Supporting Information

Pore-Bound Water at the Key Residue Histidine 37 in Influenza A M2
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Experimental Procedures

Protein expression
The M2 conductance domain (residue 18 to 60) from Influenza A was expressed and purified as previously described.[1] The M2 amino acid sequence from the Udom strain was used with a C50S mutation and an N-terminal 9xHis tag followed by TrpLE. Uniformly 15N and 13C labeled M2 expression was carried out using 13C6-glucose and 15N-ammonium chloride as carbon and nitrogen sources. Expression in Escherichia coli resulted in inclusion bodies, which were resuspended in 6M guanidinium and purified through a nickel column and cleaved using cyanogen bromide to remove the TrpLE tag. Protein was finally purified on a C4 HPLC column with gradient elution using 3:2 isopropanol:acetonitrile. The lyophilized protein was resuspended in NMR buffer (40 mM sodium phosphate, 30 mM glutamate, 3 mM sodium azide, pH 7.8) containing octyl glucoside detergent and reconstituted in d78-phytanoyl, d9-choline (DPhPC deuterated lipids from FBRagents). The lipid to protein ratio was 1:1 by weight, about 6 per monomer, or 24 per tetramer. The D2O exchange was performed by incubating the sample from a 1.3 mm rotor in NMR buffer prepared in 99 % D2O. Briefly, the sample was prepacked in a 1.3 mm rotor and then emptied in 1 mL of NMR D2O buffer. The sample was incubated for 24 hours at room temperature (~20 °C). The sample was repacked in a 1.3 mm rotor using a tabletop centrifuge, and kept at 4 °C until the NMR measurement.
NMR experiments

The ultra-fast MAS spectra were recorded using a 0.7 mm HCDN probe at a 950 MHz (22.3 T) Bruker AVANCE III HD spectrometer. The sample was spun to 100 kHz MAS and the temperature was set at 250 K (sample temperature at around 10 °C). The D2O exchange spectra were recorded at 45 kHz MAS using 1.3 mm HCN probe at an 800 MHz (18.8 T) Bruker AVANCE III HD spectrometer with the temperature set at 235 K (sample temperature below 10 °C). The DNP spectra were recorded using an HCN mode of a 2.5 mm Phoenix HFXY DNP probe at a 600 MHz (14.1 T) Bruker spectrometer with a 396 GHz gyrotron matching the TEMTrPol-1 [2] radical's cross-effect condition. The cooling was set at 90 K which results in a sample temperature of about 100 K at 24 kHz MAS. The DNP sample was prepared from a 1.3 mm rotor containing about 1 mg of reconstituted M2 protein. The pellet from the 1.3 mm rotor was resuspended in 24 µl of ‘DNP juice’, composed of 98% 13C depleted, d-8 glycerol, D2O and H2O based NMR buffer at 60:30:10 volume ratios, respectively. A final concentration of 5 to 10 mM of TEMTrPol-1 was reached by adding a 30 mM stock TEMTrPol-1 solution in DNP juice and mixing thoroughly. The final ~36 µl sample was then centrifuged into the 2.5mm zirconia rotor using the Phoenix 2.5 mm liquid sample packing tools, for 5 min at 5000 g. The sample was then frozen inside the packed and closed zirconia rotor with a liquid nitrogen bath, thawed, and repeated 3 times in order to remove dissolved oxygen.

Structural refinement and NMR chemical shift calculations using DFT and GIAO methods

Density functional theory (DFT) calculations were performed using gaussian 16 software[3]. As a starting structure, we used the de novo M2 calculated structure obtained using CYANA[4] with the experimental chemical shift and restraints shown in Table S1, S2 and S3. The NMR spectra and parameters recorded for the assignment and obtaining structural restraints are shown in Table S4. To accelerate the DFT and the Gauge-Independent Atomic Orbital (GIAO)[5] based NMR calculations, a reduced set of atoms, spanning residues G34 to W41, were used. Two starting structures were optimized with first semi-empirical and later DFT methods using different functionals (hybrid and GGA) and basis sets available in gaussian16, on either the dimer or the tetramer structure. The gaussian input file of the tetramer used for DFT is shown in Table S5. The structures were optimized stepwise, firstly by a semi-empirical PM6[6] and later by hybrid B3LYP[7] or pure generalized gradient approximation (GGA) mPW1PW91[8] level of theory with 6-311G++2d,p as basis set in both cases. One or two molecules of water were added in the dimer or tetramer, respectively. After addition of water molecule(s), the structures were reoptimized before performing the NMR calculations using GIAO method. For the NMR calculation, both B3LYP with 6-31G, 6-311G++d,p, 6-311G++d,p (pcpm,solvent=water) and MPW1PW91 with 6-311G++2d,p, 6-311G++2d,p (pcpm,solvent=water) were performed. We also tested solvation by adding water in a polarizable continuum model (PCPM)[9] and performing a Hybrid functional DFT calculation. A final calculation was performed using the same DFT parameters (basis set and functional) but removing the water molecules. The proton chemical shift is calculated using TMS (31.88 ppm) as reference for protons from the chemical shielding tensor of the GIAO results. We achieve R2=0.98 for H37s and R2=0.56 for H37a for protons without considering the H37a of H37 since the H37a is not forming a H bond with the carboxyl at the +4 residue as usually encountered in helix structures. The discrepancy on the R2 obtained for protons between the different chains is due to the H37a at the imidazole ring. Indeed, from our NMR assignments, we find an unusual proton chemical shift of ~4.1 ppm for H37a with respect to the usual values reported on the BMRB at ~ 7.8 ppm. The high field proton chemical shift could be from ring current shifts that differ in the DFT calculations. For obtaining the nitrogen chemical shift from the calculated isotropic nitrogen chemical shift, a regression method using the slope of the curve obtained by comparing the calculated isotropic chemical shift and the experimental nitrogen chemical shift of H37a, which are independent of the water, has been used for internal 15N referencing (Fig S4E and S5E), where we achieve R2=0.991 [10]. The regressions between calculated and experimental proton chemical shifts are shown in Fig S4B-C and S5B-C for dimer and tetramer, respectively.

PH of the frozen sample with phosphate buffer

A pH-indicator solution pH 4.0-10.0 from Merck (1.09175.0100) was used for measuring the pH shift after liquid nitrogen freezing of the phosphate/glutamate buffer used in DNP samples. Two conditions were tested, either with or without protein. For a total of 30 µl final solution, 24 µl of DNP juice was mixed with either 6 µl of free protein phosphate buffer or with the sample from a prepacked rotor (~6 µl), which contains about 1 mg of reconstituted M2 protein. On top of these samples, ~6 µl of pH-indicator solution was added and the solutions were frozen inside a liquid nitrogen bath.
Figure S1. Pulse sequences used for dipolar filtered (A) and reference (B) spectra. In (A) and (B), the first two CP periods polarize $^{15}$N. The delay $d_2$ (1 to several seconds) allows spin diffusion to equilibrate polarization among both protonated and non-protonated $^{15}$N spins. The third CP step transfers signal back to $^1$H for detection. These initial CP steps are made long enough (several ms) to transfer signal to (or from) protons that are remote from $^{15}$N. Polarization is also transferred across shorter distances such as a chemical bond. The final (fourth) CP step in (A) is the filter, which here is implemented for both $^{15}$N and $^{13}$C. Protons that are close to $^{15}$N or $^{13}$C lose polarization faster than those that are more remote.
**Figure S2.** (H)CH spectrum recorded with a 0.7 mm 4 channel HDCN Bruker probe with 100 kHz MAS on a 950 MHz Bruker spectrometer at ~10 °C.
Figure S3. 2D (H)NH spectra of H₂O (blue) and D₂O-washed (orange) at 45 kHz MAS on a 800 MHz Bruker spectrometer at 240 K. Negative contours are pink and green, respectively. Labels indicate proton shifts.
Figure S4. Proton chemical shift assignment of His37 side chain imidazole ring in M2 from influenza A. The left panel shows the 2D (H)NH with 4 ms CP (black) and an N-H projection of the (H)(C)NCH spectrum (red). The spectra were recorded on a 0.7 mm 4 channel HDCN Bruker probe with 100 kHz MAS on a 950 MHz Bruker spectrometer at ~10 ºC. The panels at right show selected planes from the 3D spectrum. The assignment to the tau tautomer can be made since Hδ2 correlates only to Nε2, whose chemical shift in the 160-180 ppm range is indicative of protonation.[11] On the other hand, the Hε1 proton correlates to two 15N resonances, both Nε2 and Nδ1, Nδ1 is found near 250 ppm, indicative of a deprotonated nitrogen.[11]
Figure S5: Phosphate/glutamate buffer pH upon liquid nitrogen freezing. The pH as determined by a color indicator is shown in (A) after cooling in liquid nitrogen and in (B) at room temperature for a DNP sample containing ~1 mg (6 µl) of reconstituted M2 protein resuspended in 24 µl of DNP juice frozen. Panel (C) shows the pH shift observed for the DNP buffer alone upon liquid nitrogen freezing, as compared with room temperature (D).
Figure S6: The full 2D (H)NH spectrum (black) is compared with a CP-based dipolar filtered (H)NH spectrum (red) of Figure 2B. The CP contact time for filtering was 200 µs for HN and 100 µs for HC. Both HN and NH CPs used a contact time of 2 ms. Both spectra were measured at 600 MHz with cooling set at 90 K corresponding to a sample temperature of about 100 K using 24 kHz MAS. The data were measured using a three-channel phoenix probe with a 2.5 mm rotor. With this setup, we obtained an $^1$H DNP enhancement factor, $e$, of 22 using 5 to 10 mM TEMTriPol. The enhancement factor was measured from 1D carbon CP spectra by taking the signal ratio between spectra with and without microwaves.
Figure S7: Correlation between experimental and calculated NMR chemical shifts obtained from a tetramer structure. (A) shows the dimer structures containing chain A and B from the geometry optimized M2 tetramer structures with or without water calculated from the NMR data using CYANA. Panels (B) and (C) show the correlation for proton resonances of H37 of chain B and chain A, respectively. In (D), the difference between experimental and calculated proton chemical shift obtained for the water (H\textsubscript{1}) and H\textsubscript{2} of H37 is shown. Panel (E) shows the correlation between the GIAO calculated isotropic chemical shielding and the experimental chemical shift of chain A, as used for chemical shift calibration of nitrogen, with a $R^2=0.991$. In (F), the difference between the calculated and experimental nitrogen chemical shifts are shown.
Figure S8: Correlation between experimental and calculated NMR chemical shifts starting from a dimer structure. In (A), the dimer structures with and without (No Water) a water molecule are shown. (B) and (C) shows the correlation between experimental and calculated proton chemical shifts of the H37 of chain B (B) and chain A (C). In (D), the difference between calculated and experimental chemical shifts obtained for the water proton (H1) and H37 of H37 is shown. Panel (E), shows the correlation between the isotropic chemical shielding and the experimental chemical shifts of chain A used for chemical shift calibration of nitrogen, with $R^2=0.98$. In (F), the difference between the calculated and experimental nitrogen chemical shifts are shown.
Table S1. NMR chemical shift table.

| Residue | Atom | Chemical shift | Residue | Atom | Chemical shift |
|---------|------|----------------|---------|------|----------------|
| 25      | N    | 25.496         | Chain B | 25   | 65.496         |
| 25      | CA   | 4.075          | 25      | CB   | 32.819         |
| 25      | HB2  | 2.176          | 25      | HB3  | 1.690          |
| 25      | QB   | -              | 25      | CG   | 27.608         |
| 25      | HG2  | 1.952          | 25      | HG3  | 2.010          |
| 25      | QG   | -              | 25      | CD   | 51.124         |
| 25      | HQ2  | 3.937          | 25      | HD3  | 3.765          |
| 25      | HQD  | -              | 26      | C    | 177.164        |
| 26      | N    | 118.643        | 26      | H    | 7.710          |
| 26      | CA   | 57.607         | 26      | CB   | 40.408         |
| 26      | HB2  | 1.694          | 26      | HB3  | 0.593          |
| 26      | QG   | -              | 26      | CD   | 23.937         |
| 26      | HQ2  | -              | 26      | HQD  | -              |
| 26      | HQD  | -              | 27      | C    | 178.259        |
| 27      | N    | 120.321        | 27      | H    | 8.157          |
| 27      | CA   | 67.253         | 27      | CB   | 31.536         |
| 27      | HB2  | 1.684          | 27      | HB3  | 0.593          |
| 27      | QG   | -              | 27      | CD   | 23.937         |
| 27      | HQ2  | -              | 27      | HQD  | -              |
| 27      | HQD  | -              | 28      | C    | 178.737        |
| 28      | N    | 119.425        | 28      | H    | 8.224          |
| 28      | CA   | 67.118         | 28      | HB   | 2.215          |
| 28      | HB2  | 3.345          | 28      | HB3  | 3.405          |
| 28      | QG   | -              | 28      | CD   | 51.124         |
| 28      | HQ2  | -              | 28      | HQD  | -              |
| 28      | HQD  | -              | 29      | C    | 177.835        |
| 29      | N    | 121.127        | 29      | H    | 8.399          |
| 29      | CA   | 55.910         | 29      | HB   | 3.713          |
| 29      | HB2  | 1.415          | 29      | HB3  | 1.303          |
| 35 | HG21 – | 135 | HG21 – |
| 35 | HG22 – | 135 | HG22 – |
| 35 | HG23 – | 135 | HG23 – |
| 35 | CG1 30.070 | 135 | CG1 29.719 |
| 35 | HG12 0.641 | 135 | HG12 0.877 |
| 35 | HG13 1.799 | 135 | HG13 1.655 |
| 35 | GG1 – | 135 | GG1 – |
| 35 | GD1 0.576 | 135 | GD1 0.568 |
| 35 | GD1 13.557 | 135 | GD1 13.542 |
| 35 | HD11 – | 135 | HD11 – |
| 35 | HD12 – | 135 | HD12 – |
| 35 | HD13 – | 135 | HD13 – |
| 35 | C 176.646 | 135 | C 176.646 |
| 36 | N 119.371 | 136 | N 119.787 |
| 36 | H 8.209 | 136 | H 8.549 |
| 36 | CA 56.229 | 136 | CA 56.454 |
| 36 | HA 3.806 | 136 | HA 3.792 |
| 36 | CB 41.701 | 136 | CB 41.832 |
| 36 | HB2 1.359 | 136 | HB2 1.744 |
| 36 | HB3 1.742 | 136 | HB3 1.361 |
| 36 | QB – | 136 | QB – |
| 36 | CG 30.191 | 136 | CG 30.247 |
| 36 | HG 1.716 | 136 | HG 1.525 |
| 36 | GD1 – | 136 | GD1 1.742 |
| 36 | QD2 – | 136 | QD2 0.633 |
| 36 | CD1 26.803 | 136 | CD1 26.856 |
| 36 | HD11 – | 136 | HD11 – |
| 36 | HD12 – | 136 | HD12 – |
| 36 | HD13 – | 136 | HD13 – |
| 36 | CD2 – | 136 | CD2 23.110 |
| 36 | HD21 – | 136 | HD21 – |
| 36 | HD22 – | 136 | HD22 – |
| 36 | HD23 – | 136 | HD23 – |
| 36 | QDD – | 136 | QDD – |
| 36 | C 177.564 | 136 | C 177.663 |
| 37 | N 117.271 | 137 | N 116.495 |
| 37 | H 8.022 | 137 | H 8.360 |
| 37 | CA 62.339 | 137 | CA 59.558 |
| 37 | HA 3.624 | 137 | HA 4.358 |
| 37 | CB 32.196 | 137 | CB 31.203 |
| 37 | HB2 2.964 | 137 | HB2 2.923 |
| 37 | HB3 2.796 | 137 | HB3 – |
| 37 | QB – | 137 | QB – |
| 37 | CG – | 137 | CG – |
| 37 | ND1 252.609 | 137 | ND1 249.236 |
| 37 | CD2 116.227 | 137 | CD2 118.742 |
| 37 | CE1 136.282 | 137 | CE1 137.228 |
| 37 | NE2 166.110 | 137 | NE2 172.784 |
| 37 | HD2 6.434 | 137 | HD2 7.260 |
| 37 | HE1 4.130 | 137 | HE1 6.910 |
| 37 | HE2 11.713 | 137 | HE2 14.276 |
| 37 | C 176.748 | 137 | C 175.214 |
| 37 | N 119.528 | 138 | N 117.299 |
| 37 | H 8.073 | 138 | H 7.710 |
| 37 | CA 58.171 | 138 | CA 59.024 |
| 37 | HA 3.376 | 138 | HA 3.527 |
| 37 | CB 40.642 | 138 | CB 42.469 |
| 37 | HB2 1.557 | 138 | HB2 2.119 |
| 37 | HB3 0.566 | 138 | HB3 1.396 |
| 37 | QB – | 138 | QB – |
| 37 | CG 26.507 | 138 | CG 26.591 |
| 37 | HG – | 138 | HG 1.385 |
| 38 | QD1 1.179 | 138 | QD1 0.645 |
| 38 | QD2 – | 138 | QD2 – |
| 38 | CD1 21.769 | 138 | CD1 – |
| 38 | HD11 – | 138 | HD11 – |
| 38 | HD12 – | 138 | HD12 – |
| 38 | HD13 – | 138 | HD13 – |
| 38 | CD2 – | 138 | CD2 – |
| 38 | HD21 – | 138 | HD21 – |
| 38 | HD22 – | 138 | HD22 – |
| 38 | HD23 – | 138 | HD23 – |
| 38 | QDD – | 138 | QDD – |
| 38 | C 178.370 | 138 | C 177.485 |
| 39 | N 117.391 | 139 | N 114.432 |
| 39 | H 8.259 | 139 | H 8.023 |
| 39 | CA 65.806 | 139 | CA 65.472 |
| 39 | HA 3.311 | 139 | HA 3.391 |
| 39 | CB 37.442 | 139 | CB 37.571 |
| 39 | HB 1.620 | 139 | HB 1.831 |
| 39 | QG2 0.644 | 139 | QG2 0.653 |
| 39 | CG2 17.327 | 139 | CG2 17.384 |
| 39 | HG21 – | 139 | HG21 – |
|   | HG22 |   | HG22 |   |
|---|------|---|------|---|
| 39 | 29.606 | 139 | 29.659 | 139 |
| 39 | 1.800 | 139 | 1.762 | 139 |
| 39 | 0.920 | 139 | 0.835 | 139 |
| 39 | 0.564 | 139 | 0.575 | 139 |
| 39 | 13.610 | 139 | 13.686 | 139 |
| 39 | HD11 | 139 | HD11 | 139 |
| 39 | HD12 | 139 | HD12 | 139 |
| 39 | HD13 | 139 | HD13 | 139 |
| 39 | C 177.087 | 139 | C 177.056 | 139 |
| 40 | N 118.895 | 140 | N 121.275 | 140 |
| 40 | H 7.728 | 140 | H 8.822 | 140 |
| 40 | CA 58.226 | 140 | CA 58.491 | 140 |
| 40 | HA 3.839 | 140 | HA 3.845 | 140 |
| 40 | CB 40.725 | 140 | CB 41.359 | 140 |
| 40 | HB2 1.693 | 140 | HB2 2.164 | 140 |
| 40 | HB3 0.637 | 140 | HB3 | 140 |
| 40 | QB | 140 | QB | 140 |
| 40 | CG 30.110 | 140 | CG 26.836 | 140 |
| 40 | HG 1.886 | 140 | HG | 140 |
| 40 | QD1 1.639 | 140 | QD1 1.665 | 140 |
| 40 | QD2 | 140 | QD2 0.928 | 140 |
| 40 | CD1 26.699 | 140 | CD1 25.618 | 140 |
| 40 | HD11 | 140 | HD11 | 140 |
| 40 | HD12 | 140 | HD12 | 140 |
| 40 | HD13 | 140 | HD13 | 140 |
| 40 | CD2 26.600 | 140 | CD2 22.959 | 140 |
| 40 | HD21 | 140 | HD21 | 140 |
| 40 | HD22 | 140 | HD22 | 140 |
| 40 | HD23 | 140 | HD23 | 140 |
| 40 | QQD | 140 | QQD | 140 |
| 40 | C 178.352 | 140 | C 178.703 | 140 |
| 41 | N 123.002 | 141 | N 120.804 | 141 |
| 41 | H 8.510 | 141 | H 9.459 | 141 |
| 41 | CA 62.763 | 141 | CA 61.474 | 141 |
| 41 | HA 3.750 | 141 | HA 3.654 | 141 |
| 41 | CB 28.157 | 141 | CB 27.473 | 141 |
| 41 | HB1 3.341 | 141 | HB2 2.503 | 141 |
| 41 | HB2 2.531 | 141 | HB3 | 141 |
| 41 | QB | 141 | QB | 141 |
| 41 | CG | 141 | CG | 141 |
| 41 | CD1 127.718 | 141 | CD1 126.563 | 141 |
| 41 | CD2 | 141 | CD2 | 141 |
| 41 | CE3 120.720 | 141 | CE3 119.417 | 141 |
| 41 | CE2 | 141 | CE2 | 141 |
| 41 | NE1 130.945 | 141 | NE1 131.220 | 141 |
| 41 | HD11 7.210 | 141 | HD11 6.145 | 141 |
| 41 | HE3 7.392 | 141 | HE3 | 141 |
| 41 | CZ3 120.717 | 141 | CZ3 121.646 | 141 |
| 41 | CZ2 114.559 | 141 | CZ2 114.847 | 141 |
| 41 | HE1 11.276 | 141 | HE1 10.776 | 141 |
| 41 | HZ3 6.673 | 141 | HZ3 5.172 | 141 |
| 41 | CH2 123.168 | 141 | CH2 123.900 | 141 |
| 41 | HZ2 7.812 | 141 | HZ2 7.614 | 141 |
| 41 | HH2 6.923 | 141 | HH2 7.182 | 141 |
| 41 | C 178.527 | 141 | C 178.143 | 141 |
| 42 | N 119.515 | 142 | N 117.151 | 142 |
| 42 | H 8.812 | 142 | H 7.834 | 142 |
| 42 | CA 65.022 | 142 | CA 66.579 | 142 |
| 42 | HA 3.040 | 142 | HA 3.230 | 142 |
| 42 | CB 37.620 | 142 | CB 37.638 | 142 |
| 42 | HB 1.811 | 142 | HB 1.873 | 142 |
| 42 | CG2 0.589 | 142 | CG2 0.670 | 142 |
| 42 | CG2 17.048 | 142 | CG2 17.506 | 142 |
| 42 | HG21 | 142 | HG21 | 142 |
| 42 | HG22 | 142 | HG22 | 142 |
| 42 | HG23 | 142 | HG23 | 142 |
| 42 | CG1 29.388 | 142 | CG1 29.610 | 142 |
| 42 | HG12 0.620 | 142 | HG12 1.831 | 142 |
| 42 | HG13 0.448 | 142 | HG13 0.632 | 142 |
| 42 | QG1 | 142 | QG1 | 142 |
| 42 | QD1 0.564 | 142 | QD1 0.630 | 142 |
| 42 | CD1 13.634 | 142 | CD1 13.804 | 142 |
| 42 | HD11 | 142 | HD11 | 142 |
| 42 | HD12 | 142 | HD12 | 142 |
| 42 | HD13 | 142 | HD13 | 142 |
| 42 | C 177.924 | 142 | C 177.743 | 142 |
| 43 | N 119.131 | 143 | N 117.248 | 143 |
| 43 | H 8.460 | 143 | H 8.441 | 143 |
| 43 | CA 58.150 | 143 | CA 58.071 | 143 |
| 43 | HA | 143 | HA 3.835 | 143 |
|   |   |   |   |
|---|---|---|---|
| 43 | CB  |   | 143 | CB  | 41.717 |
| 43 | HB2 |   | 143 | HB2 | 2.042 |
| 43 | HB3 |   | 143 | HB3 | 1.382 |
| 43 | QB  |   | 143 | QB  |   |
| 43 | CQ  |   | 143 | CQ  | 26.654 |
| 43 | HG  |   | 143 | HG  | 1.671 |
| 43 | QD1 |   | 143 | QD1 |   |
| 43 | QD2 |   | 143 | QD2 |   |
| 43 | CD1 |   | 143 | CD1 | 22.938 |
| 43 | HD11|   | 143 | HD11|   |
| 43 | HD12|   | 143 | HD12|   |
| 43 | HD13|   | 143 | HD13|   |
| 43 | CD2 |   | 143 | CD2 |   |
| 43 | HD21|   | 143 | HD21|   |
| 43 | HD22|   | 143 | HD22|   |
| 43 | HD23|   | 143 | HD23|   |
| 43 | QQD |   | 143 | QQD |   |
| 43 | C   |   | 143 | C   | 179.626 |
| 44 | N   |   | 120.828 |
| 44 | H   |   | 9.064  |
| 44 | CA  |   | 57.820 |
| 44 | HA  |   | 4.761  |
| 44 | CB  |   | 42.688 |
| 44 | HB2 |   | 2.571  |
| 44 | HB3 |   | 2.876  |
| 44 | QB  |   |   |
| 44 | CG  |   |   |
| 44 | QD1 |   |   |
| 44 | QD2 |   |   |
| 44 | C   |   | 178.417 |
| 45 | N   |   | 116.290 |
| 45 | H   |   | 8.329  |
| 45 | CA  |   | 57.082 |
| 45 | HA  |   | 3.515  |
| 45 | CB  |   | 30.472 |
| 45 | HB2 |   | 1.656  |
| 45 | HB3 |   | 1.535  |
| 45 | QB  |   |   |
| 45 | CG  |   | 25.154 |
| 45 | HG2 |   | 1.018  |
| 45 | HG3 |   | 0.771  |
| 45 | QG  |   |   |
| 45 | CD  |   | 43.206 |
| 45 | HD2 |   |   |
| 45 | HD3 |   |   |
| 45 | QQD |   |   |
| 45 | NE  |   |   |
| 45 | HE  |   |   |
| 45 | CZ  |   |   |
| 45 | NH1 |   |   |
| 45 | HH11|   |   |
| 45 | HH12|   |   |
| 45 | NH2 |   |   |
| 45 | HH21|   |   |
| 45 | HH22|   |   |
| 45 | QH2 |   |   |
| 45 | C   |   | 178.289 |
| 46 | N   |   | 113.319 |
| 46 | H   |   | 7.793  |
| 46 | CA  |   | 56.308 |
| 46 | HA  |   | 3.796  |
| 46 | CB  |   | 42.254 |
| 46 | HB2 |   | 0.994  |
| 46 | HB3 |   | 1.437  |
| 46 | QB  |   |   |
| 46 | CG  |   | 26.683 |
| 46 | HG  |   |   |
| 46 | QD1 |   |   |
| 46 | QD2 |   |   |
| 46 | CD1 |   |   |
| 46 | HD11|   |   |
| 46 | HD12|   |   |
| 46 | HD13|   |   |
| 46 | CD2 |   |   |
| 46 | HD21|   |   |
| 46 | HD22|   |   |
| 46 | HD23|   |   |
| 46 | QQD |   |   |
| 46 | C   |   | 177.261 |
| 47 | N   |   | 112.813 |
| 47 | H   |   | 7.536  |
| 47 | CA  |   | 58.771 |
| 47 | HA  |   | 4.616  |
| 147 | CB   | 41.510 |
|-----|------|--------|
| 147 | HB2  | 2.496  |
| 147 | HB3  | –      |
| 147 | QB   | –      |
| 147 | QD   | –      |
| 147 | QE   | –      |
| 147 | QR   | –      |
| 147 | CG   | –      |
| 147 | GD1  | –      |
| 147 | CE1  | –      |
| 147 | HE1  | –      |
| 147 | CZ   | –      |
| 147 | HZ   | –      |
| 147 | CE2  | –      |
| 147 | HE2  | –      |
| 147 | GD2  | –      |
| 147 | HD1  | –      |
| 147 | HD2  | –      |
| 148 | N    | 118.432|
| 148 | H    | 7.373  |
| 148 | CA   | 61.539 |
| 148 | HA   | 4.216  |
| 148 | CB   | 39.503 |
| 148 | HB2  | 3.521  |
| 148 | HB3  | 3.131  |
| 148 | QB   | –      |
| 148 | QD   | –      |
| 148 | QE   | –      |
| 148 | QR   | –      |
| 148 | CG   | –      |
| 148 | GD1  | –      |
| 148 | CE1  | –      |
| 148 | HE1  | –      |
| 148 | CZ   | –      |
| 148 | HZ   | –      |
| 148 | CE2  | –      |
| 148 | HE2  | –      |
| 148 | HD2  | –      |
| 148 | C    | 175.579|
| 149 | N    | 120.103|
| 149 | H    | 9.020  |
| 149 | CA   | 57.147 |
| 149 | HA   | 3.323  |
| 149 | CB   | 30.366 |
| 149 | HB2  | 1.675  |
| 149 | HB3  | 1.025  |
| 149 | QB   | –      |
| 149 | CG   | 25.281 |
| 149 | HG2  | 0.994  |
| 149 | HG3  | –      |
| 149 | QG   | –      |
| 149 | CD   | 29.297 |
| 149 | HD2  | –      |
| 149 | HD3  | –      |
| 149 | QD   | –      |
| 149 | CE   | –      |
| 149 | HE2  | –      |
| 149 | HE3  | –      |
| 149 | QE   | –      |
| 149 | NZ   | –      |
| 149 | HZ1  | –      |
| 149 | HZ2  | –      |
| 149 | HZ3  | –      |
| 149 | QZ   | –      |
| 150 | C    | 175.633|
| 150 | N    | 111.292|
| 150 | H    | 9.020  |
| 150 | CA   | 60.519 |
| 150 | HA   | 4.428  |
| 150 | CB   | 66.283 |
| 150 | HB2  | 3.512  |
| 150 | HB3  | 3.632  |
| 150 | QB   | –      |
| 150 | QG   | –      |
| 150 | HG   | –      |
| 150 | C    | 174.659|
| 151 | N    | 126.452|
| 151 | H    | 9.926  |
| 151 | CA   | 66.079 |
| 151 | HA   | 3.164  |
|   |   |   |
|---|---|---|
| 151 | CB | 38.119 |
| 151 | HB | 1.164 |
| 151 | QG2 | -0.914 |
| 151 | CG2 | 17.164 |
| 151 | HG21 | - |
| 151 | HG22 | - |
| 151 | HG23 | - |
| 151 | CG1 | 38.119 |
| 151 | HG12 | 28.621 |
| 151 | HG13 | 0.413 |
| 151 | HG1 | - |
| 151 | CD1 | 13.806 |
| 151 | HD11 | - |
| 151 | HD12 | - |
| 151 | HD13 | - |
| 151 | C | 176.078 |
| 151 | N | 117.337 |
| 151 | H | 7.911 |
| 151 | CA | 62.800 |
| 151 | HA | 3.854 |
| 151 | CB | 36.611 |
| 151 | HB2 | 2.575 |
| 151 | HB3 | 1.885 |
| 152 | QD | - |
| 152 | QE | - |
| 152 | QR | - |
| 152 | CG | - |
| 152 | CD1 | - |
| 152 | HD1 | - |
| 152 | CE1 | - |
| 152 | HE1 | - |
| 152 | CZ | - |
| 152 | CE2 | - |
| 152 | HE2 | - |
| 152 | CD2 | - |
| 152 | HD2 | - |
| 152 | OH | - |
| 152 | HH | - |
| 152 | C | 178.934 |
| 152 | N | 121.954 |
| 152 | H | 8.543 |
| 152 | CA | 58.909 |
| 152 | HA | 3.994 |
| 152 | CB | 29.381 |
| 152 | HB2 | 1.335 |
| 152 | HB3 | - |
| 153 | QB | - |
| 153 | CG | 25.241 |
| 153 | HG2 | 0.990 |
| 153 | HG3 | - |
| 153 | QG | - |
| 153 | CD | 42.646 |
| 153 | HD2 | 2.713 |
| 153 | HD3 | - |
| 153 | QD | - |
| 153 | NE | - |
| 153 | HE | - |
| 153 | CZ | - |
| 153 | NH1 | - |
| 153 | HH11 | - |
| 153 | HH12 | - |
| 153 | NH2 | - |
| 153 | HH21 | - |
| 153 | HH22 | - |
| 153 | QH2 | - |
| 153 | C | 177.941 |
| 154 | N | 120.662 |
| 154 | H | 7.312 |
| 154 | CA | 61.022 |
| 154 | HA | 4.199 |
| 154 | CB | 38.281 |
| 154 | HB2 | 2.967 |
| 154 | HB3 | 3.212 |
| 154 | QB | - |
| 154 | QD | - |
| 154 | QE | - |
| 154 | QR | - |
| 154 | CG | - |
| 154 | CD1 | - |
| 154 | HD1 | - |
| 154 | CE1 | - |
### Table S2. Manual restraints used for the structure calculation in CYANA.

| Residue number | Residue | Atom | Residue number | Residue | Atom | Distance |
|----------------|---------|------|----------------|---------|------|----------|
| 27             | VAL     | CA   | 127            | VAL     | CA   | 10.00    |
| 27             | VAL     | CA   | 327            | VAL     | CA   | 10.00    |
| 27             | VAL     | CA   | 227            | VAL     | CA   | 14.00    |
| 327            | VAL     | CA   | 127            | VAL     | CA   | 14.00    |
| 45             | ARG     | CB   | 245            | ARG     | CB   | 21.00    |
| 45             | ARG     | CB   | 345            | ARG     | CB   | 21.00    |

### Table S3. J-coupling restraints used for the structure calculation in CYANA.

| Residue number | Residue | Atom | Residue number | Residue | Atom | Distance |
|----------------|---------|------|----------------|---------|------|----------|
| 137            | HIST    | HE2  | 37             | HIST    | ND1  | 1.50     |
| 137            | HIST    | NE2  | 37             | HIST    | ND1  | 2.80     |
| 337            | HIST    | HE2  | 237            | HIST    | ND1  | 1.50     |
| 337            | HIST    | NE2  | 237            | HIST    | ND1  | 2.80     |
### Table S4. Solid-state NMR experiments and parameters.

| Experiment | (H)CNH | (H)(Co)CNH | (H)CNH | (H)(Co)NH | (H)NH in | (H)NH water |
|------------|--------|------------|--------|-----------|----------|------------|
| Transfer 1 | HN-CP  | HN-CP      | HN-CP  | HC-CP     | HN-CP    | HN-CP      |
| Max RF Field (kHz) (Ramp in H) | 149/20 (100 to 80) | 149/20 (100 to 80) | 149/20 (100 to 80) | 139/29 (80 to 80) | 149/20 (100 to 80) | 142/30 (100 to 80) |
| Time (ms)* | 1.25   | 3          | 6      | 1.2       | 1.25     | 4          |
| Transfer 2 | NH-CP  | NH-CP      | NH-CP  | CH-CP     | N-N inept | NH-CP      |
| Max RF Field (kHz) (Ramp in H) | 30/137 (80 to 100) | 30/137 (80 to 100) | 30/137 (80 to 100) | 29/127 (80 to 100) | -         | 30/140 (80 to 100) |
| Time (ms)* | 0.5    | 3          | 6      | 0.35      | Different times used | 4          |
| Transfer 3 | -      | -          | -      | -         | NH-CP    | NH-CP      |
| Max RF Field (kHz) (Ramp in H) | -      | -          | -      | -         | 30/140 (80 to 100) | 140/30 (H/N) |
| Time (ms)* | -      | -          | -      | -         | 0.5      | 0.5 (H/N)  |
| Interscan delay (s) | 1.1 | 1.1 | 1.1 | 1.1 | 1.1 | 1.1 |
| Number of scans | 4 | 40 | 46 | 4 | - | - |
| Measurement time (h) | 1.25 | 14 | 34 | 1.25 | - | - |

| Experiment | (H)CaNH | (H)(Co)Ca(N)NH | (H)CoNH | (H)(Co)NH | (H)Ca(NH) | (H)Ca(Ca)NH |
|------------|---------|----------------|---------|-----------|-----------|-------------|
| Transfer 1 | HC-CP   | HC-CP          | HC-CP   | HC-CP     | HC-CP     | HC-CP       |
| Max RF Field (kHz) (Ramp in H) | 132/29 (100 to 80) | 132/29 (100 to 80) | 121/22 (85 to 80) | 121/22 (85 to 80) | 119/22 (85 to 100) |
| Time (ms)* | 1.4     | 2.7            | 2.9     | 2.9       | 0.5       | 0.8         |
| Transfer 2 | CN-CP   | CO-CA INEPT    | CN-CP   | CO-CA INEPT | CA-CB-CA INEPT | CA-CB-CA INEPT |
| Max RF Field (kHz) (Ramp in H) | 61/42 (100 to 80) | -        | 69/42 (Tan) | -         | -          |
| Time (ms)* | 9.8     | T2 Ca and Co optimised | 4        | 4.2 (T2 optimised) | 4.5 (T2 optimised) |
| Transfer 3 | NH-CP   | CN-CP          | NH-CP   | CN-CP     | CN-CP     | CN-CP       |
| Max RF Field (kHz) (Ramp in H) | 31/126 (80 to 100) | 62/42 (Tan) | 31/130 (80 to 100) | 69/42 (80 to 100) | 69/42 (80 to 100) |
| Time (ms)* | 0.3     | 11.2           | 0.5     | 14        | 14        | 14          |
| Transfer 4 | -       | NH-CP          | -       | NH-CP     | NH-CP     | NH-CP       |
| Max RF Field (kHz) (Ramp) | -       | 31/133 (80 to 100) | -       | 31/122 (80 to 100) | 31/122 (80 to 100) |
| Time (ms)* | -       | 0.5            | 0.5     | 0.5       | 0.5       | 0.5         |
| Interscan delay (s) | 1.1 | 1.1 | 1.1 | 1.1 | 1.1 | 1.1 |
| Number of scans | 4 | 20 | 4 | 16 | 16 | 16 |
### Measurement time (h)

| Experiment | (H)NCaHa | (H)COCAHa | (HCa)Cb(Ca)N H |
|------------|----------|-----------|----------------|
| Transfer 1 | HN-CP    | HC-CP     | HC-CP          |
| Max RF Field (kHz) (Ramp) | 139/31 | 133/29 | 120/22 |
| Time (ms)* | 1.5      | 3.5       | 0.75           |
| Transfer 2 | NC-CP    | CO-CA INEPT | CA-CB INEPT |
| Max RF Field (kHz) (Ramp) | 71/42 | -        | -              |
| Time (ms)* | 13       | 4.16      | 4.3            |
| Transfer 3 | CH-CP    | CH-CP     | CN-CP          |
| Max RF Field (kHz) (Ramp) | 30/125 | 29/137 | 69/42 |
| Time (ms)* | 0.35     | 0.25      | 1.1            |
| Transfer 4 | -        | -        | NH-CP          |
| Max RF Field (kHz) (Ramp) | -        | -        | 31/122         |
| Time (ms)* | -        | -        | 0.5            |

| sw (t1) (ppm) | 30 | 52 | 30 |
| Acq.time (t1) (ms) | 15.2 | 40 | 15 |
| sw (t2) (ppm) | 30 | 30 | 60 |
| Acq.time (t2) (ms) | 6.8 | 9 | 10 |
| sw (t3) (ppm) | 52 | 15 | 52 |
| Acq.time (t3) (ms) | 20.4 | 16 | 15 |

**1H decoupling**
- slppm

| Interscan delay (s) | 1.1 | 1.1 | 1.1 |
| Number of scans    | 4   | 4   | 12  |

| Experiment | H(H)NH | H(H)CH | (H)(H)CH | (H)(H)XH |
|------------|--------|--------|----------|----------|
| Transfer 1 | HN-CP  | HC-CP  | HC-CP    | HC-CP    |
| Max RF Field (kHz) (Ramp in H) | 150/30 | 169/51 | 167/51 | 149(H)/33(C)/ 31(N) |
| Time (ms)* | 1       | 1.2    | 0.35     | 1.5 (HN-CP) |
| Transfer 2 | NH-CP  | CH-CP  | CH-CP    | CH-CP    |
| Max RF Field (kHz) (Ramp in N) | 30/137 | 51/158 | 51/156 | 138H)/32(C)/ 31(N) |
| Time (ms)* | 0.4     | 0.35   | 0.2      | 1.5 (HN-CP) |
| Transfer 3 | -       | -      | -        | -        |
| Max RF Field (kHz) (Ramp in N) | -       | -      | -        | 149(H)/33(C)/ 31(N) |
| Time (ms)* | -       | -      | -        | 1.5 (HN-CP) |
| Transfer 4 | -       | -      | -        | CH-CP    |
| Max RF Field (kHz) (Ramp) | -       | -      | -        | 138H)/32(C)/ 31(N) |
| Time (ms)* | -       | -      | -        | 0.3 (HC-CP) |
| Mixing (ms)* | -       | -      | -        | 0.45 (HN-CP) |

| sw (t1) (ppm) | 22 | 15 | 15 | 290 |
| Acq.time (t1) (ms) | 4 | 4 | 4 | 4.5 |
| sw (t2) (ppm) | 52 | 30 | 30 | 268 |
| Acq.time (t2) (ms) | 40 | 36 | 36 | 4.5 |
|                  | 1  | 2  | 3  | 4  |
|------------------|----|----|----|----|
| $^{1}H$ decoupling RF field (kHz) | 22 | 22 | 22 | 22 |
| Interscan delay (s)    | 1.1| 1.1| 1.1| 1.1|
| Number of scans        | 4  | 2  | 4  | 2  |
| Measurement time (h)   | 26 | 36 | 54 | 122|
### Table S5: CYANA table output from the structure calculation.

| Cycle | 1    | 2    | 3    | 4    | 5    | 6    | 7    | final |
|-------|------|------|------|------|------|------|------|-------|
| Peaks |      |      |      |      |      |      |      |       |
| Selected | 3095 | 3095 | 3095 | 3095 | 3095 | 3095 | 3095 | 3095  |
| Assigned | 1311 | 1389 | 1366 | 1369 | 1339 | 1319 | 1315 |       |
| Unassigned | 1784 | 1706 | 1729 | 1726 | 1756 | 1776 | 1780 |       |
| With diagonal assignment | 6    | 6    | 6    | 6    | 6    | 6    | 6    |       |
| Cross peaks |      |      |      |      |      |      |      |       |
| With off-diagonal assignment | 1305 | 1383 | 1360 | 1363 | 1333 | 1313 | 1309 |       |
| With unique assignment | 556  | 823  | 852  | 866  | 946  | 972  | 970  |       |
| With short-range assignment | 1017 | 1165 | 1141 | 1134 | 1101 | 1089 | 1091 |       |
| With medium-range assignment 1<i-j<5 | 143  | 180  | 176  | 188  | 176  | 173  | 170  |       |
| With long-range assignment | 145  | 38   | 43   | 41   | 56   | 51   | 48   |       |
| With intermolecular assignment | 0    | 8    | 15   | 13   | 14   | 13   | 13   |       |
| Upper distance limits |      |      |      |      |      |      |      |       |
| Total | 1350 | 1276 | 1216 | 1196 | 1116 | 1056 | 1084 | 1081  |
| Short-range 1<i-j<1 | 790  | 882  | 820  | 778  | 700  | 666  | 636  | 635   |
| Medium-range 1<i-j<5 | 430  | 388  | 316  | 338  | 310  | 296  | 316  | 314   |
| Long-range | 130  | 6    | 80   | 80   | 106  | 94   | 132  | 132   |
| Average assignments/restraint | 7.52 | 2.59 | 1.94 | 1.85 | 1.63 | 1.51 | 1.00 |       |
| Average target function value | 634.46 | 159.70 | 109.91 | 23.09 | 15.79 | 12.76 | 11.18 | 9.96 |
| RMSD (residues 27..43, 128..154): |      |      |      |      |      |      |      |       |
| Average backbone RMSD to mean | 4.47 | 0.69 | 0.31 | 0.34 | 0.32 | 0.32 | 0.37 | 0.35  |
| Average heavy atom RMSD to mean | 5.19 | 1.31 | 0.87 | 0.88 | 0.95 | 0.87 | 0.95 | 0.87  |
### Table S4. Tetramer PDB coordinates used for the tetramer DFT calculations.

| REMARK | Molecule | Name | created | by GaussView | 5.0.8 |
|--------|----------|------|---------|-------------|-------|
| HETATM | H        | 0    | -17,202 | 0.199       | -12.718 | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -22,710 | -9.536     | -17.717 | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -17,679 | -2.928     | -4.853  | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -25,069 | -11.670    | -4.560  | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -10,260 | -4.336     | -8.087  | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -13,393 | -15.937    | -9.386  | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -10,087 | -2.063     | -16.808 | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -10,426 | -12.075    | -22.668 | 0.00 | 0.00 | H |
| HETATM | N        | 0    | -18,156 | 0.453      | -12.504 | 0.00 | 0.00 | N |
| HETATM | H        | 0    | -18,121 | 1.298      | -12.009 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -18,776 | -0.713     | -11.900 | 0.00 | 0.00 | C |
| HETATM | H        | 0    | -18,095 | -1.548     | -11.975 | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -18,963 | -0.507     | -10.857 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -20,084 | -1.085     | -12.568 | 0.00 | 0.00 | C |
| HETATM | O        | 0    | -20,290 | -2.239     | -12.944 | 0.00 | 0.00 | O |
| HETATM | N        | 0    | -20,971 | -0.106     | -12.716 | 0.00 | 0.00 | N |
| HETATM | H        | 0    | -20,748 | 0.793      | -12.396 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -22,266 | -0.338     | -13.342 | 0.00 | 0.00 | C |
| HETATM | H        | 0    | -22,802 | -1.059     | -12.742 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -23,099 | 0.956      | -13.407 | 0.00 | 0.00 | C |
| HETATM | H        | 0    | -23,310 | 1.273      | -12.397 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -22,311 | 2.059      | -14.096 | 0.00 | 0.00 | C |
| HETATM | H        | 0    | -22,801 | 3.009      | -13.930 | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -21,311 | 2.095      | -13.691 | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -22,263 | 1.860      | -15.156 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -24,420 | 0.702      | -14.137 | 0.00 | 0.00 | C |
| HETATM | H        | 0    | -25,034 | 1.586      | -14.076 | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -24,212 | 0.483      | -15.174 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -25,212 | -0.454     | -13.567 | 0.00 | 0.00 | C |
| HETATM | H        | 0    | -24,861 | -0.674     | -12.570 | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -26,259 | -0.188     | -13.528 | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -25,085 | -1.323     | -14.195 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -22,103 | -0.894     | -14.754 | 0.00 | 0.00 | C |
| HETATM | O        | 0    | -22,784 | -1.845     | -15.140 | 0.00 | 0.00 | O |
| HETATM | N        | 0    | -21,193 | -0.298     | -15.517 | 0.00 | 0.00 | N |
| HETATM | H        | 0    | -20,681 | 0.454      | -15.153 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -20,938 | -0.736     | -16.885 | 0.00 | 0.00 | C |
| HETATM | H        | 0    | -21,887 | -0.796     | -17.396 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -20,046 | 0.276      | -17.607 | 0.00 | 0.00 | C |
| HETATM | H        | 0    | -20,329 | 0.282      | -18.648 | 0.00 | 0.00 | H |
| HETATM | H        | 0    | -20,237 | 1.249      | -17.178 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -18,541 | 0.017      | -17.532 | 0.00 | 0.00 | C |
| HETATM | H        | 0    | -18,301 | -0.391     | -16.560 | 0.00 | 0.00 | H |
| HETATM | C        | 0    | -18,121 | -0.996     | -18.584 | 0.00 | 0.00 | C |
**SUPPORTING INFORMATION**

| HETATM | 45   | H    | 0    | -18.946 | -1.182  | -19.256 | 0.00 | 0.00 | H         |
|--------|------|------|------|---------|---------|---------|------|------|-----------|
| HETATM | 46   | H    | 0    | -17.282 | -0.608  | -19.143 | 0.00 | 0.00 | H         |
| HETATM | 47   | H    | 0    | -17.836 | -1.920  | -18.101 | 0.00 | 0.00 | H         |
| HETATM | 48   | C    | 0    | -17.768 | 1.317   | -17.702 | 0.00 | 0.00 | C         |
| HETATM | 49   | H    | 0    | -16.779 | 1.204   | -17.283 | 0.00 | 0.00 | H         |
| HETATM | 50   | H    | 0    | -17.690 | 1.554   | -18.752 | 0.00 | 0.00 | H         |
| HETATM | 51   | H    | 0    | -18.286 | 2.114   | -17.190 | 0.00 | 0.00 | H         |
| HETATM | 52   | C    | 0    | -20.282 | -2.113  | -16.902 | 0.00 | 0.00 | C         |
| HETATM | 53   | O    | 0    | -20.514 | -2.911  | -17.812 | 0.00 | 0.00 | O         |
| HETATM | 54   | N    | 0    | -19.463 | -2.386  | -15.892 | 0.00 | 0.00 | N         |
| HETATM | 55   | H    | 0    | -19.318 | -1.709  | -15.198 | 0.00 | 0.00 | H         |
| HETATM | 56   | C    | 0    | -18.775 | -3.668  | -15.790 | 0.00 | 0.00 | C         |
| HETATM | 57   | H    | 0    | -18.260 | -3.844  | -16.722 | 0.00 | 0.00 | H         |
| HETATM | 58   | C    | 0    | -17.751 | -3.632  | -14.655 | 0.00 | 0.00 | C         |
| HETATM | 59   | H    | 0    | -16.923 | -3.003  | -14.946 | 0.00 | 0.00 | H         |
| HETATM | 60   | H    | 0    | -18.217 | -3.221  | -13.771 | 0.00 | 0.00 | H         |
| HETATM | 61   | C    | 0    | -17.201 | -4.980  | -14.302 | 0.00 | 0.00 | C         |
| HETATM | 62   | N    | 0    | -17.460 | -5.608  | -13.101 | 0.00 | 0.00 | N         |
| HETATM | 63   | C    | 0    | -16.405 | -5.822  | -15.001 | 0.00 | 0.00 | C         |
| HETATM | 64   | C    | 0    | -16.844 | -6.776  | -13.076 | 0.00 | 0.00 | C         |
| HETATM | 65   | N    | 0    | -16.198 | -6.931  | -14.217 | 0.00 | 0.00 | N         |
| HETATM | 66   | H    | 0    | -16.006 | -5.655  | -15.992 | 0.00 | 0.00 | H         |
| HETATM | 67   | H    | 0    | -16.865 | -7.485  | -12.262 | 0.00 | 0.00 | H         |
| HETATM | 68   | H    | 0    | -15.658 | -7.712  | -14.482 | 0.00 | 0.00 | H         |
| HETATM | 69   | C    | 0    | -19.770 | -4.801  | -15.558 | 0.00 | 0.00 | C         |
| HETATM | 70   | O    | 0    | -19.637 | -5.885  | -16.128 | 0.00 | 0.00 | O         |
| HETATM | 71   | N    | 0    | -20.767 | -4.545  | -14.718 | 0.00 | 0.00 | N         |
| HETATM | 72   | H    | 0    | -20.820 | -3.662  | -14.295 | 0.00 | 0.00 | H         |
| HETATM | 73   | C    | 0    | -21.784 | -5.543  | -14.410 | 0.00 | 0.00 | C         |
| HETATM | 74   | H    | 0    | -21.279 | -6.459  | -14.142 | 0.00 | 0.00 | H         |
| HETATM | 75   | C    | 0    | -22.640 | -5.080  | -13.230 | 0.00 | 0.00 | C         |
| HETATM | 76   | H    | 0    | -21.994 | -4.982  | -12.371 | 0.00 | 0.00 | H         |
| HETATM | 77   | H    | 0    | -23.052 | -4.113  | -13.479 | 0.00 | 0.00 | H         |
| HETATM | 78   | C    | 0    | -23.799 | -5.999  | -12.840 | 0.00 | 0.00 | C         |
| HETATM | 79   | H    | 0    | -24.050 | -5.830  | -11.802 | 0.00 | 0.00 | H         |
| HETATM | 80   | C    | 0    | -25.030 | -5.689  | -13.677 | 0.00 | 0.00 | C         |
| HETATM | 81   | H    | 0    | -24.997 | -6.262  | -14.592 | 0.00 | 0.00 | H         |
| HETATM | 82   | H    | 0    | -25.918 | -5.950  | -13.121 | 0.00 | 0.00 | H         |
| HETATM | 83   | H    | 0    | -25.049 | -4.636  | -13.913 | 0.00 | 0.00 | H         |
| HETATM | 84   | C    | 0    | -23.399 | -7.458  | -12.997 | 0.00 | 0.00 | C         |
| HETATM | 85   | H    | 0    | -23.506 | -7.752  | -14.031 | 0.00 | 0.00 | H         |
| HETATM | 86   | H    | 0    | -22.370 | -7.584  | -12.692 | 0.00 | 0.00 | H         |
| HETATM | 87   | H    | 0    | -24.036 | -8.075  | -12.390 | 0.00 | 0.00 | H         |
| HETATM | 88   | C    | 0    | -22.671 | -5.808  | -15.623 | 0.00 | 0.00 | C         |
| HETATM | 89   | O    | 0    | -22.823 | -6.951  | -16.054 | 0.00 | 0.00 | O         |
| HETATM | 90   | N    | 0    | -23.252 | -4.745  | -16.168 | 0.00 | 0.00 | N         |
| HETATM | 91   | H    | 0    | -23.093 | -3.860  | -15.779 | 0.00 | 0.00 | H         |
| HETATM | 92   | C    | 0    | -24.121 | -4.864  | -17.333 | 0.00 | 0.00 | C         |
| SUPPORTING INFORMATION |
|------------------------|
| **HETATM** | 93 | H | 0 | -24.976 | -5.462 | -17.051 | 0.00 | 0.00 | H |
| **HETATM** | 94 | C | 0 | -24.628 | -3.486 | -17.799 | 0.00 | 0.00 | C |
| **HETATM** | 95 | H | 0 | -25.126 | -3.010 | -16.969 | 0.00 | 0.00 | H |
| **HETATM** | 96 | C | 0 | -23.459 | -2.606 | -18.218 | 0.00 | 0.00 | C |
| **HETATM** | 97 | H | 0 | -23.815 | -1.606 | -18.417 | 0.00 | 0.00 | H |
| **HETATM** | 98 | H | 0 | -22.728 | -2.578 | -17.423 | 0.00 | 0.00 | H |
| **HETATM** | 99 | H | 0 | -23.005 | -3.011 | -19.110 | 0.00 | 0.00 | H |
| **HETATM** | 100 | C | 0 | -25.620 | -3.648 | -18.953 | 0.00 | 0.00 | C |
| **HETATM** | 101 | H | 0 | -25.932 | -2.671 | -19.290 | 0.00 | 0.00 | H |
| **HETATM** | 102 | H | 0 | -25.134 | -4.166 | -19.766 | 0.00 | 0.00 | H |
| **HETATM** | 103 | C | 0 | -26.860 | -4.427 | -18.578 | 0.00 | 0.00 | C |
| **HETATM** | 104 | H | 0 | -26.901 | -5.339 | -19.157 | 0.00 | 0.00 | H |
| **HETATM** | 105 | H | 0 | -26.829 | -4.670 | -17.527 | 0.00 | 0.00 | H |
| **HETATM** | 106 | H | 0 | -27.737 | -3.831 | -18.784 | 0.00 | 0.00 | H |
| **HETATM** | 107 | C | 0 | -23.401 | -5.546 | -18.489 | 0.00 | 0.00 | C |
| **HETATM** | 108 | O | 0 | -23.994 | -6.332 | -19.229 | 0.00 | 0.00 | O |
| **HETATM** | 109 | N | 0 | -22.115 | -5.244 | -18.639 | 0.00 | 0.00 | N |
| **HETATM** | 110 | H | 0 | -21.697 | -4.612 | -18.019 | 0.00 | 0.00 | H |
| **HETATM** | 111 | C | 0 | -21.310 | -5.831 | -19.706 | 0.00 | 0.00 | C |
| **HETATM** | 112 | H | 0 | -21.869 | -5.748 | -20.625 | 0.00 | 0.00 | H |
| **HETATM** | 113 | C | 0 | -19.992 | -5.070 | -19.853 | 0.00 | 0.00 | C |
| **HETATM** | 114 | H | 0 | -20.206 | -4.017 | -19.755 | 0.00 | 0.00 | H |
| **HETATM** | 115 | H | 0 | -19.340 | -5.380 | -19.049 | 0.00 | 0.00 | H |
| **HETATM** | 116 | C | 0 | -19.243 | -5.274 | -21.171 | 0.00 | 0.00 | C |
| **HETATM** | 117 | H | 0 | -18.413 | -4.583 | -21.217 | 0.00 | 0.00 | H |
| **HETATM** | 118 | C | 0 | -18.682 | -6.685 | -21.251 | 0.00 | 0.00 | C |
| **HETATM** | 119 | H | 0 | -18.597 | -7.098 | -20.257 | 0.00 | 0.00 | H |
| **HETATM** | 120 | H | 0 | -19.343 | -7.303 | -21.842 | 0.00 | 0.00 | H |
| **HETATM** | 121 | H | 0 | -17.706 | -6.659 | -21.714 | 0.00 | 0.00 | H |
| **HETATM** | 122 | C | 0 | -20.158 | -4.993 | -22.354 | 0.00 | 0.00 | C |
| **HETATM** | 123 | H | 0 | -20.965 | -4.349 | -22.039 | 0.00 | 0.00 | H |
| **HETATM** | 124 | H | 0 | -19.594 | -4.508 | -23.138 | 0.00 | 0.00 | H |
| **HETATM** | 125 | H | 0 | -20.563 | -5.924 | -22.724 | 0.00 | 0.00 | H |
| **HETATM** | 126 | C | 0 | -21.032 | -7.305 | -19.430 | 0.00 | 0.00 | C |
| **HETATM** | 127 | O | 0 | -21.045 | -8.130 | -20.343 | 0.00 | 0.00 | O |
| **HETATM** | 128 | N | 0 | -20.783 | -7.628 | -18.166 | 0.00 | 0.00 | N |
| **HETATM** | 129 | H | 0 | -20.787 | -6.925 | -17.482 | 0.00 | 0.00 | H |
| **HETATM** | 130 | C | 0 | -20.503 | -9.003 | -17.770 | 0.00 | 0.00 | C |
| **HETATM** | 131 | H | 0 | -19.688 | -9.364 | -18.379 | 0.00 | 0.00 | H |
| **HETATM** | 132 | C | 0 | -20.086 | -8.058 | -16.300 | 0.00 | 0.00 | C |
| **HETATM** | 133 | H | 0 | -19.222 | -8.427 | -16.153 | 0.00 | 0.00 | H |
| **HETATM** | 134 | H | 0 | -20.900 | -8.695 | -15.688 | 0.00 | 0.00 | H |
| **HETATM** | 135 | C | 0 | -19.736 | -10.438 | -15.831 | 0.00 | 0.00 | C |
| **HETATM** | 136 | C | 0 | -18.484 | -10.970 | -15.717 | 0.00 | 0.00 | C |
| **HETATM** | 137 | C | 0 | -20.649 | -11.460 | -15.418 | 0.00 | 0.00 | C |
| **HETATM** | 138 | C | 0 | -22.040 | -11.533 | -15.310 | 0.00 | 0.00 | C |
| **HETATM** | 139 | C | 0 | -19.880 | -12.587 | -15.065 | 0.00 | 0.00 | C |
| **HETATM** | 140 | N | 0 | -18.563 | -12.263 | -15.257 | 0.00 | 0.00 | N |
| ATOM | ELEMENT | X-VALUE | Y-VALUE | Z-VALUE | TEMP | SCALE |
|------|---------|---------|---------|---------|------|-------|
| 141  | H       | -17.574 | -10.443 | -15.958 | 0.00 | 0.00  |
| 142  | H       | -22.665 | -10.692 | -15.570 | 0.00 | 0.00  |
| 143  | C       | -22.612 | -12.708 | -14.862 | 0.00 | 0.00  |
| 144  | C       | -20.459 | -13.770 | -14.613 | 0.00 | 0.00  |
| 145  | H       | -17.799 | -12.856 | -15.092 | 0.00 | 0.00  |
| 146  | H       | -23.686 | -12.783 | -14.772 | 0.00 | 0.00  |
| 147  | C       | -21.823 | -13.813 | -14.517 | 0.00 | 0.00  |
| 148  | H       | -19.863 | -14.630 | -14.344 | 0.00 | 0.00  |
| 149  | H       | -22.313 | -14.710 | -14.172 | 0.00 | 0.00  |
| 150  | C       | -21.720 | -9.894  | -17.999 | 0.00 | 0.00  |
| 151  | O       | -21.596 | -11.012 | -18.498 | 0.00 | 0.00  |
| 152  | N       | -18.143 | -2.337  | -4.178  | 0.00 | 0.00  |
| 153  | H       | -17.615 | -1.514  | -4.111  | 0.00 | 0.00  |
| 154  | C       | -18.372 | -3.147  | -2.995  | 0.00 | 0.00  |
| 155  | H       | -17.820 | -4.070  | -3.093  | 0.00 | 0.00  |
| 156  | H       | -18.009 | -2.613  | -2.131  | 0.00 | 0.00  |
| 157  | C       | -19.838 | -3.473  | -2.790  | 0.00 | 0.00  |
| 158  | O       | -20.215 | -4.641  | -2.703  | 0.00 | 0.00  |
| 159  | N       | -20.666 | -2.436  | -2.710  | 0.00 | 0.00  |
| 160  | H       | -20.306 | -1.529  | -2.786  | 0.00 | 0.00  |
| 161  | C       | -22.099 | -2.618  | -2.511  | 0.00 | 0.00  |
| 162  | H       | -22.237 | -3.381  | -1.760  | 0.00 | 0.00  |
| 163  | C       | -22.767 | -1.322  | -2.016  | 0.00 | 0.00  |
| 164  | H       | -22.310 | -1.044  | -1.078  | 0.00 | 0.00  |
| 165  | C       | -22.536 | -0.193  | -3.009  | 0.00 | 0.00  |
| 166  | H       | -21.580 | -0.330  | -3.492  | 0.00 | 0.00  |
| 167  | H       | -23.319 | -0.201  | -3.752  | 0.00 | 0.00  |
| 168  | H       | -22.544 | 0.753   | -2.487  | 0.00 | 0.00  |
| 169  | C       | -24.264 | -1.546  | -1.796  | 0.00 | 0.00  |
| 170  | H       | -24.811 | -1.130  | -2.627  | 0.00 | 0.00  |
| 171  | H       | -24.457 | -2.609  | -1.739  | 0.00 | 0.00  |
| 172  | C       | -24.791 | -0.909  | -0.529  | 0.00 | 0.00  |
| 173  | H       | -25.020 | 0.130   | -0.716  | 0.00 | 0.00  |
| 174  | H       | -25.686 | -1.424  | -0.212  | 0.00 | 0.00  |
| 175  | H       | -24.043 | -0.979  | 0.247   | 0.00 | 0.00  |
| 176  | C       | -22.779 | -3.066  | -3.801  | 0.00 | 0.00  |
| 177  | O       | -23.608 | -3.978  | -3.793  | 0.00 | 0.00  |
| 178  | N       | -22.424 | -2.422  | -4.906  | 0.00 | 0.00  |
| 179  | H       | -21.759 | -1.705  | -4.849  | 0.00 | 0.00  |
| 180  | C       | -22.998 | -2.756  | -6.205  | 0.00 | 0.00  |
| 181  | H       | -24.048 | -2.501  | -6.178  | 0.00 | 0.00  |
| 182  | C       | -22.317 | -1.945  | -7.309  | 0.00 | 0.00  |
| 183  | H       | -22.341 | -0.906  | -7.019  | 0.00 | 0.00  |
| 184  | H       | -21.290 | -2.276  | -7.375  | 0.00 | 0.00  |
| 185  | C       | -22.937 | -2.057  | -8.702  | 0.00 | 0.00  |
| 186  | H       | -22.572 | -1.246  | -9.318  | 0.00 | 0.00  |
| 187  | C       | -22.533 | -3.366  | -9.363  | 0.00 | 0.00  |
| 188  | H       | -22.079 | -3.161  | -10.321 | 0.00 | 0.00  |
| HETATM | 189 | H | 0 | -21.825 | -3.884 | -8.733 | 0.00 | 0.00 | H |
|--------|-----|---|---|---------|--------|--------|------|------|---|
| HETATM | 190 | H | 0 | -23.408 | -3.983 | -9.505 | 0.00 | 0.00 | H |
| HETATM | 191 | C | 0 | -24.453 | -1.943 | -8.622 | 0.00 | 0.00 | C |
| HETATM | 192 | H | 0 | -24.719 | -1.175 | -7.912 | 0.00 | 0.00 | H |
| HETATM | 193 | H | 0 | -24.846 | -1.686 | -9.596 | 0.00 | 0.00 | H |
| HETATM | 194 | H | 0 | -24.868 | -2.887 | -8.304 | 0.00 | 0.00 | H |
| HETATM | 195 | C | 0 | -22.862 | -4.247 | -6.494 | 0.00 | 0.00 | C |
| HETATM | 196 | O | 0 | -23.853 | -4.937 | -6.736 | 0.00 | 0.00 | O |
| HETATM | 197 | N | 0 | -21.627 | -4.739 | -6.466 | 0.00 | 0.00 | N |
| HETATM | 198 | H | 0 | -20.878 | -4.140 | -6.266 | 0.00 | 0.00 | H |
| HETATM | 199 | C | 0 | -21.361 | -6.150 | -6.721 | 0.00 | 0.00 | C |
| HETATM | 200 | H | 0 | -21.851 | -6.417 | -7.645 | 0.00 | 0.00 | H |
| HETATM | 201 | C | 0 | -19.858 | -6.388 | -6.868 | 0.00 | 0.00 | C |
| HETATM | 202 | H | 0 | -19.337 | -5.849 | -6.922 | 0.00 | 0.00 | H |
| HETATM | 203 | H | 0 | -19.655 | -7.445 | -6.764 | 0.00 | 0.00 | H |
| HETATM | 204 | C | 0 | -19.306 | -5.942 | -8.187 | 0.00 | 0.00 | C |
| HETATM | 205 | N | 0 | -19.489 | -4.670 | -8.687 | 0.00 | 0.00 | N |
| HETATM | 206 | C | 0 | -18.571 | -6.605 | -9.110 | 0.00 | 0.00 | C |
| HETATM | 207 | C | 0 | -18.892 | -4.571 | -9.862 | 0.00 | 0.00 | C |
| HETATM | 208 | N | 0 | -18.327 | -5.731 | -10.141 | 0.00 | 0.00 | N |
| HETATM | 209 | H | 0 | -18.239 | -7.633 | -9.049 | 0.00 | 0.00 | H |
| HETATM | 210 | H | 0 | -18.866 | -3.691 | -10.487 | 0.00 | 0.00 | H |
| HETATM | 211 | H | 0 | -17.818 | -5.933 | -10.953 | 0.00 | 0.00 | H |
| HETATM | 212 | C | 0 | -21.918 | -7.021 | -5.600 | 0.00 | 0.00 | C |
| HETATM | 213 | O | 0 | -22.414 | -8.122 | -5.843 | 0.00 | 0.00 | O |
| HETATM | 214 | N | 0 | -21.834 | -6.521 | -4.371 | 0.00 | 0.00 | N |
| HETATM | 215 | H | 0 | -21.428 | -5.639 | -4.241 | 0.00 | 0.00 | H |
| HETATM | 216 | C | 0 | -22.330 | -7.254 | -3.212 | 0.00 | 0.00 | C |
| HETATM | 217 | H | 0 | -21.689 | -8.110 | -3.062 | 0.00 | 0.00 | H |
| HETATM | 218 | C | 0 | -22.280 | -6.369 | -1.966 | 0.00 | 0.00 | C |
| HETATM | 219 | H | 0 | -21.253 | -6.309 | -1.642 | 0.00 | 0.00 | H |
| HETATM | 220 | H | 0 | -22.624 | -5.383 | -2.247 | 0.00 | 0.00 | H |
| HETATM | 221 | C | 0 | -23.119 | -6.837 | -0.775 | 0.00 | 0.00 | C |
| HETATM | 222 | H | 0 | -24.121 | -7.059 | -1.115 | 0.00 | 0.00 | H |
| HETATM | 223 | C | 0 | -22.534 | -8.107 | -0.177 | 0.00 | 0.00 | C |
| HETATM | 224 | H | 0 | -21.688 | -7.855 | 0.444 | 0.00 | 0.00 | H |
| HETATM | 225 | H | 0 | -23.285 | -8.603 | 0.420 | 0.00 | 0.00 | H |
| HETATM | 226 | H | 0 | -22.214 | -8.765 | -0.972 | 0.00 | 0.00 | H |
| HETATM | 227 | C | 0 | -23.209 | -5.742 | 0.277 | 0.00 | 0.00 | C |
| HETATM | 228 | H | 0 | -23.685 | -6.133 | 1.164 | 0.00 | 0.00 | H |
| HETATM | 229 | H | 0 | -22.216 | -5.396 | 0.524 | 0.00 | 0.00 | H |
| HETATM | 230 | H | 0 | -23.791 | -4.918 | -0.109 | 0.00 | 0.00 | H |
| HETATM | 231 | C | 0 | -23.756 | -7.743 | -3.445 | 0.00 | 0.00 | C |
| HETATM | 232 | O | 0 | -24.012 | -8.947 | -3.474 | 0.00 | 0.00 | O |
| HETATM | 233 | N | 0 | -24.678 | -8.802 | -3.613 | 0.00 | 0.00 | N |
| HETATM | 234 | H | 0 | -24.412 | -5.860 | -3.581 | 0.00 | 0.00 | H |
| HETATM | 235 | C | 0 | -26.077 | -7.138 | -3.849 | 0.00 | 0.00 | C |
| HETATM | 236 | H | 0 | -26.393 | -7.815 | -3.068 | 0.00 | 0.00 | H |
SUPPORTING INFORMATION

| HETATM | 237 | C | 0 | -26.974 | -5.887 | -3.797 | 0.00 | 0.00 | C |
| HETATM | 238 | H | 0 | -27.903 | -6.115 | -4.293 | 0.00 | 0.00 | H |
| HETATM | 239 | C | 0 | -27.285 | -5.518 | -2.353 | 0.00 | 0.00 | C |
| HETATM | 240 | H | 0 | -26.548 | -4.816 | -1.994 | 0.00 | 0.00 | H |
| HETATM | 241 | H | 0 | -28.267 | -5.069 | -2.300 | 0.00 | 0.00 | H |
| HETATM | 242 | H | 0 | -27.263 | -6.409 | -1.742 | 0.00 | 0.00 | H |
| HETATM | 243 | C | 0 | -26.297 | -4.717 | -4.515 | 0.00 | 0.00 | C |
| HETATM | 244 | H | 0 | -25.896 | -4.035 | -3.782 | 0.00 | 0.00 | H |
| HETATM | 245 | H | 0 | -25.490 | -5.099 | -5.125 | 0.00 | 0.00 | H |
| HETATM | 246 | C | 0 | -27.230 | -3.939 | -5.414 | 0.00 | 0.00 | C |
| HETATM | 247 | H | 0 | -27.788 | -3.227 | -4.825 | 0.00 | 0.00 | H |
| HETATM | 248 | H | 0 | -26.656 | -3.414 | -6.163 | 0.00 | 0.00 | H |
| HETATM | 249 | H | 0 | -27.915 | -4.620 | -5.089 | 0.00 | 0.00 | H |
| HETATM | 250 | C | 0 | -26.259 | -7.823 | -5.198 | 0.00 | 0.00 | C |
| HETATM | 251 | O | 0 | -27.142 | -8.665 | -5.366 | 0.00 | 0.00 | O |
| HETATM | 252 | N | 0 | -25.416 | -7.459 | -6.159 | 0.00 | 0.00 | N |
| HETATM | 253 | H | 0 | -24.734 | -6.783 | -5.965 | 0.00 | 0.00 | H |
| HETATM | 254 | C | 0 | -25.482 | -8.040 | -7.495 | 0.00 | 0.00 | C |
| HETATM | 255 | H | 0 | -26.392 | -7.694 | -7.962 | 0.00 | 0.00 | H |
| HETATM | 256 | C | 0 | -24.286 | -7.582 | -8.332 | 0.00 | 0.00 | C |
| HETATM | 257 | H | 0 | -24.234 | -6.505 | -8.272 | 0.00 | 0.00 | H |
| HETATM | 258 | H | 0 | -23.395 | -8.009 | -7.884 | 0.00 | 0.00 | H |
| HETATM | 259 | C | 0 | -24.315 | -7.967 | -9.811 | 0.00 | 0.00 | C |
| HETATM | 260 | H | 0 | -23.597 | -7.361 | -10.347 | 0.00 | 0.00 | H |
| HETATM | 261 | C | 0 | -23.924 | -9.426 | -9.990 | 0.00 | 0.00 | C |
| HETATM | 262 | H | 0 | -23.194 | -9.508 | -10.782 | 0.00 | 0.00 | H |
| HETATM | 263 | H | 0 | -23.501 | -9.801 | -9.070 | 0.00 | 0.00 | H |
| HETATM | 264 | H | 0 | -24.799 | -10.004 | -10.246 | 0.00 | 0.00 | H |
| HETATM | 265 | C | 0 | -27.691 | -7.705 | -10.404 | 0.00 | 0.00 | C |
| HETATM | 266 | H | 0 | -24.906 | -8.626 | -10.424 | 0.00 | 0.00 | H |
| HETATM | 267 | H | 0 | -26.212 | -6.978 | -9.798 | 0.00 | 0.00 | H |
| HETATM | 268 | H | 0 | -25.584 | -7.326 | -11.410 | 0.00 | 0.00 | H |
| HETATM | 269 | C | 0 | -25.515 | -9.564 | -7.426 | 0.00 | 0.00 | C |
| HETATM | 270 | O | 0 | -26.469 | -10.195 | -7.880 | 0.00 | 0.00 | O |
| HETATM | 271 | N | 0 | -24.468 | -10.147 | -6.853 | 0.00 | 0.00 | N |
| HETATM | 272 | H | 0 | -23.739 | -9.589 | -6.509 | 0.00 | 0.00 | H |
| HETATM | 273 | C | 0 | -24.378 | -11.596 | -6.722 | 0.00 | 0.00 | C |
| HETATM | 274 | H | 0 | -24.754 | -12.035 | -7.635 | 0.00 | 0.00 | H |
| HETATM | 275 | C | 0 | -22.922 | -12.022 | -8.528 | 0.00 | 0.00 | C |
| HETATM | 276 | H | 0 | -22.592 | -11.720 | -6.545 | 0.00 | 0.00 | H |
| HETATM | 277 | H | 0 | -22.854 | -10.097 | -6.612 | 0.00 | 0.00 | H |
| HETATM | 278 | C | 0 | -21.988 | -11.420 | -7.534 | 0.00 | 0.00 | C |
| HETATM | 279 | C | 0 | -21.099 | -10.404 | -7.322 | 0.00 | 0.00 | C |
| HETATM | 280 | C | 0 | -21.854 | -11.793 | -8.910 | 0.00 | 0.00 | C |
| HETATM | 281 | C | 0 | -22.471 | -12.749 | -9.721 | 0.00 | 0.00 | C |
| HETATM | 282 | C | 0 | -20.863 | -10.964 | -9.471 | 0.00 | 0.00 | C |
| HETATM | 283 | N | 0 | -20.419 | -10.125 | -8.484 | 0.00 | 0.00 | N |
| HETATM | 284 | H | 0 | -20.962 | -9.904 | -6.376 | 0.00 | 0.00 | H |
### SUPPORTING INFORMATION

| HETATM | X  | Y  | Z   | AltLoc | Biso |
|--------|----|----|-----|--------|------|
| 285    | H  | 0  | -23.235 | -13.404 | -9.328 | 0.00 | 0.00 | H   |
| 286    | C  | 0  | -22.089 | -12.845 | -11.045 | 0.00 | 0.00 | C   |
| 287    | C  | 0  | -20.480 | -11.062 | -10.806 | 0.00 | 0.00 | C   |
| 288    | H  | 0  | -19.728 | -9.438  | -8.586  | 0.00 | 0.00 | H   |
| 289    | H  | 0  | -22.556 | -13.577 | -11.688 | 0.00 | 0.00 | H   |
| 290    | C  | 0  | -21.102 | -12.007 | -11.577 | 0.00 | 0.00 | C   |
| 291    | H  | 0  | -19.719 | -10.423 | -11.231 | 0.00 | 0.00 | H   |
| 292    | H  | 0  | -20.836 | -12.116 | -12.617 | 0.00 | 0.00 | H   |
| 293    | C  | 0  | -25.224 | -12.091 | -5.554  | 0.00 | 0.00 | C   |
| 294    | O  | 0  | -26.080 | -12.960 | -5.720  | 0.00 | 0.00 | O   |
| 295    | N  | 0  | -9.317  | -4.595  | -3.341  | 0.00 | 0.00 | N   |
| 296    | H  | 0  | -8.803  | -3.763  | -8.412  | 0.00 | 0.00 | H   |
| 297    | C  | 0  | -9.418  | -5.482  | -9.486  | 0.00 | 0.00 | C   |
| 298    | H  | 0  | -10.461 | -5.674  | -9.686  | 0.00 | 0.00 | H   |
| 299    | H  | 0  | -8.981  | -4.993  | -10.345 | 0.00 | 0.00 | H   |
| 300    | C  | 0  | -8.709  | -6.803  | -9.260  | 0.00 | 0.00 | C   |
| 301    | O  | 0  | -9.216  | -7.859  | -9.638  | 0.00 | 0.00 | O   |
| 302    | N  | 0  | -7.532  | -6.743  | -8.645  | 0.00 | 0.00 | N   |
| 303    | H  | 0  | -7.181  | -5.871  | -8.368  | 0.00 | 0.00 | H   |
| 304    | C  | 0  | -6.753  | -7.944  | -8.372  | 0.00 | 0.00 | C   |
| 305    | H  | 0  | -6.622  | -8.475  | -9.304  | 0.00 | 0.00 | H   |
| 306    | C  | 0  | -5.361  | -7.595  | -7.812  | 0.00 | 0.00 | C   |
| 307    | H  | 0  | -4.829  | -7.029  | -8.560  | 0.00 | 0.00 | H   |
| 308    | C  | 0  | -5.492  | -6.732  | -8.567  | 0.00 | 0.00 | C   |
| 309    | H  | 0  | -4.521  | -6.343  | -6.294  | 0.00 | 0.00 | H   |
| 310    | H  | 0  | -6.165  | -5.911  | -6.767  | 0.00 | 0.00 | H   |
| 311    | H  | 0  | -5.882  | -7.327  | -5.754  | 0.00 | 0.00 | H   |
| 312    | C  | 0  | -4.578  | -8.873  | -7.501  | 0.00 | 0.00 | C   |
| 313    | H  | 0  | -3.562  | -8.614  | -7.251  | 0.00 | 0.00 | H   |
| 314    | H  | 0  | -5.037  | -9.370  | -8.657  | 0.00 | 0.00 | H   |
| 315    | C  | 0  | -4.538  | -9.853  | -8.653  | 0.00 | 0.00 | C   |
| 316    | H  | 0  | -4.796  | -9.342  | -9.568  | 0.00 | 0.00 | H   |
| 317    | H  | 0  | -3.544  | -10.266 | -8.739  | 0.00 | 0.00 | H   |
| 318    | H  | 0  | -5.244  | -10.650 | -8.473  | 0.00 | 0.00 | H   |
| 319    | C  | 0  | -7.474  | -8.853  | -7.383  | 0.00 | 0.00 | C   |
| 320    | O  | 0  | -7.472  | -10.076 | -7.531  | 0.00 | 0.00 | O   |
| 321    | N  | 0  | -8.090  | -8.249  | -6.373  | 0.00 | 0.00 | N   |
| 322    | H  | 0  | -8.057  | -7.273  | -6.307  | 0.00 | 0.00 | H   |
| 323    | C  | 0  | -8.818  | -9.004  | -5.358  | 0.00 | 0.00 | C   |
| 324    | H  | 0  | -8.234  | -8.878  | -5.114  | 0.00 | 0.00 | H   |
| 325    | C  | 0  | -9.001  | -8.157  | -4.098  | 0.00 | 0.00 | C   |
| 326    | H  | 0  | -8.992  | -8.823  | -3.249  | 0.00 | 0.00 | H   |
| 327    | H  | 0  | -8.162  | -7.480  | -4.031  | 0.00 | 0.00 | H   |
| 328    | C  | 0  | -10.283 | -7.327  | -4.028  | 0.00 | 0.00 | C   |
| 329    | H  | 0  | -10.560 | -7.019  | -5.027  | 0.00 | 0.00 | H   |
| 330    | C  | 0  | -11.425 | -8.154  | -3.459  | 0.00 | 0.00 | C   |
| 331    | H  | 0  | -11.038 | -9.088  | -3.079  | 0.00 | 0.00 | H   |
| 332    | H  | 0  | -11.899 | -7.608  | -2.655  | 0.00 | 0.00 | H   |
| HETATM  | 333 | H   | 0   | -12.149 | -8.352 | -4.235 | 0.00  | 0.00  | H     |
|---------|-----|-----|-----|---------|--------|--------|-------|-------|-------|
| HETATM  | 334 | C   | 0   | -10.061 | -6.073 | -3.193 | 0.00  | 0.00  | C     |
| HETATM  | 335 | H   | 0   | -10.737 | -5.298 | -3.521 | 0.00  | 0.00  | H     |
| HETATM  | 336 | H   | 0   | -10.248 | -6.297 | -2.153 | 0.00  | 0.00  | H     |
| HETATM  | 337 | H   | 0   | -9.042  | -5.738 | -3.312 | 0.00  | 0.00  | H     |
| HETATM  | 338 | C   | 0   | -10.178 | -9.454 | -5.885 | 0.00  | 0.00  | C     |
| HETATM  | 339 | O   | 0   | -10.694 | -10.498 | -5.488 | 0.00  | 0.00  | O     |
| HETATM  | 340 | N   | 0   | -10.751 | -8.659 | -6.783 | 0.00  | 0.00  | N     |
| HETATM  | 341 | H   | 0   | -10.289 | -7.841 | -7.061 | 0.00  | 0.00  | H     |
| HETATM  | 342 | C   | 0   | -12.049 | -8.977 | -7.367 | 0.00  | 0.00  | C     |
| HETATM  | 343 | H   | 0   | -12.737 | -9.173 | -8.559 | 0.00  | 0.00  | H     |
| HETATM  | 344 | C   | 0   | -12.567 | -7.793 | -8.185 | 0.00  | 0.00  | C     |
| HETATM  | 345 | H   | 0   | -12.794 | -6.976 | -7.518 | 0.00  | 0.00  | H     |
| HETATM  | 346 | H   | 0   | -11.801 | -7.483 | -8.881 | 0.00  | 0.00  | H     |
| HETATM  | 347 | C   | 0   | -13.805 | -8.104 | -8.970 | 0.00  | 0.00  | C     |
| HETATM  | 348 | N   | 0   | -13.813 | -8.236 | -10.343 | 0.00  | 0.00  | N     |
| HETATM  | 349 | C   | 0   | -15.080 | -8.310 | -8.566 | 0.00  | 0.00  | C     |
| HETATM  | 350 | C   | 0   | -15.040 | -8.509 | -10.748 | 0.00  | 0.00  | C     |
| HETATM  | 351 | N   | 0   | -15.828 | -8.560 | -9.690 | 0.00  | 0.00  | N     |
| HETATM  | 352 | H   | 0   | -15.444 | -8.284 | -7.548 | 0.00  | 0.00  | H     |
| HETATM  | 353 | H   | 0   | -15.346 | -8.664 | -11.772 | 0.00  | 0.00  | H     |
| HETATM  | 354 | H   | 0   | -16.789 | -8.745 | -9.708 | 0.00  | 0.00  | H     |
| HETATM  | 355 | C   | 0   | -11.960 | -10.220 | -8.248 | 0.00  | 0.00  | C     |
| HETATM  | 356 | O   | 0   | -12.794 | -11.121 | -8.156 | 0.00  | 0.00  | O     |
| HETATM  | 357 | N   | 0   | -10.943 | -10.261 | -9.102  | 0.00  | 0.00  | N     |
| HETATM  | 358 | H   | 0   | -10.310 | -9.514 | -9.130  | 0.00  | 0.00  | H     |
| HETATM  | 359 | C   | 0   | -10.744 | -11.393 | -10.001 | 0.00  | 0.00  | C     |
| HETATM  | 360 | H   | 0   | -11.629 | -11.491 | -10.611 | 0.00  | 0.00  | H     |
| HETATM  | 361 | C   | 0   | -9.538  | -11.144 | -10.908 | 0.00  | 0.00  | C     |
| HETATM  | 362 | H   | 0   | -9.747  | -10.267 | -11.502 | 0.00  | 0.00  | H     |
| HETATM  | 363 | H   | 0   | -8.683  | -10.952 | -10.276 | 0.00  | 0.00  | H     |
| HETATM  | 364 | C   | 0   | -9.170  | -12.280 | -11.863 | 0.00  | 0.00  | C     |
| HETATM  | 365 | H   | 0   | -8.619  | -11.874 | -12.700 | 0.00  | 0.00  | H     |
| HETATM  | 366 | C   | 0   | -8.280  | -13.296 | -11.165 | 0.00  | 0.00  | C     |
| HETATM  | 367 | H   | 0   | -8.895  | -14.004 | -10.628 | 0.00  | 0.00  | H     |
| HETATM  | 368 | H   | 0   | -8.136  | -13.819 | -11.900 | 0.00  | 0.00  | H     |
| HETATM  | 369 | H   | 0   | -7.628  | -12.787 | -10.471 | 0.00  | 0.00  | H     |
| HETATM  | 370 | C   | 0   | -10.425 | -12.950 | -12.404 | 0.00  | 0.00  | C     |
| HETATM  | 371 | H   | 0   | -10.823 | -13.622 | -11.659 | 0.00  | 0.00  | H     |
| HETATM  | 372 | H   | 0   | -11.162 | -12.195 | -12.640 | 0.00  | 0.00  | H     |
| HETATM  | 373 | H   | 0   | -10.180 | -13.506 | -13.297 | 0.00  | 0.00  | H     |
| HETATM  | 374 | C   | 0   | -10.545 | -12.684 | -9.214  | 0.00  | 0.00  | C     |
| HETATM  | 375 | O   | 0   | -11.296 | -13.646 | -9.378  | 0.00  | 0.00  | O     |
| HETATM  | 376 | N   | 0   | -9.528  | -12.699 | -8.358  | 0.00  | 0.00  | N     |
| HETATM  | 377 | H   | 0   | -8.965  | -11.901 | -8.271  | 0.00  | 0.00  | H     |
| HETATM  | 378 | C   | 0   | -9.233  | -13.870 | -7.543  | 0.00  | 0.00  | C     |
| HETATM  | 379 | H   | 0   | -8.867  | -14.655 | -8.201  | 0.00  | 0.00  | H     |
| HETATM  | 380 | C   | 0   | -8.123  | -13.577 | -6.516  | 0.00  | 0.00  | C     |
|    |   |   |   |   |   |
|----|---|---|---|---|---|
| HETATM | 381 | H | 0 | -7.229 | -13.304 | -7.053 | 0.00 | 0.00 | H |
| HETATM | 382 | C | 0 | -8.520 | -12.404 | -5.631 | 0.00 | 0.00 | C |
| HETATM | 383 | H | 0 | -7.681 | -12.121 | -5.012 | 0.00 | 0.00 | H |
| HETATM | 384 | H | 0 | -8.810 | -11.567 | -6.249 | 0.00 | 0.00 | H |
| HETATM | 385 | H | 0 | -9.349 | -12.692 | -5.002 | 0.00 | 0.00 | H |
| HETATM | 386 | C | 0 | -7.841 | -14.819 | -5.669 | 0.00 | 0.00 | H |
| HETATM | 387 | H | 0 | -7.074 | -14.588 | -4.947 | 0.00 | 0.00 | H |
| HETATM | 388 | H | 0 | -8.744 | -15.105 | -5.149 | 0.00 | 0.00 | H |
| HETATM | 389 | C | 0 | -7.373 | -16.008 | -6.478 | 0.00 | 0.00 | C |
| HETATM | 390 | H | 0 | -8.098 | -16.805 | -6.399 | 0.00 | 0.00 | H |
| HETATM | 391 | H | 0 | -7.267 | -15.720 | -7.514 | 0.00 | 0.00 | H |
| HETATM | 392 | H | 0 | -6.420 | -16.344 | -6.101 | 0.00 | 0.00 | H |
| HETATM | 393 | C | 0 | -10.476 | -14.356 | -6.808 | 0.00 | 0.00 | C |
| HETATM | 394 | O | 0 | -10.697 | -15.560 | -6.667 | 0.00 | 0.00 | O |
| HETATM | 395 | N | 0 | -11.287 | -13.413 | -6.341 | 0.00 | 0.00 | N |
| HETATM | 396 | H | 0 | -11.059 | -12.472 | -6.484 | 0.00 | 0.00 | H |
| HETATM | 397 | C | 0 | -12.512 | -13.745 | -5.621 | 0.00 | 0.00 | C |
| HETATM | 398 | H | 0 | -12.274 | -14.511 | -4.888 | 0.00 | 0.00 | H |
| HETATM | 399 | C | 0 | -13.044 | -12.513 | -4.889 | 0.00 | 0.00 | C |
| HETATM | 400 | H | 0 | -12.196 | -11.944 | -4.538 | 0.00 | 0.00 | H |
| HETATM | 401 | H | 0 | -13.605 | -11.923 | -5.596 | 0.00 | 0.00 | H |
| HETATM | 402 | C | 0 | -13.949 | -12.788 | -3.683 | 0.00 | 0.00 | C |
| HETATM | 403 | H | 0 | -14.195 | -11.850 | -3.206 | 0.00 | 0.00 | H |
| HETATM | 404 | C | 0 | -15.247 | -13.442 | -4.131 | 0.00 | 0.00 | C |
| HETATM | 405 | H | 0 | -15.412 | -13.235 | -5.178 | 0.00 | 0.00 | H |
| HETATM | 406 | H | 0 | -15.182 | -14.509 | -3.981 | 0.00 | 0.00 | H |
| HETATM | 407 | H | 0 | -16.067 | -13.045 | -3.552 | 0.00 | 0.00 | H |
| HETATM | 408 | C | 0 | -13.232 | -13.663 | -2.665 | 0.00 | 0.00 | C |
| HETATM | 409 | H | 0 | -12.164 | -13.555 | -2.787 | 0.00 | 0.00 | H |
| HETATM | 410 | H | 0 | -13.512 | -13.359 | -1.668 | 0.00 | 0.00 | H |
| HETATM | 411 | H | 0 | -13.509 | -14.695 | -2.819 | 0.00 | 0.00 | H |
| HETATM | 412 | C | 0 | -13.575 | -14.282 | -6.573 | 0.00 | 0.00 | C |
| HETATM | 413 | O | 0 | -14.318 | -15.203 | -6.233 | 0.00 | 0.00 | O |
| HETATM | 414 | N | 0 | -13.641 | -13.701 | -7.766 | 0.00 | 0.00 | N |
| HETATM | 415 | H | 0 | -13.022 | -12.972 | -7.978 | 0.00 | 0.00 | H |
| HETATM | 416 | C | 0 | -14.613 | -14.124 | -8.768 | 0.00 | 0.00 | C |
| HETATM | 417 | H | 0 | -15.598 | -14.019 | -8.339 | 0.00 | 0.00 | H |
| HETATM | 418 | C | 0 | -14.514 | -13.236 | -10.009 | 0.00 | 0.00 | C |
| HETATM | 419 | H | 0 | -14.671 | -12.206 | -9.722 | 0.00 | 0.00 | H |
| HETATM | 420 | H | 0 | -13.528 | -13.338 | -10.439 | 0.00 | 0.00 | H |
| HETATM | 421 | C | 0 | -15.519 | -13.579 | -11.067 | 0.00 | 0.00 | C |
| HETATM | 422 | C | 0 | -16.740 | -12.999 | -11.257 | 0.00 | 0.00 | C |
| HETATM | 423 | C | 0 | -15.388 | -14.583 | -12.079 | 0.00 | 0.00 | C |
| HETATM | 424 | C | 0 | -14.388 | -15.501 | -12.412 | 0.00 | 0.00 | C |
| HETATM | 425 | C | 0 | -16.568 | -14.557 | -12.848 | 0.00 | 0.00 | C |
| HETATM | 426 | N | 0 | -17.378 | -13.582 | -12.326 | 0.00 | 0.00 | N |
| HETATM | 427 | H | 0 | -17.136 | -12.201 | -10.646 | 0.00 | 0.00 | H |
| HETATM | 428 | H | 0 | -13.469 | -15.555 | -11.848 | 0.00 | 0.00 | H |
| HETATM | 429 | C  | 0   | -14.594 | -16.350 | -13.483 | 0.00 | 0.00 | C     |
|--------|-----|----|-----|---------|---------|---------|------|------|-------|
| HETATM | 430 | C  | 0   | -16.773 | -15.413 | -13.926 | 0.00 | 0.00 | C     |
| HETATM | 431 | H  | 0   | -18.266 | -13.339 | -12.660 | 0.00 | 0.00 | H     |
| HETATM | 432 | H  | 0   | -13.833 | -17.068 | -13.755 | 0.00 | 0.00 | H     |
| HETATM | 433 | C  | 0   | -15.778 | -16.302 | -14.230 | 0.00 | 0.00 | C     |
| HETATM | 434 | H  | 0   | -17.681 | -15.386 | -14.512 | 0.00 | 0.00 | H     |
| HETATM | 435 | H  | 0   | -15.896 | -16.984 | -15.057 | 0.00 | 0.00 | H     |
| HETATM | 436 | C  | 0   | -14.398 | -15.583 | -9.154  | 0.00 | 0.00 | C     |
| HETATM | 437 | O  | 0   | -15.347 | -16.367 | -9.207  | 0.00 | 0.00 | O     |
| HETATM | 438 | N  | 0   | -9.159  | -1.760  | -17.067 | 0.00 | 0.00 | N     |
| HETATM | 439 | H  | 0   | -8.955  | -0.970  | -16.522 | 0.00 | 0.00 | H     |
| HETATM | 440 | C  | 0   | -9.137  | -1.664  | -18.515 | 0.00 | 0.00 | C     |
| HETATM | 441 | H  | 0   | -10.141 | -1.796  | -18.889 | 0.00 | 0.00 | H     |
| HETATM | 442 | H  | 0   | -8.786  | -0.680  | -18.793 | 0.00 | 0.00 | H     |
| HETATM | 443 | C  | 0   | -8.234  | -2.702  | -19.151 | 0.00 | 0.00 | C     |
| HETATM | 444 | O  | 0   | -8.422  | -3.071  | -20.309 | 0.00 | 0.00 | O     |
| HETATM | 445 | N  | 0   | -7.251  | -3.173  | -18.391 | 0.00 | 0.00 | N     |
| HETATM | 446 | H  | 0   | -7.152  | -2.841  | -17.474 | 0.00 | 0.00 | H     |
| HETATM | 447 | C  | 0   | -6.316  | -4.176  | -18.888 | 0.00 | 0.00 | C     |
| HETATM | 448 | H  | 0   | -6.576  | -4.395  | -19.914 | 0.00 | 0.00 | H     |
| HETATM | 449 | C  | 0   | -4.866  | -3.658  | -18.855 | 0.00 | 0.00 | C     |
| HETATM | 450 | H  | 0   | -4.767  | -2.831  | -19.544 | 0.00 | 0.00 | H     |
| HETATM | 451 | C  | 0   | -4.516  | -3.151  | -17.484 | 0.00 | 0.00 | C     |
| HETATM | 452 | H  | 0   | -5.293  | -2.488  | -17.116 | 0.00 | 0.00 | H     |
| HETATM | 453 | H  | 0   | -4.428  | -3.989  | -16.788 | 0.00 | 0.00 | H     |
| HETATM | 454 | H  | 0   | -3.577  | -2.618  | -17.501 | 0.00 | 0.00 | H     |
| HETATM | 455 | C  | 0   | -3.898  | -4.761  | -19.286 | 0.00 | 0.00 | C     |
| HETATM | 456 | H  | 0   | -3.402  | -5.157  | -18.414 | 0.00 | 0.00 | H     |
| HETATM | 457 | H  | 0   | -4.456  | -5.551  | -19.767 | 0.00 | 0.00 | H     |
| HETATM | 458 | C  | 0   | -2.833  | -4.288  | -20.251 | 0.00 | 0.00 | C     |
| HETATM | 459 | H  | 0   | -1.995  | -3.892  | -19.696 | 0.00 | 0.00 | H     |
| HETATM | 460 | H  | 0   | -2.502  | -5.118  | -20.857 | 0.00 | 0.00 | H     |
| HETATM | 461 | H  | 0   | -3.241  | -3.517  | -20.888 | 0.00 | 0.00 | H     |
| HETATM | 462 | C  | 0   | -6.404  | -5.461  | -18.073 | 0.00 | 0.00 | C     |
| HETATM | 463 | O  | 0   | -6.416  | -6.562  | -18.626 | 0.00 | 0.00 | O     |
| HETATM | 464 | N  | 0   | -6.466  | -5.316  | -16.754 | 0.00 | 0.00 | N     |
| HETATM | 465 | H  | 0   | -6.453  | -4.415  | -16.370 | 0.00 | 0.00 | H     |
| HETATM | 466 | C  | 0   | -6.554  | -6.465  | -15.860 | 0.00 | 0.00 | C     |
| HETATM | 467 | H  | 0   | -5.616  | -6.997  | -15.910 | 0.00 | 0.00 | H     |
| HETATM | 468 | C  | 0   | -6.788  | -6.001  | -14.421 | 0.00 | 0.00 | C     |
| HETATM | 469 | H  | 0   | -6.063  | -5.233  | -14.200 | 0.00 | 0.00 | H     |
| HETATM | 470 | H  | 0   | -7.783  | -5.582  | -14.368 | 0.00 | 0.00 | H     |
| HETATM | 471 | C  | 0   | -6.673  | -7.078  | -13.341 | 0.00 | 0.00 | C     |
| HETATM | 472 | H  | 0   | -6.583  | -6.602  | -12.375 | 0.00 | 0.00 | H     |
| HETATM | 473 | C  | 0   | -7.920  | -7.948  | -13.321 | 0.00 | 0.00 | C     |
| HETATM | 474 | H  | 0   | -8.312  | -7.990  | -12.316 | 0.00 | 0.00 | H     |
| HETATM | 475 | H  | 0   | -8.665  | -7.527  | -13.980 | 0.00 | 0.00 | H     |
| HETATM | 476 | H  | 0   | -7.669  | -8.945  | -13.651 | 0.00 | 0.00 | H     |
### HETATM

| 477 | C | 0 | -5.431 | -7.928 | -13.567 | 0.00 | 0.00 | C |
| 478 | H | 0 | -4.629 | -7.304 | -13.931 | 0.00 | 0.00 | H |
| 479 | H | 0 | -5.135 | -8.387 | -12.635 | 0.00 | 0.00 | H |
| 480 | H | 0 | -5.648 | -8.698 | -14.294 | 0.00 | 0.00 | H |
| 481 | C | 0 | -7.676 | -7.405 | -16.292 | 0.00 | 0.00 | C |
| 482 | O | 0 | -7.439 | -8.577 | -16.585 | 0.00 | 0.00 | O |
| 483 | N | 0 | -8.898 | -6.883 | -16.330 | 0.00 | 0.00 | N |
| 484 | H | 0 | -9.022 | -5.943 | -16.084 | 0.00 | 0.00 | H |
| 485 | C | 0 | -10.056 | -7.675 | -16.729 | 0.00 | 0.00 | C |
| 486 | H | 0 | -10.020 | -8.608 | -16.189 | 0.00 | 0.00 | H |
| 487 | C | 0 | -11.349 | -6.941 | -16.372 | 0.00 | 0.00 | C |
| 488 | H | 0 | -11.251 | -5.900 | -16.643 | 0.00 | 0.00 | H |
| 489 | H | 0 | -12.167 | -7.377 | -16.927 | 0.00 | 0.00 | H |
| 490 | C | 0 | -11.692 | -7.006 | -14.915 | 0.00 | 0.00 | C |
| 491 | N | 0 | -10.913 | -6.434 | -13.933 | 0.00 | 0.00 | N |
| 492 | C | 0 | -12.739 | -7.579 | -14.277 | 0.00 | 0.00 | C |
| 493 | C | 0 | -11.465 | -6.653 | -12.753 | 0.00 | 0.00 | C |
| 494 | N | 0 | -12.575 | -7.346 | -12.934 | 0.00 | 0.00 | N |
| 495 | H | 0 | -13.553 | -8.121 | -14.738 | 0.00 | 0.00 | H |
| 496 | H | 0 | -11.076 | -6.322 | -11.802 | 0.00 | 0.00 | H |
| 497 | H | 0 | -13.180 | -7.644 | -12.224 | 0.00 | 0.00 | H |
| 498 | C | 0 | -10.021 | -7.972 | -18.224 | 0.00 | 0.00 | C |
| 499 | O | 0 | -10.463 | -9.033 | -18.688 | 0.00 | 0.00 | O |
| 500 | N | 0 | -9.496 | -7.028 | -18.998 | 0.00 | 0.00 | N |
| 501 | H | 0 | -9.161 | -6.204 | -18.588 | 0.00 | 0.00 | H |
| 502 | C | 0 | -9.405 | -7.188 | -20.448 | 0.00 | 0.00 | C |
| 503 | H | 0 | -10.407 | -7.157 | -20.846 | 0.00 | 0.00 | H |
| 504 | C | 0 | -8.590 | -6.046 | -21.055 | 0.00 | 0.00 | C |
| 505 | H | 0 | -9.170 | -5.141 | -20.964 | 0.00 | 0.00 | H |
| 506 | H | 0 | -7.680 | -5.948 | -20.480 | 0.00 | 0.00 | H |
| 507 | C | 0 | -8.201 | -6.208 | -22.524 | 0.00 | 0.00 | C |
| 508 | H | 0 | -7.737 | -7.175 | -22.663 | 0.00 | 0.00 | H |
| 509 | C | 0 | -9.434 | -6.149 | -23.412 | 0.00 | 0.00 | C |
| 510 | H | 0 | -9.739 | -5.120 | -23.537 | 0.00 | 0.00 | H |
| 511 | H | 0 | -9.204 | -6.575 | -24.378 | 0.00 | 0.00 | H |
| 512 | H | 0 | -10.235 | -6.708 | -22.953 | 0.00 | 0.00 | H |
| 513 | C | 0 | -7.196 | -5.140 | -22.931 | 0.00 | 0.00 | C |
| 514 | H | 0 | -7.047 | -5.175 | -24.000 | 0.00 | 0.00 | H |
| 515 | H | 0 | -7.573 | -4.166 | -22.653 | 0.00 | 0.00 | H |
| 516 | H | 0 | -6.257 | -5.320 | -22.431 | 0.00 | 0.00 | H |
| 517 | C | 0 | -8.773 | -8.528 | -20.806 | 0.00 | 0.00 | C |
| 518 | O | 0 | -9.396 | -9.363 | -21.463 | 0.00 | 0.00 | O |
| 519 | N | 0 | -7.532 | -8.728 | -20.372 | 0.00 | 0.00 | N |
| 520 | H | 0 | -7.069 | -8.025 | -19.853 | 0.00 | 0.00 | H |
| 521 | C | 0 | -8.187 | -9.968 | -20.646 | 0.00 | 0.00 | C |
| 522 | H | 0 | -6.849 | -10.142 | -21.712 | 0.00 | 0.00 | H |
| 523 | C | 0 | -5.342 | -9.876 | -20.213 | 0.00 | 0.00 | C |
| 524 | H | 0 | -4.906 | -10.859 | -20.287 | 0.00 | 0.00 | H |
| HETATM | 573 | C  |   | -15.244 | -11.404 | -16.605 | 0.00 | 0.00 | C      |
|--------|-----|----|---|---------|---------|---------|------|------|--------|
| HETATM | 574 | H  |   | -14.228 |   -8.782 | -17.085 | 0.00 | 0.00 | H      |
| HETATM | 575 | H  |   | -15.325 | -14.514 | -17.921 | 0.00 | 0.00 | H      |
| HETATM | 576 | C  |   | -15.533 | -12.734 | -16.744 | 0.00 | 0.00 | C      |
| HETATM | 577 | H  |   | -15.605 | -10.852 | -15.748 | 0.00 | 0.00 | H      |
| HETATM | 578 | H  |   | -16.122 | -13.241 | -15.996 | 0.00 | 0.00 | H      |
| HETATM | 579 | C  |   | -11.261 | -12.547 | -22.150 | 0.00 | 0.00 | C      |
| HETATM | 580 | O  |   | -11.893 | -13.447 | -22.706 | 0.00 | 0.00 | O      |
| CONECT |  11 |  9 | 12 |  13 |  14 |                     |      |      |        |
| CONECT |  14 |  11 | 15 |  16 |      |                     |      |      |        |
| CONECT |  18 |  16 | 19 |  20 |  28 |                     |      |      |        |
| CONECT |  20 |  23 | 27 |  28 |  29 |                     |      |      |        |
| CONECT |  29 |      | 31 |  32 |      |                     |      |      |        |
| CONECT |  33 |  35 | 37 |  38 |  39 |                     |      |      |        |
| CONECT |  37 |  39 |      |  41 |  42 |                     |      |      |        |
| CONECT |  42 |  43 | 44 |  45 |  46 |                     |      |      |        |
| CONECT |  44 |      | 47 |      |      |                     |      |      |        |
| CONECT |  48 |  51 | 49 |      |  50 |                     |      |      |        |
| CONECT |  52 |  53 | 54 |      |  37 |                     |      |      |        |
| CONECT |  56 |  57 | 58 |  69 |      |                     |      |      |        |
| CONECT |  58 |  59 | 60 |  61 |      |                     |      |      |        |
| CONECT |  61 |  62 | 63 |      |      |                     |      |      |        |
| CONECT |  63 |  65 | 66 |      |      |                     |      |      |        |
| CONECT |  64 |  65 | 67 |      |      |                     |      |      |        |
| CONECT |  69 |  70 | 71 |      |      |                     |      |      |        |
| CONECT |  73 |  74 | 75 |  88 |      |                     |      |      |        |
| CONECT |  75 |  76 | 77 |  78 |      |                     |      |      |        |
| CONECT |  78 |  79 | 80 |  84 |      |                     |      |      |        |
| CONECT |  80 |  81 | 82 |  83 |      |                     |      |      |        |
| CONECT |  84 |  85 | 86 |  87 |      |                     |      |      |        |
| CONECT |  88 |  89 | 90 |      |      |                     |      |      |        |
| CONECT |  92 |  93 | 94 |      |      |                     |      |      |        |
| CONECT |  94 |  95 | 96 | 100 |      |                     |      |      |        |
| CONECT |  96 |  97 | 98 |  99 |      |                     |      |      |        |
| CONECT | 100 |  94 | 101| 102 |      |                     |      |      |        |
| CONECT | 103 | 104 | 105| 106 | 100 |                     |      |      |        |
| CONECT | 107 | 108 | 109|  92 |      |                     |      |      |        |
| CONECT | 111 | 112 | 113| 126 |      |                     |      |      |        |
| CONECT | 113 | 114 | 115| 116 |      |                     |      |      |        |
| CONECT | 116 | 117 | 118| 122 |      |                     |      |      |        |
| CONECT | 118 | 119 | 120| 121 |      |                     |      |      |        |
| CONECT | 122 | 123 | 124| 125 |      |                     |      |      |        |
| CONECT | 126 | 127 | 128|      |      |                     |      |      |        |
| CONECT | 130 | 131 | 132| 150 |      |                     |      |      |        |
| CONECT | 132 | 133 | 134| 135 |      |                     |      |      |        |
| CONECT  | 135  | 132  | 136  | 137  |
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| CONECT  | 163  | 161  | 164  | 165  | 169  |
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| CONECT  | 169  | 163  | 170  | 171  | 172  |
| CONECT  | 172  | 169  | 173  | 174  | 175  |
| CONECT  | 176  | 161  | 177  | 178  |
| CONECT  | 180  | 182  | 181  | 195  | 178  |
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| CONECT  | 185  | 191  | 187  | 182  | 186  |
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| CONECT  | 191  | 185  | 192  | 193  | 194  |
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| CONECT  | 207  | 205  | 26. Jul | 210  |
| CONECT  | 212  | 199  | 31. Jul | 214  |
| CONECT  | 216  | 214  | 04. Aug | 218  | 231  |
| CONECT  | 218  | 216  | 06. Aug | 220  | 221  |
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| CONECT  | 231  | 216  | 232  | 233  |
| CONECT  | 235  | 233  | 236  | 237  | 250  |
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| CONECT  | 261  | 259  | 262  | 263  | 264  |
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| CONECT  | 269  | 254  | 270  | 271  |
| CONECT  | 273  | 271  | 274  | 275  | 293  |
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| CONECT 278 | 275 | 279 | 280 |
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| CONECT 293 | 273 | 294 | 4 |
| CONECT 297 | 295 | 298 | 299 | 300 |
| CONECT 300 | 297 | 301 | 302 |
| CONECT 304 | 302 | 305 | 306 | 319 |
| CONECT 306 | 304 | 307 | 308 | 312 |
| CONECT 308 | 306 | 309 | 310 | 311 |
| CONECT 312 | 306 | 313 | 314 | 315 |
| CONECT 315 | 312 | 316 | 317 | 318 |
| CONECT 319 | 304 | 320 | 321 |
| CONECT 323 | 321 | 324 | 325 | 338 |
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| CONECT 328 | 325 | 329 | 330 | 334 |
| CONECT 330 | 328 | 331 | 332 | 333 |
| CONECT 334 | 328 | 335 | 336 | 337 |
| CONECT 338 | 323 | 339 | 340 |
| CONECT 342 | 340 | 343 | 344 | 355 |
| CONECT 344 | 342 | 345 | 346 | 347 |
| CONECT 347 | 344 | 348 | 349 |
| CONECT 349 | 347 | 351 | 352 |
| CONECT 350 | 348 | 351 | 353 |
| CONECT 355 | 342 | 356 | 357 |
| CONECT 359 | 357 | 360 | 361 | 374 |
| CONECT 361 | 359 | 362 | 363 | 364 |
| CONECT 364 | 361 | 365 | 366 | 370 |
| CONECT 366 | 364 | 367 | 368 | 369 |
| CONECT 370 | 364 | 371 | 372 | 373 |
| CONECT 374 | 359 | 375 | 376 |
| CONECT 378 | 376 | 379 | 380 | 393 |
| CONECT 380 | 378 | 381 | 382 | 386 |
| CONECT 382 | 380 | 383 | 384 | 385 |
| CONECT 386 | 380 | 387 | 388 | 389 |
| CONECT 389 | 386 | 390 | 391 | 392 |
| CONECT 393 | 378 | 394 | 395 |
| CONECT 397 | 412 | 395 | 398 | 399 |
| CONECT 399 | 402 | 397 | 400 | 401 |
| CONECT 402 | 403 | 404 | 408 | 399 |
| CONECT 404 | 402 | 405 | 406 | 407 |
| CONECT 408 | 402 | 409 | 410 | 411 |
| CONECT 412 | 413 | 414 | 397 |
| 416 | 414 | 417 | 418 | 436 |
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| 418 | 416 | 419 | 420 | 421 |
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| 436 | 416 | 437 |     | 6   |
| 440 | 438 | 441 | 442 | 443 |
| 443 | 440 | 444 | 445 |     |
| 447 | 445 | 448 | 449 | 462 |
| 449 | 447 | 450 | 451 | 455 |
| 451 | 449 | 452 | 453 | 454 |
| 455 | 449 | 456 | 457 | 458 |
| 458 | 455 | 459 | 460 | 461 |
| 462 | 447 | 463 | 464 |     |
| 466 | 464 | 467 | 468 | 481 |
| 468 | 466 | 469 | 470 | 471 |
| 471 | 468 | 472 | 473 | 477 |
| 473 | 471 | 474 | 475 | 476 |
| 477 | 471 | 478 | 479 | 480 |
| 481 | 466 | 482 | 483 |     |
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| 551 | 545 | 552 | 553 | 554 |
| CONECT | 555 | 540 | 556 | 557 |
|--------|-----|-----|-----|-----|
| CONECT | 559 | 557 | 560 | 561 | 579 |
| CONECT | 561 | 559 | 562 | 563 | 564 |
| CONECT | 564 | 561 | 565 | 566 |
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| CONECT | 566 | 564 | 567 | 568 |
| CONECT | 567 | 566 | 571 | 572 |
| CONECT | 568 | 566 | 569 | 573 |
| CONECT | 572 | 567 | 575 | 576 |
| CONECT | 573 | 568 | 576 | 577 |
| CONECT | 576 | 572 | 573 | 578 |
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| CONECT | 153 | 152 |
SUPPORTING INFORMATION

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| SUPPORTING INFORMATION |
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Author Contributions

KT Movellan, Dr. Rıza Dervişoğlu and Dr. Loren B. Andreas performed the experiments and analyzed the data. The manuscript was written by Dr. Loren B. Andreas and KT Movellan. Dr. Stefan Becker provided the samples. All authors revised the manuscript.