.398981| 33.294106| 30.153418| 35.274521| 36.572193| 26.937191| 34.341194|
|     | Ca       | 36.572193| 26.937191| 34.341194| 36.729782| 31.080942| 33.873383| 40.124836| 29.027260| 31.576206|
|     | Ca       | 40.124836| 29.027260| 31.576206| 39.847256| 29.093773| 36.778915| 46.698818| 29.123108| 33.119038|
|     | Ca       | 46.698818| 29.123108| 33.119038| 42.717598| 29.255426| 34.534988| 42.717598| 29.255426| 34.534988|
|    |    |    |    |
|----|----|----|----|
| S  | 27.119696 | 28.102798 | 36.847755 |
| S  | 26.963631 | 33.950554 | 34.012791 |
| S  | 30.322227 | 29.679314 | 32.546341 |
| S  | 30.143326 | 31.285717 | 36.308907 |
| S  | 33.151375 | 27.211962 | 33.945087 |
| S  | 33.877834 | 32.619110 | 32.704674 |
| S  | 36.589859 | 28.704889 | 31.412230 |
| S  | 36.418179 | 29.366467 | 36.580719 |
| S  | 39.919373 | 26.889217 | 34.187370 |
| S  | 40.328426 | 31.208748 | 33.988541 |
| S  | 43.491110 | 28.541641 | 31.458523 |
| S  | 44.769844 | 26.545811 | 38.058498 |

24 generated by VMD

| Ca  | 25.382740 | 29.839466 | 32.106956 |
| Ca  | 26.420095 | 31.356989 | 35.801506 |
| Ca  | 30.109802 | 27.880615 | 35.932335 |
| Ca  | 30.144882 | 32.658051 | 33.056286 |
| Ca  | 33.368221 | 29.328358 | 31.579134 |
| Ca  | 33.219563 | 30.221485 | 35.339874 |
| Ca  | 36.524860 | 27.105160 | 34.254185 |
| Ca  | 36.896324 | 31.484444 | 34.196396 |
| Ca  | 40.136364 | 29.637465 | 31.608280 |
| Ca  | 39.958122 | 29.306026 | 36.794174 |
| Ca  | 46.688572 | 28.379259 | 33.332001 |
| Ca  | 42.779934 | 29.223295 | 34.105743 |
| S   | 27.030230 | 27.977991 | 36.892426 |
| S   | 26.773949 | 34.024406 | 33.707031 |
| S   | 30.465744 | 29.482931 | 32.820702 |
| S   | 29.931801 | 31.156403 | 36.257042 |
| S   | 33.266098 | 27.232391 | 34.287537 |
| S   | 33.629898 | 32.565071 | 32.767784 |
| S   | 36.744877 | 28.942924 | 31.618275 |
| S   | 36.386761 | 29.460579 | 36.622978 |
| S   | 39.839806 | 27.012102 | 33.721874 |
| S   | 40.594189 | 31.499903 | 34.043243 |
| S   | 43.629086 | 28.363995 | 31.272451 |
| S   | 44.511929 | 26.252115 | 37.912453 |

24 generated by VMD

| Ca  | 25.135042 | 29.619587 | 32.237110 |
| Ca  | 26.539942 | 31.169022 | 36.052570 |
| Ca  | 30.286446 | 28.083553 | 35.817318 |
| Ca  | 30.290516 | 32.737652 | 33.151714 |
| Ca  | 33.329285 | 29.713539 | 31.452448 |
| Ca  | 33.340290 | 30.336384 | 35.255913 |
|   |   |   |   |
|---|---|---|---|
| Ca | 36.422298 | 27.220085 | 34.391644 |
| Ca | 36.816616 | 31.348709 | 34.020306 |
| Ca | 40.169327 | 29.292767 | 31.479385 |
| Ca | 39.829529 | 29.215225 | 36.498039 |
| Ca | 46.727543 | 28.403217 | 33.420746 |
| Ca | 42.681160 | 29.109446 | 34.310394 |
| S  | 27.179253 | 27.749239 | 36.617855 |
| S  | 27.004498 | 33.851707 | 33.975395 |
| S  | 30.428719 | 29.519791 | 32.734619 |
| S  | 30.052801 | 31.349062 | 36.335049 |
| S  | 33.177162 | 27.425406 | 33.872452 |
| S  | 33.693993 | 32.688850 | 32.839607 |
| S  | 36.697086 | 28.910984 | 31.592216 |
| S  | 36.252861 | 29.527054 | 36.587650 |
| S  | 39.842690 | 26.850552 | 33.864246 |
| S  | 40.423225 | 31.379801 | 33.916824 |
| S  | 43.536877 | 28.403530 | 31.447525 |
| S  | 44.576752 | 26.486277 | 38.159698 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 25.000843 | 29.868084 | 32.247833 |
| Ca | 26.553425 | 31.177803 | 35.913788 |
| Ca | 30.131683 | 27.913357 | 35.882000 |
| Ca | 30.451372 | 32.820591 | 33.350647 |
| Ca | 33.253628 | 29.738983 | 31.252682 |
| Ca | 33.176701 | 30.237896 | 35.230545 |
| Ca | 36.583813 | 26.825031 | 34.512257 |
| Ca | 36.863079 | 31.076790 | 33.826435 |
| Ca | 40.070377 | 29.168507 | 31.413277 |
| Ca | 39.950928 | 29.366003 | 36.776878 |
| Ca | 46.572315 | 29.019814 | 33.322998 |
| Ca | 42.671925 | 29.285488 | 34.481712 |
| S  | 26.938168 | 27.971409 | 36.747147 |
| S  | 27.306108 | 33.962303 | 33.929157 |
| S  | 30.460323 | 29.687077 | 32.806107 |
| S  | 29.903360 | 31.299030 | 36.291599 |
| S  | 33.165134 | 27.192318 | 33.920792 |
| S  | 33.999935 | 32.496994 | 32.673668 |
| S  | 36.527534 | 28.555016 | 31.451614 |
| S  | 36.481533 | 29.245773 | 36.624355 |
| S  | 39.857643 | 27.003904 | 33.983780 |
| S  | 40.468933 | 31.306572 | 33.794456 |
| S  | 43.574734 | 28.607666 | 31.312538 |
| S  | 44.470341 | 26.565022 | 38.284363 |

24 generated by VMD
24

generated by VMD

Ca 25.264191  29.943792  32.069633
Ca 26.438904  31.302610  35.990772
Ca 30.165092  27.911148  35.828606
Ca 30.391310  32.579613  33.506908
Ca 33.168457  29.619907  31.371088
Ca 33.200390  30.293810  35.466393
Ca 36.292587  26.953947  34.248898
Ca 36.914307  31.244713  33.667439
Ca 40.227299  29.506657  31.346388
Ca 39.769020  29.380199  36.457050
Ca 46.876411  28.631191  33.485016
Ca 42.619812  29.002178  34.360138
S  27.064341  27.847343  36.838650
S  27.124115  34.035946  34.137135
S  30.314529  29.549301  32.742577
S  29.793701  31.297676  36.530167
S  33.082314  27.143415  34.049557
S  33.941021  32.295597  32.84467
S  36.681473  28.740961  31.159420
S  36.438530  29.475094  36.400097
S  39.797260  27.102423  33.655136
S  40.693962  31.565678  33.705772
S  43.807308  28.189758  31.552177
S  44.367626  26.778458  38.617146

Ca  25.305450  29.814022  32.099056
Ca  26.431589  31.201664  35.906528
Ca  30.185944  27.927094  35.959747
Ca  30.440445  32.548172  33.203182
Ca  33.446953  29.808975  31.467716
Ca  33.064045  30.298470  35.375584
Ca  36.467937  26.906834  34.345726
Ca  36.785072  31.335979  33.713577
Ca  40.096405  29.278645  31.483303
Ca  39.785797  29.628532  36.386692
Ca  46.768829  28.633986  33.077366
Ca  42.707558  29.125359  34.478951
S  27.049501  27.920620  36.818710
S  27.115456  33.961884  33.924381
S  30.458288  29.485767  32.800072
S  29.846397  31.181122  36.417923
S  33.290627  27.140457  34.151852
S  33.858791  32.630978  33.045280
S  36.668011  28.825108  31.499542
S  36.319221  29.660702  36.384968
|    |               |               |               |
|----|---------------|---------------|---------------|
| S  | 39.963432     | 27.001333     | 33.905052     |
| S  | 40.524319     | 31.447443     | 33.778076     |
| S  | 43.675617     | 28.381020     | 31.387291     |
| S  | 44.178211     | 26.247232     | 38.420105     |

24 generated by VMD

Ca | 25.124870 | 29.547319 | 32.021671 |
Ca | 26.130119 | 31.297480 | 35.812195 |
Ca | 30.176262 | 28.039436 | 35.892643 |
Ca | 30.121222 | 32.796581 | 33.319790 |
Ca | 33.342548 | 29.696583 | 31.403303 |
Ca | 33.090309 | 30.238428 | 35.279552 |
Ca | 36.720783 | 27.155510 | 34.471424 |
Ca | 36.704357 | 31.171062 | 33.829277 |
Ca | 40.002857 | 29.397591 | 31.631659 |
Ca | 39.890522 | 29.234121 | 36.633625 |
Ca | 46.916878 | 28.638861 | 32.932091 |
Ca | 42.955463 | 29.125374 | 34.489487 |
S  | 27.115910 | 28.030548 | 36.776001 |
S  | 26.914570 | 34.004105 | 33.961201 |
S  | 30.381447 | 29.546326 | 32.772789 |
S  | 29.648594 | 31.351662 | 36.317513 |
S  | 33.391178 | 27.363129 | 34.181297 |
S  | 33.720142 | 32.616642 | 32.756485 |
S  | 36.734386 | 28.708050 | 31.384903 |
S  | 36.341728 | 29.609241 | 36.620842 |
S  | 40.051655 | 26.846634 | 34.068153 |
S  | 40.637100 | 31.334930 | 33.933033 |
S  | 43.551880 | 28.546253 | 31.420952 |
S  | 44.769161 | 26.095585 | 38.120773 |

24 generated by VMD

Ca | 24.830742 | 29.966419 | 32.341160 |
Ca | 26.137344 | 31.373745 | 35.716618 |
Ca | 29.898417 | 27.925640 | 35.812202 |
Ca | 30.454657 | 32.737026 | 33.139172 |
Ca | 33.437763 | 29.561476 | 31.290161 |
Ca | 33.297409 | 30.166729 | 35.331886 |
Ca | 36.509598 | 26.736748 | 34.558064 |
Ca | 36.693943 | 30.810917 | 33.878738 |
Ca | 40.055248 | 29.394201 | 31.788651 |
Ca | 39.843758 | 29.376415 | 36.757603 |
Ca | 46.758904 | 28.683327 | 32.740158 |
Ca | 42.914215 | 29.379078 | 34.326813 |
S  | 26.976851 | 28.147327 | 36.874596 |
S  | 27.108128 | 34.036835 | 33.653877 |
|   |   |   |   |
|---|---|---|---|
| S | 30.601315 | 29.559147 | 32.770508 |
| S | 29.729973 | 31.271084 | 36.273140 |
| S | 33.338531 | 27.167814 | 34.218784 |
| S | 33.919769 | 32.428669 | 32.710361 |
| S | 36.743744 | 28.483829 | 31.500320 |
| S | 36.469162 | 29.323620 | 36.693005 |
| S | 40.071785 | 27.111839 | 34.092934 |
| S | 40.393848 | 31.520897 | 34.087013 |
| S | 43.597267 | 28.934929 | 31.211735 |
| S | 44.651546 | 26.293659 | 38.263222 |

24 generated by VMD

| Ca | 24.778282 | 30.031395 | 32.221611 |
| Ca | 26.454298 | 31.514076 | 35.657887 |
| Ca | 30.224434 | 27.936283 | 35.989132 |
| Ca | 30.166071 | 32.665241 | 33.325348 |
| Ca | 33.311302 | 29.230961 | 31.255186 |
| Ca | 33.012352 | 30.087719 | 35.294300 |
| Ca | 36.730198 | 26.894633 | 34.397301 |
| Ca | 36.653721 | 30.793072 | 33.990665 |
| Ca | 40.143051 | 29.431011 | 31.682718 |
| Ca | 39.833427 | 29.366596 | 36.438992 |
| Ca | 47.148449 | 28.739069 | 32.689266 |
| Ca | 43.097359 | 29.471212 | 34.438713 |
| S | 27.075659 | 28.369755 | 36.993454 |
| S | 27.096512 | 34.247818 | 33.837391 |
| S | 30.275948 | 29.540501 | 32.885662 |
| S | 29.926811 | 31.319107 | 36.357906 |
| S | 33.272728 | 27.006533 | 33.992332 |
| S | 33.755157 | 32.345573 | 32.582504 |
| S | 36.743050 | 28.657278 | 31.501560 |
| S | 36.165329 | 29.168180 | 36.550449 |
| S | 40.174767 | 26.950699 | 33.893234 |
| S | 40.337124 | 31.419388 | 34.041050 |
| S | 43.926540 | 28.835115 | 31.659698 |
| S | 44.131405 | 26.370407 | 38.389183 |

24 generated by VMD

| Ca | 25.221680 | 30.072718 | 32.171989 |
| Ca | 26.327503 | 31.309177 | 35.731911 |
| Ca | 30.452421 | 27.916275 | 35.867031 |
| Ca | 30.003429 | 32.632324 | 33.329418 |
| Ca | 33.299603 | 29.310678 | 31.456959 |
| Ca | 33.173965 | 30.152784 | 35.303345 |
| Ca | 36.705540 | 26.876789 | 34.530079 |
| Ca | 36.755772 | 30.997749 | 34.002758 |
Ca  40.032784  29.393116  31.436512
Ca  39.774769  29.355717  36.684074
Ca  46.855537  28.561146  32.726051
Ca  42.572552  29.234180  34.384087
S   27.337822  28.126015  36.791138
S   26.949570  34.252460  33.662468
S   30.350189  29.508009  32.779930
S   29.912399  31.337116  36.358200
S   33.424240  27.306273  34.133614
S   33.800819  32.514278  32.844749
S   36.676205  28.536861  31.559765
S   36.405411  29.331944  36.626801
S   39.981209  26.967535  33.965218
S   40.515511  31.491833  33.863022
S   43.620846  28.705046  31.454903
S   44.284138  26.501350  38.366760

generated by VMD
Ca  25.290699  30.104809  31.977890
Ca  26.370220  31.261272  35.630836
Ca  30.115334  28.037231  35.890644
Ca  30.263586  32.691135  33.36853
Ca  33.366005  29.456066  31.568066
Ca  33.201908  30.197670  35.402512
Ca  36.473312  26.882107  34.425392
Ca  36.652920  31.168350  33.930401
Ca  40.187202  28.927443  31.254171
Ca  39.810699  29.633480  36.340141
Ca  47.037239  28.797951  32.888184
Ca  42.900810  29.080364  34.487938
S   27.030111  28.021597  36.805523
S   27.008057  34.142143  33.831207
S   30.451838  29.463558  32.824863
S   29.920713  31.315731  36.525085
S   33.141632  27.119518  34.155663
S   33.603371  32.475601  32.926418
S   36.774521  28.642990  31.836155
S   36.362720  29.359512  36.564644
S   39.940563  26.928894  33.989220
S   40.527283  31.452282  33.756912
S   43.637642  28.739674  31.153202
S   44.365555  26.492031  38.528770

generated by VMD
Ca  25.482944  29.919289  32.261696
Ca  26.503204  31.416328  35.900375
Ca  30.282007  27.921474  35.851448
Ca  30.399868  32.644386  33.487442
Ca  33.263607  30.310516  35.301872
Ca  36.461807  26.681087  34.225403
Ca  36.709221  30.838795  33.674412
Ca  40.120262  29.087372  31.562099
Ca  39.491695  29.214909  36.641346
Ca  46.622231  28.848461  33.255295
Ca  42.883339  29.147661  34.502937
S   27.105114  28.115322  36.974625
S   27.090235  34.165333  33.920395
S   30.413401  29.052834  32.820995
S   30.036972  31.229975  36.490818
S   33.195442  27.300203  33.758659
S   33.799889  32.562180  32.720234
S   36.726097  28.635040  31.294338
S   36.320131  29.219305  36.358368
S   39.915131  26.852182  34.076042
S   40.205612  31.368290  33.824654
S   43.583649  28.884264  31.302471
S   44.543022  26.850739  38.541245

24

generated by VMD
Ca  25.290174  29.979700  32.140419
Ca  26.604931  31.471966  35.642094
Ca  30.082859  27.916889  35.864521
Ca  30.259014  32.761177  33.588985
Ca  33.414890  29.627842  31.432207
Ca  33.196068  30.060734  35.586363
Ca  36.682983  26.648947  34.211449
Ca  36.730080  30.796036  33.707020
Ca  40.029034  28.885918  31.435951
Ca  39.567898  29.442873  36.515682
Ca  46.529072  28.503323  33.093307
Ca  42.716316  29.227133  34.319931
S   26.990868  28.081654  36.629887
S   27.220875  34.253307  33.967949
S   30.466309  29.577753  32.998734
S   30.097591  31.145765  36.572491
S   33.339920  27.257545  33.951553
S   33.832211  32.584431  32.930798
S   36.676319  28.546547  31.357624
S   36.521526  29.073040  36.334526
S   40.023163  26.831682  34.039246
S   40.335358  31.427988  33.568970
S  43.580750  28.866375  31.347240
S  44.245682  27.422764  38.871452

24 generated by VMD
Ca  25.138374  29.751055  32.261429
Ca  26.386272  31.383808  35.796135
Ca  30.127445  27.661720  35.589207
Ca  30.132332  32.891045  33.481903
Ca  33.391071  29.733643  31.536953
Ca  33.162628  30.332542  35.354153
Ca  36.723198  26.777874  34.425255
Ca  36.799557  31.019207  33.892441
Ca  40.164734  29.052437  31.611294
Ca  39.782516  29.408150  36.321560
Ca  46.457520  28.361170  33.049438
Ca  43.050537  29.086681  34.298466
S  27.143040  28.006332  36.707909
S  26.881691  34.235043  34.054680
S  30.420835  29.789066  32.661774
S  29.821495  31.162834  36.240971
S  33.231583  27.203114  34.038303
S  33.722115  32.618153  32.950066
S  36.690063  28.781960  31.587265
S  36.312798  29.208799  36.584587
S  40.137741  26.784006  33.931114
S  40.587978  31.453335  33.728901
S  43.617264  28.543903  31.158243
S  44.551125  27.145512  38.768555

24 generated by VMD
Ca  25.218708  30.037670  32.061615
Ca  26.600513  31.152828  35.708069
Ca  30.416061  27.795815  35.592110
Ca  30.393250  32.852497  33.647938
Ca  33.372707  29.654308  31.548832
Ca  33.157074  30.493423  35.719582
Ca  36.622314  26.660923  34.488945
Ca  36.639587  30.762148  33.700775
Ca  39.983013  29.053368  31.696423
Ca  39.678444  29.699438  36.595757
Ca  46.504372  28.724724  33.239796
Ca  42.863926  28.959702  34.228523
S  27.143061  27.956776  36.593033
S  27.100180  34.082397  33.777794
S  30.413061  29.696653  32.736019
S  29.947878  31.203392  36.526913
|   |   |   |
|---|---|---|
| S | 33.357544 | 27.333441 | 34.126205 |
| S | 33.675541 | 32.570957 | 32.861897 |
| S | 36.596401 | 28.445181 | 31.421722 |
| S | 36.331932 | 29.443256 | 36.456718 |
| S | 39.946136 | 26.872288 | 34.109322 |
| S | 40.372772 | 31.440926 | 33.635994 |
| S | 43.521652 | 28.724291 | 31.195194 |
| S | 44.577782 | 26.774998 | 38.361549 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 24.976357 | 29.954735 | 32.184910 |
| Ca | 26.508520 | 31.159060 | 35.854286 |
| Ca | 30.164715 | 27.929619 | 35.929111 |
| Ca | 30.217751 | 32.813358 | 33.321674 |
| Ca | 33.445454 | 29.805197 | 31.488291 |
| Ca | 33.314529 | 30.207817 | 35.403137 |
| Ca | 36.393597 | 26.867558 | 34.810562 |
| Ca | 36.904564 | 30.961525 | 33.870277 |
| Ca | 40.183735 | 28.995783 | 31.582491 |
| Ca | 39.872536 | 29.630201 | 36.568237 |
| Ca | 46.478149 | 28.261375 | 33.058231 |
| Ca | 42.854000 | 29.212910 | 36.547108 |
| S | 27.068684 | 27.878201 | 36.594154 |
| S | 26.858925 | 33.917648 | 33.975555 |
| S | 30.406631 | 29.686384 | 32.595863 |
| S | 29.947708 | 31.220778 | 36.469276 |
| S | 33.205402 | 27.238548 | 33.996384 |
| S | 33.692959 | 32.587151 | 32.762085 |
| S | 36.707661 | 28.641109 | 31.515942 |
| S | 36.452171 | 29.560818 | 36.543365 |
| S | 39.732166 | 27.037464 | 34.126709 |
| S | 40.536461 | 31.419680 | 33.693565 |
| S | 43.637268 | 28.733494 | 31.358887 |
| S | 44.873974 | 26.670946 | 38.116894 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 24.387321 | 30.316990 | 32.457832 |
| Ca | 26.563326 | 31.346062 | 35.932335 |
| Ca | 30.074188 | 28.045471 | 35.782776 |
| Ca | 30.274508 | 32.545464 | 33.252926 |
| Ca | 33.343079 | 29.525566 | 31.639511 |
| Ca | 33.114941 | 30.172462 | 35.409500 |
| Ca | 36.451714 | 26.565380 | 34.010124 |
| Ca | 36.826046 | 30.830570 | 33.763390 |
| Ca | 40.308327 | 29.120386 | 31.234104 |
| Ca | 39.744110 | 29.776535 | 36.759949 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 46.759003    | 28.460857    | 33.529564    |
| Ca      | 42.921654    | 29.056839    | 34.625980    |
| S       | 26.962770    | 27.965958    | 36.721893    |
| S       | 27.256718    | 34.001816    | 33.757912    |
| S       | 30.327364    | 29.547829    | 32.735909    |
| S       | 30.059578    | 31.185810    | 36.369217    |
| S       | 33.301533    | 27.187325    | 34.147377    |
| S       | 33.782207    | 32.598873    | 32.705772    |
| S       | 36.692482    | 28.624699    | 31.433676    |
| S       | 36.546219    | 29.123474    | 36.363548    |
| S       | 40.002281    | 27.145462    | 34.033676    |
| S       | 40.395393    | 31.317535    | 33.578030    |
| S       | 43.801235    | 29.089293    | 31.269312    |
| S       | 44.537933    | 26.840733    | 38.516384    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 24.741413    | 30.203657    | 32.549091    |
| Ca      | 26.403030    | 31.317116    | 36.013760    |
| Ca      | 29.837519    | 27.962528    | 35.594147    |
| Ca      | 30.268127    | 32.679947    | 33.355610    |
| Ca      | 33.548893    | 29.854008    | 31.338469    |
| Ca      | 33.035263    | 30.112741    | 35.324333    |
| Ca      | 36.614895    | 26.932051    | 34.464127    |
| Ca      | 36.752403    | 30.896671    | 33.777748    |
| Ca      | 40.170742    | 28.924419    | 31.757065    |
| Ca      | 39.735271    | 29.456440    | 36.486603    |
| Ca      | 46.756485    | 28.872944    | 33.181850    |
| Ca      | 42.953773    | 29.272381    | 34.453880    |
| S       | 26.921486    | 27.921719    | 36.586018    |
| S       | 27.019985    | 34.062088    | 33.713078    |
| S       | 30.453829    | 29.541649    | 32.616547    |
| S       | 30.025009    | 31.205406    | 36.630272    |
| S       | 33.097828    | 27.261097    | 33.855038    |
| S       | 33.789967    | 32.547867    | 32.910892    |
| S       | 36.845779    | 28.510696    | 31.358524    |
| S       | 36.256680    | 29.310680    | 36.535892    |
| S       | 40.061234    | 26.851290    | 34.212067    |
| S       | 40.595436    | 31.296602    | 33.757172    |
| S       | 43.731567    | 28.623451    | 31.325642    |
| S       | 44.817268    | 26.773945    | 38.232822    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 24.563904    | 30.603302    | 32.486794    |
| Ca      | 26.223286    | 31.374508    | 36.152527    |
| Ca      | 30.254566    | 27.633818    | 35.628574    |
| Ca      | 30.107407    | 32.536373    | 33.390076    |

916
| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 33.349869 | 29.620441 | 31.237 |
| Ca      | 32.982239 | 30.206659 | 35.304314 |
| Ca      | 36.809860 | 26.684992 | 34.301319 |
| Ca      | 36.577171 | 30.795038 | 33.584240 |
| Ca      | 40.112072 | 29.065849 | 31.895111 |
| Ca      | 39.786148 | 29.852444 | 36.595039 |
| Ca      | 46.667999 | 28.520861 | 33.218609 |
| Ca      | 43.167946 | 29.266609 | 34.573887 |
| S       | 27.078789 | 28.046707 | 36.618668 |
| S       | 27.045258 | 34.156082 | 38.816467 |
| S       | 30.370281 | 29.519407 | 32.720970 |
| S       | 29.847439 | 31.129480 | 36.461170 |
| S       | 33.333267 | 27.324680 | 33.858757 |
| S       | 33.544415 | 32.533596 | 32.709484 |
| S       | 36.869591 | 28.581491 | 31.233925 |
| S       | 36.301281 | 29.251657 | 36.323219 |
| S       | 40.323009 | 26.854269 | 34.290108 |
| S       | 40.459179 | 31.621889 | 33.803307 |
| S       | 43.640293 | 28.514744 | 31.558065 |
| S       | 45.018661 | 26.696556 | 38.268826 |

24

generated by VMD

| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 24.830341 | 29.978500 | 32.280930 |
| Ca      | 26.056633 | 31.251524 | 36.078381 |
| Ca      | 30.159483 | 28.021200 | 35.688442 |
| Ca      | 30.298092 | 32.879284 | 33.180584 |
| Ca      | 33.558422 | 29.711584 | 31.564190 |
| Ca      | 33.170528 | 30.382822 | 35.435371 |
| Ca      | 36.556232 | 26.683445 | 34.306774 |
| Ca      | 36.773422 | 30.819630 | 33.578705 |
| Ca      | 40.280849 | 28.960773 | 31.807232 |
| Ca      | 39.810768 | 29.580757 | 36.599926 |
| Ca      | 46.673683 | 28.843002 | 33.214123 |
| Ca      | 42.925568 | 29.125858 | 34.334133 |
| S       | 27.007481 | 27.954992 | 36.575314 |
| S       | 26.975159 | 33.887421 | 34.128788 |
| S       | 30.646881 | 29.684019 | 32.648502 |
| S       | 29.927992 | 31.321262 | 36.447533 |
| S       | 33.366734 | 27.332256 | 34.047615 |
| S       | 33.674454 | 32.703991 | 32.950661 |
| S       | 36.910561 | 28.505510 | 31.393915 |
| S       | 36.435417 | 29.195129 | 36.286858 |
| S       | 40.075020 | 26.805019 | 34.147987 |
| S       | 40.366444 | 31.453066 | 33.660503 |
| S       | 43.622902 | 28.571665 | 31.160824 |
| S       | 44.330864 | 26.738691 | 38.513477 |
|   | Ca     | S       |
|---|--------|---------|
| 1 | 24.697550 | 30.333168 |
| 2 | 26.106869 | 31.367537 |
| 3 | 29.975557 | 27.940449 |
| 4 | 30.226166 | 32.825203 |
| 5 | 33.394180 | 29.682180 |
| 6 | 32.965878 | 30.100574 |
| 7 | 36.629135 | 26.716900 |
| 8 | 36.871834 | 30.707214 |
| 9 | 40.327774 | 28.790136 |
|10 | 39.918091 | 29.537430 |
|11 | 46.923008 | 29.077715 |
|12 | 43.149933 | 29.418079 |
|13 | 26.535660 | 27.967743 |
|14 | 26.999542 | 34.106884 |
|15 | 30.297968 | 29.706423 |
|16 | 29.811710 | 31.269276 |
|17 | 33.231026 | 27.095284 |
|18 | 33.830147 | 32.590374 |
|19 | 36.702366 | 28.399424 |
|20 | 36.494125 | 29.244997 |
|21 | 40.162933 | 26.853180 |
|22 | 40.329033 | 31.284412 |
|23 | 43.766396 | 28.691319 |
|24 | 45.087029 | 26.685461 |

24 generated by VMD

|   | Ca     | S       |
|---|--------|---------|
| 1 | 24.963337 | 30.032118 |
| 2 | 26.530943 | 31.361338 |
| 3 | 30.327110 | 27.985701 |
| 4 | 30.274399 | 32.942104 |
| 5 | 33.324329 | 29.857597 |
| 6 | 33.179649 | 30.324987 |
| 7 | 36.673363 | 26.665567 |
| 8 | 36.582233 | 30.658749 |
| 9 | 40.119652 | 28.814228 |
|10 | 39.786366 | 29.393040 |
|11 | 46.658127 | 29.329227 |
|12 | 42.887981 | 29.353785 |
|13 | 27.014065 | 27.829378 |
|14 | 26.876509 | 34.009823 |
|15 | 30.491945 | 29.643456 |
|16 | 29.909975 | 31.475903 |
|17 | 33.339775 | 27.315205 |
|18 | 33.817741 | 32.702225 |
|   |   |   |   |
|---|---|---|---|
| S | 36.628754 | 28.417648 | 31.502155 |
| S | 36.428162 | 29.152271 | 36.515762 |
| S | 40.047291 | 26.821247 | 34.280483 |
| S | 40.332554 | 31.226444 | 33.535915 |
| S | 43.652527 | 28.639896 | 31.336441 |
| S | 44.587135 | 26.439434 | 38.091389 |

24

generated by VMD

| Ca | 25.129585 | 29.848124 | 32.060829 |
| Ca | 26.433388 | 31.813641 | 35.874008 |
| Ca | 29.990429 | 27.950735 | 35.673271 |
| Ca | 30.450426 | 32.767799 | 33.279652 |
| Ca | 33.381008 | 29.559160 | 31.259899 |
| Ca | 33.105648 | 29.976738 | 35.543999 |
| Ca | 36.482414 | 26.490440 | 34.575603 |
| Ca | 36.611610 | 30.680130 | 34.004204 |
| Ca | 39.957436 | 29.282284 | 31.841822 |
| Ca | 39.774872 | 29.317062 | 36.592999 |
| Ca | 46.655460 | 29.225491 | 33.087784 |
| Ca | 42.894287 | 29.219311 | 34.395203 |
| S | 27.151794 | 28.425152 | 36.846127 |
| S | 27.083725 | 34.057495 | 33.537876 |
| S | 30.554771 | 29.646252 | 32.753075 |
| S | 29.966206 | 31.317196 | 36.438011 |
| S | 33.313606 | 27.147539 | 34.007828 |
| S | 33.752037 | 32.362743 | 32.858727 |
| S | 36.742386 | 28.356337 | 31.339918 |
| S | 36.394382 | 28.959759 | 36.663872 |
| S | 39.958252 | 26.907139 | 34.189709 |
| S | 40.197178 | 31.453344 | 34.005283 |
| S | 43.365730 | 28.975666 | 31.220448 |
| S | 45.087288 | 26.651836 | 37.979099 |

24

generated by VMD

| Ca | 24.724419 | 30.338919 | 32.249924 |
| Ca | 26.194645 | 31.564348 | 36.217014 |
| Ca | 30.014179 | 27.971920 | 35.810204 |
| Ca | 30.400951 | 32.887280 | 33.348312 |
| Ca | 33.497551 | 29.531485 | 31.451748 |
| Ca | 33.090340 | 30.194799 | 35.409256 |
| Ca | 36.693577 | 26.543591 | 34.367645 |
| Ca | 36.797268 | 30.721096 | 33.497780 |
| Ca | 40.103664 | 28.898991 | 31.376064 |
| Ca | 39.717888 | 29.105331 | 36.481209 |
| Ca | 46.854710 | 29.437687 | 33.307129 |
| Ca | 43.142845 | 29.184500 | 34.525520 |
S  26.864525  28.022594  36.585049
S  27.069290  34.068268  33.865894
S  30.450565  29.700054  32.728027
S  29.667294  31.254530  36.501831
S  32.293499  27.264120  34.039745
S  33.794800  32.545269  32.832661
S  36.793819  28.299154  31.319035
S  36.287117  29.165291  36.446781
S  40.213604  26.685791  34.014858
S  40.230938  31.094107  33.689972
S  43.734158  28.925842  31.379324
S  44.802216  26.986473  38.585640
24
  generated by VMD
Ca  24.802563  30.214600  32.403976
Ca  26.567539  31.454865  35.918945
Ca  30.099169  28.117285  35.814301
Ca  30.117992  32.543594  33.420238
Ca  33.602638  29.499128  31.445000
Ca  33.262287  30.192190  35.420422
Ca  36.514740  26.573816  34.379490
Ca  36.624092  30.517176  33.846291
Ca  40.336346  28.924669  31.468113
Ca  39.738422  29.271074  36.636669
Ca  46.532242  29.558317  33.383194
Ca  42.654106  29.225309  34.358562
S  27.051525  28.110807  36.508183
S  27.092022  34.286594  33.619572
S  30.565796  29.557362  32.726925
S  30.115078  31.420216  36.473007
S  33.310074  27.343596  34.087391
S  33.790531  32.525265  32.797104
S  36.909775  28.402050  31.536785
S  36.476326  29.013447  36.566570
S  40.049744  26.727982  34.096748
S  40.096874  31.204550  33.702927
S  43.666119  29.009218  31.391705
S  44.457912  26.698280  38.028660
24
  generated by VMD
Ca  25.244858  30.253872  32.262630
Ca  26.575474  31.570267  35.986698
Ca  30.175613  27.934881  35.834126
Ca  30.477131  32.704227  33.354679
Ca  33.389763  29.732719  31.451717
Ca  33.153889  29.960514  35.176498
|   | Ca       | S        |
|---|----------|----------|
|   | 36.612812| 26.519051| 34.434982 |
|   | 36.641659| 30.709454| 33.886269 |
|   | 39.965027| 28.825085| 31.566536 |
|   | 39.825893| 29.314625| 36.673027 |
|   | 46.595047| 29.553806| 33.283245 |
|   | 42.710419| 29.300797| 34.396141 |
|   | 27.116444| 27.982105| 36.766747 |
|   | 27.035210| 34.314220| 33.760872 |
|   | 30.466171| 29.572330| 32.744793 |
|   | 30.111345| 31.243755| 36.438396 |
|   | 33.255226| 27.160957| 33.929825 |
|   | 33.745833| 32.615768| 32.677116 |
|   | 36.670856| 28.561760| 31.329700 |
|   | 36.190422| 29.039211| 36.550072 |
|   | 40.126007| 26.782511| 34.160969 |
|   | 40.189930| 31.209183| 33.779720 |
|   | 43.564884| 28.749817| 31.408995 |
|   | 44.595222| 26.780479| 38.171955 |

24 generated by VMD

|   | Ca       | S        |
|---|----------|----------|
|   | 24.996609| 30.192371| 31.993393 |
|   | 26.406876| 31.445631| 35.957417 |
|   | 30.224728| 27.958382| 35.882055 |
|   | 30.279984| 32.964119| 33.472088 |
|   | 33.281109| 29.535135| 31.345203 |
|   | 33.230141| 30.117176| 35.381770 |
|   | 36.652744| 26.574718| 34.397476 |
|   | 36.761509| 30.686062| 33.892894 |
|   | 40.100460| 28.876156| 31.485409 |
|   | 39.741932| 29.184278| 36.508865 |
|   | 46.680122| 29.547417| 33.256859 |
|   | 42.752892| 29.387344| 34.517490 |
|   | 27.351868| 28.116781| 37.065094 |
|   | 26.984081| 34.180534| 33.479832 |
|   | 30.455032| 29.648859| 32.909724 |
|   | 29.891340| 31.325975| 36.470539 |
|   | 33.242638| 27.240402| 33.925175 |
|   | 33.834568| 32.535000| 32.779587 |
|   | 36.635307| 28.637444| 31.313606 |
|   | 36.199162| 29.022039| 36.508255 |
|   | 40.214420| 26.682211| 34.079903 |
|   | 40.128731| 31.191154| 33.797749 |
|   | 43.745888| 28.796261| 31.342918 |
|   | 44.641689| 26.544918| 38.287041 |

24 generated by VMD
|    | Ca          | S            |        |
|----|-------------|--------------|--------|
| 24 | generated by VMD |
| Ca| 24.832150 | 30.171362 | 32.733074 |
| Ca| 26.645489 | 31.579227 | 36.169834 |
| Ca| 30.106916 | 27.852842 | 35.388866 |
| Ca| 30.345324 | 33.076786 | 33.251354 |
| Ca| 33.361683 | 29.486992 | 31.368837 |
| Ca| 33.251663 | 29.840525 | 35.441986 |
| Ca| 36.632557 | 26.683054 | 34.326954 |
| Ca| 36.544640 | 30.581797 | 33.724991 |
| Ca| 40.182148 | 29.194416 | 31.611036 |
| Ca| 39.849686 | 29.469784 | 36.467922 |
| Ca| 46.822289 | 29.150909 | 33.411709 |
| Ca| 42.886536 | 29.365864 | 34.289833 |
| S | 27.089340 | 28.050379 | 36.592339 |
| S | 27.034771 | 34.184830 | 33.776409 |
| S | 30.455648 | 29.748159 | 32.564285 |
| S | 30.050583 | 31.180416 | 36.454094 |
| S | 33.209007 | 26.974884 | 34.020508 |
| S | 33.689186 | 32.522976 | 32.880238 |
| S | 36.811005 | 28.559286 | 31.357006 |
| S | 36.353214 | 29.093502 | 36.425159 |
| S | 40.097290 | 26.889410 | 34.059471 |
| S | 40.218079 | 31.462645 | 33.691570 |
| S | 43.610092 | 28.551376 | 31.402100 |
| S | 44.354553 | 26.720032 | 38.621201 |
|   | X          | Y          | Z          |
|---|------------|------------|------------|
| S | 40.195412  | 26.603767  | 34.234192  |
| S | 40.044334  | 31.191441  | 33.629730  |
| S | 43.611824  | 28.862122  | 31.407595  |
| S | 44.647194  | 26.550304  | 38.289093  |
|   | generated by VMD |
| Ca| 25.260624  | 29.750696  | 32.447498  |
| Ca| 26.607990  | 31.738138  | 35.768768  |
| Ca| 30.020699  | 27.983295  | 35.972908  |
| Ca| 30.346096  | 32.821903  | 33.526169  |
| Ca| 33.388214  | 29.781006  | 31.447098  |
| Ca| 33.189476  | 29.988791  | 35.107315  |
| Ca| 36.539902  | 26.375277  | 34.324257  |
| Ca| 36.694569  | 30.696526  | 33.780582  |
| Ca| 40.146263  | 28.926739  | 31.557310  |
| Ca| 39.882416  | 29.071566  | 36.662746  |
| Ca| 46.570877  | 29.438583  | 33.289406  |
| Ca| 42.786419  | 29.402441  | 34.347729  |
| S | 27.020256  | 28.197350  | 36.717381  |
| S | 27.056229  | 34.141518  | 33.484200  |
| S | 30.514988  | 29.762043  | 32.903164  |
| S | 30.039146  | 31.290524  | 36.539845  |
| S | 33.103561  | 27.173439  | 33.929207  |
| S | 33.879707  | 32.763977  | 32.829105  |
| S | 36.578632  | 28.412510  | 31.488382  |
| S | 36.404167  | 28.930311  | 36.413490  |
| S | 40.104630  | 26.764265  | 34.017372  |
| S | 40.111645  | 31.223694  | 33.894638  |
| S | 43.688278  | 28.945131  | 31.275894  |
| S | 44.499180  | 26.811649  | 38.306217  |
|   | generated by VMD |
| Ca| 24.933748  | 30.201508  | 32.885784  |
| Ca| 26.578236  | 31.588268  | 36.238956  |
| Ca| 30.134178  | 27.992039  | 35.245728  |
| Ca| 30.283716  | 32.784698  | 33.382149  |
| Ca| 33.306717  | 29.272865  | 31.200863  |
| Ca| 33.175369  | 30.175621  | 35.075630  |
| Ca| 36.626347  | 26.630804  | 34.190830  |
| Ca| 36.739388  | 30.772961  | 33.551437  |
| Ca| 39.955204  | 29.105249  | 31.565203  |
| Ca| 39.681038  | 29.293892  | 36.815430  |
| Ca| 46.604897  | 29.470490  | 33.582138  |
| Ca| 42.760059  | 29.321243  | 34.734482  |
| S | 27.294762  | 28.221317  | 37.007393  |
| S | 27.239288  | 34.248680  | 34.077797  |
S    30.467611       29.723272       32.382988
S    30.061859       31.121284       36.445305
S    33.324665       27.047668       32.459183
S    36.652496       28.514811       31.052189
S    36.427597       28.967752       36.153843
S    40.122139       26.858881       34.171257
S    40.191544       31.322475       33.985344
S    43.500793       28.956924       31.585165
S    44.664955       26.502583       38.457382
24
generated by VMD
Ca   24.908802       30.090214       32.555992
Ca   26.491276       31.415354       36.095665
Ca   30.105194       28.011677       35.811604
Ca   30.425299       32.721466       33.167591
Ca   33.386379       29.777739       31.368118
Ca   33.178677       30.118359       35.161774
Ca   36.612087       26.573456       34.520943
Ca   36.745232       30.820408       33.671082
Ca   40.107010       28.984116       31.786934
Ca   39.787720       29.276020       36.672085
Ca   46.692871       29.200027       33.022476
Ca   42.925842       29.375959       34.491608
S    26.756283       28.006519       36.461418
S    27.165163       33.959583       33.968204
S    30.539940       29.629913       32.642448
S    30.030682       31.294102       36.245163
S    33.261734       27.098705       34.031601
S    33.865498       32.609833       32.613628
S    36.572342       28.414614       31.520927
S    36.394276       29.404800       36.484127
S    40.181747       26.856215       34.270241
S    40.312592       31.352386       33.838112
S    43.499561       28.942936       31.318165
S    44.487648       26.456989       38.310707
24
generated by VMD
Ca   24.680450       29.936623       32.691185
Ca   26.517048       31.399275       36.127197
Ca   30.165691       27.935101       35.706886
Ca   30.330183       32.843754       33.236912
Ca   33.397705       29.777212       31.417015
Ca   33.258217       29.981874       35.367279
Ca   36.697960       26.842897       34.348907
Ca   36.870903       31.019545       33.592793
|  | Ca       |  |    | S        |
|---|---|---|---|---|
|  | 39.942650 | 28.993912 | 31.696903 | 26.556183 | 29.392818 | 32.897583 |
|  | 39.790371 | 29.082369 | 36.818489 | 42.933887 | 29.257294 | 34.584362 |
|  | 46.556183 | 29.392818 | 32.897583 | 26.932898 | 27.881636 | 36.409245 |
|  | 31.696903 | 26.556183 | 29.392818 | 42.933887 | 29.257294 | 34.584362 |
|  | 26.932898 | 27.881636 | 36.409245 | 39.790371 | 29.082369 | 36.818489 |
|  | 29.392818 | 26.556183 | 32.897583 | 42.933887 | 29.257294 | 34.584362 |
|  | 32.897583 | 26.556183 | 32.897583 | 42.933887 | 29.257294 | 34.584362 |
|  | 39.790371 | 29.082369 | 36.818489 | 42.933887 | 29.257294 | 34.584362 |
|  | 46.556183 | 29.392818 | 32.897583 | 26.932898 | 27.881636 | 36.409245 |
|  | 31.696903 | 26.556183 | 29.392818 | 42.933887 | 29.257294 | 34.584362 |

24 generated by VMD

|  | Ca       |  |    | S        |
|---|---|---|---|---|
|  | 24.815968 | 29.769396 | 32.669312 | 24.815968 | 29.769396 | 32.669312 |
|  | 26.563622 | 31.628267 | 35.860542 | 26.563622 | 31.628267 | 35.860542 |
|  | 30.275192 | 27.942345 | 35.643723 | 30.275192 | 27.942345 | 35.643723 |
|  | 30.435818 | 32.671593 | 33.180637 | 30.435818 | 32.671593 | 33.180637 |
|  | 33.373356 | 29.592175 | 31.531488 | 33.373356 | 29.592175 | 31.531488 |
|  | 33.234070 | 30.321163 | 35.357937 | 33.234070 | 30.321163 | 35.357937 |
|  | 36.685059 | 26.806717 | 34.346962 | 36.685059 | 26.806717 | 34.346962 |
|  | 36.836009 | 30.958143 | 34.007183 | 36.836009 | 30.958143 | 34.007183 |
|  | 39.848522 | 29.097618 | 31.679405 | 39.848522 | 29.097618 | 31.679405 |
|  | 39.752304 | 29.070414 | 36.629837 | 39.752304 | 29.070414 | 36.629837 |
|  | 46.500977 | 29.523354 | 33.123535 | 46.500977 | 29.523354 | 33.123535 |
|  | 42.891224 | 29.267937 | 34.495266 | 42.891224 | 29.267937 | 34.495266 |
|  | 26.996586 | 27.879904 | 36.618263 | 26.996586 | 27.879904 | 36.618263 |
|  | 27.342834 | 34.205067 | 33.532238 | 27.342834 | 34.205067 | 33.532238 |
|  | 30.442396 | 29.624763 | 32.574032 | 30.442396 | 29.624763 | 32.574032 |
|  | 29.807549 | 31.248138 | 36.374088 | 29.807549 | 31.248138 | 36.374088 |
|  | 33.259678 | 27.159681 | 33.887203 | 33.259678 | 27.159681 | 33.887203 |
|  | 33.880581 | 32.494381 | 32.853264 | 33.880581 | 32.494381 | 32.853264 |
|  | 36.735577 | 28.656292 | 31.399616 | 36.735577 | 28.656292 | 31.399616 |
|  | 36.352604 | 29.266518 | 36.542862 | 36.352604 | 29.266518 | 36.542862 |
|  | 39.971775 | 26.806335 | 34.060040 | 39.971775 | 26.806335 | 34.060040 |
|  | 40.354946 | 31.259731 | 34.074909 | 40.354946 | 31.259731 | 34.074909 |
|  | 43.260265 | 28.784201 | 31.477192 | 43.260265 | 28.784201 | 31.477192 |
|  | 44.816391 | 26.357283 | 38.11176 | 44.816391 | 26.357283 | 38.11176 |

24 generated by VMD

|  | Ca       |  |    | S        |
|---|---|---|---|---|
|  | 24.993256 | 29.852600 | 32.720741 | 24.993256 | 29.852600 | 32.720741 |
|  | 26.395756 | 31.326563 | 36.049706 | 26.395756 | 31.326563 | 36.049706 |
| Ca   | 30.324377 | 27.996378 | 35.778313 |
|------|-----------|-----------|-----------|
| Ca   | 30.167259 | 32.894871 | 33.178913 |
| Ca   | 33.469460 | 29.595543 | 31.256968 |
| Ca   | 33.206837 | 30.248411 | 35.224564 |
| Ca   | 36.532104 | 26.759598 | 33.917038 |
| Ca   | 36.806805 | 31.110498 | 33.857224 |
| Ca   | 40.154377 | 29.028011 | 31.673319 |
| Ca   | 39.713440 | 29.422100 | 36.652180 |
| Ca   | 46.657761 | 29.266989 | 33.336048 |
| Ca   | 42.699554 | 28.896557 | 34.375595 |
| S    | 27.241423 | 27.745419 | 36.603493 |
| S    | 27.063805 | 34.175930 | 34.091522 |
| S    | 30.482220 | 29.790783 | 32.705513 |
| S    | 29.838638 | 31.230869 | 36.522602 |
| S    | 33.230934 | 27.407463 | 33.820324 |
| S    | 33.675682 | 32.577393 | 32.648705 |
| S    | 36.759247 | 28.842983 | 31.492439 |
| S    | 36.438385 | 29.174454 | 36.305946 |
| S    | 40.026974 | 26.719559 | 34.095402 |
| S    | 40.580578 | 31.286827 | 33.752296 |
| S    | 43.720234 | 28.347546 | 31.403196 |
| S    | 44.252975 | 26.694019 | 38.568710 |

24

generated by VMD

| Ca   | 24.888100 | 29.714737 | 32.791710 |
|------|-----------|-----------|-----------|
| Ca   | 26.686447 | 31.481369 | 36.254444 |
| Ca   | 30.140877 | 27.883030 | 35.643135 |
| Ca   | 30.627762 | 33.070637 | 33.295094 |
| Ca   | 33.319370 | 29.685745 | 31.246590 |
| Ca   | 33.432533 | 30.001066 | 35.079350 |
| Ca   | 36.720055 | 26.826015 | 34.007946 |
| Ca   | 36.901558 | 30.874561 | 33.587891 |
| Ca   | 39.956207 | 28.902910 | 31.651041 |
| Ca   | 39.599945 | 29.669180 | 36.924961 |
| Ca   | 46.357044 | 29.290884 | 33.398396 |
| Ca   | 42.631809 | 29.353107 | 34.751106 |
| S    | 27.081249 | 27.864113 | 36.654156 |
| S    | 27.194492 | 34.108410 | 33.949741 |
| S    | 30.530823 | 29.773533 | 32.654446 |
| S    | 30.264160 | 31.027168 | 36.247318 |
| S    | 33.209499 | 27.032213 | 33.662621 |
| S    | 33.989998 | 32.656006 | 32.674110 |
| S    | 36.590336 | 28.779839 | 31.133247 |
| S    | 36.466354 | 28.974823 | 36.234516 |
| S    | 39.821198 | 26.952816 | 34.499977 |
| S    | 40.378376 | 31.424473 | 33.905575 |
|    | 24 generated by VMD |    | 24 generated by VMD |
|----|---------------------|----|---------------------|
| S  | 43.156727 28.516182 31.603977 | S  | 43.156727 28.516182 31.603977 |
| S  | 44.488987 26.528564 38.179409 |

| Ca  | 24.844545 29.833817 32.809219 |
| Ca  | 26.687202 31.294111 36.039093 |
| Ca  | 30.233675 27.927032 35.685154 |
| Ca  | 30.450445 32.949757 33.191643 |
| Ca  | 33.460457 29.613129 31.219572 |
| Ca  | 33.220875 29.965233 35.244080 |
| Ca  | 36.652115 26.871044 34.539558 |
| Ca  | 36.871925 30.948896 33.699940 |
| Ca  | 40.104149 29.233562 31.790213 |
| Ca  | 39.698578 29.457123 36.910187 |
| Ca  | 46.334824 29.012924 33.186081 |
| Ca  | 42.808361 29.332824 34.628300 |
| S  | 26.986864 27.807642 36.368217 |
| S  | 27.375948 34.142826 33.857109 |
| S  | 30.545612 29.585558 32.603714 |
| S  | 30.020065 31.191349 36.276108 |
| S  | 33.325974 27.078886 34.016125 |
| S  | 33.829193 32.543056 32.685028 |
| S  | 36.599014 28.715015 31.243584 |
| S  | 36.478771 29.480089 36.476009 |
| S  | 39.877495 27.014076 34.281372 |
| S  | 40.384487 31.483948 33.923084 |
| S  | 43.273670 28.592785 31.530300 |
| S  | 44.369637 26.315962 37.827042 |
|     | 33.319542 | 27.351089 | 33.875893 |
|-----|-----------|-----------|-----------|
| S   | 33.765171 | 32.658958 | 32.437698 |
| S   | 36.595055 | 28.766705 | 31.211992 |
| S   | 36.476986 | 29.225811 | 36.311729 |
| S   | 40.008774 | 26.891880 | 34.175674 |
| S   | 40.337662 | 31.361399 | 33.937298 |
| S   | 43.456772 | 28.309189 | 31.631586 |
| S   | 44.388783 | 26.506256 | 38.255005 |

24 generated by VMD

| Ca  | 24.648550 | 30.066303 | 32.938049 |
|-----|-----------|-----------|-----------|
| Ca  | 26.661835 | 31.276739 | 36.229847 |
| Ca  | 30.108561 | 28.112726 | 35.593704 |
| Ca  | 30.370808 | 32.946686 | 33.304848 |
| Ca  | 33.340454 | 29.596346 | 31.238920 |
| Ca  | 33.351807 | 29.996559 | 35.180649 |
| Ca  | 36.586372 | 26.638962 | 34.220398 |
| Ca  | 36.688545 | 30.746525 | 33.55042 |
| Ca  | 40.043613 | 29.135765 | 31.758652 |
| Ca  | 39.629967 | 29.460245 | 36.841530 |
| Ca  | 46.550064 | 29.322256 | 33.144028 |
| Ca  | 42.762085 | 29.196712 | 34.657036 |
| S   | 27.142576 | 27.853041 | 36.377491 |
| S   | 27.269119 | 34.024578 | 33.959171 |
| S   | 30.505793 | 29.811710 | 32.514786 |
| S   | 30.175323 | 31.296318 | 36.274265 |
| S   | 33.265610 | 27.267365 | 33.864567 |
| S   | 33.884167 | 32.527756 | 32.674995 |
| S   | 36.690536 | 28.469292 | 31.027205 |
| S   | 36.382168 | 29.161983 | 36.380127 |
| S   | 39.922974 | 26.942440 | 34.307739 |
| S   | 40.232754 | 31.370651 | 33.988205 |
| S   | 43.514530 | 28.393539 | 31.727062 |
| S   | 44.705647 | 26.776894 | 38.272339 |

24 generated by VMD

| Ca  | 24.801399 | 30.011501 | 32.695930 |
|-----|-----------|-----------|-----------|
| Ca  | 26.577662 | 31.456383 | 36.100426 |
| Ca  | 30.512566 | 27.638563 | 35.777008 |
| Ca  | 30.421698 | 32.827217 | 33.220596 |
| Ca  | 33.239517 | 29.586035 | 31.317619 |
| Ca  | 33.306000 | 30.386848 | 35.156498 |
| Ca  | 36.730225 | 26.679970 | 34.178505 |
| Ca  | 36.792377 | 30.909870 | 33.641376 |
| Ca  | 40.033733 | 29.145313 | 31.537666 |
| Ca  | 39.532104 | 29.582722 | 36.781422 |
| Element | 1st Value 1 | 2nd Value 1 | 3rd Value 1 |
|---------|------------|------------|------------|
| Ca      | 46.403568  | 29.066566  | 33.202744  |
| Ca      | 42.694992  | 29.142546  | 34.680519  |
| S       | 27.215059  | 27.875690  | 36.403168  |
| S       | 27.150021  | 34.082901  | 33.933357  |
| S       | 30.352032  | 29.651981  | 32.803142  |
| S       | 30.112389  | 31.069901  | 36.386765  |
| S       | 33.420288  | 27.323324  | 33.82296   |
| S       | 33.832676  | 32.685909  | 32.684044  |
| S       | 36.624184  | 28.746231  | 31.201374  |
| S       | 36.435047  | 29.184893  | 36.190826  |
| S       | 39.969254  | 26.994907  | 34.170013  |
| S       | 40.298050  | 31.425499  | 33.887089  |
| S       | 43.320732  | 28.307844  | 31.650585  |
| S       | 44.658409  | 26.608746  | 38.530544  |

24 generated by VMD

| Element | 1st Value 2 | 2nd Value 2 | 3rd Value 2 |
|---------|------------|------------|------------|
| Ca      | 24.692467  | 29.902931  | 32.712875  |
| Ca      | 26.460947  | 31.261026  | 36.017300  |
| Ca      | 30.476707  | 27.897409  | 35.96741   |
| Ca      | 30.401016  | 32.808273  | 33.458733  |
| Ca      | 33.264977  | 29.703230  | 31.264271  |
| Ca      | 33.276417  | 30.298923  | 35.98499   |
| Ca      | 36.887630  | 26.825043  | 34.181862  |
| Ca      | 36.981022  | 30.732359  | 33.679520  |
| Ca      | 39.945850  | 29.013420  | 31.532757  |
| Ca      | 39.631424  | 29.708715  | 36.728725  |
| Ca      | 46.364311  | 28.928030  | 33.273495  |
| Ca      | 42.903015  | 29.420113  | 34.497650  |
| S       | 27.140789  | 27.777668  | 36.242344  |
| S       | 27.263470  | 34.032459  | 34.090660  |
| S       | 30.324867  | 29.701857  | 32.726181  |
| S       | 30.068554  | 31.146221  | 36.382286  |
| S       | 33.442516  | 27.583088  | 33.762802  |
| S       | 33.948189  | 32.641617  | 32.845367  |
| S       | 36.611809  | 28.460430  | 31.031939  |
| S       | 36.428307  | 29.228172  | 36.448627  |
| S       | 40.032639  | 27.019543  | 34.247978  |
| S       | 40.431946  | 31.411646  | 33.749142  |
| S       | 43.259869  | 28.102642  | 31.593910  |
| S       | 44.195206  | 26.786535  | 38.566994  |

24 generated by VMD

| Element | 1st Value 3 | 2nd Value 3 | 3rd Value 3 |
|---------|------------|------------|------------|
| Ca      | 24.529087  | 29.989044  | 32.847599  |
| Ca      | 26.556423  | 31.230915  | 36.172501  |
| Ca      | 30.445763  | 27.604652  | 35.525791  |
| Ca      | 30.351582  | 32.889706  | 33.536797  |
Ca  33.154949  29.801167  31.019466
Ca  33.138432  30.261530  35.042072
Ca  36.790749  26.777771  34.385437
Ca  36.598839  30.952803  33.410992
Ca  39.847233  28.942017  31.597063
Ca  39.699600  29.481464  36.696953
Ca  46.576462  28.984890  33.571632
Ca  43.058060  29.192173  34.586658
S   27.094280  27.862000  36.409428
S   27.227442  34.121563  34.298779
S   30.472927  29.848078  32.655540
S   30.031139  30.984648  36.394573
S   33.474678  27.404133  33.685402
S   33.808929  32.862820  32.613445
S   36.603232  28.826750  30.958782
S   36.349270  29.267540  36.225632
S   40.056488  26.870733  34.304516
S   40.619286  31.310080  33.874199
S   43.379276  28.086914  31.663181
S   44.566805  26.913794  38.554314

24

generated by VMD

Ca  24.788635  30.003979  33.057991
Ca  26.762177  31.076092  36.203274
Ca  30.712799  27.894785  35.767395
Ca  30.454027  32.823090  33.439304
Ca  33.119877  29.561522  31.170429
Ca  33.389053  30.443901  34.895981
Ca  36.667053  26.834345  34.034531
Ca  36.758793  30.754726  33.429321
Ca  39.925869  29.275826  31.551493
Ca  39.392441  29.535793  36.778526
Ca  46.397919  28.620359  33.554916
Ca  42.677399  29.532690  34.710556
S   27.307789  27.651171  36.414116
S   27.160179  34.077637  34.283493
S   30.303326  29.705997  32.802162
S   30.396984  31.137974  36.407635
S   33.508129  27.444159  33.667160
S   33.837589  32.743279  32.279526
S   36.589279  28.754066  30.837862
S   36.396034  29.277548  36.116043
S   40.011150  26.824436  34.184307
S   40.418175  31.541092  33.868946
S   43.401779  28.317137  31.819456
S   44.057392  26.559822  38.756264
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 24.321224 | 30.029840 | 33.019871 |
| Ca      | 26.479881 | 31.093468 | 36.200932 |
| Ca      | 30.668737 | 27.506424 | 35.500416 |
| Ca      | 30.161747 | 29.00665 | 33.390086 |
| Ca      | 33.317558 | 29.907770 | 31.261547 |
| Ca      | 33.165009 | 30.526472 | 35.153976 |
| Ca      | 36.883217 | 26.955896 | 34.178009 |
| Ca      | 36.853806 | 30.905125 | 33.697525 |
| Ca      | 39.933998 | 28.917267 | 31.268581 |
| Ca      | 39.807259 | 29.422335 | 36.743687 |
| Ca      | 46.655827 | 28.682802 | 33.083965 |
| Ca      | 42.856361 | 29.316750 | 34.739666 |
| S       | 27.259584 | 27.788364 | 36.343967 |
| S       | 26.915443 | 33.996868 | 34.099590 |
| S       | 30.478882 | 29.860777 | 32.680637 |
| S       | 29.949207 | 31.003677 | 36.254128 |
| S       | 33.675354 | 27.432676 | 33.751545 |
| S       | 33.769901 | 32.829002 | 32.517750 |
| S       | 36.584797 | 28.754820 | 31.203918 |
| S       | 36.491898 | 29.563227 | 36.340935 |
| S       | 39.994644 | 26.892616 | 34.242012 |
| S       | 40.659300 | 31.287354 | 33.764687 |
| S       | 43.433266 | 28.085400 | 31.726212 |
| S       | 44.122375 | 26.731819 | 38.857948 |

24 generated by VMD
| S   | 36.607647 | 29.019966 | 31.021099 |
|-----|-----------|-----------|-----------|
| S   | 36.527020 | 29.639935 | 36.169010 |
| S   | 40.019150 | 26.970646 | 34.477753 |
| S   | 40.729515 | 31.371634 | 33.555538 |
| S   | 43.341606 | 27.720644 | 31.536148 |
| S   | 43.816635 | 26.574221 | 39.170475 |

24 generated by VMD

| Ca  | 24.603413 | 30.037819 | 32.692299 |
|-----|-----------|-----------|-----------|
| Ca  | 26.380667 | 31.260664 | 36.334286 |
| Ca  | 30.218763 | 27.804401 | 35.561989 |
| Ca  | 30.156605 | 29.946217 | 33.398903 |
| Ca  | 33.120129 | 29.543175 | 31.239716 |
| Ca  | 33.230278 | 30.398073 | 35.076916 |
| Ca  | 36.955330 | 26.746878 | 34.304375 |
| Ca  | 36.684002 | 30.863243 | 33.584873 |
| Ca  | 40.076084 | 28.875095 | 31.681643 |
| Ca  | 39.855282 | 29.565849 | 36.640118 |
| Ca  | 46.934192 | 29.015942 | 32.635448 |
| Ca  | 42.970314 | 29.234745 | 34.426384 |
| S   | 27.047245 | 27.716373 | 36.455120 |
| S   | 26.929916 | 34.165813 | 34.266659 |
| S   | 30.264347 | 29.874426 | 32.617630 |
| S   | 32.984667 | 31.034321 | 36.430176 |
| S   | 33.575394 | 27.653841 | 33.585159 |
| S   | 33.606598 | 32.665215 | 32.538036 |
| S   | 36.808643 | 28.863205 | 31.076797 |
| S   | 36.550644 | 29.261608 | 36.271797 |
| S   | 40.154316 | 26.729162 | 34.380775 |
| S   | 40.690529 | 31.310553 | 33.825050 |
| S   | 43.500607 | 28.107584 | 31.635975 |
| S   | 44.138611 | 26.716232 | 39.376278 |

24 generated by VMD

| Ca  | 24.331020 | 30.156536 | 32.858101 |
|-----|-----------|-----------|-----------|
| Ca  | 26.697624 | 31.329643 | 36.453411 |
| Ca  | 30.206312 | 27.516876 | 35.298347 |
| Ca  | 30.255426 | 32.656528 | 33.340027 |
| Ca  | 33.128326 | 29.515882 | 31.071304 |
| Ca  | 33.166069 | 30.245155 | 35.061008 |
| Ca  | 36.821274 | 27.150379 | 34.285664 |
| Ca  | 36.815834 | 31.129429 | 33.733231 |
| Ca  | 39.993988 | 29.449520 | 31.656679 |
| Ca  | 40.067528 | 29.668665 | 36.836414 |
| Ca  | 46.765045 | 28.795303 | 32.977287 |
| Ca  | 42.764721 | 29.020618 | 34.374557 |
|   |          |          |          |
|---|----------|----------|----------|
| S | 27.15827 | 27.07376 | 36.413170|
| S | 27.001429| 34.097076| 34.152584|
| S | 30.249016| 29.634075| 32.518021|
| S | 30.083675| 31.019505| 36.346951|
| S | 33.345791| 27.425383| 33.563416|
| S | 33.802685| 32.573742| 32.417457|
| S | 36.639545| 28.982508| 31.246458|
| S | 36.563381| 29.484417| 36.493969|
| S | 39.953987| 26.931770| 34.297653|
| S | 40.670063| 31.436216| 34.019859|
| S | 43.494705| 27.795057| 31.581638|
| S | 44.457565| 26.669771| 39.036163|

24

generated by VMD

| Ca |          |          |          |
|----|----------|----------|----------|
| Ca | 24.405193| 29.945421| 32.836098|
| Ca | 26.585449| 31.255386| 36.284378|
| Ca | 30.609169| 27.482985| 35.407127|
| Ca | 30.383339| 32.851231| 33.456253|
| Ca | 33.025429| 29.803585| 31.115381|
| Ca | 33.300617| 30.229370| 35.036671|
| Ca | 36.539257| 27.232832| 34.413616|
| Ca | 36.997814| 31.149208| 33.682808|
| Ca | 39.977436| 29.052441| 31.798149|
| Ca | 39.880711| 29.446226| 36.764816|
| Ca | 46.933929| 28.957344| 32.842613|
| Ca | 42.881424| 29.037012| 34.622181|
| S  | 27.378059| 27.824591| 36.522770|
| S  | 26.936119| 33.973869| 34.101254|
| S  | 30.229927| 29.647360| 32.521385|
| S  | 30.129595| 30.983391| 36.264968|
| S  | 33.427376| 27.617554| 33.337616|
| S  | 33.726772| 32.692566| 32.510498|
| S  | 36.600700| 28.794231| 31.186474|
| S  | 36.312981| 29.634102| 36.390430|
| S  | 39.835258| 26.923973| 34.522320|
| S  | 40.542263| 31.363693| 34.174553|
| S  | 43.454102| 27.939083| 31.724262|
| S  | 44.340919| 26.555538| 38.514328|

24

generated by VMD

| Ca |          |          |          |
|----|----------|----------|----------|
| Ca | 24.144470| 30.351774| 32.990181|
| Ca | 26.672640| 31.451609| 36.226944|
| Ca | 30.477255| 27.400805| 35.401768|
| Ca | 30.423557| 32.713036| 33.367981|
| Ca | 33.089794| 29.495872| 31.152416|
| Ca | 33.248875| 30.211079| 35.168827|
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 36.793034 | 26.888561 | 34.180798 |
| Ca      | 36.915005 | 30.994568 | 33.625946 |
| Ca      | 39.643261 | 29.147131 | 31.610222 |
| Ca      | 39.827927 | 29.625271 | 36.638939 |
| Ca      | 46.986862 | 28.622526 | 33.309944 |
| Ca      | 42.864983 | 29.059555 | 34.506283 |
| S       | 27.064260 | 27.868584 | 36.345371 |
| S       | 27.090891 | 34.096817 | 34.140079 |
| S       | 30.391048 | 29.707567 | 32.639908 |
| S       | 30.210232 | 30.804428 | 36.286510 |
| S       | 33.498085 | 27.380785 | 33.562222 |
| S       | 33.711590 | 32.562157 | 32.539185 |
| S       | 36.510376 | 28.764643 | 31.226164 |
| S       | 36.515091 | 29.482382 | 36.293014 |
| S       | 39.998928 | 26.915394 | 34.373341 |
| S       | 40.442225 | 31.580494 | 33.913162 |
| S       | 43.596920 | 28.306005 | 31.652636 |
| S       | 44.314632 | 26.960354 | 38.881538 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 24.625061 | 30.287699 | 32.769852 |
| Ca      | 26.529804 | 31.427383 | 36.252220 |
| Ca      | 30.299212 | 27.614925 | 35.364861 |
| Ca      | 30.498081 | 32.740841 | 33.381523 |
| Ca      | 33.247444 | 29.678686 | 31.080763 |
| Ca      | 33.135708 | 30.059746 | 35.181396 |
| Ca      | 36.685646 | 26.568310 | 34.432499 |
| Ca      | 36.757355 | 30.904799 | 33.811520 |
| Ca      | 39.944382 | 28.983715 | 31.720230 |
| Ca      | 39.759701 | 29.298952 | 36.658413 |
| Ca      | 46.946110 | 29.412079 | 33.217934 |
| Ca      | 42.779346 | 29.293587 | 34.501968 |
| S       | 27.059195 | 28.077618 | 36.486496 |
| S       | 27.325432 | 34.213432 | 34.013016 |
| S       | 30.449657 | 29.675058 | 32.673424 |
| S       | 30.024460 | 31.143799 | 36.430836 |
| S       | 33.291130 | 27.166828 | 33.710945 |
| S       | 33.745007 | 32.569229 | 32.366390 |
| S       | 36.536343 | 28.579765 | 31.287107 |
| S       | 36.278610 | 29.197184 | 36.495968 |
| S       | 40.010666 | 26.869043 | 34.337055 |
| S       | 40.334354 | 31.454971 | 33.925404 |
| S       | 43.625099 | 28.302719 | 31.662619 |
| S       | 44.546066 | 26.871050 | 38.268295 |

24 generated by VMD
Ca | 24.448181 | 30.271030 | 32.894886  
Ca | 26.421280 | 31.510633 | 36.111122  
Ca | 30.298582 | 27.384243 | 35.472519  
Ca | 30.404009 | 32.727886 | 33.095741  
Ca | 33.235760 | 29.338890 | 31.056772  
Ca | 33.225227 | 30.232258 | 35.191780  
Ca | 36.653061 | 26.830318 | 34.377747  
Ca | 36.607750 | 30.853062 | 33.987858  
Ca | 40.037594 | 29.302216 | 31.621328  
Ca | 39.913315 | 29.377743 | 36.821129  
Ca | 46.796223 | 28.843271 | 33.169964  
Ca | 42.746956 | 29.307423 | 34.546963  
S  | 27.017212 | 28.065441 | 36.523727  
S  | 27.080952 | 34.171341 | 34.134399  
S  | 30.541727 | 29.499084 | 32.653728  
S  | 30.087696 | 30.962278 | 36.060722  
S  | 33.525608 | 27.543669 | 33.760151  
S  | 33.857533 | 32.573135 | 32.360218  
S  | 36.637974 | 28.671434 | 31.490314  
S  | 36.410778 | 29.395351 | 36.706154  
S  | 39.986427 | 27.039923 | 34.189865  
S  | 40.318836 | 31.408112 | 34.068993  
S  | 43.564133 | 28.413036 | 31.570030  
S  | 44.617088 | 26.669643 | 38.164608  

24

generated by VMD

Ca | 24.638527 | 30.390228 | 32.470436  
Ca | 26.624687 | 31.645292 | 35.948330  
Ca | 30.243591 | 27.561188 | 35.862179  
Ca | 30.286510 | 32.599777 | 33.599525  
Ca | 33.229729 | 29.428045 | 31.165344  
Ca | 33.227200 | 30.102165 | 35.205143  
Ca | 36.591415 | 26.750540 | 34.454891  
Ca | 36.652195 | 30.694973 | 33.568428  
Ca | 39.986816 | 29.031397 | 31.791138  
Ca | 39.729206 | 29.443073 | 36.714760  
Ca | 46.828484 | 29.242006 | 33.231430  
Ca | 42.946316 | 29.477455 | 34.397095  
S  | 27.045443 | 28.181345 | 36.673538  
S  | 27.327709 | 34.214668 | 33.907875  
S  | 30.389872 | 29.591984 | 32.737171  
S  | 29.963869 | 31.025368 | 36.424652  
S  | 33.412003 | 27.338200 | 33.651825  
S  | 33.743164 | 32.459251 | 32.567558  
S  | 36.739471 | 28.374647 | 31.141273  
S  | 36.321835 | 29.273287 | 36.382988
|   |   |   |   |
|---|---|---|---|
| S | 40.129456 | 26.835648 | 34.217403 |
| S | 40.266998 | 31.487850 | 34.008057 |
| S | 43.666706 | 28.635406 | 31.488182 |
| S | 44.442696 | 26.607611 | 38.421528 |

24

generated by VMD

| Ca   | Ca   | Ca   |
|------|------|------|
| 24.330412 | 30.716234 | 32.731552 |
| 26.402269 | 31.589851 | 36.171925 |
| 30.198811 | 27.683306 | 35.671440 |
| 30.425447 | 32.706295 | 33.309685 |
| 33.390038 | 29.497990 | 31.225121 |
| 33.198631 | 29.913197 | 35.147900 |
| 36.580647 | 26.712969 | 34.395412 |
| 36.870071 | 30.726450 | 33.735863 |
| 40.073494 | 29.024052 | 31.629148 |
| 39.804077 | 29.515001 | 36.795040 |
| 47.010384 | 29.341646 | 33.100739 |
| 42.892708 | 29.291439 | 34.525070 |
| 26.771656 | 28.013359 | 36.445404 |
| 27.446531 | 34.124081 | 34.047226 |
| 30.436642 | 29.544243 | 32.576141 |
| 30.004623 | 31.050303 | 36.310726 |
| 33.321560 | 27.043255 | 33.782700 |
| 33.818714 | 32.329948 | 32.583103 |
| 36.701694 | 28.484863 | 31.222092 |
| 36.277706 | 29.236897 | 36.478115 |
| 39.963669 | 26.981119 | 34.374409 |
| 40.250938 | 31.314133 | 33.772179 |
| 43.640991 | 28.508099 | 31.399467 |
| 44.622204 | 27.040140 | 38.600201 |

24

generated by VMD

| Ca   | Ca   | Ca   |
|------|------|------|
| 24.846996 | 30.396656 | 32.365753 |
| 26.310972 | 31.628765 | 36.03932 |
| 30.178322 | 27.517422 | 35.713589 |
| 30.312469 | 32.641899 | 33.517303 |
| 33.322906 | 29.659245 | 31.412983 |
| 32.958839 | 30.393051 | 35.346798 |
| 36.820072 | 26.631565 | 34.391438 |
| 36.545883 | 30.786102 | 33.716209 |
| 39.969913 | 29.065357 | 31.607422 |
| 39.793114 | 29.562904 | 36.472561 |
| 47.110481 | 29.239410 | 33.171497 |
| 42.818298 | 29.281244 | 34.349075 |
| 26.926958 | 28.086763 | 36.460098 |
| 27.215618 | 34.222649 | 33.963089 |
|  |  |  |  |
|---|---|---|---|
| S  | 30.414600 | 29.497902 | 32.723099 |
| S  | 29.851845 | 30.964111 | 32.854820 |
| S  | 33.367535 | 27.336187 | 33.958248 |
| S  | 33.721199 | 32.554688 | 32.814804 |
| S  | 36.652912 | 28.480947 | 31.227779 |
| S  | 36.466461 | 29.229633 | 36.398369 |
| S  | 40.181263 | 26.861418 | 34.039986 |
| S  | 40.408009 | 31.301506 | 33.694664 |
| S  | 43.724102 | 28.194244 | 31.607635 |
| S  | 44.515060 | 26.857712 | 38.558876 |

24

generated by VMD

| Ca  | 24.397287 | 30.360096 | 32.398785 |
| Ca  | 26.533939 | 31.600767 | 36.107933 |
| Ca  | 30.184322 | 27.615009 | 35.429672 |
| Ca  | 30.383560 | 32.655922 | 33.447952 |
| Ca  | 33.292946 | 29.428865 | 31.126730 |
| Ca  | 33.177788 | 30.150499 | 35.288136 |
| Ca  | 36.499264 | 26.844109 | 34.542656 |
| Ca  | 36.755264 | 30.897591 | 33.778767 |
| Ca  | 40.101334 | 29.195208 | 31.755636 |
| Ca  | 39.877579 | 29.369274 | 36.610771 |
| Ca  | 46.991131 | 28.916285 | 33.404659 |
| Ca  | 43.056950 | 29.394848 | 34.260487 |
| S  | 26.827303 | 28.193148 | 36.759113 |
| S  | 27.209024 | 34.107628 | 33.840157 |
| S  | 30.342342 | 29.546749 | 32.501568 |
| S  | 29.951061 | 31.022320 | 36.411453 |
| S  | 33.310600 | 27.131922 | 33.876263 |
| S  | 33.781723 | 32.315220 | 32.814804 |
| S  | 36.724323 | 28.455860 | 31.387192 |
| S  | 36.390511 | 29.303356 | 36.583763 |
| S  | 40.036098 | 26.927929 | 34.165977 |
| S  | 40.530067 | 31.413662 | 33.887299 |
| S  | 43.523552 | 28.791271 | 31.377390 |
| S  | 44.555912 | 26.753832 | 38.273575 |

24

generated by VMD

| Ca  | 24.691011 | 30.436810 | 32.371933 |
| Ca  | 26.441418 | 31.400377 | 36.011642 |
| Ca  | 30.183025 | 27.756804 | 35.640400 |
| Ca  | 30.534637 | 32.847397 | 33.521759 |
| Ca  | 33.235744 | 29.229282 | 31.283321 |
| Ca  | 33.247871 | 30.348286 | 35.201664 |
| Ca  | 36.557766 | 26.614269 | 34.523335 |
| Ca  | 36.786858 | 30.719933 | 33.597408 |
Ca  39.90171  28.983578  31.822727
Ca  39.811722  29.470825  36.553875
Ca  46.957027  29.261326  33.107738
Ca  42.887531  29.256058  34.362770
S  26.729080  28.020838  36.316444
S  27.287617  34.053478  34.196934
S  30.418303  29.773090  32.706116
S  29.952641  31.105410  36.410950
S  33.217686  27.393845  34.088303
S  33.866211  32.378334  32.595749
S  36.671761  28.332647  31.116474
S  36.337456  29.068209  36.411930
S  40.004562  26.828188  34.356716
S  40.349506  31.416792  33.909534
S  43.529335  28.620529  31.479618
S  44.775059  27.075056  38.443253

24
generated by VMD
Ca  24.579552  30.634586  32.270393
Ca  26.432343  31.471436  35.905807
Ca  30.135071  27.663534  35.483456
Ca  30.342007  32.707001  33.477669
Ca  33.265915  29.518953  31.337099
Ca  33.262894  29.794250  35.229603
Ca  36.733532  26.777033  34.733177
Ca  36.879150  30.819866  33.763962
Ca  39.973839  29.018599  31.680206
Ca  39.834370  29.742880  36.612637
Ca  46.936539  28.981220  33.398746
Ca  42.843193  29.374474  34.281479
S  26.741364  27.956749  36.427952
S  27.365845  34.399708  34.174328
S  30.328966  29.682459  32.697155
S  29.955538  30.939230  36.374443
S  33.243698  26.948275  34.014980
S  33.771397  32.435463  32.647625
S  36.579178  28.320820  31.321386
S  36.436737  29.242931  36.675159
S  40.050537  26.977621  34.154537
S  40.398689  31.377323  33.673283
S  43.580509  28.492468  31.375828
S  44.762997  27.114513  38.319752

24
generated by VMD
Ca  25.021132  30.129572  32.352863
Ca  26.395264  31.419256  35.838295
Ca   30.351475  27.565123  35.769547
Ca   30.512079  32.700169  33.685333
Ca   33.307175  29.571377  31.290260
Ca   33.105610  30.160511  35.272839
Ca   36.745445  26.789846  34.335430
Ca   36.664913  30.840271  33.620583
Ca   39.787086  29.156784  31.116772
Ca   39.671818  29.592165  36.643059
Ca   46.683247  29.962952  35.490275
Ca   42.887177  29.274408  34.439919
S    26.956936  27.907284  36.428696
S    27.537624  34.418839  34.013092
S    30.436794  29.657270  32.876377
S    29.848654  31.012957  36.433735
S    33.349869  27.296700  33.881523
S    33.833252  32.492249  32.631859
S    36.507000  28.492834  31.475250
S    36.318188  29.321844  36.405941
S    40.079506  26.844730  34.267258
S    40.422127  31.437254  33.757332
S    43.406879  28.393524  31.399830
S    44.603714  26.898455  38.498409

24
generated by VMD
Ca   24.833775  30.282785  32.407204
Ca   26.420692  31.570139  35.980495
Ca   30.203205  27.452175  35.716179
Ca   30.372149  32.810387  33.439590
Ca   33.438850  29.502947  31.407188
Ca   33.140045  29.971491  35.237755
Ca   36.632576  26.577097  34.740257
Ca   36.735973  30.790770  33.783936
Ca   40.066105  29.222971  31.595274
Ca   39.667156  29.596886  36.450275
Ca   46.604149  29.238062  33.214962
Ca   42.894169  29.356369  34.524525
S    26.740208  28.127979  36.529663
S    27.280867  34.418411  33.923386
S    30.455399  29.666252  32.687374
S    29.866104  30.970261  36.335911
S    33.222935  27.031689  33.978516
S    33.883633  32.470509  32.649147
S    36.746437  28.369431  31.378571
S    36.439835  29.237406  36.391857
S    40.075211  27.043846  34.220848
S    40.439857  31.427315  33.792191
generated by VMD

Ca  24.985958  30.339691  32.185497
Ca  26.478535  31.601219  35.934601
Ca  30.201895  27.417181  35.582630
Ca  30.421223  32.803436  33.537804
Ca  33.259964  29.552958  31.449089
Ca  33.280815  29.927658  35.450130
Ca  36.709366  26.628199  34.763100
Ca  36.679554  30.731167  33.603436
Ca  39.935760  29.041162  31.667122
Ca  39.703476  29.796337  36.899940
Ca  46.582077  28.905634  33.172970
Ca  42.895523  29.227804  34.313725
S   26.920341  28.124062  36.238003
S   27.312241  34.367451  34.116852
S   30.403416  29.702587  32.751244
S   30.016832  30.884258  36.317326
S   33.324753  27.057079  34.019451
S   33.780666  32.435589  32.751076
S   36.551952  28.383694  31.246258
S   36.507843  29.292812  36.339706
S   40.003960  27.055489  34.388123
S   40.340748  31.494331  33.751820
S   43.337345  28.461546  31.236944
S   44.799763  27.160069  38.313885

24

generated by VMD

Ca  24.897640  30.406391  32.276810
Ca  26.137207  31.328398  35.947239
Ca  30.377392  27.695063  35.732864
Ca  30.257137  32.683422  33.509251
Ca  33.663986  29.554688  31.287106
Ca  32.819252  30.402637  35.385414
Ca  36.486252  26.818377  34.489975
Ca  36.741673  30.766651  33.761570
Ca  40.212780  28.843628  31.600889
Ca  39.895580  29.719170  36.515205
Ca  47.081532  28.747721  33.497990
Ca  42.905872  29.317509  34.352657
S   26.780533  27.952545  36.396530
S   27.011749  34.076344  34.255051
S   30.405237  29.695213  32.808067
S   29.790966  31.133144  36.433617
|    | 33.350006 | 27.357872 | 34.026855 |
|----|-----------|-----------|-----------|
| S  | 33.712753 | 32.522339 | 32.625015 |
| S  | 36.863434 | 28.292982 | 31.419952 |
| S  | 36.264038 | 29.410372 | 36.463936 |
| S  | 39.959545 | 26.890413 | 34.360397 |
| S  | 40.501160 | 31.500576 | 33.564747 |
| S  | 43.603374 | 28.590563 | 31.404423 |
| S  | 44.714745 | 26.685396 | 37.915104 |
|    |           |           |           |
| 24 | generated by VMD |

|    | 24.732939 | 30.208450 | 32.495979 |
| Ca | 26.435951 | 31.642805 | 36.144444 |
| Ca | 30.330009 | 27.541082 | 35.577602 |
| Ca | 30.383263 | 32.790840 | 33.330585 |
| Ca | 33.355350 | 29.476473 | 31.395670 |
| Ca | 33.080959 | 30.165443 | 35.229820 |
| Ca | 36.536667 | 26.792444 | 34.93057 |
| Ca | 36.659851 | 30.822269 | 33.878025 |
| Ca | 40.279613 | 29.217339 | 31.440601 |
| Ca | 39.768105 | 29.465866 | 36.546505 |
| Ca | 46.632454 | 29.207243 | 33.176266 |
| Ca | 42.809433 | 29.238331 | 34.665474 |
| S  | 27.049435 | 28.253660 | 36.423698 |
| S  | 27.024536 | 34.045795 | 33.743584 |
| S  | 30.509068 | 29.538118 | 32.760117 |
| S  | 29.940912 | 31.171446 | 36.382599 |
| S  | 33.380978 | 27.208536 | 34.092426 |
| S  | 33.83740  | 32.382343 | 32.700020 |
| S  | 36.780010 | 28.311619 | 31.473913 |
| S  | 36.256351 | 29.468029 | 36.614651 |
| S  | 39.907875 | 26.832050 | 34.232712 |
| S  | 40.429302 | 31.356134 | 33.842960 |
| S  | 43.568211 | 28.766266 | 31.419012 |
| S  | 44.748894 | 26.488867 | 37.970943 |

|    | 24       |          |          |
|    | generated by VMD |

|    | 24.933832 | 30.354500 | 32.084820 |
| Ca | 26.376160 | 31.659336 | 35.733315 |
| Ca | 30.008781 | 27.804220 | 35.648994 |
| Ca | 30.382156 | 32.753334 | 33.214443 |
| Ca | 33.484772 | 29.261036 | 31.679859 |
| Ca | 33.159187 | 30.003469 | 35.414276 |
| Ca | 36.481377 | 26.732567 | 34.729939 |
| Ca | 36.739990 | 30.569225 | 34.040745 |
| Ca | 40.054161 | 28.982130 | 31.635710 |
| Ca | 39.805702 | 29.322868 | 36.625252 |
|   | Ca       | S        | Ca       | Ca       | S        | S        | S        | S        |
|---|----------|----------|----------|----------|----------|----------|----------|----------|
|   | 46.585453| 29.331928| 32.834072| 42.779026| 29.521637| 34.052010| 30.332155| 29.458113|
|   | 29.331928| 32.834072| 46.585453| 29.521637| 34.052010| 30.332155| 29.458113| 34.396561|
|   | 32.834072| 46.585453| 29.331928| 32.834072| 46.585453| 29.331928| 32.834072| 46.585453|

Generated by VMD

|   | Ca       | S        | Ca       | Ca       | S        | S        | S        | S        |
|---|----------|----------|----------|----------|----------|----------|----------|----------|
|   | 25.135805| 29.867830| 32.093796| 26.230103| 31.548000| 35.674343| 30.291771| 27.808298|
|   | 29.867830| 32.093796| 25.135805| 26.230103| 31.548000| 35.674343| 30.291771| 27.808298|
|   | 32.093796| 32.093796| 25.135805| 26.230103| 31.548000| 35.674343| 30.291771| 27.808298|
|   | 25.135805| 25.135805| 25.135805| 25.135805| 25.135805| 25.135805| 25.135805| 25.135805|

Generated by VMD

|   | Ca       | S        | Ca       | Ca       | S        | S        | S        | S        |
|---|----------|----------|----------|----------|----------|----------|----------|----------|
|   | 46.430775| 29.004732| 32.958287| 46.430775| 29.004732| 32.958287| 46.430775| 29.004732|
|   | 29.004732| 32.958287| 46.430775| 29.004732| 32.958287| 46.430775| 29.004732| 32.958287|
|   | 32.958287| 32.958287| 46.430775| 29.004732| 32.958287| 46.430775| 29.004732| 32.958287|
|   | 46.430775| 46.430775| 46.430775| 46.430775| 46.430775| 46.430775| 46.430775| 46.430775|

Generated by VMD
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 33.197929  | 29.527071  | 31.441574  |
| Ca      | 33.124641  | 30.363419  | 35.457397  |
| Ca      | 36.556534  | 26.700485  | 34.696777  |
| Ca      | 36.931370  | 30.627615  | 33.781658  |
| Ca      | 39.972507  | 28.889311  | 31.658501  |
| Ca      | 39.668270  | 29.474447  | 36.565666  |
| Ca      | 46.876568  | 29.243919  | 33.179287  |
| Ca      | 42.915581  | 29.262461  | 34.390976  |
| S       | 27.062492  | 27.878977  | 36.411922  |
| S       | 27.092606  | 34.211704  | 33.985222  |
| S       | 30.240143  | 29.801825  | 32.588917  |
| S       | 30.047394  | 31.252287  | 36.585213  |
| S       | 33.241489  | 27.141121  | 34.091652  |
| S       | 33.761219  | 32.481750  | 32.731392  |
| S       | 36.702816  | 28.195187  | 31.391783  |
| S       | 36.270603  | 29.336954  | 36.473526  |
| S       | 40.024384  | 26.737486  | 34.172096  |
| S       | 40.331326  | 31.398491  | 33.824638  |
| S       | 43.479866  | 28.700436  | 31.386715  |
| S       | 44.72725   | 26.787382  | 38.097477  |

24 generated by VMD
Ca 24.898567 30.036236 32.220123
Ca 26.522902 31.352280 35.886185
Ca 30.125420 27.956131 35.861141
Ca 30.239878 32.859219 33.306683
Ca 33.622128 29.571861 31.556856
Ca 33.109226 30.226292 35.88992
Ca 36.342461 26.580858 34.365131
Ca 36.651104 30.735008 33.881424
Ca 40.130699 29.069267 31.573586
Ca 39.680340 29.245914 36.636494
Ca 46.843582 29.052761 33.192955
Ca 42.964348 28.990089 34.201057
S 26.996588 27.898636 36.542328
S 27.121834 34.191212 33.83882
S 30.449121 29.776859 32.841640
S 29.964348 31.324738 36.407280
S 33.088100 27.233166 34.037289
S 33.849987 32.478191 32.766022
S 36.716106 28.658960 31.511421
S 36.342770 29.257124 36.527237
S 39.938236 26.761036 34.056320
S 40.468113 31.202368 33.881870
S 43.698681 28.779140 31.344656
S 44.669426 27.154015 38.205193

24

Ca 24.704334 29.724419 32.072517
Ca 26.326120 31.443596 35.632465
Ca 30.250690 28.020649 36.034641
Ca 30.465223 33.126976 33.565697
Ca 33.251575 29.565498 31.399075
Ca 33.398685 29.970739 35.338539
Ca 36.451042 26.593884 34.393784
Ca 36.919674 30.802380 33.803242
Ca 40.066635 29.090397 31.630550
Ca 39.787327 29.395586 36.867851
Ca 46.423798 29.357399 32.908516
Ca 42.837284 29.078527 34.429512
S 26.886715 27.926510 36.377926
S 27.102503 34.143913 33.537838
S 30.519833 29.896865 33.000053
S 30.007782 31.334759 36.503250
S 33.122952 27.125191 34.029396
S 33.928802 32.489685 32.964287

24

generated by VMD

Ca 24.898567 30.036236 32.220123
Ca 26.522902 31.352280 35.886185
Ca 30.125420 27.956131 35.861141
Ca 30.239878 32.859219 33.306683
Ca 33.622128 29.571861 31.556856
Ca 33.109226 30.226292 35.88992
Ca 36.342461 26.580858 34.365131
Ca 36.651104 30.735008 33.881424
Ca 40.130699 29.069267 31.573586
Ca 39.680340 29.245914 36.636494
Ca 46.843582 29.052761 33.192955
Ca 42.964348 28.990089 34.201057
S 26.996588 27.898636 36.542328
S 27.121834 34.191212 33.83882
S 30.449121 29.776859 32.841640
S 29.964348 31.324738 36.407280
S 33.088100 27.233166 34.037289
S 33.849987 32.478191 32.766022
S 36.716106 28.658960 31.511421
S 36.342770 29.257124 36.527237
S 39.938236 26.761036 34.056320
S 40.468113 31.202368 33.881870
S 43.698681 28.779140 31.344656
S 44.669426 27.154015 38.205193

24

generated by VMD
|   | X       | Y       | Z       |
|---|---------|---------|---------|
| S | 36.574722 | 28.509554 | 31.457207 |
| S | 36.439098 | 29.154558 | 36.423546 |
| S | 39.910847 | 26.748499 | 34.188961 |
| S | 40.534958 | 31.257519 | 33.985771 |
| S | 43.388096 | 28.536442 | 31.239998 |
| S | 45.135117 | 27.096045 | 38.246040 |

24

generated by VMD

| Ca | X       | Y       | Z       |
|----|---------|---------|---------|
| Ca | 24.828970 | 29.931404 | 31.922298 |
| Ca | 26.324469 | 31.251654 | 35.907360 |
| Ca | 30.305773 | 28.078432 | 35.757744 |
| Ca | 30.399393 | 32.774643 | 33.113792 |
| Ca | 33.416119 | 29.513205 | 31.698120 |
| Ca | 33.213531 | 30.416843 | 35.705063 |
| Ca | 36.356056 | 26.972832 | 34.507530 |
| Ca | 36.800236 | 31.210112 | 33.892822 |
| Ca | 40.257385 | 29.035187 | 31.579689 |
| Ca | 39.718838 | 29.228218 | 36.504452 |
| Ca | 46.641853 | 29.130657 | 32.764019 |
| Ca | 42.972034 | 28.979916 | 34.374725 |
| S  | 26.914070 | 27.844112 | 36.233124 |
| S  | 27.104088 | 34.043133 | 33.800266 |
| S  | 30.460588 | 29.436329 | 32.746765 |
| S  | 29.860340 | 31.441025 | 36.423767 |
| S  | 33.297195 | 27.241644 | 34.526176 |
| S  | 33.856117 | 32.33618 | 33.129108 |
| S  | 36.732128 | 28.702917 | 31.638937 |
| S  | 36.381561 | 29.433113 | 36.584431 |
| S  | 39.878033 | 26.868488 | 33.936333 |
| S  | 40.512043 | 31.323732 | 33.874687 |
| S  | 43.592686 | 28.486778 | 31.285898 |
| S  | 44.610291 | 26.713413 | 38.123589 |

24

generated by VMD

| Ca | X       | Y       | Z       |
|----|---------|---------|---------|
| Ca | 24.451618 | 30.002171 | 31.815731 |
| Ca | 26.479340 | 31.199999 | 35.647469 |
| Ca | 30.184074 | 28.104900 | 35.974697 |
| Ca | 30.139254 | 33.046219 | 33.409554 |
| Ca | 33.455505 | 29.417566 | 31.675808 |
| Ca | 33.480549 | 30.298357 | 35.597900 |
| Ca | 36.495300 | 26.714762 | 34.553776 |
| Ca | 37.052036 | 31.107136 | 33.928417 |
| Ca | 40.115505 | 29.169422 | 31.642246 |
| Ca | 39.910378 | 29.375603 | 36.780594 |
| Ca | 46.627995 | 28.925268 | 32.737583 |
| Ca | 42.835583 | 29.023125 | 34.281788 |
|     |         |         |         |
|-----|---------|---------|---------|
| 24  | generated by VMD |
| Ca  | 24.731697 | 29.746059 | 32.061520 |
| Ca  | 26.428522 | 31.153524 | 35.470207 |
| Ca  | 30.182461 | 28.181366 | 36.180950 |
| Ca  | 30.277733 | 32.915779 | 33.200310 |
| Ca  | 33.336006 | 29.313597 | 31.766624 |
| Ca  | 33.294701 | 30.482626 | 35.628849 |
| Ca  | 36.589497 | 26.539604 | 34.354637 |
| Ca  | 36.953945 | 30.914810 | 34.089409 |
| Ca  | 40.009327 | 29.379377 | 31.498367 |
| Ca  | 39.991814 | 29.144884 | 36.601406 |
| Ca  | 46.504372 | 28.630371 | 32.857956 |
| Ca  | 42.929413 | 29.253780 | 34.416424 |
| S   | 26.881008 | 27.829195 | 36.282116 |
| S   | 26.887848 | 34.077423 | 33.388641 |
| S   | 30.466606 | 29.745955 | 33.003574 |
| S   | 29.944984 | 31.663799 | 36.434212 |
| S   | 33.249352 | 27.291454 | 34.473930 |
| S   | 33.867992 | 32.450058 | 32.804214 |
| S   | 36.715279 | 28.604576 | 31.555683 |
| S   | 36.524303 | 29.070478 | 36.604244 |
| S   | 40.016552 | 26.911425 | 34.014706 |
| S   | 40.406807 | 31.523010 | 33.949108 |
| S   | 43.384972 | 28.899342 | 31.282009 |
| S   | 44.858765 | 26.668903 | 38.111546 |

24

generated by VMD

|     |         |         |         |
|-----|---------|---------|---------|
| Ca  | 24.898262 | 29.779697 | 32.054470 |
| Ca  | 26.447403 | 31.152565 | 35.641029 |
| Ca  | 30.299490 | 28.190567 | 35.991104 |
| Ca  | 30.405058 | 33.037170 | 33.301155 |
| Ca  | 33.368164 | 29.402153 | 31.717676 |
| Ca  | 33.379543 | 30.423918 | 35.639404 |
|    | Ca      | S        | 24 | generated by VMD |
|----|---------|----------|----|------------------|
|    | 36.415817 | 26.355747 | 34.292198 | 24 |
|    | 36.792416 | 30.750744 | 33.942482 | generated by VMD |
|    | 39.872261 | 29.225702 | 31.486126 | 24 |
|    | 40.011974 | 29.646002 | 36.893192 | generated by VMD |
|    | 46.514359 | 28.871439 | 32.826694 | 24 |
|    | 42.831627 | 28.986586 | 34.359486 | generated by VMD |
|    | 26.938332 | 27.793087 | 36.184372 | 24 |
|    | 27.023956 | 34.152138 | 33.508942 | generated by VMD |
|    | 30.456268 | 29.753984 | 32.905846 | 24 |
|    | 30.106371 | 31.428144 | 36.395157 | generated by VMD |
|    | 33.251820 | 27.447300 | 34.359325 | 24 |
|    | 33.995914 | 32.513165 | 32.844101 | generated by VMD |
|    | 36.590485 | 28.175060 | 31.666502 | 24 |
|    | 36.598198 | 29.021574 | 36.557816 | generated by VMD |
|    | 39.817001 | 26.991293 | 34.123608 | 24 |
|    | 40.393623 | 31.465427 | 33.839378 | generated by VMD |
|    | 43.220345 | 28.932734 | 31.374634 | 24 |
|    | 44.805241 | 26.895178 | 38.126007 | generated by VMD |

24

|    | generated by VMD |
|----|------------------|
|    | 24.874252 | 29.750353 | 32.026524 |
|    | 26.273211 | 31.302090 | 35.618500 |
|    | 30.178823 | 28.128357 | 35.860886 |
|    | 30.549046 | 33.052464 | 33.156601 |
|    | 33.315079 | 29.419323 | 31.853880 |
|    | 33.226379 | 30.371197 | 35.640747 |
|    | 36.518780 | 26.588924 | 34.557899 |
|    | 36.649971 | 30.810421 | 33.945709 |
|    | 39.867203 | 29.095663 | 31.581409 |
|    | 39.843544 | 29.418591 | 36.556133 |
|    | 46.478092 | 29.237144 | 32.956749 |
|    | 42.896912 | 29.041664 | 34.438755 |
|    | 26.880898 | 27.876299 | 36.115444 |
|    | 27.157431 | 34.118149 | 33.946789 |
|    | 30.519798 | 29.781469 | 32.782379 |
|    | 29.887949 | 31.505531 | 36.161953 |
|    | 33.257347 | 27.156139 | 34.562359 |
|    | 33.895988 | 32.419113 | 32.656185 |
|    | 36.594936 | 28.518206 | 31.681355 |
|    | 36.387550 | 29.105354 | 36.633484 |
|    | 39.981411 | 26.756187 | 34.125214 |
|    | 40.540203 | 31.357006 | 34.043381 |
|    | 43.318630 | 28.857880 | 31.221302 |
|    | 45.340508 | 26.723854 | 37.907040 |

generated by VMD
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| Ca      | 24.790546 | 29.815454 | 31.873661 |
| Ca      | 26.324003  | 31.379486 | 35.521370  |
| Ca      | 29.929941  | 27.950123 | 35.960690  |
| Ca      | 30.492130  | 33.150627 | 33.306763  |
| Ca      | 33.483440  | 29.285128 | 31.666380  |
| Ca      | 33.317238  | 30.004307 | 35.649479  |
| Ca      | 36.416145  | 26.708729 | 34.515881  |
| Ca      | 36.821175  | 30.695841 | 33.754021  |
| Ca      | 40.096916  | 29.209295 | 31.750771  |
| Ca      | 39.671635  | 29.597393 | 36.487801  |
| Ca      | 46.533813  | 29.338045 | 33.046501  |
| Ca      | 42.785477  | 29.172556 | 34.477898  |
| S       | 26.578251  | 28.069132 | 36.308960  |
| S       | 27.348637  | 34.452938 | 33.993568  |
| S       | 30.499561  | 29.714882 | 32.912685  |
| S       | 29.971031  | 31.209736 | 36.450516  |
| S       | 33.172569  | 26.971468 | 34.301395  |
| S       | 33.844639  | 32.290504 | 32.740356  |
| S       | 36.701290  | 28.328556 | 31.460026  |
| S       | 36.450401  | 29.251671 | 36.641159  |
| S       | 40.051498  | 26.781363 | 34.102097  |
| S       | 40.505348  | 31.483845 | 33.887024  |
| S       | 43.402977  | 28.816984 | 31.242361  |
| S       | 45.245235  | 26.713295 | 37.979321  |

24 generated by VMD

| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| Ca      | 24.983604 | 29.613693 | 31.963917 |
| Ca      | 26.385612  | 31.473158 | 35.348488 |
| Ca      | 29.875189  | 28.235765 | 36.045231 |
| Ca      | 30.499294  | 32.774090 | 33.230541 |
| Ca      | 33.393291  | 29.464966 | 31.806423 |
| Ca      | 33.299416  | 30.111250 | 35.702831 |
| Ca      | 36.411518  | 26.680290 | 34.679020 |
| Ca      | 36.838242  | 30.748140 | 34.356911 |
| Ca      | 40.032120  | 29.217129 | 31.532345 |
| Ca      | 39.869987  | 29.291248 | 36.409252 |
| Ca      | 46.644325  | 29.632898 | 32.923462 |
| Ca      | 42.831173  | 29.173414 | 34.154823 |
| S       | 26.591236  | 28.195744 | 36.298046 |
| S       | 27.333984  | 34.241798 | 33.432575 |
| S       | 30.537785  | 29.589598 | 32.901539 |
| S       | 29.983086  | 31.507584 | 36.395905 |
| S       | 33.041180  | 27.150646 | 34.445755 |
| S       | 33.919991  | 32.378448 | 32.996826 |
| S       | 36.705406  | 28.305517 | 31.661129 |
| S       | 36.365147  | 28.902229 | 36.855656 |
24 generated by VMD

Ca  24.988825  29.781559  32.184654
Ca  26.335732  31.625658  35.595982
Ca  30.070530  28.100832  35.728588
Ca  30.483269  32.926598  33.280972
Ca  33.426373  29.533688  31.743826
Ca  33.243793  30.139744  35.362400
Ca  36.495579  26.454212  34.589802
Ca  36.700764  30.629677  33.999405
Ca  39.992413  29.119123  31.760944
Ca  39.712074  28.893335  36.402332
Ca  46.484852  29.791698  33.154949
Ca  42.745956  29.425259  34.416889
S   26.842752  28.208447  36.374706
S   27.178501  34.391724  33.719234
S   30.441449  29.804062  32.791065
S   29.896852  31.407764  36.291454
S   33.194504  27.100140  34.379318
S   33.896709  32.447632  32.769154
S   36.608757  28.201000  31.632032
S   36.191498  28.849893  36.752747
S   40.104122  26.611586  33.888771
S   40.222343  31.220520  34.133629
S   43.477085  28.840820  31.365608
S   45.696442  26.887360  37.712261
24 generated by VMD

Ca  25.155519  30.082867  32.467075
Ca  26.527958  31.847496  35.877277
Ca  30.078756  27.714056  35.796051
Ca  30.436640  32.956688  33.276421
Ca  33.359093  29.307781  31.570105
Ca  33.140762  29.772495  35.430458
Ca  36.593102  26.766727  34.390121
Ca  36.695633  30.792179  33.782269
Ca  40.080742  29.167364  31.551180
Ca  39.776321  29.303108  36.629715
Ca  46.753971  29.349773  33.327316
Ca  42.819370  29.273106  34.385616
S   26.799944  28.393738  36.460854
S   27.148218  34.328041  33.422642
S  30.455816  29.599129  32.828564
S  29.952557  31.180466  36.390625
S  33.238602  26.920986  34.197250
S  33.738331  32.226406  32.885677
S  36.615597  28.437515  31.458689
S  36.197269  29.114525  36.511673
S  40.079426  26.782442  34.060868
S  40.121426  31.308743  33.935326
S  43.382683  29.238337  31.345375
S  45.286091  26.527470  38.044365

24 generated by VMD
Ca  24.951714  30.145609  32.287735
Ca  26.427650  31.645342  35.790020
Ca  29.974415  27.950079  35.765713
Ca  30.356371  32.923737  33.346794
Ca  33.432327  29.357967  31.368296
Ca  33.149284  29.974636  35.422325
Ca  36.765717  26.646055  34.724575
Ca  36.643887  30.734863  33.702366
Ca  39.995087  28.884426  31.600842
Ca  39.799496  29.172697  36.712048
Ca  46.716301  29.614252  33.335682
Ca  42.992264  29.340626  34.487530
S  26.893446  28.196884  36.432850
S  27.236767  34.260590  33.558434
S  30.576147  29.713549  32.890848
S  29.908680  31.270176  36.514317
S  33.315056  27.140091  33.984318
S  33.721245  32.270657  32.827763
S  36.611572  28.372896  31.538221
S  36.300678  29.131516  36.594875
S  40.082951  26.744202  34.258583
S  40.235142  31.142620  33.983064
S  43.324772  29.141449  31.135750
S  45.022873  26.616516  37.759697

24 generated by VMD
Ca  24.571430  29.851797  32.336845
Ca  26.625322  31.480385  35.877045
Ca  29.866051  28.186994  35.711414
Ca  30.392353  33.005188  33.415913
Ca  33.387573  29.514935  31.513733
Ca  33.264992  30.124388  35.266129
Ca  36.735096  26.656536  34.706074
Ca  36.705555  30.669571  33.810574
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 40.075592 | 29.082500 | 31.594124 |
| Ca      | 39.842611 | 28.916799 | 36.602028 |
| Ca      | 46.750168 | 29.297262 | 33.460064 |
| Ca      | 42.995434 | 29.390976 | 34.404037 |
| S       | 26.720314 | 28.118092 | 36.319363 |
| S       | 26.988768 | 34.205357 | 33.770466 |
| S       | 30.531065 | 29.733322 | 32.751717 |
| S       | 30.134783 | 31.366951 | 36.435570 |
| S       | 33.225494 | 26.987085 | 34.108738 |
| S       | 33.829750 | 32.401386 | 32.658234 |
| S       | 36.641323 | 28.485964 | 31.449642 |
| S       | 36.311989 | 29.157816 | 36.585655 |
| S       | 40.171310 | 26.841898 | 34.133736 |
| S       | 40.175579 | 31.139721 | 33.983906 |
| S       | 43.539021 | 29.051653 | 31.234280 |
| S       | 44.950718 | 26.723209 | 37.901356 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 24.995224 | 29.900311 | 32.018932 |
| Ca      | 26.612955 | 31.399433 | 35.751541 |
| Ca      | 29.967731 | 28.196154 | 35.903652 |
| Ca      | 30.610094 | 33.083710 | 33.80260 |
| Ca      | 33.390999 | 29.539635 | 31.445436 |
| Ca      | 33.105938 | 29.966282 | 35.330879 |
| Ca      | 36.656494 | 26.590822 | 34.978336 |
| Ca      | 36.610741 | 30.325245 | 33.836372 |
| Ca      | 40.068386 | 28.986519 | 31.478001 |
| Ca      | 39.874508 | 29.210367 | 36.545238 |
| Ca      | 46.532887 | 29.325491 | 32.920589 |
| Ca      | 43.028561 | 29.437332 | 34.432217 |
| S       | 26.683720 | 28.247332 | 36.407646 |
| S       | 27.133089 | 34.068558 | 33.517746 |
| S       | 30.374210 | 29.842245 | 32.800640 |
| S       | 30.049974 | 31.320433 | 36.532356 |
| S       | 33.132820 | 27.070942 | 34.193756 |
| S       | 33.922218 | 32.531929 | 32.949619 |
| S       | 36.679596 | 28.208828 | 31.700386 |
| S       | 36.250805 | 29.166637 | 36.790600 |
| S       | 40.223183 | 26.734119 | 34.080887 |
| S       | 40.244171 | 31.150030 | 33.872654 |
| S       | 43.448185 | 29.172527 | 31.031179 |
| S       | 44.837406 | 26.916540 | 38.131767 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.108559 | 30.074692 | 32.088375 |
| Ca      | 26.528900 | 31.669518 | 36.015003 |
Ca  30.021292  27.953773  35.664417
Ca  30.478796  32.984116  33.478600
Ca  33.309045  29.445448  31.230837
Ca  33.103085  29.994429  35.427277
Ca  36.499161  26.303444  34.589966
Ca  36.545383  30.399149  37.988599
Ca  40.192837  28.710741  31.677198
Ca  39.728783  29.125973  36.652908
Ca  46.641117  29.808548  33.065559
Ca  42.821186  29.488468  34.453987
S   26.854397  28.412075  36.511421
S   27.147907  34.408253  33.827950
S   30.337830  29.892170  32.755081
S   30.059479  31.212181  36.441982
S   33.192871  27.144917  33.895329
S   33.762939  32.496635  32.496635
S   36.568447  28.055609  31.498680
S   36.339397  28.928886  36.597031
S   40.038548  26.463493  34.219990
S   40.119637  31.166214  33.825855
S   43.540138  29.075129  31.435278
S   45.434132  27.177530  38.104012

24

generated by VMD

Ca  24.738394  30.048624  32.078392
Ca  26.436155  31.657526  35.903442
Ca  29.701900  28.029018  35.830162
Ca  30.310238  32.916794  33.507252
Ca  33.569305  29.722897  31.398420
Ca  33.095203  29.851881  35.321213
Ca  36.549770  26.375269  34.488777
Ca  36.673161  30.540529  33.833710
Ca  39.958614  28.692818  31.532093
Ca  39.913231  28.950457  36.670227
Ca  46.655563  29.772585  33.588802
Ca  42.770607  29.321077  34.259941
S   26.611549  28.244068  36.325012
S   27.126434  34.364914  33.628036
S   30.526535  29.879107  32.950138
S   29.940742  31.301918  36.614796
S   33.132397  27.142487  33.968281
S   33.848633  32.476112  32.858849
S   36.704380  28.160269  31.536110
S   36.488888  28.965618  36.557781
S   40.184067  26.499912  34.121071
S   40.273067  31.080412  33.808491
S  43.514961  29.059837  31.191311
S  45.710075  27.337336  38.058365

24 generated by VMD

Ca  24.962803  29.664627  32.042271
Ca  26.337458  31.658295  35.781136
Ca  29.890688  28.110481  35.685909
Ca  30.288094  32.958843  33.634945
Ca  33.409096  29.773218  31.632845
Ca  33.179134  30.111227  35.493919
Ca  36.570774  26.574089  34.719379
Ca  36.842194  30.728031  33.904175
Ca  40.149712  28.687939  31.373966
Ca  39.993202  29.197233  36.809608
Ca  46.813461  29.669756  33.095291
Ca  42.892597  29.054220  34.258503
S  26.725525  28.156105  36.230732
S  26.945019  34.233730  33.351311
S  30.521505  29.729872  32.818954
S  29.813038  31.266985  36.523819
S  33.309475  27.274097  34.164936
S  33.772537  32.618248  33.070477
S  36.615746  28.388935  31.728830
S  36.337296  29.163235  36.753433
S  40.009762  26.555603  34.250977
S  40.293747  30.981197  33.832558
S  43.511307  28.911507  31.121618
S  45.249817  26.923916  37.751137

24 generated by VMD

Ca  24.694569  29.661791  32.226425
Ca  26.265396  31.637276  35.585808
Ca  30.055851  27.825855  35.626041
Ca  30.299438  33.106979  33.408627
Ca  33.418419  29.853626  31.795250
Ca  33.054413  30.025631  35.473942
Ca  36.691540  26.615025  34.657921
Ca  36.715637  30.708458  34.050911
Ca  40.010883  28.740847  31.717016
Ca  39.909504  29.189386  36.599014
Ca  46.727364  29.292667  32.907764
Ca  43.026344  29.303101  34.358700
S  26.779867  28.179729  36.229481
S  26.879503  34.276073  33.388748
S  30.410585  29.985847  32.772102
S  29.640638  31.218878  36.476662
|    |   X    |   Y    |   Z    |
|----|-------|-------|-------|
| S  | 33.213924 | 27.239752 | 34.048172 |
| S  | 33.916092 | 32.712975 | 33.279968 |
| S  | 36.601833 | 28.235651 | 31.772453 |
| S  | 36.491753 | 29.053045 | 36.790207 |
| S  | 40.237400 | 26.478821 | 34.104797 |
| S  | 40.453468 | 31.091557 | 33.620461 |
| S  | 43.532158 | 28.772984 | 31.138676 |
| S  | 45.407330 | 27.185467 | 38.001530 |

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*generated by VMD*

|    |   X    |   Y    |   Z    |
|----|-------|-------|-------|
| Ca | 24.794191 | 29.406004 | 32.128700 |
| Ca | 26.171137 | 31.453831 | 35.701866 |
| Ca | 29.688274 | 28.229731 | 35.856766 |
| Ca | 30.464243 | 33.066879 | 33.491642 |
| Ca | 33.467922 | 29.317982 | 31.601276 |
| Ca | 33.256626 | 30.186956 | 35.462994 |
| Ca | 36.617393 | 26.678310 | 34.406742 |
| Ca | 36.898781 | 30.698963 | 33.910126 |
| Ca | 40.157677 | 29.074390 | 31.547852 |
| Ca | 39.734417 | 29.077482 | 36.585350 |
| Ca | 46.805141 | 29.383858 | 33.105999 |
| Ca | 42.999508 | 29.232042 | 34.512730 |
| S  | 26.621798 | 28.167759 | 36.349293 |
| S  | 27.016018 | 34.188164 | 33.667664 |
| S  | 30.443542 | 29.910717 | 32.858086 |
| S  | 29.872185 | 31.463381 | 36.397900 |
| S  | 33.027489 | 27.317625 | 34.204128 |
| S  | 33.814350 | 32.493011 | 32.921520 |
| S  | 36.610744 | 28.433599 | 31.565464 |
| S  | 36.462135 | 29.010902 | 36.485157 |
| S  | 40.063702 | 26.810081 | 34.003937 |
| S  | 40.462364 | 31.296503 | 33.951859 |
| S  | 43.491055 | 28.805553 | 31.383247 |
| S  | 45.493217 | 26.687695 | 37.930305 |

24

*generated by VMD*

|    |   X    |   Y    |   Z    |
|----|-------|-------|-------|
| Ca | 25.199099 | 29.507183 | 31.940056 |
| Ca | 26.307974 | 31.667416 | 35.678055 |
| Ca | 30.201233 | 28.071257 | 35.888664 |
| Ca | 30.163616 | 33.137135 | 33.504990 |
| Ca | 33.326859 | 29.548851 | 31.645557 |
| Ca | 33.109230 | 30.282129 | 35.632401 |
| Ca | 36.578381 | 26.640804 | 34.606205 |
| Ca | 36.720673 | 30.452120 | 33.975243 |
| Ca | 40.155354 | 28.949408 | 31.497837 |
| Ca | 39.949745 | 29.144670 | 36.675812 |
|     | X1   | Y1   | Z1   |
|-----|------|------|------|
| Ca  | 46.74494 | 29.38392 | 33.110619 |
| Ca  | 42.864597 | 29.047768 | 34.24164 |
| S   | 26.848154 | 28.196857 | 36.425037 |
| S   | 26.962971 | 34.134506 | 33.244164 |
| S   | 30.509768 | 29.733103 | 32.868732 |
| S   | 29.758722 | 31.384333 | 36.485588 |
| S   | 33.365585 | 27.372894 | 34.451389 |
| S   | 33.636448 | 32.630623 | 33.035503 |
| S   | 36.653137 | 28.320667 | 31.541735 |
| S   | 36.428005 | 29.108486 | 36.777428 |
| S   | 39.966118 | 26.731251 | 33.969982 |
| S   | 40.413673 | 31.252026 | 33.852043 |
| S   | 43.502754 | 29.175016 | 31.057474 |
| S   | 45.064407 | 26.519012 | 37.922974 |

24 generated by VMD

|     | X1   | Y1   | Z1   |
|-----|------|------|------|
| Ca  | 25.019566 | 29.670568 | 31.690308 |
| Ca  | 26.459703 | 31.416504 | 35.537895 |
| Ca  | 29.891546 | 28.184206 | 36.021744 |
| Ca  | 30.317957 | 32.826645 | 33.622272 |
| Ca  | 33.492043 | 29.783760 | 31.501616 |
| Ca  | 33.165184 | 30.261480 | 35.451561 |
| Ca  | 36.451084 | 26.571989 | 34.713684 |
| Ca  | 36.773544 | 30.662720 | 33.954128 |
| Ca  | 39.998302 | 29.147615 | 31.231371 |
| Ca  | 39.920708 | 29.130043 | 36.632313 |
| Ca  | 46.476643 | 29.508694 | 33.267715 |
| Ca  | 42.843220 | 29.141626 | 34.446911 |
| S   | 26.693092 | 28.163893 | 36.609550 |
| S   | 27.070436 | 33.968018 | 33.126591 |
| S   | 30.564335 | 29.650185 | 32.966347 |
| S   | 29.962204 | 31.421873 | 36.654015 |
| S   | 33.175861 | 27.290478 | 34.427223 |
| S   | 33.929516 | 32.685249 | 32.996250 |
| S   | 36.697475 | 28.383184 | 31.845640 |
| S   | 36.455345 | 29.127598 | 36.791088 |
| S   | 40.052654 | 26.743412 | 34.034168 |
| S   | 40.199379 | 31.160109 | 33.640884 |
| S   | 43.499832 | 28.976311 | 31.77258 |
| S   | 45.324242 | 26.515236 | 37.690189 |

24 generated by VMD

|     | X1   | Y1   | Z1   |
|-----|------|------|------|
| Ca  | 25.192005 | 29.435032 | 32.006996 |
| Ca  | 26.466835 | 31.484940 | 35.539833 |
| Ca  | 29.914501 | 28.030125 | 35.955326 |
| Ca  | 30.094072 | 32.869267 | 33.467056 |
| Element | Ca   | S    |
|---------|------|------|
| 956     |      |      |
| Ca      | 33.452850 | 29.762238 | 31.712357 |
| Ca      | 33.091164 | 30.453148 | 35.380322 |
| Ca      | 36.346073 | 26.653080 | 34.790871 |
| Ca      | 36.696732 | 30.875478 | 34.133274 |
| Ca      | 40.094791 | 28.837400 | 31.845627 |
| Ca      | 39.907562 | 29.148346 | 36.495079 |
| Ca      | 46.706261 | 29.620274 | 32.894096 |
| Ca      | 43.051479 | 29.122524 | 34.216270 |
| S       | 26.735504 | 28.159100 | 36.472435 |
| S       | 27.076622 | 34.007042 | 33.038731 |
| S       | 30.485382 | 29.804615 | 32.683929 |
| S       | 29.988924 | 31.337528 | 36.460567 |
| S       | 33.139091 | 27.473341 | 34.268635 |
| S       | 33.664806 | 32.742653 | 33.118862 |
| S       | 36.648003 | 28.497234 | 32.012272 |
| S       | 36.346722 | 29.187931 | 36.762447 |
| S       | 40.138191 | 26.492193 | 34.151360 |
| S       | 40.341137 | 31.213661 | 33.982349 |
| S       | 43.446316 | 29.021338 | 31.036434 |
| S       | 45.408848 | 26.162613 | 37.605545 |

24 generated by VMD

| Element | Ca   | S    |
|---------|------|------|
| 956     |      |      |
| Ca      | 24.651407 | 29.874815 | 32.113605 |
| Ca      | 26.584167 | 31.484234 | 35.620094 |
| Ca      | 30.106390 | 27.997135 | 35.759392 |
| Ca      | 30.271858 | 33.110252 | 33.366993 |
| Ca      | 33.418705 | 29.643724 | 31.746441 |
| Ca      | 33.192745 | 30.156036 | 35.470604 |
| Ca      | 36.560070 | 26.437088 | 34.628376 |
| Ca      | 36.642063 | 30.762939 | 33.769234 |
| Ca      | 39.809258 | 28.852816 | 31.583254 |
| Ca      | 40.089890 | 29.182308 | 36.811417 |
| Ca      | 46.851814 | 29.483789 | 33.157349 |
| Ca      | 42.669018 | 29.250599 | 34.275661 |
| S       | 26.750881 | 28.066772 | 36.241402 |
| S       | 27.152248 | 34.199310 | 33.422157 |
| S       | 30.525082 | 29.780407 | 32.839985 |
| S       | 29.868771 | 31.186005 | 36.353886 |
| S       | 33.245480 | 27.193731 | 34.410969 |
| S       | 33.786049 | 32.594028 | 32.970348 |
| S       | 36.621761 | 28.435745 | 31.751326 |
| S       | 36.512398 | 29.207829 | 36.620293 |
| S       | 40.099316 | 26.743530 | 34.276737 |
| S       | 40.130989 | 31.160475 | 33.722797 |
| S       | 43.494980 | 29.050436 | 31.227760 |
| S       | 45.398514 | 26.537384 | 37.890556 |
|  | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | Ca       | S        | S        | S        | S        | S        | S        |
|---|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
|   | generated by VMD | generated by VMD |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 25.033138 | 29.686193 | 32.258743 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 26.395302 | 31.436966 | 35.698212 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 29.839560 | 27.964773 | 33.703327 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 30.57727 | 32.95286 | 33.48961 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 33.565403 | 29.758158 | 31.543959 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 33.104992 | 30.191647 | 35.554008 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 36.557430 | 26.749645 | 34.798370 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 36.719414 | 30.965248 | 34.050972 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 39.923737 | 28.934376 | 31.546328 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 39.919857 | 29.275547 | 36.652889 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 46.812115 | 29.358377 | 33.099663 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| Ca | 42.717484 | 29.135525 | 34.288605 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 26.689663 | 27.895542 | 36.298813 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 27.376545 | 34.074604 | 33.404629 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 30.608641 | 29.706760 | 32.746021 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 29.756788 | 31.200203 | 36.378575 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 33.245243 | 27.234339 | 34.342442 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 33.892822 | 32.754951 | 33.029999 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 36.615074 | 28.438295 | 31.817291 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 36.338905 | 29.442749 | 36.773849 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 40.097534 | 26.765260 | 34.267277 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 40.325592 | 31.196806 | 33.612076 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 43.537132 | 28.902878 | 31.129967 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
| S  | 45.003735 | 26.365932 | 37.685539 |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |        |
|     | X   | Y   | Z   |
|-----|-----|-----|-----|
| S   | 36.552189 | 28.488239 | 31.807674 |
| S   | 36.472271 | 29.385977 | 36.697010 |
| S   | 39.950073 | 26.812317 | 34.188812 |
| S   | 40.341740 | 31.304445 | 33.933258 |
| S   | 43.305794 | 28.842997 | 31.136726 |
| S   | 45.114296 | 26.353823 | 37.846970 |

24 generated by VMD

| Ca  | X   | Y   | Z   |
|-----|-----|-----|-----|
| Ca  | 24.905277 | 29.489931 | 32.085529 |
| Ca  | 26.506834 | 31.163113 | 35.520020 |
| Ca  | 30.006477 | 28.087055 | 35.865139 |
| Ca  | 30.233412 | 33.109581 | 33.33492 |
| Ca  | 33.429447 | 29.907495 | 31.631105 |
| Ca  | 33.169136 | 30.542526 | 35.476048 |
| Ca  | 36.443932 | 26.844107 | 34.855003 |
| Ca  | 36.738255 | 30.790924 | 34.051853 |
| Ca  | 39.844742 | 28.663187 | 31.642826 |
| Ca  | 40.154110 | 29.311205 | 36.837299 |
| Ca  | 46.780769 | 29.316326 | 32.857086 |
| Ca  | 42.885494 | 29.064796 | 34.222740 |
| S   | 26.952147 | 27.747894 | 36.047993 |
| S   | 26.985783 | 33.913322 | 33.346172 |
| S   | 30.432413 | 29.882700 | 32.816429 |
| S   | 29.990446 | 31.364429 | 36.439507 |
| S   | 33.173859 | 27.472649 | 34.273281 |
| S   | 33.718723 | 32.848343 | 32.984066 |
| S   | 36.498856 | 28.531418 | 31.893421 |
| S   | 36.527805 | 29.434885 | 36.902519 |
| S   | 39.970001 | 26.710670 | 34.405804 |
| S   | 40.357452 | 31.124592 | 33.748802 |
| S   | 43.416821 | 28.852585 | 31.040245 |
| S   | 45.311729 | 26.217676 | 37.754326 |

24 generated by VMD

| Ca  | X   | Y   | Z   |
|-----|-----|-----|-----|
| Ca  | 24.582355 | 29.645086 | 31.965364 |
| Ca  | 26.269188 | 31.126307 | 35.470730 |
| Ca  | 29.745651 | 28.225151 | 35.904846 |
| Ca  | 30.297112 | 32.866333 | 33.412090 |
| Ca  | 33.410507 | 29.750214 | 31.583424 |
| Ca  | 33.118294 | 30.501928 | 35.628452 |
| Ca  | 36.454006 | 26.864393 | 34.774685 |
| Ca  | 36.844769 | 30.743687 | 33.928139 |
| Ca  | 40.205112 | 28.819580 | 31.548628 |
| Ca  | 39.961506 | 29.342926 | 36.484241 |
| Ca  | 46.835972 | 29.471579 | 32.689102 |
| Ca  | 42.951199 | 28.986717 | 34.434765 |
|    | 26.687870 | 27.880747 | 36.190830 |
|----|-----------|-----------|-----------|
| S  | 27.063213 | 33.960045 | 33.455574 |
| S  | 30.394032 | 29.827835 | 32.822685 |
| S  | 29.797516 | 31.441948 | 36.465954 |
| S  | 33.087715 | 27.551041 | 34.398693 |
| S  | 33.895161 | 32.684139 | 32.993130 |
| S  | 36.647171 | 28.380264 | 31.862007 |
| S  | 36.448841 | 29.388435 | 36.814171 |
| S  | 40.240231 | 26.672647 | 34.297050 |
| S  | 40.428307 | 31.125414 | 33.882343 |
| S  | 43.574062 | 28.806704 | 31.196650 |
| S  | 45.494095 | 26.328299 | 37.827095 |

|    | 25.136585 | 29.525345 | 31.960142 |
|----|-----------|-----------|-----------|
| Ca | 26.302799 | 31.247646 | 35.425041 |
| Ca | 29.721531 | 28.132105 | 35.838020 |
| Ca | 30.580664 | 33.102669 | 33.292175 |
| Ca | 33.309372 | 29.790005 | 31.803516 |
| Ca | 32.908207 | 30.164816 | 35.668499 |
| Ca | 36.406303 | 26.791159 | 34.632408 |
| Ca | 36.841541 | 31.019474 | 34.166470 |
| Ca | 40.096226 | 28.561684 | 31.571129 |
| Ca | 40.187897 | 29.588249 | 36.732666 |
| Ca | 46.887650 | 29.304993 | 32.556774 |
| Ca | 43.055252 | 29.171129 | 34.270252 |
| S  | 25.136585 | 29.525345 | 31.960142 |
| S  | 26.302799 | 31.247646 | 35.425041 |
| S  | 29.721531 | 28.132105 | 35.838020 |
| S  | 30.580664 | 33.102669 | 33.292175 |
| S  | 33.309372 | 29.790005 | 31.803516 |
| S  | 32.908207 | 30.164816 | 35.668499 |
| S  | 36.406303 | 26.791159 | 34.632408 |
| S  | 36.841541 | 31.019474 | 34.166470 |
| S  | 40.096226 | 28.561684 | 31.571129 |
| S  | 40.187897 | 29.588249 | 36.732666 |
| S  | 46.887650 | 29.304993 | 32.556774 |
| S  | 43.055252 | 29.171129 | 34.270252 |

24

generated by VMD

Ca  25.136585  31.960142
Ca  25.053434  31.942156
Ca  26.302799  35.425041
Ca  26.353016  35.367794
Ca  29.721531  35.838020
Ca  29.820822  35.755707
Ca  30.303127  33.421841
Ca  33.405666  31.675097
Ca  33.094299  35.506866
|    |    |    |    |
|----|----|----|----|
| Ca | 36.320118 | 26.770411 | 34.744129 |
| Ca | 36.870129 | 30.838913 | 34.177441 |
| Ca | 39.937328 | 28.718880 | 31.814823 |
| Ca | 40.232204 | 29.418377 | 36.851288 |
| Ca | 46.840584 | 29.218063 | 32.492771 |
| Ca | 43.004150 | 28.718880 | 31.814823 |
| S  | 26.679768 | 28.004936 | 36.163544 |
| S  | 26.878094 | 34.025700 | 33.516731 |
| S  | 30.344357 | 29.910223 | 32.762222 |
| S  | 29.885092 | 31.255112 | 36.349083 |
| S  | 33.134785 | 27.482876 | 34.345608 |
| S  | 33.831642 | 32.829678 | 33.170269 |
| S  | 36.550751 | 28.549152 | 31.920391 |
| S  | 36.673294 | 29.309795 | 36.879158 |
| S  | 39.959339 | 26.674627 | 34.577560 |
| S  | 40.609829 | 31.273457 | 33.763927 |
| S  | 43.522820 | 28.615383 | 30.990322 |
| S  | 45.129299 | 26.638023 | 37.672100 |

24 generated by VMD

|    |    |    |    |
|----|----|----|----|
| Ca | 25.286924 | 29.473251 | 31.818466 |
| Ca | 26.386683 | 31.067741 | 35.359505 |
| Ca | 29.958242 | 28.145554 | 35.680103 |
| Ca | 30.244127 | 33.221626 | 33.559895 |
| Ca | 33.404202 | 29.938589 | 31.605501 |
| Ca | 33.125378 | 30.551502 | 35.435154 |
| Ca | 36.544582 | 26.792582 | 35.023117 |
| Ca | 36.766247 | 30.889172 | 33.979691 |
| Ca | 39.875496 | 28.603415 | 31.804873 |
| Ca | 40.159462 | 29.493511 | 36.789391 |
| Ca | 46.686729 | 29.483000 | 32.778645 |
| Ca | 43.061790 | 29.138878 | 34.183727 |
| S  | 26.725338 | 27.719028 | 36.040756 |
| S  | 26.840332 | 33.902069 | 33.461800 |
| S  | 30.448854 | 29.903299 | 32.768250 |
| S  | 29.772085 | 31.443924 | 36.525810 |
| S  | 33.197742 | 27.487562 | 34.560284 |
| S  | 33.786095 | 32.809235 | 33.077267 |
| S  | 36.369648 | 28.274666 | 32.103046 |
| S  | 36.507717 | 29.528835 | 36.888268 |
| S  | 40.069946 | 26.717930 | 34.571564 |
| S  | 40.469017 | 31.070942 | 33.789307 |
| S  | 43.375038 | 28.659029 | 31.004499 |
| S  | 45.372261 | 26.076094 | 37.221745 |

24 generated by VMD
|     | Ca       | S        |
|-----|----------|----------|
|     | 24.948664| 29.736902| 32.083580|
|     | 26.105000| 31.329334| 35.694672|
|     | 30.095171| 28.198738| 35.861343|
|     | 29.861597| 32.862938| 33.435711|
|     | 33.343216| 29.800503| 31.616302|
|     | 33.239315| 30.374165| 35.861343|
|     | 36.646343| 26.681217| 34.746719|
|     | 36.803864| 30.957691| 33.826546|
|     | 39.963459| 28.913660| 31.676435|
|     | 40.129021| 29.349503| 36.747875|
|     | 46.565376| 29.517225| 32.824921|
|     | 43.080238| 28.862047| 34.327999|
|     | 26.764957| 27.765469| 35.964146|
|     | 26.930525| 34.018833| 33.477230|
|     | 30.439228| 29.781111| 32.791672|
|     | 29.742857| 31.382347| 36.583565|
|     | 33.463024| 27.516674| 34.204468|
|     | 33.584335| 32.813957| 33.002697|
|     | 36.581905| 28.275902| 31.909550|
|     | 36.525833| 29.490843| 36.640938|
|     | 40.160542| 26.821012| 34.508018|
|     | 40.653557| 31.111248| 33.908859|
|     | 43.479385| 28.481487| 30.960037|
|     | 45.326542| 26.348616| 37.845921|

24 generated by VMD

|     | Ca       | S        |
|-----|----------|----------|
|     | 25.285416| 29.278595| 32.166359|
|     | 26.268902| 31.260588| 35.701996|
|     | 29.997999| 27.988314| 35.688316|
|     | 30.153936| 32.992836| 33.436253|
|     | 33.653305| 29.977064| 31.438423|
|     | 33.151100| 30.414490| 35.454533|
|     | 36.592926| 26.950533| 34.764061|
|     | 36.905849| 31.015926| 34.151085|
|     | 39.960171| 28.745373| 31.748203|
|     | 40.027210| 29.461792| 36.602211|
|     | 46.395248| 29.542204| 32.840668|
|     | 42.864429| 28.823828| 34.333355|
|     | 26.917397| 27.720989| 36.189018|
|     | 26.967949| 34.073715| 33.474930|
|     | 30.485456| 29.941055| 32.882957|
|     | 29.846975| 31.195898| 36.585144|
|     | 33.233181| 27.575327| 33.895126|
|     | 33.767540| 32.988579| 33.065632|
|     | 36.632366| 28.534508| 31.869982|
|     | 36.320755| 29.394947| 36.774937|
S  39.979477  26.634312  34.486374
S  40.549667  31.194584  33.657005
S  43.339149  28.294674  31.119305
S  45.137409  26.391222  37.704834

24

generated by VMD

Ca  25.103153  29.743509  32.025696
Ca  26.561451  30.888485  35.655823
Ca  30.047789  28.253212  35.833324
Ca  30.261137  32.947586  33.90743
Ca  33.480915  29.863686  31.589806
Ca  33.173809  30.628757  35.289948
Ca  36.435303  26.746332  34.814640
Ca  36.962341  30.917387  33.879005
Ca  39.950291  28.725395  31.698891
Ca  39.950638  29.460962  36.816395
Ca  46.504131  29.341198  32.870090
Ca  42.935841  28.942326  34.350582
S  26.805790  27.548929  36.160461
S  26.876911  33.752316  33.603077
S  30.407513  29.851149  32.682106
S  29.914120  31.515808  36.546001
S  33.184624  27.588844  34.174511
S  33.736526  32.841633  33.071621
S  36.702480  28.539135  31.902222
S  36.378399  29.567165  36.754620
S  40.015961  26.794712  34.470512
S  40.480698  31.112675  33.754612
S  43.405819  28.428156  31.100025
S  45.158272  26.392065  37.595951

24

generated by VMD

Ca  25.152086  29.738312  31.797733
Ca  26.385143  30.992466  35.524200
Ca  29.865891  28.271767  35.842072
Ca  30.248581  32.936150  33.522900
Ca  33.294971  29.628624  31.602234
Ca  33.172836  30.394064  35.547829
Ca  36.464954  26.838118  34.500793
Ca  36.815651  31.073524  33.974178
Ca  40.132099  28.827656  31.601536
Ca  40.098652  29.790220  36.691204
Ca  46.747334  29.091011  32.859589
Ca  43.135918  28.969549  34.417526
S  26.579224  27.644943  36.069653
S  26.990046  33.976898  33.77576
\begin{verbatim}
S    30.385279    29.722721    32.954643
S    29.967916    31.413006    36.601833
S    33.054207    27.388298    34.355373
S    33.748005    32.627174    32.962292
S    36.602295    28.561739    31.658905
S    36.597733    29.527552    36.642303
S    39.935459    26.954788    34.556961
S    40.514050    31.204420    33.588608
S    43.365387    28.406555    31.212126
S    45.180145    26.411867    37.768661

24 generated by VMD
Ca    24.958370    29.618572    32.207111
Ca    26.378195    30.874554    35.760674
Ca    30.064091    28.255861    35.950066
Ca    30.312826    33.013275    33.258778
Ca    33.326992    29.881493    31.601822
Ca    33.279385    30.450775    35.468628
Ca    36.395782    26.908237    34.255066
Ca    36.842239    31.147589    33.943748
Ca    40.009003    28.841824    31.914675
Ca    40.080662    29.526297    36.619011
Ca    46.741329    28.841738    32.770954
Ca    43.022446    28.977348    34.453247
S    26.759121    27.558304    31.065914
S    26.989910    33.913044    33.773037
S    30.388525    29.800985    32.827724
S    29.873510    31.374781    36.380516
S    33.154011    27.544327    34.299824
S    33.641140    32.698085    32.854462
S    36.543129    28.711344    31.572147
S    36.559753    29.470219    36.651478
S    39.926849    26.720470    34.438087
S    40.662746    31.274124    33.675816
S    43.641212    28.499157    31.318583
S    44.882607    26.527304    37.969311

24 generated by VMD
Ca    25.290892    29.734623    32.011562
Ca    26.373367    31.135687    35.821114
Ca    30.239904    27.882742    35.835052
Ca    29.944832    32.918636    33.766441
Ca    33.427593    29.871307    31.401100
Ca    33.150238    30.151350    35.329102
Ca    36.515900    26.883547    34.417854
Ca    36.924019    31.088497    33.647408
\end{verbatim}
Ca       40.069679       28.797661       31.630064
Ca       39.944393       29.870174       36.549747
Ca       46.736496       29.041950       33.303047
Ca       42.973106       28.931385       34.368450
S        26.919968       27.715740       36.527580
S        27.075068       34.148560       33.948494
S        30.406698       29.927694       33.003616
S        29.923941       31.149467       36.586086
S        33.208817       27.337803       33.809307
S        33.697372       32.755100       32.804756
S        36.655693       28.493105       31.474434
S        36.321243       29.572098       36.511169
S        39.886459       26.850420       34.336117
S        40.656441       31.393074       33.494919
S        43.654190       28.302090       31.178783
S        44.437645       26.438679       38.274460

24
generated by VMD
Ca       25.278536       29.800962       31.888672
Ca       26.377022       31.189333       35.890335
Ca       30.045820       28.136738       36.051252
Ca       30.262486       32.893337       33.421825
Ca       33.390556       29.781157       31.355850
Ca       33.259209       30.182383       35.325584
Ca       36.506107       26.718739       34.104519
Ca       36.673382       31.047356       33.768124
Ca       40.061546       28.651329       31.588707
Ca       39.810162       29.606438       36.740711
Ca       46.731544       29.150105       33.111111
Ca       42.844933       29.233704       34.516418
S        26.803072       27.862076       36.542255
S        27.039730       34.025932       33.953224
S        30.489100       29.759485       32.941261
S        29.950445       31.298162       36.650890
S        33.286095       27.419670       33.892418
S        33.693394       32.622662       32.938560
S        36.639793       28.531969       31.571161
S        36.519100       29.365601       36.367371
S        39.921280       26.755333       34.487274
S        40.593739       31.255896       33.478794
S        43.599625       28.537609       31.221384
S        44.657265       26.565437       38.222706

24
generated by VMD
Ca       24.956633       29.608833       32.392719
Ca       26.481115       31.276463       35.669395
| Ca   | 30.294769 | 28.061579 | 35.766083 |
|------|-----------|-----------|-----------|
| Ca   | 29.965382 | 32.972801 | 33.784714 |
| Ca   | 33.313469 | 29.796387 | 31.508198 |
| Ca   | 33.272697 | 30.201439 | 35.285694 |
| Ca   | 36.485088 | 26.615692 | 34.204414 |
| Ca   | 36.978931 | 29.98390  | 33.714714 |
| Ca   | 39.834045 | 29.263292 | 36.878849 |
| Ca   | 46.749741 | 29.548386 | 32.952518 |
| Ca   | 42.862110 | 30.032665 | 35.01423  |
| S    | 27.116076 | 27.905151 | 36.659679 |
| S    | 26.773970 | 34.213043 | 33.907974 |
| S    | 30.376986 | 29.739532 | 32.776310 |
| S    | 29.982426 | 31.503597 | 36.305134 |
| S    | 33.188137 | 27.357954 | 34.032711 |
| S    | 33.686306 | 32.765015 | 32.73875  |
| S    | 36.688427 | 28.456156 | 31.580278 |
| S    | 36.571289 | 29.308867 | 36.42207  |
| S    | 39.975044 | 26.732555 | 34.412186 |
| S    | 40.550209 | 31.239128 | 33.981968 |
| S    | 43.683819 | 28.700962 | 31.338919 |
| S    | 44.474598 | 26.244904 | 37.861477 |

generated by VMD

| Ca   | 25.015015 | 29.534008 | 32.294853 |
|------|-----------|-----------|-----------|
| Ca   | 26.473623 | 30.983095 | 35.863850 |
| Ca   | 30.409533 | 28.219570 | 35.777390 |
| Ca   | 29.890997 | 32.954319 | 33.491417 |
| Ca   | 33.411297 | 29.930346 | 31.353771 |
| Ca   | 33.202686 | 30.510921 | 35.403351 |
| Ca   | 36.610554 | 26.575294 | 34.177624 |
| Ca   | 36.723953 | 31.020807 | 33.601246 |
| Ca   | 40.170776 | 28.776819 | 31.383352 |
| Ca   | 39.797947 | 29.365829 | 36.550289 |
| Ca   | 46.850273 | 29.274565 | 33.506626 |
| Ca   | 42.857018 | 28.928400 | 34.517639 |
| S    | 27.210407 | 27.786289 | 36.465897 |
| S    | 26.765253 | 34.083920 | 34.057655 |
| S    | 30.389647 | 29.875313 | 32.853302 |
| S    | 29.923315 | 31.518368 | 36.518894 |
| S    | 33.216530 | 27.629238 | 34.018848 |
| S    | 33.445225 | 32.870941 | 32.865608 |
| S    | 36.632950 | 28.700388 | 31.632946 |
| S    | 36.365139 | 29.366411 | 36.301811 |
| S    | 40.069920 | 26.723619 | 34.148266 |
| S    | 40.508186 | 31.144588 | 33.567978 |
|     |       |       |       |
|-----|-------|-------|-------|
| S   | 43.861275 | 28.325766 | 31.447441 |
| S   | 44.632397 | 26.292618 | 38.230618 |

24 generated by VMD

| Ca  |       |       |       |
|-----|-------|-------|-------|
| Ca  | 25.079792 | 29.612307 | 32.116158 |
| Ca  | 26.450050 | 31.130205 | 35.572735 |
| Ca  | 30.221788 | 28.049751 | 35.682297 |
| Ca  | 30.200909 | 32.957119 | 33.632629 |
| Ca  | 33.414055 | 29.948648 | 31.405188 |
| Ca  | 33.104210 | 30.405893 | 35.342606 |
| Ca  | 36.646709 | 26.655659 | 34.546608 |
| Ca  | 36.680420 | 30.880243 | 33.822601 |
| Ca  | 39.993832 | 28.659464 | 31.472048 |
| Ca  | 39.874229 | 29.349888 | 36.836857 |
| Ca  | 46.811306 | 29.262344 | 33.158024 |
| Ca  | 42.901768 | 29.113024 | 34.344326 |
| S   | 27.271761 | 27.832796 | 36.487289 |
| S   | 26.939337 | 34.111416 | 33.860641 |
| S   | 30.462061 | 29.997046 | 32.681255 |
| S   | 30.038425 | 31.371845 | 36.601044 |
| S   | 33.131592 | 27.484449 | 34.064533 |
| S   | 33.542576 | 32.801430 | 32.862537 |
| S   | 36.589260 | 28.517843 | 31.634720 |
| S   | 36.372889 | 29.426100 | 36.625240 |
| S   | 39.994846 | 26.635090 | 34.411980 |
| S   | 40.289238 | 31.117041 | 33.673954 |
| S   | 43.681023 | 28.492378 | 31.341120 |
| S   | 44.740723 | 26.579447 | 37.854359 |

24 generated by VMD

| Ca  |       |       |       |
|-----|-------|-------|-------|
| Ca  | 25.258301 | 29.602001 | 31.959248 |
| Ca  | 26.280582 | 31.370417 | 35.858494 |
| Ca  | 30.155134 | 27.999435 | 35.879276 |
| Ca  | 30.298464 | 32.813213 | 33.547646 |
| Ca  | 33.216988 | 29.987442 | 31.526312 |
| Ca  | 33.108353 | 30.216089 | 35.215862 |
| Ca  | 36.585079 | 26.529011 | 34.535267 |
| Ca  | 36.632977 | 30.657347 | 33.675125 |
| Ca  | 40.185482 | 28.977570 | 31.394947 |
| Ca  | 39.928810 | 29.411659 | 36.620518 |
| Ca  | 46.767853 | 29.057959 | 33.308807 |
| Ca  | 43.030083 | 28.959293 | 34.592144 |
| S   | 27.118906 | 28.034103 | 36.705200 |
| S   | 26.955967 | 34.242077 | 33.877552 |
| S   | 30.366261 | 29.775112 | 32.801468 |
| S   | 29.901884 | 31.401043 | 36.452675 |
|   | 33.118343 | 27.276400 | 34.146931 |
|---|-----------|-----------|-----------|
| S | 33.810066 | 32.782944 | 32.701778 |
| S | 36.378475 | 28.278187 | 31.604191 |
| S | 36.373558 | 29.349749 | 36.452206 |
| S | 40.183823 | 26.891268 | 34.254894 |
| S | 40.318295 | 31.203558 | 33.611877 |
| S | 43.746231 | 29.168087 | 31.222237 |
| S | 44.714020 | 26.407499 | 38.086052 |

24 generated by VMD

|   | 25.277948 | 29.550377 | 31.903593 |
|---|-----------|-----------|-----------|
| Ca| 26.158287 | 31.102940 | 35.821518 |
| Ca| 30.144468 | 28.188019 | 35.876381 |
| Ca| 30.325916 | 32.880039 | 33.183018 |
| Ca| 33.438503 | 29.952425 | 31.402109 |
| Ca| 33.150051 | 30.473629 | 35.240326 |
| Ca| 36.590946 | 26.687193 | 34.901680 |
| Ca| 36.678673 | 30.934996 | 33.725643 |
| Ca| 40.068073 | 28.792824 | 31.717739 |
| Ca| 39.938732 | 29.574347 | 36.736992 |
| Ca| 46.639450 | 28.754925 | 32.891148 |
| Ca| 42.931396 | 28.934731 | 34.341358 |
| S | 26.943329 | 27.683422 | 36.425404 |
| S | 26.842567 | 33.917774 | 34.038231 |
| S | 30.540234 | 29.814243 | 32.729465 |
| S | 29.928307 | 31.401001 | 36.487465 |
| S | 33.239635 | 27.413523 | 34.302059 |
| S | 33.969666 | 32.881123 | 32.756100 |
| S | 36.542030 | 28.397440 | 31.887024 |
| S | 36.339180 | 29.627831 | 36.677620 |
| S | 40.009598 | 26.866016 | 34.312103 |
| S | 40.455639 | 31.169928 | 33.708557 |
| S | 43.581585 | 29.182295 | 31.104982 |
| S | 44.699730 | 26.210350 | 37.860203 |

24 generated by VMD

|   | 24.756985 | 30.000149 | 32.058102 |
|---|-----------|-----------|-----------|
| Ca| 26.306637 | 31.149107 | 35.771164 |
| Ca| 30.251211 | 28.028091 | 35.894600 |
| Ca| 30.241999 | 32.950336 | 33.479244 |
| Ca| 33.429321 | 29.808958 | 31.421837 |
| Ca| 33.173149 | 30.150597 | 35.325203 |
| Ca| 36.516304 | 26.653082 | 34.732868 |
| Ca| 36.827377 | 30.864643 | 33.714931 |
| Ca| 40.105293 | 28.589918 | 31.418884 |
| Ca| 39.840801 | 29.542290 | 36.761330 |
|   | Ca      | 46.840454 | 28.841171 | 33.111240 |
|---|---------|-----------|-----------|-----------|
|   | Ca      | 43.112923 | 29.182011 | 34.67594  |
|   | S       | 26.926815 | 27.850471 | 36.448372 |
|   | S       | 26.856554 | 34.096790 | 34.080311 |
|   | S       | 30.489727 | 29.722260 | 32.78315  |
|   | S       | 30.011765 | 31.546148 | 36.461033 |
|   | S       | 33.180538 | 27.199081 | 33.97409  |
|   | S       | 33.816177 | 32.712051 | 32.788536 |
|   | S       | 36.526119 | 28.287188 | 31.49402  |
|   | S       | 36.368462 | 29.442383 | 36.49438  |
|   | S       | 40.12371  | 26.872536 | 34.35025  |
|   | S       | 40.401894 | 31.006748 | 33.590794 |
|   | S       | 43.794060 | 29.188438 | 31.082619 |
|   | S       | 44.534988 | 26.706928 | 38.282742 |

24 generated by VMD

|   | Ca      | 24.898212 | 29.832899 | 32.198711 |
|---|---------|-----------|-----------|-----------|
|   | Ca      | 26.701384 | 31.084963 | 35.846275 |
|   | Ca      | 30.344212 | 28.185083 | 35.813179 |
|   | Ca      | 30.053852 | 32.950153 | 33.447105 |
|   | Ca      | 33.576279 | 29.651752 | 31.092072 |
|   | Ca      | 33.188446 | 30.576206 | 35.434803 |
|   | Ca      | 36.516872 | 29.672218 | 34.664803 |
|   | Ca      | 36.615395 | 30.630438 | 33.652855 |
|   | Ca      | 40.106487 | 26.636274 | 31.404119 |
|   | Ca      | 39.851444 | 29.325829 | 36.680733 |
|   | Ca      | 46.563499 | 28.973785 | 33.149891 |
|   | Ca      | 42.936546 | 29.266285 | 34.609802 |
|   | S       | 26.975920 | 27.726166 | 36.465073 |
|   | S       | 26.954702 | 34.187771 | 34.241817 |
|   | S       | 30.440407 | 29.841137 | 32.716385 |
|   | S       | 30.029587 | 31.488338 | 36.452610 |
|   | S       | 33.249107 | 27.626280 | 33.916229 |
|   | S       | 33.867039 | 32.656578 | 32.620777 |
|   | S       | 36.663780 | 28.213730 | 31.577831 |
|   | S       | 36.284904 | 29.266689 | 36.484116 |
|   | S       | 40.043335 | 26.678705 | 34.384949 |
|   | S       | 40.198914 | 30.978172 | 33.634060 |
|   | S       | 43.656483 | 29.303478 | 31.242882 |
|   | S       | 44.717052 | 26.638454 | 38.299675 |

24 generated by VMD

|   | Ca      | 25.057356 | 29.733130 | 32.429558 |
|---|---------|-----------|-----------|-----------|
|   | Ca      | 26.508446 | 31.219196 | 35.933884 |
|   | Ca      | 30.272640 | 28.047855 | 35.809231 |
|   | Ca      | 30.437525 | 32.862068 | 33.451019 |
|     | Ca     |       |       |
|-----|--------|-------|-------|
|     | 33.375088 | 29.862432 | 31.208183 |
|     | 33.171558 | 30.329933 | 35.248688 |
|     | 36.540741 | 26.683222 | 34.361076 |
|     | 36.891132 | 30.723568 | 33.679298 |
|     | 39.948383 | 28.833887 | 31.475792 |
|     | 39.857155 | 29.676376 | 36.766327 |
|     | 46.751888 | 28.656160 | 33.463509 |
|     | 42.808384 | 29.057285 | 34.459759 |
| S   | 27.060425 | 27.992878 | 36.557648 |
| S   | 27.133369 | 33.950802 | 34.182423 |
| S   | 30.408718 | 29.685181 | 32.681919 |
| S   | 30.120670 | 31.265091 | 36.490250 |
| S   | 33.138638 | 27.303236 | 33.713768 |
| S   | 33.886337 | 32.706402 | 32.736290 |
| S   | 36.545586 | 28.523941 | 31.373575 |
| S   | 36.458675 | 29.229996 | 36.395630 |
| S   | 39.906784 | 26.901419 | 34.170025 |
| S   | 40.314175 | 31.220818 | 33.679558 |
| S   | 43.527351 | 28.989822 | 31.131767 |
| S   | 44.312851 | 26.936726 | 38.631592 |
| Element | X1, Y1, Z1 | X2, Y2, Z2 | X3, Y3, Z3 |
|---------|------------|------------|------------|
| Ca      | 24.779610  | 30.021353  | 32.518875  |
| Ca      | 26.457600  | 30.889961  | 36.050468  |
| Ca      | 30.208635  | 27.853180  | 35.721615  |
| Ca      | 30.232166  | 32.874619  | 33.471039  |
| Ca      | 33.430210  | 29.891211  | 31.029121  |
| Ca      | 32.995968  | 30.625443  | 35.104942  |
| Ca      | 36.590595  | 26.859581  | 34.358513  |
| Ca      | 36.998569  | 31.105537  | 33.482616  |
| Ca      | 40.235195  | 28.784214  | 31.402985  |
| Ca      | 39.812012  | 29.723139  | 36.343525  |
| Ca      | 46.711647  | 28.647772  | 33.546211  |
| Ca      | 43.029980  | 28.873028  | 34.662098  |
| S       | 27.044880  | 27.680592  | 36.391979  |
| S       | 27.071190  | 33.990273  | 34.889954  |
| S       | 30.498848  | 29.763805  | 32.643730  |
| S       | 29.936846  | 31.053469  | 36.491539  |
| S       | 33.140484  | 27.363659  | 33.829224  |
| S       | 33.624531  | 32.711525  | 32.578388  |
| S       | 36.564518  | 28.590221  | 31.406788  |
| S       | 36.396866  | 29.662434  | 36.184387  |
| S       | 39.936325  | 26.917189  | 34.356186  |
| S       | 40.749146  | 31.213428  | 33.469086  |
| S       | 43.847672  | 28.447521  | 31.458887  |
| S       | 44.140366  | 26.848248  | 38.638592  |
| Ca      | 24.951403  | 30.098766  | 32.779202  |
| Ca      | 26.615057  | 30.957954  | 36.232231  |
| Ca      | 30.226995  | 28.051943  | 35.432072  |
| Ca      | 30.105402  | 32.829018  | 33.237587  |
| Ca      | 33.330666  | 29.716333  | 31.031511  |
| Ca      | 33.251030  | 30.304888  | 35.087280  |
| Ca      | 36.730190  | 26.852407  | 34.360733  |
| Ca      | 36.754417  | 30.955843  | 33.543354  |
| Ca      | 40.141079  | 28.829418  | 31.616980  |
| Ca      | 39.518318  | 29.581272  | 36.611801  |
| Ca      | 46.583591  | 28.557043  | 33.580788  |
| Ca      | 42.915848  | 29.105444  | 34.649097  |
| S       | 27.403353  | 27.770117  | 36.729885  |
| S       | 26.997581  | 34.057106  | 34.555614  |
| S       | 30.319519  | 29.764336  | 32.472729  |
| S       | 30.248459  | 31.211075  | 36.309643  |
| S       | 33.342300  | 27.398849  | 33.706421  |
| S       | 33.663273  | 32.809044  | 32.526501  |
| S    | 36.692818 | 28.556759 | 31.380491 |
| S    | 36.460602 | 29.381390 | 36.310566 |
| S    | 40.069786 | 26.762737 | 34.382549 |
| S    | 40.470848 | 31.224741 | 33.601501 |
| S    | 43.628506 | 28.957582 | 31.281385 |
| S    | 44.012810 | 26.657333 | 38.610817 |

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generated by VMD

| Ca   | 25.282387 | 29.704357 | 32.488548 |
| Ca   | 26.580032 | 30.983833 | 36.217094 |
| Ca   | 30.309225 | 28.200174 | 35.736618 |
| Ca   | 30.208395 | 33.020103 | 33.197197 |
| Ca   | 33.289326 | 29.815186 | 31.037161 |
| Ca   | 33.059669 | 30.387093 | 34.996483 |
| Ca   | 36.506790 | 26.774544 | 34.520325 |
| Ca   | 36.884171 | 30.920523 | 33.542778 |
| Ca   | 40.081989 | 28.821423 | 31.556355 |
| Ca   | 39.729259 | 29.196051 | 36.479939 |
| Ca   | 46.765720 | 28.816084 | 33.566666 |
| Ca   | 42.843742 | 28.917263 | 34.516529 |
| S    | 27.332375 | 27.809898 | 36.811707 |
| S    | 27.047548 | 33.780758 | 34.692459 |
| S    | 30.323221 | 29.946167 | 32.531174 |
| S    | 30.071692 | 31.396814 | 36.311668 |
| S    | 33.151005 | 27.449057 | 33.704960 |
| S    | 33.788429 | 32.793587 | 32.543449 |
| S    | 36.597248 | 28.646606 | 31.326763 |
| S    | 36.436913 | 29.339764 | 36.295082 |
| S    | 39.896069 | 26.766083 | 34.166599 |
| S    | 40.495979 | 31.177469 | 33.856331 |
| S    | 43.685844 | 28.936537 | 31.263382 |
| S    | 44.066849 | 26.791998 | 38.671417 |

24

generated by VMD

| Ca   | 24.883497 | 29.613262 | 32.852783 |
| Ca   | 26.534039 | 31.195723 | 36.286266 |
| Ca   | 30.027567 | 28.002880 | 35.363426 |
| Ca   | 30.147442 | 33.080799 | 33.486092 |
| Ca   | 33.548138 | 29.988174 | 31.079088 |
| Ca   | 32.955994 | 30.307381 | 34.968864 |
| Ca   | 36.565361 | 26.370205 | 34.398468 |
| Ca   | 37.055134 | 30.948944 | 33.660664 |
| Ca   | 40.127914 | 28.816750 | 31.389669 |
| Ca   | 39.759090 | 29.438293 | 36.582706 |
| Ca   | 46.497917 | 28.873466 | 33.740314 |
| Ca   | 42.858501 | 28.941381 | 34.705528 |
|  |  |  |  |
|---|---|---|---|
| S | 27.296576 | 27.884621 | 36.849857 |
| S | 26.925177 | 33.936455 | 34.246342 |
| S | 30.385309 | 30.094574 | 32.431065 |
| S | 30.030478 | 31.142088 | 36.374428 |
| S | 33.212509 | 27.416491 | 33.612633 |
| S | 33.568047 | 32.879810 | 32.777748 |
| S | 36.653938 | 28.671520 | 31.343079 |
| S | 36.450562 | 29.287561 | 36.193741 |
| S | 40.099136 | 26.754829 | 34.256657 |
| S | 40.506870 | 31.204252 | 33.571728 |
| S | 43.910034 | 28.665585 | 31.392220 |
| S | 44.434689 | 26.876366 | 38.467373 |

24 generated by VMD

| Ca | 24.711796 | 30.183273 | 32.457417 |
| Ca | 26.632576 | 31.079063 | 36.344906 |
| Ca | 30.234940 | 28.042696 | 35.426601 |
| Ca | 30.188324 | 32.873707 | 33.385094 |
| Ca | 33.463085 | 29.698620 | 31.285269 |
| Ca | 33.208462 | 30.251949 | 35.124874 |
| Ca | 36.589596 | 26.827156 | 34.526787 |
| Ca | 36.809624 | 31.018429 | 33.688736 |
| Ca | 40.200180 | 28.664478 | 31.567057 |
| Ca | 39.827881 | 29.775198 | 36.499268 |
| Ca | 46.683826 | 28.834429 | 33.534321 |
| Ca | 42.901985 | 29.020420 | 34.544399 |
| S | 27.201517 | 27.751778 | 36.545689 |
| S | 26.792561 | 33.950310 | 34.391720 |
| S | 30.374233 | 29.873363 | 32.504162 |
| S | 29.973076 | 31.268269 | 36.277065 |
| S | 33.203377 | 27.167162 | 33.887154 |
| S | 33.626984 | 32.654633 | 32.614582 |
| S | 36.775173 | 28.657240 | 31.507254 |
| S | 36.463993 | 29.447765 | 36.447002 |
| S | 39.949223 | 26.696634 | 34.413776 |
| S | 40.558582 | 31.213835 | 33.446091 |
| S | 43.850777 | 28.840355 | 31.266399 |
| S | 44.212185 | 26.600613 | 38.345032 |

24 generated by VMD

| Ca | 25.065548 | 30.004234 | 32.559937 |
| Ca | 26.531986 | 31.131210 | 36.386761 |
| Ca | 30.183460 | 27.813227 | 35.397778 |
| Ca | 30.103241 | 32.888008 | 33.439106 |
| Ca | 33.517807 | 29.515768 | 31.120876 |
| Ca | 33.318867 | 30.361565 | 35.229614 |
|  | Ca     | S     |
|---|--------|-------|
| Ca | 36.501255 | 26.741413 | 34.182137 |
| Ca | 36.923882 | 30.951895 | 36.504539 |
| Ca | 40.227654 | 28.891546 | 31.461691 |
| Ca | 39.801430 | 29.569792 | 36.504539 |
| Ca | 46.566612 | 28.572546 | 33.571796 |
| Ca | 42.831287 | 29.053076 | 34.377880 |
| S  | 27.167004 | 27.779337 | 36.572014 |
| S  | 26.794621 | 34.103882 | 34.536636 |
| S  | 30.327419 | 29.933598 | 32.595535 |
| S  | 30.125830 | 31.144783 | 36.500069 |
| S  | 33.277557 | 27.492155 | 33.679298 |
| S  | 33.724571 | 32.643188 | 32.634201 |
| S  | 36.833698 | 28.584982 | 31.278872 |
| S  | 36.543716 | 29.350252 | 36.300823 |
| S  | 39.943001 | 26.922558 | 34.273300 |
| S  | 40.473854 | 31.454182 | 33.500038 |
| S  | 43.738678 | 28.436884 | 31.495327 |
| S  | 43.910988 | 27.051262 | 38.723343 |

24

generated by VMD

|  | Ca     | S     |
|---|--------|-------|
| Ca | 25.161337 | 29.722612 | 32.389744 |
| Ca | 26.499382 | 31.005465 | 36.028793 |
| Ca | 30.176048 | 28.083038 | 35.512737 |
| Ca | 30.260162 | 32.975525 | 33.793331 |
| Ca | 33.513798 | 29.883213 | 30.979345 |
| Ca | 33.186069 | 30.436943 | 35.243668 |
| Ca | 36.516296 | 26.836245 | 34.548756 |
| Ca | 36.832958 | 30.978891 | 33.462132 |
| Ca | 40.177803 | 28.778698 | 31.537165 |
| Ca | 39.596630 | 29.696596 | 36.583385 |
| Ca | 46.384232 | 28.745415 | 33.489441 |
| Ca | 42.691135 | 29.155153 | 34.683006 |
| S  | 27.152023 | 27.654009 | 36.477402 |
| S  | 27.058109 | 33.990986 | 34.633095 |
| S  | 30.513773 | 29.953129 | 32.682438 |
| S  | 30.023495 | 31.156677 | 36.523529 |
| S  | 33.234467 | 27.525236 | 33.555832 |
| S  | 33.672207 | 32.714169 | 32.589996 |
| S  | 36.664787 | 28.293804 | 31.405457 |
| S  | 36.486641 | 29.630894 | 36.267899 |
| S  | 40.078167 | 26.799063 | 34.331200 |
| S  | 40.486073 | 31.242205 | 33.557087 |
| S  | 43.597168 | 28.360962 | 31.484959 |
| S  | 44.471004 | 26.772453 | 38.270309 |

24

generated by VMD
| Ca   | 24.727850 | 29.823803 | 32.607018 |
|------|-----------|-----------|-----------|
| Ca   | 26.465111 | 30.994741 | 36.146122 |
| Ca   | 30.163094 | 27.858603 | 35.523941 |
| Ca   | 29.943279 | 33.147575 | 33.196400 |
| Ca   | 33.496845 | 29.808735 | 31.390524 |
| Ca   | 33.246029 | 30.416061 | 35.202938 |
| Ca   | 36.733280 | 26.998760 | 34.581650 |
| Ca   | 36.839443 | 31.073368 | 33.771381 |
| Ca   | 40.263977 | 28.658012 | 31.756134 |
| Ca   | 39.841125 | 29.667454 | 36.658367 |
| Ca   | 46.532734 | 28.355022 | 33.408718 |
| Ca   | 42.881203 | 29.049501 | 34.517605 |
| S    | 27.057396 | 27.678879 | 36.438770 |
| S    | 26.759699 | 33.696724 | 34.336876 |
| S    | 30.506971 | 29.897638 | 32.568264 |
| S    | 29.999220 | 31.230824 | 36.170006 |
| S    | 33.496868 | 31.424066 | 34.004410 |
| S    | 33.671680 | 28.909084 | 32.548386 |
| S    | 36.637222 | 28.788170 | 31.478439 |
| S    | 36.504055 | 29.631359 | 36.468594 |
| S    | 40.159046 | 26.595013 | 34.370708 |
| S    | 40.575863 | 31.337130 | 33.602974 |
| S    | 43.778275 | 28.834459 | 31.186199 |
| S    | 44.153587 | 26.398119 | 38.096367 |

24
generated by VMD

| Ca   | 24.948936 | 29.841293 | 32.375214 |
|------|-----------|-----------|-----------|
| Ca   | 26.172802 | 31.168684 | 36.198997 |
| Ca   | 29.986324 | 28.034508 | 35.547558 |
| Ca   | 30.237101 | 32.949024 | 33.402260 |
| Ca   | 33.144592 | 29.817368 | 31.212002 |
| Ca   | 33.158607 | 30.195055 | 35.126488 |
| Ca   | 36.810505 | 26.961235 | 34.356079 |
| Ca   | 36.797714 | 31.044128 | 33.654293 |
| Ca   | 40.080353 | 28.918610 | 31.746151 |
| Ca   | 39.877987 | 29.687548 | 36.620617 |
| Ca   | 46.765366 | 28.364304 | 33.340015 |
| Ca   | 42.851303 | 28.971756 | 34.387375 |
| S    | 27.220573 | 27.697979 | 36.624939 |
| S    | 26.879623 | 34.043579 | 34.379044 |
| S    | 30.355282 | 29.885252 | 32.598507 |
| S    | 29.950436 | 31.215210 | 36.429996 |
| S    | 33.286903 | 27.273981 | 33.824932 |
| S    | 33.532234 | 32.727909 | 32.550400 |
| S    | 36.642391 | 28.662216 | 31.373909 |
| S    | 36.549244 | 29.421295 | 36.320053 |
S  40.081551  26.794933  34.307541
S  40.604115  31.405525  33.698498
S  43.907314  28.634501  31.404823
S  44.592712  26.675585  38.550972

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generated by VMD

Ca  25.013199  29.913109  32.702873
Ca  26.651360  30.973419  36.287891
Ca  30.144653  28.052006  35.529503
Ca  30.196180  33.123360  33.550072
Ca  33.319244  29.814798  31.023111
Ca  33.207951  30.150143  34.892834
Ca  36.532570  26.895439  34.457352
Ca  36.802418  31.125278  33.516373
Ca  39.926212  28.731556  31.810936
Ca  39.905319  29.632973  36.667271
Ca  46.556141  28.354546  33.445663
Ca  42.839817  28.858837  34.538826
S  27.186852  27.623215  36.289532
S  26.914597  33.854988  34.466763
S  30.452728  30.015141  32.596504
S  30.238605  31.156696  36.523052
S  33.378700  27.418522  33.677761
S  33.534050  32.801170  32.453423
S  36.567055  28.621330  31.320013
S  36.349174  29.538851  36.219345
S  39.924664  26.786682  34.531796
S  40.330090  31.277142  33.644028
S  43.885521  28.701042  31.441292
S  44.576824  26.971167  38.444534

24

generated by VMD

Ca  24.650610  29.859741  32.615707
Ca  26.506891  30.955776  35.954109
Ca  30.298727  28.106009  35.604076
Ca  30.298370  32.942204  33.528301
Ca  33.315865  29.920368  31.067802
Ca  33.246819  30.331533  35.129810
Ca  36.413200  26.581728  34.244484
Ca  39.998234  31.177050  33.559742
Ca  40.118916  28.693611  31.654360
Ca  39.909027  29.542902  36.713341
Ca  46.639740  28.526224  33.473488
Ca  42.804981  29.032566  34.508808
S  27.204205  27.556313  36.500980
S  26.689663  33.958313  34.382153
|   |   |   |
|---|---|---|
| S | 30.514301 | 29.873413 | 32.734688 |
| S | 30.172335 | 31.264502 | 36.538834 |
| S | 33.180187 | 27.423470 | 33.605286 |
| S | 33.781269 | 32.895657 | 32.728718 |
| S | 36.739601 | 28.540304 | 31.308372 |
| S | 36.538799 | 29.464359 | 36.163017 |
| S | 39.774246 | 26.880177 | 34.445621 |
| S | 40.563046 | 31.339764 | 33.605820 |
| S | 43.625061 | 28.531490 | 31.402773 |
| S | 44.449837 | 26.993940 | 38.560425 |

24 generated by VMD

| Ca | 24.964930 | 29.681015 | 32.330124 |
| Ca | 26.451740 | 31.121651 | 35.953022 |
| Ca | 29.983665 | 28.103437 | 35.675461 |
| Ca | 30.314255 | 33.056858 | 33.792194 |
| Ca | 33.423553 | 29.911753 | 31.117653 |
| Ca | 33.161713 | 30.169016 | 35.193874 |
| Ca | 36.681519 | 26.74116 | 34.420238 |
| Ca | 36.724831 | 30.999096 | 33.393082 |
| Ca | 40.135864 | 28.586189 | 31.568157 |
| Ca | 39.760796 | 29.783165 | 36.521038 |
| Ca | 46.647461 | 28.720194 | 33.504463 |
| Ca | 42.848267 | 29.241678 | 34.663223 |
| S | 26.914742 | 27.787800 | 36.533180 |
| S | 26.921089 | 34.013638 | 34.302662 |
| S | 30.488342 | 29.983568 | 32.774384 |
| S | 29.858992 | 31.174040 | 36.681900 |
| S | 33.310329 | 27.404308 | 33.748459 |
| S | 33.559589 | 32.679745 | 32.713966 |
| S | 36.649403 | 28.450586 | 31.394684 |
| S | 36.522732 | 29.585161 | 36.254768 |
| S | 40.053322 | 26.820629 | 34.472984 |
| S | 40.551502 | 31.189610 | 33.352600 |
| S | 44.004280 | 28.780399 | 31.381510 |
| S | 44.500931 | 26.403795 | 38.286583 |

24 generated by VMD

| Ca | 24.919088 | 29.779202 | 32.508804 |
| Ca | 26.363440 | 31.324070 | 36.080978 |
| Ca | 30.070936 | 27.806480 | 35.583633 |
| Ca | 30.417934 | 32.963394 | 33.422592 |
| Ca | 33.323906 | 29.824966 | 31.260069 |
| Ca | 33.243397 | 30.168116 | 35.382294 |
| Ca | 36.591270 | 26.938828 | 34.475433 |
| Ca | 36.808445 | 30.834465 | 33.506313 |
|   | Ca   | S    | S    |
|---|------|------|------|
|   | 40.105064 | 28.780533 | 31.405619 |
|   | 39.789955 | 29.795221 | 34.690567 |
|   | 46.642010 | 28.773777 | 33.331177 |
|   | 42.935879 | 29.749272 | 34.674742 |
|   | 26.873171 | 27.869873 | 36.514442 |
|   | 26.934807 | 33.905872 | 34.98629 |
|   | 30.48758 | 29.953560 | 32.746742 |
|   | 29.986938 | 31.130232 | 36.44441 |
|   | 33.225544 | 27.365818 | 33.67408 |
|   | 33.794231 | 32.680580 | 32.816952 |
|   | 36.643227 | 28.494255 | 31.30517 |
|   | 36.501369 | 29.378984 | 36.455784 |
|   | 39.923973 | 26.954290 | 34.440411 |
|   | 40.576183 | 31.162815 | 33.600468 |
|   | 43.680668 | 28.742870 | 31.430111 |
|   | 44.597744 | 26.588282 | 38.270874 |

24

generated by VMD

|   | Ca   | S    | S    |
|---|------|------|------|
|   | 24.985344 | 29.774487 | 32.501499 |
|   | 26.592384 | 31.252542 | 35.952026 |
|   | 30.209040 | 27.850103 | 35.596611 |
|   | 30.131063 | 32.918495 | 33.573128 |
|   | 33.267642 | 29.878059 | 31.234764 |
|   | 33.267765 | 30.103607 | 35.226864 |
|   | 36.648205 | 26.760071 | 34.141514 |
|   | 36.796101 | 30.917675 | 33.80089 |
|   | 39.963539 | 28.740496 | 31.672600 |
|   | 39.828007 | 29.748920 | 36.652718 |
|   | 46.399643 | 28.409479 | 33.474319 |
|   | 42.695175 | 29.250889 | 34.674820 |
|   | 27.198183 | 27.954092 | 36.759300 |
|   | 26.899889 | 34.098759 | 34.228828 |
|   | 30.558109 | 29.895355 | 32.635586 |
|   | 30.049665 | 31.084671 | 36.415756 |
|   | 33.249834 | 32.200731 | 33.697144 |
|   | 33.701252 | 28.851700 | 32.996601 |
|   | 36.556988 | 28.512728 | 31.299711 |
|   | 36.607742 | 29.454126 | 36.156910 |
|   | 40.027111 | 26.733480 | 34.321064 |
|   | 40.463524 | 31.324257 | 33.454815 |
|   | 43.774776 | 28.868563 | 31.421055 |
|   | 44.342838 | 26.808115 | 38.562927 |

24

generated by VMD

|   | Ca   | S    | S    |
|---|------|------|------|
|   | 24.983492 | 29.355213 | 32.450993 |
|   | 26.354803 | 31.064548 | 35.714737 |
|    | Ca      | S        |
|----|---------|----------|
|    | 29.99269 | 28.28027 |
|    | 30.06398 | 33.05500 |
|    | 33.47731 | 29.92117 |
|    | 33.26245 | 30.31527 |
|    | 36.68730 | 26.57010 |
|    | 36.70287 | 30.91214 |
|    | 40.18717 | 28.78903 |
|    | 39.86086 | 29.48234 |
|    | 46.78970 | 28.35619 |
|    | 42.95443 | 29.20796 |
|    | 27.31583 | 27.99116 |
|    | 26.62061 | 34.03025 |
|    | 30.35924 | 30.05775 |
|    | 30.00814 | 31.25479 |
|    | 33.12359 | 27.53368 |
|    | 33.72920 | 32.81177 |
|    | 36.73759 | 28.54918 |
|    | 36.53218 | 29.32042 |
|    | 40.03918 | 26.78343 |
|    | 40.34025 | 31.25876 |
|    | 43.81979 | 28.80740 |
|    | 44.48979 | 26.68349 |

24

generated by VMD

|    | Ca      | S        |
|----|---------|----------|
|    | 24.98408 | 29.19088 |
|    | 26.68612 | 31.22804 |
|    | 30.22163 | 28.00302 |
|    | 30.11339 | 33.17649 |
|    | 33.20093 | 29.66099 |
|    | 33.34294 | 30.20425 |
|    | 36.50371 | 26.80780 |
|    | 36.88428 | 31.02250 |
|    | 40.10136 | 29.02011 |
|    | 39.92727 | 29.62821 |
|    | 46.65327 | 28.24230 |
|    | 42.80094 | 29.03572 |
|    | 27.40771 | 27.91198 |
|    | 26.64333 | 33.97515 |
|    | 30.49342 | 30.03227 |
|    | 30.27804 | 31.26164 |
|    | 33.17834 | 27.48963 |
|    | 33.54398 | 32.79767 |
|    | 36.61380 | 28.76011 |
|    | 36.39866 | 29.38869 |
|    | 39.98314 | 27.00118 |
|    | 40.46676 | 31.35642 |
|   |   |   |
|---|---|---|
| S | 43.724159 | 28.702671 | 31.204216 |
| S | 44.282547 | 26.493593 | 38.515236 |

24

*generated by VMD*

| Ca | 24.721430 | 29.344707 | 32.742680 |
| Ca | 26.559549 | 31.264992 | 36.220825 |
| Ca | 30.103033 | 28.240055 | 35.088261 |
| Ca | 30.117044 | 33.092842 | 33.596909 |
| Ca | 32.821200 | 29.596319 | 31.038420 |
| Ca | 33.286270 | 30.299820 | 35.186085 |
| Ca | 36.707066 | 26.794909 | 34.395214 |
| Ca | 36.737392 | 30.957521 | 33.676483 |
| Ca | 40.108555 | 28.960976 | 31.666988 |
| Ca | 39.887547 | 29.435835 | 36.659660 |
| Ca | 46.558598 | 28.453331 | 33.386803 |
| Ca | 42.830170 | 28.941305 | 34.562973 |
| S  | 27.493023 | 27.865631 | 36.670605 |
| S  | 26.669773 | 34.042286 | 34.338352 |
| S  | 30.410961 | 29.980255 | 32.394897 |
| S  | 30.043856 | 31.245617 | 36.419525 |
| S  | 33.357376 | 27.546829 | 33.584461 |
| S  | 33.670383 | 32.705200 | 32.583382 |
| S  | 36.603481 | 28.557983 | 31.413733 |
| S  | 36.552750 | 29.447109 | 36.430164 |
| S  | 40.046577 | 26.708946 | 34.167412 |
| S  | 40.492554 | 31.423876 | 33.722702 |
| S  | 43.734097 | 28.876732 | 31.414988 |
| S  | 44.461178 | 26.608318 | 38.669064 |

24

*generated by VMD*

| Ca | 25.223780 | 29.482485 | 32.266449 |
| Ca | 26.286577 | 31.046118 | 35.914551 |
| Ca | 30.161352 | 28.086430 | 35.538040 |
| Ca | 30.120897 | 33.276787 | 33.592960 |
| Ca | 33.450840 | 29.434277 | 31.415245 |
| Ca | 33.308010 | 30.280939 | 35.371002 |
| Ca | 36.578724 | 26.862474 | 34.351910 |
| Ca | 36.743092 | 31.077200 | 33.731724 |
| Ca | 39.976212 | 29.006937 | 31.823946 |
| Ca | 39.855446 | 29.367485 | 36.565811 |
| Ca | 46.699429 | 28.524942 | 33.407795 |
| Ca | 42.871712 | 29.041065 | 34.197220 |
| S  | 27.352613 | 27.865734 | 36.691353 |
| S  | 26.608253 | 33.996517 | 34.187328 |
| S  | 30.544983 | 30.066296 | 32.552895 |
| S  | 30.067705 | 31.443104 | 36.380142 |
|   |   |   |   |
|---|---|---|---|
| S | 33.319553 | 27.338537 | 33.971752 |
| S | 33.594543 | 32.724895 | 32.700211 |
| S | 36.661358 | 28.632629 | 31.519302 |
| S | 36.552624 | 29.388680 | 36.386864 |
| S | 39.913433 | 26.812510 | 34.152740 |
| S | 40.504227 | 31.354010 | 33.745724 |
| S | 43.759655 | 28.750227 | 31.287621 |
| S | 44.278957 | 26.531116 | 38.278095 |

24 generated by VMD

| Ca | 25.112413 | 29.539360 | 32.530373 |
| Ca | 26.464453 | 31.068815 | 35.838120 |
| Ca | 30.298113 | 28.098307 | 35.554024 |
| Ca | 30.310444 | 33.118195 | 33.548714 |
| Ca | 33.415653 | 29.651901 | 31.136805 |
| Ca | 33.204967 | 30.169020 | 35.319553 |
| Ca | 36.759064 | 26.839699 | 34.157776 |
| Ca | 36.731365 | 31.003519 | 33.698208 |
| Ca | 39.978195 | 29.055882 | 31.631454 |
| Ca | 39.871063 | 29.601585 | 36.629734 |
| Ca | 46.483719 | 28.586742 | 33.325874 |
| Ca | 42.726482 | 29.102058 | 34.505035 |
| S | 27.418852 | 27.890165 | 36.842644 |
| S | 26.811300 | 33.894737 | 34.145828 |
| S | 30.595757 | 29.948286 | 32.729099 |
| S | 30.037451 | 31.308575 | 36.457283 |
| S | 33.434380 | 27.267029 | 33.761959 |
| S | 33.630615 | 32.788033 | 32.640606 |
| S | 36.695656 | 28.882545 | 31.405464 |
| S | 36.508289 | 29.404354 | 36.316540 |
| S | 40.006828 | 26.777872 | 34.312824 |
| S | 40.492462 | 31.385715 | 33.672607 |
| S | 43.490608 | 28.487396 | 31.392109 |
| S | 43.955719 | 26.521576 | 38.485653 |

24 generated by VMD

| Ca | 25.264610 | 29.287741 | 32.917072 |
| Ca | 26.496201 | 31.102854 | 36.216557 |
| Ca | 30.056416 | 28.128803 | 35.637455 |
| Ca | 30.280296 | 33.148808 | 33.249313 |
| Ca | 33.320518 | 29.515800 | 31.142881 |
| Ca | 33.257133 | 30.349636 | 35.192642 |
| Ca | 36.505123 | 26.848568 | 34.048969 |
| Ca | 36.870598 | 31.187843 | 33.833904 |
| Ca | 40.104118 | 29.087337 | 31.527863 |
| Ca | 39.770317 | 29.421551 | 36.755093 |
|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 46.86 | 28.56 | 33.47 |
| Ca  | 43.09 | 29.06 | 34.59 |
| S   | 27.08 | 27.75 | 36.57 |
| S   | 26.79 | 33.89 | 34.33 |
| S   | 30.13 | 30.07 | 32.56 |
| S   | 30.03 | 31.52 | 36.41 |
| S   | 33.03 | 27.38 | 33.63 |
| S   | 33.64 | 32.68 | 34.45 |
| S   | 36.71 | 28.78 | 31.40 |
| S   | 36.29 | 29.31 | 36.32 |
| S   | 39.94 | 26.90 | 34.17 |
| S   | 40.47 | 31.41 | 33.71 |
| S   | 43.78 | 28.63 | 31.46 |
| S   | 44.39 | 26.32 | 38.42 |

24 generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 25.29 | 29.44 | 32.37 |
| Ca  | 26.47 | 31.33 | 35.82 |
| Ca  | 30.16 | 27.95 | 35.60 |
| Ca  | 30.36 | 33.09 | 33.62 |
| Ca  | 33.32 | 29.39 | 31.21 |
| Ca  | 33.26 | 30.18 | 35.43 |
| Ca  | 36.50 | 26.77 | 34.32 |
| Ca  | 36.78 | 30.97 | 33.79 |
| Ca  | 40.02 | 29.05 | 31.74 |
| Ca  | 39.91 | 29.33 | 36.57 |
| Ca  | 46.43 | 29.09 | 33.19 |
| Ca  | 42.79 | 29.13 | 34.44 |
| S   | 27.25 | 28.08 | 36.68 |
| S   | 26.74 | 34.16 | 33.92 |
| S   | 30.53 | 29.97 | 32.83 |
| S   | 30.07 | 31.28 | 36.41 |
| S   | 33.29 | 27.21 | 33.89 |
| S   | 33.71 | 32.47 | 32.65 |
| S   | 36.64 | 28.55 | 31.44 |
| S   | 36.44 | 29.24 | 36.42 |
| S   | 39.96 | 26.81 | 34.10 |
| S   | 40.50 | 31.32 | 33.86 |
| S   | 43.49 | 28.78 | 31.25 |
| S   | 44.44 | 26.51 | 38.39 |

24 generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 25.37 | 29.44 | 32.27 |
| Ca  | 26.42 | 31.16 | 35.98 |
| Ca  | 30.31 | 28.08 | 35.64 |
| Ca  | 30.26 | 32.95 | 33.45 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 33.282856 | 29.704515 | 31.032497 |
| Ca      | 32.998043 | 30.458286 | 35.414104 |
| Ca      | 36.537800 | 26.757454 | 34.181873 |
| Ca      | 36.780788 | 30.897980 | 33.810635 |
| Ca      | 40.144615 | 28.812080 | 31.462902 |
| Ca      | 39.786457 | 29.190657 | 36.629684 |
| Ca      | 46.658878 | 28.837738 | 33.335110 |
| Ca      | 43.025002 | 29.260639 | 34.629772 |
| S       | 27.270285 | 32.300000 | 31.456789 |
| S       | 26.727276 | 32.893810 | 34.156841 |
| S       | 30.512730 | 29.855171 | 32.620670 |
| S       | 30.067034 | 31.517122 | 36.409824 |
| S       | 33.153973 | 27.468191 | 33.694786 |
| S       | 33.713238 | 32.664574 | 32.640064 |
| S       | 36.626083 | 28.676535 | 31.290260 |
| S       | 36.271156 | 29.264133 | 36.420120 |
| S       | 39.955086 | 26.665306 | 34.350708 |
| S       | 40.330875 | 31.147463 | 33.868881 |
| S       | 43.701435 | 29.029652 | 31.295141 |
| S       | 44.510078 | 26.442829 | 38.299217 |

24 generated by VMD

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 25.013918 | 29.826490 | 32.409916 |
| Ca      | 26.589352 | 31.335587 | 36.089790 |
| Ca      | 30.105993 | 28.168043 | 35.424709 |
| Ca      | 30.358238 | 32.982746 | 33.480797 |
| Ca      | 33.252544 | 29.168091 | 31.231199 |
| Ca      | 33.184845 | 30.363495 | 35.361023 |
| Ca      | 36.576710 | 26.650618 | 34.363400 |
| Ca      | 36.604321 | 30.680336 | 33.546135 |
| Ca      | 40.128990 | 29.036522 | 31.631298 |
| Ca      | 39.709660 | 29.346220 | 36.725628 |
| Ca      | 46.638336 | 29.101633 | 33.414665 |
| Ca      | 42.871323 | 29.244940 | 34.673363 |
| S       | 27.025589 | 27.961716 | 36.877819 |
| S       | 26.946783 | 34.132275 | 33.863411 |
| S       | 30.409870 | 29.951721 | 32.654945 |
| S       | 30.068127 | 31.382053 | 36.530640 |
| S       | 33.314514 | 27.456526 | 34.002800 |
| S       | 33.741020 | 32.399857 | 32.558002 |
| S       | 36.669628 | 28.480846 | 31.274195 |
| S       | 36.432003 | 29.072241 | 36.379768 |
| S       | 40.103848 | 26.832663 | 34.129288 |
| S       | 40.364277 | 31.250481 | 33.917568 |
| S       | 43.717140 | 29.186625 | 31.370327 |
| S       | 44.606907 | 26.379719 | 38.120071 |
| Element | X1      | Y1      | Z1      | X2      | Y2      | Z2      |
|---------|---------|---------|---------|---------|---------|---------|
| Ca      | 24.930681 | 29.638563 | 32.606949 | 26.644678 | 31.268810 | 35.904789 |
| Ca      | 30.193188 | 28.118259 | 35.660252 | 30.373198 | 33.071983 | 33.404095 |
| Ca      | 33.271614 | 29.418484 | 31.040838 | 33.209286 | 30.458090 | 35.324322 |
| Ca      | 36.622906 | 26.519558 | 34.371601 | 36.687458 | 30.651508 | 33.752728 |
| Ca      | 40.077087 | 28.952686 | 31.602444 | 39.636768 | 29.468699 | 36.629177 |
| Ca      | 46.498035 | 29.271580 | 33.541500 | 42.887852 | 29.191351 | 34.550262 |
| S       | 27.266560 | 28.102213 | 36.960232 | 26.754162 | 33.970097 | 33.994175 |
| S       | 30.449362 | 29.857162 | 32.729594 | 30.148413 | 31.484573 | 36.340580 |
| S       | 33.302471 | 27.450069 | 33.832096 | 33.799950 | 32.498116 | 32.529324 |
| S       | 36.716724 | 28.605480 | 31.283714 | 36.445549 | 29.097908 | 36.425804 |
| S       | 40.086441 | 26.576643 | 34.066376 | 40.526245 | 31.250639 | 33.826450 |
| S       | 43.674076 | 29.319391 | 31.239380 | 44.231300 | 26.149548 | 38.420700 |
| S  | 36.656311 | 28.659439 | 31.118105 |
|----|-----------|-----------|-----------|
| S  | 36.336117 | 29.170538 | 36.379761 |
| S  | 40.201759 | 26.827629 | 34.174770 |
| S  | 40.365852 | 31.182590 | 33.868641 |
| S  | 43.779037 | 28.990656 | 31.389843 |
| S  | 44.416954 | 26.209557 | 38.317543 |

24 generated by VMD

| Ca | 25.357105 | 29.760220 | 32.375267 |
|----|-----------|-----------|-----------|
| Ca | 26.618019 | 31.618856 | 36.024029 |
| Ca | 30.259087 | 27.825542 | 35.783699 |
| Ca | 30.245052 | 32.881203 | 33.475368 |
| Ca | 33.302551 | 29.128326 | 31.308987 |
| Ca | 33.220978 | 30.181515 | 35.227009 |
| Ca | 36.528461 | 26.810310 | 34.075512 |
| Ca | 36.751270 | 30.848742 | 33.561234 |
| Ca | 40.129417 | 29.140617 | 31.572210 |
| Ca | 39.540520 | 29.318432 | 36.485840 |
| Ca | 46.675556 | 28.976864 | 33.901955 |
| Ca | 42.742657 | 29.411346 | 34.774258 |
| S  | 27.208916 | 28.253418 | 37.111458 |
| S  | 26.877674 | 34.414589 | 34.244961 |
| S  | 30.414768 | 29.631920 | 32.699959 |
| S  | 30.153229 | 31.233385 | 36.425255 |
| S  | 33.266159 | 27.233643 | 33.900040 |
| S  | 33.743763 | 32.239716 | 32.364342 |
| S  | 36.751686 | 28.758907 | 31.056087 |
| S  | 36.412800 | 29.043148 | 36.196198 |
| S  | 40.065125 | 26.839638 | 34.110130 |
| S  | 40.349262 | 31.379852 | 33.901409 |
| S  | 43.670425 | 29.310465 | 31.415310 |
| S  | 44.149429 | 26.150757 | 38.040192 |

24 generated by VMD

| Ca | 24.913122 | 29.778606 | 32.231838 |
|----|-----------|-----------|-----------|
| Ca | 26.496195 | 31.338524 | 35.663696 |
| Ca | 30.260185 | 28.001713 | 35.995583 |
| Ca | 30.326178 | 32.781422 | 33.575508 |
| Ca | 33.250317 | 29.529751 | 31.336622 |
| Ca | 33.291031 | 30.423588 | 35.325974 |
| Ca | 36.571705 | 26.496948 | 34.247963 |
| Ca | 36.745815 | 30.738792 | 33.627407 |
| Ca | 40.285931 | 29.029396 | 31.389975 |
| Ca | 39.596909 | 29.324673 | 36.747417 |
| Ca | 46.668949 | 29.348656 | 33.570972 |
| Ca | 42.771885 | 29.384867 | 34.740013 |
|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| S | 27.331816 | 28.223238 | 37.157341 |
| S | 27.115608 | 34.193329 | 33.945969 |
| S | 30.365707 | 29.628561 | 32.879421 |
| S | 30.152332 | 31.337616 | 36.332195 |
| S | 33.262760 | 27.323544 | 33.969040 |
| S | 33.660957 | 32.589409 | 32.480606 |
| S | 36.624817 | 28.579597 | 31.097488 |
| S | 36.381287 | 29.107624 | 36.220573 |
| S | 40.041641 | 26.930418 | 34.047913 |
| S | 40.244186 | 31.164875 | 33.776257 |
| S | 43.794613 | 29.142099 | 31.531723 |
| S | 44.279987 | 25.994228 | 38.137688 |

24 generated by VMD

| Ca | 24.769712 | 29.917030 | 31.984053 |
| Ca | 26.528069 | 31.093288 | 35.653427 |
| Ca | 30.247658 | 28.126728 | 35.959015 |
| Ca | 30.342943 | 32.839622 | 33.408474 |
| Ca | 33.353455 | 29.114784 | 31.136169 |
| Ca | 33.137634 | 30.291021 | 35.344048 |
| Ca | 36.570812 | 26.995296 | 34.192238 |
| Ca | 36.714935 | 30.860485 | 33.691780 |
| Ca | 40.214409 | 29.395798 | 31.660431 |
| Ca | 39.608910 | 29.517635 | 36.623306 |
| Ca | 40.908920 | 29.207588 | 33.547169 |
| Ca | 42.691139 | 29.224552 | 34.702938 |
| S | 27.362700 | 28.090282 | 37.311890 |
| S | 27.180622 | 34.109978 | 33.999481 |
| S | 30.408890 | 29.551060 | 32.851845 |
| S | 30.055304 | 31.493740 | 36.462963 |
| S | 33.117409 | 27.317242 | 34.058609 |
| S | 33.742001 | 32.332268 | 32.526714 |
| S | 36.812054 | 28.597422 | 31.198689 |
| S | 36.277096 | 29.364012 | 36.417583 |
| S | 40.059280 | 26.921852 | 33.950649 |
| S | 40.426472 | 31.416348 | 33.958351 |
| S | 43.564743 | 28.928129 | 31.368250 |
| S | 44.338806 | 25.685198 | 38.022606 |

24 generated by VMD

| Ca | 24.629053 | 29.857300 | 32.436691 |
| Ca | 26.340281 | 31.335474 | 36.199574 |
| Ca | 30.015547 | 28.043552 | 35.634258 |
| Ca | 30.272205 | 33.021935 | 32.856770 |
| Ca | 33.364452 | 28.850903 | 31.336180 |
| Ca | 33.153507 | 30.080940 | 35.223389 |
|   |   |   |   |
|---|---|---|---|
| Ca | 36.529095 | 26.819118 | 34.184418 |
| Ca | 36.642883 | 30.804386 | 33.612453 |
| Ca | 40.231678 | 29.397053 | 31.496689 |
| Ca | 39.597538 | 29.419807 | 36.639530 |
| Ca | 46.927906 | 29.170385 | 33.972385 |
| Ca | 42.852070 | 29.343725 | 34.765327 |
| S  | 27.142534 | 28.259466 | 37.356262 |
| S  | 27.381010 | 34.193497 | 34.462540 |
| S  | 30.392771 | 29.685591 | 32.687603 |
| S  | 30.034779 | 31.481712 | 36.112873 |
| S  | 33.318027 | 27.170078 | 33.993187 |
| S  | 33.630779 | 32.215279 | 32.313652 |
| S  | 36.767578 | 28.623714 | 31.130146 |
| S  | 36.374249 | 29.099953 | 36.318935 |
| S  | 40.135887 | 26.922598 | 33.810322 |
| S  | 40.623795 | 31.485962 | 33.901089 |
| S  | 43.917183 | 29.491045 | 31.483631 |
| S  | 44.159092 | 25.617928 | 38.102757 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 24.722303 | 30.175898 | 32.430962 |
| Ca | 26.543396 | 31.543008 | 36.108810 |
| Ca | 30.205648 | 27.905272 | 35.812542 |
| Ca | 30.436422 | 32.780384 | 33.113422 |
| Ca | 33.182270 | 28.878462 | 31.279972 |
| Ca | 33.146614 | 29.859161 | 35.204323 |
| Ca | 36.523693 | 26.885403 | 34.235588 |
| Ca | 36.690086 | 30.881973 | 34.017815 |
| Ca | 40.009815 | 29.361202 | 31.675011 |
| Ca | 39.768826 | 29.428226 | 36.739834 |
| Ca | 46.865009 | 29.078979 | 33.735008 |
| Ca | 42.784687 | 29.431049 | 34.448265 |
| S  | 27.321955 | 28.278831 | 36.948738 |
| S  | 27.216187 | 34.246075 | 34.005539 |
| S  | 30.426559 | 29.399296 | 32.738350 |
| S  | 30.149313 | 31.419479 | 36.241531 |
| S  | 33.384868 | 27.083527 | 33.935146 |
| S  | 33.745522 | 32.079826 | 32.264679 |
| S  | 36.768539 | 28.904610 | 31.319899 |
| S  | 36.298965 | 29.124268 | 36.547531 |
| S  | 40.024620 | 26.924549 | 33.766960 |
| S  | 40.338734 | 31.559984 | 34.004284 |
| S  | 43.741547 | 29.107563 | 31.394388 |
| S  | 44.136749 | 26.053104 | 38.062103 |

24 generated by VMD
| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 24.5453  | 29.8610   | 32.7628   |
| Ca      | 26.5689  | 31.4705   | 35.8498   |
| Ca      | 29.9559  | 27.9532   | 35.7629   |
| Ca      | 30.4588  | 32.7111   | 33.0331   |
| Ca      | 33.2439  | 29.1784   | 31.1373   |
| Ca      | 33.2314  | 30.0070   | 35.2408   |
| Ca      | 36.3409  | 26.6763   | 34.2116   |
| Ca      | 36.9282  | 30.9723   | 33.6098   |
| Ca      | 40.2496  | 29.2748   | 31.5697   |
| Ca      | 39.6488  | 29.3262   | 36.8954   |
| Ca      | 46.7506  | 29.6811   | 33.9976   |
| Ca      | 42.8305  | 29.2542   | 34.7695   |
| S       | 27.0660  | 28.3523   | 37.0898   |
| S       | 27.1483  | 34.1984   | 34.1590   |
| S       | 30.4093  | 29.6022   | 32.6421   |
| S       | 30.1276  | 31.3158   | 36.1986   |
| S       | 32.9702  | 27.1952   | 33.9787   |
| S       | 33.7721  | 32.2072   | 32.4669   |
| S       | 36.7985  | 28.8911   | 31.2595   |
| S       | 36.4759  | 29.2051   | 36.2926   |
| S       | 39.9267  | 26.7642   | 33.8361   |
| S       | 40.5213  | 31.2013   | 34.1143   |
| S       | 43.8584  | 29.1824   | 31.3754   |
| S       | 44.6055  | 25.9101   | 37.7743   |

24 generated by VMD

| Element | Value 1   | Value 2   | Value 3   |
|---------|-----------|-----------|-----------|
| Ca      | 24.8104  | 29.7439   | 32.6375   |
| Ca      | 26.4151  | 31.3626   | 35.6926   |
| Ca      | 30.3093  | 28.1735   | 35.8598   |
| Ca      | 30.5536  | 32.5725   | 33.1312   |
| Ca      | 33.2036  | 29.2092   | 31.2791   |
| Ca      | 33.2334  | 30.3339   | 35.3696   |
| Ca      | 36.2611  | 26.9057   | 34.2156   |
| Ca      | 36.8439  | 30.9518   | 33.8526   |
| Ca      | 40.0974  | 29.3271   | 31.6596   |
| Ca      | 39.6463  | 29.4061   | 36.4682   |
| Ca      | 46.5663  | 29.1909   | 33.8380   |
| Ca      | 42.8443  | 29.2167   | 34.6989   |
| S       | 27.3169  | 28.0840   | 36.9876   |
| S       | 27.2313  | 34.0426   | 33.8928   |
| S       | 30.3274  | 29.5508   | 32.7196   |
| S       | 29.9543  | 31.3716   | 36.2577   |
| S       | 33.1388  | 27.3060   | 34.0199   |
| S       | 33.8258  | 32.2408   | 32.5986   |
| S       | 36.6101  | 28.9066   | 31.2470   |
| S       | 36.4121  | 29.2954   | 36.5175   |
|   |   |   |   |
|---|---|---|---|
| S | 39.839355 | 26.836246 | 33.820412 |
| S | 40.556065 | 31.400887 | 33.975922 |
| S | 43.800098 | 29.258486 | 31.568174 |
| S | 44.636425 | 25.704086 | 37.718231 |

24 generated by VMD

| Ca | 24.777315 | 29.614891 | 32.558834 |
| Ca | 26.603230 | 31.393564 | 35.736950 |
| Ca | 30.192841 | 28.103973 | 35.905315 |
| Ca | 30.204260 | 32.759773 | 33.223145 |
| Ca | 33.363500 | 29.188721 | 31.301255 |
| Ca | 33.129436 | 30.252800 | 35.211131 |
| Ca | 36.531582 | 26.700222 | 34.206108 |
| Ca | 36.859848 | 30.898685 | 33.718636 |
| Ca | 40.355633 | 29.503403 | 31.374756 |
| Ca | 39.654667 | 29.152679 | 36.515469 |
| Ca | 46.507111 | 29.530224 | 33.959282 |
| Ca | 43.542467 | 29.150395 | 34.680946 |
| S | 27.213682 | 28.369492 | 37.115494 |
| S | 26.972364 | 34.274471 | 34.045860 |
| S | 30.349949 | 29.564312 | 32.830109 |
| S | 30.038134 | 31.523212 | 36.232262 |
| S | 33.184505 | 27.184723 | 33.994671 |
| S | 33.711323 | 32.304443 | 32.543514 |
| S | 36.973465 | 28.696737 | 31.232365 |
| S | 36.429153 | 29.164936 | 36.272957 |
| S | 40.047226 | 26.745392 | 33.740940 |
| S | 40.551418 | 31.312794 | 34.020668 |
| S | 43.720051 | 29.229149 | 31.495935 |
| S | 44.420879 | 25.771746 | 37.972282 |

24 generated by VMD

| Ca | 24.807316 | 29.765209 | 32.626266 |
| Ca | 26.618679 | 31.314074 | 35.978718 |
| Ca | 30.034702 | 28.176720 | 35.801205 |
| Ca | 30.182947 | 32.674706 | 33.312439 |
| Ca | 33.383064 | 29.261061 | 31.347433 |
| Ca | 33.316589 | 30.162754 | 35.308521 |
| Ca | 36.464935 | 26.867449 | 34.067547 |
| Ca | 36.785503 | 30.995308 | 33.735588 |
| Ca | 40.264618 | 29.355448 | 31.442503 |
| Ca | 39.558014 | 29.333416 | 36.722389 |
| Ca | 46.734764 | 29.158415 | 33.956768 |
| Ca | 42.789314 | 29.184605 | 34.564331 |
| S | 27.231167 | 28.131025 | 37.053921 |
| S | 26.937086 | 34.122448 | 33.905518 |
|   |   |   |   |
|---|---|---|---|
| S | 30.356539 | 29.579273 | 32.759331 |
| S | 30.172785 | 31.482975 | 36.404694 |
| S | 33.077503 | 27.366032 | 33.967354 |
| S | 33.664604 | 32.304588 | 32.434132 |
| S | 36.902863 | 28.765261 | 31.026508 |
| S | 36.506237 | 29.230553 | 36.328541 |
| S | 40.042587 | 26.888966 | 33.814518 |
| S | 40.491432 | 31.408625 | 33.895454 |
| S | 43.945656 | 29.089664 | 31.522068 |
| S | 44.165073 | 25.772800 | 38.054924 |

24 generated by VMD

| Ca | 24.831999 | 29.674034 | 32.738537 |
| Ca | 26.629625 | 31.212404 | 36.067329 |
| Ca | 30.315786 | 28.206284 | 35.942116 |
| Ca | 30.442839 | 32.654503 | 33.280052 |
| Ca | 33.332153 | 29.303810 | 31.252754 |
| Ca | 33.164005 | 30.334564 | 35.082737 |
| Ca | 36.602646 | 27.009747 | 34.118408 |
| Ca | 36.637841 | 30.815254 | 33.494022 |
| Ca | 40.441055 | 29.449469 | 31.416424 |
| Ca | 39.351532 | 29.192156 | 36.703617 |
| Ca | 46.569664 | 29.091557 | 34.215698 |
| Ca | 42.649174 | 29.302113 | 34.925579 |
| S | 27.209024 | 28.027761 | 37.177536 |
| S | 27.380411 | 34.165489 | 34.112152 |
| S | 30.304453 | 29.557404 | 32.765694 |
| S | 30.239826 | 31.450729 | 36.478058 |
| S | 33.267521 | 27.428467 | 33.947033 |
| S | 33.508171 | 32.267181 | 32.128151 |
| S | 36.819885 | 28.844103 | 30.868538 |
| S | 36.168453 | 29.280830 | 36.191956 |
| S | 39.915112 | 26.950443 | 33.561974 |
| S | 40.469273 | 31.435249 | 34.016899 |
| S | 44.051567 | 29.183304 | 31.709351 |
| S | 44.130936 | 25.554588 | 37.836082 |

24 generated by VMD

| Ca | 24.680319 | 29.733524 | 32.756580 |
| Ca | 26.535513 | 31.443787 | 36.065125 |
| Ca | 30.259878 | 28.019676 | 35.985439 |
| Ca | 30.237288 | 32.573669 | 33.122341 |
| Ca | 33.378799 | 29.335320 | 31.450804 |
| Ca | 33.101740 | 30.440903 | 35.187698 |
| Ca | 36.490108 | 26.966406 | 34.301426 |
| Ca | 36.830528 | 31.050888 | 33.684418 |
|    | Ca      | 29.434393 | 31.298174 |
|----|---------|-----------|-----------|
|    | Ca      | 29.380260 | 34.635918 |
|    | Ca      | 28.625593 | 34.111748 |
|    | Ca      | 29.132790 | 34.635918 |
|    | S       | 27.814659 | 36.778065 |
|    | S       | 33.987869 | 33.756191 |
|    | S       | 29.478706 | 34.370732 |
|    | S       | 27.351185 | 34.178284 |
|    | S       | 32.517403 | 32.339401 |
|    | S       | 29.004589 | 31.053942 |
|    | S       | 29.296844 | 36.342819 |
|    | S       | 27.064192 | 33.576157 |
|    | S       | 31.343113 | 34.077972 |
|    | S       | 29.337929 | 31.432753 |
|    | S       | 25.579895 | 38.041824 |

24 generated by VMD

|    | Ca      | 29.500351 | 32.356030 |
|----|---------|-----------|-----------|
|    | Ca      | 31.440712 | 35.649822 |
|    | Ca      | 28.197540 | 36.224728 |
|    | Ca      | 32.631615 | 33.220230 |
|    | Ca      | 29.168003 | 31.526896 |
|    | Ca      | 30.381260 | 35.237183 |
|    | Ca      | 26.868351 | 34.377003 |
|    | Ca      | 30.763565 | 33.921677 |
|    | Ca      | 29.594017 | 31.352570 |
|    | Ca      | 29.181614 | 36.637550 |
|    | Ca      | 29.137234 | 33.647015 |
|    | Ca      | 29.062630 | 34.656712 |
|    | S       | 28.193451 | 36.903008 |
|    | S       | 34.191689 | 33.693401 |
|    | S       | 29.422039 | 32.917770 |
|    | S       | 31.518665 | 36.271042 |
|    | S       | 27.343380 | 34.331661 |
|    | S       | 32.242634 | 32.496429 |
|    | S       | 28.833096 | 31.199099 |
|    | S       | 29.248703 | 36.526531 |
|    | S       | 26.985598 | 33.597038 |
|    | S       | 31.375084 | 34.019188 |
|    | S       | 29.487209 | 31.492805 |
|    | S       | 25.622971 | 37.775406 |

24 generated by VMD

|    | Ca      | 29.445629 | 32.599201 |
|----|---------|-----------|-----------|
|    | Ca      | 31.315510 | 35.967125 |
|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 30.120501 | 28.286375 | 35.838757 |
| Ca  | 30.400551 | 32.827030 | 33.185891 |
| Ca  | 33.306759 | 29.347122 | 31.447224 |
| Ca  | 33.212986 | 30.269951 | 35.265095 |
| Ca  | 36.496574 | 26.927246 | 34.271107 |
| Ca  | 36.874748 | 30.962656 | 33.806999 |
| Ca  | 40.347954 | 29.480282 | 31.553154 |
| Ca  | 39.589455 | 29.409691 | 36.844170 |
| Ca  | 46.774078 | 29.108622 | 33.577747 |
| Ca  | 42.767796 | 28.959740 | 34.634216 |
| S   | 27.174263 | 28.101204 | 36.995289 |
| S   | 27.237858 | 33.861931 | 33.645191 |
| S   | 30.333984 | 30.503670 | 32.717690 |
| S   | 29.983183 | 31.579052 | 36.300056 |
| S   | 33.136242 | 27.249914 | 34.141930 |
| S   | 33.644962 | 32.386192 | 32.612339 |
| S   | 36.790039 | 28.921516 | 31.267818 |
| S   | 36.280037 | 29.417969 | 36.442833 |
| S   | 40.014492 | 26.924553 | 33.656593 |
| S   | 40.479130 | 31.361713 | 33.987133 |
| S   | 43.793201 | 29.183104 | 31.398125 |
| S   | 44.198078 | 25.560705 | 37.876049 |

24 generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 24.392719 | 29.433741 | 32.319111 |
| Ca  | 26.469278 | 31.560745 | 35.668076 |
| Ca  | 30.177774 | 28.080965 | 36.067329 |
| Ca  | 30.120754 | 32.733044 | 33.125854 |
| Ca  | 33.191208 | 29.214993 | 31.458147 |
| Ca  | 33.180508 | 30.181110 | 35.198334 |
| Ca  | 36.672867 | 26.924805 | 34.336052 |
| Ca  | 36.953026 | 31.094885 | 34.136219 |
| Ca  | 40.264851 | 29.426985 | 31.773989 |
| Ca  | 39.881489 | 29.278412 | 36.570717 |
| Ca  | 47.034782 | 28.723129 | 33.530014 |
| Ca  | 43.199707 | 29.342772 | 34.528671 |
| S   | 26.952522 | 28.243725 | 36.855885 |
| S   | 26.902500 | 34.220406 | 33.606453 |
| S   | 30.305996 | 29.498119 | 32.927776 |
| S   | 29.741428 | 31.314636 | 36.407532 |
| S   | 33.248714 | 27.188213 | 34.277626 |
| S   | 33.579651 | 32.434601 | 32.328209 |
| S   | 36.823814 | 29.008520 | 31.491932 |
| S   | 36.411606 | 29.352188 | 36.669865 |
| S   | 40.104462 | 26.925573 | 33.787144 |
| S   | 40.568298 | 31.484161 | 34.160194 |
|   | 43.999134 | 29.284163 | 31.184156 |
|---|-----------|-----------|-----------|
| S | 44.256771 | 25.441494 | 37.621346 |

24 generated by VMD

| Ca | 24.731516 | 29.459839 | 32.416225 |
|----|-----------|-----------|-----------|
| Ca | 26.387602 | 31.502857 | 35.547298 |
| Ca | 30.010664 | 28.085190 | 36.059998 |
| Ca | 30.288322 | 32.678322 | 33.269299 |
| Ca | 33.289776 | 29.430859 | 31.486732 |
| Ca | 33.287067 | 30.195782 | 35.212536 |
| Ca | 36.470798 | 26.843916 | 34.721703 |
| Ca | 36.717869 | 31.111198 | 33.966576 |
| Ca | 40.535637 | 29.197289 | 31.466589 |
| Ca | 39.837536 | 29.027105 | 36.676735 |
| Ca | 46.729439 | 29.536299 | 33.191238 |
| Ca | 42.991463 | 29.270445 | 34.594753 |
| S  | 26.966774 | 28.328506 | 36.907036 |
| S  | 27.183044 | 34.149113 | 33.409645 |
| S  | 30.378876 | 29.438534 | 32.818359 |
| S  | 30.091208 | 31.459721 | 36.236069 |
| S  | 33.171169 | 27.111553 | 34.308750 |
| S  | 33.771656 | 32.480820 | 32.618313 |
| S  | 36.858921 | 28.772186 | 31.508289 |
| S  | 36.334095 | 29.297665 | 36.731674 |
| S  | 39.970509 | 26.893669 | 33.896057 |
| S  | 40.334362 | 31.321939 | 34.152916 |
| S  | 43.849091 | 29.368523 | 31.367208 |
| S  | 44.246441 | 25.430155 | 37.466614 |

24 generated by VMD

| Ca | 24.835590 | 29.757198 | 32.448509 |
|----|-----------|-----------|-----------|
| Ca | 26.475740 | 31.582035 | 35.819508 |
| Ca | 30.455822 | 28.250994 | 36.004372 |
| Ca | 30.359478 | 32.795219 | 33.176098 |
| Ca | 33.162998 | 29.147882 | 31.550388 |
| Ca | 33.292397 | 30.329239 | 35.309845 |
| Ca | 36.632996 | 26.809042 | 34.471458 |
| Ca | 36.841831 | 30.686016 | 33.831436 |
| Ca | 40.084419 | 29.429852 | 31.523346 |
| Ca | 39.766762 | 28.836960 | 36.722290 |
| Ca | 46.530010 | 29.592016 | 33.558136 |
| Ca | 42.746635 | 29.193520 | 34.665462 |
| S  | 27.070753 | 28.256573 | 36.777351 |
| S  | 27.029667 | 33.943222 | 33.363930 |
| S  | 30.197247 | 29.527712 | 32.951004 |
| S  | 29.977776 | 31.579865 | 36.269978 |
|   |          |          |          |
|---|----------|----------|----------|
| S | 33.393730 | 27.237051 | 34.282337 |
| S | 33.768940 | 32.306595 | 32.493011 |
| S | 36.726532 | 28.576591 | 31.302233 |
| S | 36.280880 | 29.272318 | 36.524998 |
| S | 40.103096 | 26.836716 | 33.741245 |
| S | 40.345741 | 31.267570 | 34.188911 |
| S | 43.733040 | 29.558666 | 31.557562 |
| S | 44.621853 | 25.621355 | 37.497253 |

24 generated by VMD

| Ca   | 25.019703 | 29.526741 | 32.239998 |
| Ca   | 26.449086 | 31.515522 | 35.685467 |
| Ca   | 30.444298 | 27.908493 | 36.198879 |
| Ca   | 30.460785 | 32.845272 | 33.046104 |
| Ca   | 33.337849 | 29.415794 | 31.492188 |
| Ca   | 33.127182 | 30.184055 | 35.495575 |
| Ca   | 36.419700 | 26.957367 | 34.491802 |
| Ca   | 36.843233 | 31.027216 | 34.048794 |
| Ca   | 40.142338 | 29.375338 | 31.641867 |
| Ca   | 39.692764 | 29.249596 | 36.752319 |
| Ca   | 46.368168 | 29.211464 | 33.274139 |
| Ca   | 42.735302 | 29.080566 | 34.510410 |
| S    | 27.495522 | 28.346766 | 36.985111 |
| S    | 26.882816 | 34.049480 | 33.345787 |
| S    | 30.542496 | 29.446545 | 32.832363 |
| S    | 30.035883 | 31.452564 | 36.229591 |
| S    | 33.288315 | 27.063454 | 34.043621 |
| S    | 33.880146 | 32.416248 | 32.868767 |
| S    | 36.685715 | 28.839249 | 31.355240 |
| S    | 36.262016 | 29.222160 | 36.652245 |
| S    | 39.791286 | 26.864475 | 33.772919 |
| S    | 40.480953 | 31.294621 | 34.155144 |
| S    | 43.585041 | 29.239529 | 31.199791 |
| S    | 44.468197 | 25.858740 | 37.712616 |

24 generated by VMD

| Ca   | 24.580818 | 29.707172 | 32.366219 |
| Ca   | 26.164083 | 31.527761 | 35.915615 |
| Ca   | 30.196255 | 28.243523 | 35.947868 |
| Ca   | 30.377563 | 32.722145 | 33.149849 |
| Ca   | 33.233582 | 29.458759 | 31.161413 |
| Ca   | 33.169380 | 30.181232 | 35.346981 |
| Ca   | 36.502193 | 26.872324 | 34.619366 |
| Ca   | 37.048519 | 30.970516 | 34.052727 |
| Ca   | 40.165306 | 29.269642 | 31.399426 |
| Ca   | 39.615192 | 29.082922 | 36.828697 |
| Element | X    | Y    | Z    |
|---------|------|------|------|
| Ca      | 46.736935 | 29.689983 | 33.536777 |
| Ca      | 42.887970 | 29.039452 | 34.588181 |
| S       | 27.074926 | 28.382906 | 36.948383 |
| S       | 26.907034 | 33.781586 | 33.439781 |
| S       | 30.348940 | 29.526718 | 32.746865 |
| S       | 29.939775 | 31.538074 | 36.356094 |
| S       | 33.200535 | 27.344872 | 33.976730 |
| S       | 33.791977 | 32.325577 | 32.751564 |
| S       | 36.780273 | 28.497337 | 31.308420 |
| S       | 36.355110 | 29.274813 | 36.622719 |
| S       | 40.023598 | 26.880762 | 33.872040 |
| S       | 40.508324 | 31.156071 | 34.122822 |
| S       | 43.885563 | 29.200748 | 31.490181 |
| S       | 44.940018 | 25.716419 | 37.480160 |

24 generated by VMD

| Element | X    | Y    | Z    |
|---------|------|------|------|
| Ca      | 25.023479 | 29.672791 | 32.596218 |
| Ca      | 26.716619 | 31.595188 | 35.709522 |
| Ca      | 29.952368 | 28.017735 | 36.093884 |
| Ca      | 30.500481 | 32.538311 | 33.196606 |
| Ca      | 33.373962 | 29.592216 | 31.160782 |
| Ca      | 33.273361 | 29.912014 | 35.406845 |
| Ca      | 36.450489 | 27.016388 | 34.336540 |
| Ca      | 36.959717 | 30.937685 | 33.839909 |
| Ca      | 40.141724 | 29.276295 | 31.596313 |
| Ca      | 39.506618 | 28.924181 | 36.650604 |
| Ca      | 46.512062 | 29.568647 | 33.591702 |
| Ca      | 42.642597 | 29.150043 | 34.663445 |
| S       | 27.042320 | 28.493000 | 37.266243 |
| S       | 27.205755 | 33.977127 | 33.430618 |
| S       | 30.432747 | 29.413372 | 32.824322 |
| S       | 30.118242 | 31.246763 | 36.379063 |
| S       | 33.147446 | 27.130770 | 33.886776 |
| S       | 33.819107 | 32.546371 | 32.529125 |
| S       | 36.672436 | 28.830334 | 31.100281 |
| S       | 36.218227 | 29.275185 | 36.442329 |
| S       | 39.799168 | 26.768936 | 33.812828 |
| S       | 40.370468 | 31.161087 | 34.175011 |
| S       | 43.773880 | 29.459747 | 31.506790 |
| S       | 44.780605 | 25.887177 | 37.834949 |

24 generated by VMD

| Element | X    | Y    | Z    |
|---------|------|------|------|
| Ca      | 24.952591 | 29.321220 | 32.584072 |
| Ca      | 26.448427 | 31.520950 | 35.757652 |
| Ca      | 30.079082 | 28.080456 | 35.933884 |
| Ca      | 30.555639 | 32.688622 | 32.986275 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 33.306576 | 29.663292 | 31.344719 |
| Ca      | 33.019409 | 30.227015 | 35.445187 |
| Ca      | 36.417545 | 26.977419 | 34.527836 |
| Ca      | 37.031761 | 30.978041 | 34.284988 |
| Ca      | 40.353745 | 29.172951 | 31.459057 |
| Ca      | 39.635208 | 29.035778 | 36.368683 |
| Ca      | 46.656616 | 29.182676 | 33.626205 |
| S       | 27.109625 | 28.294338 | 36.971039 |
| S       | 27.019257 | 33.911510 | 33.424240 |
| S       | 30.453228 | 29.556555 | 32.720558 |
| S       | 29.867287 | 31.467369 | 36.326477 |
| S       | 33.115917 | 27.260197 | 34.150719 |
| S       | 33.717339 | 32.650772 | 32.842369 |
| S       | 36.782639 | 28.922749 | 31.477808 |
| S       | 36.110241 | 29.087189 | 36.71781  |
| S       | 39.964371 | 26.840702 | 33.844276 |
| S       | 40.572117 | 31.181496 | 34.041409 |
| S       | 43.927216 | 29.301544 | 31.230331 |
| S       | 44.419941 | 25.883381 | 37.484947 |

24

generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 24.889500 | 29.625034 | 32.695847 |
| Ca      | 26.242228 | 31.532265 | 35.894909 |
| Ca      | 30.160215 | 28.120956 | 35.851372 |
| Ca      | 30.283363 | 32.673927 | 33.481194 |
| Ca      | 33.444721 | 29.432613 | 31.347443 |
| Ca      | 33.375233 | 30.166710 | 35.263988 |
| Ca      | 36.386463 | 26.651173 | 34.258034 |
| Ca      | 36.908997 | 30.941502 | 33.633724 |
| Ca      | 40.351418 | 29.270248 | 31.490910 |
| Ca      | 39.532703 | 29.197268 | 36.563904 |
| Ca      | 46.986088 | 29.222946 | 33.842598 |
| Ca      | 43.010414 | 29.359686 | 34.601707 |
| S       | 27.046448 | 28.199579 | 37.119568 |
| S       | 26.796078 | 34.106293 | 33.661873 |
| S       | 30.552059 | 29.674160 | 32.667969 |
| S       | 29.893656 | 31.445923 | 36.436401 |
| S       | 33.059605 | 27.157850 | 34.135857 |
| S       | 33.905228 | 32.465160 | 32.678802 |
| S       | 36.855026 | 28.790535 | 31.069714 |
| S       | 36.281216 | 29.130884 | 36.214233 |
| S       | 39.916267 | 26.858944 | 33.887314 |
| S       | 40.524094 | 31.367107 | 34.129749 |
| S       | 44.002235 | 29.041754 | 31.515516 |
| S       | 44.030666 | 25.958868 | 37.588020 |
| Element | X1 | Y1 | Z1 | X2 | Y2 | Z2 |
|---------|----|----|----|----|----|----|
| Ca      | 24.951389 | 29.678219 | 32.619217 |
| Ca      | 26.582924 | 31.377443 | 35.937824 |
| Ca      | 30.498831 | 27.961002 | 36.042545 |
| Ca      | 30.380222 | 32.847622 | 33.452724 |
| Ca      | 33.185196 | 29.556721 | 31.247330 |
| Ca      | 33.197353 | 30.583872 | 35.159401 |
| Ca      | 36.617004 | 26.985729 | 34.04133 |
| Ca      | 36.745243 | 30.794868 | 33.514610 |
| Ca      | 40.141121 | 28.988127 | 31.447144 |
| Ca      | 39.529015 | 28.921566 | 36.628235 |
| Ca      | 46.682594 | 29.478891 | 33.956593 |
| Ca      | 42.810589 | 29.319893 | 34.473217 |
| S       | 27.241304 | 28.003052 | 36.88931 |
| S       | 27.107708 | 33.936440 | 33.769657 |
| S       | 30.422844 | 29.681274 | 32.851357 |
| S       | 30.170605 | 31.35728 | 36.452621 |
| S       | 33.212997 | 27.52935 | 34.038307 |
| S       | 33.779411 | 32.630440 | 32.505856 |
| S       | 36.601875 | 28.600399 | 31.156130 |
| S       | 36.273182 | 29.278263 | 36.363155 |
| S       | 40.076889 | 26.700348 | 33.942947 |
| S       | 40.194588 | 31.158190 | 34.013577 |
| S       | 43.873383 | 29.218750 | 31.369843 |
| S       | 44.157604 | 25.781555 | 37.995369 |
|     | 36.723732 | 28.542439 | 31.203655 |
|-----|-----------|-----------|-----------|
| S   | 36.298126 | 29.067451 | 36.393578 |
| S   | 40.096680 | 26.879284 | 33.914421 |
| S   | 40.227036 | 31.304726 | 34.158154 |
| S   | 43.829178 | 29.561102 | 31.575287 |
| S   | 44.595497 | 25.879486 | 37.587803 |

24 generated by VMD

|     | 24.914366 | 29.906149 | 32.584969 |
|-----|-----------|-----------|-----------|
| Ca  | 26.624876 | 31.616619 | 35.934044 |
| Ca  | 30.262798 | 28.002232 | 35.915771 |
| Ca  | 30.619837 | 32.751190 | 33.431198 |
| Ca  | 33.187977 | 29.503878 | 31.194668 |
| Ca  | 33.347843 | 30.242361 | 35.222755 |
| Ca  | 36.598854 | 26.541168 | 34.393276 |
| Ca  | 36.686737 | 30.457571 | 33.387524 |
| Ca  | 39.994740 | 29.011002 | 31.543480 |
| Ca  | 39.739624 | 29.247219 | 36.847031 |
| Ca  | 46.350235 | 29.842781 | 33.830223 |
| Ca  | 42.575588 | 29.374718 | 34.654087 |
| S   | 27.049425 | 28.139141 | 36.728996 |
| S   | 27.278496 | 34.184959 | 33.827175 |
| S   | 30.431261 | 29.618961 | 32.843990 |
| S   | 30.241180 | 31.352493 | 36.508408 |
| S   | 33.262890 | 27.249542 | 33.807899 |
| S   | 33.876190 | 32.461990 | 32.411873 |
| S   | 36.609730 | 28.266399 | 31.019691 |
| S   | 36.470764 | 29.067017 | 36.262379 |
| S   | 39.989117 | 26.746300 | 34.228973 |
| S   | 40.116817 | 31.273636 | 33.972015 |
| S   | 43.569584 | 29.502441 | 31.519051 |
| S   | 44.634888 | 26.031700 | 37.961205 |

24 generated by VMD

|     | 24.741322 | 30.021759 | 32.561298 |
|-----|-----------|-----------|-----------|
| Ca  | 26.547884 | 31.441582 | 35.790489 |
| Ca  | 29.933514 | 28.251583 | 35.930477 |
| Ca  | 30.454655 | 32.888725 | 33.189831 |
| Ca  | 33.380810 | 28.959448 | 31.351200 |
| Ca  | 33.217270 | 29.889259 | 35.225281 |
| Ca  | 36.425884 | 26.702221 | 34.698174 |
| Ca  | 36.927814 | 30.863430 | 33.900620 |
| Ca  | 40.301617 | 29.286633 | 31.715492 |
| Ca  | 39.668137 | 29.205708 | 36.587807 |
| Ca  | 46.637249 | 29.737808 | 33.411827 |
| Ca  | 42.763634 | 29.254990 | 34.576950 |
24

generated by VMD

Ca  24.977020  29.269047  32.650902
Ca  26.540529  31.518799  35.841194
Ca  30.282629  28.204737  35.996235
Ca  30.226391  32.733124  33.108932
Ca  33.494961  29.305679  31.192619
Ca  33.071072  30.358419  35.320690
Ca  36.563797  26.976732  34.644501
Ca  36.714100  31.096807  33.828304
Ca  40.372307  29.554497  31.517879
Ca  39.837219  28.897743  36.533924
Ca  46.556679  29.148193  33.689064
Ca  42.785332  29.094704  34.513004
S  27.108360  27.986275  36.823875
S  27.056147  34.034859  33.732170
S  30.457920  29.620911  32.741093
S  29.991734  31.566593  36.312981
S  33.223022  27.375153  34.061249
S  33.730824  32.401016  32.530277
S  36.897915  28.778637  31.373991
S  36.321884  29.511677  36.707569
S  39.989456  26.826168  33.789772
S  40.247215  31.401314  34.131302
S  43.791374  29.380657  31.539246
S  44.196068  25.349674  37.449837

24

generated by VMD

Ca  25.018467  30.071289  32.418644
Ca  26.579842  31.773834  35.754677
Ca  30.046169  27.888090  35.918053
Ca  30.454029  32.526302  33.180519
Ca  33.271130  28.664543  31.487238
Ca  33.205963  30.172483  35.458008
|   | Ca       | 36.443253 | 26.891228 | 34.507233 |
|---|----------|-----------|-----------|-----------|
|   | Ca       | 36.695824 | 30.743626 | 33.742947 |
|   | Ca       | 39.917023 | 29.281254 | 36.799938 |
|   | Ca       | 46.627140 | 29.400356 | 33.305595 |
|   | Ca       | 42.912144 | 29.244656 | 34.542000 |
|   | S        | 27.038052 | 28.375774 | 36.710255 |
|   | S        | 27.324780 | 34.286686 | 33.597382 |
|   | S        | 30.344711 | 29.336792 | 32.782318 |
|   | S        | 30.101456 | 31.320103 | 36.425148 |
|   | S        | 33.177265 | 27.028572 | 34.251377 |
|   | S        | 33.646759 | 31.933407 | 32.475178 |
|   | S        | 36.906189 | 28.675808 | 31.293297 |
|   | S        | 36.413521 | 29.373199 | 36.526558 |
|   | S        | 39.952045 | 26.998320 | 33.893421 |
|   | S        | 40.449474 | 31.565720 | 34.221233 |
|   | S        | 43.626339 | 29.481050 | 31.360588 |
|   | S        | 44.205505 | 25.760756 | 37.631912 |

24 generated by VMD

|   | Ca       | 25.105839 | 29.873188 | 32.664669 |
|---|----------|-----------|-----------|-----------|
|   | Ca       | 26.544136 | 31.495108 | 35.882866 |
|   | Ca       | 30.113970 | 28.187878 | 35.931496 |
|   | Ca       | 30.601553 | 32.490814 | 33.096439 |
|   | Ca       | 33.333073 | 29.147186 | 31.314919 |
|   | Ca       | 33.307068 | 30.301552 | 35.296131 |
|   | Ca       | 36.545998 | 27.027111 | 34.272522 |
|   | Ca       | 36.705231 | 30.817745 | 33.571587 |
|   | Ca       | 39.966530 | 29.467728 | 31.510380 |
|   | Ca       | 39.535706 | 28.817005 | 36.722870 |
|   | Ca       | 46.340584 | 29.658916 | 33.787025 |
|   | Ca       | 42.851421 | 29.206121 | 34.779007 |
|   | S        | 27.043785 | 28.111748 | 37.114902 |
|   | S        | 27.406178 | 34.078960 | 33.582794 |
|   | S        | 30.498762 | 29.453304 | 32.707664 |
|   | S        | 30.160681 | 31.331009 | 36.418839 |
|   | S        | 33.310394 | 27.389526 | 34.103195 |
|   | S        | 33.955067 | 32.202164 | 32.404770 |
|   | S        | 36.679016 | 28.533779 | 30.984924 |
|   | S        | 36.477268 | 29.381824 | 36.478622 |
|   | S        | 40.050663 | 27.014336 | 33.889370 |
|   | S        | 40.084522 | 31.161732 | 34.428505 |
|   | S        | 43.550304 | 29.644997 | 31.567127 |
|   | S        | 44.266102 | 25.597683 | 37.520100 |

24 generated by VMD
| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 25.070072 | 29.576021 | 32.339722 |
| Ca      | 26.399305 | 31.533268 | 35.579861 |
| Ca      | 30.085394 | 28.183224 | 36.232201 |
| Ca      | 30.350410 | 32.849388 | 33.211449 |
| Ca      | 33.431992 | 29.244110 | 31.360172 |
| Ca      | 33.238789 | 30.331463 | 35.624340 |
| Ca      | 36.543823 | 26.755138 | 34.524345 |
| Ca      | 36.724087 | 30.478836 | 33.483372 |
| Ca      | 40.197212 | 29.434113 | 31.196461 |
| Ca      | 39.770988 | 28.908783 | 36.624340 |
| Ca      | 46.428020 | 29.762108 | 33.964676 |
| Ca      | 42.838047 | 29.146812 | 34.499119 |
| S       | 26.907652 | 28.271004 | 36.887939 |
| S       | 27.285019 | 34.316711 | 33.657997 |
| S       | 30.555025 | 29.564518 | 33.007965 |
| S       | 29.944544 | 31.366028 | 36.396095 |
| S       | 33.278000 | 27.188034 | 34.391464 |
| S       | 33.720470 | 32.341850 | 32.702793 |
| S       | 36.817230 | 28.439159 | 31.115948 |
| S       | 36.478420 | 29.294052 | 36.490410 |
| S       | 40.190529 | 26.863491 | 33.695930 |
| S       | 40.166355 | 31.170834 | 33.965790 |
| S       | 43.870575 | 29.746973 | 31.451696 |
| S       | 44.141937 | 25.625462 | 37.646843 |

24 generated by VMD

| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 25.064117 | 29.903719 | 32.591030 |
| Ca      | 26.730850 | 31.413376 | 35.922340 |
| Ca      | 30.144947 | 28.049713 | 35.895725 |
| Ca      | 30.224869 | 32.735004 | 32.910995 |
| Ca      | 33.323563 | 29.174599 | 31.331404 |
| Ca      | 33.358227 | 30.040913 | 35.116936 |
| Ca      | 36.411236 | 26.854345 | 34.574306 |
| Ca      | 36.800282 | 30.852634 | 33.853336 |
| Ca      | 40.183044 | 29.337290 | 31.560133 |
| Ca      | 39.856178 | 29.238531 | 36.680199 |
| Ca      | 46.530209 | 29.220665 | 33.513039 |
| Ca      | 42.725056 | 29.355213 | 34.702057 |
| S       | 27.099438 | 28.144512 | 36.950687 |
| S       | 27.118593 | 34.271034 | 34.164261 |
| S       | 30.375689 | 29.539194 | 32.689838 |
| S       | 30.181854 | 31.315351 | 36.177345 |
| S       | 33.199635 | 27.140497 | 34.149513 |
| S       | 33.747818 | 32.250778 | 32.198120 |
| S       | 36.784317 | 28.693001 | 31.265825 |
| S       | 36.279297 | 29.334175 | 36.529190 |
|   | X   | Y   | Z   |
|---|-----|-----|-----|
| S | 39.953716 | 26.943579 | 33.960171 |
| S | 40.397606 | 31.414454 | 34.012589 |
| S | 43.823151 | 29.486124 | 31.500916 |
| S | 44.120190 | 25.682673 | 37.720 |

24 generated by VMD

| Ca | 25.183117 | 29.693623 | 32.362911 |
| Ca | 26.492332 | 31.529783 | 35.758892 |
| Ca | 30.124613 | 28.141542 | 35.889050 |
| Ca | 30.315905 | 32.810616 | 33.071854 |
| Ca | 33.267223 | 29.027161 | 31.477179 |
| Ca | 33.400803 | 30.090851 | 35.623451 |
| Ca | 36.398884 | 27.016029 | 34.576584 |
| Ca | 36.664295 | 30.825344 | 33.894917 |
| Ca | 40.313511 | 29.392714 | 31.349754 |
| Ca | 39.726326 | 29.069084 | 36.616425 |
| Ca | 46.630482 | 29.208717 | 33.532040 |
| Ca | 42.737869 | 29.500057 | 34.574463 |
| S | 27.033676 | 28.247746 | 36.797180 |
| S | 27.168274 | 34.093147 | 33.514343 |
| S | 30.585808 | 29.615128 | 32.898941 |
| S | 29.994076 | 31.566055 | 36.276711 |
| S | 33.180298 | 27.166826 | 34.260895 |
| S | 33.718807 | 32.299644 | 32.680862 |
| S | 36.751686 | 28.313461 | 31.400999 |
| S | 36.181755 | 29.380905 | 36.741638 |
| S | 39.966515 | 26.929882 | 33.901295 |
| S | 40.264843 | 31.312292 | 34.082787 |
| S | 43.779198 | 29.602272 | 31.463207 |
| S | 44.553509 | 25.558516 | 37.284351 |

24 generated by VMD

| Ca | 24.866293 | 29.675106 | 32.660492 |
| Ca | 26.691406 | 31.518856 | 35.949287 |
| Ca | 30.122826 | 28.271948 | 35.936069 |
| Ca | 30.430483 | 32.561836 | 33.255085 |
| Ca | 33.317619 | 29.137718 | 30.945562 |
| Ca | 33.168098 | 30.187666 | 35.139450 |
| Ca | 36.429577 | 26.922924 | 34.390591 |
| Ca | 36.911968 | 31.000134 | 34.055077 |
| Ca | 40.100441 | 29.247089 | 31.467400 |
| Ca | 39.693283 | 29.464676 | 36.471733 |
| Ca | 46.736656 | 29.141651 | 33.631737 |
| Ca | 43.017864 | 29.329117 | 34.726528 |
| S | 27.037500 | 28.046165 | 36.739235 |
| S | 27.075531 | 34.033447 | 33.922653 |
S  30.295448  29.499096  32.680908
S  30.233206  31.456512  36.466770
S  33.038483  27.240812  33.936886
S  33.935410  32.198601  32.352039
S  36.694866  28.822142  31.375713
S  36.239182  29.313248  36.594585
S  39.866402  26.866911  33.990334
S  40.473095  31.495132  34.005829
S  43.716942  29.296093  31.665773
S  44.341339  25.664562  37.671013

24 generated by VMD
Ca  24.836760  29.532888  32.351509
Ca  26.302074  31.353306  35.540222
Ca  30.109119  28.038383  36.018265
Ca  30.228287  32.743702  33.456314
Ca  33.209385  29.498169  31.444260
Ca  33.155350  30.411921  35.260979
Ca  36.568619  27.128361  34.457157
Ca  37.000832  30.984921  33.991066
Ca  40.319901  29.219307  31.438768
Ca  39.873215  29.043229  36.378582
Ca  46.892101  29.023809  33.726566
Ca  42.856232  29.302155  34.503979
S  27.008755  28.040623  36.778816
S  26.955822  33.989235  33.821247
S  30.401464  29.491211  32.745586
S  30.013680  31.265049  36.388950
S  33.239258  27.432365  34.391239
S  33.645988  32.558086  32.548767
S  36.793858  28.897896  31.362919
S  36.234688  29.461990  36.669533
S  40.053074  26.892584  33.954571
S  40.590233  31.386627  33.775848
S  43.851788  28.921019  31.394304
S  44.293354  25.414574  37.631294

24 generated by VMD
Ca  24.595915  29.974747  32.677097
Ca  26.400759  31.194557  36.053772
Ca  30.386881  28.100847  35.665459
Ca  30.553028  32.749702  33.065807
Ca  33.133503  29.217587  31.198631
Ca  33.137390  30.546707  35.035252
Ca  36.880421  26.801918  34.493618
Ca  36.867172  31.033287  33.637955
| Element | X1   | X2   | X3   |
|---------|------|------|------|
| Ca      | 39.962029 | 29.266739 | 31.760082 |
| Ca      | 39.824615 | 29.123943 | 36.572865 |
| Ca      | 46.468357 | 29.416176 | 33.583607 |
| Ca      | 42.804356 | 29.222523 | 34.836849 |
| S       | 27.152199 | 27.890678 | 36.873394 |
| S       | 27.156170 | 33.957699 | 34.042389 |
| S       | 30.250198 | 29.665573 | 32.505630 |
| S       | 30.015514 | 31.388012 | 36.221519 |
| S       | 33.249107 | 27.353134 | 34.090702 |
| S       | 33.901436 | 32.493996 | 32.261353 |
| S       | 36.480400 | 28.528904 | 31.438442 |
| S       | 36.425846 | 29.295834 | 36.392937 |
| S       | 40.234371 | 26.752399 | 33.977001 |
| S       | 40.615906 | 31.549103 | 34.195705 |
| S       | 43.398922 | 29.195896 | 31.604706 |
| S       | 44.539406 | 25.673275 | 37.846024 |

24

generated by VMD

| Element | X1   | X2   | X3   |
|---------|------|------|------|
| Ca      | 24.805410 | 29.619873 | 32.798222 |
| Ca      | 26.454470 | 31.502302 | 36.225636 |
| Ca      | 30.303562 | 28.210846 | 35.584858 |
| Ca      | 30.330759 | 32.776302 | 33.109108 |
| Ca      | 33.302505 | 29.388878 | 31.125999 |
| Ca      | 33.470497 | 30.338043 | 35.358444 |
| Ca      | 36.514908 | 26.574989 | 34.124893 |
| Ca      | 36.886829 | 30.962433 | 33.806755 |
| Ca      | 39.961555 | 29.212614 | 31.730518 |
| Ca      | 39.914909 | 29.223564 | 36.675339 |
| Ca      | 46.671585 | 29.526022 | 33.607719 |
| Ca      | 42.712120 | 29.273832 | 34.674667 |
| S       | 27.078121 | 28.121624 | 36.715004 |
| S       | 26.872164 | 33.966053 | 33.992077 |
| S       | 30.435865 | 29.630028 | 32.477116 |
| S       | 29.983469 | 31.572798 | 36.304096 |
| S       | 33.232105 | 27.349091 | 33.953171 |
| S       | 33.661469 | 32.358833 | 32.502853 |
| S       | 36.673698 | 28.610216 | 31.360430 |
| S       | 36.568596 | 29.190861 | 36.321709 |
| S       | 39.905533 | 26.710438 | 34.068474 |
| S       | 40.499733 | 31.339546 | 33.961029 |
| S       | 43.758999 | 29.116484 | 31.621859 |
| S       | 44.434986 | 25.815765 | 37.930717 |

24

generated by VMD

| Element | X1   | X2   | X3   |
|---------|------|------|------|
| Ca      | 24.721395 | 29.492268 | 32.286102 |
| Ca      | 26.545971 | 31.190441 | 35.766495 |
| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 30.373415 | 28.155733 | 35.501514 |
| Ca      | 30.431177 | 32.831806 | 33.495159 |
| Ca      | 33.289463 | 29.438148 | 31.107370 |
| Ca      | 33.315323 | 30.552818 | 35.437527 |
| Ca      | 36.400276 | 26.828529 | 34.302029 |
| Ca      | 37.018875 | 31.147732 | 33.875690 |
| Ca      | 40.031349 | 29.066414 | 31.732161 |
| Ca      | 39.880405 | 29.574165 | 36.413410 |
| Ca      | 46.526600 | 29.014343 | 33.597160 |
| Ca      | 42.919304 | 29.180172 | 34.422401 |
| S       | 27.274754 | 27.896202 | 36.828033 |
| S       | 26.813822 | 33.984192 | 33.991764 |
| S       | 30.385521 | 29.791227 | 32.654049 |
| S       | 29.971153 | 31.224762 | 36.597157 |
| S       | 33.233231 | 27.369961 | 34.047020 |
| S       | 33.833828 | 32.524498 | 32.701180 |
| S       | 36.627567 | 28.674994 | 31.473494 |
| S       | 36.528004 | 29.358131 | 36.357243 |
| S       | 39.896107 | 26.834118 | 34.278038 |
| S       | 40.728088 | 31.503662 | 33.842323 |
| S       | 43.558235 | 28.807610 | 31.328959 |
| S       | 44.130009 | 25.949436 | 37.994450 |

24

generated by VMD

| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 24.785664 | 29.682878 | 32.471809 |
| Ca      | 26.327187 | 31.165922 | 36.165035 |
| Ca      | 30.273163 | 28.231472 | 35.698318 |
| Ca      | 30.163523 | 32.725746 | 33.306374 |
| Ca      | 33.398071 | 29.273762 | 31.288925 |
| Ca      | 33.211094 | 30.673111 | 35.306198 |
| Ca      | 36.386753 | 27.107203 | 34.250484 |
| Ca      | 37.066727 | 31.050938 | 33.797279 |
| Ca      | 40.416348 | 29.104691 | 31.390575 |
| Ca      | 39.767273 | 29.322519 | 36.421661 |
| Ca      | 46.846996 | 28.984203 | 33.871315 |
| Ca      | 42.928532 | 29.152458 | 34.555740 |
| S       | 27.034845 | 27.736624 | 36.791519 |
| S       | 26.934690 | 33.972473 | 34.299568 |
| S       | 30.458630 | 29.646366 | 32.599087 |
| S       | 29.950565 | 31.523373 | 36.466011 |
| S       | 33.270279 | 27.318714 | 34.107788 |
| S       | 33.517559 | 32.447014 | 32.354454 |
| S       | 36.769505 | 28.896484 | 31.123848 |
| S       | 36.259510 | 29.530743 | 36.447258 |
| S       | 39.967129 | 26.919514 | 33.956486 |
| S       | 40.683567 | 31.324081 | 33.846901 |
| S   | 43.948730 | 28.954548 | 31.611692 |
| S   | 44.067596 | 25.646599 | 37.902317 |

24 generated by VMD

| Ca  | 24.752262 | 29.885504 | 32.678066 |
| Ca  | 26.462843 | 30.878723 | 36.137108 |
| Ca  | 30.483700 | 28.209602 | 35.709255 |
| Ca  | 30.243481 | 32.953575 | 33.076355 |
| Ca  | 33.417870 | 29.284334 | 31.108747 |
| Ca  | 33.071426 | 30.666344 | 35.334270 |
| Ca  | 36.650414 | 26.961172 | 34.485737 |
| Ca  | 36.707458 | 31.068277 | 33.865635 |
| Ca  | 40.254570 | 29.297825 | 31.492517 |
| Ca  | 39.857159 | 29.443329 | 36.555111 |
| Ca  | 46.601711 | 28.650175 | 33.531082 |
| Ca  | 42.787117 | 29.098997 | 34.629555 |
| S   | 27.464773 | 27.671532 | 36.732143 |
| S   | 26.849377 | 33.749718 | 34.037628 |
| S   | 30.468800 | 29.826899 | 32.717888 |
| S   | 30.030127 | 31.414059 | 36.407036 |
| S   | 33.282948 | 27.436268 | 34.043709 |
| S   | 33.650257 | 32.530952 | 32.314323 |
| S   | 36.881214 | 28.838686 | 31.198645 |
| S   | 36.442974 | 29.552382 | 36.481033 |
| S   | 39.978142 | 26.798214 | 33.955200 |
| S   | 40.687752 | 31.502548 | 33.926392 |
| S   | 43.520313 | 28.817417 | 31.420946 |
| S   | 43.887238 | 25.854858 | 38.192413 |

24 generated by VMD

| Ca  | 24.564484 | 30.003000 | 33.233067 |
| Ca  | 26.533516 | 31.061409 | 36.456032 |
| Ca  | 30.624483 | 28.165802 | 35.837936 |
| Ca  | 30.465935 | 32.729172 | 33.160152 |
| Ca  | 33.424404 | 29.426960 | 31.042877 |
| Ca  | 33.305489 | 30.542667 | 35.092758 |
| Ca  | 36.468075 | 27.109888 | 34.165482 |
| Ca  | 36.763714 | 30.845512 | 33.451641 |
| Ca  | 40.375675 | 29.246838 | 31.436127 |
| Ca  | 39.477264 | 29.406731 | 36.355179 |
| Ca  | 46.662785 | 28.950628 | 34.013115 |
| Ca  | 42.732582 | 29.293936 | 34.655067 |
| S   | 27.551357 | 27.690979 | 36.828053 |
| S   | 27.045914 | 33.699516 | 34.290588 |
| S   | 30.571583 | 29.584492 | 32.508862 |
| S   | 30.207659 | 31.511787 | 36.331764 |
|  |  |  |  |
|---|---|---|---|
| S | 33.302422 | 27.341301 | 33.708839 |
| S | 33.660648 | 32.486038 | 32.339474 |
| S | 36.876984 | 28.930098 | 30.794205 |
| S | 36.223057 | 29.397366 | 36.276421 |
| S | 39.894962 | 27.045647 | 33.984001 |
| S | 40.530922 | 31.562263 | 33.866489 |
| S | 43.888031 | 28.786686 | 31.709618 |
| S | 43.281994 | 25.572695 | 38.492931 |

24 generated by VMD

| Ca | 24.667343 | 29.771545 | 32.780323 |
| Ca | 26.325535 | 30.972950 | 36.096375 |
| Ca | 30.419060 | 28.313269 | 35.837883 |
| Ca | 30.287519 | 32.906075 | 33.059319 |
| Ca | 33.419346 | 29.548578 | 30.868969 |
| Ca | 33.147209 | 30.619602 | 35.260506 |
| Ca | 36.617744 | 26.803577 | 34.457817 |
| Ca | 36.679642 | 30.854378 | 33.754074 |
| Ca | 40.235138 | 29.042772 | 31.502766 |
| Ca | 39.847363 | 29.473843 | 36.651291 |
| Ca | 46.933643 | 28.842789 | 33.417797 |
| Ca | 42.861984 | 29.152180 | 34.405663 |
| S | 27.625736 | 27.718197 | 36.929935 |
| S | 27.085548 | 33.904636 | 34.287415 |
| S | 30.505173 | 29.877777 | 32.570713 |
| S | 29.846924 | 31.455582 | 36.275925 |
| S | 33.225563 | 27.567863 | 33.828423 |
| S | 33.817337 | 32.494274 | 32.527210 |
| S | 36.873886 | 28.703835 | 31.248844 |
| S | 36.351646 | 29.120205 | 36.496849 |
| S | 40.156860 | 26.838223 | 34.008667 |
| S | 40.460457 | 31.350176 | 33.831322 |
| S | 43.781265 | 28.952221 | 31.344582 |
| S | 43.262009 | 26.106857 | 38.588013 |

24 generated by VMD

| Ca | 24.460718 | 30.065922 | 32.501446 |
| Ca | 26.505438 | 30.696203 | 35.976517 |
| Ca | 30.492002 | 28.511105 | 35.359001 |
| Ca | 30.291611 | 32.951637 | 33.172718 |
| Ca | 33.282246 | 29.461227 | 31.015411 |
| Ca | 33.334980 | 30.526024 | 35.537640 |
| Ca | 36.672558 | 26.663298 | 34.505089 |
| Ca | 36.747131 | 30.818533 | 34.002281 |
| Ca | 40.426010 | 29.000662 | 31.430882 |
| Ca | 39.616768 | 29.776949 | 36.363632 |
|      |              |              |              |
|------|--------------|--------------|--------------|
| Ca   | 46.915077    | 29.071228    | 33.352993    |
| Ca   | 42.802868    | 29.379137    | 34.392128    |
| S    | 27.488007    | 27.774101    | 37.091690    |
| S    | 27.022713    | 33.944729    | 34.196571    |
| S    | 30.408937    | 29.861696    | 32.516827    |
| S    | 29.970161    | 31.482025    | 36.391239    |
| S    | 33.199062    | 27.580034    | 33.919296    |
| S    | 33.832680    | 32.504219    | 32.515205    |
| S    | 36.615089    | 28.385075    | 31.406118    |
| S    | 36.496353    | 28.958813    | 36.542019    |
| S    | 40.270500    | 26.773739    | 34.305580    |
| S    | 40.512123    | 31.347076    | 33.806248    |
| S    | 43.864914    | 28.712107    | 31.362759    |
| S    | 43.206047    | 26.145887    | 38.367447    |

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generated by VMD

|      |              |              |              |
|------|--------------|--------------|--------------|
| Ca   | 24.813026    | 29.784519    | 32.673706    |
| Ca   | 26.479202    | 30.909723    | 35.970619    |
| Ca   | 30.591053    | 28.049803    | 35.322723    |
| Ca   | 30.423477    | 32.957001    | 33.240150    |
| Ca   | 33.403828    | 29.631197    | 31.140579    |
| Ca   | 33.146816    | 30.746098    | 35.262825    |
| Ca   | 36.489162    | 26.817444    | 34.704330    |
| Ca   | 36.565765    | 30.564510    | 33.734322    |
| Ca   | 40.303471    | 28.887575    | 31.475388    |
| Ca   | 39.971436    | 29.419968    | 36.595295    |
| Ca   | 46.740555    | 29.377563    | 32.885292    |
| Ca   | 42.823097    | 29.420868    | 34.605656    |
| S    | 27.547972    | 27.907061    | 37.189919    |
| S    | 26.934521    | 33.816490    | 34.019474    |
| S    | 30.411045    | 29.894857    | 32.500412    |
| S    | 30.019663    | 31.439594    | 36.272171    |
| S    | 33.364780    | 27.725327    | 34.025917    |
| S    | 34.005482    | 32.677719    | 32.437618    |
| S    | 36.665554    | 28.275993    | 31.341759    |
| S    | 36.361443    | 29.296333    | 36.703880    |
| S    | 40.196205    | 26.865892    | 34.198971    |
| S    | 40.332329    | 31.249149    | 33.877186    |
| S    | 43.670456    | 29.060280    | 31.327782    |
| S    | 43.173573    | 25.616425    | 38.524727    |

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generated by VMD

|      |              |              |              |
|------|--------------|--------------|--------------|
| Ca   | 24.647572    | 30.187534    | 32.633133    |
| Ca   | 26.331902    | 30.878765    | 36.020409    |
| Ca   | 30.580473    | 28.314957    | 35.495090    |
| Ca   | 30.382547    | 32.738174    | 33.325329    |
| Element | Ca 1 | Ca 2 | Ca 3 | Ca 4 | Ca 5 | Ca 6 | Ca 7 | Ca 8 |
|---------|------|------|------|------|------|------|------|------|
| Ca      | 33.637012 | 29.335205 | 31.220345 | 33.186329 | 30.834394 | 35.181 | 36.884361 | 26.713619 |
| Ca      | 40.193501 | 28.891899 | 31.390154 | 39.609505 | 29.215538 | 36.288521 | 46.495255 | 29.019417 |
| S       | 27.519455 | 27.681625 | 37.148643 | 26.996895 | 33.923119 | 34.230415 | 30.477999 | 29.690735 |
| S       | 29.918615 | 31.443531 | 36.241051 | 33.773338 | 27.911482 | 32.854195 | 36.762733 | 28.230606 |
| S       | 36.346794 | 29.286961 | 36.525352 | 40.316566 | 26.851730 | 34.088455 | 40.185123 | 31.299044 |
| S       | 43.581963 | 29.139368 | 31.389816 | 43.243729 | 25.880722 | 38.639893 |

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generated by VMD

| Element | Ca 9 | Ca 10 | Ca 11 | Ca 12 | Ca 13 | Ca 14 | Ca 15 | Ca 16 |
|---------|------|------|------|------|------|------|------|------|
| Ca      | 24.622196 | 30.036449 | 32.483601 | 26.555325 | 30.986942 | 36.085968 | 30.386400 | 28.267029 |
| Ca      | 30.313591 | 32.853870 | 33.007687 | 33.589878 | 29.230148 | 31.398138 | 33.264225 | 30.332096 |
| Ca      | 36.674969 | 26.916275 | 34.528671 | 36.618114 | 30.636744 | 33.943649 | 40.176098 | 29.135727 |
| Ca      | 39.896061 | 29.844723 | 36.558895 | 46.511375 | 28.942097 | 33.060181 | 42.894310 | 29.362759 |
| S       | 27.397219 | 27.936159 | 37.078182 | 27.100679 | 33.937328 | 34.269257 | 30.400213 | 29.628418 |
| S       | 30.159372 | 31.446316 | 36.106834 | 33.633560 | 27.430378 | 34.137791 | 33.759342 | 32.454475 |
| S       | 36.843494 | 28.427462 | 31.553040 | 36.445404 | 29.344294 | 36.751842 | 40.229588 | 27.066364 |
| S       | 40.293541 | 31.337883 | 33.691849 | 43.666962 | 28.961197 | 31.123920 | 43.001984 | 25.876171 |

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|   | Ca           | S            | S            |
|---|--------------|--------------|--------------|
| 24| 24.257677    | 30.141159    | 32.745026    |
|   | 26.376842    | 31.148651    | 36.267948    |
|   | 30.541027    | 27.948826    | 35.254158    |
|   | 30.305965    | 33.090527    | 33.371532    |
|   | 33.449146    | 29.261511    | 31.302673    |
|   | 33.209251    | 30.624592    | 35.364906    |
|   | 36.743271    | 26.731327    | 34.417072    |
|   | 36.734802    | 30.610903    | 33.659157    |
|   | 40.261425    | 28.894907    | 31.267035    |
|   | 39.831383    | 29.876472    | 36.493862    |
|   | 46.548218    | 29.090698    | 33.446815    |
|   | 42.948723    | 29.429005    | 34.658985    |
|   | 27.253723    | 27.570339    | 36.760590    |
|   | 27.127886    | 34.017483    | 34.268368    |
|   | 30.517818    | 29.783009    | 32.422863    |
|   | 30.146467    | 31.193325    | 36.309639    |
|   | 33.561455    | 27.613501    | 33.999207    |
|   | 33.827045    | 32.465584    | 32.558067    |
|   | 36.820545    | 28.347719    | 31.347597    |
|   | 36.659157    | 29.379169    | 36.401039    |
|   | 40.325008    | 26.872093    | 34.312553    |
|   | 40.437649    | 31.380157    | 33.325123    |
|   | 43.775040    | 29.005775    | 31.423977    |
|   | 42.774315    | 25.914700    | 38.652508    |

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|   | Ca           | S            | S            |
|---|--------------|--------------|--------------|
|   | 24.623394    | 29.617205    | 32.889172    |
|   | 26.743504    | 31.450050    | 36.241337    |
|   | 30.459915    | 27.876068    | 35.109344    |
|   | 30.285316    | 33.085789    | 33.349220    |
|   | 33.420052    | 29.666401    | 31.317177    |
|   | 33.402569    | 30.425747    | 35.166122    |
|   | 36.834591    | 26.568558    | 34.614662    |
|   | 36.623219    | 30.665398    | 33.621346    |
|   | 40.383018    | 29.085377    | 31.376335    |
|   | 39.553875    | 29.868763    | 36.505859    |
|   | 46.648106    | 28.971313    | 33.389206    |
|   | 42.743401    | 29.429470    | 34.555233    |
|   | 27.507469    | 27.676022    | 37.120579    |
|   | 26.979532    | 34.156139    | 34.248928    |
|   | 30.518101    | 29.849575    | 32.412331    |
|   | 30.242371    | 31.130953    | 36.218006    |
|   | 33.628494    | 27.591827    | 33.693779    |
|   | 33.794777    | 32.681725    | 32.447029    |
S  36.952686  28.347120  31.488140
S  36.418499  29.165022  36.397820
S  40.240337  26.901230  34.146099
S  40.277584  31.462257  33.758469
S  43.609150  28.858189  31.429020
S  42.543983  25.861179  38.535561

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generated by VMD

Ca  24.238920  30.016256  32.825645
Ca  26.508560  31.132452  36.197361
Ca  30.554214  27.723677  35.542820
Ca  30.000269  32.984509  33.241619
Ca  33.250080  29.554195  31.236389
Ca  33.036053  30.570377  35.107685
Ca  36.943195  26.938345  34.372257
Ca  36.807755  30.828396  33.648720
Ca  40.431656  29.089781  31.404051
Ca  39.766113  29.737720  36.291172
Ca  47.318310  28.720840  33.800278
Ca  43.059719  29.310328  34.620049
S  27.307621  27.819649  37.104706
S  26.812359  33.926109  34.375092
S  30.239027  29.683992  32.588005
S  30.048368  31.201954  36.254074
S  33.588303  27.656881  33.716774
S  33.767700  32.742516  32.540916
S  36.953728  28.675238  31.210709
S  36.324448  29.280270  36.314606
S  40.280277  26.899973  34.097519
S  40.652447  31.461899  33.484375
S  43.929359  28.668690  31.679604
S  42.615459  25.767365  38.376255

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generated by VMD

Ca  24.071121  30.200062  33.158695
Ca  26.643143  30.922583  36.299484
Ca  30.339935  28.078506  34.998005
Ca  30.214312  32.916534  32.955807
Ca  33.458645  29.424515  30.937283
Ca  33.360977  30.584217  35.225246
Ca  36.686993  26.797338  34.775467
Ca  36.661125  30.702717  33.758247
Ca  40.205105  29.070133  31.627892
Ca  39.753532  29.875778  36.450459
Ca  46.902740  28.570974  33.254944
Ca  43.088737  29.522724  34.679520
|  | X  | Y  | Z  |
|---|---|---|---|
| S | 27.139915 | 27.445442 | 36.615158 |
| S | 27.153505 | 33.860016 | 34.699009 |
| S | 30.467905 | 29.710155 | 32.391479 |
| S | 30.205803 | 31.258791 | 36.113449 |
| S | 33.767616 | 27.747683 | 33.708393 |
| S | 33.641243 | 32.495697 | 32.316216 |
| S | 36.794739 | 28.555248 | 31.418407 |
| S | 36.554695 | 29.390320 | 36.663429 |
| S | 40.134914 | 27.208979 | 34.356735 |
| S | 40.618256 | 31.586769 | 33.684650 |
| S | 43.688946 | 28.488434 | 31.500923 |
| S | 42.880081 | 25.977781 | 38.441696 |

24 generated by VMD

| Ca  | 24.224758 | 30.345818 | 32.683643 |
|---|---|---|---|
| Ca  | 26.721306 | 30.960148 | 36.201527 |
| Ca  | 30.340834 | 28.062355 | 35.426861 |
| Ca  | 30.444738 | 30.24097 | 33.112816 |
| Ca  | 33.292953 | 29.330173 | 31.342972 |
| Ca  | 33.296879 | 30.389221 | 35.302170 |
| Ca  | 36.887650 | 26.900326 | 34.332825 |
| Ca  | 36.797344 | 30.876724 | 33.763279 |
| Ca  | 40.267429 | 29.143114 | 31.403889 |
| Ca  | 39.935841 | 30.020800 | 36.808498 |
| Ca  | 46.660217 | 28.616608 | 33.138939 |
| Ca  | 43.046024 | 29.435410 | 34.590500 |
| S  | 27.142595 | 27.329697 | 36.743568 |
| S  | 27.097088 | 33.851238 | 34.390987 |
| S  | 30.369444 | 29.731205 | 32.516361 |
| S  | 30.189732 | 31.254906 | 36.267677 |
| S  | 33.531044 | 27.415512 | 33.942120 |
| S  | 33.668411 | 32.369919 | 32.245308 |
| S  | 36.866222 | 28.714314 | 31.246117 |
| S  | 36.620426 | 29.426601 | 36.465336 |
| S  | 40.327515 | 27.231731 | 34.261414 |
| S  | 40.513069 | 31.499319 | 33.643898 |
| S  | 43.458080 | 28.377197 | 31.405558 |
| S  | 42.734306 | 26.084940 | 38.794525 |

24 generated by VMD

| Ca  | 24.549723 | 30.360188 | 32.914127 |
|---|---|---|---|
| Ca  | 26.659225 | 31.318836 | 36.318733 |
| Ca  | 30.331232 | 27.958435 | 35.456730 |
| Ca  | 30.358824 | 32.754356 | 33.272362 |
| Ca  | 33.499844 | 29.525379 | 31.323051 |
| Ca  | 33.213291 | 30.220604 | 35.324684 |
| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 36.812229 | 26.630800 | 34.487694 |
| Ca      | 36.600311  | 30.684631  | 33.501381  |
| Ca      | 40.231602  | 28.886626  | 31.486607  |
| Ca      | 39.766430  | 29.949875  | 36.633289  |
| Ca      | 46.631088  | 29.115715  | 33.658176  |
| Ca      | 42.741020  | 29.694752  | 34.540657  |
| S       | 27.153917  | 27.794655  | 36.216824  |
| S       | 27.268402  | 34.024864  | 34.458702  |
| S       | 30.557125  | 29.693550  | 32.490692  |
| S       | 30.145609  | 31.232174  | 36.356571  |
| S       | 33.488972  | 27.394951  | 33.894844  |
| S       | 33.665257  | 32.393864  | 32.444683  |
| S       | 36.712357  | 28.358219  | 31.376949  |
| S       | 36.527580  | 29.197222  | 36.429798  |
| S       | 40.302952  | 26.981838  | 34.365742  |
| S       | 40.361431  | 31.410252  | 33.283169  |
| S       | 43.680172  | 28.650425  | 31.425560  |
| S       | 43.175312  | 26.157137  | 38.369667  |

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generated by VMD

| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 24.522076 | 30.161392 | 32.664600 |
| Ca      | 26.280506  | 31.162945  | 36.292892  |
| Ca      | 30.198635  | 27.912155  | 35.546532  |
| Ca      | 30.334017  | 32.744614  | 33.249744  |
| Ca      | 33.840652  | 29.525967  | 31.145540  |
| Ca      | 33.107025  | 30.106089  | 34.929134  |
| Ca      | 36.696136  | 26.855177  | 34.412407  |
| Ca      | 36.885727  | 31.226892  | 33.735672  |
| Ca      | 40.315468  | 28.931606  | 31.788401  |
| Ca      | 39.915436  | 29.809822  | 36.685738  |
| Ca      | 46.739697  | 28.555458  | 32.736454  |
| Ca      | 43.359741  | 29.556416  | 34.658207  |
| S       | 26.985065  | 27.644711  | 36.702278  |
| S       | 27.129126  | 33.876076  | 34.545357  |
| S       | 30.705839  | 29.774414  | 32.455093  |
| S       | 29.962280  | 31.134407  | 36.370430  |
| S       | 33.200317  | 27.154230  | 33.870636  |
| S       | 33.682056  | 32.627815  | 32.221481  |
| S       | 36.840485  | 28.795532  | 31.584620  |
| S       | 36.357471  | 29.619055  | 36.336708  |
| S       | 40.062237  | 26.980888  | 34.571991  |
| S       | 40.529202  | 31.587822  | 33.563583  |
| S       | 43.562950  | 28.406788  | 31.419514  |
| S       | 43.221752  | 26.241085  | 38.543724  |

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generated by VMD
| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 24.409784 | 30.268261 | 32.823391 |
| Ca      | 26.711870 | 31.182249 | 36.319294 |
| Ca      | 30.181330 | 27.998997 | 35.337452 |
| Ca      | 30.102720 | 32.827465 | 33.139290 |
| Ca      | 33.519363 | 29.197447 | 31.001987 |
| Ca      | 33.149239 | 30.194775 | 35.128414 |
| Ca      | 36.664089 | 26.786432 | 34.323360 |
| Ca      | 36.943478 | 31.134359 | 33.912430 |
| Ca      | 40.241928 | 28.718367 | 31.712448 |
| Ca      | 40.016434 | 29.824406 | 36.785282 |
| Ca      | 46.716324 | 28.824673 | 32.974041 |
| Ca      | 43.108200 | 29.453236 | 34.622314 |
| S       | 27.056549 | 27.714565 | 36.698868 |
| S       | 27.006521 | 34.037682 | 34.533058 |
| S       | 30.415655 | 29.676443 | 32.401218 |
| S       | 30.183208 | 31.204815 | 36.175007 |
| S       | 33.270260 | 27.232588 | 33.802010 |
| S       | 33.678169 | 32.457134 | 32.313442 |
| S       | 36.844418 | 28.971270 | 31.608221 |
| S       | 36.427151 | 29.331089 | 36.424080 |
| S       | 40.095757 | 26.992706 | 34.485924 |
| S       | 40.639767 | 31.413155 | 33.629532 |
| S       | 43.778854 | 28.636160 | 31.310318 |
| S       | 43.272739 | 26.313068 | 38.569340 |

**Generated by VMD**

| Element | Value1 | Value2 | Value3 |
|---------|--------|--------|--------|
| Ca      | 24.957163 | 30.214542 | 32.485653 |
| Ca      | 26.533070 | 31.275589 | 36.348877 |
| Ca      | 30.198343 | 28.018349 | 35.304581 |
| Ca      | 30.203573 | 32.783859 | 33.303940 |
| Ca      | 33.512234 | 29.311323 | 31.179125 |
| Ca      | 33.220024 | 30.413288 | 35.251610 |
| Ca      | 36.697155 | 26.777653 | 34.654224 |
| Ca      | 36.722599 | 30.932812 | 33.513130 |
| Ca      | 40.155575 | 28.806850 | 31.754814 |
| Ca      | 39.944687 | 29.831547 | 36.883354 |
| Ca      | 46.919792 | 28.888844 | 32.714005 |
| Ca      | 43.060642 | 29.456612 | 34.589119 |
| S       | 26.973665 | 27.745625 | 36.624454 |
| S       | 27.031897 | 33.899384 | 34.272583 |
| S       | 30.304064 | 29.668415 | 32.487686 |
| S       | 30.086748 | 31.281303 | 36.472813 |
| S       | 33.476009 | 27.395561 | 33.817978 |
| S       | 33.642780 | 32.482887 | 32.479584 |
| S       | 36.746868 | 28.486773 | 31.560307 |
| S       | 36.395142 | 29.542912 | 36.398361 |
| Element | X (Angstroms) | Y (Angstroms) | Z (Angstroms) |
|---------|---------------|---------------|---------------|
| S       | 40.133808     | 27.056147     | 34.570080     |
| S       | 40.351913     | 31.329163     | 33.548820     |
| S       | 43.685295     | 28.862350     | 31.386127     |
| S       | 43.480789     | 25.929573     | 38.429482     |
| Ca      | 25.099222     | 29.855349     | 32.007744     |
| Ca      | 26.312723     | 31.101803     | 35.909679     |
| Ca      | 30.205713     | 28.151779     | 35.480644     |
| Ca      | 30.104734     | 32.755486     | 33.503517     |
| Ca      | 33.859821     | 29.836117     | 31.225544     |
| Ca      | 33.043442     | 30.499882     | 35.405033     |
| Ca      | 36.788361     | 26.920992     | 34.933113     |
| Ca      | 36.624516     | 30.979509     | 33.708702     |
| Ca      | 40.073200     | 28.636383     | 31.782194     |
| Ca      | 39.821381     | 29.365728     | 36.445919     |
| Ca      | 46.790985     | 28.872818     | 32.551723     |
| Ca      | 42.989151     | 29.341446     | 34.314762     |
| S       | 27.001196     | 27.689875     | 36.452511     |
| S       | 26.972607     | 33.888199     | 34.211185     |
| S       | 30.518076     | 29.870367     | 32.696262     |
| S       | 29.872223     | 31.293491     | 36.700272     |
| S       | 33.543159     | 27.698469     | 33.842743     |
| S       | 33.623199     | 32.592171     | 32.791252     |
| S       | 36.598824     | 28.592039     | 31.711348     |
| S       | 36.460796     | 29.643692     | 36.679100     |
| S       | 40.285046     | 26.805218     | 34.428555     |
| S       | 40.335796     | 31.231195     | 33.515617     |
| S       | 43.558331     | 28.324089     | 31.131281     |
| S       | 43.951447     | 26.445286     | 38.601921     |

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generated by VMD

| Element | X (Angstroms) | Y (Angstroms) | Z (Angstroms) |
|---------|---------------|---------------|---------------|
| Ca      | 24.850687     | 29.854177     | 32.252678     |
| Ca      | 26.326292     | 31.289711     | 35.974926     |
| Ca      | 30.152725     | 28.130562     | 35.571079     |
| Ca      | 30.276770     | 32.802547     | 33.506386     |
| Ca      | 33.721031     | 29.670660     | 31.212896     |
| Ca      | 33.056641     | 30.386827     | 35.434338     |
| Ca      | 36.614235     | 26.679340     | 34.838032     |
| Ca      | 36.724442     | 30.952381     | 33.778954     |
| Ca      | 40.062317     | 28.721458     | 31.592627     |
| Ca      | 40.154911     | 29.357559     | 36.609520     |
| Ca      | 46.579868     | 28.892284     | 32.531601     |
| Ca      | 43.047611     | 29.578224     | 34.336998     |
| S       | 27.242920     | 27.880728     | 36.446369     |
| S       | 26.850023     | 33.888943     | 33.869713     |
|    | S    | Ca   | S    | Ca   |
|----|------|------|------|------|
| S  | 30.557713 | 29.863102 | 32.488590 |
| S  | 29.902744 | 31.312708 | 36.519394 |
| S  | 33.357277 | 27.435349 | 33.971882 |
| S  | 33.528061 | 32.506111 | 32.713829 |
| S  | 36.583092 | 28.554337 | 31.751583 |
| S  | 36.482151 | 29.510986 | 36.718586 |
| S  | 40.140137 | 26.845364 | 34.421135 |
| S  | 40.457932 | 31.314156 | 33.695995 |
| S  | 43.559608 | 28.702404 | 31.130123 |
| S  | 44.204704 | 26.261467 | 38.663517 |

24 generated by VMD

|    | Ca   | S    | Ca   | S    |
|----|------|------|------|------|
| Ca | 24.564669 | 29.519867 | 32.644806 |
| Ca | 26.435116 | 31.263821 | 35.977798 |
| Ca | 30.095047 | 28.082043 | 35.504696 |
| Ca | 30.001846 | 32.817162 | 33.278671 |
| Ca | 33.645996 | 29.610207 | 31.074680 |
| Ca | 32.987236 | 30.435131 | 34.986393 |
| Ca | 36.770172 | 26.997395 | 34.591965 |
| Ca | 36.896130 | 31.253086 | 33.841454 |
| Ca | 40.375713 | 28.921318 | 31.695477 |
| Ca | 39.944843 | 28.926205 | 36.557220 |
| Ca | 46.852356 | 28.913109 | 32.659588 |
| Ca | 43.147881 | 29.247787 | 34.618919 |
| S  | 27.223431 | 27.927120 | 36.725349 |
| S  | 26.771616 | 33.997162 | 34.188042 |
| S  | 30.368557 | 29.692318 | 32.558964 |
| S  | 29.935755 | 31.248348 | 36.392590 |
| S  | 33.182789 | 27.481974 | 33.834145 |
| S  | 33.497360 | 32.694527 | 32.432274 |
| S  | 36.757927 | 28.998251 | 31.616871 |
| S  | 36.449371 | 29.716778 | 36.665581 |
| S  | 40.192875 | 26.889544 | 34.270679 |
| S  | 40.407516 | 31.291225 | 34.027790 |
| S  | 43.728405 | 28.557613 | 31.354286 |
| S  | 44.201298 | 25.909351 | 38.532509 |

24 generated by VMD

|    | Ca   | S    | Ca   | S    |
|----|------|------|------|------|
| Ca | 25.086533 | 29.723972 | 32.551018 |
| Ca | 26.399733 | 31.245459 | 35.926582 |
| Ca | 29.998745 | 28.172821 | 35.767857 |
| Ca | 29.933468 | 32.785622 | 33.353359 |
| Ca | 33.570137 | 29.698425 | 31.093538 |
| Ca | 33.120609 | 30.387775 | 35.106689 |
| Ca | 36.601089 | 26.910946 | 34.582840 |
| Ca | 36.941635 | 31.190086 | 33.736732 |
|   | Ca    | S    | S    |
|---|-------|------|------|
|   | 40.366146 | 28.87 | 31.482040 |
|   | 39.807468 | 29.02 | 35.04303 |
|   | 46.859287 | 29.14 | 33.053497 |
|   | 43.038120 | 29.12 | 34.504303 |
| S | 27.122477 | 27.573303 | 36.646866 |
| S | 26.806641 | 34.06 | 32.37759 |
| S | 30.515690 | 29.85 | 32.63502 |
| S | 29.848421 | 31.33 | 36.462036 |
| S | 33.103355 | 27.36 | 34.01714 |
| S | 33.401707 | 32.68 | 32.421219 |
| S | 36.854496 | 28.89 | 31.692518 |
| S | 36.599655 | 29.73 | 36.562717 |
| S | 40.281307 | 26.83 | 34.120674 |
| S | 40.543480 | 31.19 | 33.848045 |
| S | 43.678169 | 28.56 | 31.309933 |
| S | 43.965492 | 25.99 | 38.496727 |

24 generated by VMD

|   | Ca    | S    | S    |
|---|-------|------|------|
|   | 25.160694 | 29.89 | 32.558617 |
|   | 26.512257 | 31.21 | 35.722622 |
|   | 30.208519 | 27.99 | 35.775482 |
|   | 30.040424 | 32.88 | 33.468731 |
|   | 33.375378 | 29.17 | 31.076792 |
|   | 33.178097 | 30.22 | 35.248260 |
|   | 36.882420 | 26.71 | 34.402290 |
|   | 36.548584 | 31.10 | 33.630634 |
|   | 40.319260 | 29.02 | 31.551491 |
|   | 39.913414 | 29.18 | 36.284843 |
|   | 46.659801 | 30.09 | 32.987041 |
|   | 43.010590 | 29.25 | 34.430543 |
| S | 27.256695 | 28.02 | 36.82152 |
| S | 27.133451 | 34.22 | 34.189651 |
| S | 30.437796 | 29.74 | 32.835304 |
| S | 30.104980 | 31.44 | 36.530849 |
| S | 33.412315 | 27.36 | 33.839561 |
| S | 33.495586 | 32.41 | 32.400021 |
| S | 36.751846 | 28.78 | 31.555422 |
| S | 36.389091 | 29.39 | 36.420151 |
| S | 40.308495 | 26.83 | 34.152222 |
| S | 40.217724 | 31.43 | 33.869774 |
| S | 43.630020 | 28.89 | 31.339050 |
| S | 43.486378 | 26.07 | 38.940090 |

24 generated by VMD

|   | Ca    | S    | S    |
|---|-------|------|------|
|   | 24.859550 | 29.72 | 32.279549 |
|   | 26.555752 | 31.12 | 35.897907 |
| Element | Ca 30.160007 | 27.931793 | 35.720718 |
|---------|--------------|-----------|-----------|
|         | Ca 30.228123 | 32.741692 | 33.288990 |
|         | Ca 33.408150 | 29.358242 | 31.197203 |
|         | Ca 33.163502 | 30.324574 | 35.321308 |
|         | Ca 36.816204 | 26.906265 | 34.382046 |
|         | Ca 36.825195 | 31.582870 | 33.781235 |
|         | Ca 40.231709 | 28.873158 | 31.520445 |
|         | Ca 39.829166 | 29.106018 | 36.435020 |
|         | Ca 46.773888 | 28.993439 | 33.205212 |
|         | Ca 42.831440 | 29.226324 | 34.203796 |
|         | S 27.094635  | 27.847260 | 36.864288 |
|         | S 26.921770  | 34.112965 | 34.196548 |
|         | S 30.511246  | 29.636076 | 32.767399 |
|         | S 30.207483  | 31.242130 | 36.320389 |
|         | S 33.445774  | 27.480164 | 34.156738 |
|         | S 33.611641  | 32.693424 | 32.431259 |
|         | S 36.799149  | 29.060844 | 31.742479 |
|         | S 36.470627  | 29.665817 | 36.608929 |
|         | S 40.133976  | 26.844391 | 34.001068 |
|         | S 40.297161  | 31.309967 | 33.752586 |
|         | S 43.792728  | 28.848896 | 31.189405 |
|         | S 43.465054  | 25.756502 | 38.766186 |
|         | 24 generated by VMD |
|         | Ca 24.651880 | 29.783352 | 32.369678 |
|         | Ca 26.396973 | 31.417431 | 36.136986 |
|         | Ca 30.152952 | 28.005728 | 35.547520 |
|         | Ca 29.771936 | 32.617996 | 33.415642 |
|         | Ca 33.462440 | 29.187916 | 31.202673 |
|         | Ca 33.110504 | 30.647539 | 35.165710 |
|         | Ca 36.850533 | 26.729465 | 34.255344 |
|         | Ca 36.704655 | 31.525345 | 33.579304 |
|         | Ca 40.489674 | 28.886269 | 31.705236 |
|         | Ca 39.900936 | 29.190571 | 36.644604 |
|         | Ca 46.892414 | 29.116423 | 32.934601 |
|         | Ca 43.151897 | 29.087696 | 34.571914 |
|         | S 27.134161  | 27.760210 | 36.778214 |
|         | S 26.607866  | 34.111031 | 34.263874 |
|         | S 30.375370  | 29.717962 | 32.461277 |
|         | S 30.004829  | 31.313032 | 36.512081 |
|         | S 33.251820  | 27.472952 | 34.143688 |
|         | S 33.562439  | 32.604156 | 32.284901 |
|         | S 36.702618  | 29.066540 | 31.630314 |
|         | S 36.555717  | 29.670815 | 36.289833 |
|         | S 40.145897  | 26.803936 | 34.384201 |
|         | S 40.702431  | 31.259596 | 34.141251 |
|     | 43.929443 | 28.667822 | 31.320063 |
|-----|-----------|-----------|-----------|
| S   | 43.924622 | 25.747587 | 38.286484 |

24

generated by VMD

|     | 24.821692 | 29.633778 | 32.683891 |
|-----|-----------|-----------|-----------|
| Ca  | 26.502525 | 31.282265 | 36.372177 |
| Ca  | 29.914425 | 28.140789 | 35.689289 |
| Ca  | 30.000145 | 32.792080 | 33.191139 |
| Ca  | 33.629375 | 29.503494 | 31.092236 |
| Ca  | 33.013828 | 30.318806 | 35.208775 |
| Ca  | 36.893059 | 26.928907 | 34.577240 |
| Ca  | 36.679012 | 31.340668 | 33.258526 |
| Ca  | 40.247692 | 28.894928 | 31.633171 |
| Ca  | 39.849617 | 29.051880 | 36.343567 |
| Ca  | 46.805820 | 29.157812 | 33.131424 |
| Ca  | 43.046253 | 29.030041 | 34.619526 |
| S   | 26.980318 | 27.762491 | 36.583225 |
| S   | 26.819351 | 34.092747 | 34.316624 |
| S   | 30.640804 | 29.719955 | 32.574711 |
| S   | 29.946190 | 31.371950 | 36.331654 |
| S   | 33.305290 | 27.425034 | 33.880356 |
| S   | 33.550568 | 32.721001 | 32.408348 |
| S   | 36.803062 | 28.649538 | 31.470207 |
| S   | 36.500340 | 29.717319 | 36.495152 |
| S   | 40.248669 | 26.866779 | 34.216602 |
| S   | 40.486656 | 31.289995 | 33.884689 |
| S   | 43.716000 | 29.173054 | 31.511505 |
| S   | 44.033306 | 25.526045 | 38.556599 |

24

generated by VMD

|     | 24.963947 | 29.673326 | 32.381355 |
|-----|-----------|-----------|-----------|
| Ca  | 26.477175 | 31.436590 | 35.619354 |
| Ca  | 30.055710 | 27.818274 | 35.740543 |
| Ca  | 30.311859 | 32.726601 | 33.265671 |
| Ca  | 33.674671 | 29.535713 | 31.329765 |
| Ca  | 33.103737 | 30.397278 | 35.322899 |
| Ca  | 36.476131 | 26.795370 | 34.613216 |
| Ca  | 36.789352 | 30.962379 | 33.950020 |
| Ca  | 40.181190 | 29.032688 | 31.631012 |
| Ca  | 39.801155 | 29.128555 | 36.559677 |
| Ca  | 46.657539 | 29.149233 | 32.624485 |
| Ca  | 42.981052 | 29.066238 | 34.400501 |
| S   | 27.104818 | 28.008480 | 36.658230 |
| S   | 26.769407 | 34.261040 | 33.948254 |
| S   | 30.465332 | 29.699905 | 32.647327 |
| S   | 30.019026 | 31.248718 | 36.350597 |
S     33.188328       27.385954       34.080936
S     33.805523       32.580593       32.620987
S     36.731567       28.620930       31.819016
S     36.462444       29.502811       36.766434
S     40.091045       26.850281       34.118031
S     40.331890       31.240263       34.031929
S     43.583954       28.895662       31.255695
S     44.407032       26.374521       38.294788

generated by VMD

Ca    25.187160       29.862961       32.182022
Ca    26.491350       31.433495       35.695179
Ca    30.188221       27.890806       35.783871
Ca    30.283653       32.808582       33.578545
Ca    33.703293       29.798517       31.057913
Ca    33.061756       30.401251       35.496784
Ca    36.867329       26.607779       34.680069
Ca    36.642166       30.785570       33.779774
Ca    40.048817       28.648239       31.767084
Ca    39.608112       29.138901       36.384747
Ca    46.585091       29.340508       32.840664
Ca    42.863922       29.233259       34.440914
S     27.217512       28.112152       36.681564
S     26.911125       33.999538       33.701180
S     30.614435       29.771717       32.718517
S     30.019835       31.296099       36.586026
S     33.425461       27.475321       33.862835
S     33.743137       32.712769       32.870155
S     36.625511       28.485844       31.601715
S     36.243744       29.295746       36.686596
S     40.199539       26.686468       34.449608
S     40.078823       31.254032       33.837124
S     43.400791       28.772327       31.274721
S     44.423126       26.579527       38.073338

generated by VMD

Ca    24.679371       29.990231       32.324753
Ca    26.313488       31.355343       35.602619
Ca    30.249588       28.065474       35.930626
Ca    30.247820       32.724701       33.112545
Ca    33.375927       29.166925       31.400368
Ca    33.029427       30.479395       35.516544
Ca    36.689110       26.571152       34.442497
Ca    36.706928       31.202755       34.066151
Ca    40.228432       28.862528       31.642788
Ca    39.782707       29.369713       36.246857
|   |       |       |       |
|---|-------|-------|-------|
| Ca| 46.882141| 29.121094| 33.131805 |
| Ca| 42.906731| 29.189018| 34.475250 |
| S | 26.976204| 27.902555| 32.863667 |
| S | 27.030529| 34.137287| 33.889755 |
| S | 30.418726| 29.564541| 32.863667 |
| S | 29.953741| 31.479458| 36.314835 |
| S | 33.278351| 27.270180| 34.280083 |
| S | 33.679947| 32.611359| 32.715256 |
| S | 36.656105| 28.899717| 31.675550 |
| S | 36.332314| 29.259140| 36.727417 |
| S | 40.204979| 26.786926| 34.239220 |
| S | 40.346134| 31.268877| 33.744408 |
| S | 43.760834| 29.073555| 31.191931 |
| S | 44.704411| 26.039488| 38.084259 |

24 generated by VMD

|   |       |       |       |
|---|-------|-------|-------|
| Ca| 24.936436| 29.451410| 32.239166 |
| Ca| 26.232498| 31.292223| 35.825325 |
| Ca| 30.224161| 28.040833| 36.094269 |
| Ca| 30.249872| 32.915314| 33.376167 |
| Ca| 33.288052| 29.474781| 31.253523 |
| Ca| 33.228801| 30.444563| 35.433998 |
| Ca| 36.630463| 26.980440| 34.362526 |
| Ca| 36.812710| 31.412289| 33.787506 |
| Ca| 40.279350| 28.734606| 31.451263 |
| Ca| 39.839241| 29.158945| 36.376522 |
| Ca| 46.845951| 29.152580| 33.477993 |
| Ca| 42.912117| 29.075640| 34.356884 |
| S | 27.013264| 27.850809| 36.359711 |
| S | 26.795938| 33.993027| 33.852353 |
| S | 30.459558| 29.731304| 32.990696 |
| S | 29.915676| 31.490147| 36.394939 |
| S | 33.271408| 27.478567| 34.190711 |
| S | 33.731808| 32.583801| 32.726696 |
| S | 36.733200| 28.961796| 31.542137 |
| S | 36.462357| 29.473560| 36.684895 |
| S | 40.010159| 26.726345| 34.253235 |
| S | 40.386894| 31.148426| 33.838089 |
| S | 43.731518| 29.036644| 31.257122 |
| S | 44.448555| 25.783352| 37.946484 |

24 generated by VMD

|   |       |       |       |
|---|-------|-------|-------|
| Ca| 24.899891| 29.805973| 32.010605 |
| Ca| 26.334122| 31.407345| 35.609261 |
| Ca| 30.096264| 27.970894| 35.797775 |
| Ca| 30.178692| 32.559906| 33.490292 |
| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 33.596561| 29.448618| 31.398373|
| Ca      | 32.913551| 30.549366| 35.470470|
| Ca      | 36.637650| 26.869839| 34.085003|
| Ca      | 40.235088| 28.762535| 31.877832|
| Ca      | 39.944798| 29.475554| 36.226585|
| Ca      | 46.922607| 28.868155| 33.049290|
| Ca      | 42.990807| 29.110048| 34.171738|
| S       | 26.965000| 27.806999| 36.411274|
| S       | 26.954561| 34.262939| 33.879501|
| S       | 30.364037| 29.440977| 32.680733|
| S       | 29.820858| 31.266165| 36.503204|
| S       | 33.283970| 27.489283| 34.315018|
| S       | 33.592445| 32.549095| 32.715481|
| S       | 36.917835| 29.025211| 31.981833|
| S       | 36.487144| 29.565060| 36.723259|
| S       | 40.118710| 26.709484| 34.269516|
| S       | 40.344822| 31.336761| 33.667480|
| S       | 43.878895| 28.899179| 31.206526|
| S       | 44.623356| 25.872353| 37.784245|

24 generated by VMD

| Element | X1       | Y1       | Z1       |
|---------|----------|----------|----------|
| Ca      | 24.917809| 29.552761| 32.388439|
| Ca      | 26.238796| 31.142548| 35.901550|
| Ca      | 30.023376| 28.019611| 35.758469|
| Ca      | 30.320190| 32.815716| 33.372086|
| Ca      | 33.617886| 29.510748| 31.271873|
| Ca      | 32.988995| 30.331703| 35.239803|
| Ca      | 36.678146| 27.121798| 34.430542|
| Ca      | 36.626190| 31.435673| 34.101524|
| Ca      | 40.258801| 28.736320| 31.226130|
| Ca      | 39.754627| 29.501556| 36.262165|
| Ca      | 46.982838| 28.850426| 33.203651|
| Ca      | 42.906013| 29.007954| 34.573128|
| S       | 26.989475| 27.856579| 36.663502|
| S       | 26.940479| 33.967079| 34.108639|
| S       | 30.370129| 29.585722| 32.654762|
| S       | 29.985596| 31.474972| 36.339775|
| S       | 33.222889| 27.326775| 34.052040|
| S       | 33.724941| 32.585541| 32.573978|
| S       | 36.910793| 29.252087| 31.824432|
| S       | 36.594707| 29.588917| 36.705399|
| S       | 39.913464| 26.833771| 34.056984|
| S       | 40.473911| 31.254559| 33.790447|
| S       | 43.828648| 28.711025| 31.376184|
| S       | 44.165245| 25.927532| 38.155197|
| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 25.077101 | 29.971050 | 31.766331 |
| Ca      | 26.374672 | 31.410900 | 35.787849 |
| Ca      | 29.990934 | 27.967838 | 35.868851 |
| Ca      | 30.333994 | 32.752178 | 33.399551 |
| Ca      | 33.536629 | 29.215698 | 31.439465 |
| Ca      | 32.979740 | 30.360113 | 35.494312 |
| Ca      | 36.588455 | 26.712757 | 34.678364 |
| Ca      | 36.624954 | 31.067368 | 34.273457 |
| Ca      | 40.112011 | 28.878845 | 31.750603 |
| Ca      | 39.898266 | 29.409369 | 36.361702 |
| Ca      | 46.886341 | 29.043438 | 33.140579 |
| Ca      | 42.947235 | 29.002420 | 34.072884 |
| S       | 26.876413 | 27.834946 | 36.449543 |
| S       | 26.762730 | 34.296085 | 34.047390 |
| S       | 30.507488 | 29.691122 | 32.738934 |
| S       | 29.952557 | 31.400766 | 36.349915 |
| S       | 33.176571 | 27.267382 | 34.398705 |
| S       | 33.699554 | 32.480915 | 32.607540 |
| S       | 36.752983 | 28.893929 | 31.773176 |
| S       | 36.647186 | 29.295359 | 36.761219 |
| S       | 40.099064 | 26.741879 | 34.081806 |
| S       | 40.179131 | 31.369030 | 33.610168 |
| S       | 43.862286 | 28.848505 | 31.181931 |
| S       | 44.567577 | 26.479506 | 37.996490 |

24

generated by VMD

| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 25.153778 | 29.742346 | 32.018181 |
| Ca      | 26.325815 | 31.224239 | 35.639923 |
| Ca      | 30.215748 | 28.011883 | 35.905426 |
| Ca      | 30.237856 | 32.698139 | 33.465839 |
| Ca      | 33.507259 | 29.264959 | 31.198959 |
| Ca      | 32.979588 | 30.560930 | 35.518734 |
| Ca      | 36.532959 | 26.896618 | 34.722321 |
| Ca      | 36.779385 | 31.228447 | 33.865467 |
| Ca      | 40.118996 | 28.848673 | 31.535145 |
| Ca      | 39.587078 | 28.917034 | 36.333111 |
| Ca      | 46.919712 | 29.188375 | 33.118237 |
| Ca      | 42.837349 | 29.153463 | 34.433159 |
| S       | 27.299610 | 27.822666 | 36.501801 |
| S       | 27.149250 | 34.228619 | 34.127441 |
| S       | 30.608221 | 29.755501 | 32.774651 |
| S       | 29.827299 | 31.465008 | 36.463623 |
| S       | 33.217102 | 27.257629 | 34.401859 |
| S       | 33.690887 | 32.522449 | 32.445045 |
|  |  |  |  |
|---|---|---|---|
| S | 36.727821 | 28.901564 | 31.821527 |
| S | 36.284492 | 29.640900 | 36.584698 |
| S | 39.879265 | 26.817707 | 34.057770 |
| S | 40.335426 | 31.262264 | 33.865032 |
| S | 43.684059 | 28.945257 | 31.410473 |
| S | 44.534954 | 26.036734 | 37.822296 |
| Ca | 25.103437 | 29.778309 | 32.379108 |
| Ca | 26.332298 | 31.113708 | 35.848972 |
| Ca | 29.974846 | 28.113411 | 35.981674 |
| Ca | 30.145117 | 32.708668 | 33.337185 |
| Ca | 33.569828 | 29.058258 | 31.156418 |
| Ca | 33.004955 | 30.700378 | 35.266369 |
| Ca | 36.492992 | 27.005455 | 34.986800 |
| Ca | 36.824276 | 31.210228 | 33.634224 |
| Ca | 40.489071 | 28.952423 | 31.473057 |
| Ca | 39.486015 | 29.012783 | 36.231419 |
| Ca | 46.778229 | 29.054985 | 33.477104 |
| Ca | 42.771168 | 29.073730 | 34.469704 |
| S | 26.872690 | 27.798971 | 36.721794 |
| S | 26.971983 | 34.168358 | 34.453735 |
| S | 30.665943 | 29.671806 | 32.721428 |
| S | 30.099421 | 31.358509 | 36.419811 |
| S | 33.219471 | 27.367905 | 34.313881 |
| S | 33.833416 | 32.360592 | 32.257511 |
| S | 36.929714 | 28.981823 | 31.497782 |
| S | 36.449551 | 29.718136 | 36.591721 |
| S | 39.993320 | 26.854294 | 33.891712 |
| S | 40.463402 | 31.248253 | 33.877113 |
| S | 43.950397 | 29.317238 | 31.449451 |
| S | 44.012352 | 25.763229 | 38.080837 |

24 generated by VMD

| Ca | 25.196337 | 29.670654 | 32.123020 |
| Ca | 26.519075 | 31.042290 | 35.554478 |
| Ca | 30.210043 | 28.164953 | 35.822849 |
| Ca | 30.014229 | 32.940990 | 33.260704 |
| Ca | 33.425629 | 29.167913 | 31.143007 |
| Ca | 33.190891 | 30.721645 | 35.267963 |
| Ca | 36.603619 | 26.633427 | 34.457577 |
| Ca | 36.677025 | 31.137390 | 33.852451 |
| Ca | 40.138508 | 28.727844 | 31.742413 |
| Ca | 39.714973 | 29.305534 | 36.524796 |
| Ca | 46.593590 | 29.364929 | 32.998440 |
| Ca | 42.841103 | 29.269913 | 34.457378 |
|   |      |      |      |
|---|------|------|------|
| S | 27.167160 | 27.949741 | 36.523365 |
| S | 27.017157 | 34.247265 | 34.787766 |
| S | 30.584196 | 29.734257 | 32.700306 |
| S | 29.991562 | 31.469921 | 36.244370 |
| S | 33.360939 | 27.538227 | 34.396568 |
| S | 33.570469 | 32.479301 | 32.312668 |
| S | 36.748451 | 28.773636 | 31.691324 |
| S | 36.402863 | 29.295284 | 36.618565 |
| S | 40.011536 | 26.712645 | 34.336739 |
| S | 40.303860 | 31.216412 | 33.749084 |
| S | 43.745872 | 28.915491 | 31.405449 |
| S | 44.404839 | 25.911804 | 38.059483 |

24 generated by VMD

| Ca |      |      |      |
|----|------|------|------|
| Ca | 25.261091 | 29.639210 | 32.062981 |
| Ca | 26.195663 | 31.006186 | 35.805775 |
| Ca | 30.029652 | 28.383606 | 35.928288 |
| Ca | 30.111431 | 32.980854 | 33.44633 |
| Ca | 33.485744 | 29.125931 | 31.345291 |
| Ca | 33.040272 | 30.580395 | 35.342834 |
| Ca | 36.568562 | 26.776417 | 34.343098 |
| Ca | 36.825924 | 31.097221 | 33.898933 |
| Ca | 40.414307 | 28.772953 | 31.451465 |
| Ca | 39.918537 | 29.159481 | 36.373421 |
| Ca | 46.782589 | 29.33515 | 33.311203 |
| Ca | 43.030579 | 29.167828 | 34.286957 |
| S | 26.905178 | 27.639326 | 36.301926 |
| S | 26.925896 | 34.200981 | 34.642136 |
| S | 30.601933 | 29.882975 | 32.823711 |
| S | 29.713970 | 31.586235 | 36.502213 |
| S | 33.202606 | 27.615767 | 34.375732 |
| S | 33.697727 | 32.374676 | 32.460037 |
| S | 36.817955 | 28.917267 | 31.579012 |
| S | 36.493629 | 29.414833 | 36.504883 |
| S | 40.133827 | 26.816074 | 34.114166 |
| S | 40.336128 | 31.186672 | 33.569981 |
| S | 43.833786 | 28.516922 | 31.277502 |
| S | 44.106937 | 26.216080 | 38.281822 |

24 generated by VMD

| Ca |      |      |      |
|----|------|------|------|
| Ca | 25.069361 | 29.789564 | 31.917625 |
| Ca | 26.152287 | 31.094250 | 35.608982 |
| Ca | 29.799231 | 28.042320 | 35.771027 |
| Ca | 30.209705 | 32.957706 | 33.418613 |
| Ca | 33.806427 | 29.367897 | 31.406900 |
| Ca | 32.987488 | 30.368340 | 35.305706 |
|   |   |   |   |
|---|---|---|---|
| Ca | 36.658154 | 26.662386 | 34.627571 |
| Ca | 36.422268 | 31.008686 | 34.191055 |
| Ca | 40.291660 | 28.819763 | 31.478062 |
| Ca | 39.806515 | 29.466789 | 36.232628 |
| Ca | 46.932426 | 28.950714 | 32.875637 |
| Ca | 43.205906 | 29.233271 | 34.111244 |
| S  | 26.726810 | 27.775921 | 36.592541 |
| S  | 27.224598 | 34.191120 | 34.482384 |
| S  | 30.590458 | 29.819426 | 32.771393 |
| S  | 29.824377 | 31.435204 | 36.399342 |
| S  | 33.225094 | 27.413979 | 34.344986 |
| S  | 33.685551 | 32.514660 | 32.586262 |
| S  | 36.828236 | 28.847982 | 31.912727 |
| S  | 36.478264 | 29.378910 | 36.763847 |
| S  | 40.186718 | 26.876879 | 34.098034 |
| S  | 40.437073 | 31.406033 | 33.441422 |
| S  | 43.870220 | 28.469658 | 31.196653 |
| S  | 44.015091 | 26.499964 | 38.496044 |

24

generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 25.525776 | 29.651239 | 31.872250 |
| Ca | 26.335768 | 31.286108 | 35.424564 |
| Ca | 30.167349 | 27.911919 | 35.846401 |
| Ca | 30.169029 | 32.747581 | 33.286922 |
| Ca | 33.583870 | 29.308968 | 31.446270 |
| Ca | 32.970837 | 30.332048 | 35.459885 |
| Ca | 36.661053 | 26.829456 | 34.607731 |
| Ca | 36.881485 | 31.113186 | 34.079514 |
| Ca | 39.984447 | 29.011345 | 31.728100 |
| Ca | 40.041702 | 29.548023 | 36.491211 |
| Ca | 46.516857 | 28.555586 | 32.680328 |
| Ca | 43.030689 | 29.235146 | 34.209705 |
| S  | 26.780924 | 28.052971 | 36.505367 |
| S  | 27.051163 | 34.262093 | 34.274475 |
| S  | 30.555195 | 29.617226 | 32.705357 |
| S  | 29.759722 | 31.218994 | 36.388454 |
| S  | 33.329021 | 27.212683 | 34.316822 |
| S  | 33.708332 | 32.499645 | 32.843304 |
| S  | 36.771244 | 28.941427 | 31.821917 |
| S  | 36.510796 | 29.444195 | 36.848106 |
| S  | 39.992722 | 26.915354 | 34.308178 |
| S  | 40.396549 | 31.506557 | 33.610809 |
| S  | 43.372040 | 28.679199 | 30.993410 |
| S  | 44.337379 | 26.510437 | 38.281635 |

24

generated by VMD
| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| Ca      | 25.232561 | 29.449034 | 31.934429 |
| Ca      | 26.347725 | 31.022049 | 35.548832 |
| Ca      | 29.930929 | 28.233330 | 35.770405 |
| Ca      | 30.179333 | 32.772926 | 33.162037 |
| Ca      | 33.517628 | 29.365788 | 31.738752 |
| Ca      | 33.068611 | 30.285217 | 35.542198 |
| Ca      | 36.686893 | 27.087107 | 34.913338 |
| Ca      | 36.738663 | 31.530809 | 33.845825 |
| Ca      | 40.373337 | 29.147030 | 31.483778 |
| Ca      | 39.934708 | 28.900650 | 36.465374 |
| Ca      | 46.755936 | 28.483995 | 32.730350 |
| Ca      | 42.884205 | 29.310062 | 34.262619 |
| S       | 26.585150 | 27.853798 | 36.298458 |
| S       | 27.231258 | 34.101086 | 34.142719 |
| S       | 30.389261 | 29.586525 | 32.759739 |
| S       | 29.897623 | 31.371738 | 36.310757 |
| S       | 33.376434 | 27.290642 | 34.636951 |
| S       | 33.557369 | 32.545490 | 32.773552 |
| S       | 36.810169 | 29.006073 | 31.779354 |
| S       | 36.750942 | 30.065344 | 36.814026 |
| S       | 40.130730 | 26.869198 | 33.951328 |
| S       | 40.281082 | 31.275389 | 34.050781 |
| S       | 43.650497 | 28.737556 | 31.144527 |
| S       | 44.122887 | 26.100491 | 37.970551 |

24 generated by VMD

| Element | X      | Y      | Z      |
|---------|--------|--------|--------|
| Ca      | 25.111429 | 29.497463 | 32.147621 |
| Ca      | 26.223303 | 31.285549 | 35.519974 |
| Ca      | 29.952562 | 28.246307 | 35.918407 |
| Ca      | 30.229057 | 32.670204 | 33.207684 |
| Ca      | 33.274971 | 29.069454 | 31.358637 |
| Ca      | 33.347683 | 30.269444 | 35.473896 |
| Ca      | 36.591408 | 27.109123 | 34.688858 |
| Ca      | 36.819313 | 31.407127 | 34.223461 |
| Ca      | 40.029655 | 29.146267 | 31.587881 |
| Ca      | 39.950043 | 29.161623 | 36.408295 |
| Ca      | 47.010117 | 28.790092 | 33.049507 |
| Ca      | 43.105740 | 28.932974 | 34.242233 |
| S       | 26.750128 | 27.765890 | 36.344727 |
| S       | 27.075336 | 34.193367 | 34.062923 |
| S       | 30.456060 | 29.503162 | 32.739250 |
| S       | 30.047243 | 31.403101 | 36.266186 |
| S       | 33.154148 | 27.304306 | 34.476231 |
| S       | 33.761341 | 32.358627 | 32.650753 |
| S       | 36.665150 | 29.270685 | 31.889658 |
| S       | 36.688431 | 29.671839 | 36.846424 |
|   | X       | Y       | Z       |
|---|---------|---------|---------|
| S | 30.425520 | 29.757559 | 32.804398 |
| S | 29.833689 | 31.634226 | 36.212238 |
| S | 33.150291 | 27.353889 | 34.305176 |
| S | 33.637245 | 32.496162 | 32.628803 |
| S | 36.799683 | 29.152344 | 31.779692 |
| S | 36.189606 | 29.304405 | 36.612011 |
| S | 40.096489 | 26.807995 | 34.117176 |
| S | 40.479427 | 31.294205 | 34.021797 |
| S | 43.632790 | 28.693256 | 31.282532 |
| S | 44.495296 | 25.892231 | 38.023972 |

generated by VMD

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| Ca | 25.313549 | 29.579296 | 31.935570 |
| Ca | 26.368584 | 31.318153 | 35.640697 |
| Ca | 29.929964 | 28.075542 | 35.645359 |
| Ca | 30.222342 | 32.692406 | 33.491238 |
| Ca | 33.499687 | 29.365929 | 31.302006 |
| Ca | 33.193245 | 30.313669 | 35.310078 |
| Ca | 36.538525 | 26.809856 | 34.274330 |
| Ca | 36.678627 | 31.213219 | 33.853382 |
| Ca | 40.287075 | 28.852156 | 31.425947 |
| Ca | 39.887981 | 29.350361 | 36.517681 |
| Ca | 46.793900 | 29.415062 | 32.934452 |
| Ca | 42.765045 | 29.085438 | 34.451859 |
| S | 26.921925 | 28.190945 | 36.847885 |
| S | 27.223721 | 34.333511 | 34.500973 |
| S | 30.384161 | 29.565847 | 32.729477 |
| S | 29.852802 | 31.283218 | 36.529915 |
| S | 33.228653 | 27.361834 | 34.238632 |
| S | 33.732323 | 32.408302 | 32.421516 |
| S | 36.784649 | 28.952133 | 31.648573 |
| S | 36.453465 | 29.236361 | 36.569901 |
| S | 40.057541 | 26.719975 | 34.115875 |
| S | 40.383919 | 31.285305 | 33.836010 |
| S | 43.571411 | 28.590446 | 31.337158 |
| S | 44.360771 | 26.392433 | 38.472202 |

generated by VMD

|   | X       | Y       | Z       |
|---|---------|---------|---------|
| Ca | 25.024067 | 29.562910 | 32.049828 |
| Ca | 26.235535 | 31.330982 | 35.404312 |
| Ca | 29.917366 | 28.321035 | 35.833786 |
| Ca | 30.041492 | 32.661728 | 33.396343 |
| Ca | 33.519958 | 28.947174 | 31.490242 |
| Ca | 33.127110 | 30.370335 | 35.561954 |
| Ca | 36.487465 | 26.785496 | 34.156178 |
| Ca | 36.683460 | 31.378811 | 33.911213 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 40.360733 | 29.070879 | 31.441174 |
| Ca      | 39.818905 | 29.138027 | 36.260170 |
| Ca      | 47.105515 | 28.811016 | 33.128891 |
| Ca      | 42.926453 | 29.424639 | 34.316040 |
| S       | 26.930920 | 28.198046 | 36.757748 |
| S       | 27.001225 | 34.236832 | 34.326488 |
| S       | 30.448687 | 29.549547 | 32.725422 |
| S       | 32.02473 | 27.369896 | 34.589397 |
| S       | 33.703014 | 32.266132 | 32.550385 |
| S       | 37.031445 | 29.063461 | 31.71442 |
| S       | 36.461521 | 29.274712 | 36.618423 |
| S       | 40.151722 | 26.773792 | 33.954269 |
| S       | 40.395107 | 31.420742 | 34.060589 |
| S       | 43.782127 | 28.855747 | 31.261034 |
| S       | 44.216064 | 26.103874 | 38.157936 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.298649 | 29.383606 | 32.192421 |
| Ca      | 26.590773 | 31.222198 | 35.637432 |
| Ca      | 29.968483 | 28.366684 | 36.008980 |
| Ca      | 30.146023 | 32.864697 | 33.239536 |
| Ca      | 33.700497 | 29.260344 | 31.42955 |
| Ca      | 33.016300 | 30.470907 | 35.590672 |
| Ca      | 36.449738 | 26.36105 | 34.203907 |
| Ca      | 36.633286 | 31.11553 | 33.838226 |
| Ca      | 40.248608 | 29.029472 | 31.348490 |
| Ca      | 39.714264 | 29.074551 | 36.331619 |
| Ca      | 46.839100 | 29.306454 | 33.497238 |
| Ca      | 42.683060 | 29.099199 | 34.381210 |
| S       | 26.805822 | 27.986240 | 36.514175 |
| S       | 27.135181 | 34.163776 | 34.303528 |
| S       | 30.708210 | 29.663183 | 32.876442 |
| S       | 29.993288 | 31.501720 | 36.509048 |
| S       | 33.206966 | 27.325115 | 34.372810 |
| S       | 33.815037 | 32.535671 | 32.633175 |
| S       | 36.867535 | 28.978420 | 31.370691 |
| S       | 36.339432 | 29.186874 | 36.624512 |
| S       | 39.955177 | 26.808830 | 33.935410 |
| S       | 40.278069 | 31.194698 | 33.778477 |
| S       | 43.699184 | 28.782860 | 31.330307 |
| S       | 44.341194 | 26.238214 | 38.089386 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.529608 | 29.39054 | 32.074139 |
| Ca      | 26.173361 | 31.224268 | 35.602055 |
|   | Ca     |       |       |
|---|--------|-------|-------|
|   | 29.899431 | 28.009842 | 36.114101 |
|   | 30.290924 | 32.785835 | 35.721066 |
|   | 33.714741 | 29.068516 | 31.432505 |
|   | 32.821297 | 30.767838 | 35.417839 |
|   | 36.599789 | 31.445770 | 33.774136 |
|   | 40.466751 | 29.134342 | 31.334019 |
|   | 39.736862 | 29.299263 | 36.562210 |
|   | 46.786907 | 29.163553 | 33.175919 |
|   | 42.932137 | 29.121826 | 34.393223 |
|   | 26.644552 | 27.992722 | 36.719566 |
| S | 27.244209 | 34.115547 | 34.228035 |
|   | 30.601728 | 29.553429 | 32.953922 |
|   | 29.764206 | 31.469475 | 36.461720 |
|   | 33.180046 | 27.356901 | 34.505440 |
|   | 33.790127 | 32.266758 | 32.372738 |
|   | 36.893753 | 29.127890 | 31.535904 |
|   | 36.439102 | 29.459160 | 36.726246 |
|   | 39.880585 | 26.979908 | 33.822926 |
|   | 40.380383 | 31.268669 | 33.993786 |
| S | 44.011623 | 28.815002 | 31.357090 |
|   | 44.411713 | 25.624744 | 37.840279 |

24 generated by VMD

|   | Ca     |       |       |
|---|--------|-------|-------|
|   | 25.458263 | 29.468071 | 32.252594 |
|   | 26.277340 | 31.295071 | 35.624428 |
|   | 30.268045 | 28.062996 | 35.920944 |
|   | 30.219645 | 32.890453 | 32.975521 |
|   | 33.710423 | 29.301567 | 31.652012 |
|   | 33.027760 | 30.597672 | 35.620636 |
|   | 36.392006 | 26.925949 | 34.195801 |
|   | 36.620571 | 31.324238 | 34.064575 |
|   | 40.252632 | 29.189037 | 31.695847 |
|   | 39.438580 | 28.937065 | 36.350155 |
|   | 46.830963 | 29.125912 | 33.058575 |
|   | 42.916107 | 28.945137 | 34.356117 |
| S | 27.039637 | 28.007120 | 36.741188 |
|   | 27.049397 | 34.192772 | 34.120895 |
|   | 30.674377 | 29.471279 | 32.870201 |
|   | 29.787443 | 31.421021 | 36.119591 |
|   | 33.317001 | 27.300476 | 34.527058 |
|   | 33.626869 | 32.493183 | 32.382339 |
|   | 36.857426 | 29.243275 | 31.593767 |
|   | 36.273701 | 29.397411 | 36.702797 |
|   | 39.943439 | 26.698988 | 33.838936 |
|   | 40.243938 | 31.197817 | 34.151539 |
|  | X          | Y          | Z          |
|---|------------|------------|------------|
| S | 43.581226  | 28.904659  | 31.293760  |
| S | 44.627151  | 26.000256  | 37.921505  |

generated by VMD

| Ca | 25.349197  | 29.228518  | 31.924969  |
| Ca | 26.205294  | 31.271877  | 35.537861  |
| Ca | 29.979458  | 28.267353  | 36.203316  |
| Ca | 30.202320  | 32.856056  | 33.326115  |
| Ca | 33.651764  | 29.205311  | 31.549072  |
| Ca | 32.998985  | 30.330860  | 35.559040  |
| Ca | 36.457047  | 26.780182  | 34.524235  |
| Ca | 36.73996   | 31.450418  | 34.110298  |
| Ca | 40.254681  | 29.032019  | 31.444288  |
| Ca | 39.587521  | 28.919922  | 36.130898  |
| Ca | 46.939323  | 29.240433  | 33.341187  |
| Ca | 43.041019  | 29.287846  | 34.224319  |
| S  | 26.782003  | 28.167393  | 36.577827  |
| S  | 26.862810  | 34.268101  | 34.068790  |
| S  | 30.652870  | 29.624355  | 32.822556  |
| S  | 29.819500  | 31.630600  | 36.345268  |
| S  | 33.035374  | 27.157455  | 34.552383  |
| S  | 33.797043  | 32.327194  | 32.650055  |
| S  | 36.914780  | 29.019444  | 31.716761  |
| S  | 36.544529  | 29.557835  | 36.795509  |
| S  | 40.019806  | 26.808670  | 33.627796  |
| S  | 40.487038  | 31.136936  | 34.078220  |
| S  | 43.915276  | 29.028034  | 31.151346  |
| S  | 44.262241  | 25.794575  | 37.768623  |

24

generated by VMD

| Ca | 25.329662  | 29.183329  | 32.008945  |
| Ca | 26.350363  | 31.155937  | 35.400257  |
| Ca | 30.144075  | 28.322613  | 36.129745  |
| Ca | 30.288033  | 33.031586  | 33.155186  |
| Ca | 33.449768  | 29.089417  | 31.391615  |
| Ca | 33.079941  | 30.426708  | 35.516964  |
| Ca | 36.543491  | 26.915318  | 34.590160  |
| Ca | 36.633011  | 31.308918  | 34.230732  |
| Ca | 40.280609  | 29.112846  | 31.504839  |
| Ca | 39.378193  | 28.788759  | 35.986073  |
| Ca | 46.528652  | 29.465694  | 33.332794  |
| Ca | 42.868015  | 29.069542  | 34.527649  |
| S  | 26.989441  | 27.900677  | 36.775944  |
| S  | 27.077673  | 34.215591  | 33.939194  |
| S  | 30.566334  | 29.759773  | 32.953812  |
| S  | 29.795664  | 31.636906  | 36.232761  |
|   | X    | Y    | Z    |
|---|------|------|------|
| S | 33.180016 | 27.455215 | 34.528538 |
| S | 33.816483 | 32.451664 | 32.636040 |
| S | 36.871819 | 29.072979 | 31.930759 |
| S | 36.350845 | 29.528122 | 36.644196 |
| S | 40.136650 | 26.543064 | 33.643082 |
| S | 40.349846 | 31.215797 | 34.075985 |
| S | 43.662094 | 29.127214 | 31.214590 |
| S | 44.763176 | 25.613724 | 37.680820 |

24 generated by VMD

| Ca  | X    | Y    | Z    |
|-----|------|------|------|
| Ca  | 25.432482 | 29.526535 | 32.183891 |
| Ca  | 26.292620 | 31.118813 | 35.725578 |
| Ca  | 30.110762 | 28.498899 | 35.868584 |
| Ca  | 30.163877 | 32.847736 | 32.897423 |
| Ca  | 33.540104 | 29.036385 | 31.509499 |
| Ca  | 33.166355 | 30.599617 | 35.581223 |
| Ca  | 36.428551 | 26.796551 | 34.413307 |
| Ca  | 36.719372 | 31.353092 | 34.052696 |
| Ca  | 40.298309 | 29.154329 | 31.777143 |
| Ca  | 39.446754 | 29.019104 | 36.406654 |
| Ca  | 46.699203 | 29.236679 | 32.910965 |
| Ca  | 43.033562 | 29.064611 | 34.226738 |
| S   | 26.606087 | 27.769442 | 36.450153 |
| S   | 27.059467 | 34.026997 | 33.947060 |
| S   | 30.551565 | 29.588259 | 32.807388 |
| S   | 29.872473 | 31.676952 | 36.311050 |
| S   | 33.242401 | 27.547607 | 34.602657 |
| S   | 33.686565 | 32.358803 | 32.547729 |
| S   | 36.837818 | 29.068420 | 31.811262 |
| S   | 36.253593 | 29.338203 | 36.823425 |
| S   | 40.156975 | 26.875397 | 34.167797 |
| S   | 40.415638 | 31.165134 | 34.227261 |
| S   | 43.600639 | 28.961449 | 31.180695 |
| S   | 44.818722 | 25.762356 | 37.600548 |

24 generated by VMD

| Ca  | X    | Y    | Z    |
|-----|------|------|------|
| Ca  | 25.170845 | 29.512724 | 32.111809 |
| Ca  | 26.104307 | 31.364895 | 35.653179 |
| Ca  | 29.946316 | 28.172493 | 35.735287 |
| Ca  | 30.145859 | 32.874348 | 33.094833 |
| Ca  | 33.503853 | 29.357765 | 31.545906 |
| Ca  | 33.111927 | 30.430191 | 35.485107 |
| Ca  | 36.747456 | 26.600176 | 34.473484 |
| Ca  | 36.689911 | 31.176805 | 34.024704 |
| Ca  | 40.387039 | 28.747242 | 31.375675 |
| Ca  | 39.845970 | 29.048206 | 36.499039 |
|   |        |        |        |
|---|--------|--------|--------|
| Ca | 46.654030 | 29.579811 | 33.257877 |
| Ca | 42.846478 | 29.097267 | 34.249863 |
| S  | 26.582167 | 27.951317 | 36.477531 |
| S  | 27.139900 | 34.293549 | 34.174419 |
| S  | 30.524256 | 29.696985 | 32.721535 |
| S  | 29.786930 | 31.462337 | 36.391846 |
| S  | 33.236012 | 27.364323 | 34.500069 |
| S  | 33.572670 | 32.679352 | 32.735233 |
| S  | 36.786335 | 28.831141 | 31.887850 |
| S  | 36.508301 | 29.241858 | 36.692989 |
| S  | 40.179108 | 26.765411 | 34.011623 |
| S  | 40.357376 | 31.177254 | 33.799442 |
| S  | 43.799370 | 28.817907 | 31.301361 |
| S  | 44.807495 | 26.148060 | 37.830017 |

24

 generated by VMD

|   |        |        |        |
|---|--------|--------|--------|
| Ca | 24.941950 | 29.588814 | 32.142960 |
| Ca | 26.187546 | 31.222252 | 35.547710 |
| Ca | 30.020844 | 28.366213 | 36.255867 |
| Ca | 30.283726 | 32.703064 | 33.000118 |
| Ca | 33.636707 | 29.298462 | 31.400852 |
| Ca | 32.920620 | 30.659031 | 35.467670 |
| Ca | 36.510815 | 26.727486 | 34.472740 |
| Ca | 36.781635 | 31.078667 | 34.317429 |
| Ca | 40.397324 | 29.079903 | 31.460781 |
| Ca | 39.755245 | 28.960348 | 36.232919 |
| Ca | 46.629738 | 29.583767 | 33.287018 |
| Ca | 42.863541 | 29.321812 | 34.428932 |
| S  | 26.875462 | 27.825493 | 36.617020 |
| S  | 27.065693 | 34.096592 | 33.819595 |
| S  | 30.545773 | 29.503332 | 32.903870 |
| S  | 29.895191 | 31.670746 | 36.285179 |
| S  | 33.246582 | 27.437019 | 34.592075 |
| S  | 33.861389 | 32.413307 | 32.533279 |
| S  | 36.837864 | 29.009031 | 31.770332 |
| S  | 36.474129 | 29.296196 | 36.690849 |
| S  | 40.058975 | 26.731659 | 33.820480 |
| S  | 40.345695 | 31.296608 | 33.957787 |
| S  | 43.607800 | 29.005695 | 31.322674 |
| S  | 44.689751 | 25.515884 | 37.703152 |

24

 generated by VMD

|   |        |        |        |
|---|--------|--------|--------|
| Ca | 25.206360 | 29.904446 | 32.149532 |
| Ca | 26.055813 | 31.271074 | 35.761780 |
| Ca | 29.942984 | 28.133579 | 36.097427 |
| Ca | 30.205664 | 32.667526 | 33.047680 |
|     |       |       |       |       |
|-----|-------|-------|-------|-------|
|     | 33.746803 | 29.107389 | 31.427095 |       |
| Ca  | 32.992851  | 30.472771  | 35.451393  |       |
| Ca  | 36.544945  | 26.857407  | 34.515663  |       |
| Ca  | 36.825577  | 31.373789  | 34.032700  |       |
| Ca  | 40.410175  | 28.929779  | 31.415398  |       |
| Ca  | 39.603218  | 29.225628  | 36.179558  |       |
| Ca  | 46.646080  | 29.633339  | 33.398167  |       |
| Ca  | 42.939571  | 29.045769  | 34.334976  |       |
| S   | 26.802258  | 27.939367  | 36.403587  |       |
| S   | 27.011433  | 34.024635  | 34.034142  |       |
| S   | 30.635942  | 29.631815  | 32.863499  |       |
| S   | 29.702677  | 31.621666  | 36.443680  |       |
| S   | 33.151112  | 27.335142  | 34.622169  |       |
| S   | 33.716339  | 32.387989  | 32.579525  |       |
| S   | 36.936749  | 28.909449  | 31.909779  |       |
| S   | 36.378418  | 29.302519  | 36.698227  |       |
| S   | 40.082588  | 26.746069  | 33.938526  |       |
| S   | 40.376396  | 31.240721  | 33.773952  |       |
| S   | 43.824398  | 28.924519  | 31.331778  |       |
| S   | 44.695583  | 25.705082  | 37.620457  |       |

24

generated by VMD

|     |       |       |       |       |
|-----|-------|-------|-------|-------|
|     | 25.369837 | 29.756115 | 32.022884 |       |
| Ca  | 26.334114  | 31.109600  | 35.731415  |       |
| Ca  | 30.055340  | 28.447617  | 35.997204  |       |
| Ca  | 30.308617  | 32.765755  | 32.994736  |       |
| Ca  | 33.442135  | 28.943935  | 31.353243  |       |
| Ca  | 33.079926  | 30.462460  | 35.503254  |       |
| Ca  | 36.645832  | 26.852879  | 34.458630  |       |
| Ca  | 36.711979  | 31.286079  | 34.006466  |       |
| Ca  | 40.325565  | 29.089670  | 31.422855  |       |
| Ca  | 39.378246  | 28.907665  | 36.245392  |       |
| Ca  | 46.474274  | 29.404831  | 33.473732  |       |
| Ca  | 42.806763  | 29.157661  | 34.446247  |       |
| S   | 26.975742  | 27.899277  | 36.824158  |       |
| S   | 27.174902  | 34.045490  | 34.132881  |       |
| S   | 30.498386  | 29.678202  | 32.736095  |       |
| S   | 29.843168  | 31.596996  | 36.332352  |       |
| S   | 33.248161  | 27.452427  | 34.472282  |       |
| S   | 33.716354  | 32.382122  | 32.654011  |       |
| S   | 36.795418  | 29.046219  | 31.703491  |       |
| S   | 36.421070  | 29.331924  | 36.647804  |       |
| S   | 40.061100  | 26.699051  | 33.824764  |       |
| S   | 40.225952  | 31.216610  | 33.969055  |       |
| S   | 43.848335  | 28.967335  | 31.301218  |       |
| S   | 44.692680  | 25.891510  | 37.776512  |       |
|  |  |  |  |
|---|---|---|---|
| Ca | 25.111759 | 29.846848 | 31.787258 |
| Ca | 25.905165 | 31.257113 | 35.644833 |
| Ca | 29.835976 | 28.277843 | 36.029438 |
| Ca | 30.310957 | 32.856697 | 33.085438 |
| Ca | 33.698158 | 29.135635 | 31.470444 |
| Ca | 32.969482 | 30.548094 | 35.463398 |
| Ca | 36.577393 | 26.700787 | 34.601730 |
| Ca | 36.498108 | 31.017542 | 34.206184 |
| Ca | 40.384686 | 28.912842 | 31.489954 |
| Ca | 39.685215 | 29.003609 | 36.242146 |
| Ca | 46.803413 | 29.652203 | 33.287064 |
| Ca | 43.061909 | 29.139740 | 34.232811 |
| S  | 26.733379 | 27.969799 | 36.630138 |
| S  | 27.144451 | 34.066830 | 34.061485 |
| S  | 30.496588 | 29.643280 | 32.866413 |
| S  | 29.588947 | 31.631153 | 36.361309 |
| S  | 33.161469 | 27.506891 | 34.697147 |
| S  | 33.847610 | 32.459900 | 32.526695 |
| S  | 36.807663 | 28.741108 | 31.946684 |
| S  | 36.459530 | 29.068439 | 36.873642 |
| S  | 40.295834 | 26.670307 | 33.908600 |
| S  | 40.354809 | 31.297062 | 33.883499 |
| S  | 43.870419 | 28.909027 | 31.097548 |
| S  | 44.831039 | 26.078625 | 37.639364 |

24

|  |  |  |  |
|---|---|---|---|
| Ca | 25.019770 | 29.810316 | 32.051559 |
| Ca | 26.273563 | 31.497377 | 35.541222 |
| Ca | 29.905964 | 28.179571 | 35.963497 |
| Ca | 30.375013 | 32.788513 | 33.210197 |
| Ca | 33.416077 | 28.984238 | 31.463902 |
| Ca | 33.034752 | 30.372589 | 35.386166 |
| Ca | 36.551750 | 26.425432 | 34.637676 |
| Ca | 36.664314 | 30.881969 | 34.075844 |
| Ca | 40.369102 | 29.208073 | 31.585115 |
| Ca | 39.640957 | 29.084988 | 36.393051 |
| Ca | 46.604996 | 30.141884 | 33.311054 |
| Ca | 42.875927 | 29.194145 | 34.392094 |
| S  | 26.727154 | 28.244179 | 36.756706 |
| S  | 27.220104 | 34.229588 | 33.779724 |
| S  | 30.496777 | 29.643280 | 32.889992 |
| S  | 29.857220 | 31.530027 | 36.407162 |
| S  | 33.202003 | 27.211391 | 34.575760 |
| S  | 33.930527 | 32.277107 | 32.498426 |
|  |  |  |  |
|---|---|---|---|
| S | 36.766140 | 28.676012 | 31.774097 |
| S | 36.413422 | 29.066225 | 36.657196 |
| S | 40.306801 | 26.856144 | 33.897064 |
| S | 40.247463 | 31.273937 | 33.909988 |
| S | 43.794209 | 29.129467 | 31.356110 |
| S | 44.739914 | 25.682285 | 37.526104 |

24 generated by VMD

| Ca | 24.952791 | 29.811342 | 32.311115 |
| Ca | 26.391022 | 31.221123 | 35.638565 |
| Ca | 30.021646 | 28.572712 | 35.811428 |
| Ca | 30.452503 | 32.588144 | 32.671337 |
| Ca | 33.528206 | 29.055534 | 31.388510 |
| Ca | 33.172806 | 30.491416 | 35.425766 |
| Ca | 36.383400 | 26.311445 | 34.579212 |
| Ca | 36.772617 | 31.011116 | 34.348808 |
| Ca | 40.158466 | 29.001312 | 31.741371 |
| Ca | 39.752632 | 29.010048 | 36.475643 |
| Ca | 46.493656 | 29.705467 | 33.285709 |
| Ca | 42.795155 | 29.247446 | 34.468887 |
| S | 26.757446 | 27.917662 | 36.829422 |
| S | 27.365036 | 33.986179 | 33.948097 |
| S | 30.495029 | 29.445269 | 32.531784 |
| S | 29.926357 | 31.669125 | 36.016956 |
| S | 33.210587 | 27.419230 | 34.503437 |
| S | 34.030716 | 32.413246 | 32.632294 |
| S | 36.785198 | 28.930141 | 31.940044 |
| S | 36.331547 | 29.037373 | 36.891312 |
| S | 39.915649 | 26.648567 | 34.066620 |
| S | 40.294930 | 31.337337 | 34.062084 |
| S | 43.591099 | 29.391323 | 31.255840 |
| S | 44.855484 | 25.845749 | 37.206478 |

24 generated by VMD

| Ca | 25.179813 | 29.777203 | 31.969597 |
| Ca | 25.866732 | 31.100941 | 35.507645 |
| Ca | 30.056623 | 28.337660 | 35.965511 |
| Ca | 30.361629 | 32.770546 | 32.857254 |
| Ca | 33.557076 | 29.093672 | 31.459433 |
| Ca | 32.955276 | 30.497734 | 35.406483 |
| Ca | 36.500240 | 26.913912 | 34.981369 |
| Ca | 36.758461 | 31.043083 | 34.439835 |
| Ca | 40.392715 | 29.022827 | 31.520782 |
| Ca | 39.619656 | 29.186108 | 36.517151 |
| Ca | 46.937092 | 29.349739 | 33.040997 |
| Ca | 43.149750 | 29.149139 | 34.257801 |
|  | 26.570246 | 27.921890 | 36.567692 |
|---|---|---|---|
| S | 27.087111 | 33.966072 | 33.793266 |
| S | 30.467920 | 29.664345 | 32.777790 |
| S | 29.426878 | 31.651089 | 36.268303 |
| S | 33.121571 | 27.483381 | 34.720955 |
| S | 33.744678 | 32.410759 | 32.591583 |
| S | 36.745201 | 28.952715 | 32.042370 |
| S | 36.499123 | 29.351120 | 37.085342 |
| S | 40.173691 | 26.948835 | 34.198109 |
| S | 40.486439 | 31.158138 | 34.049686 |
| S | 43.723022 | 29.054798 | 30.980059 |
| S | 45.052917 | 25.585777 | 37.031693 |

24

generated by VMD

| Ca | 25.026928 | 29.513758 | 31.912109 |
| Ca | 26.112276 | 31.059763 | 35.577675 |
| Ca | 29.874483 | 28.511497 | 35.959739 |
| Ca | 30.140678 | 33.029236 | 32.876614 |
| Ca | 33.514771 | 29.194992 | 31.612814 |
| Ca | 33.123882 | 30.855553 | 35.431587 |
| Ca | 36.544353 | 26.466215 | 34.744465 |
| Ca | 36.786419 | 31.084927 | 34.414703 |
| Ca | 40.292480 | 28.846752 | 31.480904 |
| Ca | 39.623539 | 28.765636 | 36.293274 |
| Ca | 46.671730 | 29.488361 | 33.243874 |
| Ca | 42.842049 | 29.287323 | 34.599445 |
| S | 26.827168 | 27.757988 | 36.448498 |
| S | 26.948986 | 34.237057 | 33.960564 |
| S | 30.559397 | 29.854296 | 32.885635 |
| S | 29.639711 | 31.681650 | 36.233696 |
| S | 33.140648 | 27.527817 | 34.711895 |
| S | 33.802719 | 32.525482 | 32.612148 |
| S | 36.799515 | 28.748692 | 32.029938 |
| S | 36.373764 | 29.085293 | 36.806187 |
| S | 40.280724 | 26.605797 | 34.019058 |
| S | 40.364368 | 31.127319 | 33.863487 |
| S | 43.801289 | 29.147682 | 31.160873 |
| S | 45.341942 | 25.988346 | 37.153316 |

24

generated by VMD

| Ca | 25.001266 | 29.585293 | 32.138409 |
| Ca | 26.152626 | 31.292114 | 35.731026 |
| Ca | 30.151892 | 28.494783 | 36.055862 |
| Ca | 30.235401 | 32.860428 | 32.727566 |
| Ca | 33.498878 | 29.218163 | 31.446484 |
| Ca | 33.132042 | 30.609348 | 35.590965 |
|   |   |   |   |
|---|---|---|---|
| Ca | 36.547775 | 26.587040 | 34.709034 |
| Ca | 36.895363 | 31.256992 | 34.384514 |
| Ca | 40.211201 | 29.050270 | 31.504791 |
| Ca | 39.515633 | 28.851652 | 36.283340 |
| Ca | 46.568748 | 29.659534 | 33.220982 |
| Ca | 42.934902 | 29.155487 | 34.533028 |
| S  | 27.011154 | 27.808159 | 36.529560 |
| S  | 26.828571 | 33.931957 | 33.568752 |
| S  | 30.466806 | 29.858875 | 32.844639 |
| S  | 29.749165 | 31.652328 | 36.247356 |
| S  | 33.288467 | 27.550718 | 34.375252 |
| S  | 33.635040 | 32.462708 | 32.595051 |
| S  | 36.745296 | 28.739910 | 31.913671 |
| S  | 36.490517 | 29.237404 | 36.954815 |
| S  | 40.083912 | 26.740002 | 34.042938 |
| S  | 40.347954 | 31.136894 | 34.091255 |
| S  | 43.607559 | 29.142132 | 31.360119 |
| S  | 45.337771 | 25.509233 | 37.181282 |

24

generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 24.972567 | 29.850714 | 31.792088 |
| Ca | 26.295361 | 31.220898 | 35.541428 |
| Ca | 30.193247 | 28.483179 | 36.188076 |
| Ca | 30.208153 | 32.823872 | 33.108257 |
| Ca | 33.433739 | 29.052069 | 31.610271 |
| Ca | 33.288532 | 30.758846 | 35.563274 |
| Ca | 36.462070 | 26.705994 | 34.670670 |
| Ca | 36.807549 | 31.324123 | 34.354912 |
| Ca | 40.258507 | 28.814535 | 31.476114 |
| Ca | 39.730980 | 28.948936 | 36.284653 |
| Ca | 46.559937 | 29.725189 | 33.188957 |
| Ca | 42.822361 | 29.055920 | 34.249046 |
| S  | 26.792168 | 27.650639 | 36.05592 |
| S  | 26.838779 | 33.989433 | 33.960239 |
| S  | 30.651609 | 29.579807 | 33.006001 |
| S  | 29.808317 | 31.650766 | 36.382854 |
| S  | 33.225258 | 27.544956 | 34.733555 |
| S  | 33.705044 | 32.307407 | 32.505512 |
| S  | 36.838305 | 28.961504 | 32.066833 |
| S  | 36.52169 | 29.345644 | 36.765476 |
| S  | 40.003952 | 26.635637 | 33.907097 |
| S  | 40.412811 | 31.130856 | 33.924358 |
| S  | 43.705795 | 28.810558 | 31.626980 |
| S  | 44.891159 | 26.019884 | 37.568489 |

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generated by VMD
| Element | Value 1 | Value 2 | Value 3 |
|---------|---------|---------|---------|
| Ca      | 25.097057 | 30.262177 | 31.807724 |
| Ca      | 26.037920 | 31.163918 | 35.695232 |
| Ca      | 30.061905 | 28.262381 | 36.063210 |
| Ca      | 30.319262 | 32.769310 | 33.112030 |
| Ca      | 33.326630 | 28.872473 | 31.597216 |
| Ca      | 33.061066 | 30.497368 | 35.455673 |
| Ca      | 36.640938 | 26.912575 | 34.0010 |
| Ca      | 36.832874 | 31.264359 | 34.349621 |
| Ca      | 40.297554 | 28.673828 | 31.403008 |
| Ca      | 39.645592 | 29.306259 | 36.321053 |
| Ca      | 46.489658 | 29.521568 | 33.156403 |
| Ca      | 42.905266 | 29.247446 | 34.434753 |
| S       | 26.767046 | 27.759445 | 36.198559 |
| S       | 27.000816 | 33.983227 | 33.957367 |
| S       | 30.463158 | 29.707928 | 32.850189 |
| S       | 29.635056 | 31.517654 | 36.433128 |
| S       | 33.348343 | 27.351131 | 34.737518 |
| S       | 33.727783 | 32.213127 | 32.380455 |
| S       | 36.827381 | 29.040081 | 31.934734 |
| S       | 36.487274 | 29.478298 | 36.888779 |
| S       | 40.326843 | 26.754824 | 34.086353 |
| S       | 40.370983 | 31.108902 | 33.774033 |
| S       | 43.705170 | 28.890949 | 31.148382 |
| S       | 45.058273 | 25.832212 | 37.483227 |

Generated by VMD
|   |          |          |          |
|---|----------|----------|----------|
| S | 40.028111 | 26.602039 | 34.136326 |
| S | 40.484238 | 31.101505 | 33.897396 |
| S | 43.928139 | 28.750710 | 31.148811 |
| S | 44.899467 | 25.999348 | 37.478584 |
|   | generated by VMD |
| Ca| 25.317917 | 29.904720 | 31.668079 |
| Ca| 26.173702 | 31.057476 | 35.388683 |
| Ca| 29.908176 | 28.625790 | 36.034081 |
| Ca| 30.363539 | 32.861946 | 33.008396 |
| Ca| 33.571793 | 29.032316 | 31.686390 |
| Ca| 32.922871 | 30.812527 | 35.672791 |
| Ca| 36.582096 | 26.445951 | 34.752499 |
| Ca| 36.690559 | 31.103853 | 34.338940 |
| Ca| 40.364223 | 28.734291 | 31.595917 |
| Ca| 39.589516 | 29.397783 | 36.616615 |
| Ca| 46.635742 | 29.716434 | 32.793324 |
| Ca| 42.896221 | 29.113705 | 34.300629 |
| S | 26.820051 | 27.656918 | 36.523262 |
| S | 27.306311 | 33.989979 | 33.917717 |
| S | 30.530239 | 29.670067 | 32.893745 |
| S | 29.646305 | 31.854507 | 36.252846 |
| S | 33.282360 | 27.509150 | 34.771851 |
| S | 33.735195 | 32.195179 | 32.580345 |
| S | 36.894836 | 28.824532 | 31.948000 |
| S | 36.338100 | 29.170456 | 36.893674 |
| S | 39.985256 | 26.553654 | 34.005142 |
| S | 40.296394 | 31.104633 | 34.095032 |
| S | 43.658070 | 29.021854 | 31.095448 |
| S | 44.924381 | 26.033646 | 37.194653 |
|   | generated by VMD |
| Ca| 25.121178 | 30.014130 | 31.646172 |
| Ca| 26.178013 | 31.023449 | 35.485130 |
| Ca| 30.067236 | 28.463758 | 35.967522 |
| Ca| 30.119892 | 32.870796 | 33.284828 |
| Ca| 33.466362 | 28.944157 | 31.565590 |
| Ca| 33.054142 | 30.681280 | 35.603291 |
| Ca| 36.396324 | 26.692911 | 34.911201 |
| Ca| 36.889496 | 31.216022 | 34.019123 |
| Ca| 40.492092 | 28.829741 | 31.298817 |
| Ca| 39.786121 | 28.942265 | 36.574490 |
| Ca| 46.645344 | 29.758936 | 33.077576 |
| Ca| 42.906708 | 28.886168 | 34.234688 |
| S | 26.772186 | 27.808216 | 36.549301 |
| S | 26.935720 | 34.059921 | 34.134869 |
|  | S          | Ca         | S          |
|---|------------|------------|------------|
| 1 | 30.450470  | 25.213886  | 29.634823  |
| 2 | 29.725771  | 26.352674  | 31.742500  |
| 3 | 33.165916  | 30.259705  | 27.511333  |
| 4 | 33.541691  | 30.199764  | 32.256073  |
| 5 | 36.857231  | 33.434010  | 28.823275  |
| 6 | 36.481869  | 33.024017  | 29.496954  |
| 7 | 39.994476  | 36.669601  | 31.723333  |
| 8 | 40.309368  | 36.572563  | 31.150913  |
| 9 | 44.080849  | 40.141315  | 28.879555  |
|10 | 44.995502  | 42.900566  | 30.078175  |
|11 |            |            | 29.930904  |
|12 |            |            | 31.150913  |
|13 |            |            | 30.259705  |
|14 |            |            | 30.199764  |
|15 |            |            | 33.434010  |
|16 |            |            | 33.024017  |
|17 |            |            | 36.669601  |
|18 |            |            | 36.572563  |
|19 |            |            | 40.141315  |
|20 |            |            | 39.802124  |
|21 |            |            | 46.430759  |
|22 |            |            | 42.900566  |
|23 |            |            | 29.059212  |
|24 |            |            | 30.078175  |
|25 |            |            | 29.930904  |
|26 |            |            | 31.150913  |
|27 |            |            | 30.259705  |
|28 |            |            | 30.199764  |
|29 |            |            | 33.434010  |
|30 |            |            | 33.024017  |
|31 |            |            | 36.669601  |
|32 |            |            | 36.572563  |
|33 |            |            | 40.141315  |

24 generated by VMD
|   |      |      |      |
|---|------|------|------|
|Ca| 40.285736 | 29.058212 | 31.765841 |
|Ca| 39.737736 | 28.969776 | 36.480976 |
|Ca| 46.598869 | 29.573576 | 33.092941 |
|Ca| 42.902294 | 29.084900 | 34.373554 |
|S | 27.014072 | 27.635523 | 36.069092 |
|S | 27.176399 | 34.056610 | 34.034088 |
|S | 30.385317 | 29.765369 | 33.006004 |
|S | 29.545921 | 31.548462 | 36.315231 |
|S | 33.318047 | 27.538914 | 34.811119 |
|S | 33.666214 | 32.351536 | 32.462833 |
|S | 36.680222 | 28.846149 | 31.981499 |
|S | 36.668739 | 29.687378 | 36.597359 |
|S | 40.035633 | 26.622059 | 34.016506 |
|S | 40.291660 | 31.248592 | 34.282059 |
|S | 43.591747 | 28.596646 | 31.295280 |
|S | 45.331657 | 25.916573 | 37.257496 |

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generated by VMD

|   |      |      |      |
|---|------|------|------|
|Ca| 40.285736 | 29.058212 | 31.765841 |
|Ca| 42.902294 | 29.084900 | 34.373554 |
|Ca| 33.459245 | 28.901890 | 31.480459 |
|Ca| 33.214264 | 30.507393 | 35.533501 |
|Ca| 36.729061 | 26.322983 | 34.606651 |
|Ca| 36.462723 | 31.247131 | 33.990997 |
|Ca| 40.010223 | 28.796539 | 31.889261 |
|Ca| 39.708721 | 29.194408 | 36.644260 |
|Ca| 46.538269 | 29.720953 | 32.994755 |
|S | 42.864079 | 29.290257 | 34.392242 |
|S | 36.798010 | 27.509834 | 35.751888 |
|S | 27.347933 | 33.978153 | 34.186325 |
|S | 30.744423 | 29.815514 | 32.875656 |
|S | 29.674383 | 31.669836 | 36.286777 |
|S | 33.356079 | 27.407272 | 34.760353 |
|S | 33.769997 | 32.295769 | 32.293312 |
|S | 36.660980 | 28.624210 | 31.906637 |
|S | 36.520481 | 29.245253 | 36.712181 |
|S | 40.218906 | 26.615086 | 34.335598 |
|S | 40.125580 | 31.215534 | 33.900223 |
|S | 43.365551 | 28.623680 | 31.293480 |
|S | 45.377922 | 26.465710 | 37.403370 |

24

generated by VMD

|   |      |      |      |
|---|------|------|------|
|Ca| 45.377922 | 26.465710 | 37.403370 |
|Ca| 42.864079 | 29.290257 | 34.392242 |
|Ca| 36.798010 | 27.509834 | 35.751888 |
|Ca| 36.462723 | 31.247131 | 33.990997 |
|Ca| 40.010223 | 28.796539 | 31.889261 |
|Ca| 39.708721 | 29.194408 | 36.644260 |
|Ca| 46.538269 | 29.720953 | 32.994755 |
|S | 42.864079 | 29.290257 | 34.392242 |
|S | 26.798010 | 27.509834 | 35.751888 |
|S | 27.347933 | 33.978153 | 34.186325 |
|S | 30.744423 | 29.815514 | 32.875656 |
|S | 29.674383 | 31.669836 | 36.286777 |
|S | 33.356079 | 27.407272 | 34.760353 |
|S | 33.769997 | 32.295769 | 32.293312 |
|S | 36.660980 | 28.624210 | 31.906637 |
|S | 36.520481 | 29.245253 | 36.712181 |
|S | 40.218906 | 26.615086 | 34.335598 |
|S | 40.125580 | 31.215534 | 33.900223 |
|S | 43.365551 | 28.623680 | 31.293480 |
|S | 45.377922 | 26.465710 | 37.403370 |
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 30.084496     | 28.471405     | 36.411697     |
| Ca      | 30.185318     | 32.801743     | 33.025402     |
| Ca      | 33.006851     | 30.475052     | 35.530193     |
| Ca      | 36.867573     | 26.212997     | 34.793510     |
| Ca      | 36.498550     | 31.158286     | 33.025402     |
| Ca      | 40.233471     | 28.749393     | 31.582258     |
| Ca      | 39.906719     | 29.090317     | 36.469395     |
| Ca      | 46.376877     | 29.901958     | 32.889755     |
| Ca      | 42.890156     | 29.321499     | 34.101986     |
| S       | 26.593277     | 27.833279     | 35.617092     |
| S       | 27.056355     | 34.201717     | 33.979198     |
| S       | 30.565947     | 29.654745     | 33.039886     |
| S       | 29.723305     | 31.690502     | 36.352798     |
| S       | 33.359962     | 27.307083     | 35.070637     |
| S       | 33.660313     | 32.132343     | 32.497101     |
| S       | 36.738289     | 28.520199     | 32.188255     |
| S       | 36.577555     | 29.064056     | 36.803497     |
| S       | 40.358921     | 26.566023     | 34.233223     |
| S       | 40.169678     | 31.146221     | 33.922588     |
| S       | 43.514687     | 28.900955     | 31.036827     |
| S       | 45.322533     | 26.552967     | 37.495354     |

24 generated by VMD

| Ca      | 25.096102     | 30.252335     | 31.760420     |
| Ca      | 26.476036     | 31.243637     | 35.759178     |
| Ca      | 30.266136     | 28.317928     | 36.116673     |
| Ca      | 30.412249     | 32.785954     | 33.296158     |
| Ca      | 33.443874     | 28.812113     | 31.370281     |
| Ca      | 33.170429     | 30.510075     | 35.409924     |
| Ca      | 36.895729     | 26.418953     | 34.800789     |
| Ca      | 36.459583     | 31.241896     | 33.501286     |
| Ca      | 39.947598     | 28.977432     | 31.936218     |
| Ca      | 39.744778     | 28.979885     | 36.570847     |
| Ca      | 46.352043     | 29.843498     | 33.076450     |
| Ca      | 42.691456     | 29.127283     | 34.609531     |
| S       | 26.903004     | 27.798279     | 35.910805     |
| S       | 27.233181     | 34.191780     | 34.410152     |
| S       | 30.571629     | 29.703804     | 32.911205     |
| S       | 30.084343     | 31.581833     | 36.511044     |
| S       | 33.332935     | 27.433022     | 34.499302     |
| S       | 33.644100     | 32.157642     | 31.998306     |
| S       | 36.613647     | 28.510801     | 31.781254     |
| S       | 36.593910     | 29.439619     | 36.628399     |
| S       | 40.297768     | 26.448566     | 34.106846     |
| S       | 40.060871     | 31.287415     | 34.197929     |
|   | 43.33698 | 28.967430 | 31.332779 |
|---|---------|-----------|-----------|
| S | 44.808765 | 26.360254 | 37.534935 |

24 generated by VMD

| Ca | 24.940311 | 30.233131 | 31.698198 |
|---|-----------|-----------|-----------|
| Ca | 26.380510 | 31.314995 | 35.489357 |
| Ca | 30.225346 | 28.390209 | 36.272114 |
| Ca | 30.346642 | 33.027618 | 33.115025 |
| Ca | 33.272610 | 28.761147 | 31.566296 |
| Ca | 33.192226 | 30.444065 | 35.469589 |
| Ca | 36.674530 | 26.263987 | 34.635277 |
| Ca | 36.630974 | 30.884918 | 34.002048 |
| Ca | 39.978191 | 28.791170 | 31.571659 |
| Ca | 39.660442 | 28.873039 | 36.410336 |
| Ca | 46.462860 | 30.199642 | 33.105217 |
| Ca | 42.900730 | 29.301144 | 34.303505 |
| S  | 26.957487 | 27.904694 | 36.094391 |
| S  | 27.067478 | 34.262402 | 34.186127 |
| S  | 30.524446 | 29.824139 | 32.964348 |
| S  | 29.859026 | 31.625494 | 36.331932 |
| S  | 33.235626 | 27.402191 | 34.754501 |
| S  | 33.949272 | 32.168022 | 32.361610 |
| S  | 36.631607 | 28.512569 | 31.902245 |
| S  | 36.433044 | 28.963543 | 36.738350 |
| S  | 40.247303 | 26.545628 | 34.033989 |
| S  | 40.229149 | 31.226679 | 34.057808 |
| S  | 43.598118 | 28.972374 | 31.250084 |
| S  | 45.035923 | 26.498653 | 37.716671 |

24 generated by VMD

| Ca | 24.970520 | 30.307196 | 31.942999 |
|---|-----------|-----------|-----------|
| Ca | 26.544870 | 31.226589 | 35.893406 |
| Ca | 30.205986 | 28.292833 | 36.176201 |
| Ca | 30.326578 | 32.898048 | 33.235695 |
| Ca | 33.289928 | 28.716917 | 31.278011 |
| Ca | 33.000084 | 30.611298 | 35.374832 |
| Ca | 36.708439 | 26.528316 | 34.220764 |
| Ca | 36.699371 | 31.112316 | 33.768997 |
| Ca | 40.214394 | 28.878521 | 31.734612 |
| Ca | 39.557095 | 28.893055 | 36.494293 |
| Ca | 46.444294 | 29.846985 | 33.488560 |
| Ca | 42.868114 | 29.156883 | 34.708065 |
| S  | 26.753866 | 27.726151 | 36.317116 |
| S  | 27.069111 | 34.096573 | 34.088570 |
| S  | 30.407623 | 29.713509 | 32.887783 |
| S  | 30.140614 | 31.642181 | 36.449104 |
|   |   |   |   |
|---|---|---|---|
| S | 33.234936 | 27.455462 | 34.565964 |
| S | 33.672615 | 32.119560 | 32.177681 |
| S | 36.723007 | 28.865326 | 31.541288 |
| S | 36.353699 | 29.267975 | 36.548252 |
| S | 40.301285 | 26.710293 | 34.209457 |
| S | 40.231220 | 31.145126 | 34.086792 |
| S | 43.545868 | 29.061861 | 31.451382 |
| S | 45.170433 | 26.118397 | 37.390907 |
| 24 | generated by VMD |
| Ca | 24.767788 | 30.309496 | 31.995836 |
| Ca | 26.263557 | 31.194008 | 35.905834 |
| Ca | 30.205721 | 28.128477 | 35.747726 |
| Ca | 30.164351 | 32.939899 | 33.37823 |
| Ca | 33.540359 | 29.005518 | 31.342491 |
| Ca | 32.945778 | 30.709484 | 35.502838 |
| Ca | 36.732304 | 26.443596 | 34.455352 |
| Ca | 36.620583 | 31.361052 | 34.126228 |
| Ca | 40.330315 | 28.477177 | 31.623283 |
| Ca | 39.554218 | 28.999678 | 36.438786 |
| Ca | 46.634529 | 29.986238 | 32.965389 |
| Ca | 42.854336 | 29.121166 | 34.327888 |
| S | 26.725512 | 27.924194 | 35.997532 |
| S | 26.992516 | 34.163448 | 34.065399 |
| S | 30.447515 | 29.667612 | 32.817326 |
| S | 29.888029 | 31.518486 | 36.319847 |
| S | 33.210789 | 27.557423 | 34.602192 |
| S | 33.748764 | 32.216080 | 32.447311 |
| S | 36.814129 | 28.707333 | 31.941341 |
| S | 36.524910 | 29.263031 | 36.825916 |
| S | 40.311756 | 26.456593 | 34.152084 |
| S | 40.144058 | 31.027184 | 33.958157 |
| S | 43.737591 | 28.644379 | 31.263149 |
| S | 45.274399 | 26.569893 | 37.829857 |
| 24 | generated by VMD |
| Ca | 24.954775 | 30.282602 | 32.054836 |
| Ca | 26.549265 | 31.370756 | 35.650230 |
| Ca | 30.139877 | 28.501526 | 36.278381 |
| Ca | 30.435846 | 32.757065 | 33.022987 |
| Ca | 33.309814 | 28.714987 | 31.407959 |
| Ca | 33.141876 | 30.585501 | 35.463726 |
| Ca | 36.557175 | 26.191551 | 34.406315 |
| Ca | 36.584385 | 31.081484 | 33.965538 |
| Ca | 40.133926 | 29.056871 | 31.772141 |
| Ca | 39.627899 | 28.815514 | 36.455555 |
|   |   |   |
|---|---|---|
| Ca | 46.518993 | 29.940861 | 33.038429 |
| Ca | 42.908497 | 29.113115 | 34.528137 |
| S  | 26.787464 | 27.788631 | 36.111465 |
| S  | 27.251099 | 34.240185 | 34.039394 |
| S  | 30.393040 | 29.555635 | 33.084686 |
| S  | 30.045343 | 31.785717 | 36.343510 |
| S  | 33.330292 | 27.306366 | 34.566536 |
| S  | 33.803692 | 31.970215 | 32.270885 |
| S  | 36.751980 | 28.641695 | 31.805683 |
| S  | 36.443790 | 29.113121 | 36.578590 |
| S  | 40.204792 | 26.554419 | 33.897766 |
| S  | 40.198147 | 31.258194 | 34.105499 |
| S  | 43.541080 | 29.303398 | 31.518950 |
| S  | 44.820835 | 26.462036 | 37.663536 |

24 generated by VMD

| Ca | 24.989244 | 30.367727 | 31.785681 |
| Ca | 26.475281 | 31.099094 | 35.721230 |
| Ca | 30.080767 | 28.475498 | 35.951511 |
| Ca | 30.274811 | 32.701576 | 33.121479 |
| Ca | 33.525787 | 28.982586 | 31.515514 |
| Ca | 33.153229 | 30.803444 | 35.502098 |
| Ca | 36.591660 | 26.356153 | 34.518608 |
| Ca | 36.580708 | 31.051542 | 34.002258 |
| Ca | 40.169807 | 28.767368 | 31.690126 |
| Ca | 39.737797 | 28.856298 | 36.419090 |
| Ca | 46.568535 | 29.826534 | 32.794022 |
| Ca | 42.879650 | 29.075497 | 34.306450 |
| S  | 26.602058 | 27.787893 | 36.087685 |
| S  | 27.089813 | 33.907436 | 34.111500 |
| S  | 30.530228 | 29.518147 | 32.918205 |
| S  | 29.853827 | 31.703426 | 36.353493 |
| S  | 33.211998 | 27.613255 | 34.725437 |
| S  | 33.842720 | 32.504807 | 32.469753 |
| S  | 36.694092 | 28.526409 | 32.015362 |
| S  | 36.597538 | 29.302551 | 36.786812 |
| S  | 40.265671 | 26.497702 | 34.180988 |
| S  | 40.069126 | 31.061008 | 33.915695 |
| S  | 43.644371 | 28.992538 | 31.277264 |
| S  | 45.005119 | 26.612883 | 37.860443 |

24 generated by VMD

| Ca | 24.649500 | 30.599638 | 32.036758 |
| Ca | 26.384008 | 31.232088 | 35.878181 |
| Ca | 30.052811 | 28.442867 | 35.874413 |
| Ca | 30.324474 | 32.759293 | 33.220169 |
| Element | Ca    | S     |
|---------|-------|-------|
|         | 33.494492 | 28.873514 | 31.414230 |
|         | 33.131115  | 30.525961  | 35.426403  |
|         | 36.800213  | 26.171148  | 34.457481  |
|         | 36.568272  | 31.160336  | 33.916637  |
|         | 40.197403  | 28.797148  | 31.815088  |
|         | 39.497856  | 28.948017  | 36.306664  |
|         | 46.493759  | 29.983322  | 33.039413  |
|         | 42.931519  | 29.268799  | 34.374321  |
|         | 26.631071  | 27.788136  | 36.171494  |
|         | 27.195709  | 34.093582  | 34.145714  |
|         | 30.375994  | 29.612488  | 32.730381  |
|         | 29.852476  | 31.698444  | 36.381443  |
|         | 33.478912  | 27.390068  | 34.579872  |
|         | 33.688656  | 32.229683  | 32.259327  |
|         | 36.856842  | 28.496084  | 31.767435  |
|         | 36.561962  | 29.217344  | 36.689194  |
|         | 40.445217  | 26.584055  | 34.214382  |
|         | 40.099174  | 31.134207  | 34.176483  |
|         | 43.718636  | 28.883881  | 31.345200  |
|         | 45.003788  | 26.501392  | 37.810089  |

24

generated by VMD

| Element | Ca    | S     |
|---------|-------|-------|
|         | 24.903788 | 30.440060 | 31.748913 |
|         | 26.362707 | 31.314032 | 35.646370 |
|         | 30.100906 | 28.344959 | 36.189632 |
|         | 30.439117 | 32.748657 | 33.060028 |
|         | 33.565063 | 28.744282 | 31.625282 |
|         | 33.050873 | 30.316841 | 35.502476 |
|         | 36.482838 | 26.562607 | 34.408592 |
|         | 36.689095 | 31.105644 | 34.175629 |
|         | 40.123169 | 28.851337 | 31.669460 |
|         | 39.903248 | 29.076574 | 36.400787 |
|         | 46.470726 | 30.046295 | 32.993439 |
|         | 42.860130 | 29.236782 | 34.266644 |
|         | 26.608044 | 27.875954 | 35.916477 |
|         | 27.309429 | 34.206676 | 34.281364 |
|         | 30.467216 | 29.503431 | 32.912071 |
|         | 29.742634 | 31.574730 | 36.240154 |
|         | 33.073425 | 27.178001 | 34.717663 |
|         | 33.754059 | 32.028370 | 32.483376 |
|         | 36.700569 | 28.742794 | 32.028763 |
|         | 36.601379 | 29.415045 | 36.750351 |
|         | 40.208908 | 26.555828 | 34.139130 |
|         | 40.318241 | 31.275696 | 33.956902 |
|         | 43.654865 | 28.707138 | 31.227333 |
|         | 45.043503 | 26.539654 | 37.689842 |
| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Ca      | 25.054174  | 30.576283  | 31.926245  |
| Ca      | 26.373022  | 31.516613  | 35.528793  |
| Ca      | 29.857477  | 28.263184  | 36.027767  |
| Ca      | 30.54134   | 32.689457  | 33.289169  |
| Ca      | 33.38840   | 28.708050  | 31.350891  |
| Ca      | 33.05914   | 30.360125  | 35.731213  |
| Ca      | 36.56279   | 26.194458  | 34.676613  |
| Ca      | 36.76307   | 30.835857  | 33.977295  |
| Ca      | 40.25607   | 28.774960  | 31.444828  |
| Ca      | 39.64629   | 28.975758  | 36.350468  |
| Ca      | 46.47419   | 30.054909  | 32.918167  |
| Ca      | 42.93871   | 29.515362  | 34.575294  |
| S       | 26.49737   | 27.982651  | 36.086308  |
| S       | 27.39544   | 34.381657  | 34.177582  |
| S       | 30.42141   | 29.659828  | 32.897018  |
| S       | 29.78454   | 31.459663  | 36.446003  |
| S       | 33.22055   | 27.174153  | 34.584084  |
| S       | 33.85661   | 32.037151  | 32.434810  |
| S       | 36.69962   | 28.429426  | 31.808704  |
| S       | 36.35138   | 29.044151  | 36.744221  |
| S       | 40.36692   | 26.777405  | 34.107220  |
| S       | 40.19973   | 31.165936  | 33.839555  |
| S       | 43.61200   | 28.916523  | 31.330120  |
| S       | 45.10817   | 26.898930  | 37.788481  |

| Element | X          | Y          | Z          |
|---------|------------|------------|------------|
| Ca      | 25.772335  | 29.918097  | 31.601236  |
| Ca      | 26.305189  | 31.310102  | 35.557503  |
| Ca      | 29.960831  | 28.353388  | 35.915501  |
| Ca      | 30.312935  | 32.910172  | 33.320747  |
| Ca      | 33.597645  | 29.013136  | 31.631178  |
| Ca      | 33.085712  | 30.20930   | 35.59839   |
| Ca      | 36.517334  | 26.511213  | 34.769764  |
| Ca      | 36.556396  | 31.065250  | 34.069891  |
| Ca      | 40.284744  | 28.751564  | 31.692249  |
| Ca      | 39.796318  | 29.180241  | 36.459492  |
| Ca      | 46.320255  | 30.078617  | 32.510002  |
| Ca      | 42.713936  | 29.140640  | 34.260082  |
| S       | 26.659012  | 28.069683  | 36.050240  |
| S       | 27.103901  | 34.385803  | 34.178570  |
| S       | 30.558472  | 29.698179  | 32.862011  |
| S       | 29.988422  | 31.509525  | 36.322929  |
| S       | 33.205173  | 27.052248  | 34.670433  |
| S       | 33.776592  | 32.337574  | 32.716858  |
|  | X       | Y       | Z       |
|---|--------|--------|--------|
| S | 36.739429 | 28.582790 | 32.078629 |
| S | 36.430290 | 29.339813 | 36.875210 |
| S | 39.990330 | 26.608385 | 34.100990 |
| S | 40.178371 | 31.185905 | 33.934929 |
| S | 43.520981 | 28.518232 | 31.286282 |
| S | 45.059193 | 26.669903 | 37.567955 |

24 generated by VMD

|  | X       | Y       | Z       |
|---|--------|--------|--------|
| Ca | 25.001835 | 29.971127 | 32.278946 |
| Ca | 26.459578 | 31.277275 | 35.597679 |
| Ca | 29.724161 | 28.177038 | 35.686562 |
| Ca | 30.315449 | 32.843845 | 33.236763 |
| Ca | 33.697128 | 28.849262 | 31.367161 |
| Ca | 33.133457 | 30.223301 | 35.335373 |
| Ca | 36.608501 | 26.752995 | 35.000370 |
| Ca | 36.445065 | 31.498562 | 34.049370 |
| Ca | 40.305851 | 28.768108 | 31.559929 |
| Ca | 39.721142 | 29.014044 | 36.475197 |
| Ca | 46.356346 | 30.178673 | 32.747543 |
| Ca | 43.009270 | 28.776831 | 34.275665 |
| S | 26.579678 | 28.02242 | 36.053886 |
| S | 27.068699 | 34.215160 | 34.315273 |
| S | 30.532000 | 29.762115 | 32.611977 |
| S | 29.980431 | 31.330540 | 36.318279 |
| S | 33.200130 | 27.190948 | 34.354321 |
| S | 33.685448 | 32.403439 | 32.607021 |
| S | 36.777557 | 28.823956 | 32.042953 |
| S | 36.501579 | 29.555134 | 36.777641 |
| S | 40.112198 | 26.725681 | 34.283752 |
| S | 40.536140 | 31.096386 | 34.079338 |
| S | 43.659100 | 28.544058 | 31.220142 |
| S | 45.023144 | 26.390644 | 37.755630 |

24 generated by VMD

|  | X       | Y       | Z       |
|---|--------|--------|--------|
| Ca | 25.186028 | 30.350914 | 32.078697 |
| Ca | 26.305008 | 31.207411 | 35.925907 |
| Ca | 29.965096 | 28.016289 | 35.963455 |
| Ca | 30.455557 | 32.873703 | 33.421558 |
| Ca | 33.365364 | 29.175758 | 31.200293 |
| Ca | 33.287750 | 30.229939 | 35.362503 |
| Ca | 36.602627 | 26.720791 | 34.386341 |
| Ca | 36.735123 | 31.327698 | 33.510330 |
| Ca | 40.170116 | 28.838825 | 31.442001 |
| Ca | 39.748764 | 28.897453 | 36.556957 |
| Ca | 46.692188 | 30.012791 | 33.496716 |
| Ca | 42.959480 | 29.142729 | 34.346458 |
|     | X      | Y      | Z      |
|-----|--------|--------|--------|
| S   | 26.708652 | 27.675734 | 36.259323 |
| S   | 27.164902 | 34.051651 | 34.436855 |
| S   | 30.554758 | 29.793221 | 32.845367 |
| S   | 30.003456 | 31.370148 | 36.584309 |
| S   | 33.155552 | 27.264069 | 34.342148 |
| S   | 33.691132 | 32.362267 | 32.283146 |
| S   | 36.672680 | 28.725004 | 31.644554 |
| S   | 36.547653 | 29.715187 | 36.438358 |
| S   | 40.069130 | 26.681063 | 34.297619 |
| S   | 40.252357 | 31.065762 | 33.728374 |
| S   | 43.670059 | 28.502541 | 31.452133 |
| S   | 44.470463 | 26.390503 | 38.027260 |

24 generated by VMD

| Ca  | 24.949211 | 30.234976 | 32.077507 |
| Ca  | 26.532236 | 31.491098 | 35.677723 |
| Ca  | 29.667490 | 28.232288 | 35.700695 |
| Ca  | 30.272425 | 32.787205 | 33.397141 |
| Ca  | 33.527359 | 28.981928 | 31.196045 |
| Ca  | 33.056370 | 30.266212 | 35.437126 |
| Ca  | 36.851997 | 26.464334 | 34.545033 |
| Ca  | 36.732700 | 31.065241 | 33.841751 |
| Ca  | 40.024033 | 28.758675 | 31.974857 |
| Ca  | 39.756668 | 29.217163 | 36.440552 |
| Ca  | 46.603039 | 30.058043 | 32.604523 |
| Ca  | 43.032135 | 29.355858 | 34.622051 |
| S   | 26.345684 | 28.022655 | 36.508801 |
| S   | 27.169392 | 34.280376 | 34.344875 |
| S   | 30.422338 | 29.626022 | 32.702465 |
| S   | 30.087456 | 31.315575 | 36.453835 |
| S   | 33.382694 | 27.249161 | 34.210079 |
| S   | 33.607891 | 32.232475 | 32.303829 |
| S   | 36.776672 | 28.561367 | 31.762751 |
| S   | 36.420643 | 29.247282 | 36.546276 |
| S   | 40.242493 | 26.602064 | 34.224915 |
| S   | 40.309631 | 31.240513 | 33.895683 |
| S   | 43.815083 | 28.704777 | 31.481171 |
| S   | 44.848362 | 26.396065 | 38.080959 |

24 generated by VMD

| Ca  | 25.042393 | 30.099850 | 32.209564 |
| Ca  | 26.422161 | 31.097076 | 35.678303 |
| Ca  | 29.697002 | 28.354931 | 35.691479 |
| Ca  | 30.332874 | 32.820938 | 33.129253 |
| Ca  | 33.645157 | 29.329609 | 31.445896 |
| Ca  | 33.002903 | 30.173016 | 35.356308 |
Ca       36.748627       26.633377       34.717388
Ca       36.679451       31.036554       33.957153
Ca       40.238895       28.826908       31.646626
Ca       39.732224       29.249063       36.254456
Ca       46.299564       30.097214       32.904797
Ca       43.077953       29.102634       34.342888
S        26.585466       27.681499       36.403954
S        27.222610       34.118065       34.473591
S        30.589479       29.849621       32.558571
S        29.895399       31.439451       36.368202
S        33.212784       27.276836       34.232971
S        33.903034       32.438248       32.647968
S        36.829323       28.588762       31.905075
S        36.447247       29.458731       36.647568
S        40.184620       26.874535       34.235260
S        40.419132       31.234646       33.881626
S        43.629528       28.186893       31.416084
S        44.596088       26.423010       37.925732

generated by VMD
Ca       24.829477       30.219055       32.295162
Ca       26.493530       31.117748       35.771824
Ca       29.970293       28.193153       35.966206
Ca       30.287788       32.712578       33.133121
Ca       33.443752       29.139326       31.152042
Ca       33.121418       30.330313       35.246048
Ca       36.558403       26.810747       34.321556
Ca       36.768707       31.279861       33.843552
Ca       40.11714        28.985672       31.699850
Ca       39.723064       29.173916       36.434654
Ca       46.584072       29.732563       33.036186
Ca       43.049500       29.152897       34.537968
S        26.809128       27.811529       36.335999
S        27.444969       34.170269       34.635101
S        30.376278       29.467255       32.921059
S        29.915960       31.388153       36.188213
S        33.252338       27.219612       34.194237
S        33.748337       32.353405       32.225163
S        36.725246       28.976742       31.792240
S        36.450642       29.456743       36.453293
S        40.179493       26.695984       34.192841
S        40.289097       31.275366       33.984779
S        43.750671       28.378738       31.482693
S        44.543991       26.349791       38.186867

generated by VMD
|       |       |       |
|-------|-------|-------|
| Ca    | 24.976501 | 30.291794 | 32.206421 |
| Ca    | 26.430546 | 31.062174 | 35.979122 |
| Ca    | 29.998474 | 27.975353 | 35.693851 |
| Ca    | 30.245674 | 32.980759 | 32.998363 |
| Ca    | 33.537941 | 29.103973 | 31.315784 |
| Ca    | 33.168102 | 30.302879 | 35.2796765|
| Ca    | 36.638020 | 26.651829 | 34.687447 |
| Ca    | 36.530155 | 31.269297 | 33.820404 |
| Ca    | 40.299820 | 29.011189 | 31.579765 |
| Ca    | 39.791229 | 29.421566 | 36.563477 |
| Ca    | 46.650257 | 29.490814 | 32.820499 |
| Ca    | 42.923916 | 29.340580 | 34.531181 |
| S     | 26.813271 | 27.738335 | 36.507927 |
| S     | 27.197041 | 34.110603 | 34.635098 |
| S     | 30.417086 | 29.821537 | 32.624428 |
| S     | 29.897097 | 31.385601 | 36.127495 |
| S     | 33.096661 | 27.274544 | 34.254822 |
| S     | 33.612160 | 32.392570 | 32.355518 |
| S     | 36.862293 | 28.674355 | 31.847998 |
| S     | 36.429928 | 29.480612 | 36.516857 |
| S     | 40.147373 | 26.789654 | 34.192585 |
| S     | 40.366043 | 31.316227 | 33.807041 |
| S     | 43.766785 | 28.321110 | 31.575150 |
| S     | 44.637466 | 26.184029 | 38.109726 |

24 generated by VMD

|       |       |       |
|-------|-------|-------|
| Ca    | 25.032494 | 29.996052 | 32.236378 |
| Ca    | 26.527557 | 31.335035 | 35.999302 |
| Ca    | 29.864105 | 28.193207 | 35.721672 |
| Ca    | 30.639412 | 32.844151 | 33.152702 |
| Ca    | 33.617012 | 29.255909 | 31.258490 |
| Ca    | 33.038799 | 30.119953 | 35.328838 |
| Ca    | 36.399025 | 26.739731 | 34.422741 |
| Ca    | 36.502136 | 30.943132 | 33.706100 |
| Ca    | 40.166725 | 29.055216 | 31.703321 |
| Ca    | 39.712513 | 29.006569 | 36.464680 |
| Ca    | 46.678562 | 29.882278 | 33.209221 |
| Ca    | 42.881428 | 29.220606 | 34.474766 |
| S     | 26.673668 | 27.753880 | 36.539663 |
| S     | 27.419319 | 34.240223 | 34.651611 |
| S     | 30.389229 | 29.723812 | 32.727501 |
| S     | 30.058712 | 31.459972 | 36.376911 |
| S     | 33.040165 | 27.251167 | 34.129768 |
| S     | 33.834728 | 32.315342 | 32.303719 |
| S     | 36.781578 | 28.716969 | 31.570793 |
| S     | 36.318481 | 29.276609 | 36.498863 |
|   | X     | Y     | Z     |
|---|-------|-------|-------|
| S | 40.154537 | 26.693506 | 34.024944 |
| S | 40.258690 | 31.303322 | 33.768528 |
| S | 43.874756 | 28.485285 | 31.562859 |
| S | 44.570282 | 26.579456 | 38.197029 |

24 generated by VMD

| Ca  | X     | Y     | Z     |
|-----|-------|-------|-------|
| Ca  | 24.801331 | 30.032913 | 32.099380 |
| Ca  | 26.344257 | 31.064133 | 35.729675 |
| Ca  | 30.296787 | 28.079273 | 35.801624 |
| Ca  | 30.272266 | 32.979389 | 33.153160 |
| Ca  | 33.380703 | 29.193508 | 31.374933 |
| Ca  | 33.058495 | 30.506456 | 35.395115 |
| Ca  | 36.618679 | 26.821743 | 34.722912 |
| Ca  | 36.830025 | 31.029804 | 33.982719 |
| Ca  | 40.224609 | 28.893692 | 31.638342 |
| Ca  | 39.754360 | 29.017570 | 36.388710 |
| Ca  | 46.488918 | 29.726583 | 32.700901 |
| Ca  | 42.941471 | 29.044222 | 34.561695 |
| S   | 27.071741 | 27.844391 | 36.298950 |
| S   | 27.096252 | 34.231102 | 34.617157 |
| S   | 30.522345 | 29.636246 | 32.797016 |
| S   | 29.862053 | 31.431923 | 36.039543 |
| S   | 33.249672 | 27.329422 | 34.255287 |
| S   | 33.893936 | 32.435436 | 32.390797 |
| S   | 36.662930 | 28.739033 | 31.723244 |
| S   | 36.339771 | 29.410034 | 36.714230 |
| S   | 40.082344 | 26.766689 | 34.162079 |
| S   | 40.420132 | 31.191381 | 33.907299 |
| S   | 43.571949 | 28.444321 | 31.293358 |
| S   | 44.648907 | 26.542168 | 38.282654 |

24 generated by VMD

| Ca  | X     | Y     | Z     |
|-----|-------|-------|-------|
| Ca  | 25.101498 | 29.865294 | 31.989353 |
| Ca  | 26.292372 | 31.299150 | 35.621849 |
| Ca  | 29.951979 | 28.427944 | 36.122597 |
| Ca  | 30.429493 | 32.759029 | 33.130718 |
| Ca  | 33.295963 | 28.908981 | 31.353355 |
| Ca  | 33.084076 | 30.236572 | 35.392857 |
| Ca  | 36.637592 | 26.824455 | 34.437592 |
| Ca  | 36.637539 | 30.940594 | 33.897270 |
| Ca  | 40.067101 | 29.262383 | 31.580198 |
| Ca  | 39.919968 | 28.926271 | 36.611450 |
| Ca  | 46.532207 | 30.015081 | 33.227802 |
| Ca  | 42.941666 | 29.055141 | 34.363777 |
| S   | 26.737694 | 28.038218 | 36.474941 |
| S   | 27.327244 | 34.202957 | 34.083286 |
S  30.416922       29.543674       32.836754
S  29.929476       31.685040       36.118092
S  33.148422       27.228065       34.553032
S  33.763748       32.311569       32.680721
S  36.653648       28.916784       31.502594
S  36.398750       29.018934       36.846478
S  40.123428       26.997276       33.996719
S  40.230507       31.109928       34.098217
S  43.684113       28.686415       31.380056
S  45.128433       26.131590       37.730965
24 generated by VMD
Ca  25.075768       30.328163       31.821291
Ca  26.354710       31.345516       35.852676
Ca  29.994633       28.133751       35.923233
Ca  30.184319       32.601742       32.989986
Ca  33.479317       28.951054       31.389341
Ca  32.989601       30.464392       35.585510
Ca  36.669479       26.607382       34.699486
Ca  36.581940       31.177147       33.632862
Ca  40.265175       29.106321       31.808245
Ca  39.918999       29.053764       36.570572
Ca  46.536880       29.706131       32.972855
Ca  43.032654       29.209015       34.389091
S  26.711700       27.842056       36.068806
S  27.264076       34.211472       34.811268
S  30.426018       29.584391       32.702015
S  29.878902       31.542927       36.314301
S  33.173180       27.206020       34.394009
S  33.730705       32.323570       32.310513
S  36.800377       28.569714       31.806435
S  36.291389       29.416664       36.495575
S  40.126831       26.875549       34.300339
S  40.129837       31.329556       34.013580
S  43.538612       28.410332       31.313107
S  45.278805       26.394772       37.865597
24 generated by VMD
Ca  25.048201       30.003990       31.938906
Ca  26.346205       31.234245       35.702034
Ca  30.119833       28.512707       35.964741
Ca  30.322271       32.940956       33.208412
Ca  33.282013       28.859539       31.197880
Ca  32.953449       30.456238       35.420639
Ca  36.480701       26.522976       34.636543
Ca  36.845081       30.885836       34.139214
| Element | Ca    | S     | Ca    |
|---------|-------|-------|-------|
|         | 40.089771 | 29.012079 | 31.524811 |
|         | 39.772530 | 28.846134 | 36.391098 |
|         | 46.536827 | 30.008373 | 33.154270 |
|         | 42.786434 | 29.299171 | 34.474361 |
|         | 26.828083 | 27.890656 | 36.217243 |
|         | 27.183081 | 34.147835 | 34.336937 |
|         | 30.430029 | 29.764969 | 32.774143 |
|         | 29.833481 | 31.635132 | 36.465866 |
|         | 33.106697 | 27.393436 | 34.449242 |
|         | 33.775913 | 32.169785 | 32.366768 |
|         | 36.574661 | 28.724297 | 31.791307 |
|         | 36.422340 | 29.138756 | 36.773567 |
|         | 40.033260 | 26.736712 | 34.035275 |
|         | 40.263275 | 31.297459 | 33.943287 |
|         | 43.690308 | 28.464613 | 31.461052 |
|         | 45.349361 | 26.445526 | 37.663116 |

generated by VMD

| Element | Ca    | S     | Ca    |
|---------|-------|-------|-------|
|         | 25.142467 | 29.84563 | 32.112137 |
|         | 26.310801 | 31.136505 | 35.565056 |
|         | 30.045280 | 28.263546 | 35.993874 |
|         | 30.156239 | 32.798164 | 33.283092 |
|         | 33.548210 | 29.078938 | 31.294479 |
|         | 33.040123 | 30.447887 | 35.431309 |
|         | 36.479954 | 26.874018 | 34.358723 |
|         | 36.538582 | 31.418316 | 34.001423 |
|         | 40.279980 | 29.116646 | 31.546993 |
|         | 39.697655 | 28.919479 | 36.383038 |
|         | 46.773563 | 29.470110 | 33.019226 |
|         | 42.899254 | 29.126709 | 34.355533 |
|         | 26.968863 | 27.768324 | 36.501278 |
|         | 26.985907 | 34.064568 | 34.133438 |
|         | 30.440674 | 29.703651 | 32.833958 |
|         | 29.851231 | 31.690247 | 36.370068 |
|         | 33.096073 | 27.440636 | 34.335480 |
|         | 33.822334 | 32.268330 | 32.451321 |
|         | 36.877731 | 29.116241 | 31.737446 |
|         | 36.404343 | 29.467693 | 36.738827 |
|         | 40.017208 | 26.727520 | 33.995892 |
|         | 40.275143 | 31.143198 | 34.252625 |
|         | 43.577225 | 28.338003 | 31.442818 |
|         | 45.205025 | 26.167252 | 37.892647 |

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generated by VMD

| Element | Ca    | S     | Ca    |
|---------|-------|-------|-------|
|         | 25.174084 | 29.912640 | 32.07732 |
|         | 26.476921 | 31.036797 | 35.792259 |
| Element | Ca       | 30.206869 | 28.473713 | 35.936275 |
|---------|----------|-----------|-----------|-----------|
|         | 30.298515| 30.845097 | 35.359692 |
|         | 36.440956| 26.816051 | 34.722336 |
|         | 36.619217| 31.385544 | 34.128803 |
|         | 40.248756| 28.978954 | 31.820139 |
|         | 39.530052| 28.851984 | 36.451714 |
|         | 46.530170| 29.590057 | 32.584488 |
|         | 42.964729| 29.112934 | 34.465179 |
|         | 26.977381| 27.446850 | 36.021038 |
|         | 27.008101| 34.028805 | 34.092972 |
|         | 30.445171| 29.640339 | 32.790737 |
|         | 29.896208| 31.643402 | 36.221626 |
|         | 33.253365| 27.675285 | 34.694206 |
|         | 33.548313| 32.518337 | 32.380310 |
|         | 36.741867| 28.825558 | 31.956799 |
|         | 36.485046| 29.372890 | 36.928230 |
|         | 40.160450| 26.570049 | 34.074295 |
|         | 40.275845| 31.160519 | 34.248848 |
|         | 43.510712| 28.552834 | 31.393280 |
|         | 45.038593| 26.055763 | 37.462318 |

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generated by VMD

| Element | Ca       | 25.308903 | 29.522684 | 31.807850 |
|---------|----------|-----------|-----------|-----------|
|         | 26.407005| 31.172768 | 35.908669 |
|         | 30.094193| 28.668901 | 36.082203 |
|         | 30.219353| 33.003899 | 33.315674 |
|         | 33.563427| 28.999676 | 31.486084 |
|         | 33.155556| 30.669785 | 35.471981 |
|         | 36.482693| 26.831306 | 34.309994 |
|         | 36.681705| 31.236694 | 33.814232 |
|         | 40.290768| 28.982239 | 31.466473 |
|         | 39.641739| 28.817081 | 36.531467 |
|         | 46.700108| 29.501627 | 33.029999 |
|         | 42.785702| 28.977924 | 34.460800 |
|         | 26.793549| 27.628826 | 36.180683 |
|         | 26.846981| 33.874710 | 34.114601 |
|         | 30.494045| 29.808891 | 32.952637 |
|         | 29.849133| 31.747772 | 36.549343 |
|         | 33.222828| 27.564930 | 34.582001 |
|         | 33.692307| 32.471054 | 32.575516 |
|         | 36.832428| 28.832062 | 31.540504 |
|         | 36.551937| 29.442215 | 36.617596 |
|         | 40.018551| 26.589737 | 33.890583 |
|         | 40.352928| 31.164557 | 34.019379 |
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| S       | 43.605141     | 28.587269     | 31.279057     |
| S       | 44.842918     | 26.294760     | 38.043308     |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 25.132103     | 29.423069     | 32.151836     |
| Ca      | 26.304211     | 30.894808     | 35.539612     |
| Ca      | 29.980286     | 28.540779     | 35.932209     |
| Ca      | 30.382334     | 33.082466     | 33.345551     |
| Ca      | 33.397011     | 29.372860     | 31.151661     |
| Ca      | 32.918255     | 30.665665     | 35.480164     |
| Ca      | 36.370125     | 26.902878     | 34.409947     |
| Ca      | 36.867500     | 31.307356     | 34.154915     |
| Ca      | 40.411144     | 28.740732     | 31.349657     |
| Ca      | 39.803272     | 28.881779     | 36.372704     |
| Ca      | 46.953758     | 29.387859     | 33.102829     |
| Ca      | 42.962303     | 28.778034     | 34.372566     |
| S       | 26.919445     | 27.719883     | 36.563606     |
| S       | 26.974895     | 33.888752     | 34.016277     |
| S       | 30.388847     | 29.862570     | 32.878235     |
| S       | 29.678450     | 31.699963     | 36.357777     |
| S       | 32.991875     | 27.381536     | 34.415009     |
| S       | 33.863136     | 32.446007     | 32.736237     |
| S       | 36.710121     | 29.212421     | 31.954878     |
| S       | 36.428104     | 29.331131     | 36.658195     |
| S       | 39.844864     | 26.648487     | 33.892712     |
| S       | 40.471027     | 31.136583     | 34.028477     |
| S       | 43.905685     | 28.579407     | 31.282297     |
| S       | 44.775101     | 26.506378     | 37.883804     |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 25.221771     | 29.536823     | 32.203751     |
| Ca      | 26.532322     | 31.270294     | 35.635651     |
| Ca      | 30.157249     | 28.449430     | 36.105228     |
| Ca      | 30.370199     | 32.748112     | 33.194031     |
| Ca      | 33.552059     | 29.521603     | 31.316025     |
| Ca      | 33.031105     | 30.626352     | 35.588116     |
| Ca      | 36.572937     | 26.711905     | 34.328957     |
| Ca      | 36.540466     | 31.175497     | 34.095757     |
| Ca      | 40.145393     | 29.149021     | 31.477352     |
| Ca      | 39.540188     | 28.813034     | 36.395340     |
| Ca      | 46.820217     | 29.372375     | 33.003483     |
| Ca      | 42.641502     | 29.173794     | 34.373772     |
| S       | 26.929245     | 27.783232     | 36.345650     |
| S       | 26.956228     | 33.956085     | 33.848942     |
| S       | 30.558147     | 29.574493     | 32.997746     |
| S       | 29.837233     | 31.605742     | 36.412476     |
S  33.501564  27.582735  34.601624
S  33.673000  32.515465  32.636852
S  36.688431  29.054329  31.639015
S  36.417477  29.368546  36.603264
S  39.957058  26.617210  33.736847
S  40.221405  31.168949  33.975208
S  43.856972  28.419678  31.509174
S  44.711678  26.196665  38.006485

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Ca  25.289701  29.357712  31.999588
Ca  26.219662  31.203169  35.702988
Ca  30.256874  28.481449  36.155178
Ca  30.207657  32.828613  33.244087
Ca  33.561665  29.236086  31.297543
Ca  33.137230  30.822186  35.413445
Ca  36.555527  26.717377  33.949902
Ca  36.617668  31.358410  33.899300
Ca  40.035221  29.198807  31.643131
Ca  39.518353  28.611273  36.479904
Ca  46.740196  29.137821  33.205135
Ca  42.817734  29.261566  34.548080
S  27.097399  27.850576  36.643600
S  26.865265  34.009842  34.154499
S  30.416374  29.656406  32.987968
S  29.844658  31.689346  36.450188
S  33.394512  27.471170  34.454128
S  33.591759  32.540020  32.448311
S  36.803013  29.152248  31.492735
S  36.375263  29.368038  36.411060
S  39.963398  26.689484  33.825489
S  40.284813  31.134359  34.194168
S  43.879723  28.534910  31.502209
S  44.960289  26.080515  37.928120

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generated by VMD

Ca  25.071722  29.582851  32.138695
Ca  26.310543  31.284992  35.684769
Ca  30.022005  28.193642  35.748322
Ca  29.978355  32.775639  33.490425
Ca  33.675072  29.497250  31.283989
Ca  32.937435  30.421215  35.495579
Ca  36.506638  26.665424  34.311203
Ca  36.535423  31.402147  33.956848
Ca  40.432400  28.760296  31.687174
Ca  39.440750  29.018368  36.272961
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 46.954220 | 29.269548 | 33.251740 |
| Ca      | 42.769970 | 29.199957 | 34.330341 |
| S       | 27.140295 | 28.084602 | 36.670200 |
| S       | 26.822634 | 34.207771 | 33.875282 |
| S       | 30.484436 | 29.836628 | 32.659294 |
| S       | 29.721411 | 31.447796 | 36.608601 |
| S       | 33.296597 | 27.414360 | 34.435551 |
| S       | 33.770302 | 32.527679 | 32.818031 |
| S       | 36.846672 | 28.932323 | 31.773544 |
| S       | 39.976574 | 26.530140 | 33.761215 |
| S       | 40.286716 | 31.157875 | 34.067451 |
| S       | 44.042049 | 28.485683 | 31.534483 |
| S       | 45.031265 | 26.361790 | 37.658134 |

24 generated by VMD

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 25.079363 | 29.412958 | 32.104889 |
| Ca      | 26.538055 | 30.928795 | 35.605572 |
| Ca      | 30.107285 | 28.704357 | 36.162056 |
| Ca      | 30.159586 | 32.819714 | 33.364185 |
| Ca      | 33.513313 | 29.511084 | 31.341936 |
| Ca      | 33.149330 | 30.707657 | 35.594440 |
| Ca      | 36.536011 | 26.420517 | 34.202034 |
| Ca      | 36.679367 | 31.302055 | 34.057137 |
| Ca      | 40.164810 | 29.090147 | 31.321602 |
| Ca      | 39.508411 | 28.808212 | 36.156952 |
| Ca      | 46.768570 | 29.329248 | 33.326797 |
| Ca      | 42.879425 | 29.101830 | 34.486141 |
| S       | 26.733500 | 27.738163 | 36.328518 |
| S       | 26.806019 | 33.975666 | 33.943306 |
| S       | 30.450630 | 29.757214 | 32.992252 |
| S       | 30.039175 | 31.872631 | 36.571686 |
| S       | 33.314651 | 27.608259 | 34.629852 |
| S       | 33.654942 | 32.612278 | 32.529194 |
| S       | 36.665657 | 28.982784 | 31.622169 |
| S       | 36.365334 | 29.162754 | 36.304226 |
| S       | 40.116913 | 26.621178 | 33.570316 |
| S       | 40.352489 | 31.182459 | 34.218601 |
| S       | 43.835110 | 28.311911 | 31.409985 |
| S       | 45.015892 | 26.429527 | 38.186840 |

24 generated by VMD

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 24.864857 | 29.753250 | 32.339638 |
| Ca      | 26.204414 | 30.952240 | 35.941399 |
| Ca      | 30.230787 | 28.405518 | 35.826359 |
| Ca      | 30.214012 | 33.117168 | 33.239613 |
|   | 1st Value   | 2nd Value   | 3rd Value   |
|---|-------------|-------------|-------------|
| Ca | 33.757393   | 29.418388   | 31.343557   |
| Ca | 33.116611   | 30.510578   | 34.105587   |
| Ca | 36.617279   | 26.818958   | 34.470695   |
| Ca | 40.108147   | 28.908377   | 31.526693   |
| Ca | 39.628235   | 29.133450   | 36.048645   |
| Ca | 46.785461   | 29.200485   | 33.321564   |
| Ca | 42.911892   | 28.934557   | 34.430473   |
| S  | 27.018955   | 27.656496   | 36.356297   |
| S  | 26.508133   | 33.874092   | 34.203907   |
| S  | 30.641140   | 29.935299   | 32.669441   |
| S  | 29.810299   | 31.460827   | 36.482262   |
| S  | 33.272587   | 27.449001   | 34.328007   |
| S  | 33.744919   | 32.691536   | 32.557701   |
| S  | 36.891491   | 28.950016   | 31.853191   |
| S  | 36.291660   | 29.433033   | 36.570564   |
| S  | 40.068115   | 26.620121   | 33.761696   |
| S  | 40.382645   | 31.220085   | 33.744286   |
| S  | 43.928143   | 28.248753   | 31.413706   |
| S  | 44.795601   | 26.355362   | 38.185867   |

24 generated by VMD

|   | 1st Value   | 2nd Value   | 3rd Value   |
|---|-------------|-------------|-------------|
| Ca | 24.802465   | 29.428459   | 32.291706   |
| Ca | 26.442253   | 31.041357   | 35.998154   |
| Ca | 30.368294   | 28.555874   | 36.144226   |
| Ca | 30.207272   | 32.929310   | 33.075512   |
| Ca | 33.352512   | 29.677195   | 31.241718   |
| Ca | 33.215385   | 30.766182   | 35.392956   |
| Ca | 36.472809   | 26.757553   | 34.249561   |
| Ca | 36.664082   | 31.314562   | 33.849163   |
| Ca | 40.338669   | 29.208000   | 31.233364   |
| Ca | 39.537521   | 28.720543   | 36.361645   |
| Ca | 46.849983   | 29.448473   | 33.466438   |
| Ca | 42.916531   | 28.984915   | 34.586185   |
| S  | 27.035868   | 27.746990   | 36.462433   |
| S  | 26.608322   | 33.744736   | 33.918289   |
| S  | 30.387762   | 29.752548   | 32.807125   |
| S  | 29.82871    | 31.782555   | 36.452316   |
| S  | 33.178741   | 27.473892   | 34.411266   |
| S  | 33.729485   | 32.640839   | 32.621265   |
| S  | 36.717075   | 29.113573   | 31.545681   |
| S  | 36.450745   | 29.332464   | 36.636539   |
| S  | 39.967049   | 26.604836   | 33.543720   |
| S  | 40.360104   | 30.904278   | 34.123974   |
| S  | 44.070782   | 28.365271   | 31.609169   |
| S  | 44.931259   | 26.096937   | 38.008350   |
|    |      |      |      |
|----|------|------|------|
| Ca | 25.043297 | 29.551310 | 32.416176 |
| Ca | 26.414982 | 30.780035 | 36.240005 |
| Ca | 30.162857 | 28.794048 | 35.842518 |
| Ca | 30.082897 | 33.160564 | 33.108002 |
| Ca | 33.513889 | 29.259644 | 31.189137 |
| Ca | 33.114815 | 30.751633 | 35.336411 |
| Ca | 36.538723 | 26.556944 | 34.260368 |
| Ca | 36.678612 | 31.203016 | 34.003109 |
| Ca | 40.374939 | 29.093525 | 31.456280 |
| Ca | 39.642769 | 28.795883 | 36.155563 |
| Ca | 46.645351 | 29.325630 | 33.411766 |
| Ca | 42.830185 | 29.093838 | 34.486645 |
| S  | 27.040600 | 27.595737 | 36.355965 |
| S  | 26.658730 | 33.816895 | 34.229965 |
| S  | 30.436531 | 29.914948 | 32.730629 |
| S  | 29.939482 | 31.962082 | 36.297596 |
| S  | 33.199863 | 27.636475 | 34.299351 |
| S  | 33.744202 | 32.508781 | 32.472057 |
| S  | 36.839390 | 28.784050 | 31.707081 |
| S  | 36.487000 | 29.277090 | 36.605068 |
| S  | 40.089317 | 26.662605 | 33.742363 |
| S  | 40.353180 | 31.081696 | 34.056404 |
| S  | 43.924801 | 28.576725 | 31.415928 |
| S  | 44.677490 | 26.208244 | 38.212219 |
|     |       |       |       |
|-----|-------|-------|-------|
| S   | 36.897133 | 28.656908 | 31.684710 |
| S   | 36.612457 | 29.419411 | 36.688454 |
| S   | 40.070938 | 26.480396 | 33.523041 |
| S   | 40.112431 | 30.980751 | 33.992615 |
| S   | 43.861015 | 28.392231 | 31.464169 |
| S   | 44.565758 | 26.373135 | 38.091900 |

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generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 24.658495 | 29.909620 | 32.500904 |
| Ca  | 26.560532 | 30.760994 | 36.137936 |
| Ca  | 30.154154 | 28.455482 | 35.456863 |
| Ca  | 30.109159 | 33.063271 | 33.346081 |
| Ca  | 33.765877 | 29.539722 | 31.122902 |
| Ca  | 33.192688 | 30.577152 | 35.376759 |
| Ca  | 36.657871 | 26.808729 | 34.396446 |
| Ca  | 36.646702 | 31.172970 | 33.770050 |
| Ca  | 40.227386 | 28.854204 | 31.455563 |
| Ca  | 39.698360 | 29.014185 | 36.488029 |
| Ca  | 46.706867 | 29.298067 | 33.395821 |
| Ca  | 42.717865 | 28.983398 | 34.526218 |
| S   | 26.934029 | 27.565966 | 36.327896 |
| S   | 26.809504 | 33.859268 | 34.301773 |
| S   | 30.592915 | 29.969337 | 32.611099 |
| S   | 29.963476 | 31.617685 | 36.363525 |
| S   | 33.184391 | 27.617496 | 34.071846 |
| S   | 33.665535 | 32.516144 | 32.590061 |
| S   | 36.734512 | 28.807644 | 31.470055 |
| S   | 36.536842 | 29.451508 | 36.552002 |
| S   | 40.041843 | 26.539698 | 34.026386 |
| S   | 40.236969 | 31.060467 | 34.006203 |
| S   | 43.559029 | 28.178667 | 31.480515 |
| S   | 45.078934 | 26.769753 | 38.255722 |

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generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 24.497652 | 29.850506 | 32.330708 |
| Ca  | 26.636034 | 30.827057 | 36.036644 |
| Ca  | 30.179817 | 28.447384 | 35.524242 |
| Ca  | 30.240749 | 33.039974 | 33.277687 |
| Ca  | 33.678757 | 29.423893 | 31.291189 |
| Ca  | 33.021355 | 30.611866 | 35.463383 |
| Ca  | 36.776741 | 26.808313 | 34.614071 |
| Ca  | 36.521400 | 31.286327 | 33.708691 |
| Ca  | 40.219826 | 28.801277 | 31.509705 |
| Ca  | 39.826950 | 29.124443 | 36.620537 |
| Ca  | 46.560692 | 29.206768 | 33.263214 |
| Ca  | 42.659172 | 28.977438 | 34.387497 |
|  | S | Ca |
|---|---|---|
| 24 | generated by VMD | generated by VMD |
| S | 26.866423 | 24.260492 |
| S | 26.805294 | 29.753229 |
| S | 30.415806 | 30.945007 |
| S | 30.029318 | 28.527672 |
| S | 33.314354 | 33.104389 |
| S | 33.630234 | 29.207544 |
| S | 36.653942 | 30.790442 |
| S | 36.724171 | 26.426889 |
| S | 40.126766 | 31.203583 |
| S | 40.175240 | 28.908508 |
| S | 43.648304 | 29.840567 |
| S | 45.224945 | 29.359173 |
| S | 26.835110 | 29.126692 |
| S | 26.817762 | 27.585762 |
| S | 30.249296 | 29.993855 |
| S | 30.021843 | 31.577551 |
| S | 33.391411 | 27.782169 |
| S | 33.645435 | 32.657009 |
| S | 36.634247 | 28.774429 |
| S | 36.718498 | 29.329733 |
| S | 40.213326 | 26.535442 |
| S | 40.220932 | 31.074715 |
| S | 43.762554 | 28.301701 |
| S | 45.014603 | 26.557766 |
| Element | X1     | Y1     | Z1     |
|---------|--------|--------|--------|
| Ca      | 36.68854 | 26.661879 | 34.522690 |
| Ca      | 36.621620 | 31.274967 | 33.934826 |
| Ca      | 40.045609 | 28.832653 | 31.458729 |
| Ca      | 39.734810 | 29.040569 | 36.482525 |
| Ca      | 46.606750 | 29.347324 | 33.108372 |
| Ca      | 42.897625 | 29.284624 | 34.440079 |
| S       | 26.999172 | 27.672478 | 34.169144 |
| S       | 26.803280 | 33.788006 | 34.095230 |
| S       | 30.288046 | 29.901899 | 32.435272 |
| S       | 30.214931 | 31.502481 | 36.120785 |
| S       | 33.340950 | 27.738468 | 34.037819 |
| S       | 33.570831 | 32.535633 | 32.514095 |
| S       | 36.549652 | 28.878160 | 31.911119 |
| S       | 36.633907 | 29.421368 | 36.852257 |
| S       | 39.984192 | 26.664865 | 34.102844 |
| S       | 40.329792 | 31.197704 | 34.008366 |
| S       | 43.601135 | 28.305103 | 31.510681 |
| S       | 44.839722 | 26.295502 | 38.138969 |

24

generated by VMD

| Element | X1     | Y1     | Z1     |
|---------|--------|--------|--------|
| Ca      | 24.474033 | 30.194534 | 32.353958 |
| Ca      | 26.469942 | 30.999172 | 36.027130 |
| Ca      | 29.819973 | 28.415228 | 35.487328 |
| Ca      | 30.158905 | 32.808479 | 33.569702 |
| Ca      | 33.631325 | 29.152187 | 31.360878 |
| Ca      | 33.262711 | 30.192402 | 35.582394 |
| Ca      | 36.495674 | 26.874458 | 34.553646 |
| Ca      | 36.684700 | 31.483620 | 33.827477 |
| Ca      | 40.342243 | 28.699284 | 31.506836 |
| Ca      | 39.901253 | 29.073048 | 36.187016 |
| Ca      | 46.699001 | 29.170660 | 33.262581 |
| Ca      | 42.792934 | 29.276186 | 34.353073 |
| S       | 26.718044 | 27.715588 | 36.080173 |
| S       | 27.035189 | 33.917454 | 34.184155 |
| S       | 30.501362 | 29.768772 | 32.592445 |
| S       | 29.956240 | 31.477823 | 36.427402 |
| S       | 33.175663 | 27.489183 | 34.081425 |
| S       | 33.601814 | 32.302017 | 32.645870 |
| S       | 36.895523 | 29.013229 | 31.800531 |
| S       | 36.589424 | 29.454361 | 36.689327 |
| S       | 40.064220 | 26.626040 | 33.923916 |
| S       | 40.312714 | 31.340279 | 33.649605 |
| S       | 43.890633 | 28.177784 | 31.503304 |
| S       | 44.986629 | 26.769606 | 38.380547 |

24

generated by VMD
|   |   |   |
|---|---|---|
| Ca | 24.608973 | 29.879339 | 32.402233 |
| Ca | 26.617920 | 30.848675 | 36.096828 |
| Ca | 30.012779 | 28.386932 | 35.634640 |
| Ca | 30.363194 | 32.971405 | 33.163239 |
| Ca | 33.556507 | 29.246593 | 31.355009 |
| Ca | 32.979912 | 30.680614 | 35.536606 |
| Ca | 36.232059 | 26.813995 | 34.485744 |
| Ca | 36.709610 | 31.318626 | 34.041206 |
| Ca | 40.324532 | 29.013374 | 31.472265 |
| Ca | 39.766960 | 28.944214 | 36.160477 |
| Ca | 46.869202 | 29.223103 | 33.297607 |
| Ca | 42.840824 | 29.132401 | 34.335762 |
| S  | 26.659718 | 27.584942 | 35.937492 |
| S  | 26.757864 | 33.803684 | 34.343559 |
| S  | 30.543489 | 29.844059 | 32.678883 |
| S  | 30.058945 | 31.707651 | 36.314831 |
| S  | 33.102051 | 27.416298 | 34.295544 |
| S  | 33.743176 | 32.475811 | 32.528015 |
| S  | 36.838120 | 28.945080 | 31.723148 |
| S  | 36.521271 | 29.521301 | 36.766338 |
| S  | 39.782028 | 26.584438 | 33.875217 |
| S  | 40.423817 | 31.224285 | 33.907253 |
| S  | 43.830494 | 28.192364 | 31.516373 |
| S  | 45.290501 | 26.632191 | 38.162422 |

24 generated by VMD

|   |   |   |
|---|---|---|
| Ca | 24.743788 | 29.941689 | 32.498856 |
| Ca | 26.355114 | 30.926373 | 35.979263 |
| Ca | 30.056652 | 28.603065 | 35.423794 |
| Ca | 30.192684 | 33.117451 | 33.045906 |
| Ca | 33.371510 | 29.084816 | 31.326963 |
| Ca | 33.162876 | 30.358578 | 35.498280 |
| Ca | 36.569866 | 26.579220 | 34.388657 |
| Ca | 36.693279 | 31.112644 | 34.065380 |
| Ca | 40.227390 | 28.905792 | 31.721613 |
| Ca | 39.883652 | 28.948914 | 36.405479 |
| Ca | 46.812889 | 29.291214 | 32.868393 |
| Ca | 42.964443 | 29.184923 | 34.438034 |
| S  | 26.875036 | 27.679798 | 36.174526 |
| S  | 26.925848 | 34.095490 | 34.221970 |
| S  | 30.292395 | 30.023413 | 32.454472 |
| S  | 29.915016 | 31.666588 | 36.229488 |
| S  | 33.218422 | 27.335598 | 34.315880 |
| S  | 33.636040 | 32.369938 | 32.547256 |
| S  | 36.707428 | 28.973858 | 31.751503 |
| S  | 36.509815 | 29.143381 | 36.834000 |
|  |  |  |  |
|---|---|---|---|
| S | 40.041534 | 26.722605 | 33.992195 |
| S | 40.236721 | 31.207624 | 34.102329 |
| S | 43.577267 | 28.291405 | 31.436106 |
| S | 45.464249 | 26.827055 | 38.310371 |

24

generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 24.995770 | 29.878906 | 32.189140 |
| Ca | 26.630848 | 31.013962 | 35.784267 |
| Ca | 29.656555 | 28.389568 | 35.430771 |
| Ca | 30.326248 | 33.074051 | 33.323242 |
| Ca | 33.633789 | 29.183784 | 31.493279 |
| Ca | 33.010017 | 30.198944 | 35.546116 |
| Ca | 36.575974 | 26.649734 | 34.519974 |
| Ca | 36.567028 | 31.115196 | 34.051468 |
| Ca | 40.071114 | 29.009212 | 31.401651 |
| Ca | 39.758778 | 29.100842 | 36.519104 |
| Ca | 46.711834 | 29.461861 | 33.003113 |
| Ca | 42.860916 | 29.202261 | 34.170544 |
| S | 26.447872 | 27.821941 | 36.263012 |
| S | 27.077583 | 34.058849 | 34.248775 |
| S | 30.497980 | 29.813583 | 32.628521 |
| S | 30.135820 | 31.538086 | 36.321495 |
| S | 33.316826 | 27.323544 | 34.352455 |
| S | 33.598312 | 32.385380 | 32.704643 |
| S | 36.771919 | 28.850124 | 31.784081 |
| S | 36.611557 | 29.544016 | 36.882553 |
| S | 40.097191 | 26.727781 | 33.912140 |
| S | 40.272041 | 31.144798 | 33.866001 |
| S | 43.790009 | 28.142490 | 31.244133 |
| S | 45.017906 | 26.762501 | 38.390244 |

24

generated by VMD

|  |  |  |  |
|---|---|---|---|
| Ca | 24.755648 | 29.957798 | 32.305450 |
| Ca | 26.526031 | 30.831741 | 35.879379 |
| Ca | 30.157925 | 28.468372 | 35.328552 |
| Ca | 30.095600 | 33.159931 | 33.218811 |
| Ca | 33.404949 | 29.031090 | 31.565010 |
| Ca | 33.211109 | 30.470509 | 35.704628 |
| Ca | 36.570183 | 26.846390 | 34.771698 |
| Ca | 36.575630 | 31.004200 | 34.125378 |
| Ca | 40.051651 | 28.861813 | 31.543972 |
| Ca | 39.852371 | 29.188942 | 36.331745 |
| Ca | 46.900822 | 29.059675 | 32.725922 |
| Ca | 42.794807 | 29.145435 | 34.097248 |
| S | 26.877327 | 27.602871 | 35.926586 |
| S | 26.778896 | 33.845211 | 33.970551 |
S  30.418650  29.915382  32.530682
S  29.937748  31.609806  36.164616
S  33.368088  27.717701  34.436508
S  33.562943  32.726822  32.770824
S  36.657356  28.859690  31.825420
S  36.474735  29.350838  37.224281
S  40.008568  26.742596  34.040798
S  40.401508  31.305531  33.922390
S  43.707966  28.104202  31.210846
S  45.343369  26.584881  38.409462

generated by VMD

Ca  25.267351  29.705990  32.003422
Ca  26.374187  31.077574  35.918159
Ca  30.067036  28.429367  35.579308
Ca  30.229517  33.021687  33.074123
Ca  33.502598  29.321423  31.298595
Ca  33.041492  30.625156  35.578491
Ca  36.517857  26.681692  34.709003
Ca  36.550854  30.703144  34.128632
Ca  40.250042  29.014297  31.590469
Ca  39.835934  28.905502  36.694130
Ca  46.735466  29.638741  32.285698
Ca  42.780972  28.973858  34.245312
S  26.877165  27.765285  36.366947
S  26.735983  33.911919  34.145294
S  30.411978  29.897194  32.672993
S  29.913378  31.728512  36.250107
S  33.307091  27.809059  34.176762
S  33.793720  32.559353  32.717632
S  36.735291  28.897049  31.676109
S  36.663109  29.103443  37.065048
S  39.868137  26.528284  33.980698
S  40.191380  31.184803  34.036190
S  43.528423  27.951588  31.339310
S  45.254921  26.956501  38.498257

generated by VMD

Ca  24.739738  30.113621  31.869507
Ca  26.554934  31.303707  35.934002
Ca  30.235367  27.878035  35.233765
Ca  30.118477  32.930931  33.421398
Ca  33.324215  29.190613  31.681538
Ca  33.141579  30.347366  35.479797
Ca  36.789787  26.745884  34.590076
Ca  36.747696  31.450539  34.243378
| Element | X-position | Y-position | Z-position |
|---------|------------|------------|------------|
| Ca      | 40.121956  | 28.593357  | 31.789156  |
| Ca      | 39.936733  | 28.017372  | 36.495728  |
| Ca      | 46.521660  | 29.226749  | 32.591011  |
| Ca      | 42.953369  | 29.185944  | 34.053402  |
| S       | 26.886415  | 27.832081  | 36.013588  |
| S       | 26.635626  | 34.166588  | 34.137920  |
| S       | 30.300688  | 29.656538  | 32.521107  |
| S       | 30.005615  | 31.361132  | 36.283405  |
| S       | 33.434532  | 27.406826  | 34.246445  |
| S       | 33.628880  | 32.642395  | 32.873528  |
| S       | 36.667812  | 29.075216  | 32.092850  |
| S       | 36.504456  | 29.407234  | 36.791695  |
| S       | 40.214649  | 26.578552  | 34.291992  |
| S       | 40.396523  | 31.239235  | 33.906887  |
| S       | 43.463699  | 27.837271  | 31.235130  |
| S       | 45.109550  | 27.204185  | 38.253349  |

24 generated by VMD

| Element | X-position | Y-position | Z-position |
|---------|------------|------------|------------|
| Ca      | 24.884775  | 29.906363  | 32.157997  |
| Ca      | 26.387320  | 30.912960  | 35.931385  |
| Ca      | 29.980700  | 28.464958  | 35.587551  |
| Ca      | 30.120872  | 33.227962  | 32.971409  |
| Ca      | 33.446064  | 29.141457  | 31.628031  |
| Ca      | 33.200691  | 30.496105  | 35.560287  |
| Ca      | 36.638561  | 26.618225  | 34.589130  |
| Ca      | 36.674149  | 31.301718  | 34.200497  |
| Ca      | 40.224609  | 28.803749  | 31.654245  |
| Ca      | 39.646194  | 29.069622  | 36.088165  |
| Ca      | 47.062744  | 29.186014  | 32.718071  |
| Ca      | 42.794708  | 28.918800  | 34.287243  |
| S       | 26.756748  | 27.619598  | 35.993420  |
| S       | 26.772715  | 33.837379  | 34.236458  |
| S       | 30.411385  | 29.871521  | 32.633461  |
| S       | 29.813206  | 31.582985  | 36.245403  |
| S       | 33.318478  | 27.508621  | 34.348831  |
| S       | 33.764278  | 32.671749  | 32.871216  |
| S       | 36.752209  | 28.978168  | 32.026459  |
| S       | 36.493530  | 29.446573  | 36.896584  |
| S       | 40.078854  | 26.581020  | 34.020012  |
| S       | 40.453659  | 31.307419  | 33.819542  |
| S       | 43.669216  | 28.095272  | 31.257259  |
| S       | 45.087673  | 26.843172  | 38.308025  |

24 generated by VMD

| Element | X-position | Y-position | Z-position |
|---------|------------|------------|------------|
| Ca      | 24.769299  | 29.884911  | 31.960011  |
| Ca      | 26.433958  | 30.922623  | 35.699520  |
| Ca       | 29.838667 | 28.448792 | 35.486462 |
|----------|-----------|-----------|-----------|
| Ca       | 30.284809 | 33.074600 | 33.213409 |
| Ca       | 33.657719 | 29.667965 | 31.627934 |
| Ca       | 33.145786 | 30.317732 | 35.453197 |
| Ca       | 36.527733 | 26.691845 | 35.074314 |
| Ca       | 36.842968 | 31.114393 | 34.257557 |
| Ca       | 40.152069 | 28.482164 | 31.488869 |
| Ca       | 40.021038 | 29.195038 | 36.290218 |
| Ca       | 46.607327 | 29.361465 | 32.572281 |
| Ca       | 42.925060 | 29.172091 | 34.108734 |
| S        | 26.747108 | 27.622181 | 35.755714 |
| S        | 26.974340 | 33.986393 | 34.388145 |
| S        | 30.582211 | 29.908195 | 32.580544 |
| S        | 29.837021 | 31.490461 | 36.242085 |
| S        | 33.183647 | 27.326660 | 34.315028 |
| S        | 33.625641 | 32.657989 | 32.980495 |
| S        | 36.697124 | 28.730080 | 32.132286 |
| S        | 36.619350 | 29.496563 | 37.000183 |
| S        | 39.960247 | 26.564842 | 34.202499 |
| S        | 40.319275 | 31.153694 | 33.719566 |
| S        | 43.552189 | 27.967564 | 31.271374 |
| S        | 45.379356 | 27.153255 | 38.210098 |
| 24 generated by VMD |
| Ca       | 24.789112 | 29.805573 | 32.044937 |
| Ca       | 26.480457 | 31.043530 | 35.699448 |
| Ca       | 29.959003 | 28.381994 | 35.505047 |
| Ca       | 30.182720 | 33.271271 | 33.273746 |
| Ca       | 33.741112 | 29.396633 | 31.807362 |
| Ca       | 33.024521 | 30.518093 | 35.619347 |
| Ca       | 36.592724 | 26.495213 | 34.573318 |
| Ca       | 36.752876 | 31.346237 | 34.363941 |
| Ca       | 40.057129 | 28.394989 | 31.593800 |
| Ca       | 39.796360 | 29.065517 | 36.165386 |
| Ca       | 46.724339 | 29.433834 | 32.724682 |
| Ca       | 42.699512 | 28.979965 | 34.112644 |
| S        | 26.811131 | 27.643181 | 35.794937 |
| S        | 26.901665 | 33.920399 | 34.021198 |
| S        | 30.497946 | 30.071978 | 32.762856 |
| S        | 29.761530 | 31.473217 | 36.399647 |
| S        | 33.300655 | 27.500854 | 34.308247 |
| S        | 33.665359 | 32.645382 | 33.082527 |
| S        | 36.946903 | 28.845018 | 32.123383 |
| S        | 36.525536 | 29.256668 | 36.790123 |
| S        | 39.960007 | 26.330849 | 34.082760 |
| S        | 40.383327 | 31.049702 | 33.679123 |
|    |    |    |    |    |    |
|---|---|---|---|---|---|
| S  | 43.474773 | 28.113499 | 31.148643 |
| S  | 45.405300 | 27.407827 | 38.353607 |

24

generated by VMD

| Ca   |    |    |    |    |    |
|------|---|---|---|---|---|
|      | 25.039307 | 30.119831 | 32.142536 |
|      | 26.437874 | 30.954861 | 35.830585 |
|      | 29.760208 | 28.327732 | 35.466251 |
|      | 30.285454 | 32.906387 | 33.545982 |
|      | 33.626312 | 29.757206 | 31.415956 |
|      | 32.887596 | 30.614666 | 35.441902 |
|      | 36.404797 | 26.406101 | 34.751358 |
|      | 36.640049 | 30.868996 | 34.110447 |
|      | 40.177937 | 28.320654 | 31.789307 |
|      | 39.869450 | 29.015575 | 36.338253 |
|      | 46.882450 | 29.490425 | 32.775089 |
|      | 43.002926 | 29.110472 | 34.044693 |
| S    | 26.704626 | 27.622410 | 35.961491 |
| S    | 26.990660 | 33.990093 | 34.187248 |
| S    | 30.424089 | 30.050934 | 32.453190 |
| S    | 29.786554 | 31.397972 | 36.414604 |
| S    | 32.979824 | 27.648960 | 34.236561 |
| S    | 33.808903 | 32.865433 | 32.953102 |
| S    | 36.710110 | 28.558283 | 31.948919 |
| S    | 36.419624 | 29.127174 | 36.835655 |
| S    | 40.081600 | 26.432426 | 34.222946 |
| S    | 40.316319 | 31.050678 | 33.722015 |
| S    | 43.696857 | 27.970097 | 31.257839 |
| S    | 45.500374 | 27.784008 | 38.184776 |

24

generated by VMD

| Ca   |    |    |    |    |    |
|------|---|---|---|---|---|
|      | 25.275036 | 29.561186 | 31.657269 |
|      | 26.363396 | 30.875662 | 35.757671 |
|      | 29.846947 | 28.614582 | 35.555138 |
|      | 30.392275 | 33.378094 | 33.447250 |
|      | 33.767410 | 29.827499 | 31.564983 |
|      | 32.952324 | 30.617901 | 35.605583 |
|      | 36.370632 | 26.170769 | 34.558605 |
|      | 36.671455 | 31.182755 | 34.445221 |
|      | 40.302364 | 28.189056 | 31.385214 |
|      | 39.937729 | 29.024170 | 36.418648 |
|      | 46.727718 | 29.570662 | 32.539055 |
|      | 42.837837 | 28.957478 | 34.097527 |
| S    | 26.551929 | 27.584658 | 36.168934 |
| S    | 26.855907 | 33.751141 | 33.962528 |
| S    | 30.488297 | 30.185497 | 32.622143 |
| S    | 29.683081 | 31.776894 | 36.441933 |
|    |          |          |          |
|----|----------|----------|----------|
|    | 33.116329| 27.794765| 34.226688|
|    | 33.751934| 32.799030| 33.186737|
|    | 36.694866| 28.684187| 32.092892|
|    | 36.393372| 37.039944|
|    | 39.978992| 34.273106|
|    | 40.202686| 33.798897|
|    | 43.552261| 31.189005|
|    | 45.719120| 37.995678|
| 24 |          |          |          |
|    | generated by VMD |
| Ca | 25.550671| 29.991116| 31.739412|
| Ca | 26.193026| 30.849751| 35.804878|
| Ca | 29.894508| 35.845890|
| Ca | 30.321095| 33.324150| 33.385036|
| Ca | 33.795273| 31.405067|
| Ca | 32.986263| 35.641273|
| Ca | 36.295109| 34.621635|
| Ca | 36.678482| 34.167652|
| Ca | 40.255589| 31.666119|
| Ca | 39.682644| 36.280510|
| Ca | 46.757835| 32.448185|
| Ca | 43.094414| 34.180492|
|    | generated by VMD |
| S  | 26.838301| 27.545418| 36.173843|
| S  | 26.733093| 34.239143|
| S  | 30.537924| 32.913158|
| S  | 29.650414| 36.441967|
| S  | 33.062767| 34.062737|
| S  | 33.719776| 32.764381|
| S  | 36.781525| 31.883789|
| S  | 36.265850| 36.805496|
| S  | 39.959637| 34.307148|
| S  | 40.338375| 33.740707|
| S  | 43.532433| 31.187878|
| S  | 45.008835| 38.324245|
| 24 |          |          |          |
|    | generated by VMD |
| Ca | 25.176058| 32.069656|
| Ca | 26.424576| 35.772007|
| Ca | 30.110550| 35.337349|
| Ca | 30.135948| 33.630714|
| Ca | 33.613308| 31.454967|
| Ca | 33.144215| 35.332436|
| Ca | 36.631290| 34.898006|
| Ca | 36.719166| 34.090122|
| Ca | 40.112305| 31.505598|
| Ca | 39.871960| 36.266579|
| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 46.735420 | 29.528587 | 32.821693 |
| Ca      | 42.890728 | 28.848833 | 34.186527 |
| S       | 26.996321 | 27.549915 | 36.115543 |
| S       | 26.700188 | 34.099072 | 34.495308 |
| S       | 30.382524 | 30.064518 | 32.626945 |
| S       | 29.961353 | 31.342690 | 36.358192 |
| S       | 33.127541 | 27.583084 | 33.909359 |
| S       | 33.506031 | 32.989120 | 32.794888 |
| S       | 36.778385 | 28.524879 | 32.041126 |
| S       | 36.369499 | 29.273605 | 36.768761 |
| S       | 40.011177 | 26.124451 | 34.095444 |
| S       | 40.303860 | 30.949818 | 33.498074 |
| S       | 43.515831 | 28.018795 | 31.386755 |
| S       | 45.215614 | 27.884657 | 38.574684 |

24 generated by VMD

| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 25.777941 | 30.149122 | 31.976261 |
| Ca      | 26.073338 | 30.740225 | 36.052990 |
| Ca      | 30.026449 | 28.384472 | 35.528297 |
| Ca      | 30.551445 | 33.076035 | 33.458233 |
| Ca      | 33.799515 | 29.542242 | 31.222778 |
| Ca      | 33.217659 | 30.393078 | 35.313164 |
| Ca      | 36.374454 | 26.716892 | 34.682625 |
| Ca      | 36.598412 | 31.417423 | 34.238667 |
| Ca      | 39.944111 | 27.980637 | 31.278700 |
| Ca      | 39.956406 | 29.438301 | 36.394203 |
| Ca      | 46.501194 | 29.839346 | 33.084076 |
| Ca      | 42.553070 | 28.784170 | 34.176956 |
| S       | 26.743036 | 27.400627 | 36.031631 |
| S       | 27.043373 | 33.819775 | 34.625156 |
| S       | 30.626154 | 30.118027 | 32.703751 |
| S       | 29.791998 | 31.388767 | 36.446831 |
| S       | 33.223469 | 27.602592 | 33.879642 |
| S       | 33.794373 | 32.825188 | 32.729271 |
| S       | 36.716599 | 28.854900 | 32.032784 |
| S       | 36.450165 | 29.434006 | 36.760971 |
| S       | 39.972851 | 26.433395 | 34.362030 |
| S       | 40.143494 | 30.657425 | 33.280312 |
| S       | 43.378178 | 27.963375 | 31.118855 |
| S       | 45.176155 | 27.431370 | 38.556164 |

24 generated by VMD

| Element | X1 | Y1 | Z1 |
|---------|----|----|----|
| Ca      | 25.542479 | 30.014893 | 31.734255 |
| Ca      | 26.331951 | 30.779922 | 35.859070 |
| Ca      | 30.139404 | 28.467861 | 35.601379 |
| Ca      | 30.377974 | 33.172569 | 33.707596 |
| Element | Ca  | 33.763855 | 29.407475 | 31.164352 |
|---------|-----|-----------|-----------|-----------|
|         | Ca  | 33.043713 | 30.759800 | 35.693993 |
|         | Ca  | 36.346790 | 26.560913 | 34.540123 |
|         | Ca  | 36.656242 | 31.049038 | 34.081963 |
|         | Ca  | 40.268623 | 28.066063 | 31.386131 |
|         | Ca  | 39.936302 | 29.386703 | 36.547256 |
|         | Ca  | 46.349236 | 29.829395 | 32.713684 |
|         | Ca  | 42.610840 | 28.691242 | 34.308876 |
|         | S   | 26.860281 | 27.481480 | 36.052338 |
|         | S   | 26.945744 | 33.838337 | 34.405045 |
|         | S   | 30.629648 | 30.189564 | 32.777306 |
|         | S   | 29.819984 | 31.461754 | 36.666931 |
|         | S   | 33.125740 | 27.726387 | 34.130760 |
|         | S   | 33.771469 | 32.739105 | 32.755951 |
|         | S   | 36.703175 | 28.548573 | 31.834238 |
|         | S   | 36.429199 | 29.226467 | 36.699776 |
|         | S   | 39.862564 | 26.417965 | 34.376575 |
|         | S   | 40.272148 | 30.905376 | 33.372829 |
|         | S   | 43.499344 | 28.067142 | 31.239973 |
|         | S   | 45.147171 | 27.603374 | 38.386356 |

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generated by VMD

| Element | Ca  | 25.327030 | 30.161299 | 31.872547 |
|---------|-----|-----------|-----------|-----------|
|         | Ca  | 26.340200 | 30.998503 | 35.842262 |
|         | Ca  | 30.147947 | 28.243874 | 35.443207 |
|         | Ca  | 30.402409 | 33.321358 | 33.748932 |
|         | Ca  | 33.588993 | 29.337885 | 31.238335 |
|         | Ca  | 32.984280 | 30.184591 | 35.496666 |
|         | Ca  | 36.457279 | 26.670349 | 34.639622 |
|         | Ca  | 36.542873 | 31.065548 | 33.981529 |
|         | Ca  | 40.239285 | 28.213634 | 31.465324 |
|         | Ca  | 39.842396 | 29.114286 | 36.315086 |
|         | Ca  | 46.445354 | 29.900890 | 32.978146 |
|         | Ca  | 42.860191 | 28.612251 | 34.092121 |
|         | S   | 26.877727 | 27.529942 | 36.142059 |
|         | S   | 26.926533 | 34.187855 | 34.607464 |
|         | S   | 30.506184 | 30.123266 | 32.672680 |
|         | S   | 29.982128 | 31.471889 | 36.540333 |
|         | S   | 33.170284 | 27.437515 | 33.986900 |
|         | S   | 33.610218 | 32.616516 | 32.653111 |
|         | S   | 36.869579 | 28.643429 | 32.078709 |
|         | S   | 36.402397 | 29.302799 | 36.796181 |
|         | S   | 40.018242 | 26.290241 | 34.319046 |
|         | S   | 40.292542 | 31.010588 | 33.407383 |
|         | S   | 43.660820 | 28.159615 | 31.142899 |
|         | S   | 44.939445 | 27.793308 | 38.570164 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.361794    | 29.965729    | 32.186146    |
| Ca      | 26.313957    | 30.940548    | 36.245533    |
| Ca      | 29.891628    | 28.271160    | 35.441193    |
| Ca      | 30.172726    | 33.192356    | 33.491352    |
| Ca      | 33.856632    | 29.545012    | 31.127151    |
| Ca      | 36.279808    | 26.702961    | 34.390831    |
| Ca      | 36.756760    | 31.281820    | 33.972382    |
| Ca      | 40.334438    | 28.253033    | 31.325989    |
| Ca      | 39.779709    | 29.134745    | 36.341225    |
| Ca      | 46.323414    | 29.725605    | 33.372322    |
| Ca      | 42.708221    | 28.643702    | 34.300259    |
| Ca      | 26.879269    | 27.591745    | 36.347797    |
| Ca      | 26.935976    | 33.943123    | 34.648296    |
| Ca      | 30.603292    | 30.082195    | 32.631218    |
| Ca      | 29.981054    | 31.467827    | 36.448307    |
| Ca      | 33.028236    | 27.488449    | 33.787792    |
| Ca      | 33.769341    | 32.591049    | 32.676056    |
| Ca      | 36.913876    | 28.798965    | 31.753654    |
| Ca      | 36.500969    | 29.378628    | 36.625359    |
| Ca      | 39.881363    | 26.241734    | 33.985603    |
| Ca      | 40.481735    | 30.951786    | 33.621208    |
| Ca      | 43.719074    | 28.166553    | 31.212109    |
| Ca      | 44.935982    | 27.701324    | 38.593155    |

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generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.278521    | 30.391098    | 32.162903    |
| Ca      | 26.218054    | 31.081684    | 36.201984    |
| Ca      | 29.816692    | 28.277618    | 35.578487    |
| Ca      | 30.168301    | 33.013756    | 33.453018    |
| Ca      | 33.690071    | 29.265724    | 31.016119    |
| Ca      | 33.062031    | 30.078239    | 35.070934    |
| Ca      | 36.591755    | 26.495436    | 34.471405    |
| Ca      | 36.722553    | 31.355944    | 34.164440    |
| Ca      | 40.269279    | 28.203585    | 31.658642    |
| Ca      | 39.821678    | 29.204926    | 36.380562    |
| Ca      | 46.623466    | 29.972519    | 32.869854    |
| Ca      | 43.077278    | 28.908913    | 34.209457    |
| S       | 26.714079    | 27.723370    | 36.249577    |
| S       | 27.027512    | 34.124302    | 34.523457    |
| S       | 30.450338    | 29.907654    | 32.732548    |
| S       | 29.889549    | 31.557446    | 36.569565    |
| S       | 33.100349    | 27.199295    | 33.905819    |
| S       | 33.700806    | 32.508446    | 32.562244    |
| X  | Y     | Z     |
|----|-------|-------|
| S  | 36.87300 | 28.837427 | 31.937557 |
| S  | 36.311089 | 29.247288 | 36.518105 |
| S  | 39.975052 | 26.193909 | 34.471855 |
| S  | 40.355740 | 31.181730 | 33.529675 |
| S  | 43.822849 | 28.263544 | 31.267857 |
| S  | 44.868591 | 27.397526 | 38.524574 |

24 generated by VMD

| X  | Y     | Z     |
|----|-------|-------|
| Ca | 25.210579 | 30.113998 | 32.006851 |
| Ca | 26.735998 | 30.570210 | 36.140728 |
| Ca | 30.079056 | 28.427746 | 35.528366 |
| Ca | 30.023796 | 33.073940 | 33.396393 |
| Ca | 33.894707 | 29.299950 | 31.260868 |
| Ca | 33.004318 | 30.529045 | 35.659096 |
| Ca | 36.364437 | 26.972130 | 34.472939 |
| Ca | 36.546032 | 31.285656 | 33.881084 |
| Ca | 40.362141 | 28.212181 | 31.452141 |
| Ca | 39.778744 | 29.244987 | 36.248409 |
| Ca | 46.620991 | 29.618591 | 32.973846 |
| Ca | 42.849506 | 28.589878 | 34.216408 |
| S  | 26.739756 | 27.522099 | 35.882664 |
| S  | 26.962091 | 33.791374 | 34.796482 |
| S  | 30.500454 | 30.066799 | 32.618912 |
| S  | 29.959656 | 31.611866 | 36.402466 |
| S  | 33.091248 | 27.652964 | 34.394840 |
| S  | 33.634132 | 32.607258 | 32.637093 |
| S  | 36.889568 | 28.801674 | 31.813971 |
| S  | 36.436787 | 29.558271 | 36.661995 |
| S  | 39.801075 | 26.436172 | 34.220127 |
| S  | 40.401402 | 31.174160 | 33.504631 |
| S  | 43.721535 | 28.071484 | 31.250422 |
| S  | 44.825924 | 27.159000 | 38.609928 |

24 generated by VMD

| X  | Y     | Z     |
|----|-------|-------|
| Ca | 25.136276 | 29.933556 | 32.330547 |
| Ca | 26.579441 | 30.566734 | 36.036697 |
| Ca | 29.976278 | 28.364771 | 35.411324 |
| Ca | 30.279171 | 33.059952 | 33.532906 |
| Ca | 33.709652 | 29.571304 | 31.241045 |
| Ca | 33.136776 | 30.518927 | 35.338631 |
| Ca | 36.397221 | 26.936798 | 34.624851 |
| Ca | 36.716599 | 31.419395 | 33.862656 |
| Ca | 40.185261 | 28.289377 | 31.294043 |
| Ca | 39.975151 | 29.262119 | 36.517597 |
| Ca | 46.393066 | 29.545387 | 33.333984 |
| Ca | 42.700985 | 28.374615 | 34.157063 |
| S   | 26.839802 | 27.402611 | 35.941914 |
|----|-----------|-----------|-----------|
| S   | 26.930428 | 33.748554 | 34.705414 |
| S   | 30.537861 | 30.123135 | 32.540951 |
| S   | 30.020149 | 31.395611 | 36.565987 |
| S   | 33.168743 | 27.683208 | 34.056793 |
| S   | 33.595314 | 32.831184 | 32.644108 |
| S   | 36.843136 | 28.837238 | 31.811020 |
| S   | 36.454147 | 29.680784 | 36.642197 |
| S   | 39.757191 | 26.575623 | 34.251163 |
| S   | 40.509590 | 30.991409 | 33.387154 |
| S   | 43.739487 | 28.072407 | 31.201134 |
| S   | 44.852158 | 27.206715 | 38.601521 |

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generated by VMD

| Ca  | 25.395515 | 29.912495 | 31.927620 |
|-----|-----------|-----------|-----------|
| Ca  | 26.346554 | 30.723976 | 36.040691 |
| Ca  | 29.926319 | 28.299107 | 35.696190 |
| Ca  | 30.172045 | 33.056885 | 33.725159 |
| Ca  | 33.794037 | 29.519058 | 31.406006 |
| Ca  | 33.137592 | 30.585131 | 35.510944 |
| Ca  | 36.338726 | 27.074757 | 34.514374 |
| Ca  | 36.778328 | 31.383438 | 33.760574 |
| Ca  | 40.293465 | 28.123425 | 31.159973 |
| Ca  | 39.815304 | 28.988451 | 36.239319 |
| Ca  | 46.595818 | 29.703274 | 33.464787 |
| Ca  | 42.705437 | 28.826675 | 34.002125 |
| S   | 26.610697 | 27.444374 | 36.090576 |
| S   | 26.889555 | 33.755280 | 34.619133 |
| S   | 30.666382 | 30.073463 | 32.819199 |
| S   | 30.134439 | 31.460392 | 36.608860 |
| S   | 33.240738 | 27.424831 | 34.220230 |
| S   | 33.716919 | 32.730316 | 32.707977 |
| S   | 36.877449 | 28.993088 | 31.804985 |
| S   | 36.494938 | 29.754932 | 36.405861 |
| S   | 39.751953 | 26.494499 | 33.987549 |
| S   | 40.486732 | 31.074657 | 33.440392 |
| S   | 43.910118 | 27.998177 | 31.178946 |
| S   | 44.354820 | 26.990715 | 38.699280 |

24

generated by VMD

| Ca  | 24.740269 | 29.995573 | 32.357311 |
|-----|-----------|-----------|-----------|
| Ca  | 26.519470 | 30.845100 | 36.038082 |
| Ca  | 30.021397 | 28.477962 | 35.559475 |
| Ca  | 30.225328 | 32.962578 | 33.538582 |
| Ca  | 34.003601 | 29.356579 | 31.237171 |
| Ca  | 32.979572 | 30.694912 | 35.470566 |
|   |   |   |   |
|---|---|---|---|
| Ca | 36.440918 | 26.740265 | 34.497196 |
| Ca | 36.703300 | 31.007944 | 33.956379 |
| Ca | 40.409748 | 28.376492 | 31.144676 |
| Ca | 39.868389 | 28.928558 | 36.337498 |
| Ca | 46.551712 | 29.996925 | 33.330456 |
| Ca | 42.856533 | 28.657160 | 34.155895 |
| S  | 26.825014 | 27.589165 | 36.092289 |
| S  | 26.835857 | 33.923975 | 34.653912 |
| S  | 30.619095 | 29.992586 | 32.673798 |
| S  | 30.017727 | 31.517925 | 36.476471 |
| S  | 33.178425 | 27.722670 | 34.246590 |
| S  | 33.611145 | 32.598392 | 32.469173 |
| S  | 36.929203 | 28.735107 | 31.649555 |
| S  | 36.441410 | 29.423306 | 36.560051 |
| S  | 40.030258 | 26.497471 | 33.957680 |
| S  | 40.406635 | 30.987547 | 33.541386 |
| S  | 43.833752 | 28.317722 | 31.163870 |
| S  | 44.385170 | 27.040112 | 38.922623 |

24

generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 24.920115 | 30.362230 | 32.330448 |
| Ca | 26.441536 | 31.056587 | 36.156452 |
| Ca | 29.928431 | 28.115326 | 35.570744 |
| Ca | 30.139095 | 32.885281 | 33.381058 |
| Ca | 33.999874 | 29.365479 | 31.562820 |
| Ca | 33.025169 | 30.451176 | 35.508831 |
| Ca | 36.463112 | 26.866047 | 34.519459 |
| Ca | 36.706554 | 31.730602 | 33.903641 |
| Ca | 40.507599 | 28.162329 | 31.174870 |
| Ca | 39.459911 | 28.906422 | 35.872406 |
| Ca | 46.698013 | 30.119125 | 33.247925 |
| Ca | 42.761898 | 28.670197 | 34.307419 |
| S  | 26.602608 | 27.642632 | 35.984222 |
| S  | 27.066605 | 34.095776 | 34.575092 |
| S  | 30.464794 | 29.754837 | 32.762634 |
| S  | 29.899517 | 31.177631 | 36.398136 |
| S  | 33.271324 | 27.447380 | 34.294586 |
| S  | 33.523903 | 32.486511 | 32.581100 |
| S  | 37.174675 | 28.922081 | 31.907206 |
| S  | 36.505112 | 29.642509 | 36.541927 |
| S  | 40.021259 | 26.301708 | 33.786297 |
| S  | 40.333504 | 31.111982 | 33.567719 |
| S  | 43.964523 | 28.107643 | 31.462471 |
| S  | 44.554794 | 27.009943 | 38.633297 |

24

generated by VMD
|  | Ca       | 24.638662 | 30.208866 | 32.418056 |
|  | Ca       | 26.566467 | 31.362019 | 35.606369 |
|  | Ca       | 30.177654 | 28.027151 | 35.603409 |
|  | Ca       | 30.215240 | 32.734093 | 33.545258 |
|  | Ca       | 33.660378 | 28.968370 | 31.307693 |
|  | Ca       | 33.069729 | 30.724865 | 35.514229 |
|  | Ca       | 36.361294 | 26.642937 | 34.261147 |
|  | Ca       | 36.625114 | 31.423800 | 34.333183 |
|  | Ca       | 40.379097 | 28.540394 | 31.139677 |
|  | Ca       | 39.535198 | 28.812445 | 36.216415 |
|  | Ca       | 46.789875 | 30.001736 | 33.085892 |
|  | Ca       | 42.766350 | 28.929329 | 34.363914 |
|  | S        | 26.760941 | 27.718084 | 36.138741 |
|  | S        | 27.024946 | 34.288109 | 34.216362 |
|  | S        | 30.560209 | 29.711319 | 32.72016 |
|  | S        | 30.098068 | 31.557697 | 36.461407 |
|  | S        | 33.281383 | 27.464323 | 34.551888 |
|  | S        | 33.558643 | 32.351898 | 32.616566 |
|  | S        | 36.958233 | 28.956545 | 31.922476 |
|  | S        | 36.427792 | 29.036076 | 36.530312 |
|  | S        | 39.87329 | 26.435600 | 33.811378 |
|  | S        | 40.338348 | 31.048914 | 33.698940 |
|  | S        | 43.891239 | 28.324871 | 31.436348 |
|  | S        | 44.875839 | 27.121952 | 38.524063 |

24 generated by VMD

|  | Ca       | 24.683102 | 30.240421 | 32.520256 |
|  | Ca       | 26.564102 | 31.203300 | 36.265736 |
|  | Ca       | 30.205976 | 28.103722 | 35.690010 |
|  | Ca       | 30.261965 | 32.667328 | 33.249908 |
|  | Ca       | 33.736660 | 29.150818 | 31.016678 |
|  | Ca       | 33.037231 | 30.597908 | 35.127056 |
|  | Ca       | 36.419102 | 26.577553 | 34.160484 |
|  | Ca       | 36.714348 | 31.333324 | 33.985058 |
|  | Ca       | 40.307060 | 28.866449 | 31.465553 |
|  | Ca       | 39.660339 | 29.079273 | 36.492897 |
|  | Ca       | 46.607361 | 29.314581 | 33.225403 |
|  | Ca       | 42.779499 | 28.860126 | 34.476101 |
|  | S        | 26.752964 | 27.782845 | 36.206635 |
|  | S        | 27.071606 | 34.123886 | 34.534775 |
|  | S        | 30.378969 | 29.535217 | 32.551304 |
|  | S        | 30.137384 | 31.448971 | 36.368366 |
|  | S        | 33.199585 | 27.470726 | 34.083817 |
|  | S        | 33.665894 | 32.329376 | 32.309593 |
|  | S        | 36.930878 | 29.025629 | 31.892799 |
|  | S        | 36.412823 | 29.226509 | 36.494026 |
| S  | 39.906010  | 26.594181  | 33.941250 |
|----|------------|------------|-----------|
| S  | 40.361626  | 31.237719  | 33.948044 |
| S  | 43.590015  | 28.462954  | 31.478401 |
| S  | 45.049477  | 27.158556  | 38.546570 |

24

generated by VMD

| Ca | 24.613129  | 30.018776  | 32.612934 |
|----|------------|------------|-----------|
| Ca | 26.493906  | 31.281677  | 35.958954 |
| Ca | 30.097454  | 28.117218  | 35.609100 |
| Ca | 30.435844  | 32.900887  | 33.338047 |
| Ca | 33.903938  | 28.903824  | 31.033791 |
| Ca | 32.974552  | 30.454853  | 35.426975 |
| Ca | 36.564156  | 26.810635  | 34.192261 |
| Ca | 36.667622  | 31.201294  | 34.075752 |
| Ca | 40.245964  | 28.888657  | 31.626087 |
| Ca | 39.466511  | 28.816574  | 36.271202 |
| Ca | 46.648098  | 29.563469  | 33.057434 |
| Ca | 42.950405  | 29.032022  | 34.433449 |
| S  | 26.873650  | 27.930149  | 36.445015 |
| S  | 27.093472  | 34.019100  | 34.197968 |
| S  | 30.640585  | 29.787598  | 32.561939 |
| S  | 29.941967  | 31.453049  | 36.323845 |
| S  | 33.274593  | 27.451374  | 34.189671 |
| S  | 33.759315  | 32.405544  | 32.622223 |
| S  | 36.937809  | 29.022919  | 31.787407 |
| S  | 36.374672  | 29.181271  | 36.666962 |
| S  | 40.025322  | 26.485807  | 33.683926 |
| S  | 40.222820  | 31.161163  | 34.009502 |
| S  | 43.632652  | 28.402458  | 31.274883 |
| S  | 44.595390  | 27.101116  | 38.631390 |

24

generated by VMD

| Ca | 24.915253  | 30.130093  | 32.435795 |
|----|------------|------------|-----------|
| Ca | 26.432262  | 30.792843  | 36.296585 |
| Ca | 29.895266  | 28.355167  | 35.646080 |
| Ca | 30.436380  | 32.985378  | 33.337757 |
| Ca | 33.657650  | 29.050407  | 31.073290 |
| Ca | 33.131550  | 30.495148  | 35.396683 |
| Ca | 36.365974  | 26.905575  | 34.463104 |
| Ca | 36.782894  | 31.398245  | 33.886051 |
| Ca | 40.435192  | 28.658192  | 31.518108 |
| Ca | 39.570843  | 29.093521  | 36.169292 |
| Ca | 46.802311  | 29.435757  | 33.066307 |
| Ca | 42.860344  | 29.025713  | 34.368053 |
| S  | 26.574594  | 27.619041  | 36.049438 |
| S  | 27.185602  | 33.822624  | 34.594879 |
|   | 30.584414 | 29.826315 | 32.641464 |
|---|-----------|-----------|-----------|
| S | 29.952127 | 31.503366 | 36.426670 |
| S | 33.132542 | 27.403111 | 34.234715 |
| S | 33.712589 | 32.389832 | 32.400150 |
| S | 37.028328 | 28.928043 | 31.787292 |
| S | 36.448446 | 29.614677 | 36.551971 |
| S | 39.868446 | 31.359123 | 33.739033 |
| S | 43.862217 | 28.258465 | 31.418089 |
| S | 44.431301 | 26.764557 | 38.584049 |

24 generated by VMD

| Ca  | 25.034863 | 30.204851 | 32.436905 |
|-----|-----------|-----------|-----------|
| Ca  | 26.307640 | 30.594429 | 36.257202 |
| Ca  | 30.090929 | 28.443621 | 35.726711 |
| Ca  | 30.408619 | 33.108627 | 33.198662 |
| Ca  | 33.701969 | 29.184284 | 31.248802 |
| Ca  | 33.029377 | 30.528345 | 35.375374 |
| Ca  | 36.479832 | 26.968153 | 34.467556 |
| Ca  | 36.845158 | 31.278320 | 34.023659 |
| Ca  | 40.443111 | 28.622473 | 31.326237 |
| Ca  | 39.459171 | 29.009365 | 36.198425 |
| Ca  | 46.632286 | 29.636406 | 33.282520 |
| Ca  | 42.861427 | 28.862198 | 34.315140 |
| S   | 26.877600 | 27.271084 | 36.047455 |
| S   | 27.017324 | 33.985054 | 34.662369 |
| S   | 30.558048 | 29.917501 | 32.698586 |
| S   | 29.780149 | 31.606884 | 36.433266 |
| S   | 33.127979 | 27.487141 | 34.292789 |
| S   | 33.757637 | 32.510750 | 32.092808 |
| S   | 37.082520 | 28.934259 | 32.005135 |
| S   | 36.384373 | 29.516310 | 36.609425 |
| S   | 39.907951 | 26.543087 | 33.999992 |
| S   | 40.525314 | 31.223585 | 33.498966 |
| S   | 43.714165 | 28.296309 | 31.371395 |
| S   | 44.406399 | 26.658367 | 38.461273 |

24 generated by VMD

| Ca  | 24.948982 | 29.880909 | 32.803623 |
|-----|-----------|-----------|-----------|
| Ca  | 26.532396 | 30.674583 | 36.269352 |
| Ca  | 29.858130 | 28.487015 | 35.688862 |
| Ca  | 30.201296 | 33.044018 | 33.065914 |
| Ca  | 33.728611 | 29.276852 | 31.086372 |
| Ca  | 33.147038 | 30.363110 | 35.268471 |
| Ca  | 36.552685 | 26.941212 | 34.381817 |
| Ca  | 36.721497 | 31.506405 | 34.151459 |
| Element | X Cords  | Y Cords  | Z Cords  |
|---------|----------|----------|----------|
| Ca      | 40.381966| 28.583572| 31.374317|
| Ca      | 39.555874| 28.958305| 36.089203|
| Ca      | 46.797325| 29.482256| 33.358932|
| Ca      | 42.777515| 28.798893| 34.275925|
| S       | 26.645176| 27.615520| 35.775688|
| S       | 27.026096| 33.773529| 34.596741|
| S       | 30.393333| 29.915833| 35.725100|
| S       | 30.054323| 31.609791| 36.384449|
| S       | 33.056435| 27.463699| 34.189747|
| S       | 33.728893| 32.625610| 32.575951|
| S       | 36.993690| 29.135895| 31.994300|
| S       | 36.544971| 29.596668| 36.649540|
| S       | 40.024506| 26.414381| 33.765564|
| S       | 40.475025| 31.295063| 33.646816|
| S       | 43.705078| 28.100437| 31.388958|
| S       | 44.582977| 26.847828| 38.670986|

24 generated by VMD

| Element | X Cords  | Y Cords  | Z Cords  |
|---------|----------|----------|----------|
| Ca      | 25.175875| 29.987621| 32.435204|
| Ca      | 26.361109| 30.712128| 36.468765|
| Ca      | 29.889034| 28.309532| 35.591736|
| Ca      | 30.113203| 32.859016| 33.232849|
| Ca      | 33.665512| 29.308363| 31.281143|
| Ca      | 33.156776| 30.547459| 35.202721|
| Ca      | 36.441673| 27.119617| 34.496910|
| Ca      | 36.869205| 31.514435| 33.839470|
| Ca      | 40.463310| 28.771223| 31.085850|
| Ca      | 39.572865| 28.957878| 36.064156|
| Ca      | 46.766678| 29.254076| 33.765549|
| Ca      | 42.763496| 28.537952| 34.254333|
| S       | 26.776186| 27.469013| 36.113564|
| S       | 26.876476| 33.752876| 34.679794|
| S       | 30.431583| 29.828514| 32.645111|
| S       | 30.047344| 31.500526| 36.599724|
| S       | 33.088615| 27.540123| 34.279221|
| S       | 33.607445| 32.641132| 32.400459|
| S       | 37.019588| 29.166405| 31.762817|
| S       | 36.675446| 29.902660| 36.385765|
| S       | 39.826427| 26.635204| 33.660656|
| S       | 40.627689| 31.129734| 33.656338|
| S       | 43.842434| 28.328648| 31.426142|
| S       | 44.375977| 26.617325| 38.702415|

24 generated by VMD

| Element | X Cords  | Y Cords  | Z Cords  |
|---------|----------|----------|----------|
| Ca      | 25.260590| 29.879221| 32.462658|
| Ca      | 26.493685| 30.817453| 36.338436|
|  | Ca       | 29.966339 | 28.398159 | 35.779045 |
|  | Ca       | 30.319666 | 33.141464 | 33.139080 |
|  | Ca       | 33.601051 | 30.526476 | 35.233006 |
|  | Ca       | 36.303146 | 26.799961 | 34.399296 |
|  | Ca       | 36.688168 | 31.345072 | 33.898224 |
|  | Ca       | 40.457142 | 28.693340 | 31.386328 |
|  | Ca       | 39.643200 | 28.847219 | 36.130074 |
|  | Ca       | 46.828972 | 29.631935 | 33.636593 |
|  | Ca       | 42.807281 | 28.676296 | 34.354662 |
|  | S        | 26.754162 | 27.478008 | 36.247429 |
|  | S        | 27.111570 | 33.887474 | 34.822968 |
|  | S        | 30.409155 | 29.838867 | 32.700542 |
|  | S        | 29.991583 | 31.617622 | 36.415142 |
|  | S        | 33.030724 | 27.436981 | 34.098877 |
|  | S        | 33.608391 | 32.517639 | 32.415005 |
|  | S        | 36.934750 | 29.046293 | 31.725819 |
|  | S        | 36.425320 | 29.519138 | 36.340508 |
|  | S        | 40.041962 | 26.553921 | 33.778801 |
|  | S        | 40.503403 | 31.161125 | 33.911324 |
|  | S        | 43.773399 | 28.200886 | 31.321106 |
|  | S        | 44.435051 | 26.922100 | 38.543064 |

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generated by VMD

|  | Ca       | 25.030159 | 30.099730 | 32.426552 |
|  | Ca       | 26.697304 | 30.757360 | 36.345119 |
|  | Ca       | 29.897402 | 28.709534 | 35.514256 |
|  | Ca       | 30.258837 | 32.777679 | 33.243610 |
|  | Ca       | 33.665726 | 29.053137 | 30.983301 |
|  | Ca       | 33.169384 | 30.648201 | 35.450977 |
|  | Ca       | 36.337624 | 26.860096 | 34.368824 |
|  | Ca       | 36.646481 | 31.263550 | 34.095978 |
|  | Ca       | 40.383438 | 28.604328 | 31.291431 |
|  | Ca       | 39.637810 | 28.829720 | 36.332813 |
|  | Ca       | 46.423965 | 29.796108 | 33.151241 |
|  | Ca       | 42.710964 | 28.858643 | 34.517750 |
|  | S        | 26.692108 | 27.592941 | 36.194908 |
|  | S        | 27.037344 | 33.806564 | 34.415421 |
|  | S        | 30.489494 | 29.748554 | 32.469280 |
|  | S        | 30.047342 | 31.715042 | 36.451389 |
|  | S        | 33.216354 | 27.787476 | 34.158241 |
|  | S        | 33.791008 | 32.393719 | 32.511066 |
|  | S        | 36.973927 | 29.016933 | 31.816269 |
|  | S        | 36.444717 | 29.323812 | 36.701614 |
|  | S        | 39.973827 | 26.333172 | 33.894707 |
|  | S        | 40.381878 | 31.026274 | 33.746250 |
S  43.579010  28.395344  31.424309
S  44.947819  26.993471  38.525486

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generated by VMD
Ca  25.318851  29.977127  32.565338
Ca  26.574570  30.978981  36.329880
Ca  30.060322  28.506031  35.668884
Ca  30.141787  32.786140  33.379921
Ca  33.717865  29.234524  31.087734
Ca  33.060745  30.715544  35.206902
Ca  36.272957  26.742682  34.143608
Ca  36.624718  31.333645  34.017586
Ca  40.388824  28.457554  31.204851
Ca  39.613037  28.787060  36.283958
Ca  46.645245  29.717224  32.940899
Ca  42.764725  28.696445  34.546677
S  26.855558  27.672348  36.176323
S  26.902805  33.796215  34.385475
S  30.411695  29.829414  32.568748
S  30.270638  31.650410  36.569656
S  33.030220  27.606050  34.047226
S  33.654308  32.635662  32.358910
S  36.908691  29.038013  31.783468
S  36.245533  29.289181  36.578785
S  39.885956  26.461369  33.928051
S  40.363602  30.968235  33.828552
S  43.631443  28.422924  31.482971
S  45.089855  27.088608  38.946297

24
generated by VMD
Ca  25.108391  29.946463  32.448566
Ca  26.293537  30.859795  36.081196
Ca  30.025593  28.744740  35.599937
Ca  30.127991  33.095497  33.224892
Ca  33.825226  29.131908  31.269802
Ca  33.104240  30.786709  35.655842
Ca  36.388416  26.483776  34.093258
Ca  36.789574  31.562096  34.107445
Ca  40.336082  28.502048  31.078472
Ca  39.667526  28.639347  36.286602
Ca  46.913837  29.428474  32.992378
Ca  42.799812  28.770622  34.245270
S  26.675091  27.631550  36.102982
S  26.793819  33.695141  34.443977
S  30.460251  29.800023  32.697681
S  29.772005  31.833649  36.472389
|  | X    | Y    | Z    |
|---|------|------|------|
| S | 33.131340 | 27.599831 | 34.433975 |
| S | 33.589115 | 32.546234 | 32.658653 |
| S | 36.837749 | 28.969269 | 31.880440 |
| S | 36.568779 | 29.222612 | 36.438873 |
| S | 39.941727 | 26.349472 | 33.665867 |
| S | 40.549774 | 30.989109 | 33.684586 |
| S | 43.886044 | 28.449078 | 31.278889 |
| S | 44.848000 | 27.353939 | 39.188702 |

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generated by VMD

| Ca  | X    | Y    | Z    |
|-----|------|------|------|
| Ca  | 25.119343 | 30.008173 | 32.197704 |
| Ca  | 26.419409 | 31.004978 | 35.850616 |
| Ca  | 30.038248 | 28.518984 | 35.880005 |
| Ca  | 30.194908 | 33.023952 | 33.244652 |
| Ca  | 33.655529 | 29.242172 | 31.345287 |
| Ca  | 33.141212 | 30.418022 | 35.608963 |
| Ca  | 36.401630 | 26.724211 | 34.335464 |
| Ca  | 36.894676 | 31.388992 | 34.198780 |
| Ca  | 40.286053 | 28.656658 | 31.493225 |
| Ca  | 39.459164 | 28.610703 | 35.820168 |
| Ca  | 46.676605 | 29.560474 | 33.135376 |
| Ca  | 42.901737 | 28.873058 | 34.198959 |
| S   | 26.525965 | 27.570671 | 36.208088 |
| S   | 26.851404 | 33.966934 | 34.104065 |
| S   | 30.488503 | 29.860777 | 32.813332 |
| S   | 29.915482 | 31.588699 | 36.594963 |
| S   | 33.201534 | 27.406151 | 34.227318 |
| S   | 33.559471 | 32.531982 | 32.792473 |
| S   | 36.931480 | 28.927944 | 31.986427 |
| S   | 36.571690 | 29.423641 | 36.638500 |
| S   | 39.992340 | 26.444641 | 33.625496 |
| S   | 40.519329 | 31.090599 | 33.844658 |
| S   | 43.860676 | 28.333994 | 31.171900 |
| S   | 44.827488 | 27.214977 | 38.714348 |

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generated by VMD

| Ca  | X    | Y    | Z    |
|-----|------|------|------|
| Ca  | 25.145893 | 30.202637 | 32.214558 |
| Ca  | 26.281090 | 31.017895 | 35.950565 |
| Ca  | 29.801620 | 28.609764 | 35.809654 |
| Ca  | 30.241737 | 32.908009 | 33.179207 |
| Ca  | 33.986900 | 29.127230 | 31.427315 |
| Ca  | 33.124619 | 30.544415 | 35.674721 |
| Ca  | 36.342827 | 26.630882 | 34.363163 |
| Ca  | 36.863823 | 31.364235 | 34.307308 |
| Ca  | 40.457314 | 28.554796 | 31.198273 |
| Ca  | 39.492100 | 28.498962 | 36.141857 |
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 46.890526     | 29.741055     | 33.271267     |
| Ca      | 42.776981     | 28.808535     | 34.013008     |
| S       | 26.556236     | 27.731777     | 36.083775     |
| S       | 27.061718     | 33.891666     | 34.375721     |
| S       | 30.473078     | 29.750170     | 32.699089     |
| S       | 29.760447     | 31.556684     | 36.480614     |
| S       | 33.125340     | 27.494520     | 34.451477     |
| S       | 33.734344     | 32.363441     | 32.701969     |
| S       | 37.072033     | 29.069530     | 32.082838     |
| S       | 36.379433     | 29.270473     | 36.576130     |
| S       | 39.795040     | 26.210581     | 33.628883     |
| S       | 40.353729     | 31.055498     | 33.744335     |
| S       | 43.917477     | 28.300873     | 31.180216     |
| S       | 44.799618     | 27.687809     | 38.469360     |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 25.268559     | 29.913500     | 32.154743     |
| Ca      | 26.514189     | 31.093481     | 36.032259     |
| Ca      | 30.061380     | 28.403843     | 35.781338     |
| Ca      | 30.294617     | 32.791138     | 33.371864     |
| Ca      | 33.880501     | 29.331657     | 31.500919     |
| Ca      | 33.046185     | 30.485445     | 35.651035     |
| Ca      | 36.311890     | 26.810791     | 34.356689     |
| Ca      | 36.786911     | 31.481277     | 34.131748     |
| Ca      | 40.370914     | 28.590045     | 31.175770     |
| Ca      | 39.308598     | 28.388817     | 35.810822     |
| Ca      | 46.713997     | 29.919250     | 33.363335     |
| Ca      | 42.707977     | 28.807602     | 34.258018     |
| S       | 26.766903     | 27.903496     | 36.413704     |
| S       | 26.933552     | 33.970409     | 34.035809     |
| S       | 30.578201     | 29.697359     | 32.730743     |
| S       | 29.953365     | 31.534300     | 36.510822     |
| S       | 33.193428     | 27.343916     | 34.386726     |
| S       | 33.701878     | 32.488155     | 32.777199     |
| S       | 37.130772     | 29.063747     | 31.929178     |
| S       | 36.404984     | 29.435093     | 36.595398     |
| S       | 39.986984     | 26.274166     | 33.423901     |
| S       | 40.360291     | 31.213409     | 33.813675     |
| S       | 43.764072     | 28.382774     | 31.334436     |
| S       | 44.393764     | 27.058762     | 38.490582     |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 25.218376     | 30.013273     | 32.070385     |
| Ca      | 26.294731     | 30.959866     | 36.073627     |
| Ca      | 29.943489     | 28.395073     | 35.939548     |
| Ca      | 30.220818     | 33.020554     | 33.220516     |
| Element | First Value | Second Value | Third Value |
|---------|-------------|--------------|-------------|
| Ca      | 33.588242   | 29.309074    | 31.429428   |
| Ca      | 33.051098   | 30.623764    | 35.445301   |
| Ca      | 36.442814   | 26.654078    | 34.427094   |
| Ca      | 36.619774   | 31.505726    | 34.250664   |
| Ca      | 40.536057   | 28.686251    | 31.332357   |
| Ca      | 39.63856    | 28.490479    | 36.063675   |
| Ca      | 46.65909    | 29.679260    | 32.967571   |
| Ca      | 42.82291    | 28.577026    | 34.099049   |
| S       | 26.650543   | 27.678644    | 36.113625   |
| S       | 26.98690    | 33.917065    | 34.264015   |
| S       | 30.386015   | 29.842371    | 32.857025   |
| S       | 29.812244   | 31.609241    | 36.393494   |
| S       | 33.074131   | 27.488583    | 34.415546   |
| S       | 33.596291   | 32.496212    | 32.441647   |
| S       | 37.152374   | 28.977491    | 32.137981   |
| S       | 36.437756   | 29.397436    | 36.645302   |
| S       | 40.09690    | 26.198666    | 33.666248   |
| S       | 40.520699   | 31.113422    | 34.018021   |
| S       | 43.878761   | 28.328011    | 31.144434   |
| S       | 44.815155   | 27.429819    | 38.614193   |

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generated by VMD

| Element | First Value | Second Value | Third Value |
|---------|-------------|--------------|-------------|
| Ca      | 25.198805   | 30.218006    | 32.230839   |
| Ca      | 26.446392   | 30.716984    | 36.045952   |
| Ca      | 29.775440   | 28.632431    | 35.759911   |
| Ca      | 30.140068   | 32.886665    | 33.134270   |
| Ca      | 33.848228   | 29.268795    | 31.400703   |
| Ca      | 33.071594   | 30.622608    | 35.483715   |
| Ca      | 36.248657   | 26.811100    | 34.514603   |
| Ca      | 36.805222   | 31.396923    | 34.253273   |
| Ca      | 40.046644   | 28.608116    | 31.002666   |
| Ca      | 39.413208   | 28.484779    | 35.954601   |
| Ca      | 46.881130   | 29.571198    | 33.190498   |
| Ca      | 42.615631   | 28.675209    | 34.258423   |
| S       | 26.559111   | 27.508266    | 36.189110   |
| S       | 26.957039   | 33.830318    | 34.432743   |
| S       | 30.488379   | 29.748463    | 32.727970   |
| S       | 29.940868   | 31.803743    | 36.307198   |
| S       | 33.112656   | 27.551563    | 34.583553   |
| S       | 33.612595   | 32.459759    | 32.693546   |
| S       | 37.051720   | 29.003538    | 32.023026   |
| S       | 36.577438   | 29.432201    | 36.667686   |
| S       | 39.856232   | 26.355284    | 33.468174   |
| S       | 40.539421   | 31.039368    | 33.743420   |
| S       | 43.893394   | 28.364876    | 31.327877   |
| S       | 44.796017   | 27.401188    | 38.636955   |
|    | Ca          | S           |
|----|-------------|-------------|
| 24 | 25.317499   | 29.971672   |
|    | 26.466963   | 30.846077   |
|    | 29.835159   | 28.393261   |
|    | 30.501369   | 32.976845   |
|    | 33.791775   | 29.233810   |
|    | 32.915340   | 30.600868   |
|    | 36.235043   | 26.896854   |
|    | 36.705292   | 31.267565   |
|    | 40.472618   | 28.612270   |
|    | 39.347790   | 28.362091   |
|    | 46.838837   | 29.581852   |
|    | 42.905064   | 28.775970   |
|    | 26.585836   | 27.649120   |
|    | 27.293856   | 33.916546   |
|    | 30.600183   | 29.818773   |
|    | 29.894230   | 31.538342   |
|    | 33.016171   | 27.561241   |
|    | 33.752857   | 32.503681   |
|    | 37.061893   | 29.035633   |
|    | 36.328171   | 29.465702   |
|    | 39.793552   | 26.292980   |
|    | 40.460217   | 31.021376   |
|    | 43.917099   | 28.371391   |
|    | 44.397015   | 27.697502   |

|    | Ca          | S           |
|----|-------------|-------------|
| 24 | 25.098248   | 29.884895   |
|    | 26.426647   | 30.942307   |
|    | 30.049013   | 28.372944   |
|    | 30.214838   | 33.021156   |
|    | 33.797127   | 29.285145   |
|    | 33.067162   | 30.575714   |
|    | 36.261314   | 26.722233   |
|    | 36.939171   | 31.398647   |
|    | 40.544586   | 28.690603   |
|    | 39.283077   | 28.443514   |
|    | 46.828186   | 29.396017   |
|    | 42.821648   | 28.796082   |
|    | 26.689425   | 27.606289   |
|    | 26.962646   | 33.985550   |
|    | 30.539667   | 29.840124   |
|    | 30.050611   | 31.662922   |
|    | 33.031223   | 27.537956   |
|    | 33.683056   | 32.475895   |
| S   | 37.025944 | 29.060768 | 31.744251 |
|-----|-----------|-----------|-----------|
| S   | 36.377811 | 29.379023 | 36.575134 |
| S   | 39.772453 | 26.410936 | 33.577374 |
| S   | 40.435272 | 31.025352 | 33.970768 |
| S   | 43.869164 | 28.163170 | 31.464752 |
| S   | 44.665543 | 27.714134 | 38.572552 |

24 generated by VMD

| Ca  | 25.081575 | 30.283012 | 32.227142 |
|-----|-----------|-----------|-----------|
| Ca  | 26.326355 | 30.807199 | 36.243439 |
| Ca  | 29.858719 | 28.219543 | 35.753387 |
| Ca  | 30.156349 | 32.922436 | 33.417957 |
| Ca  | 34.089901 | 29.343399 | 31.288319 |
| Ca  | 32.955441 | 30.595022 | 35.489052 |
| Ca  | 36.215260 | 26.929453 | 34.328575 |
| Ca  | 36.832085 | 31.585732 | 33.980759 |
| Ca  | 40.527435 | 28.648422 | 31.202366 |
| Ca  | 39.594265 | 28.716208 | 35.923561 |
| Ca  | 46.977673 | 29.125053 | 33.339638 |
| Ca  | 42.858143 | 28.650322 | 34.193920 |
| S   | 26.390762 | 27.518284 | 36.223824 |
| S   | 27.029354 | 33.741222 | 34.651283 |
| S   | 30.557146 | 29.874981 | 32.792912 |
| S   | 29.777367 | 31.532314 | 36.504700 |
| S   | 33.090034 | 27.386627 | 34.259056 |
| S   | 33.499847 | 32.415798 | 32.439560 |
| S   | 37.139553 | 29.119553 | 31.833818 |
| S   | 36.536304 | 29.730339 | 36.420193 |
| S   | 39.836361 | 26.453602 | 33.504204 |
| S   | 40.463749 | 31.161079 | 33.739204 |
| S   | 44.062710 | 28.067432 | 31.404917 |
| S   | 44.577503 | 27.564354 | 38.868942 |

24 generated by VMD

| Ca  | 25.286541 | 30.101871 | 32.285767 |
|-----|-----------|-----------|-----------|
| Ca  | 26.505972 | 30.983849 | 36.187325 |
| Ca  | 30.045380 | 28.385891 | 35.719273 |
| Ca  | 30.415199 | 32.954025 | 33.306393 |
| Ca  | 33.797821 | 29.185835 | 31.159998 |
| Ca  | 33.092102 | 30.375454 | 35.641624 |
| Ca  | 36.176888 | 26.794804 | 34.006947 |
| Ca  | 36.895271 | 31.424194 | 34.253353 |
| Ca  | 40.314583 | 28.613979 | 31.047112 |
| Ca  | 39.285172 | 28.558016 | 35.568382 |
| Ca  | 46.806484 | 29.367359 | 33.457787 |
| Ca  | 42.651909 | 28.881721 | 34.148033 |
S 26.615566 27.560526 36.415752
S 26.987936 33.928459 34.479507
S 30.007492 31.633831 36.592930
S 32.994175 27.272873 34.339317
S 33.819511 32.625557 32.634434
S 37.077942 29.074184 31.920786
S 36.350655 29.151188 36.421619
S 39.910675 26.336994 33.327240
S 40.332302 31.297714 33.792076
S 43.987480 28.096827 31.380333
S 44.375195 27.883215 39.196602

24 generated by VMD
Ca 24.950951 30.164921 32.704292
Ca 24.739136 31.188881 36.186642
Ca 29.997730 28.236877 35.580441
Ca 30.436028 32.955158 33.435486
Ca 33.669785 29.175659 31.105122
Ca 33.174141 30.180094 35.360092
Ca 36.312801 26.525120 34.058594
Ca 36.527740 31.252464 33.956894
Ca 40.349945 29.004622 31.32218
Ca 39.647335 28.548382 36.033829
Ca 46.668800 29.703396 33.603954
Ca 42.759335 28.840149 34.266911
S 26.847614 27.892311 36.555832
S 27.030720 34.081444 34.245045
S 30.523230 29.832338 32.684170
S 30.367935 31.529987 36.44805
S 33.058025 27.165680 34.160015
S 33.763836 32.421677 32.518829
S 36.895535 28.968178 31.667542
S 36.396038 28.967075 36.359882
S 39.867275 26.425886 33.372765
S 40.392624 31.215916 33.864746
S 43.857307 28.387070 31.364647
S 44.200138 27.728134 39.187912

24 generated by VMD
Ca 24.959515 30.228664 32.210007
Ca 26.625931 31.177145 36.090340
Ca 30.156393 28.336628 35.680515
Ca 30.299646 32.922386 33.530540
Ca 33.740913 29.216635 31.460484
Ca 33.048477 30.253151 35.502235
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 36.463142    | 26.444569    | 33.787308    |
| Ca      | 36.768982    | 31.070040    | 34.176147    |
| Ca      | 40.452610    | 28.784210    | 31.405453    |
| Ca      | 39.708420    | 28.894142    | 35.897659    |
| Ca      | 46.689175    | 29.805695    | 33.348236    |
| Ca      | 42.892872    | 28.891499    | 34.224537    |
| S       | 26.643896    | 28.011421    | 36.497417    |
| S       | 26.829430    | 34.045841    | 34.174461    |
| S       | 30.415127    | 29.806458    | 32.796162    |
| S       | 30.101749    | 31.539627    | 36.509964    |
| S       | 33.050449    | 27.277611    | 34.236137    |
| S       | 33.629070    | 32.427883    | 32.706387    |
| S       | 36.978146    | 28.907684    | 31.913452    |
| S       | 36.266190    | 28.843983    | 36.343021    |
| S       | 39.924988    | 26.389751    | 33.518379    |
| S       | 40.494522    | 31.358269    | 33.666283    |
| S       | 43.925137    | 27.954554    | 31.382324    |
| S       | 44.369106    | 27.803537    | 38.973179    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.273808    | 29.762285    | 32.238998    |
| Ca      | 26.438976    | 30.961761    | 36.267921    |
| Ca      | 30.024271    | 28.494370    | 35.661530    |
| Ca      | 30.297649    | 33.190552    | 33.373970    |
| Ca      | 33.610794    | 29.203163    | 30.954960    |
| Ca      | 33.069916    | 30.552441    | 35.346600    |
| Ca      | 36.479500    | 26.552761    | 33.992420    |
| Ca      | 36.851845    | 31.174053    | 34.226566    |
| Ca      | 40.262928    | 28.651119    | 31.406700    |
| Ca      | 39.618904    | 28.587713    | 36.388535    |
| Ca      | 46.507206    | 29.758453    | 33.102619    |
| Ca      | 42.815269    | 28.820004    | 34.223225    |
| S       | 26.452326    | 27.664768    | 36.559517    |
| S       | 26.987019    | 33.993988    | 34.393658    |
| S       | 30.505501    | 30.075918    | 32.676651    |
| S       | 29.908131    | 31.486576    | 36.604485    |
| S       | 33.054440    | 27.652153    | 34.210972    |
| S       | 33.674957    | 32.574127    | 32.467735    |
| S       | 36.996643    | 29.112015    | 31.668247    |
| S       | 36.400169    | 28.990349    | 36.424644    |
| S       | 40.093422    | 26.202171    | 33.638092    |
| S       | 40.598812    | 31.130405    | 33.970863    |
| S       | 43.932587    | 27.985134    | 31.333115    |
| S       | 44.578846    | 27.815130    | 38.898663    |

24 generated by VMD
| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 25.272396 | 29.906754 | 32.133003 |
| Ca      | 26.327023 | 31.060135 | 35.906029 |
| Ca      | 29.876377 | 28.463497 | 35.950325 |
| Ca      | 30.340919 | 32.970203 | 33.446037 |
| Ca      | 33.846855 | 29.397434 | 31.231960 |
| Ca      | 33.040165 | 30.561512 | 35.771110 |
| Ca      | 36.335712 | 26.573463 | 33.84156 |
| Ca      | 36.843628 | 31.082359 | 34.010948 |
| Ca      | 40.587776 | 28.490738 | 31.285803 |
| Ca      | 39.472763 | 28.764320 | 35.970589 |
| Ca      | 46.831520 | 30.032894 | 32.974632 |
| Ca      | 42.805943 | 28.969954 | 34.301712 |
| S       | 26.383759 | 27.709446 | 36.547005 |
| S       | 27.046404 | 33.861671 | 34.391163 |
| S       | 30.616770 | 29.861687 | 32.901455 |
| S       | 30.012062 | 31.552204 | 36.626404 |
| S       | 33.083996 | 27.466354 | 34.287308 |
| S       | 33.825409 | 32.719669 | 32.833557 |
| S       | 37.134964 | 28.916054 | 31.671268 |
| S       | 36.282101 | 29.144003 | 36.472477 |
| S       | 39.909660 | 26.309475 | 33.612358 |
| S       | 40.552418 | 31.088642 | 33.631699 |
| S       | 43.912338 | 27.911673 | 31.521992 |
| S       | 44.093029 | 27.577190 | 38.897736 |

24 generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 25.081469 | 30.151541 | 32.284824 |
| Ca      | 26.408546 | 30.945530 | 35.980705 |
| Ca      | 30.028683 | 28.503237 | 35.491512 |
| Ca      | 30.241196 | 32.810211 | 33.657310 |
| Ca      | 33.743587 | 29.342279 | 31.312862 |
| Ca      | 33.114395 | 30.634327 | 35.572338 |
| Ca      | 36.300423 | 26.506279 | 34.145668 |
| Ca      | 36.749207 | 31.045088 | 34.058510 |
| Ca      | 40.460835 | 28.532747 | 31.447514 |
| Ca      | 39.720474 | 28.752914 | 36.071251 |
| Ca      | 46.711857 | 29.890701 | 33.147392 |
| Ca      | 42.986866 | 28.595322 | 34.220375 |
| S       | 26.565123 | 27.807796 | 36.217670 |
| S       | 26.729820 | 34.027916 | 34.279053 |
| S       | 30.380135 | 29.824797 | 32.630436 |
| S       | 30.195362 | 31.638433 | 36.625435 |
| S       | 33.050034 | 27.595318 | 34.222767 |
| S       | 33.649277 | 32.489243 | 32.689423 |
| S       | 37.127735 | 28.767801 | 31.938984 |
| S       | 36.222797 | 29.102358 | 36.550343 |
|    | 39.866280 | 26.290236 | 33.725727 |
|----|-----------|-----------|-----------|
| S  | 40.469215 | 31.127817 | 33.847252 |
| S  | 43.849152 | 28.075325 | 31.261463 |
| S  | 44.781372 | 27.934208 | 38.651958 |

24 generated by VMD

| Ca  | 25.142210 | 30.050739 | 32.580532 |
|-----|-----------|-----------|-----------|
| Ca  | 26.463324 | 30.853504 | 36.133553 |
| Ca  | 29.998919 | 28.330746 | 35.499466 |
| Ca  | 30.400084 | 33.201714 | 33.338932 |
| Ca  | 33.632290 | 29.523304 | 31.188612 |
| Ca  | 33.124828 | 30.234934 | 35.178627 |
| Ca  | 36.593391 | 26.646027 | 34.177631 |
| Ca  | 36.713596 | 31.300995 | 33.910309 |
| Ca  | 40.467304 | 28.582191 | 31.506611 |
| Ca  | 39.455830 | 28.564291 | 36.185665 |
| Ca  | 46.744064 | 29.838190 | 32.922932 |
| Ca  | 42.677544 | 28.518597 | 34.429703 |
| S   | 26.759033 | 27.631561 | 36.471474 |
| S   | 26.971260 | 33.998863 | 34.543266 |
| S   | 30.363600 | 30.036463 | 32.564888 |
| S   | 30.181179 | 31.608707 | 36.530434 |
| S   | 33.073082 | 27.362576 | 33.969875 |
| S   | 33.644318 | 32.725647 | 32.457085 |
| S   | 36.886841 | 28.760799 | 31.837482 |
| S   | 36.420990 | 29.362490 | 36.419163 |
| S   | 39.996933 | 26.274891 | 33.788261 |
| S   | 40.348537 | 31.016491 | 33.930820 |
| S   | 43.840286 | 28.170801 | 31.528244 |
| S   | 44.534477 | 27.796871 | 38.937183 |

24 generated by VMD

| Ca  | 25.010138 | 30.257957 | 32.438885 |
|-----|-----------|-----------|-----------|
| Ca  | 26.658499 | 31.008976 | 36.276585 |
| Ca  | 30.023708 | 28.403957 | 35.420151 |
| Ca  | 30.178967 | 33.060791 | 33.438393 |
| Ca  | 33.673294 | 29.192640 | 31.110203 |
| Ca  | 33.135345 | 30.280807 | 35.181843 |
| Ca  | 36.367531 | 26.447468 | 34.335136 |
| Ca  | 36.894348 | 31.173374 | 33.996529 |
| Ca  | 40.320103 | 28.467033 | 31.376030 |
| Ca  | 39.560085 | 28.568119 | 36.250843 |
| Ca  | 46.593018 | 30.011475 | 33.416626 |
| Ca  | 42.732445 | 28.894848 | 34.317661 |
| S   | 26.705063 | 27.778111 | 36.307850 |
| S   | 26.818382 | 34.235165 | 34.544067 |
|     | S       | Ca       | S       |
|-----|---------|----------|---------|
| S   | 30.454552 | 30.22263 | 32.515556 |
| S   | 30.142715 | 31.546101 | 36.431923 |
| S   | 33.083435 | 27.275301 | 34.007942 |
| S   | 33.630013 | 32.516335 | 32.657993 |
| S   | 36.921490 | 28.731983 | 31.870092 |
| S   | 36.325092 | 29.052629 | 36.525902 |
| S   | 39.994461 | 26.364731 | 33.929195 |
| S   | 40.386852 | 31.076881 | 33.653229 |
| S   | 43.857620 | 28.274918 | 31.421448 |
| S   | 44.966747 | 27.749573 | 38.606544 |
| 24  | generated by VMD | Ca       | S       |
| Ca  | 25.581020 | 30.159107 | 31.941238 |
| Ca  | 26.516493 | 30.909409 | 36.305622 |
| Ca  | 29.959242 | 28.443140 | 35.553501 |
| Ca  | 30.335428 | 33.168976 | 33.463215 |
| Ca  | 33.541885 | 29.183336 | 31.147701 |
| Ca  | 33.222008 | 30.278027 | 35.44931 |
| Ca  | 36.340218 | 26.575384 | 34.424896 |
| Ca  | 36.880333 | 31.228624 | 34.062920 |
| Ca  | 40.441677 | 28.595579 | 31.204453 |
| Ca  | 39.532631 | 28.463408 | 36.043465 |
| Ca  | 46.539764 | 29.639837 | 33.368546 |
| Ca  | 42.515747 | 28.809216 | 34.276672 |
| S   | 26.537405 | 27.696560 | 36.334663 |
| S   | 27.043865 | 34.050472 | 36.574885 |
| S   | 30.502338 | 30.011730 | 32.627453 |
| S   | 30.022064 | 31.442287 | 36.477745 |
| S   | 33.042629 | 27.365643 | 34.154732 |
| S   | 33.610321 | 32.447018 | 33.662910 |
| S   | 36.840839 | 28.848110 | 31.845112 |
| S   | 36.606808 | 29.345486 | 36.590263 |
| S   | 39.856873 | 26.422258 | 33.582642 |
| S   | 40.453362 | 31.101177 | 33.589203 |
| S   | 43.654308 | 28.125134 | 31.427853 |
| S   | 44.856491 | 28.081537 | 38.826073 |

24 | generated by VMD | Ca       | S       |
| Ca  | 25.260754 | 30.368938 | 31.945610 |
| Ca  | 26.413815 | 30.977556 | 36.183334 |
| Ca  | 29.912079 | 28.554783 | 35.351479 |
| Ca  | 30.128763 | 32.989830 | 33.685127 |
| Ca  | 33.576866 | 29.246548 | 31.170044 |
| Ca  | 33.155304 | 30.261703 | 35.323074 |
| Ca  | 36.521118 | 26.512814 | 34.433876 |
| Ca  | 36.726284 | 31.040598 | 34.009064 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 40.302277    | 28.324627    | 31.466045    |
| Ca      | 39.815620    | 28.861099    | 36.230453    |
| Ca      | 46.579594    | 29.898018    | 33.088242    |
| Ca      | 42.953800    | 28.682091    | 34.112099    |
| S       | 26.509035    | 27.785164    | 36.057415    |
| S       | 26.956463    | 34.233192    | 34.772465    |
| S       | 30.372700    | 29.990875    | 32.609783    |
| S       | 29.987411    | 31.500158    | 36.567062    |
| S       | 33.124069    | 27.359955    | 34.009605    |
| S       | 33.516422    | 32.371925    | 32.609627    |
| S       | 36.774189    | 28.517515    | 32.009846    |
| S       | 36.612335    | 29.232183    | 36.558239    |
| S       | 40.092880    | 26.280293    | 34.052315    |
| S       | 40.393761    | 31.071299    | 33.781689    |
| S       | 43.808937    | 28.085114    | 31.339249    |
| S       | 44.939419    | 28.245121    | 38.664902    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.414167    | 30.419746    | 32.135540    |
| Ca      | 26.305151    | 30.685814    | 36.258560    |
| Ca      | 29.902851    | 28.576786    | 35.586113    |
| Ca      | 30.270779    | 33.078079    | 33.422714    |
| Ca      | 33.433044    | 29.181650    | 31.364254    |
| Ca      | 33.101387    | 30.419651    | 35.412594    |
| Ca      | 36.460205    | 26.820206    | 34.360344    |
| Ca      | 36.864674    | 31.357571    | 33.805660    |
| Ca      | 40.190292    | 28.473572    | 31.210516    |
| Ca      | 39.688965    | 28.737411    | 36.371925    |
| Ca      | 46.593269    | 29.401821    | 32.273243    |
| Ca      | 42.866264    | 28.715118    | 34.187271    |
| S       | 26.469351    | 27.583511    | 35.704369    |
| S       | 27.071911    | 33.763809    | 34.892532    |
| S       | 30.538588    | 29.867474    | 32.609589    |
| S       | 30.010708    | 31.574387    | 36.566521    |
| S       | 33.155495    | 27.410286    | 34.347832    |
| S       | 33.633881    | 32.452324    | 32.644588    |
| S       | 36.774746    | 28.743076    | 31.606361    |
| S       | 36.647827    | 29.519737    | 36.607132    |
| S       | 39.956093    | 26.433109    | 33.893967    |
| S       | 40.510708    | 31.038784    | 33.631039    |
| S       | 43.733898    | 28.010351    | 31.314621    |
| S       | 44.839581    | 28.127106    | 38.824421    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.199089    | 29.795641    | 32.243721    |
| Ca      | 26.373333    | 30.780581    | 36.017418    |
|   |   |   |   |
|---|---|---|---|
| Ca | 30.155899 | 28.568819 | 35.641254 |
| Ca | 30.216856 | 33.259781 | 33.566269 |
| Ca | 33.621437 | 30.377399 | 35.374809 |
| Ca | 36.450508 | 26.428646 | 34.362789 |
| Ca | 36.713886 | 31.125469 | 33.838242 |
| Ca | 40.264755 | 28.377899 | 31.219322 |
| Ca | 39.572803 | 28.564091 | 36.077843 |
| Ca | 46.543655 | 29.721355 | 33.340134 |
| Ca | 42.885914 | 28.804604 | 34.169735 |
| S  | 26.507050 | 27.605684 | 36.083340 |
| S  | 26.966564 | 34.220230 | 34.682663 |
| S  | 30.559950 | 30.191433 | 32.712402 |
| S  | 30.095966 | 31.587423 | 36.603168 |
| S  | 33.051338 | 27.383495 | 34.212715 |
| S  | 33.663422 | 32.723591 | 32.682983 |
| S  | 36.837086 | 28.686014 | 31.741055 |
| S  | 36.501419 | 29.117760 | 36.502220 |
| S  | 40.143322 | 26.315603 | 33.926273 |
| S  | 40.383347 | 30.901674 | 33.548462 |
| S  | 43.907646 | 28.354256 | 31.322681 |
| S  | 44.634300 | 27.932083 | 38.979866 |

24

generated by VMD

|   |   |   |   |
|---|---|---|---|
| Ca | 24.865528 | 30.570667 | 32.012550 |
| Ca | 26.181078 | 30.572376 | 36.142815 |
| Ca | 29.864288 | 28.675879 | 35.441528 |
| Ca | 30.177292 | 33.216576 | 33.316162 |
| Ca | 33.485237 | 29.139570 | 31.080338 |
| Ca | 33.021027 | 30.520039 | 35.529037 |
| Ca | 36.534977 | 26.472630 | 34.459553 |
| Ca | 36.732998 | 31.124153 | 34.033218 |
| Ca | 40.044247 | 28.364511 | 31.319714 |
| Ca | 39.957607 | 28.541374 | 36.185654 |
| Ca | 46.719460 | 30.139923 | 33.210484 |
| Ca | 43.076473 | 28.726748 | 34.119068 |
| S  | 26.694502 | 27.365612 | 36.088539 |
| S  | 27.017197 | 34.171917 | 34.711178 |
| S  | 30.309734 | 29.997612 | 32.588760 |
| S  | 29.897896 | 31.661518 | 36.483150 |
| S  | 33.289169 | 27.555805 | 34.383839 |
| S  | 33.638451 | 32.461178 | 32.554573 |
| S  | 36.809006 | 28.747213 | 31.823639 |
| S  | 36.569210 | 29.237778 | 36.617966 |
| S  | 40.145489 | 26.374886 | 33.961658 |
| S  | 40.387840 | 30.935566 | 33.880100 |
|     |          |          |          |
|-----|----------|----------|----------|
| S   | 43.879005| 27.950773| 31.269064|
| S   | 45.136230| 27.867119| 38.818142|

24 generated by VMD

| Ca  |          |          |          |
|-----|----------|----------|----------|
|     | 25.419659| 30.186314| 32.144699|
| Ca  | 26.341408| 31.032570| 36.136322|
| Ca  | 29.855440| 28.600868| 35.529068|
| Ca  | 30.241732| 33.229538| 33.425327|
| Ca  | 33.727108| 29.269672| 31.149364|
| Ca  | 33.108711| 30.424355| 35.531387|
| Ca  | 36.291862| 26.485470| 34.287663|
| Ca  | 36.667492| 30.824736| 33.845398|
| Ca  | 40.317692| 28.468933| 31.366844|
| Ca  | 39.794128| 28.587404| 36.261646|
| Ca  | 46.692009| 29.800591| 33.158535|
| Ca  | 43.015793| 28.886555| 34.240921|
| S   | 26.634737| 27.526827| 36.178665|
| S   | 26.970285| 34.068146| 34.745171|
| S   | 30.450478| 30.038471| 32.615906|
| S   | 29.874645| 31.736904| 36.486877|
| S   | 33.147846| 27.467388| 34.142204|
| S   | 33.691208| 32.438461| 32.777706|
| S   | 36.805626| 28.560940| 31.675333|
| S   | 36.453007| 29.075356| 36.637897|
| S   | 39.886864| 26.458694| 33.798985|
| S   | 40.245010| 30.924286| 33.830624|
| S   | 43.825623| 28.096592| 31.223045|
| S   | 44.975578| 28.202351| 38.841164|

24 generated by VMD

| Ca  |          |          |          |
|-----|----------|----------|----------|
|     | 25.435593| 29.921719| 32.039314|
| Ca  | 26.569651| 30.749662| 36.011562|
| Ca  | 29.995062| 28.619360| 35.858223|
| Ca  | 30.435278| 33.164963| 33.304501|
| Ca  | 33.646351| 29.372513| 31.055214|
| Ca  | 33.091690| 30.418133| 35.349350|
| Ca  | 36.272579| 26.782284| 34.468155|
| Ca  | 36.842529| 31.160511| 33.866276|
| Ca  | 40.049583| 28.567247| 31.702782|
| Ca  | 39.801811| 28.740736| 36.377968|
| Ca  | 46.514687| 29.897091| 32.862419|
| Ca  | 42.871685| 28.545937| 34.369804|
| S   | 26.679045| 27.524790| 36.203098|
| S   | 27.097878| 33.828949| 34.464249|
| S   | 30.417828| 30.009720| 32.837177|
| S   | 30.081501| 31.670185| 36.445484|
|          |          |          |          |
|----------|----------|----------|----------|
| S        | 32.970440| 27.502228| 34.218204|
| S        | 33.777512| 32.501720| 32.705967|
| S        | 36.861111| 28.838272| 31.635521|
| S        | 36.399525| 29.289263| 36.601559|
| S        | 39.639744| 26.291389| 33.865082|
| S        | 40.500000| 30.958609| 33.966568|
| S        | 43.595814| 28.320066| 31.225811|
| S        | 44.886967| 27.716061| 38.596420|
| 24       |          |          |          |
|          | generated by VMD |
| Ca       | 25.669670 | 30.216145 | 31.895657 |
| Ca       | 26.519110 | 30.899239 | 35.914604 |
| Ca       | 29.887226 | 28.537128 | 35.685673 |
| Ca       | 30.249657 | 33.055798 | 33.350788 |
| Ca       | 33.716125 | 29.211037 | 31.337784 |
| Ca       | 33.154114 | 30.550474 | 35.364132 |
| Ca       | 36.201099 | 26.490686 | 34.587067 |
| Ca       | 36.799721 | 31.173531 | 33.946400 |
| Ca       | 39.975517 | 28.345648 | 31.884716 |
| Ca       | 39.521057 | 28.511044 | 36.154327 |
| Ca       | 46.703754 | 30.021233 | 32.799591 |
| Ca       | 43.013863 | 28.766239 | 34.162121 |
| S        | 26.373198 | 27.674225 | 36.138336 |
| S        | 27.119686 | 33.868782 | 34.748901 |
| S        | 30.459568 | 29.955996 | 32.682304 |
| S        | 29.904196 | 31.643318 | 36.475376 |
| S        | 32.858910 | 27.532631 | 34.272423 |
| S        | 33.779701 | 32.598038 | 32.612473 |
| S        | 36.760891 | 28.595819 | 31.930166 |
| S        | 36.481461 | 29.275906 | 36.522839 |
| S        | 39.638317 | 26.033112 | 33.949299 |
| S        | 40.422516 | 30.939449 | 34.014835 |
| S        | 43.980110 | 28.414169 | 31.117870 |
| S        | 45.244404 | 28.081770 | 38.482986 |
| 24       |          |          |          |
|          | generated by VMD |
| Ca       | 25.545113 | 30.154934 | 32.224243 |
| Ca       | 26.493830 | 31.069151 | 36.076302 |
| Ca       | 30.066547 | 28.475552 | 35.581291 |
| Ca       | 30.147503 | 33.189911 | 33.521828 |
| Ca       | 33.591934 | 29.521645 | 31.166695 |
| Ca       | 33.253857 | 30.297340 | 35.452667 |
| Ca       | 36.494602 | 26.492821 | 34.193401 |
| Ca       | 36.711319 | 30.830288 | 33.642868 |
| Ca       | 40.204021 | 28.423500 | 31.485909 |
| Ca       | 39.840118 | 28.672943 | 36.405331 |
|  | Ca  | S   | S   |
|---|-----|-----|-----|
|  | 46.565269 | 30.197643 | 33.430515 |
|  | 42.882511 | 28.532299 | 34.323124 |
|  | 26.518696 | 27.579819 | 36.295372 |
|  | 26.969168 | 34.077499 | 34.723824 |
|  | 30.322535 | 29.986393 | 32.730774 |
|  | 30.118296 | 31.615295 | 36.574390 |
|  | 32.990723 | 27.569546 | 33.974377 |
|  | 33.637497 | 32.605640 | 32.639236 |
|  | 36.696608 | 28.562378 | 31.448505 |
|  | 36.535137 | 29.147316 | 36.394089 |
|  | 39.966366 | 26.208595 | 34.008049 |
|  | 40.243263 | 30.778156 | 33.602787 |
|  | 43.860317 | 28.378239 | 31.345199 |
|  | 44.775665 | 28.024525 | 38.789711 |

24 generated by VMD

|  | Ca  | S   | S   |
|---|-----|-----|-----|
|  | 25.400455 | 30.145374 | 32.030960 |
|  | 26.460047 | 30.816769 | 35.951073 |
|  | 29.999319 | 28.681894 | 35.854454 |
|  | 30.406094 | 33.156883 | 33.432571 |
|  | 33.459049 | 29.280525 | 31.312607 |
|  | 33.044941 | 30.613045 | 35.508514 |
|  | 36.393532 | 26.400110 | 34.202305 |
|  | 36.688839 | 31.006403 | 33.988792 |
|  | 40.063885 | 28.312248 | 31.584942 |
|  | 39.797424 | 28.840736 | 36.263798 |
|  | 46.749050 | 29.723030 | 33.432220 |
|  | 42.781303 | 28.772509 | 34.114136 |
|  | 26.562450 | 27.498447 | 35.873127 |
|  | 27.027586 | 33.943298 | 34.752190 |
|  | 30.353775 | 29.931240 | 32.787365 |
|  | 30.005663 | 31.652702 | 36.518040 |
|  | 33.095879 | 27.618645 | 34.261490 |
|  | 33.815758 | 32.580563 | 32.561783 |
|  | 36.676682 | 28.829615 | 31.639431 |
|  | 36.442127 | 29.180206 | 36.496536 |
|  | 39.967430 | 26.190020 | 34.067268 |
|  | 40.288971 | 30.868984 | 33.541172 |
|  | 43.737400 | 28.495075 | 31.162083 |
|  | 45.216251 | 27.853077 | 38.693813 |

24 generated by VMD

|  | Ca  | S   | S   |
|---|-----|-----|-----|
|  | 25.205914 | 30.335106 | 31.882156 |
|  | 26.552683 | 30.749166 | 35.882103 |
|  | 30.167971 | 28.649139 | 35.880482 |
|  | 30.207451 | 33.030212 | 33.514309 |
|       |       |       |
|-------|-------|-------|
| Ca    | 33.508118 | 29.171173 | 31.349771 |
| Ca    | 33.290527 | 30.521133 | 35.412052 |
| Ca    | 36.516727 | 26.508533 | 34.474674 |
| Ca    | 36.758301 | 31.161545 | 33.944405 |
| Ca    | 40.068062 | 28.747320 | 31.521603 |
| Ca    | 39.699802 | 28.730099 | 36.272133 |
| Ca    | 46.798237 | 29.118885 | 32.961838 |
| Ca    | 42.712543 | 28.857378 | 34.179737 |
| S     | 26.591864 | 27.488300 | 35.845917 |
| S     | 26.977291 | 33.892899 | 34.606148 |
| S     | 30.599882 | 29.980965 | 32.785156 |
| S     | 29.991163 | 31.588781 | 36.684669 |
| S     | 33.023911 | 27.496445 | 34.382225 |
| S     | 33.569981 | 32.559013 | 32.473171 |
| S     | 36.784981 | 28.741590 | 31.854279 |
| S     | 36.442013 | 29.269091 | 36.441544 |
| S     | 39.938152 | 26.418129 | 33.997261 |
| S     | 40.438622 | 31.138172 | 33.596725 |
| S     | 43.664696 | 28.176449 | 31.401417 |
| S     | 44.924957 | 28.061863 | 38.686935 |

24

generated by VMD

|       |       |       |
|-------|-------|-------|
| Ca    | 25.505068 | 29.893837 | 31.889528 |
| Ca    | 26.551659 | 30.663364 | 36.382721 |
| Ca    | 30.011776 | 28.634613 | 35.855785 |
| Ca    | 30.382757 | 33.194782 | 33.415249 |
| Ca    | 33.299286 | 29.325146 | 30.843193 |
| Ca    | 33.265079 | 30.567842 | 35.492508 |
| Ca    | 36.353729 | 26.715260 | 34.060097 |
| Ca    | 36.781715 | 31.351130 | 33.723278 |
| Ca    | 40.007034 | 28.613518 | 31.587215 |
| Ca    | 39.834297 | 28.678099 | 36.551384 |
| Ca    | 46.747494 | 29.439770 | 33.444141 |
| Ca    | 42.838024 | 28.730307 | 34.414078 |
| S     | 26.786394 | 27.388634 | 36.131233 |
| S     | 27.082762 | 33.808998 | 34.819641 |
| S     | 30.519444 | 29.950151 | 32.733322 |
| S     | 30.132561 | 31.672874 | 36.571518 |
| S     | 33.033192 | 27.556103 | 34.286381 |
| S     | 33.692764 | 32.616695 | 32.378052 |
| S     | 36.652283 | 29.034615 | 31.303385 |
| S     | 36.408482 | 29.313530 | 36.345871 |
| S     | 39.847332 | 26.456743 | 34.036110 |
| S     | 40.441174 | 30.955235 | 33.701313 |
| S     | 43.417435 | 28.222115 | 31.322445 |
| S     | 44.842197 | 27.608051 | 38.742283 |
|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| Ca | 25.663795 | 30.161797 | 31.884708 |
| Ca | 26.439190 | 30.840570 | 35.859962 |
| Ca | 29.826305 | 28.649101 | 35.691303 |
| Ca | 30.444448 | 33.148453 | 33.417355 |
| Ca | 33.614342 | 29.254395 | 31.336432 |
| Ca | 33.008137 | 30.519696 | 35.561501 |
| Ca | 36.296188 | 26.335304 | 34.449745 |
| Ca | 36.783436 | 31.040060 | 33.930725 |
| Ca | 40.156055 | 28.648193 | 31.433224 |
| Ca | 39.697205 | 28.652077 | 36.248825 |
| Ca | 46.826855 | 29.678633 | 33.133068 |
| Ca | 42.670029 | 28.837967 | 34.250259 |
| S  | 26.535772 | 27.536350 | 36.204906 |
| S  | 27.202568 | 33.919365 | 34.594364 |
| S  | 30.494812 | 29.987705 | 32.860348 |
| S  | 29.964571 | 31.649700 | 36.715328 |
| S  | 33.067871 | 27.422058 | 34.297928 |
| S  | 33.736118 | 32.514561 | 32.478306 |
| S  | 36.804810 | 28.765656 | 31.645693 |
| S  | 36.474529 | 29.304295 | 36.552284 |
| S  | 39.883739 | 26.367290 | 33.885056 |
| S  | 40.166046 | 30.938129 | 33.775299 |
| S  | 43.612389 | 28.281965 | 31.169312 |
| S  | 45.064697 | 27.942802 | 38.654709 |

24

generated by VMD

| Ca | 25.327061 | 30.044903 | 31.721905 |
| Ca | 26.639717 | 31.077333 | 35.802433 |
| Ca | 30.091623 | 28.429747 | 35.697586 |
| Ca | 30.148354 | 32.988800 | 33.574856 |
| Ca | 33.493874 | 29.322813 | 31.389940 |
| Ca | 33.247265 | 30.420040 | 35.559624 |
| Ca | 36.387970 | 26.556271 | 34.518127 |
| Ca | 36.771366 | 30.935524 | 34.112606 |
| Ca | 40.033630 | 28.629974 | 31.453865 |
| Ca | 39.923843 | 28.845814 | 36.168228 |
| Ca | 46.481907 | 29.774494 | 33.022911 |
| Ca | 42.665600 | 28.824413 | 34.180420 |
| S  | 26.795441 | 27.703526 | 36.171043 |
| S  | 26.830744 | 34.068531 | 34.222198 |
| S  | 30.452007 | 29.940117 | 32.696827 |
| S  | 30.147921 | 31.630859 | 36.452744 |
| S  | 33.160915 | 27.469635 | 34.500732 |
| S  | 33.599758 | 32.459606 | 32.664948 |
|   |                  |                  |                  |
|---|-----------------|-----------------|-----------------|
| S | 36.708073       | 28.821335       | 31.873657       |
| S | 36.650082       | 29.137419       | 36.796337       |
| S | 39.849758       | 26.315266       | 33.925804       |
| S | 40.385574       | 31.052084       | 33.777416       |
| S | 43.552551       | 28.384638       | 31.037514       |
| S | 45.088982       | 27.558304       | 38.708996       |

24

generated by VMD

|   |                  |                  |                  |
|---|-----------------|-----------------|-----------------|
| Ca| 25.643133       | 29.872053       | 31.775593       |
| Ca| 26.575960       | 30.704960       | 35.938923       |
| Ca| 29.990238       | 28.756390       | 35.817009       |
| Ca| 30.278589       | 33.201996       | 33.475044       |
| Ca| 33.731506       | 29.393597       | 31.426062       |
| Ca| 33.238876       | 30.584824       | 35.729923       |
| Ca| 36.165852       | 26.588354       | 34.499908       |
| Ca| 36.668301       | 31.243368       | 34.145100       |
| Ca| 40.118740       | 28.502634       | 31.335245       |
| Ca| 39.855270       | 28.624182       | 36.251812       |
| Ca| 46.787285       | 29.504536       | 32.975052       |
| Ca| 42.806767       | 28.595480       | 34.032730       |

S 26.571407       27.388803       35.919552       S 26.931198       33.843582       34.269508 |
| S 30.537457       29.993546       32.946705       S 30.126530       31.822716       36.602200 |
| S 33.065334       27.645266       34.400040       S 33.553577       32.558929       32.618629 |
| S 36.684273       28.698744       31.942873       S 36.516991       29.268387       36.636707 |
| S 39.846592       26.408749       33.863930       S 40.403690       30.997635       33.657959 |
| S 43.662476       28.413696       31.106991       S 44.673767       27.778950       38.663181 |

24

generated by VMD

|   |                  |                  |                  |
|---|-----------------|-----------------|-----------------|
| Ca| 25.727962       | 29.887356       | 31.846104       |
| Ca| 26.412296       | 30.715446       | 35.981041       |
| Ca| 30.127413       | 28.703192       | 35.962627       |
| Ca| 30.412754       | 33.220543       | 33.350483       |
| Ca| 33.675720       | 29.213432       | 31.397038       |
| Ca| 33.137371       | 30.825161       | 35.813320       |
| Ca| 36.247223       | 26.818848       | 34.479584       |
| Ca| 36.793545       | 31.116676       | 34.072990       |
| Ca| 40.071682       | 28.614433       | 31.553013       |
| Ca| 39.511497       | 28.514343       | 36.199066       |
| Ca| 46.859627       | 29.337193       | 32.829556       |
| Ca| 42.847359       | 28.656052       | 34.086189       |
|   |     |     |     |
|---|-----|-----|-----|
| S | 26.707893 | 27.240717 | 35.934452 |
| S | 26.934958 | 33.754974 | 34.009279 |
| S | 30.698969 | 30.006741 | 32.844166 |
| S | 29.938581 | 31.688772 | 36.405338 |
| S | 33.177528 | 27.732426 | 34.487148 |
| S | 33.747414 | 32.530151 | 32.647076 |
| S | 36.774616 | 29.001072 | 31.644455 |
| S | 36.271645 | 29.375614 | 36.762249 |
| S | 39.675858 | 26.485361 | 33.845665 |
| S | 40.278912 | 31.153530 | 33.723068 |
| S | 43.617538 | 28.144810 | 31.080978 |
| S | 44.785545 | 27.654545 | 38.675690 |

24 generated by VMD

|   |     |
|---|-----|
| Ca | 25.131844 |
| Ca | 26.576277 |
| Ca | 29.957743 |
| Ca | 30.174797 |
| Ca | 33.402077 |
| Ca | 33.153820 |
| Ca | 36.448170 |
| Ca | 36.868095 |
| Ca | 40.163853 |
| Ca | 39.915821 |
| Ca | 46.574661 |
| Ca | 42.870041 |
| S  | 26.502277 |
| S  | 26.890768 |
| S  | 30.455894 |
| S  | 29.988726 |
| S  | 33.165932 |
| S  | 33.783897 |
| S  | 36.747032 |
| S  | 36.470867 |
| S  | 39.801876 |
| S  | 40.524727 |
| S  | 43.541325 |
| S  | 45.323441 |

24 generated by VMD

|   |     |     |
|---|-----|-----|
| Ca | 25.275505 | 30.048912 |
| Ca | 26.629204 | 30.738480 |
| Ca | 29.971323 | 28.592209 |
| Ca | 30.220425 | 33.328102 |
| Ca | 33.471813 | 28.890739 |
| Ca | 32.992893 | 30.501318 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 36.405670    | 26.764210    | 34.610146    |
| Ca      | 36.790810    | 31.300976    | 34.134804    |
| Ca      | 40.374107    | 28.666685    | 31.300987    |
| Ca      | 39.696762    | 28.862785    | 36.204613    |
| Ca      | 46.727299    | 29.085087    | 32.957428    |
| Ca      | 42.852459    | 28.675774    | 34.240929    |
| S       | 26.427595    | 27.644199    | 35.687317    |
| S       | 27.019415    | 33.882874    | 34.826065    |
| S       | 30.270485    | 29.980930    | 32.600719    |
| S       | 30.050789    | 31.616825    | 36.520866    |
| S       | 33.121277    | 27.307255    | 34.453762    |
| S       | 33.548729    | 32.373928    | 32.520367    |
| S       | 36.916332    | 29.040747    | 31.930202    |
| S       | 36.491581    | 29.422485    | 36.749702    |
| S       | 39.878834    | 26.530712    | 33.852711    |
| S       | 40.485085    | 31.011066    | 33.628456    |
| S       | 43.467655    | 28.093082    | 31.165314    |
| S       | 45.347786    | 28.032011    | 38.765690    |

24

generated by VMD

Ca  | 25.462357    | 29.630756    | 31.872841    |
Ca  | 26.482447    | 30.831509    | 35.724239    |
Ca  | 29.971638    | 28.558125    | 35.803932    |
Ca  | 30.071501    | 33.138794    | 33.300358    |
Ca  | 33.710606    | 29.135860    | 31.367628    |
Ca  | 33.102291    | 30.517731    | 35.690739    |
Ca  | 36.313278    | 26.815292    | 34.743217    |
Ca  | 36.669434    | 31.124846    | 34.130260    |
Ca  | 40.272011    | 29.065727    | 31.570911    |
Ca  | 39.608990    | 28.996750    | 36.515007    |
Ca  | 46.726051    | 29.062027    | 32.704174    |
Ca  | 42.912777    | 28.566307    | 34.237537    |
S   | 26.463392    | 27.683817    | 35.951855    |
S   | 26.855812    | 33.879910    | 34.407776    |
S   | 30.670315    | 30.047337    | 32.774055    |
S   | 30.019716    | 31.701139    | 36.352989    |
S   | 32.991192    | 27.398739    | 34.463799    |
S   | 33.765621    | 32.460545    | 32.552235    |
S   | 36.727016    | 28.942631    | 31.765366    |
S   | 36.331810    | 29.414429    | 36.830338    |
S   | 39.826824    | 26.608204    | 34.077263    |
S   | 40.460213    | 31.331245    | 34.083340    |
S   | 43.453831    | 28.110977    | 31.157295    |
S   | 45.564846    | 27.368721    | 37.953545    |

24

generated by VMD
Ca  25.466154  29.662270  31.957340
Ca  26.370985  30.740559  35.855896
Ca  29.823868  28.658880  31.783260
Ca  30.372776  33.252274  33.147911
Ca  33.771526  29.223583  31.614588
Ca  33.112438  30.326355  35.443344
Ca  36.421024  26.805876  34.888271
Ca  36.689522  31.391029  34.188377
Ca  40.173874  28.852825  31.440607
Ca  39.414745  28.820274  36.041965
Ca  46.838959  29.071854  32.609520
Ca  42.673092  28.843243  34.201832
S   26.493914  27.610935  35.814095
S   26.805971  33.787743  34.363590
S   30.611979  29.957745  32.763309
S   29.949055  31.904026  36.367416
S   33.039257  27.377472  34.669144
S   33.757633  32.552887  32.659447
S   36.940620  28.784264  32.079933
S   36.394550  29.558846  36.966393
S   39.988766  26.408319  33.773064
S   40.519547  31.199043  33.981873
S   43.600224  28.431072  31.276424
S   45.203457  27.169991  38.143166

24 generated by VMD
Ca  25.004810  30.025364  31.477102
Ca  26.619213  30.820461  36.235184
Ca  29.817360  28.469326  35.910309
Ca  30.338013  32.809193  33.354515
Ca  33.402328  29.181465  31.247272
Ca  33.213730  30.348747  35.294270
Ca  36.310749  26.701757  34.539021
Ca  36.638905  31.651437  34.013443
Ca  40.195972  28.841747  31.581497
Ca  39.900269  28.928318  36.559212
Ca  46.635345  29.272997  32.867245
Ca  42.930069  28.625664  34.391823
S   26.247162  27.750954  35.952595
S   27.050653  33.865921  34.430935
S   30.435694  29.767979  32.869308
S   30.267282  31.716492  36.460056
S   32.957916  27.147411  34.528290
S   33.609917  32.440304  32.295219
S   36.819530  29.028694  31.893333
S   36.595360  29.588057  36.515656
|   |   |   |   |
|---|---|---|---|
| S | 39.969463 | 26.362492 | 34.017342 |
| S | 40.506607 | 31.278275 | 34.100590 |
| S | 43.499321 | 28.402836 | 31.341949 |
| S | 45.468147 | 27.401505 | 38.154633 |
|   |   |   |   |
| Ca | 25.230757 | 30.218130 | 31.793016 |
| Ca | 26.725645 | 30.624674 | 36.002888 |
| Ca | 29.918377 | 28.834656 | 35.902252 |
| Ca | 30.176853 | 33.076656 | 33.313831 |
| Ca | 33.439789 | 29.161777 | 31.309088 |
| Ca | 33.228653 | 30.682041 | 35.446026 |
| Ca | 36.303276 | 26.618820 | 34.411816 |
| Ca | 36.633087 | 31.030079 | 33.958439 |
| Ca | 40.096581 | 28.680464 | 31.817583 |
| Ca | 39.633659 | 28.676537 | 36.060333 |
| Ca | 46.649502 | 29.412701 | 33.099712 |
| Ca | 43.130276 | 28.695263 | 34.228241 |
| S | 26.421118 | 27.405544 | 35.868599 |
| S | 26.911636 | 33.884460 | 34.571114 |
| S | 30.461220 | 29.929739 | 32.816360 |
| S | 30.016834 | 31.902016 | 36.515705 |
| S | 33.005833 | 27.508968 | 34.417221 |
| S | 33.576065 | 32.349636 | 32.544575 |
| S | 36.602242 | 28.727484 | 31.761421 |
| S | 36.685150 | 29.444683 | 36.622765 |
| S | 40.056789 | 26.244514 | 33.950066 |
| S | 40.463215 | 30.976988 | 33.987247 |
| S | 43.778328 | 28.600866 | 31.024616 |
| S | 45.288982 | 27.704742 | 38.607773 |

24 generated by VMD

|   |   |   |   |
|---|---|---|---|
| S | 26.582493 | 27.741552 | 36.106552 |
| S | 26.754951 | 33.957977 | 34.281326 |

24 generated by VMD
| S     | 30.315399 | 29.927151 | 32.852139 |
|-------|-----------|-----------|-----------|
| S     | 30.091557 | 31.713476 | 36.547138 |
| S     | 32.906567 | 27.182388 | 34.661224 |
| S     | 33.620808 | 32.198711 | 32.503006 |
| S     | 36.771801 | 29.016346 | 31.662157 |
| S     | 36.489006 | 29.483210 | 36.498798 |
| S     | 39.985355 | 26.452311 | 33.912182 |
| S     | 40.605595 | 31.099609 | 33.994514 |
| S     | 43.837872 | 28.600784 | 30.980478 |
| S     | 45.210629 | 27.058905 | 38.510216 |

24 generated by VMD

| Ca    | 25.387894 | 30.049206 | 31.251049 |
|-------|-----------|-----------|-----------|
| Ca    | 26.542418 | 30.952152 | 35.906509 |
| Ca    | 29.867533 | 28.626171 | 35.784943 |
| Ca    | 30.140921 | 33.050102 | 33.334309 |
| Ca    | 33.416702 | 28.796461 | 31.741051 |
| Ca    | 33.116596 | 30.420542 | 35.517769 |
| Ca    | 36.358490 | 26.809378 | 34.475761 |
| Ca    | 36.633301 | 31.006023 | 34.091190 |
| Ca    | 40.228935 | 28.928761 | 31.596628 |
| Ca    | 40.026981 | 28.796764 | 36.351788 |
| Ca    | 46.532032 | 29.549999 | 33.081394 |
| Ca    | 43.010891 | 28.551243 | 34.089600 |
| S     | 26.458145 | 27.794376 | 36.007256 |
| S     | 26.955111 | 33.921394 | 34.403008 |
| S     | 30.358570 | 29.971958 | 32.755402 |
| S     | 30.019323 | 31.820240 | 36.568027 |
| S     | 33.109692 | 27.416027 | 34.836029 |
| S     | 33.515984 | 32.202534 | 32.475113 |
| S     | 36.768723 | 28.799927 | 31.915684 |
| S     | 36.622246 | 29.205927 | 36.888386 |
| S     | 39.936481 | 26.555134 | 33.878658 |
| S     | 40.452839 | 31.222660 | 33.939548 |
| S     | 43.559437 | 28.494015 | 30.881897 |
| S     | 45.414673 | 27.450377 | 38.259762 |

24 generated by VMD

| Ca    | 25.381859 | 29.991516 | 31.306120 |
|-------|-----------|-----------|-----------|
| Ca    | 26.779362 | 30.959133 | 36.066196 |
| Ca    | 29.805252 | 28.731331 | 35.733429 |
| Ca    | 30.435932 | 32.978970 | 33.406246 |
| Ca    | 33.566113 | 28.864849 | 31.415775 |
| Ca    | 33.283546 | 30.319653 | 35.821743 |
| Ca    | 36.243965 | 26.743759 | 34.625744 |
| Ca    | 36.867111 | 30.995132 | 34.041603 |
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 40.208511  | 28.971081  | 31.551147  |
| Ca      | 39.762589  | 28.523132  | 36.330194  |
| Ca      | 46.318737  | 29.638844  | 32.950554  |
| Ca      | 42.626614  | 28.676346  | 34.182655  |
| S       | 26.426548  | 27.640274  | 35.857235  |
| S       | 27.104113  | 34.034424  | 34.488686  |
| S       | 30.475624  | 29.782953  | 32.736233  |
| S       | 30.323502  | 31.739742  | 36.509144  |
| S       | 32.998241  | 27.354689  | 34.508858  |
| S       | 33.754757  | 32.227066  | 32.520103  |
| S       | 36.731861  | 28.855366  | 31.910320  |
| S       | 36.427269  | 29.454071  | 36.816605  |
| S       | 39.693737  | 26.578552  | 33.751274  |
| S       | 40.295197  | 31.125906  | 33.939953  |
| S       | 43.221214  | 28.354221  | 31.122612  |
| S       | 45.702324  | 27.850407  | 38.438274  |

24 generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.573433  | 30.024487  | 31.251591  |
| Ca      | 26.705997  | 30.924343  | 35.756031  |
| Ca      | 29.894165  | 28.815306  | 35.821537  |
| Ca      | 30.250505  | 33.069336  | 33.392067  |
| Ca      | 33.239449  | 28.633888  | 31.736546  |
| Ca      | 33.297131  | 30.306034  | 35.763947  |
| Ca      | 36.212540  | 26.722046  | 34.584984  |
| Ca      | 36.851330  | 30.902130  | 34.363602  |
| Ca      | 40.159710  | 28.969139  | 31.700245  |
| Ca      | 39.879665  | 28.965252  | 36.445076  |
| Ca      | 46.620964  | 29.281651  | 32.109215  |
| Ca      | 42.711483  | 29.032166  | 34.254997  |
| S       | 26.568165  | 27.864029  | 35.784863  |
| S       | 26.753914  | 34.078938  | 34.109634  |
| S       | 30.289463  | 29.655323  | 32.789474  |
| S       | 30.291626  | 31.832737  | 36.436104  |
| S       | 33.086136  | 27.344254  | 34.635101  |
| S       | 33.601044  | 32.168526  | 32.756233  |
| S       | 36.720257  | 28.843281  | 32.030704  |
| S       | 36.602051  | 29.201096  | 36.890156  |
| S       | 39.884232  | 26.646069  | 33.907566  |
| S       | 40.533409  | 31.340090  | 33.966221  |
| S       | 43.200512  | 28.160751  | 31.097282  |
| S       | 45.506779  | 27.610546  | 38.447456  |

24 generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.671249  | 29.832745  | 31.034386  |
| Ca      | 26.488091  | 30.863352  | 35.730183  |
| Element | x-axis value | y-axis value | z-axis value |
|---------|--------------|--------------|--------------|
| Ca      | 29.784529    | 28.679447    | 35.894764    |
| Ca      | 30.396257    | 32.908836    | 33.523727    |
| Ca      | 33.669827    | 30.464443    | 35.699135    |
| Ca      | 36.287308    | 26.795391    | 34.759003    |
| Ca      | 36.843559    | 31.149994    | 34.393635    |
| Ca      | 40.185261    | 29.101345    | 31.590206    |
| Ca      | 39.900589    | 29.105469    | 36.319153    |
| Ca      | 46.639992    | 28.708603    | 32.543118    |
| Ca      | 42.687149    | 28.781940    | 33.920574    |
| S       | 26.345236    | 27.719391    | 35.768639    |
| S       | 26.915567    | 33.991646    | 34.138817    |
| S       | 30.473679    | 29.765137    | 32.818314    |
| S       | 29.877626    | 31.774557    | 36.694214    |
| S       | 32.913994    | 27.272720    | 34.742180    |
| S       | 33.757874    | 32.285728    | 32.873848    |
| S       | 36.857483    | 28.943743    | 32.115982    |
| S       | 36.518295    | 29.322136    | 36.960502    |
| S       | 39.825871    | 26.676212    | 33.827137    |
| S       | 40.425922    | 31.374283    | 33.865738    |
| S       | 43.250164    | 28.089596    | 31.028751    |
| S       | 45.607178    | 27.868385    | 38.092182    |

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generated by VMD

| Element | x-axis value | y-axis value | z-axis value |
|---------|--------------|--------------|--------------|
| Ca      | 25.469854    | 29.719316    | 31.207695    |
| Ca      | 26.750975    | 30.554239    | 35.889603    |
| Ca      | 30.056623    | 28.880257    | 35.845119    |
| Ca      | 30.271015    | 33.203049    | 33.038284    |
| Ca      | 33.684029    | 28.941700    | 31.771931    |
| Ca      | 33.109318    | 30.777239    | 35.762409    |
| Ca      | 36.159782    | 26.892370    | 34.515682    |
| Ca      | 36.835178    | 31.176144    | 34.335640    |
| Ca      | 40.070198    | 29.164917    | 31.631256    |
| Ca      | 39.780579    | 28.602760    | 36.324875    |
| Ca      | 46.479378    | 29.238575    | 32.516361    |
| Ca      | 43.040054    | 28.502548    | 34.099182    |
| S       | 26.563938    | 27.429178    | 36.091022    |
| S       | 26.916061    | 33.767101    | 34.249516    |
| S       | 30.639170    | 29.830137    | 32.867596    |
| S       | 29.823385    | 31.985586    | 36.320381    |
| S       | 33.064781    | 27.548124    | 34.752148    |
| S       | 33.780548    | 32.421852    | 32.659538    |
| S       | 36.767330    | 28.913574    | 32.175072    |
| S       | 36.467232    | 29.337372    | 36.953197    |
| S       | 39.782700    | 26.525570    | 33.709522    |
| S       | 40.486168    | 31.174145    | 34.161472    |
|     |       |       |       |
|-----|-------|-------|-------|
| S   | 43.296597 | 28.217094 | 30.982624 |
| S   | 45.139019  | 27.588551  | 38.170536  |

24 generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 25.679245 | 30.109327 | 31.325806 |
| Ca  | 26.358656  | 30.913212  | 35.884773  |
| Ca  | 29.905483  | 28.725548  | 35.936779  |
| Ca  | 30.176155  | 32.966499  | 33.218246  |
| Ca  | 33.587986  | 28.639820  | 31.685814  |
| Ca  | 32.997330  | 30.539505  | 35.904980  |
| Ca  | 36.337273  | 26.874882  | 34.586758  |
| Ca  | 36.634018  | 31.196369  | 34.216869  |
| Ca  | 40.138889  | 29.055574  | 31.544600  |
| Ca  | 39.670597  | 28.858501  | 36.073761  |
| Ca  | 46.576797  | 29.172741  | 32.702141  |
| Ca  | 42.948746  | 28.748478  | 34.185349  |
| S   | 26.456173  | 27.617651  | 35.831699  |
| S   | 26.985378  | 33.976959  | 34.209667  |
| S   | 30.609308  | 29.609741  | 32.876099  |
| S   | 29.929083  | 31.928699  | 36.430641  |
| S   | 32.967655  | 27.411797  | 34.814796  |
| S   | 33.664864  | 32.283092  | 32.836620  |
| S   | 36.712898  | 28.835197  | 31.992504  |
| S   | 36.442875  | 29.292299  | 36.779346  |
| S   | 39.814262  | 26.498718  | 33.552879  |
| S   | 40.610695  | 31.249771  | 34.051632  |
| S   | 43.419243  | 28.350952  | 31.069263  |
| S   | 45.810291  | 27.536055  | 38.319756  |

24 generated by VMD

|     |       |       |       |
|-----|-------|-------|-------|
| Ca  | 25.442635 | 29.974052 | 31.520815 |
| Ca  | 26.827442  | 30.814945  | 35.856495  |
| Ca  | 29.963730  | 28.572149  | 35.961281  |
| Ca  | 30.595495  | 33.048901  | 33.158348  |
| Ca  | 33.657642  | 29.023445  | 31.845047  |
| Ca  | 33.054668  | 30.462914  | 35.646420  |
| Ca  | 36.026299  | 26.697334  | 34.449490  |
| Ca  | 36.688614  | 31.280869  | 34.279778  |
| Ca  | 40.138210  | 29.087484  | 31.565010  |
| Ca  | 39.526791  | 28.463911  | 36.061813  |
| Ca  | 46.606056  | 29.395687  | 32.863556  |
| Ca  | 42.929958  | 28.826256  | 34.157787  |
| S   | 26.656212  | 27.550892  | 36.146225  |
| S   | 27.222855  | 34.018742  | 34.298820  |
| S   | 30.552422  | 29.821995  | 32.732475  |
| S   | 30.066151  | 31.746027  | 36.358601  |
|    | X   | Y   | Z   |
|----|-----|-----|-----|
| S  | 32.865646 | 27.368343 | 34.734112 |
| S  | 33.896111 | 32.335262 | 32.376835 |
| S  | 36.813477 | 28.895235 | 32.201702 |
| S  | 36.328636 | 29.097660 | 36.699242 |
| S  | 39.605762 | 26.534355 | 33.503525 |
| S  | 40.351273 | 31.193230 | 34.139999 |
| S  | 43.362080 | 28.368938 | 31.063759 |
| S  | 45.255783 | 27.812750 | 38.409500 |

24

-generated by VMD

| Ca  | X   | Y   | Z   |
|-----|-----|-----|-----|
| Ca  | 25.677505 | 29.634102 | 31.533031 |
| Ca  | 26.690653 | 30.868452 | 35.975655 |
| Ca  | 29.800114 | 28.683563 | 36.033638 |
| Ca  | 30.118580 | 33.063320 | 33.334305 |
| Ca  | 33.746323 | 28.999329 | 31.750929 |
| Ca  | 33.197487 | 30.212181 | 35.760342 |
| Ca  | 36.147926 | 27.087776 | 34.453392 |
| Ca  | 36.759285 | 31.566944 | 34.388542 |
| Ca  | 40.264542 | 28.948801 | 31.014774 |
| Ca  | 36.308613 | 29.340427 | 33.314617 |
| Ca  | 42.596161 | 28.624849 | 34.047062 |
| S  | 26.469837 | 27.559942 | 35.881733 |
| S  | 26.845501 | 33.961716 | 34.119289 |
| S  | 30.692673 | 29.862129 | 32.989742 |
| S  | 30.104469 | 31.764402 | 36.541092 |
| S  | 32.888397 | 27.181133 | 34.713531 |
| S  | 33.726131 | 32.502731 | 32.593998 |
| S  | 36.971363 | 29.353664 | 32.176994 |
| S  | 36.706245 | 29.351383 | 36.758461 |
| S  | 39.679306 | 26.894902 | 33.361595 |
| S  | 40.543613 | 31.156971 | 33.793732 |
| S  | 43.654701 | 28.125587 | 30.979870 |
| S  | 45.226215 | 27.393791 | 38.552586 |

24

-generated by VMD

| Ca  | X   | Y   | Z   |
|-----|-----|-----|-----|
| Ca  | 25.443829 | 29.802822 | 31.513821 |
| Ca  | 26.621588 | 30.702286 | 35.976810 |
| Ca  | 29.988089 | 28.729269 | 35.734219 |
| Ca  | 30.214117 | 33.107841 | 33.482216 |
| Ca  | 33.687759 | 29.194189 | 31.730488 |
| Ca  | 33.227390 | 30.527851 | 35.730965 |
| Ca  | 36.484070 | 26.894705 | 34.692574 |
| Ca  | 36.663658 | 31.368979 | 33.965645 |
| Ca  | 40.246712 | 28.965874 | 31.143276 |
| Ca  | 39.659863 | 28.371557 | 36.153725 |
|    | Ca       | 45.832760 | 29.855295 | 33.481026 |
|----|----------|-----------|-----------|-----------|
|    | Ca       | 42.588173 | 28.389187 | 34.099335 |
|    | S        | 26.714296 | 27.452106 | 35.796494 |
|    | S        | 26.963402 | 33.804802 | 34.177299 |
|    | S        | 30.655870 | 29.830618 | 32.885948 |
|    | S        | 30.171223 | 31.971769 | 36.635880 |
|    | S        | 33.191452 | 27.348930 | 34.860474 |
|    | S        | 33.613022 | 32.446640 | 32.582542 |
|    | S        | 36.916103 | 29.015594 | 31.910191 |
|    | S        | 36.833248 | 29.667816 | 36.731674 |
|    | S        | 39.665150 | 26.383009 | 33.316628 |
|    | S        | 40.436768 | 30.872458 | 33.865738 |
|    | S        | 43.310444 | 28.353836 | 31.081505 |
|    | S        | 45.304977 | 27.333918 | 38.482208 |

24 generated by VMD

|    | Ca       | 25.156897 | 29.792196 | 31.359234 |
|----|----------|-----------|-----------|-----------|
|    | Ca       | 26.217882 | 30.893864 | 35.980484 |
|    | Ca       | 29.796196 | 28.887875 | 36.050373 |
|    | Ca       | 30.508753 | 33.076813 | 33.406582 |
|    | Ca       | 33.633942 | 28.953392 | 31.785002 |
|    | Ca       | 33.150318 | 30.629988 | 35.718239 |
|    | Ca       | 36.290817 | 26.747023 | 34.698200 |
|    | Ca       | 36.944653 | 30.997561 | 34.262264 |
|    | Ca       | 40.206707 | 28.688412 | 31.103184 |
|    | Ca       | 39.842682 | 28.476301 | 36.254089 |
|    | Ca       | 46.065857 | 30.116968 | 33.260410 |
|    | Ca       | 42.742756 | 28.662518 | 34.091164 |

S | 26.445145 | 27.584082 | 35.653458 |
S | 27.010481 | 33.992752 | 34.104687 |
S | 30.559782 | 29.989183 | 32.897366 |
S | 30.013075 | 31.916204 | 36.620377 |
S | 33.128799 | 27.306549 | 34.851631 |
S | 33.914139 | 32.272461 | 32.620758 |
S | 36.805580 | 28.722424 | 31.873131 |
S | 36.652035 | 29.164547 | 36.849182 |
S | 39.846600 | 26.348028 | 33.663338 |
S | 40.443424 | 30.900928 | 33.645390 |
S | 43.622871 | 28.831673 | 30.990986 |
S | 45.434555 | 27.439604 | 38.291237 |

24 generated by VMD

|    | Ca       | 25.277187 | 29.645784 | 31.624825 |
|----|----------|-----------|-----------|-----------|
|    | Ca       | 26.351807 | 30.866247 | 35.995258 |
|    | Ca       | 30.016136 | 28.868525 | 36.013229 |
|    | Ca       | 30.174572 | 33.031178 | 33.265797 |
|  | Ca    |  |  |
|---|-------|---|---|
| Ca | 33.735321 | 28.994173 | 31.545555 |
| Ca | 33.235462 | 30.569468 | 35.617683 |
| Ca | 36.597031 | 26.917051 | 34.585670 |
| Ca | 36.774967 | 31.205931 | 34.354023 |
| Ca | 40.350571 | 28.726944 | 31.075821 |
| Ca | 39.764580 | 28.611473 | 36.134480 |
| Ca | 46.097538 | 29.991806 | 33.422455 |
| Ca | 42.745388 | 28.673637 | 34.156647 |
| S  | 26.231493 | 27.738260 | 35.580040 |
| S  | 27.006756 | 33.987976 | 34.027599 |
| S  | 30.542316 | 29.743626 | 32.981266 |
| S  | 29.978117 | 31.984320 | 36.571835 |
| S  | 33.125443 | 27.345510 | 34.854588 |
| S  | 33.733669 | 32.284348 | 32.887810 |
| S  | 36.804543 | 28.880144 | 31.938705 |
| S  | 36.866611 | 29.252752 | 36.867943 |
| S  | 39.828018 | 26.345448 | 33.478001 |
| S  | 40.459209 | 31.010420 | 33.757778 |
| S  | 43.394409 | 28.663795 | 31.167301 |
| S  | 45.342770 | 27.052603 | 38.126476 |

24 generated by VMD

|  | Ca    |  |  |
|---|-------|---|---|
| Ca | 25.292385 | 29.656513 | 31.128746 |
| Ca | 26.446218 | 30.933296 | 36.022598 |
| Ca | 30.019960 | 28.701591 | 36.137978 |
| Ca | 30.373079 | 33.117523 | 33.248566 |
| Ca | 33.568977 | 29.180481 | 31.782444 |
| Ca | 33.068787 | 30.423538 | 35.685837 |
| Ca | 36.456394 | 26.881294 | 34.765800 |
| Ca | 36.742161 | 31.334584 | 34.142452 |
| Ca | 40.158916 | 28.640610 | 31.065756 |
| Ca | 39.715340 | 28.692131 | 36.384098 |
| Ca | 46.091423 | 29.941685 | 33.294563 |
| Ca | 42.665436 | 28.583801 | 34.062557 |
| S  | 26.633097 | 27.608585 | 35.788971 |
| S  | 27.095711 | 33.926918 | 33.841724 |
| S  | 30.541134 | 29.815857 | 33.070866 |
| S  | 29.933510 | 31.902590 | 36.626244 |
| S  | 33.162460 | 27.332706 | 35.070129 |
| S  | 33.756134 | 32.438477 | 32.606873 |
| S  | 36.828495 | 28.844330 | 31.867168 |
| S  | 36.732903 | 29.350163 | 36.893280 |
| S  | 39.970966 | 26.452461 | 33.691235 |
| S  | 40.218605 | 31.055868 | 33.823006 |
| S  | 43.538219 | 28.907333 | 30.938236 |
| S  | 45.423584 | 26.670176 | 38.091579 |
| Element | X-coord | Y-coord | Z-coord |
|---------|---------|---------|---------|
| Ca      | 25.497160 | 29.400446 | 31.500605 |
| Ca      | 26.581221 | 31.107899 | 35.843956 |
| Ca      | 29.896814 | 28.815565 | 36.007183 |
| Ca      | 30.236435 | 32.875015 | 33.344269 |
| Ca      | 33.598091 | 28.968410 | 31.583212 |
| Ca      | 33.174488 | 30.432232 | 35.776180 |
| Ca      | 36.305652 | 27.170736 | 34.566277 |
| Ca      | 36.850557 | 31.090740 | 34.219467 |
| Ca      | 40.293217 | 28.792030 | 31.165901 |
| Ca      | 39.967323 | 28.482969 | 36.510132 |
| Ca      | 46.144554 | 30.230808 | 33.332711 |
| Ca      | 42.773109 | 28.397005 | 34.041283 |
| S       | 26.473083 | 27.735308 | 36.055916 |
| S       | 26.831610 | 34.129906 | 33.759552 |
| S       | 30.456797 | 29.761993 | 32.842396 |
| S       | 30.043899 | 31.968397 | 36.594162 |
| S       | 33.040977 | 27.417002 | 34.872192 |
| S       | 33.836376 | 32.127548 | 32.920536 |
| S       | 36.848808 | 29.183105 | 31.858444 |
| S       | 36.775135 | 29.134611 | 36.847282 |
| S       | 39.661621 | 26.551613 | 33.518311 |
| S       | 40.410145 | 31.037769 | 33.748947 |
| S       | 43.539524 | 28.886492 | 30.972605 |
| S       | 45.231415 | 26.693792 | 38.148640 |

24

generated by VMD
|    |      |      |      |
|----|------|------|------|
| S  | 36.959465 | 29.264893 | 32.063644 |
| S  | 36.606426 | 29.52068 | 36.692314 |
| S  | 39.675926 | 26.32465 | 33.507278 |
| S  | 40.456589 | 31.32505 | 36.320412 |
| S  | 43.482712 | 28.370428 | 31.116768 |
| S  | 45.146935 | 27.021534 | 38.193745 |
| Ca | 25.379213 | 29.317436 | 31.071321 |
| Ca | 26.511211 | 30.81647 | 36.121284 |
| Ca | 30.047516 | 28.930431 | 35.915859 |
| Ca | 30.261703 | 33.087234 | 33.389835 |
| Ca | 33.612362 | 29.184025 | 31.959805 |
| Ca | 33.232197 | 30.626225 | 35.772278 |
| Ca | 36.401619 | 26.32932 | 34.560478 |
| Ca | 36.804138 | 31.122244 | 34.285049 |
| Ca | 40.292011 | 28.765963 | 31.265671 |
| Ca | 39.763115 | 28.662514 | 36.010910 |
| Ca | 46.144127 | 29.820267 | 33.272263 |
| Ca | 42.733952 | 28.536636 | 34.054817 |
| S  | 26.416964 | 27.534552 | 35.790417 |
| S  | 26.775198 | 33.922279 | 33.940933 |
| S  | 30.463320 | 29.83023 | 33.004044 |
| S  | 29.985123 | 31.993217 | 36.632156 |
| S  | 33.303970 | 27.547276 | 35.045193 |
| S  | 33.798454 | 32.443001 | 32.892643 |
| S  | 36.869755 | 29.068144 | 31.910423 |
| S  | 36.802254 | 29.330814 | 36.738525 |
| S  | 39.773888 | 26.383137 | 33.406803 |
| S  | 40.553108 | 31.076538 | 33.715549 |
| S  | 43.509670 | 28.473488 | 30.933096 |
| S  | 44.999046 | 26.970428 | 38.341263 |

24 generated by VMD

|    |      |      |      |
|----|------|------|------|
| Ca | 25.469776 | 29.221096 | 31.267704 |
| Ca | 26.463228 | 30.962955 | 36.058876 |
| Ca | 30.080219 | 28.847878 | 36.191608 |
| Ca | 30.330637 | 33.045364 | 33.493546 |
| Ca | 33.486511 | 29.271023 | 31.544844 |
| Ca | 33.152042 | 30.760151 | 35.822350 |
| Ca | 36.403866 | 26.892452 | 34.559589 |
| Ca | 36.650391 | 31.117842 | 34.312256 |
| Ca | 40.181385 | 28.988880 | 31.170067 |
| Ca | 39.721825 | 28.448669 | 36.072025 |
| Ca | 46.473415 | 29.859999 | 33.772751 |
| Ca | 42.945263 | 28.481148 | 33.880730 |
|   | 26.521711 | 27.593868 | 35.983009 |
|---|-----------|-----------|-----------|
| S | 26.723576 | 33.934846 | 33.915482 |
| S | 30.364822 | 29.849926 | 32.905289 |
| S | 30.066883 | 31.979366 | 36.810055 |
| S | 33.013130 | 27.659126 | 34.702168 |
| S | 33.584500 | 32.586933 | 32.679283 |
| S | 36.695206 | 28.999722 | 31.810135 |
| S | 36.831497 | 29.121670 | 36.587509 |
| S | 39.876068 | 26.370384 | 33.335575 |
| S | 40.518276 | 30.951046 | 33.768030 |
| S | 43.784279 | 28.573664 | 30.967712 |
| S | 45.085426 | 26.873772 | 38.427238 |
|   | 24        |           |           |
| generated by VMD |
| Ca | 25.621792 | 29.437321 | 31.281826 |
| Ca | 26.559645 | 30.974720 | 35.967617 |
| Ca | 29.742170 | 28.692179 | 36.122837 |
| Ca | 30.350458 | 32.887123 | 33.401184 |
| Ca | 33.745644 | 29.194891 | 31.690899 |
| Ca | 33.156414 | 30.650784 | 35.804577 |
| Ca | 36.393299 | 27.116020 | 34.762955 |
| Ca | 36.731781 | 31.282875 | 34.142639 |
| Ca | 40.149712 | 29.035442 | 31.216228 |
| Ca | 39.691826 | 28.617743 | 36.134914 |
| Ca | 42.62127 | 29.902306 | 33.600353 |
| Ca | 42.807259 | 28.378023 | 33.980598 |
| S | 26.605103 | 27.438190 | 35.858879 |
| S | 26.979061 | 33.871658 | 33.859032 |
| S | 30.629723 | 29.709768 | 33.078064 |
| S | 29.989799 | 31.786953 | 36.617744 |
| S | 33.157814 | 27.544888 | 34.849506 |
| S | 33.739075 | 32.509911 | 32.812851 |
| S | 36.679676 | 28.913780 | 31.850994 |
| S | 36.876984 | 29.653671 | 36.848473 |
| S | 39.651917 | 26.630081 | 33.454553 |
| S | 40.500015 | 31.117508 | 33.804310 |
| S | 43.545399 | 28.505501 | 30.902481 |
| S | 44.867229 | 26.540123 | 37.987289 |
|   | 24        |           |           |
| generated by VMD |
| Ca | 25.468760 | 29.461660 | 31.321045 |
| Ca | 26.556707 | 30.914545 | 36.097229 |
| Ca | 29.958950 | 28.719374 | 36.041683 |
| Ca | 30.361347 | 33.114086 | 33.350426 |
| Ca | 33.503090 | 29.050850 | 31.588573 |
| Ca | 33.252502 | 30.724676 | 35.763809 |
| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 36.475807 | 26.781303 | 34.564068 |
| Ca      | 36.645164 | 31.150608 | 34.091942 |
| Ca      | 40.179916 | 28.889915 | 31.119709 |
| Ca      | 39.717510 | 28.290005 | 36.114166 |
| Ca      | 46.141251 | 30.317593 | 33.844292 |
| Ca      | 42.824944 | 28.747190 | 34.120533 |
| S       | 26.495714 | 27.546219 | 36.060692 |
| S       | 27.101009 | 33.901165 | 34.110573 |
| S       | 30.547813 | 30.005611 | 32.954613 |
| S       | 30.216246 | 31.917315 | 36.666710 |
| S       | 33.132126 | 27.500355 | 34.753723 |
| S       | 33.897411 | 32.328571 | 32.417789 |
| S       | 36.665321 | 28.876226 | 31.764744 |
| S       | 36.771484 | 29.350460 | 36.800690 |
| S       | 39.810490 | 26.520601 | 33.435539 |
| S       | 40.319080 | 30.986153 | 33.942757 |
| S       | 43.540253 | 28.649019 | 30.830894 |
| S       | 44.852692 | 26.647863 | 38.274529 |

generated by VMD

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| Ca      | 25.413670 | 29.709389 | 31.802231 |
| Ca      | 26.368412 | 30.783455 | 36.331596 |
| Ca      | 29.941183 | 28.733601 | 35.971607 |
| Ca      | 30.337940 | 32.941856 | 33.013260 |
| Ca      | 33.763557 | 29.092482 | 31.693451 |
| Ca      | 33.152607 | 30.835384 | 35.540848 |
| Ca      | 36.307610 | 26.854977 | 34.533764 |
| Ca      | 36.763260 | 31.213331 | 34.026714 |
| Ca      | 40.251030 | 29.009533 | 31.257189 |
| Ca      | 39.572361 | 28.342077 | 36.044212 |
| Ca      | 46.286896 | 30.489126 | 34.233551 |
| Ca      | 42.800938 | 28.458324 | 34.080208 |
| S       | 26.408852 | 27.557819 | 36.032154 |
| S       | 27.158554 | 33.679688 | 34.301037 |
| S       | 30.647259 | 29.780191 | 32.791107 |
| S       | 30.037649 | 31.953817 | 36.469139 |
| S       | 32.945442 | 27.566948 | 34.770035 |
| S       | 33.853264 | 32.493233 | 32.389500 |
| S       | 36.830620 | 28.775633 | 31.870199 |
| S       | 36.644009 | 29.592081 | 36.682816 |
| S       | 39.749043 | 26.363853 | 33.271339 |
| S       | 40.459072 | 30.965256 | 33.995312 |
| S       | 43.628933 | 28.830788 | 30.971031 |
| S       | 45.111679 | 26.368584 | 37.958416 |

generated by VMD
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.366894 | 29.558353 | 31.617773 |
| Ca      | 26.466309 | 31.006762 | 36.214962 |
| Ca      | 30.005074 | 28.958727 | 36.086823 |
| Ca      | 30.245390 | 32.771656 | 33.307335 |
| Ca      | 33.475124 | 29.137733 | 31.510336 |
| Ca      | 33.067024 | 30.798496 | 35.387932 |
| Ca      | 36.314091 | 26.602465 | 34.469257 |
| Ca      | 36.908913 | 31.258080 | 33.985371 |
| Ca      | 40.504925 | 28.961082 | 31.144287 |
| Ca      | 39.626740 | 28.307924 | 36.075626 |
| Ca      | 46.212097 | 30.185440 | 34.156502 |
| Ca      | 42.830452 | 28.399797 | 34.231438 |
| S       | 26.738928 | 27.646091 | 36.228859 |
| S       | 27.021540 | 34.031002 | 34.449932 |
| S       | 30.294479 | 29.655312 | 32.984818 |
| S       | 30.086262 | 32.019051 | 36.557049 |
| S       | 33.063717 | 27.419899 | 34.560009 |
| S       | 33.604420 | 32.290230 | 34.417263 |
| S       | 36.043640 | 29.092999 | 31.518311 |
| S       | 36.489048 | 29.267769 | 36.490269 |
| S       | 39.918114 | 26.435171 | 33.239288 |
| S       | 40.568832 | 30.858826 | 33.964542 |
| S       | 43.630192 | 28.956982 | 31.052502 |
| S       | 45.061066 | 26.771458 | 38.380222 |

24 generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 25.541590 | 29.531193 | 31.621071 |
| Ca      | 26.517029 | 30.929941 | 36.466927 |
| Ca      | 30.073324 | 28.769581 | 35.974640 |
| Ca      | 30.269012 | 33.010517 | 33.265831 |
| Ca      | 33.456707 | 29.025158 | 31.256359 |
| Ca      | 33.328014 | 31.063452 | 35.611214 |
| Ca      | 36.386673 | 26.486259 | 33.983231 |
| Ca      | 36.631157 | 31.038357 | 33.949509 |
| Ca      | 40.070454 | 28.779530 | 31.247746 |
| Ca      | 39.537224 | 28.118872 | 35.993935 |
| Ca      | 45.951054 | 30.512199 | 34.383888 |
| Ca      | 42.736183 | 28.651564 | 34.300354 |
| S       | 26.934704 | 27.702555 | 36.359745 |
| S       | 27.170277 | 33.965492 | 34.568241 |
| S       | 30.510218 | 29.998550 | 32.877689 |
| S       | 30.116482 | 32.048889 | 36.611111 |
| S       | 33.232048 | 27.674860 | 34.386063 |
| S       | 33.697071 | 32.336266 | 32.368347 |
| S       | 36.653938 | 28.795404 | 31.500332 |
| S       | 36.499737 | 29.088043 | 36.359154 |
|  |  |  |  |
|---|---|---|---|
| S | 40.078251 | 26.242899 | 33.356861 |
| S | 40.295372 | 30.742889 | 33.894783 |
| S | 43.762726 | 29.001005 | 31.101837 |
| S | 44.984596 | 26.877888 | 38.591808 |

24

*generated by VMD*

| Ca | 25.484863 | 29.501484 | 31.692963 |
| Ca | 26.386898 | 31.116760 | 36.238281 |
| Ca | 30.332275 | 28.571804 | 36.149273 |
| Ca | 29.974575 | 33.058620 | 33.162376 |
| Ca | 33.526806 | 29.249710 | 31.502043 |
| Ca | 33.285175 | 30.650543 | 35.565655 |
| Ca | 36.683392 | 26.693338 | 34.248627 |
| Ca | 36.774178 | 31.141239 | 34.121639 |
| Ca | 40.120525 | 29.012661 | 31.125685 |
| Ca | 39.580956 | 28.157848 | 35.782890 |
| Ca | 46.109299 | 30.367403 | 34.313747 |
| Ca | 42.716927 | 28.578112 | 34.166473 |

| S | 26.721052 | 27.772726 | 36.305832 |
| S | 26.871656 | 34.117058 | 34.274471 |

| S | 30.570648 | 29.875477 | 32.977634 |
| S | 29.898960 | 31.881884 | 36.405746 |
| S | 33.414040 | 27.453690 | 34.529205 |
| S | 33.561165 | 32.441753 | 32.595966 |
| S | 36.698719 | 29.153574 | 31.586891 |
| S | 36.713951 | 29.168827 | 36.628841 |
| S | 39.954575 | 26.375051 | 32.943855 |
| S | 40.360634 | 30.834291 | 33.905296 |
| S | 43.761314 | 28.519564 | 31.338608 |
| S | 45.031349 | 26.722004 | 38.468601 |

24

*generated by VMD*

| Ca | 25.701176 | 29.666622 | 32.020504 |
| Ca | 26.538460 | 30.871164 | 36.237961 |
| Ca | 30.143995 | 28.837788 | 36.264214 |
| Ca | 30.367962 | 33.143623 | 33.088676 |
| Ca | 33.580574 | 28.818554 | 31.285614 |
| Ca | 33.393978 | 30.917751 | 35.482468 |
| Ca | 36.347656 | 26.625322 | 34.286118 |
| Ca | 36.650215 | 31.140127 | 33.812302 |
| Ca | 40.291992 | 29.177801 | 31.363262 |
| Ca | 39.480354 | 28.267649 | 36.255894 |
| Ca | 45.957783 | 30.259552 | 34.014999 |
| Ca | 42.487999 | 28.775837 | 34.219379 |
| S | 26.840479 | 27.524561 | 36.207573 |
| S | 27.101761 | 33.988289 | 34.383495 |
S    30.677586  29.925026  32.874344
S    30.112907  31.856773  36.552238
S    33.248230  27.560863  34.616146
S    33.763065  32.169334  32.262135
S    36.823776  28.848171  31.357243
S    36.523746  29.219492  36.552238
S    39.808441  26.470627  33.210915
S    40.219788  30.953241  34.126377
S    43.687241  28.854073  31.357943
S    44.739285  26.519159  38.197910

24 generated by VMD
Ca    25.275278  29.764221  31.795435
Ca    26.764847  30.848036  36.548332
Ca    30.156898  28.794081  35.882252
Ca    30.203520  33.188179  33.029980
Ca    33.259308  28.697691  31.540497
Ca    33.289494  31.057657  35.357224
Ca    36.635807  26.819994  34.232147
Ca    36.696983  31.160162  33.966686
Ca    40.124474  29.175591  31.339481
Ca    39.639835  28.206850  36.310810
Ca    46.266121  30.254837  34.354008
Ca    42.701454  28.502583  34.051483
S    26.885143  27.481373  36.334454
S    27.007673  33.830769  34.125805
S    30.418854  29.787827  32.793247
S    30.060341  32.038239  36.436268
S    33.190132  27.781610  34.605663
S    33.629234  32.260612  32.368481
S    36.617249  29.122076  31.644619
S    36.534367  29.037985  36.632927
S    39.923431  26.405176  33.166477
S    40.389732  30.777094  34.159512
S    43.749580  28.937416  31.049644
S    45.014122  26.461376  38.305267

24 generated by VMD
Ca    25.409847  29.434803  31.631096
Ca    26.887611  30.984547  36.249374
Ca    30.100273  28.752098  36.089340
Ca    30.302322  32.858757  33.130898
Ca    33.231262  28.912222  31.236481
Ca    33.336685  30.991346  35.397701
Ca    36.343441  26.869434  34.326027
Ca    36.908176  31.207264  33.852341
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 40.1.42014 | 29.1.29400 | 31.6.22524 |
| Ca      | 39.4.00921 | 28.2.68709 | 36.3.08144 |
| Ca      | 46.0.84366 | 30.2.70100 | 33.7.10434 |
| Ca      | 42.8.99822 | 28.5.98816 | 34.3.07774 |
| S       | 26.7.64277 | 27.5.32419 | 36.1.57532 |
| S       | 27.1.75709 | 33.9.85809 | 34.3.74973 |
| S       | 30.3.37700 | 29.7.39969 | 32.8.53027 |
| S       | 30.2.34661 | 31.8.58131 | 36.6.29398 |
| S       | 33.0.02501 | 27.6.58049 | 34.5.36942 |
| S       | 33.7.29828 | 32.2.57083 | 32.2.25525 |
| S       | 36.6.64295 | 29.0.36411 | 31.4.69210 |
| S       | 36.4.91470 | 29.3.90038 | 36.5.46680 |
| S       | 39.8.74397 | 26.5.80170 | 33.6.36288 |
| S       | 40.3.74603 | 30.8.56552 | 34.4.41113 |
| S       | 43.4.50409 | 28.8.74981 | 31.2.18615 |
| S       | 45.2.64297 | 26.3.20993 | 38.0.79193 |

24 generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.7.45979 | 29.6.35069 | 31.7.92652 |
| Ca      | 26.6.10477 | 30.9.42736 | 36.2.82059 |
| Ca      | 30.1.31388 | 28.6.82413 | 35.9.77528 |
| Ca      | 30.1.48724 | 32.9.74628 | 32.8.67096 |
| Ca      | 33.3.85109 | 28.9.35654 | 31.3.65074 |
| Ca      | 33.2.77336 | 30.7.89482 | 35.6.34571 |
| Ca      | 36.3.89275 | 26.7.49689 | 34.2.05521 |
| Ca      | 36.6.38206 | 31.2.36003 | 33.7.90119 |
| Ca      | 40.1.57269 | 29.1.69472 | 31.2.89906 |
| Ca      | 39.6.46851 | 28.4.73764 | 36.1.95320 |
| Ca      | 46.2.01775 | 30.0.82529 | 34.2.26284 |
| Ca      | 42.6.46549 | 28.6.61617 | 34.1.41632 |
| S       | 26.9.58096 | 27.7.58680 | 36.7.64267 |
| S       | 27.1.24565 | 33.9.01894 | 34.3.58829 |
| S       | 30.4.54412 | 29.7.22111 | 32.8.93063 |
| S       | 30.0.86796 | 31.9.59286 | 36.2.54539 |
| S       | 33.1.99074 | 27.6.09158 | 34.6.53805 |
| S       | 33.5.52330 | 32.2.44408 | 32.3.68034 |
| S       | 36.7.22630 | 28.9.31740 | 31.4.91297 |
| S       | 36.6.02730 | 29.2.37757 | 36.4.77566 |
| S       | 39.9.78413 | 26.4.81728 | 33.2.14844 |
| S       | 40.2.40860 | 31.0.58489 | 34.3.08167 |
| S       | 43.8.48724 | 29.1.77204 | 31.3.30811 |
| S       | 44.6.86275 | 25.9.75254 | 38.1.47720 |

24 generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.0.55077 | 29.8.80474 | 31.8.29510 |
| Ca      | 26.6.98755 | 30.8.86841 | 36.3.77556 |
| Element | X-coordinate 1 | Y-coordinate 1 | Z-coordinate 1 | X-coordinate 2 | Y-coordinate 2 | Z-coordinate 2 |
|---------|----------------|----------------|----------------|----------------|----------------|----------------|
| Ca      | 30.192936      | 28.808130      | 36.024540      | 30.142239      | 32.839996      | 33.151520      |
| Ca      | 33.373871      | 30.871611      | 35.356728      | 33.375622      | 29.026478      | 31.162037      |
| S       | 26.972933      | 27.496679      | 36.528736      | 26.971779      | 33.873577      | 34.469231      |
| S       | 30.419178      | 29.641243      | 32.787575      | 30.133259      | 31.876303      | 36.369392      |
| S       | 33.177219      | 27.541143      | 34.605843      | 33.653950      | 32.366364      | 32.264893      |
| S       | 36.853157      | 28.908257      | 31.458191      | 36.471418      | 29.282354      | 36.304337      |
| S       | 39.920738      | 26.553707      | 33.480225      | 40.335945      | 30.968290      | 34.212029      |
| S       | 43.784771      | 28.851490      | 31.374701      | 44.774643      | 26.202696      | 38.425407      |

24 generated by VMD

| Element | X-coordinate 1 | Y-coordinate 1 | Z-coordinate 1 | X-coordinate 2 | Y-coordinate 2 | Z-coordinate 2 |
|---------|----------------|----------------|----------------|----------------|----------------|----------------|
| Ca      | 25.288866      | 29.880182      | 31.907080      | 26.483562      | 30.836002      | 36.610210      |
| Ca      | 30.316120      | 28.736607      | 36.046928      | 30.257353      | 32.830177      | 33.059471      |
| Ca      | 33.375622      | 29.026478      | 31.162037      | 33.111515      | 31.169317      | 35.260338      |
| Ca      | 36.242607      | 27.016182      | 33.835381      | 36.704926      | 31.238827      | 33.920605      |
| Ca      | 40.257301      | 28.915585      | 31.332859      | 39.682316      | 28.280626      | 36.313858      |
| Ca      | 46.311630      | 30.208073      | 34.344135      | 42.895752      | 28.588329      | 34.467087      |
| S       | 27.091938      | 27.525618      | 36.692066      | 27.048361      | 33.791088      | 34.532562      |
| S       | 30.268793      | 29.652180      | 32.822216      | 29.885637      | 31.849527      | 36.428444      |
| S       | 33.204567      | 27.647154      | 34.412186      | 33.687199      | 32.364944      | 32.166641      |
| S       | 36.937748      | 29.295626      | 31.182341      | 36.567200      | 29.181055      | 36.320183      |
| S       | 39.924812      | 26.418385      | 33.333229      | 40.362595      | 30.857418      | 34.170815      |
S  43.725338  28.657457  31.346512
S  44.902206  26.424578  38.363541

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generated by VMD

Ca   25.188272  29.717756  32.201508
Ca   26.754164  30.816004  36.335518
Ca   30.182920  28.809715  35.841118
Ca   30.468575  32.947281  33.067932
Ca   33.525364  29.097094  31.212765
Ca   33.395821  30.951105  35.367691
Ca   36.274006  26.637918  33.992100
Ca   36.623119  30.814785  33.806934
Ca   40.037476  29.121016  31.353235
Ca   39.413231  28.109331  36.224873
Ca   46.237690  30.391798  34.367207
Ca   42.813026  28.673306  34.343864
S    27.125660  27.659334  36.595333
S    27.287865  33.999695  34.487934
S    30.489048  29.853901  32.709385
S    30.128099  31.951536  36.351765
S    33.184643  27.674852  34.383640
S    33.825447  32.397129  32.228992
S    36.712605  28.753803  31.286175
S    36.344250  28.845821  36.593185
S    39.874245  26.556124  33.397537
S    40.107996  30.844542  34.289688
S    43.604805  28.921659  31.304531
S    44.842804  26.845892  38.287788

24

generated by VMD

Ca   25.108055  29.968338  32.148750
Ca   26.818905  30.680050  36.475178
Ca   30.206749  28.805168  35.849342
Ca   30.109615  33.030571  33.036453
Ca   33.323032  29.032982  31.163929
Ca   33.401276  30.929684  35.395668
Ca   36.472687  26.601887  34.002380
Ca   36.627262  31.032524  33.677139
Ca   40.284924  28.747719  31.114491
Ca   39.768188  28.334702  36.297752
Ca   46.271500  30.347385  34.353577
Ca   42.531292  28.797447  34.284546
S    27.100954  27.602764  36.656261
S    27.062756  33.968853  34.720070
S    30.252924  29.818985  32.527767
S    30.137522  31.942844  36.388569
S  33.229443  27.803083  34.301838
S  33.457905  32.302116  32.325050
S  36.865658  29.005463  31.370850
S  36.667419  28.943821  36.454262
S  40.042988  26.340328  33.402863
S  40.384281  31.050499  33.898567
S  43.955936  28.750481  31.516346
S  44.352654  26.554132  38.669014

24

generated by VMD

Ca  25.210779  29.881760  31.818932
Ca  26.408081  30.952221  36.455307
Ca  30.219173  28.862684  36.054470
Ca  30.591940  32.812077  33.072723
Ca  33.358208  28.970375  31.393116
Ca  33.237808  30.763409  35.355301
Ca  36.363293  26.464638  34.237774
Ca  36.664143  31.154745  33.769993
Ca  40.286972  28.995567  31.400873
Ca  39.490929  28.443888  36.227936
Ca  46.094696  30.448391  34.035412
Ca  42.817646  28.602272  34.083687
S  27.086733  27.747025  36.322731
S  27.384750  33.931709  34.438869
S  30.450600  29.669437  32.832069
S  30.185728  32.028866  36.289726
S  33.183865  27.523590  34.623783
S  33.755600  32.212803  32.298340
S  36.807362  28.814152  31.653709
S  36.445015  28.989084  36.570782
S  39.883839  26.283825  33.412254
S  40.256275  30.829990  34.116951
S  43.741669  29.303993  31.221317
S  44.508804  26.704956  38.344566

24
generated by VMD

Ca  25.285397  29.758411  31.954834
Ca  26.596445  31.088818  36.317593
Ca  30.340977  28.824646  36.255833
Ca  30.466795  32.917183  32.799004
Ca  33.414150  28.921059  31.257444
Ca  33.148102  30.821787  35.369926
Ca  36.242287  26.85436  33.986866
Ca  36.610466  31.029739  33.861286
Ca  40.233215  29.139027  31.458731
Ca  39.581573  28.357952  36.338596
Ca  46.065445  30.325258  34.114182
Ca  42.594707  28.570892  34.260494
S   27.092125  27.640705  36.667786
S   27.429529  33.980049  34.324505
S   30.546516  29.623371  32.941685
S   29.989220  31.943886  36.244732
S   33.200768  27.477671  34.489677
S   33.966610  32.230862  32.356174
S   36.799526  29.016979  31.284042
S   36.403088  28.875483  36.508041
S   40.000397  26.319019  33.492882
S   40.129230  30.903152  34.282814
S   43.578125  29.393574  31.306410
S   44.719185  26.546412  38.157227

24
generated by VMD
Ca  25.423740  29.538355  31.890774
Ca  26.298958  30.986979  36.680054
Ca  30.312767  28.765495  36.290424
Ca  30.593861  33.177868  32.969372
Ca  33.520809  28.917934  31.050205
Ca  33.277576  30.846027  35.514236
Ca  36.536331  26.559940  34.093147
Ca  36.521282  31.064526  33.929512
Ca  40.250175  28.962498  31.374002
Ca  39.485497  28.410446  36.491440
Ca  46.084259  30.567591  33.734489
Ca  42.710911  28.436256  34.178913
S   27.187540  27.654451  36.251057
S   27.200251  34.015079  34.328377
S   30.646221  30.004173  32.957016
S   29.863918  31.913364  36.379528
S   33.350719  27.642796  34.407253
S   33.758514  32.204620  32.144821
S   36.905323  28.838785  31.560482
S   36.434746  28.928364  36.536247
S   39.899105  26.338116  33.575657
S   40.311005  31.037422  34.168575
S   43.573811  28.941696  31.181118
S   44.286495  26.638662  38.344021

24
generated by VMD
Ca  25.691389  29.358360  31.782810
Ca  26.371840  31.000816  36.366138
Ca  30.344225  28.730900  36.322163
Ca  30.312639  33.042847  33.232185
|   | Ca       | S        | 24  |
|---|----------|----------|-----|
|   | 33.636391| 29.191895| 31.193817|
| Ca| 33.312374| 30.908379| 35.507362|
| Ca| 36.292171| 26.504494| 33.716534|
| Ca| 36.636238| 31.217178| 33.871811|
| Ca| 40.206783| 28.792751| 31.517450|
| Ca| 39.461395| 28.420918| 36.019974|
| Ca| 46.186737| 30.070358| 34.001217|
| Ca| 42.787735| 28.616119| 34.370903|
| S | 27.216885| 27.536438| 36.525688|
| S | 27.206738| 34.026276| 36.368675|
| S | 30.564125| 30.005081| 33.108479|
| S | 30.042068| 31.902081| 36.613037|
| S | 33.232803| 27.651764| 34.406555|
| S | 33.724102| 32.501659| 32.198715|
| S | 36.875481| 28.959011| 31.357536|
| S | 36.413673| 28.844688| 36.318985|
| S | 39.939533| 26.335553| 33.370640|
| S | 40.248604| 31.007664| 33.931053|
| S | 43.480915| 29.001076| 31.429142|
| S | 44.249062| 26.767029| 38.499790|

24 generated by VMD

|   | Ca       | S        |
|---|----------|----------|
| Ca| 25.560297| 29.524799| 31.592360|
| Ca| 26.703608| 31.052452| 36.314911|
| Ca| 30.190699| 28.901562| 35.983875|
| Ca| 30.259136| 33.030567| 33.249222|
| Ca| 33.551109| 29.040928| 31.343264|
| Ca| 33.489738| 30.968472| 35.597721|
| Ca| 36.271206| 26.510481| 34.100975|
| Ca| 36.587723| 30.726406| 33.778687|
| Ca| 40.178795| 28.937496| 31.347103|
| Ca| 39.636936| 28.443920| 36.261154|
| Ca| 46.230595| 30.239595| 34.075214|
| Ca| 42.753967| 28.740730| 34.198891|
| S | 26.768547| 27.608011| 36.686386|
| S | 26.887486| 33.881523| 34.130795|
| S | 30.548973| 29.911900| 32.986824|
| S | 30.200644| 32.181667| 36.577015|
| S | 33.151497| 27.743538| 34.498985|
| S | 33.715767| 32.237652| 32.320766|
| S | 36.763889| 28.768763| 31.266747|
| S | 36.505714| 28.674305| 36.617889|
| S | 39.887424| 26.507847| 33.482162|
| S | 40.355843| 30.929272| 34.148842|
| S | 43.519600| 29.270973| 31.208454|
| S | 44.714714| 26.558584| 38.262524|
|        |                  |                  |                  |
|--------|-----------------|-----------------|-----------------|
| Ca     | 25.418587       | 29.730129       | 31.962332       |
| Ca     | 26.510042       | 31.160988       | 36.584698       |
| Ca     | 30.152725       | 29.079180       | 35.969841       |
| Ca     | 30.407940       | 33.098038       | 33.116375       |
| Ca     | 33.459488       | 28.717113       | 31.210680       |
| Ca     | 33.448021       | 30.782421       | 35.445122       |
| Ca     | 36.428238       | 26.416874       | 33.767891       |
| Ca     | 36.635609       | 30.676565       | 33.676659       |
| Ca     | 40.327019       | 28.965231       | 31.470715       |
| Ca     | 39.451092       | 28.296871       | 36.113770       |
| Ca     | 45.999619       | 30.458546       | 34.555889       |
| Ca     | 42.558277       | 28.688141       | 34.258595       |
| S      | 26.996731       | 27.778133       | 36.502991       |
| S      | 27.000549       | 33.821930       | 34.552883       |
| S      | 30.489019       | 29.876541       | 32.914677       |
| S      | 30.295630       | 32.104565       | 36.477829       |
| S      | 33.308960       | 27.479977       | 34.391468       |
| S      | 33.770481       | 32.226967       | 32.331856       |
| S      | 36.796852       | 28.771145       | 31.217663       |
| S      | 36.469196       | 28.772955       | 36.369873       |
| S      | 39.879150       | 26.424782       | 33.373489       |
| S      | 40.256741       | 30.997742       | 34.042431       |
| S      | 43.714233       | 29.287899       | 31.453506       |
| S      | 44.659710       | 26.778656       | 38.269405       |

|        |                  |                  |                  |
|--------|-----------------|-----------------|-----------------|
| Ca     | 25.182976       | 29.352268       | 32.134197       |
| Ca     | 26.512907       | 31.132349       | 36.566902       |
| Ca     | 30.306267       | 28.797594       | 36.000778       |
| Ca     | 30.396101       | 33.188679       | 33.122620       |
| Ca     | 33.487137       | 29.185616       | 31.000168       |
| Ca     | 33.325897       | 30.987160       | 35.503471       |
| Ca     | 36.302250       | 26.499634       | 33.733467       |
| Ca     | 36.611031       | 30.961262       | 33.857777       |
| Ca     | 40.248138       | 28.975704       | 31.408852       |
| Ca     | 39.447697       | 28.254389       | 36.096306       |
| Ca     | 46.107498       | 30.429932       | 34.418091       |
| Ca     | 42.758598       | 28.579279       | 34.381073       |
| S      | 27.300098       | 27.674152       | 36.643795       |
| S      | 27.122410       | 33.732540       | 34.317776       |
| S      | 30.557446       | 29.961864       | 32.967915       |
| S      | 29.992165       | 31.939697       | 36.526611       |
| S      | 33.204590       | 27.656731       | 34.248936       |
| S      | 33.766045       | 32.458527       | 32.146530       |
|   | 36.763920 | 28.958000 | 31.266796 |
|---|-----------|-----------|-----------|
| S | 36.341236 | 28.867989 | 36.357559 |
| S | 39.813198 | 26.358528 | 33.268639 |
| S | 40.429081 | 30.802526 | 34.146355 |
| S | 43.661438 | 29.062674 | 31.453716 |
| S | 44.795742 | 26.574396 | 38.462330 |

24

generated by VMD

| Ca | 25.635136 | 29.199621 | 31.995211 |
|----|-----------|-----------|-----------|
| Ca | 26.712873 | 30.964190 | 36.803101 |
| Ca | 30.256964 | 29.160908 | 35.922775 |
| Ca | 30.537659 | 33.163254 | 33.308598 |
| Ca | 33.471764 | 29.188780 | 31.046425 |
| Ca | 33.412003 | 31.011028 | 35.323009 |
| Ca | 36.188179 | 26.136469 | 33.928093 |
| Ca | 36.504585 | 30.703537 | 33.538628 |
| Ca | 40.126904 | 28.919613 | 31.386686 |
| Ca | 39.358601 | 28.253780 | 36.052158 |
| Ca | 45.819614 | 30.379625 | 34.550938 |
| Ca | 42.686298 | 28.547947 | 34.446598 |

| S  | 27.186314 | 27.658573 | 36.566551 |
|----|-----------|-----------|-----------|
| S  | 27.042572 | 33.933952 | 34.621544 |
| S  | 30.500269 | 30.072460 | 32.831238 |
| S  | 30.360376 | 32.152580 | 36.676044 |
| S  | 33.201447 | 27.621038 | 34.019375 |
| S  | 33.778198 | 32.347542 | 32.089348 |
| S  | 36.761097 | 28.697729 | 31.151121 |
| S  | 36.238796 | 28.863955 | 36.227169 |
| S  | 39.866268 | 26.338449 | 33.354683 |
| S  | 40.027229 | 30.888348 | 34.027908 |
| S  | 43.662678 | 29.491291 | 31.518412 |
| S  | 45.098053 | 26.696722 | 38.645111 |

24

generated by VMD

| Ca | 25.459936 | 29.521235 | 31.916138 |
|----|-----------|-----------|-----------|
| Ca | 26.318256 | 31.088020 | 36.696365 |
| Ca | 30.150846 | 28.813585 | 35.995686 |
| Ca | 30.534292 | 33.086971 | 33.322433 |
| Ca | 33.715446 | 29.120621 | 31.129591 |
| Ca | 33.283607 | 30.706995 | 35.413033 |
| Ca | 36.374496 | 26.592978 | 33.940010 |
| Ca | 36.694603 | 31.014925 | 33.666325 |
| Ca | 40.241886 | 28.639351 | 31.297670 |
| Ca | 39.408852 | 28.321829 | 36.013000 |
| Ca | 45.769104 | 30.645927 | 34.371269 |
| Ca | 42.611958 | 28.671608 | 34.297112 |
|     |        |        |        |
|-----|--------|--------|--------|
| S   | 27.202726 | 27.708824 | 36.549557 |
| S   | 27.268326 | 33.770679 | 34.435047 |
| S   | 30.610561 | 30.071774 | 32.849117 |
| S   | 30.130884 | 31.920664 | 36.689606 |
| S   | 33.148422 | 27.619757 | 34.330345 |
| S   | 33.881626 | 32.439568 | 32.226883 |
| S   | 36.810886 | 28.745522 | 31.315292 |
| S   | 36.430126 | 28.983778 | 36.399261 |
| S   | 40.061649 | 26.128792 | 33.313778 |
| S   | 40.216049 | 30.738628 | 33.900856 |
| S   | 43.764675 | 29.294216 | 31.275604 |
| S   | 44.344654 | 26.745142 | 38.686707 |

24

generated by VMD

| Ca  | 25.411221 | 29.835121 | 32.132130 |
| Ca  | 26.749350 | 30.970819 | 36.451717 |
| Ca  | 30.179781 | 28.829544 | 36.099915 |
| Ca  | 30.192583 | 33.107826 | 33.266792 |
| Ca  | 33.517044 | 28.903084 | 31.115427 |
| Ca  | 33.427761 | 30.689985 | 35.338383 |
| Ca  | 36.397240 | 26.542845 | 33.893944 |
| Ca  | 36.476822 | 31.223803 | 33.641449 |
| Ca  | 40.361691 | 28.648308 | 31.142805 |
| Ca  | 39.428921 | 28.359385 | 35.987969 |
| Ca  | 46.064919 | 30.351233 | 34.506268 |
| Ca  | 42.633278 | 28.647179 | 34.348175 |
| S   | 26.930178 | 27.660505 | 36.374619 |
| S   | 27.197441 | 33.887867 | 34.846809 |
| S   | 30.382212 | 29.923941 | 32.801338 |
| S   | 30.402096 | 31.954647 | 36.608681 |
| S   | 33.232525 | 27.581825 | 34.390186 |
| S   | 33.448013 | 32.294094 | 32.008224 |
| S   | 36.809483 | 28.881023 | 31.264065 |
| S   | 36.587818 | 29.089884 | 36.189381 |
| S   | 40.005371 | 26.232157 | 33.392242 |
| S   | 40.125492 | 30.866692 | 33.942909 |
| S   | 43.940002 | 29.265463 | 31.487389 |
| S   | 44.532703 | 26.644197 | 38.799976 |

24

generated by VMD

| Ca  | 25.205904 | 30.248949 | 32.488140 |
| Ca  | 26.900410 | 30.760298 | 36.426624 |
| Ca  | 30.152473 | 28.889051 | 36.116512 |
| Ca  | 30.399780 | 33.016983 | 32.888268 |
| Ca  | 33.379955 | 28.781523 | 31.334008 |
| Ca  | 33.317444 | 30.568045 | 35.183399 |
|  | 36.299431 | 26.652927 | 33.862770 |
| Ca | 36.659111 | 30.848930 | 33.546974 |
| Ca | 40.456909 | 28.976707 | 30.932940 |
| Ca | 39.437672 | 28.557777 | 36.264786 |
| Ca | 45.781353 | 30.616777 | 34.590725 |
| Ca | 42.621174 | 28.732927 | 34.315205 |
| S  | 26.754467 | 27.547098 | 36.426033 |
| S  | 27.558199 | 33.994415 | 34.807236 |
| S  | 30.345652 | 29.853846 | 32.826210 |
| S  | 30.451832 | 32.056374 | 36.330204 |
| S  | 33.166096 | 27.368759 | 34.401375 |
| S  | 33.741985 | 32.047821 | 32.019817 |
| S  | 36.736866 | 28.875742 | 31.109819 |
| S  | 36.217632 | 28.748390 | 36.521511 |
| S  | 39.991173 | 26.470997 | 33.384842 |
| S  | 40.268299 | 30.851833 | 34.117390 |
| S  | 43.916615 | 29.150757 | 31.295010 |
| S  | 44.673424 | 26.774534 | 38.840519 |

24 generated by VMD

|  | 25.198503 | 30.409063 | 32.465240 |
| Ca | 27.044727 | 31.057137 | 36.418098 |
| Ca | 30.110695 | 28.697212 | 36.079548 |
| Ca | 30.418926 | 32.784306 | 33.182930 |
| Ca | 33.510735 | 28.830456 | 31.364677 |
| Ca | 33.412907 | 30.417736 | 35.122032 |
| Ca | 36.309177 | 26.568344 | 33.905304 |
| Ca | 36.684212 | 30.889702 | 33.379150 |
| Ca | 40.177757 | 29.124731 | 31.016834 |
| Ca | 39.488316 | 28.553076 | 36.466003 |
| Ca | 45.483189 | 30.985596 | 34.552208 |
| Ca | 42.565502 | 28.803997 | 34.355568 |
| S  | 26.853094 | 27.845926 | 36.343796 |
| S  | 27.567865 | 33.897507 | 34.703705 |
| S  | 30.589533 | 29.634705 | 32.686893 |
| S  | 30.541378 | 31.764509 | 36.399349 |
| S  | 33.125950 | 27.264486 | 34.469193 |
| S  | 33.835461 | 32.237293 | 32.065872 |
| S  | 36.667332 | 28.537497 | 31.196850 |
| S  | 36.450329 | 28.995081 | 36.275429 |
| S  | 39.991196 | 26.364967 | 33.492622 |
| S  | 40.157383 | 30.815035 | 33.836304 |
| S  | 43.773228 | 29.204514 | 31.429264 |
| S  | 44.476624 | 26.708544 | 38.823814 |

24 generated by VMD
| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 25.128260 | 30.397078 | 32.440033 |
| Ca      | 26.614998  | 30.751892 | 36.421097 |
| Ca      | 30.393415  | 28.890553 | 35.774345 |
| Ca      | 30.300217  | 32.914093 | 33.031853 |
| Ca      | 33.338142  | 28.925440 | 31.192249 |
| Ca      | 33.324505  | 30.733580 | 35.774345 |
| Ca      | 36.497936  | 26.629276 | 34.283447 |
| Ca      | 36.861168  | 31.037817 | 33.656174 |
| Ca      | 40.272182  | 28.854116 | 31.077877 |
| Ca      | 39.584896  | 28.654684 | 36.262657 |
| Ca      | 45.631531  | 30.919174 | 34.210354 |
| Ca      | 42.655106  | 28.881641 | 34.341202 |
| S       | 27.108440  | 27.599258 | 36.609852 |
| S       | 27.375170  | 33.849968 | 34.798706 |
| S       | 30.351761  | 29.523668 | 32.562943 |
| S       | 30.284361  | 31.844299 | 36.331387 |
| S       | 33.343330  | 27.600336 | 34.385883 |
| S       | 33.635490  | 32.064259 | 32.117783 |
| S       | 36.784851  | 28.855667 | 31.359282 |
| S       | 36.457970  | 29.256042 | 36.430649 |
| S       | 39.961868  | 26.386211 | 33.698982 |
| S       | 40.224026  | 30.693745 | 33.896832 |
| S       | 43.962105  | 29.144825 | 31.342957 |
| S       | 44.342140  | 25.983713 | 38.838997 |

24 generated by VMD

| Element | X1   | Y1   | Z1   |
|---------|------|------|------|
| Ca      | 25.490499 | 30.162708 | 32.135590 |
| Ca      | 26.644938 | 31.171539 | 36.418282 |
| Ca      | 30.156649 | 28.827631 | 35.782814 |
| Ca      | 30.483503 | 32.927601 | 32.904198 |
| Ca      | 33.370911 | 28.694012 | 31.299969 |
| Ca      | 33.309998 | 30.278002 | 35.226929 |
| Ca      | 36.390545 | 26.520296 | 34.065853 |
| Ca      | 36.683517 | 30.658758 | 33.826500 |
| Ca      | 40.058201 | 29.198500 | 31.176456 |
| Ca      | 39.478554 | 28.660587 | 36.180439 |
| Ca      | 45.505928 | 30.910358 | 33.952190 |
| Ca      | 42.606998 | 28.823288 | 34.553883 |
| S       | 26.938503 | 27.948856 | 36.799911 |
| S       | 27.358562 | 33.983906 | 34.539360 |
| S       | 30.374607 | 29.645176 | 32.731037 |
| S       | 30.420000 | 31.778214 | 36.358345 |
| S       | 33.217510 | 27.271259 | 34.411739 |
| S       | 33.845680 | 32.177139 | 32.215118 |
| S       | 36.613342 | 28.956493 | 31.239588 |
| S       | 36.373489 | 28.877937 | 36.475891 |
|   |   |   |   |
|---|---|---|---|
| S | 40.020741 | 26.447008 | 33.481602 |
| S | 40.296471 | 30.932838 | 34.028984 |
| S | 43.792992 | 28.961872 | 31.432610 |
| S | 45.001778 | 26.577402 | 38.793434 |

24 generated by VMD

| Ca  |   |   |   |
|-----|---|---|---|
| 25.042469 | 30.218990 | 32.450123 |
| 26.632784 | 30.829046 | 36.336121 |
| 30.211880 | 28.760168 | 35.884430 |
| 30.294720 | 32.852585 | 33.175072 |

| Ca  |   |   |   |
|-----|---|---|---|
| 33.513256 | 28.868425 | 31.331352 |
| 33.420429 | 30.739120 | 35.344692 |
| 36.345844 | 26.852358 | 34.226852 |
| 36.777264 | 31.208620 | 33.539516 |

| Ca  |   |   |   |
|-----|---|---|---|
| 40.390228 | 28.993992 | 30.966286 |
| 39.651573 | 28.097815 | 36.186462 |
| 45.739872 | 30.649725 | 34.159836 |
| 42.614048 | 28.711723 | 34.430444 |

| S   |   |   |   |
|-----|---|---|---|
| 26.888739 | 27.594927 | 36.408813 |
| 27.157450 | 33.879807 | 34.590370 |
| 30.326210 | 29.790504 | 32.581039 |
| 30.137142 | 31.754835 | 36.444389 |

| S   |   |   |   |
|-----|---|---|---|
| 33.183033 | 27.486893 | 34.367126 |
| 33.726364 | 32.178890 | 32.098938 |
| 36.837566 | 28.835024 | 31.389053 |
| 36.685822 | 29.499922 | 36.424500 |
| 40.021080 | 26.429792 | 33.294098 |
| 40.239037 | 30.738817 | 34.087791 |
| 43.877411 | 28.949080 | 31.422630 |
| 44.719620 | 26.470320 | 38.887222 |

24 generated by VMD

| Ca  |   |   |   |
|-----|---|---|---|
| 25.247871 | 30.300842 | 32.346283 |
| 26.583677 | 31.151297 | 36.177425 |
| 30.312225 | 28.545130 | 36.161045 |
| 30.465992 | 32.642109 | 32.988174 |
| 33.457397 | 29.133873 | 31.207664 |
| 33.196537 | 30.884510 | 35.283913 |

| Ca  |   |   |   |
|-----|---|---|---|
| 36.443733 | 26.643969 | 34.127457 |
| 36.565857 | 30.854433 | 33.654297 |
| 40.359081 | 29.111267 | 31.064930 |
| 39.570030 | 28.048170 | 36.174858 |
| 46.063099 | 30.636581 | 34.396103 |
| 42.472782 | 28.862375 | 34.167824 |

| S   |   |   |   |
|-----|---|---|---|
| 27.046967 | 27.689257 | 36.724266 |
| 27.542984 | 33.895607 | 34.513908 |
| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| S       | 30.557095    | 29.576107    | 32.783684    |
| S       | 30.043884    | 31.675417    | 36.454403    |
| S       | 33.189148    | 27.460466    | 34.34566     |
| S       | 33.824345    | 32.433998    | 32.134861    |
| S       | 36.642395    | 28.739326    | 31.232048    |
| S       | 36.64694     | 29.272511    | 36.549877    |
| S       | 39.917400    | 26.266821    | 33.128315    |
| S       | 39.959793    | 30.793007    | 34.171722    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.264858    | 30.432148    | 32.195511    |
| Ca      | 26.663609    | 31.029295    | 36.422173    |
| Ca      | 30.287788    | 28.689037    | 35.783688    |
| Ca      | 30.271347    | 32.955627    | 33.106075    |
| Ca      | 33.392933    | 28.732155    | 31.338331    |
| Ca      | 33.219700    | 30.739643    | 35.458443    |
| Ca      | 36.350910    | 26.685316    | 34.088596    |
| Ca      | 36.652473    | 30.769310    | 33.927635    |

24 generated by VMD

| Element | X-coordinate | Y-coordinate | Z-coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 25.005709    | 30.584690    | 32.237213    |
| Ca      | 26.429024    | 31.016659    | 36.311634    |
| Ca      | 30.127937    | 28.549990    | 35.943970    |
| Ca      | 30.171726    | 33.028790    | 33.188587    |
| Ca      | 33.274044    | 28.724648    | 31.300018    |
| Ca      | 33.195961    | 30.444031    | 35.32214     |
| Ca      | 36.604721    | 26.572258    | 34.227203    |
| Ca      | 36.681870    | 31.069618    | 33.753899    |
| Element | X Coord | Y Coord | Z Coord |
|---------|---------|---------|---------|
| Ca      | 40.460640 | 28.851906 | 31.121080 |
| Ca      | 39.708183 | 28.341579 | 36.016846 |
| Ca      | 46.151794 | 30.643763 | 34.436565 |
| Ca      | 42.518101 | 28.760201 | 34.148487 |
| S       | 26.808582 | 27.775272 | 36.478279 |
| S       | 27.173595 | 34.153809 | 34.567635 |
| S       | 30.454000 | 29.841534 | 32.724663 |
| S       | 29.986652 | 31.799034 | 36.322887 |
| S       | 33.167261 | 27.105808 | 34.593312 |
| S       | 33.702393 | 32.020813 | 32.242279 |
| S       | 36.953373 | 28.897053 | 31.451168 |
| S       | 36.597496 | 29.119274 | 36.377548 |
| S       | 40.127823 | 26.321362 | 33.343999 |
| S       | 40.284275 | 30.979137 | 33.973486 |
| S       | 44.014786 | 28.980217 | 31.462490 |
| S       | 44.836468 | 26.809374 | 38.555977 |

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generated by VMD

| Element | X Coord | Y Coord | Z Coord |
|---------|---------|---------|---------|
| Ca      | 25.030807 | 30.420567 | 32.197304 |
| Ca      | 26.484524 | 31.086128 | 35.988468 |
| Ca      | 30.319620 | 28.554829 | 35.840229 |
| Ca      | 30.474470 | 32.887466 | 33.011246 |
| Ca      | 33.174583 | 28.647350 | 31.461168 |
| Ca      | 33.172523 | 30.563004 | 35.634186 |
| Ca      | 36.503151 | 26.520107 | 34.299896 |
| Ca      | 36.739787 | 31.014328 | 34.153542 |
| Ca      | 40.299812 | 28.855003 | 30.986509 |
| Ca      | 39.750954 | 28.548477 | 36.138588 |
| Ca      | 46.195190 | 30.872812 | 34.063774 |
| Ca      | 42.675426 | 28.718765 | 34.104794 |
| S       | 26.816143 | 27.878904 | 36.328209 |
| S       | 27.428656 | 34.113870 | 34.478027 |
| S       | 30.191746 | 29.694580 | 32.698170 |
| S       | 30.203865 | 31.886482 | 36.313976 |
| S       | 33.129944 | 27.290264 | 34.563526 |
| S       | 33.678013 | 31.898510 | 32.383705 |
| S       | 36.758919 | 28.936190 | 31.659645 |
| S       | 36.436665 | 28.930075 | 36.593109 |
| S       | 40.006565 | 26.366642 | 33.461334 |
| S       | 40.434635 | 30.821678 | 33.919907 |
| S       | 44.021595 | 28.993513 | 31.247877 |
| S       | 44.512131 | 26.887344 | 38.503422 |

24

generated by VMD

| Element | X Coord | Y Coord | Z Coord |
|---------|---------|---------|---------|
| Ca      | 25.034698 | 30.697216 | 32.026283 |
| Ca      | 26.347075 | 31.187281 | 35.697617 |
| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| Ca      | 30.224468 | 28.304127 | 36.230862 |
| Ca      | 30.355076 | 32.802437 | 31.980129 |
| Ca      | 33.089550 | 28.805862 | 31.623848 |
| Ca      | 33.138161 | 30.261425 | 35.356281 |
| Ca      | 36.612747 | 26.562389 | 34.159950 |
| Ca      | 36.693768 | 31.154995 | 33.758087 |
| Ca      | 40.072891 | 29.097628 | 31.261591 |
| Ca      | 39.854015 | 28.801558 | 36.359241 |
| Ca      | 45.939781 | 30.354240 | 34.007824 |
| Ca      | 42.694954 | 28.739698 | 34.172104 |
| S       | 26.879406 | 27.874660 | 36.505573 |
| S       | 27.241894 | 34.131191 | 34.236256 |
| S       | 30.351258 | 29.530191 | 32.950329 |
| S       | 30.147102 | 31.528751 | 36.400528 |
| S       | 33.373569 | 27.095692 | 34.577339 |
| S       | 33.867447 | 32.086655 | 32.373539 |
| S       | 36.555798 | 29.058232 | 31.436953 |
| S       | 36.646896 | 29.155298 | 36.646523 |
| S       | 40.039326 | 26.567165 | 33.518261 |
| S       | 40.332684 | 30.982895 | 34.072861 |
| S       | 43.953342 | 28.866137 | 31.290981 |
| S       | 44.987022 | 26.745071 | 38.387768 |
S  44.243103  28.92137  31.535805
S  44.697132  26.432117  38.317043

24 generated by VMD
Ca  24.612272  30.380289  32.568336
Ca  26.640429  31.499958  35.932159
Ca  30.047874  28.450031  36.062347
Ca  30.281269  32.576893  33.169811
Ca  33.147877  28.737667  31.387691
Ca  33.098587  30.306313  35.217850
Ca  36.500103  26.798260  34.038200
Ca  36.921970  30.862885  33.852516
Ca  40.276024  29.450249  31.172573
Ca  39.693993  28.261040  36.080086
Ca  46.153034  30.434717  34.128258
Ca  42.967243  28.862875  34.670166
S  26.720058  28.127890  36.66458
S  27.248991  34.244247  33.834621
S  30.266375  29.358208  32.938248
S  30.053913  31.649134  36.425175
S  33.102158  27.124249  34.442394
S  33.665993  31.886353  32.389126
S  36.766964  29.083277  31.334541
S  36.792690  28.980595  36.465370
S  40.313820  26.589750  33.154499
S  40.377823  30.925606  34.098576
S  44.053860  29.242699  31.404924
S  44.730579  26.558195  38.596672

24 generated by VMD
Ca  24.990080  30.384365  32.425583
Ca  26.567535  31.394569  36.103828
Ca  30.182487  27.984455  36.034069
Ca  30.380869  32.560696  33.160332
Ca  32.295284  29.124453  31.222488
Ca  33.145691  30.332870  35.308189
Ca  36.271667  26.928085  34.317455
Ca  36.752556  30.959373  33.791500
Ca  40.202427  29.278818  31.054276
Ca  39.677055  28.553520  36.295425
Ca  46.085583  30.214993  34.524677
Ca  42.873627  28.815138  34.142159
S  26.819969  28.003744  36.560459
S  27.382185  34.098869  34.263969
S  30.373255  29.475548  32.904873
S  30.103729  31.447218  36.245815
|   |   |   |   |
|---|---|---|---|
| S | 33.018230 | 27.152874 | 34.319736 |
| S | 33.808743 | 32.136662 | 32.411911 |
| S | 36.740150 | 29.312111 | 31.179946 |
| S | 36.563293 | 29.124557 | 36.549072 |
| S | 39.966404 | 26.668671 | 33.481033 |
| S | 40.363285 | 30.862022 | 33.952393 |
| S | 43.952431 | 28.835119 | 31.167124 |
| S | 44.916775 | 26.742706 | 38.616333 |

24 generated by VMD

| Ca |   |   |   |
|----|---|---|---|
| Ca | 24.975048 | 30.449480 | 31.989773 |
| Ca | 26.418325 | 31.35946 | 35.917236 |
| Ca | 30.252138 | 28.335888 | 36.141838 |
| Ca | 30.372974 | 32.651371 | 33.089298 |
| Ca | 33.281181 | 28.784981 | 31.435400 |
| Ca | 33.217667 | 30.434143 | 35.267262 |
| Ca | 36.624939 | 26.687542 | 34.430447 |
| Ca | 36.764935 | 31.332985 | 33.792786 |
| Ca | 40.268875 | 29.247013 | 31.108681 |
| Ca | 39.708443 | 28.463825 | 36.020130 |
| Ca | 46.074352 | 30.311296 | 34.224106 |
| Ca | 42.653450 | 28.988306 | 34.249161 |
| S | 26.712383 | 28.045923 | 36.607742 |
| S | 27.352840 | 34.060810 | 34.197952 |
| S | 30.292904 | 29.292164 | 32.864227 |
| S | 30.003738 | 31.52774 | 36.458473 |
| S | 33.165119 | 27.105804 | 34.584003 |
| S | 33.788361 | 32.025970 | 32.415073 |
| S | 36.753353 | 28.997486 | 31.429749 |
| S | 36.754921 | 29.308918 | 36.661118 |
| S | 40.126461 | 26.593872 | 33.250275 |
| S | 40.234329 | 31.036009 | 34.026203 |
| S | 43.714851 | 29.152802 | 31.330959 |
| S | 44.922348 | 26.206062 | 38.538857 |

24 generated by VMD

| Ca |   |   |   |
|----|---|---|---|
| Ca | 25.280529 | 30.383724 | 32.011070 |
| Ca | 26.456497 | 31.186119 | 36.041096 |
| Ca | 30.101894 | 28.615858 | 36.018990 |
| Ca | 30.536537 | 32.843388 | 33.134930 |
| Ca | 33.443790 | 28.827520 | 31.482759 |
| Ca | 33.255985 | 30.418152 | 35.497948 |
| Ca | 36.423145 | 26.608574 | 34.290459 |
| Ca | 36.697342 | 31.017229 | 33.957890 |
| Ca | 40.433796 | 29.025093 | 31.053629 |
| Ca | 39.603794 | 28.483482 | 35.929527 |
| Ca    | 45.865425 | 31.036379 | 34.775581 |
|------|-----------|-----------|-----------|
| Ca    | 42.771675 | 28.928812 | 34.216904 |
| S     | 26.814732 | 27.885294 | 36.554298 |
| S     | 27.219217 | 34.100967 | 34.158901 |
| S     | 30.299950 | 29.538420 | 32.951603 |
| S     | 29.923048 | 31.668060 | 36.468544 |
| S     | 33.143097 | 27.293797 | 34.693878 |
| S     | 33.787193 | 32.086716 | 32.295208 |
| S     | 36.869251 | 28.877813 | 31.453659 |
| S     | 36.561081 | 28.947506 | 36.692745 |
| S     | 40.024635 | 26.508919 | 33.451496 |
| S     | 40.258831 | 30.962406 | 33.903946 |
| S     | 43.826817 | 28.916492 | 31.166496 |
| S     | 44.835613 | 26.230684 | 37.829208 |

24 generated by VMD

| Ca    | 25.283039 | 30.415859 | 31.929626 |
|------|-----------|-----------|-----------|
| Ca    | 26.531036 | 31.272814 | 36.090927 |
| Ca    | 30.341770 | 28.497066 | 36.165939 |
| Ca    | 30.466223 | 32.690483 | 33.316319 |
| Ca    | 33.355988 | 28.832340 | 31.276665 |
| Ca    | 33.153027 | 30.418951 | 35.417877 |
| Ca    | 36.523285 | 26.585737 | 34.345131 |
| Ca    | 36.701759 | 31.059881 | 33.814667 |
| Ca    | 40.381184 | 29.063082 | 31.053232 |
| Ca    | 39.439896 | 28.505703 | 35.788807 |
| Ca    | 45.750095 | 30.802574 | 34.324081 |
| Ca    | 42.807285 | 28.768333 | 34.224442 |
| S     | 26.753708 | 27.932251 | 36.569511 |
| S     | 27.266262 | 34.237740 | 34.433708 |
| S     | 30.412037 | 29.495518 | 32.979500 |
| S     | 29.999033 | 31.615021 | 36.463242 |
| S     | 33.394680 | 27.096447 | 34.700909 |
| S     | 33.749481 | 32.092606 | 32.290333 |
| S     | 36.885513 | 28.822800 | 31.330900 |
| S     | 36.484261 | 29.235947 | 36.534897 |
| S     | 40.074306 | 26.468954 | 33.262939 |
| S     | 40.403328 | 30.793924 | 33.951042 |
| S     | 44.041340 | 29.112133 | 31.097382 |
| S     | 44.235359 | 26.575237 | 38.668537 |

24 generated by VMD

| Ca    | 25.068592 | 30.128086 | 32.381042 |
|------|-----------|-----------|-----------|
| Ca    | 26.595337 | 31.381437 | 35.898754 |
| Ca    | 30.076956 | 28.417948 | 35.934593 |
| Ca    | 30.307852 | 32.957413 | 33.277004 |
|   |       |       |       |
|---|-------|-------|-------|
| Ca | 33.218002 | 28.964870 | 31.411701 |
| Ca | 33.294449 | 30.335026 | 35.406639 |
| Ca | 36.216763 | 26.708225 | 34.267815 |
| Ca | 36.602646 | 30.901783 | 33.937733 |
| Ca | 40.575695 | 28.996914 | 31.033651 |
| Ca | 39.633251 | 28.407749 | 36.012268 |
| Ca | 45.966625 | 30.709850 | 34.430286 |
| Ca | 42.761478 | 29.126183 | 34.396530 |
| S  | 26.849625 | 27.997669 | 36.630783 |
| S  | 27.304466 | 34.175461 | 34.184376 |
| S  | 30.289185 | 29.634548 | 32.800117 |
| S  | 30.080002 | 31.515591 | 36.350666 |
| S  | 33.094875 | 27.270599 | 34.549755 |
| S  | 33.884441 | 32.077793 | 32.393005 |
| S  | 36.768269 | 28.812912 | 31.445791 |
| S  | 36.574825 | 29.052238 | 36.539635 |
| S  | 40.117577 | 26.421532 | 33.215332 |
| S  | 40.256157 | 31.048748 | 33.961487 |
| S  | 44.179058 | 28.916718 | 31.463247 |
| S  | 44.717815 | 26.432127 | 38.108505 |

24

generated by VMD

|   |       |       |       |
|---|-------|-------|-------|
| Ca | 24.957972 | 30.414551 | 31.939095 |
| Ca | 26.542877 | 31.329548 | 35.892647 |
| Ca | 30.235344 | 28.274593 | 36.087528 |
| Ca | 30.390905 | 32.712448 | 32.983433 |
| Ca | 33.433018 | 29.046520 | 31.399357 |
| Ca | 33.149120 | 30.488546 | 35.569180 |
| Ca | 36.422691 | 26.607933 | 34.333183 |
| Ca | 36.677658 | 31.031315 | 34.122002 |
| Ca | 40.254169 | 29.040806 | 31.342445 |
| Ca | 39.586502 | 28.324970 | 36.104027 |
| Ca | 45.834976 | 30.834469 | 34.086971 |
| Ca | 42.605862 | 28.786400 | 34.109207 |
| S  | 27.032644 | 27.960236 | 36.576542 |
| S  | 27.210323 | 34.212936 | 33.989609 |
| S  | 30.522736 | 29.536331 | 32.871819 |
| S  | 30.023500 | 31.524704 | 36.356964 |
| S  | 33.331959 | 27.261349 | 34.647964 |
| S  | 33.804657 | 32.139122 | 32.500832 |
| S  | 36.382649 | 28.897570 | 31.626747 |
| S  | 36.556435 | 29.132599 | 36.687695 |
| S  | 39.975090 | 26.352753 | 33.484180 |
| S  | 40.162579 | 30.942059 | 34.063591 |
| S  | 43.862247 | 28.918137 | 31.225395 |
| S  | 45.027416 | 26.621502 | 38.030342 |
| Element | X-Coordinate | Y-Coordinate | Z-Coordinate |
|---------|--------------|--------------|--------------|
| Ca      | 24.726084    | 30.382572    | 32.462280    |
| Ca      | 26.468006    | 31.288540    | 35.988113    |
| Ca      | 30.218683    | 28.187244    | 35.925087    |
| Ca      | 30.368404    | 32.639202    | 33.244560    |
| Ca      | 33.451683    | 29.179663    | 31.493189    |
| Ca      | 33.062241    | 30.528692    | 35.240906    |
| Ca      | 36.377571    | 26.908268    | 34.084961    |
| Ca      | 36.754234    | 30.976837    | 33.666042    |
| Ca      | 40.486546    | 29.027161    | 31.159634    |
| Ca      | 39.607105    | 28.438370    | 36.451981    |
| Ca      | 46.129955    | 30.571968    | 34.317009    |
| Ca      | 42.797382    | 28.805866    | 34.418888    |
| S       | 26.931440    | 27.960445    | 36.601692    |
| S       | 26.920652    | 34.054070    | 34.110741    |
| S       | 30.221237    | 29.488249    | 32.873192    |
| S       | 29.992689    | 31.637825    | 36.264221    |
| S       | 33.131203    | 27.283634    | 34.444942    |
| S       | 33.822113    | 32.201366    | 32.417152    |
| S       | 36.891808    | 28.983891    | 31.200783    |
| S       | 36.648926    | 29.278175    | 36.477833    |
| S       | 40.135204    | 26.623888    | 33.652393    |
| S       | 40.204781    | 30.828508    | 34.032597    |
| S       | 43.863621    | 28.868116    | 31.367538    |
| S       | 45.222328    | 26.248873    | 38.134968    |
S  36.907223  29.127888  31.394436
S  36.587914  29.251083  36.460945
S  40.034489  26.536602  33.395897
S  40.537655  30.933334  34.023346
S  44.174030  28.998037  31.536032
S  45.185703  26.579411  38.303482

24 generated by VMD
Ca  24.873970  30.305622  32.160500
Ca  26.503988  31.409498  35.976753
Ca  30.164829  28.000639  35.914433
Ca  30.386473  32.811283  33.279076
Ca  33.226147  28.960743  31.381502
Ca  33.187332  30.327574  35.367542
Ca  36.276829  27.103218  34.497227
Ca  36.819752  30.961090  33.928787
Ca  40.256466  29.193985  31.499765
Ca  39.662403  28.398018  36.145767
Ca  46.479862  30.449684  33.809784
Ca  42.900303  28.928890  34.464211

S  27.021385  27.979286  36.664444
S  26.968552  34.029472  33.652626
S  30.380671  29.568401  32.890263
S  29.992222  31.449821  36.416035
S  33.162880  27.194229  34.293907
S  33.820057  32.141731  32.602932
S  36.794041  29.138872  31.420933
S  36.704247  29.554771  36.672508
S  39.990662  26.698999  33.485619
S  40.290234  30.930779  34.214546
S  43.702610  28.624752  31.240070
S  44.868057  26.230076  38.057323

24 generated by VMD
Ca  25.218729  30.237457  31.931297
Ca  26.404737  31.352924  35.919563
Ca  30.068037  28.195229  35.960194
Ca  30.264229  32.998276  33.450027
Ca  33.368679  28.965925  31.394156
Ca  33.274342  30.056730  35.463322
Ca  36.367542  26.778238  34.471321
Ca  36.699348  31.041126  33.928211
Ca  40.195168  29.085392  31.468399
Ca  39.670525  28.425983  35.926788
Ca  46.402683  30.234283  33.850761
Ca  42.767933  29.113796  34.349186
|    |        |        |        |
|----|--------|--------|--------|
| S  | 26.958904 | 28.070717 | 36.592266 |
| S  | 26.936312 | 34.192917 | 33.892296 |
| S  | 30.418043 | 29.729460 | 32.818714 |
| S  | 30.140755 | 31.639931 | 36.388374 |
| S  | 33.013977 | 27.121143 | 34.505211 |
| S  | 33.631737 | 32.166660 | 32.577454 |
| S  | 36.708385 | 28.790010 | 31.649326 |
| S  | 36.656601 | 29.183315 | 36.575600 |
| S  | 40.094070 | 26.574417 | 33.396687 |
| S  | 40.231136 | 31.072191 | 33.936520 |
| S  | 43.858582 | 28.794527 | 31.399031 |
| S  | 45.083447 | 26.570791 | 38.186020 |

24

generated by VMD

|    |        |        |        |
|----|--------|--------|--------|
| Ca | 24.908134 | 29.948870 | 32.269966 |
| Ca | 26.487280 | 31.125565 | 36.003742 |
| Ca | 30.101948 | 28.390728 | 35.904404 |
| Ca | 30.233702 | 32.959694 | 33.131683 |
| Ca | 33.384125 | 29.052856 | 31.368511 |
| Ca | 33.340973 | 30.069790 | 35.279156 |
| Ca | 36.325802 | 26.908295 | 34.622120 |
| Ca | 36.903698 | 31.022575 | 33.902657 |
| Ca | 40.224091 | 29.425611 | 31.342617 |
| Ca | 39.796364 | 28.696182 | 36.247833 |
| Ca | 46.265903 | 30.221336 | 34.190693 |
| Ca | 42.859268 | 29.194130 | 34.393806 |
| S  | 26.840000 | 27.946497 | 36.654995 |
| S  | 27.019524 | 34.112225 | 33.982769 |
| S  | 30.500637 | 29.636953 | 32.730122 |
| S  | 30.265137 | 31.510101 | 36.312706 |
| S  | 33.018723 | 27.116817 | 34.291283 |
| S  | 33.840961 | 32.155537 | 32.543270 |
| S  | 36.851131 | 28.794872 | 31.560898 |
| S  | 36.781708 | 29.550346 | 36.705765 |
| S  | 40.175163 | 26.849880 | 33.447685 |
| S  | 40.440617 | 31.202938 | 34.150299 |
| S  | 43.667130 | 28.626797 | 31.219418 |
| S  | 44.201836 | 25.872799 | 37.774303 |

24

generated by VMD

|    |        |        |        |
|----|--------|--------|--------|
| Ca | 25.552443 | 30.297264 | 32.074223 |
| Ca | 26.243416 | 31.529339 | 35.788872 |
| Ca | 29.977871 | 28.135513 | 36.036030 |
| Ca | 30.409506 | 32.672626 | 33.170162 |
| Ca | 33.260902 | 28.781212 | 31.522194 |
| Ca | 32.969971 | 30.258324 | 35.380714 |
| Ca  | 36.415417 | 26.642994 | 34.321590 |
| Ca  | 36.826805 | 31.048668 | 34.315422 |
| Ca  | 40.177341 | 29.068279 | 31.199017 |
| Ca  | 39.707794 | 28.774645 | 36.067795 |
| Ca  | 46.559361 | 30.375879 | 33.874386 |
| Ca  | 42.801521 | 29.056515 | 34.204845 |
| S   | 26.867384 | 28.311790 | 36.806206 |
| S   | 26.951401 | 34.166611 | 33.721718 |
| S   | 30.281248 | 29.629017 | 35.833229 |
| S   | 29.800280 | 31.516909 | 36.471924 |
| S   | 32.972187 | 27.190502 | 34.473724 |
| S   | 33.863537 | 31.999084 | 32.554098 |
| S   | 36.857090 | 28.976768 | 31.687477 |
| S   | 36.563606 | 28.948811 | 36.739624 |
| S   | 40.153805 | 26.516048 | 33.475220 |
| S   | 40.462513 | 31.278931 | 34.150578 |
| S   | 43.742760 | 28.816540 | 31.216049 |
| S   | 45.015701 | 26.399197 | 37.945583 |

24

generated by VMD

| Ca  | 25.387127 | 30.250122 | 31.682003 |
| Ca  | 26.323618 | 31.403545 | 35.493790 |
| Ca  | 29.970669 | 28.343479 | 36.286919 |
| Ca  | 30.469427 | 32.821384 | 33.323574 |
| Ca  | 33.391018 | 28.799149 | 31.618368 |
| Ca  | 33.240276 | 30.347858 | 35.504856 |
| Ca  | 36.607410 | 26.506605 | 34.672981 |
| Ca  | 36.741829 | 30.903416 | 34.173740 |
| Ca  | 40.050411 | 29.185413 | 31.259346 |
| Ca  | 39.743737 | 28.872946 | 36.207390 |
| Ca  | 46.226704 | 30.552902 | 33.683815 |
| Ca  | 42.736687 | 28.911972 | 34.152031 |
| S   | 26.642231 | 28.036438 | 36.439339 |
| S   | 26.964703 | 34.175339 | 33.615467 |
| S   | 30.449228 | 29.471893 | 33.059650 |
| S   | 29.942825 | 31.551105 | 36.474815 |
| S   | 33.277119 | 27.321136 | 34.707603 |
| S   | 33.846001 | 32.095333 | 32.503143 |
| S   | 36.769554 | 28.740967 | 31.862064 |
| S   | 36.607689 | 29.243488 | 36.870399 |
| S   | 40.104794 | 26.626173 | 33.587055 |
| S   | 40.288387 | 31.192848 | 34.056049 |
| S   | 43.547813 | 28.929012 | 31.187084 |
| S   | 45.104019 | 26.108826 | 37.613842 |

24

generated by VMD
| Ca         | 25.090704 | 30.279665 | 32.044544 |
| Ca         | 26.392282 | 31.709164 | 35.716747 |
| Ca         | 29.854403 | 28.167547 | 35.766941 |
| Ca         | 30.475376 | 32.586189 | 33.531151 |
| Ca         | 33.386871 | 28.867353 | 31.481834 |
| Ca         | 33.163036 | 29.874367 | 35.581028 |
| Ca         | 36.495338 | 26.731598 | 34.413036 |
| Ca         | 36.862648 | 31.167755 | 34.068672 |
| Ca         | 40.254364 | 29.105339 | 31.301643 |
| Ca         | 39.621887 | 28.880638 | 36.089882 |
| Ca         | 46.388836 | 30.486986 | 33.882179 |
| Ca         | 42.816814 | 29.117224 | 34.379765 |
| S          | 26.882977 | 28.349997 | 36.749577 |
| S          | 26.951302 | 34.253746 | 33.492950 |
| S          | 30.215641 | 29.518852 | 32.818199 |
| S          | 30.142227 | 31.489223 | 36.523109 |
| S          | 33.105309 | 26.892109 | 34.438129 |
| S          | 33.805843 | 32.030872 | 32.614540 |
| S          | 36.781258 | 28.849178 | 31.747002 |
| S          | 36.495083 | 29.108486 | 36.760971 |
| S          | 40.088554 | 26.660042 | 33.637783 |
| S          | 40.386826 | 31.153111 | 34.011982 |
| S          | 43.737312 | 28.893234 | 31.263947 |
| S          | 45.038967 | 26.218676 | 37.715050 |

24 generated by VMD

| Ca         | 25.297356 | 29.972649 | 32.094574 |
| Ca         | 26.518396 | 31.612503 | 35.648003 |
| Ca         | 30.024578 | 28.116652 | 35.771820 |
| Ca         | 30.546654 | 32.761559 | 33.197472 |
| Ca         | 33.272655 | 28.932247 | 31.583580 |
| Ca         | 33.098904 | 30.109266 | 35.532078 |
| Ca         | 36.506599 | 26.598236 | 34.487610 |
| Ca         | 36.657391 | 30.976347 | 34.360554 |
| Ca         | 40.250511 | 29.206474 | 31.218262 |
| Ca         | 39.490555 | 29.077665 | 36.236748 |
| Ca         | 46.593094 | 30.126110 | 33.694851 |
| Ca         | 42.781067 | 29.197014 | 34.319153 |
| S          | 27.019663 | 28.399601 | 36.915146 |
| S          | 27.233202 | 34.259430 | 33.348099 |
| S          | 30.363167 | 29.447346 | 32.844372 |
| S          | 30.102886 | 31.488857 | 36.324806 |
| S          | 33.103600 | 26.866051 | 34.559746 |
| S          | 33.872463 | 32.054810 | 32.746986 |
| S          | 36.671154 | 28.940922 | 31.816971 |
| S          | 36.440094 | 29.117794 | 36.890724 |
|   |      |      |      |
|---|------|------|------|
|  S | 40.014030 | 26.851095 | 33.641388 |
|  S | 40.315094 | 31.180279 | 34.118828 |
|  S | 43.710072 | 29.179771 | 31.260754 |
|  S | 44.550789 | 25.918777 | 37.418179 |

24

generated by VMD

|   |      |      |      |
|---|------|------|------|
|  Ca | 25.210562 | 30.305264 | 31.975620 |
|  Ca | 26.563093 | 31.601860 | 35.880455 |
|  Ca | 30.075413 | 28.235418 | 35.982746 |
|  Ca | 30.363707 | 32.730087 | 33.258297 |
|  Ca | 33.531315 | 28.868938 | 31.512054 |
|  Ca | 33.032967 | 29.964806 | 35.491344 |
|  Ca | 36.724564 | 26.750910 | 34.197983 |
|  Ca | 36.520081 | 30.962196 | 33.994347 |
|  Ca | 40.293613 | 29.184811 | 31.338005 |
|  Ca | 39.647030 | 28.842081 | 36.145363 |
|  Ca | 46.194016 | 30.127605 | 34.066662 |
|  Ca | 42.819019 | 29.076488 | 34.341251 |
|  S | 26.612587 | 28.31607 | 36.806820 |
|  S | 27.097630 | 34.282158 | 33.748909 |
|  S | 30.414986 | 29.538368 | 32.852200 |
|  S | 29.991531 | 31.360744 | 36.429138 |
|  S | 33.275749 | 26.993813 | 34.516632 |
|  S | 33.638565 | 31.951702 | 32.787746 |
|  S | 36.759335 | 29.076946 | 31.489914 |
|  S | 36.640110 | 29.051266 | 36.706177 |
|  S | 40.242832 | 26.611502 | 33.564159 |
|  S | 40.375156 | 31.055794 | 33.982010 |
|  S | 43.915016 | 28.864565 | 31.237522 |
|  S | 44.495083 | 26.637497 | 37.725292 |

24

generated by VMD

|   |      |      |      |
|---|------|------|------|
|  Ca | 25.016579 | 30.354794 | 32.140041 |
|  Ca | 26.393421 | 31.570480 | 35.857338 |
|  Ca | 29.883932 | 28.234362 | 35.871078 |
|  Ca | 30.408808 | 32.619019 | 33.296242 |
|  Ca | 33.402355 | 29.100624 | 31.508366 |
|  Ca | 33.269173 | 29.997252 | 35.447170 |
|  Ca | 36.542473 | 26.597748 | 34.407272 |
|  Ca | 36.774162 | 31.167933 | 34.238441 |
|  Ca | 40.324635 | 28.976318 | 31.316410 |
|  Ca | 39.736671 | 28.981655 | 36.314182 |
|  Ca | 46.396385 | 30.044785 | 33.691635 |
|  Ca | 42.792698 | 29.229858 | 34.198174 |
|  S | 26.625427 | 28.116898 | 36.518620 |
|  S | 27.286964 | 34.172928 | 33.595222 |
|     | S     |          |          |
|-----|-------|----------|----------|
|     | 30.336157 | 29.341469 | 32.858818 |
|     | 29.926777 | 31.532043 | 34.375614 |
|     | 33.074986 | 26.931206 | 32.788116 |
|     | 33.828247 | 32.146511 |          |
|     | 36.796444 | 28.922523 | 31.685276 |
|     | 36.537060 | 29.155195 | 36.858437 |
|     | 40.266724 | 26.660784 | 33.602901 |
|     | 40.364006 | 31.099348 | 33.979042 |
|     | 43.823727 | 28.747648 | 31.076225 |
|     | 44.626114 | 26.690018 | 37.965500 |

24 generated by VMD

|     | Ca    |          |          |
|-----|-------|----------|----------|
|     | 25.014008 | 30.417395 | 31.895639 |
|     | 26.342865 | 31.466730 | 35.728996 |
|     | 29.825188 | 28.211937 | 35.943035 |
|     | 30.234936 | 32.560211 | 33.120300 |
|     | 33.511703 | 28.956650 | 31.709997 |
|     | 33.055439 | 30.186577 | 35.551170 |
|     | 36.383881 | 26.718351 | 34.637650 |
|     | 36.681965 | 31.183826 | 34.265583 |
|     | 40.354015 | 29.185217 | 31.178310 |
|     | 39.681725 | 28.832190 | 36.147881 |
|     | 46.665836 | 29.786434 | 33.791252 |
|     | 42.910572 | 29.272755 | 34.042088 |
|     | 26.652863 | 28.202692 | 36.665352 |
|     | 26.989443 | 34.211750 | 33.678699 |
|     | 30.437141 | 29.324085 | 32.760391 |
|     | 29.970129 | 31.459061 | 36.289093 |
|     | 33.034081 | 26.963108 | 34.595165 |
|     | 33.776897 | 32.071918 | 32.754742 |
|     | 36.882191 | 29.111973 | 31.897572 |
|     | 36.624889 | 29.248322 | 36.981514 |
|     | 40.161850 | 26.739080 | 33.563873 |
|     | 40.275280 | 31.125666 | 34.047054 |
|     | 43.984592 | 28.813091 | 31.130285 |
|     | 44.982430 | 26.342388 | 37.655060 |

24 generated by VMD

|     | Ca    |          |          |
|-----|-------|----------|----------|
|     | 24.545076 | 30.653326 | 32.133526 |
|     | 26.419287 | 31.520845 | 35.713402 |
|     | 29.900675 | 28.178102 | 36.011826 |
|     | 30.208281 | 32.352970 | 33.157192 |
|     | 33.444721 | 28.931942 | 31.578068 |
|     | 33.022831 | 30.292427 | 35.340164 |
|     | 36.692696 | 26.903706 | 34.553467 |
|     | 36.759563 | 31.065086 | 34.100548 |
| Ca       | 40.286140 | 29.212708 | 31.378414 |
| Ca       | 39.816051 | 28.828804 | 36.182301 |
| Ca       | 46.602077 | 30.176186 | 33.838799 |
| Ca       | 42.919464 | 29.045200 | 34.369770 |
| S        | 26.419970 | 28.143177 | 36.589703 |
| S        | 27.209949 | 33.988609 | 33.625900 |
| S        | 30.344021 | 29.207861 | 32.801373 |
| S        | 29.837276 | 31.338856 | 36.449524 |
| S        | 32.15336  | 27.267193 | 34.623470 |
| S        | 33.792358 | 32.026947 | 32.481052 |
| S        | 36.799919 | 29.070862 | 31.693146 |
| S        | 36.721451 | 29.423828 | 36.840839 |
| S        | 40.207619 | 26.629478 | 33.577667 |
| S        | 40.539761 | 31.152817 | 34.133202 |
| S        | 43.809467 | 28.894358 | 31.126125 |
| S        | 44.919949 | 26.086178 | 37.731285 |

24
generated by VMD

| Ca       | 24.874517 | 30.646717 | 32.122616 |
| Ca       | 26.206944 | 31.554371 | 35.857216 |
| Ca       | 29.918407 | 28.035622 | 36.102459 |
| Ca       | 30.386015 | 32.500137 | 33.085690 |
| Ca       | 33.337910 | 28.809811 | 31.552280 |
| Ca       | 33.127277 | 30.386131 | 35.611668 |
| Ca       | 36.597591 | 26.807350 | 34.347614 |
| Ca       | 36.907841 | 31.059637 | 34.347191 |
| Ca       | 40.374214 | 29.327702 | 31.277287 |
| Ca       | 39.753113 | 28.930895 | 36.256733 |
| Ca       | 47.024712 | 29.341179 | 33.692165 |
| Ca       | 42.949905 | 29.198605 | 34.257965 |
| S        | 26.387501 | 28.104954 | 36.668621 |
| S        | 26.938972 | 34.037872 | 33.452767 |
| S        | 30.072037 | 29.152012 | 32.812160 |
| S        | 29.783064 | 31.428291 | 36.229984 |
| S        | 33.225304 | 27.292629 | 34.681320 |
| S        | 33.727303 | 32.031342 | 32.692444 |
| S        | 36.786419 | 29.237522 | 31.587175 |
| S        | 36.539608 | 29.122929 | 36.781460 |
| S        | 40.315620 | 26.909256 | 33.716526 |
| S        | 40.412571 | 31.224930 | 34.057461 |
| S        | 43.955395 | 28.895214 | 31.125687 |
| S        | 44.831676 | 26.356266 | 37.731682 |

24
generated by VMD

| Ca       | 24.618538 | 30.790482 | 32.253487 |
| Ca       | 26.025751 | 31.508366 | 35.867886 |
| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 30.097359 | 27.905411 | 35.995968 |
| Ca      | 30.244894 | 32.668274 | 33.072144 |
| Ca      | 33.398243 | 28.991154 | 31.664661 |
| Ca      | 33.093929 | 30.108002 | 35.563934 |
| Ca      | 36.509064 | 26.616173 | 34.286289 |
| Ca      | 36.739185 | 31.239399 | 34.071766 |
| Ca      | 40.492996 | 29.234936 | 31.117290 |
| Ca      | 39.562706 | 28.834557 | 35.925682 |
| Ca      | 46.870541 | 29.634571 | 33.943256 |
| Ca      | 42.796680 | 29.225231 | 34.291523 |
| Ca      | 26.682104 | 28.177704 | 36.599640 |
| Ca      | 27.301765 | 34.334373 | 33.701176 |
| Ca      | 30.458288 | 29.291296 | 32.849564 |
| Ca      | 29.662598 | 31.315231 | 36.250195 |
| Ca      | 33.268566 | 26.903481 | 34.774197 |
| Ca      | 33.770569 | 32.044346 | 32.637642 |
| Ca      | 36.868233 | 28.916458 | 31.754234 |
| Ca      | 36.499046 | 29.213875 | 36.687485 |
| Ca      | 40.285496 | 26.582943 | 33.712334 |
| Ca      | 40.336231 | 31.273054 | 33.820648 |
| Ca      | 44.103092 | 29.060507 | 31.383305 |
| Ca      | 44.748093 | 26.521616 | 37.806297 |

24

generated by VMD

| Element | X | Y | Z |
|---------|---|---|---|
| Ca      | 24.975422 | 30.610430 | 32.093739 |
| Ca      | 26.215561 | 31.307701 | 35.825317 |
| Ca      | 30.143572 | 28.126503 | 36.159538 |
| Ca      | 30.222485 | 32.726128 | 33.184887 |
| Ca      | 33.199005 | 28.771278 | 31.434361 |
| Ca      | 32.926804 | 30.442610 | 35.451656 |
| Ca      | 36.567276 | 26.649879 | 34.414291 |
| Ca      | 36.594151 | 31.235058 | 33.979557 |
| Ca      | 40.249470 | 29.333759 | 31.073002 |
| Ca      | 39.479408 | 28.893005 | 36.164848 |
| Ca      | 47.120880 | 29.468990 | 33.945126 |
| Ca      | 42.801800 | 29.165104 | 34.218166 |
| S       | 26.896143 | 28.012991 | 36.708462 |
| S       | 26.956902 | 33.968605 | 33.769230 |
| S       | 30.372534 | 29.483585 | 32.892036 |
| S       | 29.917526 | 31.473415 | 36.393494 |
| S       | 33.232388 | 27.281471 | 34.570366 |
| S       | 33.787834 | 32.193741 | 32.530258 |
| S       | 36.777966 | 29.004183 | 31.681299 |
| S       | 36.484665 | 29.382669 | 36.676460 |
| S       | 40.152443 | 26.731194 | 33.588371 |
| S       | 40.325970 | 31.145325 | 34.076328 |
|   |       |       |       |
|---|-------|-------|-------|
| S | 44.261780 | 28.801701 | 31.543945 |
| S | 44.771954 | 26.182081 | 37.655926 |

24 generated by VMD

| Ca | 24.372187 | 30.416603 | 32.195168 |
| Ca | 26.215752 | 31.321983 | 35.960861 |
| Ca | 30.038174 | 28.143078 | 35.953064 |
| Ca | 30.540998 | 32.893562 | 33.244068 |
| Ca | 33.502483 | 28.819679 | 31.441547 |
| Ca | 33.142563 | 30.347511 | 35.658791 |
| Ca | 36.624519 | 26.807035 | 34.592968 |
| Ca | 36.700699 | 31.288254 | 33.910244 |
| Ca | 40.305958 | 29.272057 | 31.208008 |
| Ca | 39.646721 | 28.940651 | 36.144657 |
| Ca | 46.808453 | 29.280716 | 33.723946 |
| Ca | 42.743774 | 29.200342 | 34.242336 |

S | 26.549673 | 27.15515 | 36.299698 |
S | 27.058416 | 33.754704 | 33.822609 |
S | 30.444412 | 29.671570 | 32.828850 |
S | 29.850031 | 31.474030 | 36.511131 |
S | 33.394127 | 27.364330 | 34.450512 |
S | 33.856640 | 32.189384 | 32.453735 |
S | 36.844730 | 28.876465 | 31.852551 |
S | 36.575752 | 29.632254 | 36.684582 |
S | 40.156429 | 26.628876 | 33.561974 |
S | 40.324646 | 31.156122 | 33.909676 |
S | 44.089706 | 28.818104 | 31.293118 |
S | 44.646999 | 26.378593 | 38.086647 |

24 generated by VMD

| Ca | 24.481125 | 30.583487 | 32.321533 |
| Ca | 25.846821 | 30.975134 | 36.309395 |
| Ca | 30.081985 | 28.129152 | 35.753216 |
| Ca | 30.407236 | 32.610092 | 33.183762 |
| Ca | 33.505234 | 29.110226 | 31.409403 |
| Ca | 33.143664 | 30.836876 | 35.658791 |
| Ca | 36.375885 | 27.211786 | 34.565014 |
| Ca | 36.885651 | 31.370079 | 33.784065 |
| Ca | 40.421848 | 29.234398 | 31.213818 |
| Ca | 39.714821 | 29.320469 | 36.200890 |
| Ca | 47.049114 | 28.930897 | 33.810654 |
| Ca | 42.913879 | 29.102310 | 34.350544 |
| S | 26.697258 | 27.769241 | 36.341156 |
| S | 27.087547 | 33.863831 | 34.188881 |
| S | 30.522139 | 29.497650 | 32.682194 |
| S | 29.729568 | 31.341394 | 36.302063 |
S  33.069321  27.126648  34.459427
S  33.817223  32.239578  32.584938
S  36.995651  29.087387  31.635014
S  36.596703  29.748596  36.635883
S  39.848438  26.853218  33.863720
S  40.697235  31.322985  33.781708
S  44.171730  28.404640  31.469406
S  44.430153  26.426317  37.789528

24 generated by VMD
Ca  24.629730  30.616137  32.416618
Ca  25.999903  31.213493  36.097839
Ca  30.206692  28.251482  35.955231
Ca  30.185316  32.604313  33.071301
Ca  33.237415  28.929785  31.374622
Ca  33.126511  30.288898  35.159851
Ca  36.555897  26.810818  34.575794
Ca  36.682182  31.007845  33.907326
Ca  40.391666  29.409039  31.320032
Ca  39.979458  29.224209  36.267147
Ca  46.886566  28.665897  33.626526
Ca  42.883850  29.299503  34.230515
S  26.758698  27.674267  36.198204
S  27.051350  34.007355  34.118969
S  30.276052  29.478111  32.790413
S  29.678633  31.529684  36.287830
S  33.296642  27.262163  34.295326
S  33.768978  32.479683  32.572765
S  36.702034  28.893162  31.694935
S  36.567085  29.364323  36.844978
S  40.283714  26.884109  33.822983
S  40.392124  31.291088  33.816856
S  44.056343  28.626438  31.385025
S  44.836948  26.579636  38.199604

24 generated by VMD
Ca  24.514885  30.261599  32.053936
Ca  26.250835  31.110270  35.946842
Ca  30.036671  28.157825  35.995148
Ca  30.208992  32.540257  33.117184
Ca  33.288559  29.214626  31.463724
Ca  33.034340  30.298065  35.391109
Ca  36.443836  27.034540  34.819439
Ca  36.874195  31.364506  34.102745
Ca  40.504845  29.267738  31.110659
Ca  39.962563  29.247257  36.269115
| Element | X1     | Y1     | Z1     |
|---------|--------|--------|--------|
| Ca      | 46.974113 | 28.694874 | 33.447723 |
| Ca      | 43.001225 | 29.054144 | 34.137894 |
| S       | 26.588335 | 27.878773 | 36.108994 |
| S       | 26.866352 | 33.931988 | 33.965168 |
| S       | 30.292559 | 29.492115 | 32.841663 |
| S       | 29.721836 | 31.351513 | 36.331566 |
| S       | 33.000217 | 27.179476 | 34.384064 |
| S       | 33.685947 | 32.374710 | 32.899021 |
| S       | 36.783695 | 29.227327 | 31.820274 |
| S       | 36.561062 | 29.709415 | 36.807205 |
| S       | 40.126976 | 26.898148 | 33.945668 |
| S       | 40.613312 | 31.278193 | 33.842197 |
| S       | 44.059032 | 28.327499 | 31.177530 |
| S       | 45.039558 | 26.496555 | 38.050972 |

generated by VMD

| Element | X1     | Y1     | Z1     |
|---------|--------|--------|--------|
| Ca      | 24.616404 | 30.051891 | 32.064625 |
| Ca      | 25.884781 | 31.230770 | 35.925629 |
| Ca      | 29.978828 | 28.259274 | 35.803699 |
| Ca      | 30.156788 | 32.959122 | 33.307102 |
| Ca      | 33.803253 | 29.426979 | 31.614716 |
| Ca      | 33.148247 | 30.374393 | 35.388680 |
| Ca      | 36.634327 | 26.669720 | 34.713215 |
| Ca      | 36.765133 | 31.310457 | 34.189323 |
| Ca      | 40.391373 | 29.094643 | 31.105450 |
| Ca      | 39.910099 | 29.063671 | 36.356739 |
| Ca      | 47.114265 | 28.780373 | 33.091305 |
| Ca      | 43.189770 | 29.176338 | 34.169937 |
| S       | 26.579594 | 27.871542 | 36.318134 |
| S       | 26.545168 | 33.794254 | 33.683121 |
| S       | 30.580303 | 29.884243 | 32.904259 |
| S       | 29.466322 | 31.448748 | 36.359032 |
| S       | 32.933430 | 27.195415 | 34.414108 |
| S       | 33.578304 | 32.573078 | 32.835693 |
| S       | 36.906952 | 28.866692 | 32.061733 |
| S       | 36.430164 | 29.471025 | 36.734177 |
| S       | 40.265255 | 26.710909 | 33.910255 |
| S       | 40.262009 | 31.140419 | 33.808025 |
| S       | 44.104294 | 28.307213 | 31.302170 |
| S       | 45.188831 | 26.730249 | 37.969570 |

generated by VMD

| Element | X1     | Y1     | Z1     |
|---------|--------|--------|--------|
| Ca      | 24.727774 | 30.150345 | 31.972542 |
| Ca      | 26.165215 | 31.083946 | 35.784172 |
| Ca      | 30.049133 | 28.110754 | 35.797916 |
| Ca      | 30.238573 | 32.831562 | 33.326843 |
| Element | X (histogram) | Y (histogram) | Z (histogram) |
|---------|---------------|---------------|---------------|
| Ca      | 33.450054     | 29.599741     | 31.557058     |
| Ca      | 33.205059     | 30.203058     | 35.368225     |
| Ca      | 36.693363     | 26.944872     | 34.762917     |
| Ca      | 36.836060     | 31.176998     | 34.026665     |
| Ca      | 40.066933     | 29.151203     | 31.281195     |
| Ca      | 40.065659     | 29.230293     | 36.536575     |
| Ca      | 46.830883     | 28.562962     | 33.435047     |
| Ca      | 42.975002     | 29.205286     | 34.073215     |
| S       | 26.811630     | 27.699909     | 36.251671     |
| S       | 26.854033     | 33.946724     | 33.992195     |
| S       | 30.468384     | 29.675510     | 32.742893     |
| S       | 29.668419     | 31.323927     | 36.338863     |
| S       | 33.344639     | 27.313814     | 34.347862     |
| S       | 33.644424     | 32.623753     | 32.851234     |
| S       | 36.648911     | 28.771008     | 31.837065     |
| S       | 36.659176     | 29.579422     | 36.837021     |
| S       | 40.116787     | 26.888865     | 33.845734     |
| S       | 40.479527     | 31.232121     | 33.830280     |
| S       | 43.635166     | 28.167212     | 31.105335     |
| S       | 44.799053     | 26.918173     | 38.128216     |

24 generated by VMD

| Element | X (histogram) | Y (histogram) | Z (histogram) |
|---------|---------------|---------------|---------------|
| Ca      | 24.881725     | 30.321289     | 31.671638     |
| Ca      | 26.020329     | 31.105185     | 35.829479     |
| Ca      | 29.909660     | 28.259169     | 35.996906     |
| Ca      | 30.336710     | 32.832798     | 33.379253     |
| Ca      | 33.632893     | 29.353523     | 31.739445     |
| Ca      | 33.112236     | 30.278790     | 35.613880     |
| Ca      | 36.631001     | 26.709515     | 34.697380     |
| Ca      | 36.758366     | 31.299551     | 33.958546     |
| Ca      | 40.078304     | 29.119072     | 31.123951     |
| Ca      | 39.890209     | 29.082874     | 36.339088     |
| Ca      | 46.754051     | 28.889254     | 33.320000     |
| Ca      | 42.906773     | 29.057774     | 34.073292     |
| S       | 26.600998     | 27.744705     | 36.088657     |
| S       | 26.940243     | 33.827564     | 33.792782     |
| S       | 30.454491     | 29.723255     | 32.887833     |
| S       | 29.714962     | 31.372154     | 36.521385     |
| S       | 33.177650     | 27.235191     | 34.694820     |
| S       | 33.693489     | 32.587669     | 32.823429     |
| S       | 36.659561     | 28.759237     | 31.930067     |
| S       | 36.806332     | 29.434217     | 36.652679     |
| S       | 40.145500     | 26.816143     | 33.828091     |
| S       | 40.376774     | 31.258316     | 33.631348     |
| S       | 43.815735     | 28.308605     | 31.149363     |
| S       | 45.136005     | 27.015562     | 38.287312     |
|  |  |  |  |
|---|---|---|---|
| Ca | 25.112640 | 30.211800 | 31.682209 |
| Ca | 25.920010 | 31.339035 | 35.624832 |
| Ca | 29.857504 | 28.161169 | 36.148937 |
| Ca | 30.303295 | 32.760368 | 33.325958 |
| Ca | 33.582844 | 29.292807 | 31.653059 |
| Ca | 32.993496 | 30.243416 | 35.570549 |
| Ca | 36.787266 | 26.724808 | 34.596466 |
| Ca | 36.778996 | 30.754509 | 34.183365 |
| Ca | 40.081486 | 28.984058 | 31.197132 |
| Ca | 40.010246 | 29.086740 | 36.109455 |
| Ca | 46.451244 | 28.921032 | 33.580070 |
| Ca | 42.978676 | 29.488693 | 34.027302 |
| S  | 26.562325 | 27.965698 | 36.363022 |
| S  | 27.069012 | 34.092079 | 33.678123 |
| S  | 30.315741 | 29.650433 | 32.846375 |
| S  | 29.602922 | 31.363041 | 36.557816 |
| S  | 33.240707 | 27.351124 | 34.477043 |
| S  | 33.763435 | 32.465244 | 33.080620 |
| S  | 36.682056 | 28.733414 | 31.840889 |
| S  | 36.828217 | 29.205029 | 36.908508 |
| S  | 40.288372 | 26.777702 | 33.656696 |
| S  | 40.230053 | 31.258102 | 33.693977 |
| S  | 43.858021 | 28.612587 | 30.986324 |
| S  | 45.135269 | 26.948593 | 38.242001 |

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|  |  |  |  |
|---|---|---|---|
| Ca | 25.349976 | 30.636925 | 31.829351 |
| Ca | 25.965586 | 31.294885 | 35.652187 |
| Ca | 30.053366 | 28.130424 | 35.668911 |
| Ca | 30.204390 | 32.846069 | 33.539227 |
| Ca | 33.671074 | 29.781380 | 31.567936 |
| Ca | 33.076164 | 30.302408 | 35.666801 |
| Ca | 36.652393 | 26.686690 | 34.635307 |
| Ca | 36.587360 | 30.988770 | 34.019566 |
| Ca | 40.127407 | 28.851702 | 31.401859 |
| Ca | 39.884212 | 29.033352 | 36.300346 |
| Ca | 46.596577 | 29.226219 | 33.265041 |
| Ca | 42.869873 | 29.207451 | 34.023129 |
| S  | 26.910158 | 28.049801 | 36.461113 |
| S  | 26.923725 | 34.095482 | 33.810791 |
| S  | 30.542610 | 29.759954 | 32.655468 |
| S  | 29.483368 | 31.411777 | 36.430325 |
| S  | 33.231167 | 27.430771 | 34.472275 |
| S  | 33.669743 | 32.782001 | 33.114407 |
| S   | 36.618130 | 28.779402 | 31.788044 |
| S   | 36.565708 | 29.333843 | 36.752449 |
| S   | 40.075558 | 26.562475 | 33.937805 |
| S   | 40.289112 | 31.109501 | 33.934341 |
| S   | 43.758385 | 28.230961 | 31.179686 |
| S   | 45.327854 | 26.857550 | 37.924324 |

24 generated by VMD

| Ca  | 25.295441 | 29.970676 | 31.407923 |
| Ca  | 25.949615 | 31.013489 | 35.525120 |
| Ca  | 30.192266 | 28.198406 | 35.999802 |
| Ca  | 30.200285 | 32.878193 | 33.184273 |
| Ca  | 33.600834 | 29.774588 | 31.992897 |
| Ca  | 32.907734 | 30.471699 | 35.683720 |
| Ca  | 36.647720 | 26.682312 | 34.699043 |
| Ca  | 36.741257 | 31.001854 | 34.066002 |
| Ca  | 40.028530 | 28.877453 | 31.381617 |
| Ca  | 40.025909 | 28.940144 | 36.135139 |
| Ca  | 46.490040 | 29.344870 | 33.204548 |
| Ca  | 42.855465 | 29.345314 | 34.007320 |
| S   | 26.749460 | 27.937399 | 36.349152 |
| S   | 26.857325 | 34.101345 | 33.864090 |
| S   | 30.568216 | 29.670832 | 32.795700 |
| S   | 29.479639 | 31.464878 | 36.372780 |
| S   | 33.257919 | 27.459206 | 34.642670 |
| S   | 33.707981 | 32.660988 | 33.239319 |
| S   | 36.601032 | 28.545300 | 31.982561 |
| S   | 36.752167 | 29.300526 | 36.869537 |
| S   | 40.102654 | 26.621462 | 33.778603 |
| S   | 40.327850 | 31.141148 | 33.770359 |
| S   | 43.695229 | 28.186487 | 31.092247 |
| S   | 45.399326 | 26.802828 | 37.986210 |

24 generated by VMD

| Ca  | 25.167620 | 29.863707 | 32.008167 |
| Ca  | 26.025915 | 31.065357 | 35.856525 |
| Ca  | 30.093779 | 28.379187 | 35.759853 |
| Ca  | 30.196049 | 32.938271 | 33.223843 |
| Ca  | 33.699169 | 29.569841 | 31.774757 |
| Ca  | 33.298000 | 30.468945 | 35.533966 |
| Ca  | 36.506001 | 26.760645 | 34.480503 |
| Ca  | 36.773724 | 31.192888 | 33.911591 |
| Ca  | 40.163776 | 29.010708 | 31.287828 |
| Ca  | 39.699551 | 28.741913 | 36.078705 |
| Ca  | 46.569496 | 29.476812 | 33.604271 |
| Ca  | 42.715385 | 29.089413 | 34.284100 |
|    |       |       |       |
|----|-------|-------|-------|
| S  | 26.872314 | 27.773390 | 36.355324 |
| S  | 27.015514 | 33.884296 | 33.990520 |
| S  | 30.633705 | 29.769800 | 32.695171 |
| S  | 29.567341 | 31.519421 | 36.478371 |
| S  | 33.266354 | 27.322653 | 34.536404 |
| S  | 33.799702 | 32.682613 | 32.783287 |
| S  | 36.667686 | 28.694704 | 31.843868 |
| S  | 36.519608 | 29.461971 | 36.699421 |
| S  | 40.038242 | 26.651478 | 33.727585 |
| S  | 40.268074 | 31.130686 | 33.951374 |
| S  | 43.701599 | 28.319920 | 31.224270 |
| S  | 45.175320 | 26.622778 | 37.940968 |

24

| Ca  |       |       |       |
|-----|-------|-------|-------|
| Ca  | 24.540001 | 29.991734 | 32.067875 |
| Ca  | 26.336323 | 31.042376 | 35.638962 |
| Ca  | 30.126144 | 28.270327 | 35.899773 |
| Ca  | 30.045290 | 32.686638 | 33.286076 |
| Ca  | 33.697613 | 29.723343 | 31.766239 |
| Ca  | 33.003387 | 30.505644 | 35.460392 |
| Ca  | 36.814026 | 26.767326 | 34.573444 |
| Ca  | 36.752972 | 31.195215 | 34.006329 |
| Ca  | 40.148979 | 29.155857 | 31.233513 |
| Ca  | 39.829788 | 28.692135 | 36.108356 |
| Ca  | 46.740047 | 29.398325 | 33.599663 |
| Ca  | 42.962090 | 29.015341 | 34.192314 |
| S   | 26.918552 | 27.829487 | 36.392319 |
| S   | 26.499855 | 33.857216 | 33.799423 |
| S   | 30.524403 | 29.726019 | 32.762314 |
| S   | 29.816330 | 31.586138 | 36.362743 |
| S   | 33.384281 | 27.523642 | 34.585514 |
| S   | 33.592896 | 32.774971 | 32.892712 |
| S   | 36.649410 | 28.914158 | 31.672230 |
| S   | 36.804550 | 29.435596 | 36.736843 |
| S   | 40.197132 | 26.585041 | 33.667526 |
| S   | 40.373669 | 31.047619 | 33.920521 |
| S   | 43.836185 | 28.127569 | 31.286118 |
| S   | 44.840038 | 26.539661 | 38.119446 |

24

| Ca  |       |       |       |
|-----|-------|-------|-------|
| Ca  | 24.888115 | 29.866535 | 32.277340 |
| Ca  | 26.069698 | 31.130592 | 35.692142 |
| Ca  | 30.168745 | 28.190348 | 35.830139 |
| Ca  | 30.109154 | 32.935593 | 33.269150 |
| Ca  | 33.668594 | 29.635054 | 31.343525 |
| Ca  | 32.893505 | 30.647501 | 35.429901 |
Ca    36.772724  26.657520  34.577026
Ca    36.667641  30.895166  34.032276
Ca    40.235634  29.010359  31.290871
Ca    39.834690  28.917625  36.463928
Ca    46.878506  29.251200  33.430836
Ca    42.820312  29.242437  34.136940
S     26.871691  27.790485  36.553139
S     26.861296  34.168968  34.134590
S     30.407946  29.777641  32.714970
S     29.598618  31.443230  36.238014
S     33.346066  27.605347  34.392178
S     33.680534  32.714664  32.697765
S     36.646103  28.776146  31.480042
S     36.509918  29.063534  36.707417
S     40.092041  26.704176  33.835915
S     40.225845  31.093464  34.020920
S     44.005829  28.217285  34.354492
S     45.180649  26.656578  38.127083

24 generated by VMD
Ca    24.756264  30.282215  32.267338
Ca    26.259159  31.447062  35.789238
Ca    30.335135  27.922394  35.866104
Ca    30.207748  32.677681  33.098976
Ca    33.341629  29.767511  31.520916
Ca    32.830456  30.429081  35.481182
Ca    36.949097  26.332223  34.378284
Ca    36.427479  30.694910  33.968807
Ca    40.042023  28.927511  31.132315
Ca    39.690140  28.954010  36.207615
Ca    46.788849  29.317965  33.764034
Ca    42.947952  29.303686  34.207298
S     26.666357  27.970404  36.391514
S     27.180538  34.352463  34.041389
S     30.356056  29.580591  32.734570
S     29.757689  31.417662  36.240665
S     33.484146  27.429131  34.264538
S     33.740044  32.675003  32.961601
S     36.373993  28.512260  31.642767
S     36.484161  28.949102  36.827969
S     40.394760  26.609465  33.869560
S     40.215366  31.091722  33.737606
S     43.937386  28.635803  31.267334
S     45.267467  27.110525  38.369102

24 generated by VMD
|   | Ca       |         |         |         | Ca       |         |         |         | Ca       |         |         |         | Ca       |         |         |         | Ca       |         |         |         |
|---|----------|---------|---------|---------|----------|---------|---------|---------|----------|---------|---------|---------|----------|---------|---------|---------|----------|---------|---------|---------|
|   | 24.596910| 30.207836| 32.150322|
|   | 26.336010| 31.012699| 35.838211|
|   | 30.020784| 28.247986| 35.836876|
|   | 30.368904| 32.788574| 33.461266|
|   | 33.505856| 29.585957| 31.440367|
|   | 33.036583| 30.479977| 35.368286|
|   | 36.523293| 26.523653| 34.216927|
|   | 36.713776| 31.089199| 33.942066|
|   | 40.221954| 28.858953| 31.403555|
|   | 39.390339| 28.998480| 36.208057|
|   | 46.904331| 29.246487| 33.389351|
|   | 42.866375| 29.111259| 34.342621|
|   | 26.721613| 27.753773| 36.489277|
|   | 27.018377| 34.035919| 33.893429|
|   | 30.532261| 29.741234| 32.740005|
|   | 29.728680| 31.500443| 36.464634|
|   | 33.208309| 27.291796| 34.230350|
|   | 33.802486| 32.628368| 32.689041|
|   | 36.738968| 29.013949| 31.644325|
|   | 36.330669| 29.241890| 36.721951|
|   | 40.084236| 26.564255| 33.936127|
|   | 40.306255| 31.140965| 33.981968|
|   | 43.784691| 28.205914| 31.496113|
|   | 45.692265| 27.122564| 38.145576|

24 generated by VMD

|   | Ca       |         |         |         | Ca       |         |         |         | Ca       |         |         |         | Ca       |         |         |         | Ca       |         |         |         |
|---|----------|---------|---------|---------|----------|---------|---------|---------|----------|---------|---------|---------|----------|---------|---------|---------|----------|---------|---------|---------|
|   | 24.699604| 30.047188| 32.019264|
|   | 25.949772| 31.011595| 35.601768|
|   | 30.048008| 28.369709| 35.892174|
|   | 30.415504| 32.794033| 33.073238|
|   | 33.749844| 29.571396| 31.765867|
|   | 33.083992| 30.511253| 35.536664|
|   | 36.519764| 26.764885| 34.311388|
|   | 36.682926| 31.123590| 34.242462|
|   | 40.181103| 28.600508| 31.273426|
|   | 39.819469| 28.766172| 36.342258|
|   | 46.588219| 29.300785| 33.363129|
|   | 42.844662| 29.267855| 34.074060|
|   | 26.658609| 27.764458| 36.482967|
|   | 27.022139| 33.905869| 33.891586|
|   | 30.607048| 29.612503| 32.823975|
|   | 29.611717| 31.609299| 36.232456|
|   | 33.274384| 27.428955| 34.617928|
|   | 33.825893| 32.740818| 32.743179|
|   | 36.775684| 29.023401| 31.814005|
|   | 36.493259| 29.071844| 36.813511|
# Natural Text

## Table of Structural Data

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| S    | 40.222843 | 26.687346 | 33.920864 |
| S    | 40.198486 | 31.118702 | 33.944286 |
| S    | 43.683189 | 28.565638 | 31.191891 |
| S    | 45.477852 | 26.733196 | 38.059185 |

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24 generated by VMD

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| Ca   | 25.057468 | 30.316471 | 32.151855 |
| Ca   | 26.309551 | 31.190708 | 35.449146 |
| Ca   | 30.044958 | 28.139402 | 35.891991 |
| Ca   | 30.405058 | 32.556023 | 32.911663 |
| Ca   | 33.630917 | 29.561739 | 31.765125 |
| Ca   | 33.182362 | 30.357855 | 35.631348 |
| Ca   | 36.532753 | 26.625187 | 34.382912 |
| Ca   | 36.723312 | 31.047989 | 34.108929 |
| Ca   | 40.047638 | 29.056984 | 31.064211 |
| Ca   | 39.747829 | 28.835228 | 36.487473 |
| Ca   | 46.389786 | 29.456009 | 33.597832 |
| Ca   | 42.669064 | 29.167036 | 34.119194 |
| S    | 26.746752 | 27.954954 | 36.548313 |
| S    | 27.145452 | 34.164158 | 33.956745 |
| S    | 30.696337 | 29.370306 | 32.878841 |
| S    | 29.681408 | 31.528645 | 36.211739 |
| S    | 33.306877 | 27.210354 | 34.580746 |
| S    | 33.693718 | 32.569283 | 32.877918 |
| S    | 36.620338 | 28.818027 | 31.753088 |
| S    | 36.440529 | 29.162968 | 36.726093 |
| S    | 40.129719 | 26.742569 | 33.769684 |
| S    | 40.128654 | 31.148384 | 33.982929 |
| S    | 43.786655 | 28.521898 | 31.297073 |
| S    | 45.316719 | 26.889248 | 37.885929 |

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24 generated by VMD

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| Ca   | 25.398941 | 30.013916 | 32.142967 |
| Ca   | 26.474802 | 31.300610 | 35.864761 |
| Ca   | 30.339817 | 28.315048 | 36.020287 |
| Ca   | 30.483395 | 32.842297 | 33.136452 |
| Ca   | 33.414925 | 29.531080 | 31.343338 |
| Ca   | 33.011227 | 30.471512 | 35.341866 |
| Ca   | 36.564873 | 26.505100 | 34.179066 |
| Ca   | 36.490147 | 30.633007 | 33.818665 |
| Ca   | 39.876698 | 29.135849 | 31.118849 |
| Ca   | 39.595703 | 28.597214 | 36.346832 |
| Ca   | 46.548470 | 29.491888 | 33.813251 |
| Ca   | 42.676399 | 29.203415 | 34.211769 |
| S    | 26.950237 | 27.818588 | 36.538712 |
| S    | 27.497786 | 34.215630 | 34.214535 |
|    | 30.416555 | 29.691029 | 32.882618 |
|----|-----------|-----------|-----------|
| S  | 29.875931 | 31.435907 | 36.647755 |
| S  | 33.262897 | 27.508720 | 34.172764 |
| S  | 33.870327 | 32.608398 | 32.639610 |
| S  | 36.503101 | 28.553978 | 31.416847 |
| S  | 36.300800 | 28.914347 | 36.709908 |
| S  | 40.113956 | 26.646673 | 33.710899 |
| S  | 39.941010 | 30.896774 | 33.950592 |
| S  | 43.933628 | 28.656744 | 31.285069 |
| S  | 44.892326 | 27.403679 | 38.523312 |

24 generated by VMD

| Ca  | 24.806936 | 30.454437 | 32.148540 |
|-----|-----------|-----------|-----------|
| Ca  | 26.207148 | 31.127966 | 35.764603 |
| Ca  | 29.991003 | 28.251570 | 35.884117 |
| Ca  | 30.435720 | 32.657497 | 33.204334 |
| Ca  | 33.768139 | 29.203270 | 31.292542 |
| Ca  | 33.114353 | 30.474926 | 35.380013 |
| Ca  | 36.504951 | 26.582230 | 34.414078 |
| Ca  | 36.587051 | 31.045937 | 33.894737 |
| Ca  | 40.243092 | 29.001238 | 31.183863 |
| Ca  | 39.630890 | 28.492970 | 36.516823 |
| Ca  | 46.581100 | 30.034885 | 33.476421 |
| Ca  | 42.683208 | 29.181545 | 34.390694 |
| S  | 26.805353 | 27.924170 | 36.658882 |
| S  | 27.246582 | 34.199387 | 34.217796 |
| S  | 30.584797 | 29.649630 | 32.752937 |
| S  | 29.856012 | 31.510426 | 36.315022 |
| S  | 33.086952 | 27.362101 | 34.261883 |
| S  | 33.752708 | 32.528820 | 32.560852 |
| S  | 36.730919 | 28.536388 | 31.648600 |
| S  | 36.404591 | 29.076738 | 36.713322 |
| S  | 40.068546 | 26.618296 | 33.887585 |
| S  | 40.083660 | 30.958208 | 34.021286 |
| S  | 43.900459 | 28.455193 | 31.470179 |
| S  | 45.359749 | 27.063585 | 37.971554 |

24 generated by VMD

| Ca  | 24.769140 | 29.936169 | 32.075226 |
|-----|-----------|-----------|-----------|
| Ca  | 26.028431 | 31.458338 | 35.592251 |
| Ca  | 30.117540 | 28.146646 | 35.839481 |
| Ca  | 30.266085 | 32.984398 | 33.305038 |
| Ca  | 33.968662 | 29.801863 | 31.597000 |
| Ca  | 33.118137 | 30.250816 | 35.460396 |
| Ca  | 36.924259 | 26.407089 | 34.424767 |
| Ca  | 36.613342 | 30.843840 | 34.097794 |
|    |    |    |    |
|----|----|----|----|
| Ca | 39.986362 | 28.636641 | 31.162815 |
| Ca | 39.676357 | 28.731915 | 36.449207 |
| Ca | 46.278591 | 29.978834 | 33.122536 |
| Ca | 42.642342 | 29.262520 | 34.345993 |
| S  | 26.895912 | 28.077625 | 36.345520 |
| S  | 26.956381 | 34.378086 | 33.998360 |
| S  | 30.743408 | 29.637398 | 32.792839 |
| S  | 33.489948 | 27.301147 | 34.511848 |
| S  | 33.853237 | 32.627651 | 32.943253 |
| S  | 36.654755 | 28.448771 | 31.712816 |
| S  | 36.624687 | 28.950283 | 36.823051 |
| S  | 40.205814 | 26.428608 | 33.684868 |
| S  | 39.981365 | 30.919514 | 34.006313 |
| S  | 43.621284 | 28.384321 | 31.272308 |
| S  | 45.095894 | 27.375679 | 38.272057 |
| 24 |    |    |    |
| generated by VMD |
| Ca | 24.813513 | 29.899374 | 32.008686 |
| Ca | 26.019102 | 31.316902 | 35.713387 |
| Ca | 29.894714 | 28.310886 | 35.961483 |
| Ca | 30.264627 | 32.762566 | 33.143898 |
| Ca | 33.768852 | 29.565807 | 31.846600 |
| Ca | 33.168957 | 30.473507 | 35.450314 |
| Ca | 36.615952 | 26.594948 | 34.022442 |
| Ca | 36.895565 | 30.976919 | 34.145901 |
| Ca | 40.352509 | 28.960514 | 30.833448 |
| Ca | 39.535351 | 28.932291 | 36.151234 |
| Ca | 46.142670 | 30.130939 | 33.788223 |
| Ca | 42.701885 | 28.738213 | 34.269852 |
| S  | 26.836985 | 27.959776 | 36.572071 |
| S  | 27.149487 | 33.943176 | 34.116608 |
| S  | 30.625364 | 29.690681 | 32.783409 |
| S  | 29.550182 | 31.586094 | 36.400749 |
| S  | 33.211788 | 27.352833 | 34.683670 |
| S  | 33.882210 | 32.587639 | 32.999588 |
| S  | 36.818039 | 28.871910 | 31.684385 |
| S  | 36.481148 | 29.006081 | 36.592987 |
| S  | 40.064533 | 26.493773 | 33.477707 |
| S  | 40.452446 | 30.912271 | 33.749996 |
| S  | 44.024834 | 28.264521 | 31.286613 |
| S  | 45.163193 | 27.059801 | 38.347473 |
| 24 |    |    |    |
| generated by VMD |
| Ca | 25.163176 | 30.093430 | 32.285984 |
| Ca | 26.119268 | 31.005840 | 35.803249 |
| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 30.256388 | 28.160244 | 35.599129 |
| Ca      | 30.370783 | 32.934841 | 33.122406 |
| Ca      | 33.501339 | 29.865692 | 31.529133 |
| Ca      | 33.176285 | 30.414867 | 35.343636 |
| Ca      | 36.692070 | 26.534399 | 34.439308 |
| Ca      | 36.703667 | 31.018661 | 33.986710 |
| Ca      | 40.021038 | 28.704922 | 31.194229 |
| Ca      | 39.631424 | 28.950092 | 36.248096 |
| Ca      | 46.323082 | 30.020390 | 33.223820 |
| Ca      | 42.663006 | 28.844620 | 34.411407 |
| Ca      | 27.193218 | 27.773582 | 36.496864 |
| Ca      | 27.188614 | 33.997429 | 34.414890 |
| Ca      | 30.508579 | 29.798168 | 32.670982 |
| Ca      | 29.750248 | 31.357376 | 36.247128 |
| Ca      | 33.347260 | 27.495640 | 34.163239 |
| Ca      | 33.787006 | 32.824871 | 32.796188 |
| Ca      | 36.504990 | 28.791229 | 31.647760 |
| Ca      | 36.406994 | 29.312691 | 36.737812 |
| Ca      | 40.089897 | 26.395058 | 33.941990 |
| Ca      | 40.327271 | 30.925297 | 33.796444 |
| Ca      | 43.732899 | 27.937040 | 31.441811 |
| Ca      | 44.975311 | 27.235077 | 38.488533 |

24 generated by VMD

| Element | Value 1  | Value 2  | Value 3  |
|---------|---------|---------|---------|
| Ca      | 25.137589 | 30.368919 | 31.824396 |
| Ca      | 26.277412 | 31.297222 | 35.706852 |
| Ca      | 29.985273 | 28.158279 | 36.034885 |
| Ca      | 30.290779 | 32.768368 | 33.434578 |
| Ca      | 33.517681 | 29.446428 | 31.382210 |
| Ca      | 33.114307 | 30.306358 | 35.477093 |
| Ca      | 36.616096 | 26.535183 | 34.461128 |
| Ca      | 36.727249 | 31.020880 | 34.018829 |
| Ca      | 40.397263 | 28.634371 | 30.972937 |
| Ca      | 39.679825 | 29.057615 | 36.175629 |
| Ca      | 46.058689 | 30.380554 | 33.261417 |
| Ca      | 42.748341 | 28.972939 | 34.198063 |
| S       | 26.784637 | 27.934563 | 36.337311 |
| S       | 27.018780 | 34.243889 | 34.330444 |
| S       | 30.608135 | 29.664267 | 32.886986 |
| S       | 29.790052 | 31.277515 | 36.469837 |
| S       | 33.188530 | 27.260002 | 34.530659 |
| S       | 33.773918 | 32.523346 | 32.624275 |
| S       | 36.654713 | 28.615276 | 31.745056 |
| S       | 36.454781 | 29.251772 | 36.785778 |
| S       | 40.085094 | 26.478638 | 33.675335 |
| S       | 40.411884 | 30.929337 | 33.683186 |
| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| S       | 44.006367 | 28.188940 | 31.493752 |
| S       | 45.106514 | 27.076717 | 38.520061 |

24 generated by VMD

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 25.048824 | 29.933613 | 31.937426 |
| Ca      | 26.172977 | 31.450966 | 35.499275 |
| Ca      | 29.971437 | 28.354099 | 35.751087 |
| Ca      | 30.261337 | 32.798656 | 33.295494 |
| Ca      | 33.522064 | 31.450966 | 35.499275 |
| Ca      | 33.002064 | 30.167244 | 35.674114 |
| Ca      | 36.567223 | 26.482906 | 34.339054 |
| Ca      | 36.720989 | 30.836853 | 34.206528 |
| Ca      | 40.369087 | 28.875111 | 31.015314 |
| Ca      | 39.885803 | 28.745392 | 36.468834 |
| Ca      | 45.890179 | 30.646435 | 32.743530 |
| Ca      | 42.741444 | 28.946169 | 34.280590 |
| S       | 26.941399 | 28.094225 | 36.637314 |
| S       | 27.155333 | 34.315723 | 34.067928 |
| S       | 30.451714 | 29.677486 | 32.677891 |
| S       | 29.794384 | 31.484308 | 36.296658 |
| S       | 33.053921 | 27.357971 | 34.336327 |
| S       | 33.699142 | 32.548985 | 32.885906 |
| S       | 36.949570 | 28.709148 | 31.775936 |
| S       | 36.488281 | 28.950890 | 36.802227 |
| S       | 40.186321 | 26.474998 | 33.904018 |
| S       | 40.262257 | 30.867458 | 34.028198 |
| S       | 43.883926 | 27.942905 | 31.249249 |
| S       | 46.411510 | 27.265696 | 38.575024 |

24 generated by VMD

| Element | X   | Y   | Z   |
|---------|-----|-----|-----|
| Ca      | 25.144440 | 30.367477 | 31.920504 |
| Ca      | 26.307537 | 31.450146 | 35.584534 |
| Ca      | 30.197186 | 28.372463 | 36.081081 |
| Ca      | 30.288439 | 32.910683 | 33.285770 |
| Ca      | 33.485462 | 29.205103 | 31.267387 |
| Ca      | 33.123714 | 30.530310 | 35.433098 |
| Ca      | 36.845440 | 26.292427 | 34.452713 |
| Ca      | 36.378305 | 30.540419 | 33.827877 |
| Ca      | 40.163994 | 28.877796 | 31.395733 |
| Ca      | 39.711086 | 28.782139 | 36.449242 |
| Ca      | 46.070312 | 30.586897 | 32.951752 |
| Ca      | 42.696140 | 29.185774 | 34.219200 |
| S       | 27.053797 | 27.899979 | 36.247711 |
| S       | 27.281916 | 34.338734 | 34.225784 |
| S       | 30.625952 | 29.660727 | 32.911732 |
| S       | 29.761911 | 31.643211 | 36.403976 |
S    33.368893  27.327660  34.538219
S    33.651085  32.461678  32.731274
S    36.649860  28.358004  31.506878
S    36.556480  28.733244  36.887482
S    40.295879  26.440876  33.792992
S    40.048111  31.042734  34.002426
S    43.648407  28.270941  31.375717
S    45.082802  27.198311  38.537670

24

generated by VMD

Ca   24.779884  30.296860  32.511909
Ca   26.371681  31.179575  35.858925
Ca   30.235165  28.142363  35.882843
Ca   30.334127  33.013092  33.256744
Ca   33.502266  29.315748  30.910877
Ca   33.109749  30.384441  35.277802
Ca   36.861214  26.444218  33.891876
Ca   36.612305  30.799007  33.683296
Ca   40.263889  29.027779  31.359856
Ca   39.463879  28.854883  36.208553
Ca   46.242721  30.362196  33.775200
Ca   42.686722  28.813980  34.478546
S    27.114161  27.890440  36.804573
S    27.266560  34.88984  34.685429
S    30.625238  29.806568  32.756752
S    29.850721  31.387297  36.376965
S    33.315979  27.454762  34.084824
S    33.807079  32.521492  32.479435
S    36.669559  28.771877  31.311523
S    36.446228  28.932447  36.401440
S    40.216805  26.460297  33.721912
S    40.181133  31.050119  33.950806
S    43.940582  28.034885  31.735321
S    44.536716  27.227554  38.625294

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Ca   25.150320  30.324133  32.098595
Ca   26.442408  31.196060  35.681232
Ca   30.238796  28.169952  35.777012
Ca   30.340361  32.912781  33.252491
Ca   33.621983  29.375235  31.145203
Ca   33.210583  30.595739  35.740654
Ca   36.709518  26.355553  34.415012
Ca   36.454624  30.428368  33.721024
Ca   40.076588  28.897497  30.918863
Ca   39.459381  28.998081  36.504368
| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| Ca      | 46.039188 | 30.405399 | 33.340160 |
| Ca      | 42.627090 | 29.195709 | 34.450417 |
| S       | 27.165804 | 27.870956 | 36.723213 |
| S       | 27.432301 | 34.312737 | 34.394020 |
| S       | 30.714911 | 29.733507 | 32.671005 |
| S       | 29.953104 | 31.492548 | 36.455074 |
| S       | 33.396294 | 27.454651 | 34.278671 |
| S       | 33.900146 | 32.390106 | 32.562637 |
| S       | 36.563225 | 28.426773 | 31.326778 |
| S       | 36.341473 | 28.877205 | 36.691284 |
| S       | 40.078972 | 26.715149 | 33.863346 |
| S       | 39.951389 | 30.932877 | 33.996254 |
| S       | 43.669308 | 28.296671 | 31.561012 |
| S       | 44.896244 | 27.033760 | 38.462418 |

24 generated by VMD

| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| Ca      | 25.112688 | 29.916210 | 32.002628 |
| Ca      | 26.251335 | 31.104721 | 35.518688 |
| Ca      | 30.025585 | 28.432575 | 35.841301 |
| Ca      | 30.400984 | 32.864441 | 33.164024 |
| Ca      | 33.486950 | 29.079487 | 31.208904 |
| Ca      | 33.186733 | 30.585991 | 35.559544 |
| Ca      | 36.602783 | 26.552801 | 34.315109 |
| Ca      | 36.694244 | 31.013714 | 34.146271 |
| Ca      | 40.233658 | 29.185093 | 31.356785 |
| Ca      | 39.449226 | 28.687679 | 36.445118 |
| Ca      | 46.085823 | 30.334658 | 33.132790 |
| Ca      | 42.683758 | 28.848785 | 34.400970 |
| S       | 27.121378 | 27.970470 | 36.876038 |
| S       | 27.188555 | 34.059658 | 33.983555 |
| S       | 30.433363 | 29.794582 | 32.789028 |
| S       | 29.779037 | 31.677750 | 36.324997 |
| S       | 33.242409 | 27.500942 | 34.316250 |
| S       | 33.898190 | 32.405506 | 32.666458 |
| S       | 36.790340 | 29.001080 | 31.665474 |
| S       | 36.491035 | 28.936501 | 36.837563 |
| S       | 39.941784 | 26.424007 | 33.780273 |
| S       | 40.165607 | 30.860847 | 34.306602 |
| S       | 43.677925 | 28.263710 | 31.456362 |
| S       | 45.490620 | 26.890228 | 37.935986 |

24 generated by VMD

| Element | X     | Y     | Z     |
|---------|-------|-------|-------|
| Ca      | 25.200573 | 30.559149 | 31.967817 |
| Ca      | 26.151524 | 31.353714 | 35.853973 |
| Ca      | 30.135159 | 28.293610 | 35.816795 |
| Ca      | 30.177147 | 32.713322 | 33.264019 |
|    |     |     |     |
|----|-----|-----|-----|
| Ca | 33.501202 | 28.869030 | 31.202431 |
| Ca | 33.169262 | 30.292765 | 35.468391 |
| Ca | 36.496197 | 26.382370 | 34.397175 |
| Ca | 36.554749 | 30.796539 | 33.903706 |
| Ca | 40.169643 | 29.134201 | 31.488110 |
| Ca | 39.811886 | 28.793476 | 36.448071 |
| Ca | 46.185047 | 30.454929 | 33.049149 |
| Ca | 42.793022 | 29.031418 | 34.394669 |
| S  | 27.009195 | 28.068390 | 36.598763 |
| S  | 27.255571 | 34.359676 | 32.212837 |
| S  | 30.413857 | 29.687689 | 32.763264 |
| S  | 29.823416 | 31.454975 | 36.423172 |
| S  | 33.304234 | 27.321308 | 34.196770 |
| S  | 33.727573 | 32.180660 | 32.594391 |
| S  | 36.589565 | 28.387793 | 31.560215 |
| S  | 36.453701 | 29.126991 | 36.730045 |
| S  | 40.012653 | 26.641045 | 33.694260 |
| S  | 40.310020 | 31.185017 | 34.169418 |
| S  | 43.847904 | 28.192219 | 31.567707 |
| S  | 45.340813 | 27.111120 | 38.265610 |

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|    |     |     |     |
|----|-----|-----|-----|
| Ca | 24.976454 | 30.443432 | 32.006737 |
| Ca | 26.144728 | 31.195068 | 35.579426 |
| Ca | 30.177166 | 28.147463 | 35.788383 |
| Ca | 30.247160 | 32.911335 | 33.366932 |
| Ca | 33.591438 | 29.201773 | 31.484821 |
| Ca | 33.073021 | 30.350491 | 35.332451 |
| Ca | 36.527328 | 26.530750 | 34.355217 |
| Ca | 36.654316 | 30.740969 | 34.197693 |
| Ca | 40.075531 | 29.003143 | 31.123741 |
| Ca | 39.769711 | 28.633062 | 36.312000 |
| Ca | 46.166393 | 30.022507 | 33.265007 |
| Ca | 42.787663 | 29.035620 | 34.197144 |
| S  | 27.119345 | 28.044155 | 36.438446 |
| S  | 27.091152 | 34.345573 | 34.354450 |
| S  | 30.446173 | 29.621159 | 32.707371 |
| S  | 29.710316 | 31.473347 | 36.279018 |
| S  | 33.235844 | 27.292381 | 34.439369 |
| S  | 33.831532 | 32.462570 | 32.670952 |
| S  | 36.747471 | 28.621286 | 31.895052 |
| S  | 36.493984 | 28.984674 | 36.786808 |
| S  | 40.102428 | 26.476139 | 33.755966 |
| S  | 40.362747 | 30.989792 | 33.835503 |
| S  | 43.692745 | 28.199234 | 31.271553 |
| S  | 45.409264 | 27.665493 | 38.586693 |
| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 25.163975     | 30.173111     | 32.011070     |
| Ca      | 26.399864     | 31.365364     | 35.579609     |
| Ca      | 30.008972     | 28.001841     | 35.765675     |
| Ca      | 30.232992     | 32.888443     | 33.344200     |
| Ca      | 33.440628     | 29.174793     | 31.436977     |
| Ca      | 33.080929     | 30.226629     | 35.341675     |
| Ca      | 36.743408     | 26.421024     | 34.44576      |
| Ca      | 36.503056     | 30.831751     | 34.244854     |
| Ca      | 40.264984     | 29.049355     | 31.104586     |
| Ca      | 39.689205     | 28.666555     | 36.584763     |
| Ca      | 46.364910     | 29.665850     | 33.238892     |
| Ca      | 42.824654     | 29.113276     | 34.059345     |
| S       | 26.917877     | 28.046236     | 36.628761     |
| S       | 27.048079     | 34.391468     | 34.012043     |
| S       | 30.526003     | 29.841379     | 32.910488     |
| S       | 29.931078     | 31.528240     | 36.368893     |
| S       | 33.316460     | 27.274101     | 34.208267     |
| S       | 33.642315     | 32.549622     | 32.706524     |
| S       | 35.677711     | 28.807308     | 31.776981     |
| S       | 36.368946     | 28.924559     | 36.796242     |
| S       | 40.163174     | 26.748655     | 33.849575     |
| S       | 40.117912     | 30.967772     | 34.064140     |
| S       | 43.750111     | 28.235870     | 31.161476     |
| S       | 45.256554     | 27.498158     | 38.391029     |

24 generated by VMD

| Element | X-coordinates | Y-coordinates | Z-coordinates |
|---------|---------------|---------------|---------------|
| Ca      | 25.389944     | 30.072618     | 32.208916     |
| Ca      | 26.396383     | 31.322582     | 35.765446     |
| Ca      | 30.145929     | 28.198090     | 35.692383     |
| Ca      | 30.068707     | 32.899811     | 33.366749     |
| Ca      | 33.492710     | 29.186743     | 31.276424     |
| Ca      | 33.168896     | 30.135807     | 35.370716     |
| Ca      | 36.520649     | 26.417393     | 34.065777     |
| Ca      | 36.658165     | 31.108597     | 34.009911     |
| Ca      | 40.175961     | 29.153095     | 31.302681     |
| Ca      | 39.653339     | 28.688335     | 36.395130     |
| Ca      | 46.174847     | 29.974361     | 33.036057     |
| Ca      | 42.730476     | 28.923708     | 34.341080     |
| S       | 27.119877     | 28.025364     | 36.751842     |
| S       | 27.040695     | 34.352715     | 34.252491     |
| S       | 30.443079     | 29.799517     | 32.697632     |
| S       | 30.083445     | 31.393944     | 36.436485     |
| S       | 33.279072     | 27.371683     | 34.068954     |
| S       | 33.758827     | 32.396381     | 32.656498     |
|   |   |   |   |
|---|---|---|---|
| S | 36.795628 | 28.831804 | 31.687355 |
| S | 36.382633 | 28.984669 | 36.685257 |
| S | 39.936607 | 26.638405 | 33.718021 |
| S | 40.445560 | 30.978294 | 34.102352 |
| S | 43.676231 | 27.931000 | 31.364010 |
| S | 44.896233 | 27.606472 | 38.778645 |

24 generated by VMD

| Ca | 25.350334 | 30.195417 | 32.023743 |
| Ca | 26.277895 | 31.290588 | 35.792225 |
| Ca | 30.052120 | 28.111691 | 35.711674 |
| Ca | 30.396023 | 33.087387 | 33.378067 |
| Ca | 33.618710 | 29.134691 | 31.220671 |
| Ca | 33.073608 | 30.498417 | 35.449547 |
| Ca | 36.648884 | 26.416994 | 34.622513 |
| Ca | 36.708412 | 30.639380 | 34.155216 |
| Ca | 40.145317 | 29.025829 | 31.209618 |
| Ca | 39.724072 | 28.876375 | 36.173393 |
| Ca | 46.298447 | 30.096262 | 33.312107 |
| Ca | 42.711899 | 29.096066 | 34.314236 |
| S | 26.873531 | 27.917257 | 36.576721 |
| S | 27.020817 | 34.280544 | 34.321438 |
| S | 30.601730 | 29.890915 | 32.704727 |
| S | 29.765192 | 31.406841 | 36.475533 |
| S | 33.203369 | 27.393427 | 34.121006 |
| S | 33.816086 | 32.431820 | 32.505249 |
| S | 36.648918 | 28.417889 | 31.794590 |
| S | 36.334488 | 29.010681 | 36.877571 |
| S | 40.086548 | 26.620378 | 33.730015 |
| S | 40.267395 | 31.024179 | 33.952446 |
| S | 43.655533 | 28.240498 | 31.183346 |
| S | 45.154583 | 27.287872 | 38.425049 |

24 generated by VMD

| Ca | 25.594589 | 30.150261 | 31.771755 |
| Ca | 26.211632 | 31.340015 | 35.685791 |
| Ca | 30.191420 | 28.263065 | 35.886055 |
| Ca | 30.388847 | 32.961586 | 33.268372 |
| Ca | 33.396835 | 29.168877 | 31.354584 |
| Ca | 32.919044 | 30.572281 | 35.589371 |
| Ca | 36.634193 | 26.265154 | 34.356327 |
| Ca | 36.490528 | 30.488678 | 34.248940 |
| Ca | 40.106449 | 28.948668 | 31.051029 |
| Ca | 39.642910 | 28.880638 | 36.370396 |
| Ca | 46.324360 | 29.977663 | 32.979042 |
| Ca | 42.636318 | 29.047161 | 34.339867 |
|    | x      | y      | z      |
|----|--------|--------|--------|
| S  | 26.998220 | 28.176910 | 36.684761 |
| S  | 27.064587 | 34.256882 | 34.082928 |
| S  | 30.463108 | 29.736607 | 32.855457 |
| S  | 29.689802 | 31.527010 | 36.495598 |
| S  | 33.390831 | 27.578188 | 34.367863 |
| S  | 33.977833 | 32.341984 | 32.688892 |
| S  | 36.597748 | 28.640213 | 31.624304 |
| S  | 36.345272 | 28.579773 | 36.843838 |
| S  | 40.190723 | 26.450108 | 33.44427 |
| S  | 40.224247 | 31.163055 | 34.206821 |
| S  | 43.627159 | 28.101639 | 31.287575 |
| S  | 45.327267 | 27.774967 | 38.546688 |
|    | S      |        |        |

24 generated by VMD

|    | x      | y      | z      |
|----|--------|--------|--------|
| Ca | 25.275671 | 30.048388 | 31.835527 |
| Ca | 26.363644 | 31.270660 | 35.966789 |
| Ca | 30.008636 | 28.297716 | 35.974354 |
| Ca | 30.225641 | 32.949085 | 33.296455 |
| Ca | 33.452400 | 29.036282 | 31.252647 |
| Ca | 33.048161 | 30.581203 | 35.440823 |
| Ca | 36.502583 | 26.562534 | 34.395130 |
| Ca | 36.428425 | 30.820780 | 33.748379 |
| Ca | 40.307926 | 28.937408 | 30.945099 |
| Ca | 39.602764 | 28.618057 | 36.476387 |
| Ca | 46.148148 | 30.164000 | 33.198467 |
| Ca | 42.841965 | 29.111774 | 34.718372 |
| S  | 26.908974 | 27.881016 | 36.508244 |
| S  | 27.184694 | 34.270931 | 34.399494 |
| S  | 30.617914 | 29.857368 | 32.755089 |
| S  | 29.868799 | 31.554436 | 36.438435 |
| S  | 33.234715 | 27.541786 | 34.356365 |
| S  | 33.785290 | 32.370743 | 32.433586 |
| S  | 36.594746 | 28.686075 | 31.520761 |
| S  | 36.507511 | 28.931911 | 36.717251 |
| S  | 40.031727 | 26.611084 | 33.545780 |
| S  | 40.158455 | 30.855095 | 34.189522 |
| S  | 43.736641 | 28.262341 | 31.634262 |
| S  | 45.598461 | 27.170681 | 38.283470 |

24 generated by VMD

|    | x      | y      | z      |
|----|--------|--------|--------|
| Ca | 25.129353 | 29.892866 | 31.802876 |
| Ca | 26.354345 | 31.253958 | 35.496391 |
| Ca | 30.234753 | 28.205997 | 36.097916 |
| Ca | 30.148329 | 32.945164 | 33.361725 |
| Ca | 33.362183 | 29.299911 | 31.450544 |
| Ca | 32.966709 | 30.514084 | 35.633102 |
| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 36.570518  | 26.624863  | 34.483139  |
| Ca      | 36.662865  | 26.987635  | 34.338257  |
| Ca      | 40.350018  | 29.152618  | 31.015007  |
| Ca      | 39.778358  | 28.056923  | 34.090290  |
| Ca      | 46.612335  | 29.251448  | 33.166439  |
| Ca      | 42.845997  | 29.059692  | 34.079559  |
| Ca      | 29.152618  | 29.007879  | 35.360344  |
| Ca      | 26.883444  | 27.727621  | 36.141548  |
| Ca      | 26.900965  | 34.264694  | 33.930061  |
| Ca      | 30.436426  | 29.738422  | 33.107769  |
| Ca      | 39.708963  | 31.653908  | 36.549355  |
| Ca      | 33.211445  | 27.314228  | 34.631660  |
| Ca      | 33.640926  | 32.575760  | 32.882095  |
| Ca      | 36.581982  | 28.774330  | 31.789758  |
| Ca      | 36.639214  | 29.103884  | 36.825184  |
| Ca      | 40.102638  | 26.655577  | 33.559990  |
| Ca      | 40.280396  | 31.040199  | 33.928265  |
| Ca      | 43.950214  | 28.169716  | 31.160421  |
| Ca      | 45.081528  | 27.104160  | 38.509300  |

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generated by VMD

| Element | X Position | Y Position | Z Position |
|---------|------------|------------|------------|
| Ca      | 25.526604  | 29.966896  | 31.678074  |
| Ca      | 26.331461  | 31.007879  | 35.360344  |
| Ca      | 30.058531  | 28.283314  | 36.181290  |
| Ca      | 30.233328  | 32.970070  | 33.213911  |
| Ca      | 33.523911  | 29.353832  | 31.219654  |
| Ca      | 33.114201  | 30.415462  | 35.741169  |
| Ca      | 36.394524  | 26.815134  | 34.551662  |
| Ca      | 36.551910  | 30.805193  | 33.947163  |
| Ca      | 40.103870  | 29.202587  | 31.319336  |
| Ca      | 39.659676  | 28.988260  | 36.073376  |
| Ca      | 46.450962  | 29.326630  | 33.354862  |
| Ca      | 42.732754  | 28.850744  | 34.013165  |
| Ca      | 26.925648  | 27.737900  | 36.345383  |
| Ca      | 26.996273  | 34.185760  | 34.424408  |
| Ca      | 30.624372  | 29.784372  | 33.110600  |
| Ca      | 29.743835  | 31.563560  | 36.465935  |
| Ca      | 33.213100  | 27.401958  | 34.337021  |
| Ca      | 33.663727  | 32.408569  | 32.676010  |
| Ca      | 36.637070  | 28.751068  | 31.525120  |
| Ca      | 36.567314  | 29.290508  | 36.892010  |
| Ca      | 39.841480  | 26.855165  | 33.656677  |
| Ca      | 40.441120  | 31.237572  | 33.881260  |
| Ca      | 43.670120  | 28.059189  | 31.185005  |
| Ca      | 45.428143  | 27.129753  | 38.639481  |

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generated by VMD
| Ca   | 25.447247 | 30.195759 | 31.687033 |
|-----|-----------|-----------|-----------|
| Ca   | 26.246826 | 31.338074 | 35.642906 |
| Ca   | 30.165468 | 28.212547 | 36.131966 |
| Ca   | 30.390413 | 32.950264 | 33.532410 |
| Ca   | 33.298843 | 29.168638 | 31.144722 |
| Ca   | 33.052536 | 30.342144 | 35.565088 |
| Ca   | 36.542709 | 26.576591 | 34.382450 |
| Ca   | 36.597664 | 30.738520 | 33.875847 |
| Ca   | 40.045490 | 29.112673 | 31.182159 |
| Ca   | 39.725140 | 28.879639 | 36.249104 |
| Ca   | 46.763554 | 29.144489 | 33.433685 |
| Ca   | 42.685551 | 29.104668 | 34.155861 |
| S    | 26.855232 | 27.880102 | 36.176159 |
| S    | 27.046808 | 34.369724 | 34.450748 |
| S    | 30.464294 | 29.730856 | 32.972153 |
| S    | 29.808540 | 31.366753 | 36.576321 |
| S    | 33.068901 | 27.205570 | 34.342976 |
| S    | 33.680084 | 32.351940 | 32.671986 |
| S    | 36.521420 | 28.715015 | 31.549658 |
| S    | 36.456779 | 29.159822 | 36.662319 |
| S    | 39.917633 | 26.808685 | 33.734653 |
| S    | 40.246002 | 31.153517 | 33.895348 |
| S    | 43.585033 | 28.235958 | 31.271923 |
| S    | 45.821693 | 27.649487 | 38.743256 |
| Ca   | 25.437819 | 30.037992 | 31.737949 |
| Ca   | 26.353251 | 31.182417 | 35.615791 |
| Ca   | 29.978895 | 28.108391 | 35.877407 |
| Ca   | 30.114883 | 33.137173 | 33.633118 |
| Ca   | 33.398071 | 29.965550 | 31.394024 |
| Ca   | 33.006901 | 30.302795 | 35.578850 |
| Ca   | 36.613087 | 26.726994 | 34.394325 |
| Ca   | 36.050777 | 30.886154 | 34.073147 |
| Ca   | 40.177822 | 28.857624 | 31.297979 |
| Ca   | 39.696918 | 28.973225 | 36.284786 |
| Ca   | 46.398121 | 29.386463 | 32.830421 |
| Ca   | 42.877022 | 29.086628 | 34.246864 |
| S    | 26.868580 | 27.834705 | 36.301842 |
| S    | 26.782133 | 34.310932 | 34.248745 |
| S    | 30.443672 | 30.033102 | 32.927994 |
| S    | 29.843048 | 31.504311 | 36.478012 |
| S    | 33.323788 | 27.308081 | 34.254597 |
| S    | 33.809208 | 32.307468 | 32.802841 |
| S    | 36.695824 | 28.879477 | 31.645729 |
| S    | 36.329731 | 29.156239 | 36.716469 |
S  40.097424  26.740845  33.837345
S  40.470016  31.087898  33.805511
S  43.518631  27.922819  31.090782
S  45.540428  27.523087  38.956207

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generated by VMD
Ca  25.680443  30.050295  31.799377
Ca  26.204702  31.361401  35.766872
Ca  29.981033  28.082973  35.954720
Ca  30.301441  33.124733  33.339020
Ca  33.697559  29.103331  31.335186
Ca  33.074444  30.226797  35.640335
Ca  36.383125  26.638758  34.463974
Ca  36.746151  30.874214  34.066063
Ca  40.141483  29.284809  31.281990
Ca  39.622971  28.824539  36.105118
Ca  46.361813  29.582878  33.022919
Ca  42.779701  29.102020  34.105782
S  26.994116  27.855728  36.579266
S  26.871834  34.404831  34.083755
S  30.597939  29.846123  32.866817
S  29.790091  31.480690  36.466412
S  33.165657  27.126541  34.234234
S  33.671207  32.348175  32.808189
S  36.774811  28.784531  31.790165
S  36.409870  28.970329  36.830231
S  39.961666  26.762268  33.680870
S  40.327652  31.144146  33.917904
S  43.634731  28.054701  31.074167
S  45.259491  27.356609  38.817337

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generated by VMD
Ca  25.426750  30.059328  31.881271
Ca  26.136236  31.362467  35.897243
Ca  29.928520  28.394680  35.788448
Ca  30.244797  33.016495  33.508305
Ca  33.445148  29.209663  31.329584
Ca  33.078754  30.245987  35.547394
Ca  36.552406  26.663702  34.465687
Ca  36.671722  31.235409  34.130959
Ca  40.268124  29.159716  31.169823
Ca  39.783371  28.390839  36.078781
Ca  46.233143  28.898073  34.124943
S  26.700607  27.762932  36.10167
S  26.897757  34.087540  34.071465
|   | S     | Ca    |
|---|-------|-------|
| 1  | 30.382612 | 25.572876 |
| 2  | 29.821962 | 25.915495 |
| 3  | 33.095844 | 29.899777 |
| 4  | 33.646149 | 30.175814 |
| 5  | 36.710403 | 33.544441 |
| 6  | 36.435688 | 33.245544 |
| 7  | 39.877636 | 36.533424 |
| 8  | 40.512318 | 40.058014 |
| 9  | 43.597679 | 42.664745 |
| 10 | 46.270363 | 42.640303 |

24

generated by VMD

|   | S     | Ca    |
|---|-------|-------|
| 11 | 26.743092 | 25.357241 |
| 12 | 26.852024 | 25.382589 |
| 13 | 30.530556 | 29.746719 |
| 14 | 29.637211 | 30.287792 |
| 15 | 33.231392 | 33.64482 |
| 16 | 33.682941 | 33.068207 |
| 17 | 36.488094 | 36.723385 |
| 18 | 40.202770 | 36.495945 |
| 19 | 40.368301 | 30.382589 |
| 20 | 43.538525 | 29.747619 |
| 21 | 46.222122 | 30.530556 |

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generated by VMD
|   |          |          |          |
|---|----------|----------|----------|
| Ca| 40.021248| 29.219999| 31.154869|
| Ca| 39.706318| 29.070986| 36.317516|
| Ca| 46.368618| 29.026773| 33.526562|
| Ca| 42.669601| 28.971127| 34.175858|
| S | 26.550320| 27.866764| 36.278725|
| S | 27.035986| 34.226688| 34.422523|
| S | 30.568300| 29.737392| 32.868675|
| S | 29.788036| 31.367733| 36.504219|
| S | 33.317150| 27.323250| 34.242531|
| S | 33.540302| 32.422680| 32.735237|
| S | 36.750835| 28.664558| 31.683331|
| S | 36.481953| 29.172197| 36.759811|
| S | 40.037453| 26.730911| 33.498520|
| S | 40.277592| 31.257999| 33.915394|
| S | 43.664131| 28.158512| 31.110023|
| S | 45.949615| 27.532328| 38.817390|

24

generated by VMD

|   |          |          |          |
|---|----------|----------|----------|
| Ca| 25.458225| 30.153719| 31.769112|
| Ca| 26.381205| 31.440840| 35.630127|
| Ca| 30.087555| 28.205635| 36.297375|
| Ca| 30.089081| 32.963661| 33.337273|
| Ca| 33.469265| 28.944471| 31.545382|
| Ca| 33.050846| 30.097275| 35.687431|
| Ca| 36.304188| 26.509960| 34.162647|
| Ca| 36.543915| 31.013433| 33.978630|
| Ca| 40.177071| 29.327023| 30.979485|
| Ca| 39.756157| 28.966516| 36.156685|
| Ca| 46.508198| 29.233713| 33.360088|
| Ca| 42.689175| 29.041986| 34.208961|
| S | 26.776442| 27.926491| 36.296692|
| S | 26.706709| 34.364323| 34.222221|
| S | 30.625839| 29.816875| 33.044704|
| S | 29.845516| 31.623056| 36.514301|
| S | 33.161152| 27.131481| 34.384861|
| S | 33.703922| 32.335258| 32.637913|
| S | 36.817532| 28.745575| 31.693699|
| S | 36.450241| 28.977209| 36.566341|
| S | 39.938244| 26.767113| 33.540146|
| S | 40.229889| 31.095802| 33.918411|
| S | 43.782444| 28.309044| 31.122793|
| S | 45.881165| 27.400969| 38.975403|

24

generated by VMD

|   |          |          |          |
|---|----------|----------|----------|
| Ca| 25.238106| 30.239967| 31.705574|
| Ca| 26.111998| 31.196638| 35.784161|
|   |   |   |
|---|---|---|
| Ca | 29.771503 | 28.240564 | 36.039787 |
| Ca | 30.400921 | 32.861374 | 33.584248 |
| Ca | 33.479172 | 30.310093 | 35.643406 |
| Ca | 36.535580 | 26.792223 | 34.343025 |
| Ca | 36.77977 | 31.137890 | 33.930862 |
| Ca | 40.345406 | 29.224897 | 31.148123 |
| Ca | 39.798431 | 28.950739 | 36.126598 |
| Ca | 46.674706 | 28.552465 | 33.378338 |
| Ca | 42.791515 | 29.159103 | 34.067345 |
| S  | 26.486191 | 27.733959 | 36.148376 |
| S  | 26.821144 | 34.098888 | 34.183487 |
| S  | 30.435690 | 29.877287 | 32.994030 |
| S  | 29.688169 | 31.350945 | 36.792866 |
| S  | 33.162907 | 27.136295 | 34.371635 |
| S  | 33.807434 | 32.356743 | 32.613762 |
| S  | 36.844334 | 29.012457 | 31.585060 |
| S  | 36.434052 | 29.268681 | 36.668617 |
| S  | 39.960270 | 26.705288 | 33.658268 |
| S  | 40.460854 | 31.336481 | 33.854187 |
| S  | 43.620167 | 28.003141 | 31.163170 |
| S  | 45.662724 | 27.798693 | 38.787575 |

24

generated by VMD

|   |   |   |
|---|---|---|
| Ca | 25.082249 | 30.280365 | 31.666386 |
| Ca | 26.389355 | 31.168074 | 35.611202 |
| Ca | 30.063789 | 28.194996 | 35.936207 |
| Ca | 30.322426 | 33.061836 | 33.466320 |
| Ca | 33.539146 | 29.197582 | 31.486855 |
| Ca | 33.248217 | 30.288502 | 35.509003 |
| Ca | 36.538784 | 26.482513 | 34.606094 |
| Ca | 36.734825 | 31.065557 | 34.233379 |
| Ca | 40.041409 | 29.017122 | 31.134636 |
| Ca | 39.670948 | 29.016319 | 36.207012 |
| Ca | 46.429096 | 29.247438 | 33.197765 |
| Ca | 42.760414 | 29.002907 | 34.117405 |
| S  | 26.658886 | 27.725010 | 35.842171 |
| S  | 26.937248 | 34.143688 | 34.314945 |
| S  | 30.584055 | 29.997471 | 32.985359 |
| S  | 29.842958 | 31.340212 | 36.673714 |
| S  | 33.153503 | 27.339502 | 34.464928 |
| S  | 33.798546 | 32.485279 | 32.548138 |
| S  | 36.646835 | 28.614178 | 31.979259 |
| S  | 36.454781 | 29.151340 | 36.826607 |
| S  | 39.979691 | 26.483080 | 33.633827 |
| S  | 40.249916 | 31.113708 | 33.853203 |
| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| S       | 43.552338| 27.871675| 31.187389|
| S       | 45.749954| 28.103039| 38.548893|

generated by VMD

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| Ca      | 25.277428| 30.110676| 31.865273|
| Ca      | 26.235857| 31.224857| 35.591353|
| Ca      | 30.019154| 28.447660| 35.778137|
| Ca      | 30.359592| 32.885605| 33.738140|
| Ca      | 33.658165| 29.362576| 31.425200|
| Ca      | 33.136551| 30.240208| 35.594707|
| Ca      | 36.439247| 26.505365| 34.381008|
| Ca      | 36.754559| 30.862680| 34.037060|
| Ca      | 40.119843| 28.965342| 31.239538|
| Ca      | 39.833309| 28.912647| 36.328758|
| Ca      | 46.420254| 29.071999| 33.408688|
| Ca      | 42.729694| 29.242870| 34.015884|
| S       | 26.802431| 27.860938| 36.217930|
| S       | 26.818985| 34.138664| 34.144047|
| S       | 30.516529| 29.954231| 32.842964|
| S       | 29.817940| 31.437969| 36.655338|
| S       | 32.960091| 27.190483| 34.409073|
| S       | 33.891357| 32.370323| 32.786522|
| S       | 36.748943| 28.772995| 31.680237|
| S       | 36.529716| 29.024836| 36.685848|
| S       | 40.165359| 26.524481| 33.701481|
| S       | 40.419468| 31.113077| 33.920589|
| S       | 43.574966| 28.038063| 31.079908|
| S       | 45.204498| 28.133503| 38.502468|

generated by VMD

| Element | X        | Y        | Z        |
|---------|----------|----------|----------|
| Ca      | 25.388479| 29.925793| 31.414259|
| Ca      | 26.165733| 31.126631| 35.684872|
| Ca      | 30.036867| 28.259161| 36.112740|
| Ca      | 30.227831| 33.000946| 33.588799|
| Ca      | 33.340004| 29.393261| 31.478384|
| Ca      | 33.065964| 30.373758| 35.605919|
| Ca      | 36.642437| 26.830540| 34.364971|
| Ca      | 36.633255| 31.267572| 33.834023|
| Ca      | 40.086674| 28.994942| 31.093214|
| Ca      | 39.931561| 28.796848| 36.427937|
| Ca      | 46.617638| 28.885134| 33.262482|
| Ca      | 42.616505| 28.700876| 34.125481|
| S       | 26.787853| 27.736403| 36.257584|
| S       | 27.000301| 34.163723| 34.244526|
| S       | 30.394190| 29.881546| 32.933292|
| S       | 29.714731| 31.294716| 36.689472|
| S       | 33.098988 | 27.431040 | 34.368195 |
|---------|-----------|-----------|-----------|
| S       | 33.804451 | 32.419674 | 32.829739 |
| S       | 36.669510 | 28.988396 | 31.555988 |
| S       | 36.695900 | 29.348896 | 36.728916 |
| S       | 40.038010 | 26.475494 | 33.660515 |
| S       | 40.398834 | 30.984972 | 34.051785 |
| S       | 43.774410 | 28.032915 | 31.130392 |
| S       | 45.303787 | 28.078613 | 38.587238 |

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generated by VMD

| Ca      | 25.651442 | 30.032288 | 31.484772 |
|---------|-----------|-----------|-----------|
| Ca      | 26.191338 | 31.179266 | 35.699562 |
| Ca      | 29.919018 | 28.179575 | 35.963211 |
| Ca      | 30.102333 | 32.994434 | 33.587555 |
| Ca      | 33.649609 | 29.435041 | 31.632656 |
| Ca      | 33.077648 | 30.484360 | 35.813782 |
| Ca      | 36.483425 | 26.581114 | 34.604553 |
| Ca      | 36.693737 | 30.803560 | 34.070892 |
| Ca      | 40.039471 | 29.055563 | 30.802505 |
| Ca      | 40.020580 | 28.866356 | 36.262451 |
| Ca      | 46.533031 | 28.984983 | 33.323444 |
| Ca      | 42.820709 | 28.762093 | 34.015034 |
| S       | 26.528267 | 27.827801 | 36.163013 |
| S       | 26.803551 | 34.211655 | 34.016087 |
| S       | 30.471701 | 29.917561 | 32.986992 |
| S       | 29.718960 | 31.286800 | 36.697937 |
| S       | 33.189865 | 27.378696 | 34.282143 |
| S       | 33.720482 | 32.717621 | 33.025616 |
| S       | 36.703857 | 28.735643 | 31.748062 |
| S       | 36.504410 | 29.029600 | 36.805847 |
| S       | 39.976765 | 26.622759 | 33.574585 |
| S       | 40.562870 | 30.943970 | 33.735229 |
| S       | 43.560066 | 27.934145 | 31.094486 |
| S       | 45.510799 | 28.426514 | 38.640278 |

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generated by VMD

| Ca      | 25.230787 | 30.461432 | 31.571566 |
|---------|-----------|-----------|-----------|
| Ca      | 26.216293 | 31.144125 | 35.644077 |
| Ca      | 30.189146 | 28.212898 | 36.035378 |
| Ca      | 30.326923 | 33.114571 | 33.601166 |
| Ca      | 33.369530 | 29.367977 | 31.522963 |
| Ca      | 33.264484 | 30.253019 | 35.588417 |
| Ca      | 36.683296 | 26.424984 | 34.351925 |
| Ca      | 36.672226 | 30.717463 | 33.882732 |
| Ca      | 40.038181 | 28.920486 | 31.260874 |
| Ca      | 39.633480 | 28.886753 | 36.223927 |
|   |   |   |
|---|---|---|
| Ca | 46.508896 | 29.181376 | 33.381203 |
| Ca | 42.789062 | 28.955193 | 34.060539 |
| S  | 26.758104 | 27.694372 | 36.025528 |
| S  | 26.992422 | 34.348904 | 34.192318 |
| S  | 30.529140 | 29.903444 | 33.137344 |
| S  | 29.765388 | 31.352016 | 36.652290 |
| S  | 33.146603 | 27.287941 | 34.531601 |
| S  | 33.815800 | 32.516701 | 32.951546 |
| S  | 36.523670 | 28.567417 | 31.543951 |
| S  | 36.466656 | 29.026808 | 36.577808 |
| S  | 40.187065 | 26.549654 | 33.522301 |
| S  | 40.297348 | 30.891167 | 33.868607 |
| S  | 43.697056 | 28.005739 | 31.115973 |
| S  | 45.332249 | 28.606983 | 38.786629 |

24 generated by VMD

| Ca | 25.344000 | 30.176895 | 31.657024 |
| Ca | 26.345434 | 31.097607 | 35.597816 |
| Ca | 30.181078 | 28.262928 | 35.881859 |
| Ca | 30.290325 | 33.227844 | 33.462181 |
| Ca | 33.728947 | 29.533459 | 31.601398 |
| Ca | 33.175652 | 30.276821 | 35.557690 |
| Ca | 36.548107 | 26.396820 | 34.584305 |
| Ca | 36.690224 | 30.833267 | 34.138638 |
| Ca | 39.988041 | 28.742109 | 31.168091 |
| Ca | 39.824245 | 28.922802 | 36.328255 |
| Ca | 46.286499 | 29.450027 | 33.126526 |
| Ca | 42.697918 | 29.075239 | 34.247326 |
| S  | 26.871355 | 27.704969 | 36.145199 |
| S  | 26.841785 | 34.179012 | 34.231552 |
| S  | 30.628204 | 30.073624 | 32.814709 |
| S  | 29.781097 | 31.341379 | 36.555820 |
| S  | 33.117905 | 27.433216 | 34.318329 |
| S  | 33.755192 | 32.734364 | 32.803783 |
| S  | 36.573700 | 28.474155 | 31.799633 |
| S  | 36.551491 | 28.973557 | 36.847328 |
| S  | 39.960487 | 26.536854 | 33.821072 |
| S  | 40.140560 | 30.769146 | 33.736164 |
| S  | 43.501003 | 27.978792 | 31.111645 |
| S  | 45.610649 | 28.196531 | 38.494362 |

24 generated by VMD

| Ca | 25.071573 | 30.333105 | 31.660244 |
| Ca | 26.393208 | 31.411594 | 35.768391 |
| Ca | 30.147854 | 27.936928 | 35.708057 |
| Ca | 30.011314 | 33.180439 | 33.805508 |
|   |   |   |
|---|---|---|
| Ca | 33.651978 | 29.295448 | 31.206047 |
| Ca | 33.195694 | 30.299145 | 35.602142 |
| Ca | 36.537624 | 26.208879 | 34.464897 |
| Ca | 36.607605 | 30.798512 | 33.927269 |
| Ca | 40.047729 | 28.749018 | 31.218830 |
| Ca | 39.869507 | 28.854959 | 36.429565 |
| Ca | 46.554832 | 29.452026 | 33.215027 |
| Ca | 42.669708 | 28.999533 | 34.111652 |
| S  | 26.810982 | 27.847485 | 36.125191 |
| S  | 26.707451 | 34.476025 | 34.242928 |
| S  | 30.640112 | 30.168549 | 33.004593 |
| S  | 29.693689 | 31.277731 | 36.514008 |
| S  | 33.273769 | 27.467951 | 34.176933 |
| S  | 33.855614 | 32.617783 | 32.971207 |
| S  | 36.605637 | 28.382030 | 31.714680 |
| S  | 36.444450 | 28.829056 | 36.727783 |
| S  | 40.135757 | 26.285297 | 33.918110 |
| S  | 40.175674 | 30.827047 | 33.850548 |
| S  | 45.528076 | 28.816647 | 38.473782 |

24

generated by VMD
|   |   |   |
|---|---|---|
| **Ca** | 25.536184 | 30.226505 | 31.608501 |
| **Ca** | 26.298201 | 31.388134 | 35.672581 |
| **Ca** | 29.673134 | 27.951868 | 35.690720 |
| **Ca** | 30.233112 | 33.149368 | 33.498756 |
| **Ca** | 33.458767 | 29.274958 | 31.322464 |
| **Ca** | 33.004498 | 30.159027 | 35.563194 |
| **Ca** | 36.507263 | 26.338533 | 34.414993 |
| **Ca** | 36.533390 | 30.596239 | 34.236031 |
| **Ca** | 40.032112 | 28.727154 | 31.318918 |
| **Ca** | 39.831913 | 29.051157 | 36.401783 |
| **Ca** | 46.681072 | 29.448492 | 33.040421 |
| **Ca** | 42.700401 | 28.908081 | 34.176277 |
| **S**  | 26.562027 | 28.062981 | 36.259300 |
| **S**  | 26.994986 | 34.385246 | 34.398956 |
| **S**  | 30.628344 | 30.115625 | 32.803565 |
| **S**  | 29.802483 | 31.293125 | 36.375817 |
| **S**  | 33.001995 | 27.383703 | 34.163849 |
| **S**  | 33.889175 | 32.600300 | 33.013527 |
| **S**  | 36.527245 | 28.567440 | 31.871168 |
| **S**  | 36.332909 | 28.627558 | 36.914169 |
| **S**  | 39.997555 | 26.482079 | 33.924141 |
| **S**  | 40.280170 | 30.975170 | 33.866005 |
| **S**  | 43.645149 | 27.792442 | 31.221203 |
| **S**  | 46.281830 | 28.886192 | 38.271461 |

|   |   |   |
|---|---|---|
| **Ca** | 25.102074 | 30.607193 | 31.851297 |
| **Ca** | 26.294130 | 31.49385 | 35.759323 |
| **Ca** | 30.150982 | 27.827204 | 35.874821 |
| **Ca** | 30.040003 | 32.834644 | 33.526360 |
| **Ca** | 33.502995 | 29.384178 | 31.372602 |
| **Ca** | 33.104401 | 30.171164 | 35.470169 |
| **Ca** | 36.450031 | 26.519779 | 34.624695 |
| **Ca** | 36.651157 | 30.810953 | 33.984200 |
| **Ca** | 40.161167 | 29.145575 | 31.150047 |
| **Ca** | 39.922298 | 28.578186 | 36.476784 |
| **Ca** | 46.585377 | 29.081226 | 33.206902 |
| **Ca** | 42.805840 | 28.944788 | 34.084148 |
| **S**  | 26.763597 | 28.041361 | 36.098511 |
| **S**  | 27.033243 | 34.276161 | 34.152454 |
| **S**  | 30.469269 | 29.738232 | 32.840839 |
| **S**  | 29.746424 | 31.164972 | 36.505764 |
| **S**  | 33.130844 | 27.322756 | 34.105991 |
| **S**  | 33.720901 | 32.605469 | 32.854977 |
S   36.511086  28.591421  31.677242
S   36.562946  29.149046  36.685493
S   40.116119  26.582077  33.897270
S   40.095669  30.947802  33.911602
S   43.557308  28.012796  31.248629
S   45.956055  28.604980  38.670452

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generated by VMD
Ca  24.794865  30.630129  31.694729
Ca  26.249645  31.208143  35.801277
Ca  30.033714  28.054911  35.791092
Ca  30.292479  32.923149  33.561485
Ca  33.511612  29.370501  31.465836
Ca  33.113201  30.401522  35.462578
Ca  36.599377  26.394886  34.576134
Ca  36.713596  30.691439  34.104420
Ca  40.215103  28.818338  31.271574
Ca  39.934319  29.164112  36.555096
Ca  46.599899  29.195301  32.842213
Ca  42.784611  28.834789  33.990238
S   26.464420  27.833990  35.735348
S   27.144360  34.184528  34.258171
S   30.396173  29.802052  32.807434
S   29.714342  31.245157  36.393974
S   33.313702  27.472694  34.274658
S   33.920399  32.521381  32.987457
S   36.523693  28.473259  31.798120
S   36.317558  29.097404  37.002071
S   40.019768  26.525187  34.125580
S   40.124634  30.910252  33.919029
S   43.621441  27.833902  31.088238
S   46.030975  28.804390  38.523949

24

generated by VMD
Ca  25.588600  30.371655  31.502197
Ca  26.149006  31.400902  36.072819
Ca  29.808327  28.076920  35.655731
Ca  30.214159  32.994110  33.626171
Ca  33.581444  29.291407  31.265841
Ca  32.821121  30.324886  35.658684
Ca  36.474174  26.524637  34.394218
Ca  36.515106  30.811039  34.108875
Ca  40.252666  29.069307  31.194262
Ca  39.760017  29.121035  36.191692
Ca  46.778427  28.219894  33.052113
Ca  42.868942  29.004337  34.334824
|     |          |          |          |
|-----|----------|----------|----------|
| S   | 26.639870 | 27.830227 | 36.133129 |
| S   | 27.012022 | 34.356918 | 34.350037 |
| S   | 30.481287 | 29.979080 | 32.893677 |
| S   | 29.599403 | 31.193756 | 36.731533 |
| S   | 33.177887 | 27.230616 | 34.064407 |
| S   | 33.743282 | 32.350395 | 32.937660 |
| S   | 36.631348 | 28.654818 | 31.633619 |
| S   | 36.246693 | 28.904179 | 36.733589 |
| S   | 40.116356 | 26.611898 | 33.935612 |
| S   | 40.314034 | 31.118509 | 33.942734 |
| S   | 43.625214 | 27.711838 | 31.195374 |
| S   | 46.034531 | 29.239088 | 38.421829 |
| 24  |          |          |          |
| S   | 26.375536 | 27.715555 | 35.830971 |
| S   | 26.831757 | 34.238491 | 34.087688 |
| S   | 30.556253 | 29.862347 | 32.856712 |
| S   | 29.572653 | 31.493504 | 36.494484 |
| S   | 33.044834 | 27.424381 | 34.434483 |
| S   | 33.778408 | 32.372150 | 32.709908 |
| S   | 36.759186 | 28.753740 | 32.097729 |
| S   | 36.561787 | 29.093777 | 37.198639 |
| S   | 39.975388 | 26.673817 | 33.945602 |
| S   | 40.315445 | 31.033638 | 34.141518 |
| S   | 43.718781 | 27.947922 | 30.985577 |
| S   | 46.179302 | 28.490906 | 37.985607 |

24 generated by VMD

|     |          |          |          |
|-----|----------|----------|----------|
| Ca  | 24.840645 | 30.140354 | 31.568642 |
| Ca  | 26.197083 | 31.223610 | 35.738789 |
| Ca  | 29.775151 | 28.351322 | 35.712360 |
| Ca  | 30.297449 | 32.954952 | 33.345417 |
| Ca  | 33.679520 | 29.152674 | 31.331322 |
| Ca  | 33.001091 | 30.453928 | 35.565136 |
| Ca  | 36.364468 | 26.556417 | 34.738541 |
| Ca  | 36.648106 | 30.831188 | 34.412022 |
| Ca  | 40.129829 | 29.033031 | 31.472996 |
| Ca  | 39.942837 | 28.957071 | 36.778751 |
| Ca  | 46.971348 | 28.567476 | 32.327679 |
| Ca  | 42.916779 | 29.069151 | 34.270119 |
| S   | 26.375536 | 27.715555 | 35.830971 |
| S   | 26.831757 | 34.238491 | 34.087688 |
| S   | 30.556253 | 29.862347 | 32.856712 |
| S   | 29.572653 | 31.493504 | 36.494484 |
| S   | 33.044834 | 27.424381 | 34.434483 |
| S   | 33.778408 | 32.372150 | 32.709908 |
| S   | 36.759186 | 28.753740 | 32.097729 |
| S   | 36.561787 | 29.093777 | 37.198639 |
| S   | 39.975388 | 26.673817 | 33.945602 |
| S   | 40.315445 | 31.033638 | 34.141518 |
| S   | 43.718781 | 27.947922 | 30.985577 |
| S   | 46.179302 | 28.490906 | 37.985607 |
