Supplementary Information

Computational Study on the Binding of Mango-II RNA Aptamer and Fluorogen Using the Polarizable Force Field AMOEBA

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(TO1-Biotin parameters: 24; TO3-Biotin parameters: 45)
I. Tables

Table S1. The details of the system used for simulation.

| Complex                  | Number of K⁺ a) | Number of Cl⁻ b) | Range of restraint c)         |
|--------------------------|-----------------|------------------|------------------------------|
| Mango-II-WT TO1-Biotin   | 58              | 27               | 5.00 ~ 6.00                  |
| Mango-II-WT TO3-Biotin   | 58              | 27               | 5.00 ~ 6.00                  |
| Mango-II-A22U TO1-Biotin | 57              | 27               | 5.00 ~ 6.00 (Config. A)      |
|                          |                 |                  | 5.00 ~ 6.20 (Config. B)      |
| Mango-II-A22U TO3-Biotin | 57              | 27               | 5.50 ~ 6.80 (Config. A)      |
|                          |                 |                  | 5.00 ~ 6.80 (Config. B)      |

a). K⁺ in solvation (The number of K⁺ inside the G-quadruplex is 2 and they are not counted here). b). Cl⁻ in solvation. c). The harmonic restraint will be removed only if the distance between COM of ligands and K2 (the K⁺ between T3 and T2 layers) is inside the range mentioned here.

Table S2. Statistics of the position of K⁺ in three-layer G-quadruplex during the equilibration.

| Complex                  | T3-K2 b) | T2-K2 b) | T2-K1 b) | T1-K1 b) |
|--------------------------|----------|----------|----------|----------|
| Mango-II-WT              | 1.45±0.19| 1.99±0.18| 1.84±0.19| 1.53±0.20|
| Mango-II-WT TO1-Biotin   | 1.29±0.17| 2.12±0.17| 1.68±0.19| 1.69±0.20|
| Mango-II-WT TO3-Biotin   | 1.36±0.17| 2.07±0.17| 1.76±0.19| 1.57±0.20|
| Mango-II-A22U TO1-Biotin (A) | 1.44±0.21| 2.01±0.20| 1.85±0.21| 1.50±0.21|
| Mango-II-A22U TO1-Biotin (B) | 1.25±0.22| 2.18±0.21| 1.70±0.21| 1.60±0.22|
| Mango-II-A22U TO3-Biotin (A) | 1.39±0.19| 2.07±0.19| 1.82±0.24| 1.56±0.23|
| Mango-II-A22U TO3-Biotin (B) | 1.22±0.19| 2.15±0.18| 1.71±0.18| 1.63±0.19|

a). (A)/(B) mean the configuration A or B. b). The specific definition of the abbreviations can be found in Figure 1. The data has been shown in the format as: Average ± standard deviation (Unit: Å).
Table S3. Statistics of the position of K+ in three-layer G-quadruplex during the FEP alchemical calculation (126ns).

| Complex\(^{a)}\) | T3-K\(^{b)}\) (Å) | T2-K\(^{b)}\) (Å) | T2-K1\(^{b)}\) (Å) | T1-K1\(^{b)}\) (Å) |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| Mango-II-WT TO1-Biotin | 1.16±0.37 | 2.32±0.23 | 1.55±0.22 | 1.85±0.22 |
| Mango-II-WT TO3-Biotin | 1.23±0.20 | 2.20±0.20 | 1.68±0.08 | 1.66±0.21 |
| Mango-II-A22U TO1-Biotin (A) | 1.35±0.23 | 2.08±0.22 | 1.80±0.21 | 1.55±0.22 |
| Mango-II-A22U TO1-Biotin (B) | 1.13±0.21 | 2.31±0.21 | 1.59±0.21 | 1.71±0.22 |
| Mango-II-A22U TO3-Biotin (A) | 1.31±0.20 | 2.14±0.20 | 1.75±0.22 | 1.62±0.22 |
| Mango-II-A22U TO3-Biotin (B) | 1.14±0.27 | 2.41±0.71 | 1.66±0.23 | 1.71±0.24 |

\(^{a)}\) (A)/(B) mean the configuration A or B. \(^{b)}\) The specific definition of the abbreviations can be found in Figure 1. The data has been shown in the format as: Average ± standard deviation (Unit: Å).

Table S4. The alchemical states used for the calculation of free energy

| Index of state | \(\lambda_{vdw}\) | \(\lambda_{ele}\) | Force constant of harmonic restraint \(k_R\) (kcal/(mol·Å\(^2\))) |
|----------------|----------------|-----------------|-----------------|
| 1              | 0.00           | 0.00            | 15              |
| 2              | 0.50           | 0.00            | 15              |
| 3              | 0.55           | 0.00            | 15              |
| 4              | 0.60           | 0.00            | 15              |
| 5              | 0.62           | 0.00            | 15              |
| 6              | 0.65           | 0.00            | 15              |
| 7              | 0.70           | 0.00            | 15              |
| 8              | 0.75           | 0.00            | 15              |
| 9              | 0.80           | 0.00            | 15              |
| 10             | 0.90           | 0.00            | 15              |
| 11             | 1.00           | 0.00            | 15              |
| 12             | 1.00           | 0.10            | 15              |
| 13             | 1.00           | 0.20            | 15              |
| 14             | 1.00           | 0.30            | 15              |
| 15             | 1.00           | 0.40            | 15              |
| 16             | 1.00           | 0.50            | 15              |
| 17             | 1.00           | 0.60            | 10              |
| 18             | 1.00           | 0.70            | 5               |
Table S5. Statistics of the interstage free energy change in the annihilation of TO1-Biotin from wild-type Mango-II_TO1-Biotin complex. (The states here are represented by corresponding indices mentioned in Table S4. Unit: kcal/mol)

| State change | Δ\( \mathcal{G} \) | RMSD |
|--------------|----------------|------|
| 1 to 2       | 5.106          | 0.055|
| 2 to 3       | 7.9549         | 0.0478|
| 3 to 4       | 13.9947        | 0.1602|
| 4 to 5       | 4.2996         | 0.1079|
| 5 to 6       | 3.1671         | 0.078 |
| 6 to 7       | 2.1343         | 0.1204|
| 7 to 8       | -0.2994        | 0.0681|
| 8 to 9       | -2.4445        | 0.0627|
| 9 to 10      | -11.9338       | 0.0948|
| 10 to 11     | -24.5045       | 0.1109|
| 11 to 12     | -0.7262        | 0.0375|
| 12 to 13     | -1.9454        | 0.0405|
| 13 to 14     | -3.2742        | 0.0384|
| 14 to 15     | -4.7055        | 0.0438|
| 15 to 16     | -6.0603        | 0.037 |
| 16 to 17     | -7.5918        | 0.0477|
| 17 to 18     | -9.6083        | 0.0483|
| 18 to 19     | -11.9364       | 0.0597|
| 19 to 20     | -14.6174       | 0.0572|
| 20 to 21     | -17.5225       | 0.0693|
| Restrained Correction | | 0.6913 |

Table S6. Statistics of the interstage free energy change in the annihilation of TO1-Biotin from the configuration A of Mango-II-A22U_TO1-Biotin complex. (The states here are represented by corresponding indices mentioned in Table S4. Unit: kcal/mol)

| State change | Δ\( \mathcal{G} \) | RMSD |
|--------------|----------------|------|
| 1 to 2       | 1.9359         | 0.0091|
| 2 to 3       | 3.7139         | 0.0131|
| 3 to 4       | 7.9712         | 0.0313|
| 4 to 5       | 4.7967         | 0.0217|
| 5 to 6       | 8.5257         | 0.0548|
| 6 to 7       | 12.2082        | 0.2782|
Table S7. Statistics of the interstage free energy change in the annihilation of TO1-Biotin from the configuration B of Mango-II-A22U_TO1-Biotin complex. (The states here are represented by corresponding indices mentioned in Table S4. Unit: kcal/mol)

| State change | $\Delta G$ kcal/mol | RMSD kcal/mol |
|--------------|----------------------|---------------|
| 1 to 2       | 5.1753               | 0.0526        |
| 2 to 3       | 7.8988               | 0.0557        |
| 3 to 4       | 13.4672              | 0.165         |
| 4 to 5       | 3.8369               | 0.1007        |
| 5 to 6       | 2.287                | 0.0834        |
| 6 to 7       | 1.1154               | 0.0769        |
| 7 to 8       | -0.643               | 0.0682        |
| 8 to 9       | -2.7028              | 0.0547        |
| 9 to 10      | -13.7957             | 0.0625        |
| 10 to 11     | -23.7263             | 0.0776        |
| 11 to 12     | -0.0529              | 0.0427        |
| 12 to 13     | -1.3402              | 0.052         |
| 13 to 14     | -2.4986              | 0.0449        |
| 14 to 15     | -3.9358              | 0.0442        |
| 15 to 16     | -5.4716              | 0.0461        |
| 16 to 17     | -7.2293              | 0.0479        |
| 17 to 18     | -9.0417              | 0.0478        |
| 18 to 19     | -11.3286             | 0.0641        |
| 19 to 20     | -13.7957             | 0.0625        |
| 20 to 21     | -16.6278             | 0.064         |
| Restrain Correction | 0.6913 |               |
Table S8. Statistics of the interstage free energy change in the solvation of TO1-Biotin. (The states here are represented by corresponding indices mentioned in Table S4. Unit: kcal/mol)

| State change | Δ\(G\) | RMSD |
|--------------|---------|------|
| 1 to 2       | 3.2544  | 0.0182 |
| 2 to 3       | 5.994   | 0.0317 |
| 3 to 4       | 10.5201 | 0.1414 |
| 4 to 5       | 3.1783  | 0.0744 |
| 5 to 6       | 2.4685  | 0.0716 |
| 6 to 7       | 1.744   | 0.0795 |
| 7 to 8       | 0.1795  | 0.0591 |
| 8 to 9       | -1.1372 | 0.0442 |
| 9 to 10      | -6.4516 | 0.0795 |
| 10 to 11     | -14.4784 | 0.0888 |
| 11 to 12     | -0.0249 | 0.0445 |
| 12 to 13     | -1.3465 | 0.0472 |
| 13 to 14     | -2.7753 | 0.0443 |
| 14 to 15     | -4.1272 | 0.0458 |
| 15 to 16     | -5.6486 | 0.0483 |
| 16 to 17     | -7.3282 | 0.0492 |
| 17 to 18     | -9.2552 | 0.055 |
| 18 to 19     | -11.434 | 0.0576 |
| 19 to 20     | -13.9842 | 0.0657 |
| 20 to 21     | -17.2574 | 0.0798 |

Table S9. Statistics of the interstage free energy change in the annihilation of TO3-Biotin from wild-type Mango-II_TO3-Biotin complex. (The states here are represented by corresponding indices mentioned in Table S4. Unit: kcal/mol)

| State change | Δ\(G\) | RMSD |
|--------------|---------|------|
| 1 to 2       | 5.6047  | 0.0425 |
| 2 to 3       | 8.6706  | 0.0687 |
| 3 to 4       | 14.3202 | 0.156 |
| 4 to 5       | 4.8909  | 0.124 |
| 5 to 6       | 3.4468  | 0.0857 |
| 6 to 7       | 2.5624  | 0.1083 |
| 7 to 8       | -0.021  | 0.0903 |
| 8 to 9       | -2.674  | 0.0628 |
| 9 to 10      | -13.6573 | 0.1419 |
| 10 to 11     | -27.1263 | 0.0757 |
| 11 to 12     | -0.2698 | 0.0366 |
| 12 to 13     | -0.9386 | 0.0338 |
| State change | $\Delta G$ | RMSD |
|--------------|------------|------|
| 13 to 14     | -1.8874    | 0.041|
| 14 to 15     | -2.9836    | 0.0353|
| 15 to 16     | -4.3279    | 0.0499|
| 16 to 17     | -5.7511    | 0.0381|
| 17 to 18     | -6.8371    | 0.0413|
| 18 to 19     | -8.1012    | 0.0421|
| 19 to 20     | -9.7248    | 0.0488|
| 20 to 21     | -11.7511   | 0.0546|
| Restrain Correction | 0.6913 |      |

Table S10. Statistics of the interstage free energy change in the annihilation of TO3-Biotin from the configuration A of Mango-II-A22U_TO3-Biotin complex. (The states here are represented by corresponding indices mentioned in Table S4. Unit: kcal/mol)

| State change | $\Delta G$ | RMSD |
|--------------|------------|------|
| 1 to 2       | 4.8775     | 0.0534|
| 2 to 3       | 7.6464     | 0.0484|
| 3 to 4       | 13.6055    | 0.1509|
| 4 to 5       | 4.2185     | 0.0982|
| 5 to 6       | 3.0746     | 0.0899|
| 6 to 7       | 1.7182     | 0.1039|
| 7 to 8       | -0.7575    | 0.0739|
| 8 to 9       | -2.839     | 0.0488|
| 9 to 10      | -12.3229   | 0.1074|
| 10 to 11     | -26.3573   | 0.1284|
| 11 to 12     | -0.5565    | 0.0413|
| 12 to 13     | -1.6898    | 0.0366|
| 13 to 14     | -2.6647    | 0.0356|
| 14 to 15     | -3.6047    | 0.0372|
| 15 to 16     | -4.642     | 0.0379|
| 16 to 17     | -5.7927    | 0.0421|
| 17 to 18     | -6.9909    | 0.04|
| 18 to 19     | -8.1808    | 0.0436|
| 19 to 20     | -9.6719    | 0.0561|
| 20 to 21     | -11.9472   | 0.0578|
| Restrain Correction | 0.4398 |      |

Table S11. Statistics of the interstage free energy change in the annihilation of TO3-Biotin from the configuration B of Mango-II-A22U_TO3-Biotin complex. (The states here are represented by corresponding indices mentioned in Table S4. Unit: kcal/mol)
| State change | $\Delta G$  | RMSD  |
|--------------|-------------|-------|
| 1 to 2       | 5.2736      | 0.0366|
| 2 to 3       | 8.2494      | 0.0449|
| 3 to 4       | 14.2153     | 0.1186|
| 4 to 5       | 5.3124      | 0.0712|
| 5 to 6       | 4.1662      | 0.0793|
| 6 to 7       | 2.6974      | 0.1183|
| 7 to 8       | -0.3375     | 0.0542|
| 8 to 9       | -2.4511     | 0.0446|
| 9 to 10      | -11.8772    | 0.0805|
| 10 to 11     | -25.1459    | 0.1092|
| 11 to 12     | -0.4573     | 0.0275|
| 12 to 13     | -1.3929     | 0.0346|
| 13 to 14     | -2.3161     | 0.0262|
| 14 to 15     | -3.3461     | 0.0367|
| 15 to 16     | -4.7802     | 0.0321|
| 16 to 17     | -5.9471     | 0.0313|
| 17 to 18     | -7.1036     | 0.0313|
| 18 to 19     | -8.2823     | 0.0335|
| 19 to 20     | -9.8166     | 0.0378|
| 20 to 21     | -11.6017    | 0.0396|
| Restrain     | 0.3294      |       |

Table S12. Statistics of the interstage free energy change in the solvation of TO3-Biotin. (The states here are represented by corresponding indices mentioned in Table S4. Unit: kcal/mol)
|       | Value  | SD    |
|-------|--------|-------|
| 16 to 17 | -5.1851 | 0.0435 |
| 17 to 18 | -6.5626 | 0.0448 |
| 18 to 19 | -8.1086 | 0.0492 |
| 19 to 20 | -9.9617 | 0.0537 |
| 20 to 21 | -12.1937 | 0.058  |
II. Figures

Figure S1. RMSD trajectory of core G-quadruplex (the heavy atoms from bases of 10~29) from the MD simulation of single wild type Mango-II.

Figure S2. RMSD trajectory of core G-quadruplex (the heavy atoms from bases of 10~29) from the MD simulation of single wild type Mango-II without polarization.
**Figure S3.** RMSD trajectories of core G-quadruplex (the heavy atoms from bases of 10–29) from the MD simulations on 4 aptamer-fluorogen complexes (Mango-II-A22U complexes choose the configuration A).

**Figure S4.** The trajectories of important structural parameters in MD simulation (N-H denotes the distance of N of A12 and the H on G24, see the 4ns snapshot of the Figure
Figure S5. RMSD trajectories of core G-quadruplex (the heavy atoms from bases of 10~29) from the MD simulation on the configuration B of Mango-II-A22U_TO1-Biotin.

Figure S6. Trajectories of important structural parameters from the MD simulation on the configuration B of Mango-II-A22U_TO1-Biotin.
Figure S7. RMSD trajectories of core G-quadruplex (the heavy atoms from bases of 10~29) from the MD simulation on the configuration B of Mango-II-A22U_TO3-Biotin.

Figure S8. Trajectories of important structural parameters from the MD simulation on the configuration B of Mango-II-A22U_TO3-Biotin.
Figure S9. Statistics of the position of K⁺ in three-layer G-quadruplex of wild-type Mango-II during the 10ns equilibration.

Figure S10. Statistics of the position of K⁺ in three-layer G-quadruplex of wild-type Mango-II during the 10ns equilibration with no polarization.
Figure S11. Statistics of the position of K\(^+\) in three-layer G-quadruplex of wild-type Mango-II_TO1-Biotin complex during the 10ns equilibration.

Figure S12. Statistics of the position of K\(^+\) in three-layer G-quadruplex of wild-type Mango-II_TO3-Biotin complex during the 10ns equilibration.
**Figure S13.** Statistics of the position of K⁺ in three-layer G-quadruplex from configuration A of Mango-II-A22U_TO1-Biotin complex during the 10ns equilibration.

**Figure S14.** Statistics of the position of K⁺ in three-layer G-quadruplex from configuration B of Mango-II-A22U_TO1-Biotin complex during the 35ns equilibration.
**Figure S15.** Statistics of the position of K\(^+\) in three-layer G-quadruplex from configuration A of Mango-II-A22U_TO3-Biotin complex during the 10ns equilibration.

**Figure S16.** Statistics of the position of K\(^+\) in three-layer G-quadruplex from configuration B of Mango-II-A22U_TO3-Biotin complex during the 10ns equilibration.
III. Deduction of Equation
The deduction of the Equation 3

\[ K_D = \frac{[R][L]}{[RL]} \Rightarrow [RL] = \frac{[R][L]}{K_D} \]

\[ K_D^* = \frac{[R^*][L]}{[R^*L]} \Rightarrow [R^*L] = \frac{[R^*][L]}{K_D^*} \]

\[ K_{eq}^R = \frac{[R^*]}{[R]} \]

\[ K_D^{app} = \frac{( [R] + [R^*][L] )}{[RL] + [R^*L]} = \frac{[R] + [R^*]}{K_D} + \frac{[R^*]}{K_D^*} = K_D K_D^* \frac{1 + K_{eq}^R}{K_D + K_D K_{eq}^R} \]

IV. QM and AMOEBA geometries of ligands
QM optimized geometry of TO1-Biotin (charge: 2)

| C   | X         | Y         | Z           |
|-----|-----------|-----------|-------------|
| 1   | -0.998818978622 | -0.185918954587 | 0.530002383579 |
| 2   | -1.963549127011  | 1.384379580966  |
| 3   | -3.391955323401  | -0.058349374291 |
| 4   | 6.030877920694   | -1.324460246607 |
| 5   | 5.93902707390    | 0.573956937976  |
| 6   | 4.523832945947   | 1.003439761675  |
| 7   | 2.129059490923   | 1.412620725232  |
| 8   | 0.795574556665   | 1.243582069525  |
| 9   | -4.068154225733  | 1.896224011781  |
| 10  | -5.423936666970  | 1.680140424820  |
| 11  | -7.546279688641  | 0.557129231319  |
| 12  | -5.503019399443  | -0.077953092555 |
| 13  | -6.243362003610  | -1.06018566615  |
| 14  | -5.613222638703  | -1.836638341604 |
| 15  | -4.247653293261  | -1.645700795884 |
| 16  | -3.507597256710  | -0.49851385303 |
| 17  | -4.112910774053  | 0.66776418988  |
| 18  | 0.465168125424   | 0.759241395365 |
| 19  | 1.039212024108   | -1.433203879320 |
| 20  | 2.296974138269   | 1.018527547735 |
| 21  | 2.951893463816   | 0.071447383863 |
| 22  | 2.392327622506   | 0.742830908361 |
| 23  | 1.175954817529   | 0.261038186022 |
AMOEBa optimized geometry of TO1-Biotin (charge: 2) (.txyz file)

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 24 | N | 3.271657474525 | 1.293987324841 | 1.055033824462 |
| 25 | N | 0.415223497784 | 0.58874797601 | 0.787028901250 |
| 26 | N | -6.106676153516 | -0.568901230270 | 0.731443672867 |
| 27 | O | 5.165984735015 | 0.617204736258 | -0.702126483613 |
| 28 | O | 0.415223497784 | 0.58874797601 | 0.787028901250 |
| 29 | S | -5.165984735015 | 0.617204736258 | -0.702126483613 |
| 30 | H | 5.165984735015 | 0.617204736258 | -0.702126483613 |
| 31 | H | 0.415223497784 | 0.58874797601 | 0.787028901250 |
| 32 | H | -6.106676153516 | -0.568901230270 | 0.731443672867 |
| 33 | H | 5.165984735015 | 0.617204736258 | -0.702126483613 |
| 34 | H | 0.415223497784 | 0.58874797601 | 0.787028901250 |
| 35 | H | -6.106676153516 | -0.568901230270 | 0.731443672867 |
| 36 | H | 5.165984735015 | 0.617204736258 | -0.702126483613 |
| 37 | H | 0.415223497784 | 0.58874797601 | 0.787028901250 |
| 38 | H | -6.106676153516 | -0.568901230270 | 0.731443672867 |
| 39 | H | 6.085322836019 | -1.254905325636 | -0.714192529726 |

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|   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|
| 33  | 34  | C | 4.63802924 | 1.89320884 | 1.32178825 | 403 | 5 | 24 |
| 35  | 36  | C | 2.17668831 | 1.63831895 | 1.39318463 | 408 | 8 | 24 |
| 28  | 8   | C | 0.84871034 | 0.90921279 | 1.20236044 | 411 | 7 | 25 |
| 56  | 9   | C | -4.22660615 | -0.53695857 | 2.15439343 | 414 | 3 | 10 |
| 37  | 10  | C | -5.60515509 | -0.71734158 | 2.03294725 | 410 | 9 | 26 |
| 38  | 11  | C | -7.75844640 | -0.52885153 | 0.88115041 | 405 | 26 | 39 |
| 40  | 12  | C | -5.65209674 | 0.43950944 | -0.07039131 | 409 | 13 | 17 |
| 26  | 13  | C | -6.38345650 | 1.00309565 | -1.17998759 | 413 | 12 | 14 |
| 42  | 14  | C | -5.70956634 | 1.72544669 | -2.15956417 | 417 | 13 | 15 |
| 43  | 15  | C | -4.31282011 | 1.92811808 | -2.07746233 | 424 | 14 | 16 |
| 44  | 16  | C | -3.58411662 | 1.40240407 | -1.01741900 | 416 | 15 | 17 |
| 16  | 17  | C | -4.22892762 | 0.62839686 | 0.01335856 | 412 | 3 | 12 |
| 29  | 18  | C | 0.16411873 | -2.16513183 | -0.66796708 | 425 | 19 | 23 |
| 19  | 19  | C | 0.62700694 | -3.31285663 | -1.32941925 | 420 | 18 | 20 |
| 46  | 20  | C | 1.97120375 | -3.70020732 | -1.16514002 | 427 | 19 | 21 |
| 47  | 21  | C | 2.82771339 | -2.96161269 | -0.32858160 | 421 | 20 | 22 |
| 48  | 22  | C | 2.37254632 | -1.81958230 | 0.34871095 | 426 | 21 | 23 |
| 49  | 23  | C | 1.03241534 | -1.39280097 | 0.13062391 | 418 | 18 | 22 |
| 25  | 24  | N | 0.37332260 | -0.24708158 | 0.71578948 | 422 | 1 | 8 |
| 26  | 25  | N | -6.29195445 | -0.27365785 | 0.93781050 | 407 | 10 | 11 |
| 12  | 27  | O | 5.51836441 | -0.65818233 | 0.96914657 | 429 | 4 | 5 |
QM optimized geometry of TO3-Biotin (charge: 2)

1 C -8.311832562926 -0.920443135638 0.411793438441
2 C -6.413746683550 0.586126895554 0.497733249872
3 C -5.054484302805 0.879403422247 0.504547763197
4 C -4.102756140989 -0.133684115521 0.470238175842
5 C -2.709908274110 0.270465310889 0.29379781382
6 C -1.789896029170 -0.416396186818 -0.441960287481
7 C -0.403296225598 -0.093846898446 -0.65394472454
8 C 0.320394038028 0.965820508342 -0.178433093204
9 C 1.582854891239 2.372581817101 1.404630379396
10 C 2.070642274651 3.20765641845 2.407507322838
11 C 3.43139071480 3.495708800184 2.424083050256
12 C 4.28162856292 2.993937060812 1.42653403026
13 C 3.802254741639 2.17324550669 0.414647590027
The table contains the AMOEBA optimized geometry of TO3-Biotin (charge: 2) in the .txyz file format.
|   | C     | -8.42642347 | -1.04459087 | 0.91645676 | 403 | 22 | 25 |
|---|-------|-------------|-------------|------------|-----|----|----|
| 2 | C     | -6.47728422 | 0.43046644  | 1.06645699 | 409 | 3  | 22 |
| 3 | C     | -5.11772846 | 0.73148477  | 0.97982117 | 413 | 2  | 4  |
| 4 | C     | -4.16832933 | -0.24000306 | 0.63040848 | 415 | 3  | 5  |
| 5 | C     | -2.77888909 | 0.25736188  | 0.44364760 | 420 | 4  | 6  |
| 6 | C     | -1.87984147 | -0.16548930 | -0.50776888| 422 | 5  | 7  | 31 |
| 7 | C     | -0.50016236 | 0.21955994  | -0.79265872| 425 | 6  | 8  |
| 8 | C     | 0.37724943  | 1.14236561  | -0.20309076| 419 | 7  | 23 |
| 9 | C     | 1.73656669  | 2.66459444  | 1.23179265 | 427 | 10 | 14 |
| 10| C     | 2.28842082  | 3.51329116  | 2.20549488 | 423 | 9  | 11 |
| 11| C     | 3.62908992  | 3.90505289  | 2.08279253 | 428 | 10 | 12 |
| 12| C     | 4.40482965  | 3.46436626  | 0.99295286 | 424 | 11 | 13 |
| 13| C     | 3.85902578  | 2.61646911  | 0.01171032 | 426 | 12 | 14 |
| 14| C     | 2.50686026  | 2.19550337  | 0.14967015 | 418 | 9  | 13 |
| 15| C     | 2.17875007  | 0.63085836  | -1.77369766| 410 | 23 | 37 |
| 16| C     | -4.66218162 | -1.60378299 | 0.42693096 | 411 | 4  | 17 |
| 17| C     | -3.79379730 | -2.73380774 | 0.18248825 | 416 | 16 | 18 |
| 18| C     | -4.30381491 | -4.00815041 | -0.03875333| 421 | 17 | 19 |
| 19| C     | -5.70156777 | -4.22432279 | -0.00125248| 417 | 18 | 20 |
| 20| C     | -6.57870599 | -3.17880377 | 0.27607855 | 412 | 19 | 21 |
| 21| C     | -6.08829948 | -1.86812627 | 0.50845269 | 408 | 16 | 20 |
| 22| N     | -6.95510406 | -0.82444785 | 0.81931731 | 406 | 1  | 2  |
| 23|       |             |             |            |     |    |    |
|   | N     | 1.75096284 | 1.33967121 | -0.71107306 | 414 | 8 | 14 |
|---|-------|------------|------------|-------------|-----|---|----|
| 24| S     | 0.08080504 | 2.12251306 | 1.20703580  | 430 | 8 | 9 |
| 25| H     | -8.77100509| -1.43074511| -0.04591061 | 433 | 1 |
| 26| H     | -8.60157850| -1.4308325  | 1.7340673   | 433 | 1 |
| 27| H     | -7.20396095| 1.19447733  | 1.32341921  | 437 | 2 |
| 28| H     | -4.82934726| 1.76796398  | 1.17360661  | 440 | 3 |
| 29| H     | -2.48323248| 0.99439127  | -1.22864535 | 448 | 6 |
| 30| H     | -2.24413557| -0.90365192 | -1.64832798 | 446 | 7 |
| 31| H     | -1.69238901| 3.87501845  | 3.04604018  | 450 | 10 |
| 32| H     | 4.07506083 | 4.56269890  | 2.83137108  | 447 | 11 |
| 33| H     | 5.44773054 | 3.76875764  | 0.88800997  | 449 | 12 |
| 34| H     | 4.47409611 | 2.32032910  | -0.8269214  | 445 | 13 |
| 35| H     | 1.51932668 | 0.65574813  | -2.64407258 | 438 | 15 |
| 36| H     | -2.72266487| -2.59508143 | 0.19004461  | 441 | 17 |
| 37| H     | -3.62849747| 4.84290774  | -0.23501954 | 444 | 18 |
| 38| H     | -6.09749844| -5.22597032 | -0.18222114 | 442 | 19 |
| 39| H     | -7.63688930| -3.40327392 | 0.31224433  | 439 | 20 |
| 40| C     | 3.43625864 | -0.09400965 | -2.18129032 | 407 | 15 |
| 41| O     | 3.47915148 | -0.3583195  | -3.38961430 | 436 | 42 |
| 42| N     | 4.44232224 | -0.35911255 | -1.29236206 | 405 | 42 |
| 43| C     | 5.67454024 | -1.0250887  | -1.79055632 | 401 | 44 |
| 44| H     | 4.32647752 | -0.13388180 | -0.30764448 | 435 | 44 |
| 45| C     | 6.68588937 | -1.2336442  | -0.6446465  | 402 | 46 |
| 46| H     | 5.41272773 | -1.97948870 | -2.24885942 | 432 | 46 |
| 47| H     | 6.11997460 | -0.41582037 | -2.58274832 | 432 | 46 |
| 48| C     | 6.68588937 | -1.2336442  | -0.6446465  | 402 | 46 |
| 49| H     | 8.52122751 | -2.79347206 | 0.50011936  | 434 | 53 |
| 50| H     | 9.68122938 | -2.66633707 | -0.83754968 | 434 | 53 |
| 51| H     | 9.27001434 | -1.22440286 | 0.11241682  | 434 | 53 |

V. Parameters in Tinker format

TO1-Biotin parameters

| atom | 419 | 419 | C | "TO1-E" | 6 |

Page 24 of 66
12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  4
atom  12.011  4
atom  12.011  4
atom  12.011  4
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  4
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom  12.011  3
atom
| Atom | Z | Atom | Z | Atom | Z | Atom | Z |
|------|---|------|---|------|---|------|---|
| 12.011 | 3 | 14.007 | 3 | 14.007 | 3 | 14.007 | 3 |
| 15.999 | 2 | 15.999 | 1 | 32.066 | 2 | 1.008 | 1 |
| 1.008 | 1 | 1.008 | 1 | 1.008 | 1 | 1.008 | 1 |
| 1.008 | 1 | 1.008 | 1 | 1.008 | 1 | 1.008 | 1 |
| 1.008 | 1 | 1.008 | 1 | 1.008 | 1 | 1.008 | 1 |
| 1.008 | 1 | 1.008 | 1 | 1.008 | 1 | 1.008 | 1 |
| 1.008 | 1 | 1.008 | 1 | 1.008 | 1 | 1.008 | 1 |
| 1.008 | 1 | 1.008 | 1 | 1.008 | 1 | 1.008 | 1 |
| 1.008 | 1 | 1.008 | 1 | 1.008 | 1 | 1.008 | 1 |
| 1.008 | 1 | 1.008 | 1 | 1.008 | 1 | 1.008 | 1 |
| 1.008 | 1 | 1.008 | 1 | 1.008 | 1 | 1.008 | 1 |
| 1.008 | 1 | 1.008 | 1 | 1.008 | 1 | 1.008 | 1 |

| atom | Z | atom | Z | atom | Z | atom | Z |
|------|---|------|---|------|---|------|---|
| 406  | N | "TO1-E" | "  | 7 |
| 422  | N | "TO1-E" | "  | 7 |
| 407  | N | "TO1-E" | "  | 7 |
| 429  | O | "TO1-E" | "  | 8 |
| 437  | O | "TO1-E" | "  | 8 |
| 430  | S | "TO1-E" | "  | 16 |
| 442  | H | "TO1-E" | "  | 1 |
| 432  | H | "TO1-E" | "  | 1 |
| 433  | H | "TO1-E" | "  | 1 |
| 434  | H | "TO1-E" | "  | 1 |
| 440  | H | "TO1-E" | "  | 1 |
| 438  | H | "TO1-E" | "  | 1 |
| 435  | H | "TO1-E" | "  | 1 |
| 439  | H | "TO1-E" | "  | 1 |
| 445  | H | "TO1-E" | "  | 1 |
| 446  | H | "TO1-E" | "  | 1 |
| 444  | H | "TO1-E" | "  | 1 |
| 448  | H | "TO1-E" | "  | 1 |
| 447  | H | "TO1-E" | "  | 1 |
| 449  | H | "TO1-E" | "  | 1 |
| 441  | H | "TO1-E" | "  | 1 |
| 436  | H | "TO1-E" | "  | 1 |
| Atom | Z | Charge | Element | Bond | VDW Distance | VDW Energy |
|------|---|--------|---------|------|--------------|------------|
| 1    | C | 1      | 402     | TO1-E | 6            |            |
| 4    | H | 1      | 431     | TO1-E | 1            |            |
| 1    | O | 1      | 428     | TO1-E | 8            |            |
| 2    | H | 1      | 450     | TO1-E | 1            |            |
| 1    | H | 1      | 443     | TO1-E | 1            |            |
| vdw 418 | 3.8200 | 0.1010 |
| vdw 429 | 3.4050 | 0.1100 |
| vdw 428 | 3.4050 | 0.1100 |
| vdw 450 | 2.6550 | 0.0135  |
| vdw 432 | 2.8700 | 0.0240  |
| vdw 433 | 2.8700 | 0.0240  |
| vdw 431 | 2.8700 | 0.0240  |
| vdw 401 | 3.8200 | 0.1010  |
| vdw 404 | 3.8200 | 0.1010  |
| vdw 403 | 3.8200 | 0.1010  |
| vdw 405 | 3.8200 | 0.1010  |
| vdw 402 | 3.8200 | 0.1010  |
| vdw 435 | 2.9800 | 0.0240  |
| vdw 434 | 2.9600 | 0.0220  |
| vdw 423 | 3.8200 | 0.1060  |
| vdw 408 | 3.8200 | 0.1060  |
| vdw 411 | 3.8200 | 0.1060  |
| vdw 437 | 3.3000 | 0.1120  |
| vdw 406 | 3.7100 | 0.1100  |
| vdw 436 | 2.5900 | 0.0220  |
| vdw 442 | 2.9200 | 0.0300  |
| vdw 443 | 2.9200 | 0.0300  |
| vdw 430 | 4.0050 | 0.3550  |
| vdw 419 | 3.8000 | 0.0890  |
| vdw 420 | 3.8000 | 0.0890  |
| vdw 438 | 2.9800 | 0.0260  |
| vdw 439 | 2.9800 | 0.0260  |
| vdw 444 | 2.9800 | 0.0260  |
| vdw 448 | 2.9800 | 0.0260  |
| vdw 441 | 2.9800 | 0.0260  |
| vdw 414 | 3.8000 | 0.0910  |
| vdw 426 | 3.8000 | 0.0910  |
| vdw 440 | 2.9800 | 0.0260  |
vdw 445 2.9800 0.0260 0.920
vdw 446 2.9800 0.0260 0.920
vdw 447 2.9800 0.0260 0.920
vdw 449 2.9800 0.0260 0.920
vdw 407 3.7100 0.1050
vdw 415 3.8000 0.1010
vdw 410 3.8000 0.1010
vdw 409 3.8000 0.1010
vdw 413 3.8000 0.1010
vdw 417 3.8000 0.1010
vdw 424 3.8000 0.1010
vdw 416 3.8000 0.1010
vdw 412 3.8000 0.1010
vdw 425 3.8000 0.1010
vdw 427 3.8000 0.1010
vdw 421 3.8000 0.1010
vdw 422 3.7100 0.1050
bond 419 430 216.0 1.76
bond 411 422 400.0 1.31
bond 407 410 381.30 1.34
bond 408 411 385.0 1.51
bond 430 425 250.0 1.77
bond 437 408 601.80 1.24
bond 442 423 400.0 1.09
bond 443 411 400.0 1.09
bond 415 423 385.0 1.48
bond 423 419 385.0 1.34
bond 422 419 600.0 1.46
bond 422 418 600.0 1.43
bond 409 407 400.0 1.3471999999999997
bond 414 415 379.094345 1.38
bond 412 415 337.112301 1.42
bond 429 401 274.968492 1.43
bond 432 401 340.532535 1.1
bond 402 401 205.758598 1.52
bond 403 404 205.758598 1.51
bond 429 404 274.968492 1.42
bond 433 404 340.532535 1.1
bond 406 403 232.730342 1.47
bond 434 403 340.532535 1.09
bond 406 408 363.15688 1.35
bond 410 414 375.678112 1.39
bond 440 414 368.093365 1.09
bond 438 410 375.586577 1.08
bond 407 405 295.419463 1.4494
bond 435 405 345.97894 1.09
bond 413 409 375.678112 1.41
bond 412 409 375.678112 1.3990999999999998
bond 417 413 379.094345 1.38
bond 439 413 368.093365 1.08
bond 424 417 379.094345 1.41
bond 445 417 368.093365 1.09
bond 416 424 379.094345 1.38
bond 446 424 368.093365 1.09
bond 412 416 337.112301 1.42
bond 444 416 368.093365 1.09
bond 420 425 378.323984 1.39
bond 418 425 375.678112 1.4
bond 427 420 379.094345 1.4
bond 448 420 368.093365 1.09
bond 421 427 379.094345 1.4
bond 447 427 368.093365 1.09
bond 426 421 379.094345 1.39
bond 449 421 368.093365 1.09
bond 418 426 375.678112 1.4
bond 441 426 368.093365 1.08
bond 436 406 475.798234 1.02
bond 431 402 340.532535 1.1
bond 428 402 216.835083 1.42
bond 450 428 497.050438 0.97
angle 419 423 442 50.0 119.9
angle 419 422 411 65.0 119.52
angle 419 430 425 80.0 85.2493
angle 423 419 422 80.0 120.96719999999999
angle 423 419 430 53.2 132.0401
angle 408 411 422 80.0 134.33
angle 411 422 418 65.0 134.19639999999998
angle 418 425 430 53.2 113.39
angle 422 419 430 60.0 107.0648
angle 422 411 443 60.0 115.08
angle 403 404 429 88.0 104.62
angle 402 401 429 88.0 112.949
angle 430 425 420 60.0 126.68
angle 438 410 407 58.99 116.8
angle 443 411 408 38.0 110.4
angle 405 407 410 51.80 118.48
angle 437 408 411 65.0 114.075500000000002
angle 406 408 411 60.0 119.83359999999999
| angle | 406 | 408 | 437 | 76.98 | 126.23 |
| angle | 415 | 423 | 442 | 50.0  | 119.396 |
| angle | 409 | 407 | 405 | 65.0  | 118.536 |
| angle | 415 | 423 | 419 | 60.0  | 120.366 |
| angle | 407 | 410 | 414 | 60.0  | 121.38  |
| angle | 422 | 418 | 425 | 60.0  | 108.795 |
| angle | 422 | 418 | 426 | 60.0  | 127.04  |
| angle | 409 | 407 | 410 | 65.0  | 121.66  |
| angle | 412 | 415 | 423 | 60.0  | 122.08  |
| angle | 413 | 409 | 407 | 80.0  | 118.975 |
| angle | 412 | 409 | 407 | 80.0  | 118.67  |
| angle | 414 | 415 | 423 | 60.0  | 118.81  |
| angle | 418 | 422 | 419 | 65.0  | 105.639 |
| angle | 410 | 414 | 415 | 89.183 | 120.2  |
| angle | 440 | 414 | 415 | 36.771 | 121.32 |
| angle | 409 | 412 | 415 | 89.183 | 119.02 |
| angle | 416 | 412 | 415 | 78.148 | 122.67 |
| angle | 404 | 429 | 401 | 88.187 | 112.085 |
| angle | 431 | 402 | 401 | 48.261 | 110.71 |
| angle | 428 | 402 | 401 | 94.530 | 103.89 |
| angle | 406 | 403 | 404 | 99.687 | 104.746 |
| angle | 434 | 403 | 404 | 48.260 | 111.22 |
| angle | 433 | 404 | 403 | 48.260 | 110.26 |
| angle | 408 | 406 | 403 | 87.947 | 116.052 |
| angle | 436 | 406 | 403 | 29.797 | 111.62 |
| angle | 436 | 406 | 408 | 40.855 | 114.678 |
| angle | 412 | 415 | 414 | 59.085 | 119.0  |
| angle | 438 | 410 | 414 | 59.926 | 123.491 |
| angle | 440 | 414 | 410 | 47.266 | 118.47 |
| angle | 417 | 413 | 409 | 89.183 | 119.36 |
| angle | 439 | 413 | 409 | 47.266 | 119.642 |
| angle | 416 | 412 | 409 | 89.183 | 118.3  |
| angle | 412 | 409 | 413 | 59.085 | 121.746 |
| angle | 424 | 417 | 413 | 74.630 | 120.9  |
| angle | 445 | 417 | 413 | 36.770 | 119.35 |
| angle | 439 | 413 | 417 | 36.770 | 121.798 |
| angle | 416 | 424 | 417 | 74.630 | 120.59 |
| angle | 446 | 424 | 417 | 36.770 | 119.52 |
| angle | 445 | 417 | 424 | 36.770 | 119.73 |
| angle | 412 | 416 | 424 | 59.085 | 120.44 |
| angle | 444 | 416 | 424 | 36.770 | 122.930 |
| angle | 446 | 424 | 416 | 36.770 | 119.89 |
| angle | 444 | 416 | 412 | 26.510 | 116.906 |
| angle | 427 | 420 | 425 | 68.376 | 118.24 |
angle 448 420 425 29.804975 121.03
angle 426 418 425 76.194709 122.2
angle 418 425 420 89.183524 119.9
angle 421 427 420 74.630713 121.21
angle 447 427 420 36.770174 119.18
angle 448 420 427 36.770174 120.69
angle 426 421 427 74.630713 120.94
angle 449 421 427 36.770174 119.78
angle 447 427 421 36.770174 119.57
angle 418 426 421 89.183524 117.09
angle 441 426 421 36.770174 122.97119999999998
angle 449 421 426 36.770174 119.25
angle 441 426 418 47.265893 121.66
angle 434 403 406 57.622801 109.71
angle 435 405 407 53.335255 106.86390000000002
angle 432 401 429 54.887155 107.82
angle 433 404 429 54.887155 111.69
angle 432 401 432 30.490529 110.2527
angle 402 401 432 48.260518 108.71
angle 433 404 433 30.490529 108.3
angle 434 403 434 30.490529 110.709
angle 435 405 435 36.406852 112.96910000000001
angle 450 428 402 48.760726 106.30720000000001
angle 431 402 431 30.490529 108.27
angle 428 402 431 60.032562 111.64
strbnd 419 423 442 0 0
strbnd 419 422 411 0 0
strbnd 419 430 425 0 0
strbnd 423 419 422 0 0
strbnd 423 419 430 0 0
strbnd 408 411 422 0 0
strbnd 411 422 418 0 0
strbnd 418 425 430 0 0
strbnd 422 419 430 0 0
strbnd 422 411 443 0 0
strbnd 403 404 429 0 0
strbnd 402 401 429 0 0
strbnd 430 425 420 0 0
strbnd 438 410 407 11.50 11.50
strbnd 443 411 408 0 0
strbnd 405 407 410 7.20 7.20
strbnd 437 408 411 0 0
strbnd 406 408 411 0 0
strbnd 406 408 437 18.70 18.70
| strbnd | 415 | 423 | 442 | 0  | 0  |
|--------|-----|-----|-----|----|----|
| strbnd | 409 | 407 | 405 | 0  | 0  |
| strbnd | 415 | 423 | 419 | 0  | 0  |
| strbnd | 407 | 410 | 414 | 0  | 0  |
| strbnd | 422 | 418 | 425 | 0  | 0  |
| strbnd | 422 | 418 | 426 | 0  | 0  |
| strbnd | 409 | 407 | 410 | 0  | 0  |
| strbnd | 412 | 415 | 423 | 0  | 0  |
| strbnd | 413 | 409 | 407 | 0  | 0  |
| strbnd | 412 | 409 | 407 | 0  | 0  |
| strbnd | 414 | 415 | 423 | 0  | 0  |
| strbnd 410 414 415 20.4528 20.4528 |
| strbnd 440 414 415 20.4528 20.4528 |
| strbnd 409 412 415 20.4528 20.4528 |
| strbnd 416 412 415 20.4528 20.4528 |
| strbnd 404 429 401 6.8713 6.8713 |
| strbnd 431 402 401 5.7126 5.7126 |
| strbnd 428 402 401 5.7126 5.7126 |
| strbnd 406 403 404 5.7126 5.7126 |
| strbnd 434 403 404 5.7126 5.7126 |
| strbnd 433 404 403 5.7126 5.7126 |
| strbnd 408 406 403 25.9516 25.9516 |
| strbnd 436 406 403 25.9516 25.9516 |
| strbnd 436 406 408 25.9516 25.9516 |
| strbnd 412 415 414 20.4528 20.4528 |
| strbnd 438 410 414 36.8955 36.8955 |
| strbnd 440 414 410 20.4528 20.4528 |
| strbnd 417 413 409 20.4528 20.4528 |
| strbnd 439 413 409 20.4528 20.4528 |
| strbnd 416 412 409 20.4528 20.4528 |
| strbnd 412 409 413 20.4528 20.4528 |
| strbnd 424 417 413 20.4528 20.4528 |
| strbnd 445 417 413 20.4528 20.4528 |
| strbnd 439 413 417 20.4528 20.4528 |
| strbnd 416 424 417 20.4528 20.4528 |
| strbnd 446 424 417 20.4528 20.4528 |
| strbnd 445 417 424 20.4528 20.4528 |
| strbnd 412 416 424 20.4528 20.4528 |
| strbnd 444 416 424 20.4528 20.4528 |
| strbnd 446 424 416 20.4528 20.4528 |
| strbnd 444 416 412 20.4528 20.4528 |
| strbnd 427 420 425 20.4528 20.4528 |
| strbnd 448 420 425 20.4528 20.4528 |
| strbnd 426 418 425 20.4528 20.4528 |
| Start  | End   | Width | Height | Angle  |
|--------|-------|-------|--------|--------|
| 418    | 420   | 20.4528 | 20.4528 | 0      |
| 421    | 420   | 20.4528 | 20.4528 | 0      |
| 447    | 420   | 20.4528 | 20.4528 | 0      |
| 448    | 420   | 20.4528 | 20.4528 | 0      |
| 426    | 420   | 20.4528 | 20.4528 | 0      |
| 449    | 420   | 20.4528 | 20.4528 | 0      |
| 418    | 420   | 20.4528 | 20.4528 | 0      |
| 449    | 420   | 20.4528 | 20.4528 | 0      |
| 441    | 420   | 20.4528 | 20.4528 | 0      |
| 441    | 420   | 20.4528 | 20.4528 | 0      |
| 434    | 406   | 5.7126  | 5.7126 | 0      |
| 435    | 407   | 5.7126  | 5.7126 | 0      |
| 432    | 407   | 5.7126  | 5.7126 | 0      |
| 433    | 407   | 5.7126  | 5.7126 | 0      |
| 443    | 407   | 5.7126  | 5.7126 | 0      |
| 405    | 407   | 5.7126  | 5.7126 | 0      |
| 435    | 407   | 5.7126  | 5.7126 | 0      |
| 402    | 407   | 5.7126  | 5.7126 | 0      |
| 443    | 407   | 5.7126  | 5.7126 | 0      |
| 449    | 420   | 5.7126  | 5.7126 | 0      |
| 422    | 419   | 5.7126  | 5.7126 | 0      |
| 422    | 418   | 5.7126  | 5.7126 | 0      |
| 423    | 415   | 5.7126  | 5.7126 | 0      |
| 407    | 409   | 5.7126  | 5.7126 | 0      |
| 419    | 422   | 5.7126  | 5.7126 | 0      |
| 418    | 422   | 5.7126  | 5.7126 | 0      |
| 414    | 415   | 5.7126  | 5.7126 | 0      |
| 415    | 414   | 5.7126  | 5.7126 | 0      |
| 412    | 415   | 5.7126  | 5.7126 | 0      |
| 415    | 412   | 5.7126  | 5.7126 | 0      |
| 403    | 406   | 5.7126  | 5.7126 | 0      |
| 406    | 408   | 5.7126  | 5.7126 | 0      |
| 408    | 406   | 5.7126  | 5.7126 | 0      |
| 437    | 408   | 5.7126  | 5.7126 | 0      |
| 410    | 414   | 5.7126  | 5.7126 | 0      |
opbend 414 410 0 0 34.0822
opbend 440 414 0 0 72.8135
opbend 438 410 0 0 72.8135
opbend 413 409 0 0 47.0937
opbend 409 413 0 0 47.0937
opbend 412 409 0 0 47.0937
opbend 409 412 0 0 47.0937
opbend 417 413 0 0 84.8861
opbend 413 417 0 0 84.8861
opbend 413 413 0 0 72.8135
opbend 424 417 0 0 84.8861
opbend 417 424 0 0 84.8861
opbend 445 417 0 0 72.8135
opbend 416 424 0 0 84.8861
opbend 424 416 0 0 84.8861
opbend 446 424 0 0 72.8135
opbend 412 416 0 0 100.1116
opbend 416 412 0 0 100.1116
opbend 444 416 0 0 72.8135
opbend 420 425 0 0 14.9839
opbend 425 420 0 0 14.9839
opbend 418 425 0 0 47.0937
opbend 425 418 0 0 47.0937
opbend 427 420 0 0 84.8861
opbend 420 427 0 0 84.8861
opbend 448 420 0 0 72.8135
opbend 421 427 0 0 84.8861
opbend 427 421 0 0 84.8861
opbend 447 427 0 0 72.8135
opbend 426 421 0 0 84.8861
opbend 421 426 0 0 84.8861
opbend 449 421 0 0 72.8135
opbend 418 426 0 0 39.6142
opbend 426 418 0 0 39.6142
opbend 441 426 0 0 72.8135
opbend 436 406 0 0 26.8945
opbend 423 419 0 0 14.39
opbend 430 419 0 0 14.39
opbend 422 411 0 0 14.39
opbend 411 422 0 0 3.6
opbend 408 411 0 0 14.39
opbend 407 410 0 0 14.39
opbend 410 407 0 0 3.6
opbend 409 407 0 0 3.6
opbend 430 425 0 0 14.39
torsion 414 415 423 419 -0.480 0.0 1 14.422 180.0 2 4.720 0.0 3
torsion 412 415 423 419 -2.723 0.0 1 -16.439 180.0 2 3.870 0.0 3
torsion 408 411 422 419 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 443 411 422 419 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 420 425 430 419 0.854 0.0 1 -0.374 180.0 2 0.108 0.0 3
torsion 418 425 430 419 0.854 0.0 1 -0.374 180.0 2 0.108 0.0 3
torsion 411 422 419 423 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 418 422 419 423 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 425 430 419 423 0.854 0.0 1 -0.374 180.0 2 0.108 0.0 3
torsion 422 419 423 415 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 418 422 411 408 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 411 422 419 415 -0.374 180.0 2 0.108 0.0 3
torsion 425 418 422 411 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 426 418 422 411 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 418 422 411 408 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 442 419 423 415 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 425 430 425 418 0.854 0.0 1 -0.374 180.0 2 0.108 0.0 3
torsion 422 419 423 415 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 435 405 407 410 0.121 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 438 410 407 405 1.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 437 408 411 422 0.063 0.0 1 -0.102 180.0 2 -0.807 0.0 3
torsion 430 425 418 426 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 430 419 422 418 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 443 411 422 418 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 406 403 404 429 -0.628 0.0 1 -0.391 180.0 2 0.534 0.0 3
torsion 406 408 411 422 0.924 0.0 1 -0.102 180.0 2 0.514 0.0 3
torsion 442 423 419 422 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 437 408 411 422 0.063 0.0 1 -0.102 180.0 2 -0.807 0.0 3
torsion 430 425 418 422 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 442 423 419 430 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 430 425 420 427 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 430 425 420 448 0.55 0.0 1 6.187 180.0 2 -0.55 0.0 3
torsion 405 407 410 414 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 435 405 407 410 0.072 0.0 1 -0.012 180.0 2 0.563 0.0 3
torsion 438 410 407 405 1.000 0.0 1 -0.648 180.0 2 0.199 0.0 3
torsion 437 408 411 443 0 0.0 1 0 180.0 2 0.108 0.0 3
torsion 406 408 411 443 0 0.0 1 0 180.0 2 0.108 0.0 3
torsion 435 405 407 409 0 0.0 1 0 180.0 2 0.108 0.0 3
torsion 403 406 408 411 -1.000 0.0 1 4.283333333333333 180.0 2 2.050 0.0 3
torsion 405 407 409 413 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 436 406 408 411 0.000 0.0 1 3.483333333333333 180.0 2 0.800 0.0 3
torsion 437 408 406 403 1.000 0.0 1 9.1 180.0 2 -2.250 0.0 3
torsion 436 406 408 437 0.000 0.0 1 1.619333333333333 180.0 2 -0.357 0.0 3
torsion 412 415 423 442 0 0.0 1 0 180.0 2 0.108 0.0 3
torsion 407 410 414 415 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 422 418 425 420 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 422 418 426 421 -0.67 0.0 1 6.287 180.0 2 0.0 0.0 3
torsion 438 410 414 440 0.000 0.0 1 6.355333333333333 180.0 2 0.000 0.0 3
torsion 422 418 426 441 0.55 0.0 1 6.187 180.0 2 -0.55 0.0 3
torsion 407 410 414 440 0.55 0.0 1 6.187 180.0 2 -0.55 0.0 3
torsion 419 422 418 426 -0.67 0.0 1 6.287 180.0 2 -0.67 0.0 3
torsion 421 426 418 426 -0.67 0.0 1 6.287 180.0 2 -0.67 0.0 3
torsion 418 425 420 427 -0.67 0.0 1 6.287 180.0 2 -0.67 0.0 3
torsion 418 426 421 427 -0.67 0.0 1 6.287 180.0 2 -0.67 0.0 3
torsion 447 427 420 425 0.55 0.0 1 6.187 180.0 2 -0.55 0.0 3
torsion 449 421 426 418 -0.67 0.0 1 6.287 180.0 2 -0.67 0.0 3

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| Torsion | Atom 1 | Atom 2 | Atom 3 | Atom 4 | Value 1 | Value 2 | Value 3 | Value 4 | Value 5 | Value 6 | Value 7 |
|---------|--------|--------|--------|--------|---------|---------|---------|---------|---------|---------|---------|
| torsion 424 416 412 409 | -0.670 | 0.0 | 1 | 4.304 | 180.0 | 2 | 0.000 | 0.0 | 3 |
| torsion 416 412 409 413 | -0.670 | 0.0 | 1 | 4.304 | 180.0 | 2 | 0.000 | 0.0 | 3 |
| torsion 416 424 417 413 | -0.670 | 0.0 | 1 | 4.304 | 180.0 | 2 | 0.000 | 0.0 | 3 |
| torsion 412 409 413 417 | -0.670 | 0.0 | 1 | 4.304 | 180.0 | 2 | 0.000 | 0.0 | 3 |
| torsion 412 416 424 417 | -0.670 | 0.0 | 1 | 4.304 | 180.0 | 2 | 0.000 | 0.0 | 3 |
| torsion 421 427 420 425 | -0.67 | 0.0 | 1 | 6.287 | 180.0 | 2 | 0.000 | 0.0 | 3 |
| torsion 426 421 427 420 | -0.670 | 0.0 | 1 | 4.304 | 180.0 | 2 | 0.000 | 0.0 | 3 |
| torsion 414 415 412 409 | -0.610 | 0.0 | 1 | 4.212 | 180.0 | 2 | 0.000 | 0.0 | 3 |
| torsion 414 415 412 416 | -0.610 | 0.0 | 1 | 4.212 | 180.0 | 2 | 0.000 | 0.0 | 3 |
| torsion 423 415 414 440 | 0.55 | 0.0 | 1 | 6.187 | 180.0 | 2 | -0.55 | 0.0 | 3 |
| torsion 412 415 414 440 | 0.000 | 0.0 | 1 | 0.000 | 180.0 | 2 | 0.341 | 0.0 | 3 |
| torsion 410 414 415 423 | -0.67 | 0.0 | 1 | 6.287 | 180.0 | 2 | 0.000 | 0.0 | 3 |
| torsion 410 414 415 412 | 0.260 | 0.0 | 1 | -0.255 | 180.0 | 2 | 0.260 | 0.0 | 3 |
| torsion 415 414 410 438 | 0.000 | 0.0 | 1 | 0.000 | 180.0 | 2 | 0.341 | 0.0 | 3 |
| torsion 436 406 403 434 | 1.397 | 0 | 1 | 0.709 | 180.0 | 2 | -0.436 | 0 | 3 |
| torsion 450 428 402 431 | -0.448 | 0 | 1 | 0.493 | 180.0 | 2 | -0.096 | 0 | 3 |
| torsion 434 403 404 429 | 0.0 | 0 | 1 | 0.0 | 180.0 | 2 | 0.108 | 0 | 3 |
| torsion 434 403 404 433 | 0.0 | 0 | 1 | 0.0 | 180.0 | 2 | 0.299 | 0 | 3 |
| torsion 434 403 404 408 | 0.0 | 0 | 1 | 0.0 | 180.0 | 2 | 0.108 | 0 | 3 |
| torsion 431 402 401 429 | 0.0 | 0 | 1 | 0.0 | 180.0 | 2 | 0.108 | 0 | 3 |
| torsion 431 402 401 432 | 0.0 | 0 | 1 | 0.0 | 180.0 | 2 | 0.299 | 0 | 3 |
| torsion 406 403 404 433 | 0.195 | 0.0 | 1 | -0.098 | 180.0 | 2 | 0.176 | 0.0 | 3 |
| torsion 436 406 403 404 | 0.0 | 0 | 1 | 0.0 | 180.0 | 2 | 0.108 | 0 | 3 |
| torsion 408 406 403 404 | -0.879 | 0 | 1 | -0.305 | 180.0 | 2 | -1.398 | 0 | 3 |
| torsion 414 415 423 442 | 0.0 | 0 | 1 | 0.0 | 180.0 | 2 | 0.108 | 0 | 3 |
| torsion 433 404 429 401 | 0.0 | 0 | 1 | 0.0 | 180.0 | 2 | 0.108 | 0 | 3 |
| torsion 403 404 429 401 | -0.508 | 0 | 1 | 0.088 | 180.0 | 2 | 1.122 | 0 | 3 |
| torsion 402 401 429 404 | 1.298 | 0 | 1 | -0.514 | 180.0 | 2 | 1.129 | 0 | 3 |
| torsion 432 401 429 404 | 0.0 | 0 | 1 | 0.0 | 180.0 | 2 | 0.108 | 0 | 3 |
| torsion 428 402 401 429 | 0.912 | 0 | 1 | -1.127 | 180.0 | 2 | 2.601 | 0 | 3 |
| torsion 428 402 401 432 | 0.0 | 0 | 1 | 0.0 | 180.0 | 2 | 0.108 | 0 | 3 |
| torsion 450 428 402 401 | -0.416 | 0 | 1 | 0.144 | 180.0 | 2 | 1.086 | 0 | 3 |

SOLUTE 450 2.6533 3.392 2.9044
SOLUTE 442 2.574 2.758 2.9054
SOLUTE 440 2.574 2.758 2.9054
SOLUTE 438 2.9059 2.602 2.5726
SOLUTE 439 2.574 2.758 2.9054
SOLUTE 445 2.574 2.758 2.9054
SOLUTE 446 2.574 2.758 2.9054
SOLUTE 444 2.574 2.758 2.9054
SOLUTE 448 2.574 2.758 2.9054
SOLUTE 447 2.574 2.758 2.9054
SOLUTE 449 2.574 2.758 2.9054
| SOLUTE   | 441 | 2.574 | 2.758 | 2.9054 |
|----------|-----|-------|-------|--------|
| SOLUTE   | 443 | 2.574 | 2.758 | 2.9054 |
| SOLUTE   | 434 | 3.0556| 2.996 | 4.032 |
| SOLUTE   | 436 | 3.6491| 3.404 | 2.9894 |
| SOLUTE   | 431 | 3.6491| 3.404 | 2.9894 |
| SOLUTE   | 432 | 3.0205| 3.885 | 4.0505|
| SOLUTE   | 433 | 3.9912| 4.144 | 3.8925|
| SOLUTE   | 435 | 3.143 | 3.374 | 4.144 |
| SOLUTE   | 410 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 419 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 409 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 418 | 3.8585| 3.766 | 3.8448|
| SOLUTE   | 415 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 414 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 413 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 416 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 425 | 3.8585| 3.766 | 3.8448|
| SOLUTE   | 420 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 426 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 408 | 2.9301| 4.506 | 4.2118|
| SOLUTE   | 417 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 424 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 412 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 427 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 421 | 3.8286| 3.893 | 4.5084|
| SOLUTE   | 423 | 2.9301| 4.506 | 4.2118|
| SOLUTE   | 411 | 2.9301| 4.506 | 4.2118|
| SOLUTE   | 405 | 3.5062| 3.309 | 4.536 |
| SOLUTE   | 401 | 3.3025| 2.854 | 4.9016|
| SOLUTE   | 404 | 3.3025| 2.854 | 4.9016|
| SOLUTE   | 403 | 3.3025| 2.854 | 4.9016|
| SOLUTE   | 402 | 3.3025| 2.854 | 4.9016|
| SOLUTE   | 422 | 3.4243| 3.491 | 4.2676|
| SOLUTE   | 407 | 3.4243| 3.491 | 4.2676|
| SOLUTE   | 406 | 2.8836| 2.99  | 3.218 |
| SOLUTE   | 437 | 2.9835| 3.356 | 2.9616|
| SOLUTE   | 429 | 3.1684| 3.134 | 3.0999|
| SOLUTE   | 428 | 3.1684| 3.134 | 3.0999|
| SOLUTE   | 430 | 4.4346| 4.194 | 4.5431|

| polarize | 419 | 2.0645 | 0.3900 | 422 430 |
| polarize | 423 | 1.4150 | 0.3900 | 442   |
| polarize | 415 | 2.0645 | 0.3900 | 414 412 |
| polarize | 401 | 1.6196 | 0.3900 | 429 432 |
| polarize | 404 | 1.6196 | 0.3900 | 429 433 |
| Polarize | Value 1 | Value 2 | Value 3 | Value 4 |
|----------|---------|---------|---------|---------|
| 403      | 1.6196  | 0.3900  | 434     |
| 408      | 2.0645  | 0.3900  | 437     |
| 411      | 1.4150  | 0.3900  | 443     |
| 414      | 2.0645  | 0.3900  | 440     |
| 410      | 2.0645  | 0.3900  | 438     |
| 405      | 1.6196  | 0.3900  | 435     |
| 409      | 2.0645  | 0.3900  | 447     |
| 413      | 2.0645  | 0.3900  | 439     |
| 417      | 2.0645  | 0.3900  | 445     |
| 424      | 2.0645  | 0.3900  | 446     |
| 416      | 2.0645  | 0.3900  | 444     |
| 412      | 2.0645  | 0.3900  | 444     |
| 425      | 2.0645  | 0.3900  | 430     |
| 420      | 2.0645  | 0.3900  | 448     |
| 427      | 2.0645  | 0.3900  | 447     |
| 421      | 2.0645  | 0.3900  | 449     |
| 426      | 2.0645  | 0.3900  | 441     |
| 418      | 2.0645  | 0.3900  | 422     |
| 406      | 1.2433  | 0.3900  | 436     |
| 422      | 1.7018  | 0.3900  | 418     |
| 407      | 1.7018  | 0.3900  | 409     |
| 429      | 0.8122  | 0.3900  | 404     |
| 437      | 0.9138  | 0.3900  | 408     |
| 430      | 3.2059  | 0.3900  | 425     |
| 442      | 0.4803  | 0.3900  | 423     |
| 432      | 0.4803  | 0.3900  | 401     |
| 433      | 0.4803  | 0.3900  | 404     |
| 434      | 0.4803  | 0.3900  | 403     |
| 440      | 0.4318  | 0.3900  | 414     |
| 438      | 0.4318  | 0.3900  | 410     |
| 435      | 0.4803  | 0.3900  | 405     |
| 439      | 0.4318  | 0.3900  | 413     |
| 445      | 0.4318  | 0.3900  | 417     |
| 446      | 0.4318  | 0.3900  | 424     |
| 444      | 0.4318  | 0.3900  | 416     |
| 448      | 0.4318  | 0.3900  | 420     |
| 447      | 0.4318  | 0.3900  | 427     |
| 449      | 0.4318  | 0.3900  | 421     |
| 441      | 0.4318  | 0.3900  | 426     |
| 436      | 0.4573  | 0.3900  | 406     |
| 402      | 1.6196  | 0.3900  | 428     |
| 431      | 0.4803  | 0.3900  | 402     |
| 428      | 0.8122  | 0.3900  | 450     |
| 450      | 0.4573  | 0.3900  | 428     |
| Polarization | Multipole | Coefficients |
|-------------|-----------|--------------|
| Polarize    | 419 430 422 | -0.22823     |
|             |           | 0.18994      |
|             |           | 0.00000      |
|             |           | -0.38505     |
| Multipole   | 423 442 415 | -0.14327     |
|             |           | -0.03283     |
|             |           | -0.21202     |
|             |           | 0.00000      |
|             |           | 0.23935      |
| Multipole   | 415 412 414 | -0.07777     |
|             |           | -0.28161     |
|             |           | -0.08134     |
|             |           | 0.00000      |
|             |           | 0.00000      |
| Multipole   | 401 402 429 | 0.07114      |
|             |           | 0.42578      |
|             |           | 0.39558      |
|             |           | 0.00000      |
|             |           | -0.36574     |
| Multipole   | 404 429 403 | 0.06569      |
|             |           | 0.25578      |
|             |           | 0.00125      |
|             |           | 0.00000      |
|             |           | -0.05230     |
| Multipole   | 403 406 404 | -0.04002     |
|             |           | 0.20620      |
|             |           | 0.12238      |
|             |           | 0.00000      |
|             |           | -0.20156     |
| Multipole   | 408 437 406 | 0.71246      |
|             |           | -0.07646     |
|             |           | -0.00000     |
|             |           | 0.07472      |
|             |           | 0.00000      |
|             |           | -0.09823     |
| Multipole   | 411 443 422 | 0.04500      |
|             |           | 0.14958      |
|             |           | 0.16370      |
|             |           | 0.00000      |
|             |           | -0.32747     |
| Multipole   | 414 440 410 | -0.10584     |
|             |           | -0.11618     |
|             |           | 0.04056      |
| Multipole | Coefficients          |
|-----------|-----------------------|
| 410 438 407 | 0.00000 0.15954 -0.05380 0.00000 -0.20010 |
|           | 0.26395               |
|           | 0.25601 0.00000 -0.19513 |
|           | -0.11635              |
|           | 0.00000 -0.52155      |
|           | -0.20792 0.00000 0.63790 |
| 405 407 409 | -0.07500              |
|           | -0.06928 0.00000 0.49814 |
|           | -0.46189              |
|           | 0.00000 -0.50082      |
|           | -0.07817 0.00000 0.96271 |
| 409 407 412 | 0.08054               |
|           | -0.09848 0.00000 0.06035 |
|           | -0.85295              |
|           | 0.00000 -0.08638      |
|           | -0.00035 0.00000 0.93933 |
| 413 439 417 | -0.10830              |
|           | -0.16453 0.00000 0.23837 |
|           | 0.13298               |
|           | 0.00000 -0.01324      |
|           | 0.14099 0.00000 -0.11974 |
| 417 445 424 | 0.30169               |
|           | 0.01313 0.00000 -0.40834 |
|           | -0.80929              |
|           | 0.00000 -0.76050      |
|           | -0.06625 0.00000 1.56979 |
| 424 446 416 | -0.00401              |
|           | 0.00630 0.00000 0.17381 |
|           | 0.21423               |
|           | 0.00000 0.00438       |
|           | -0.07560 0.00000 -0.21861 |
| 416 444 412 | -0.19528              |
|           | -0.17316 0.00000 0.26512 |
|           | -0.11654              |
|           | 0.00000 0.11648       |
|           | 0.19812 0.00000 0.00006 |
| 412 416 409 | 0.01011               |
|           | -0.07833 0.00000 0.07784 |
|           | -0.15988              |
|           | 0.00000 0.70605       |
|           | -0.25498 0.00000 -0.54617 |
| 425 430 418 | -0.25554              |
|           | -0.01764 0.00000 0.04851 |
| Multipole  | 420 448 427 | 427 447 421 | 421 449 426 | 426 441 418 | 418 422 426 | 406 436 408 | 422 418 411 | 407 409 405 | 429 404 401 |
|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
|            | 0.20411     | -0.07002    | 0.04608     | -0.02429    | -0.11301    | -0.18300    | 0.22996     | -0.20500    | -0.33032    |
|            | 0.00000     | 0.05627     | 0.03159     | -0.03498    | 0.12946     | -0.03987    | 0.08389     | -0.13587    | 0.00000     |
|            | 0.10046     | 0.00000     | 0.00000     | 0.00000     | 0.11695     | 0.00000     | 0.00000     | 0.00000     | 0.10046     |
|            | -0.19759    | 0.04495     | 0.00000     | 0.00000     | 0.11344     | 0.00000     | 0.00000     | 0.00000     | -0.10046    |
|            | -0.30457    | -0.19759    | -0.20524    | -0.03520    | -0.18300    | -1.16989    | -0.13837    | 0.82593     | -0.33032    |
|            | -0.07002    | 0.05627     | 0.03159     | 0.04608     | 0.12946     | 0.47895     | 0.08389     | 0.18492     | 0.00000     |
|            | 0.00000     | 0.00000     | 0.00000     | 0.00000     | -0.03725    | 0.00000     | 0.00000     | -0.23041    | -0.33032    |
|            | 0.10046     | 0.20446     | -0.00587    | 0.07370     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
|            | -0.30457    | -0.10245    | 0.00000     | 0.00000     | 0.00000     | -1.24307    | 0.00000     | 0.00000     | -0.33032    |
|            | -0.07002    | 0.20446     | -0.00587    | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | -0.64906    |
|            | 0.00000     | -0.03498    | 0.10175     | 0.00000     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
|            | 0.10046     | -0.03498    | 0.10175     | 0.00000     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
|            | -0.19759    | 0.16116     | 0.00000     | 0.00000     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
|            | -0.30457    | -0.03520    | 0.07370     | 0.00000     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
|            | -0.07002    | 0.16116     | 0.00000     | 0.00000     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
|            | 0.00000     | -0.03520    | 0.07370     | 0.00000     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
|            | 0.00000     | 0.10175     | 0.00000     | 0.00000     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
|            | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
|            | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
|            | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.17794     | 2.26847     | 0.10942     | 0.05299     | -0.64906    |
| Multipole | Coefficients |
|----------|--------------|
|          | 0.34821      | 0.00000 | 0.17891 |
|          | 0.16531      | 0.00000 | -1.00658 |
|          | -0.55006     | 0.00000 | 0.84127 |
| 437  408 406 | -0.60533   | 0.00000 | -0.07788 |
|          | 0.03837      | 0.00000 | 0.20499 |
|          | 0.04325      | 0.00000 | 0.24944 |
|          | 0.53116      | 0.00000 | 0.51435 |
| 430  425 419 | 0.59624   | 0.00000 | 1.12713 |
|          | 0.00000      | -2.15635| 1.02922 |
|          | 0.01138      | 0.00000 | 1.02922 |
|          | 0.12022      | 0.00000 | -0.19068 |
| 442  423 415 | 0.05061   | 0.00000 | 0.13375 |
|          | 0.00000      | 0.06535 | -0.19910 |
|          | 0.09409      | 0.00000 | 0.01541 |
| 432  401 402 | 0.04779   | 0.00000 | -0.08574 |
|          | 0.04084      | 0.00000 | 0.03838 |
|          | 0.00000      | 0.01541 | -0.05379 |
| 433  404 433 | 0.04192   | 0.00000 | -0.10510 |
|          | 0.00505      | 0.00000 | 0.05296 |
|          | 0.00000      | 0.00101 | -0.05397 |
|          | 0.02418      | 0.00000 | -0.02440 |
| 434  403 434 | 0.09207   | 0.00000 | -0.04721 |
|          | -0.04721     | 0.00000 | 0.09422 |
|          | 0.00000      | 0.03951 | -0.02511 |
|          | -0.02511     | 0.00000 | -0.13373 |
|          | 0.09150      | 0.00000 | -0.11411 |
| 440  414 410 | -0.01030  | 0.00000 | 0.07275 |
|          | 0.00000      | -0.04835| 0.01069 |
|          | 0.01069      | 0.00000 | -0.02440 |
|          | -0.01544     | 0.00000 | -0.04568 |
| 438  410 407 | 0.08191   | 0.00000 | 0.01857 |
|          | -0.01544     | 0.00000 | 0.01857 |
|          | 0.00000      | -0.06506| -0.02963 |
|          | -0.02963     | 0.00000 | 0.04649 |
| Multipole | 435 405 407 | 0.10504 | 0.03232 | 0.00000 | -0.00173 |
|-----------|-------------|---------|---------|---------|-----------|
| Multipole | 439 413 417 | -0.05159 | 0.00000 | -0.17562 |
| Multipole | 445 417 424 | 0.05556 | 0.00732 | 0.00000 | 0.04164 |
| Multipole | 446 424 416 | 0.05501 | -0.00503 | 0.00000 | -0.11867 |
| Multipole | 444 416 412 | 0.10631 | 0.15131 | 0.00000 | -0.15273 |
| Multipole | 448 420 427 | 0.04689 | 0.01769 | 0.00000 | -0.14689 |
| Multipole | 447 427 421 | 0.05597 | -0.01212 | 0.00000 | -0.11751 |
| Multipole | 449 421 426 | 0.05801 | 0.02672 | 0.00000 | -0.14513 |
| Multipole | 441 426 418 | 0.05912 | -0.03292 | 0.00000 | -0.19646 |
multipoles: 436 406 408
-0.00751 0.00000 -0.20638
0.15183
-0.12467 0.00000 -0.12334
-0.03581

0.00000 0.10862
-0.07126 0.00000 -0.07281

multipoles: 402 428 401
0.11936
0.19945 0.00000 0.16810
-0.01740

0.00000 -0.34885
-0.29032 0.00000 0.36625

multipoles: 431 402 428
0.03463
0.01460 0.00000 -0.04069
0.02305

0.00000 -0.02844
-0.00863 0.00000 0.00539

multipoles: 428 450 402
-0.39391
0.39572 0.00000 -0.08327
0.56124

0.00000 -0.66438
-0.43514 0.00000 0.10314

multipoles: 450 428 402
0.23855
-0.07521 0.00000 -0.14168
-0.00949

0.00000 0.00186
-0.06292 0.00000 0.00763

multipoles: 443 411 422
0.08813
0.07024 0.00000 -0.11076
0.11547

0.00000 0.00615
0.05162 0.00000 -0.12162

TO3-Biotin parameters

| atom | 403 403 | C | "TO3-E" | 6 |
|------|---------|---|---------|--|
| 12.011 | 4 | | | |
| atom  | 409 409 | C | "TO3-E" | 6 |
| 12.011 | 3 | | | |
| atom  | 413 413 | C | "TO3-E" | 6 |
| 12.011 | 3 | | | |
| atom  | 415 415 | C | "TO3-E" | 6 |
| 12.011 | 3 | | | |
| atom  | 420 420 | C | "TO3-E" | 6 |
| 12.011 | 3 | | | |
| atom  | 422 422 | C | "TO3-E" | 6 |
| 12.011 | 3 | | | |
atom           425    425    C     "TO3-E   "       6
atom           419    419    C     "TO3-E   "       6
atom           427    427    C     "TO3-E   "       6
atom           423    423    C     "TO3-E   "       6
atom           428    428    C     "TO3-E   "       6
atom           424    424    C     "TO3-E   "       6
atom           426    426    C     "TO3-E   "       6
atom           418    418    C     "TO3-E   "       6
atom           410    410    C     "TO3-E   "       6
atom           411    411    C     "TO3-E   "       6
atom           416    416    C     "TO3-E   "       6
atom           421    421    C     "TO3-E   "       6
atom           417    417    C     "TO3-E   "       6
atom           412    412    C     "TO3-E   "       6
atom           408    408    C     "TO3-E   "       6
atom           406    406    N     "TO3-E   "       7
atom           414    414    N     "TO3-E   "       7
atom           430    430    S     "TO3-E   "      16
atom           433    433    H     "TO3-E   "       1
atom           437    437    H     "TO3-E   "       1
atom           440    440    H     "TO3-E   "       1
atom           443    443    H     "TO3-E   "       1
| vdw   | 3.4050 | 0.1100 |
|-------|--------|--------|
| vdw   | 2.8700 | 0.0240 | 0.910 |
| vdw   | 3.8200 | 0.1010 |
| vdw   | 3.8200 | 0.1010 |
| vdw   | 3.8200 | 0.1010 |
| vdw   | 3.8200 | 0.1010 |
| vdw   | 2.9800 | 0.0240 | 0.920 |
| vdw   | 2.8900 | 0.0240 | 0.910 |
| vdw   | 2.9600 | 0.0220 | 0.920 |
| vdw   | 3.8200 | 0.1060 |
| vdw   | 3.8200 | 0.1060 |
| vdw   | 3.8200 | 0.1060 |
| vdw   | 3.8200 | 0.1060 |
| vdw   | 3.3000 | 0.1120 |
| vdw   | 3.7100 | 0.1100 |
| vdw   | 2.5900 | 0.0220 | 0.900 |
| vdw   | 2.9200 | 0.0300 | 0.920 |
| vdw   | 2.9200 | 0.0300 | 0.920 |
| vdw   | 2.9200 | 0.0300 | 0.920 |
| vdw   | 2.9200 | 0.0300 | 0.920 |
| vdw   | 4.0050 | 0.3550 |
| vdw   | 3.8200 | 0.1060 |
| vdw   | 3.8000 | 0.0890 |
| vdw   | 3.8000 | 0.0890 |
| vdw   | 2.9800 | 0.0260 | 0.920 |
| vdw   | 2.9800 | 0.0260 | 0.920 |
| vdw   | 2.9800 | 0.0260 | 0.920 |
| vdw   | 2.9800 | 0.0260 | 0.920 |
| vdw   | 2.9800 | 0.0260 | 0.920 |
| vdw   | 3.8000 | 0.0910 |
| vdw   | 3.8000 | 0.0910 |
| vdw   | 2.9800 | 0.0260 | 0.920 |
| vdw   | 2.9800 | 0.0260 | 0.920 |
| vdw   | 2.9800 | 0.0260 | 0.920 |
| vdw   | 2.9800 | 0.0260 | 0.920 |
| vdw   | 2.9800 | 0.0260 | 0.920 |
| vdw   | 3.7100 | 0.1050 |
| vdw   | 3.8000 | 0.1010 |
| vdw   | 3.8000 | 0.1010 |
| vdw   | 3.8000 | 0.1010 |
| vdw   | 3.8000 | 0.1010 |
| vdw   | 3.8000 | 0.1010 |
| vdw   | 3.8000 | 0.1010 |
vdw 416 3.8000 0.1010
vdw 421 3.8000 0.1010
vdw 417 3.8000 0.1010
vdw 412 3.8000 0.1010
vdw 408 3.8000 0.1010
vdw 414 3.7100 0.1050

bond 419 430 216.0 1.74
bond 410 414 400.0 1.33
bond 406 409 381.30 1.34
bond 407 410 385.0 1.5
bond 425 422 385.0 1.44
bond 430 427 250.0 1.75
bond 436 407 601.80 1.24
bond 446 425 400.0 1.09
bond 438 410 400.0 1.09
bond 415 420 385.0 1.46
bond 425 419 385.0 1.37
bond 414 419 600.0 1.45
bond 414 418 600.0 1.42
bond 408 406 400.0 1.3469999999999998
bond 406 403 295.419463 1.4472
bond 433 403 345.97894 1.09
bond 413 409 375.678112 1.39
bond 437 409 375.586577 1.08
bond 415 413 379.094345 1.39
bond 440 413 368.093365 1.09
bond 411 415 337.112301 1.43
bond 422 420 485.389179 1.36
bond 443 420 365.16166 1.09
bond 448 422 365.16166 1.09
bond 418 427 375.678112 1.4
bond 423 427 378.323984 1.39
bond 428 423 379.094345 1.39
bond 450 423 368.093365 1.09
bond 424 428 379.094345 1.4
bond 447 428 368.093365 1.09
bond 426 424 379.094345 1.39
bond 449 424 368.093365 1.09
bond 418 426 375.678112 1.4
bond 445 426 368.093365 1.08
bond 416 411 337.112301 1.42
bond 408 411 337.112301 1.4021
bond 421 416 379.094345 1.38
bond 441 416 368.093365 1.08
| Bond 1   | Bond 2   | Bond Length | Bond Angle |
|---------|---------|-------------|------------|
| 417 421 | 379.094345 | 1.41        |
| 444 421 | 368.093365 | 1.09        |
| 412 417 | 379.094345 | 1.38        |
| 442 417 | 368.093365 | 1.09        |
| 408 412 | 375.678112 | 1.3817      |
| 439 412 | 368.093365 | 1.08        |
| 405 407 | 363.15688  | 1.36        |
| 435 405 | 475.798234 | 1.02        |
| 401 405 | 232.730342 | 1.47        |
| 432 401 | 340.532535 | 1.09        |
| 402 401 | 205.758598 | 1.52        |
| 431 402 | 340.532535 | 1.1         |
| 429 402 | 274.968492 | 1.4         |
| 404 429 | 291.912992 | 1.43        |
| 434 404 | 345.97894  | 1.09        |

| Angle 1 | Angle 2 | Angle 3 | Angle Value | Angle Value |
|---------|---------|---------|-------------|-------------|
| 425     | 419     | 414     | 80.0        | 116.24440000000001 |
| 425     | 419     | 430     | 53.2        | 130.2004     |
| 419     | 425     | 446     | 50.0        | 116.2        |
| 419     | 414     | 410     | 65.0        | 116.2248     |
| 419     | 430     | 427     | 80.0        | 89.85        |
| 418     | 427     | 430     | 53.2        | 114.01       |
| 418     | 414     | 410     | 65.0        | 131.4245     |
| 414     | 419     | 430     | 60.0        | 111.7        |
| 414     | 410     | 438     | 60.0        | 114.77       |
| 414     | 410     | 407     | 60.0        | 133.53       |
| 404     | 429     | 402     | 88.5        | 107.8052     |
| 401     | 402     | 429     | 88.0        | 105.22       |
| 430     | 427     | 423     | 60.0        | 124.8        |
| 437     | 409     | 406     | 58.99       | 116.8        |
| 438     | 410     | 407     | 38.0        | 111.21       |
| 446     | 425     | 422     | 38.0        | 114.61       |
| 409     | 406     | 403     | 51.80       | 118.57       |
| 436     | 407     | 410     | 65.0        | 116.47529999999999 |
| 405     | 407     | 410     | 60.0        | 119.6379     |
| 405     | 407     | 436     | 76.98       | 124.7        |
| 415     | 420     | 443     | 50.0        | 114.39       |
| 408     | 406     | 403     | 65.0        | 118.3764     |
| 448     | 422     | 425     | 38.0        | 113.99       |
| 422     | 420     | 415     | 60.0        | 123.08210000000001 |
| 425     | 422     | 420     | 60.0        | 126.68280000000001 |
| 419     | 425     | 422     | 60.0        | 129.18       |
| 406     | 409     | 413     | 60.0        | 121.29       |
| 414     | 418     | 427     | 60.0        | 111.02       |
| 414     | 418     | 426     | 60.0        | 127.39       |
angle 433 403 433 36.406852 113.00880000000001
angle 435 405 407 40.855201 115.76610000000001
angle 401 405 407 87.947117 114.61710000000001
angle 432 401 405 57.622801 108.3487
angle 402 401 405 9.687701 108.4788
angle 401 405 435 29.797294 116.85
angle 431 402 401 48.260518 110.6
angle 432 401 432 30.490529 108.8989
angle 402 401 432 48.260518 110.06
angle 431 402 431 30.490529 107.64
angle 429 402 431 54.887155 111.41
angle 434 404 429 57.322419 109.45
angle 434 404 434 72.813704 109.48
strbnd 425 419 414 0 0
strbnd 425 419 430 0 0
strbnd 419 425 446 0 0
strbnd 419 414 410 0 0
strbnd 419 430 427 0 0
strbnd 418 427 430 0 0
strbnd 418 414 410 0 0
strbnd 414 419 430 0 0
strbnd 414 410 438 0 0
strbnd 414 410 407 0 0
strbnd 404 429 402 0 0
strbnd 401 402 429 0 0
strbnd 430 427 423 0 0
strbnd 437 409 406 11.50 11.50
strbnd 438 410 407 0 0
strbnd 446 425 422 0 0
strbnd 409 406 403 7.20 7.20
strbnd 436 407 410 0 0
strbnd 405 407 410 0 0
strbnd 405 407 436 18.70 18.70
strbnd 415 420 443 0 0
strbnd 408 406 403 0 0
strbnd 448 422 425 0 0
strbnd 422 420 415 0 0
strbnd 425 422 420 0 0
strbnd 419 425 422 0 0
strbnd 406 409 413 0 0
strbnd 414 418 427 0 0
strbnd 414 418 426 0 0
strbnd 408 406 409 0 0
strbnd 411 415 420 0 0
| strbnd | 411 | 408 | 406 | 0 | 0 |
|--------|-----|-----|-----|---|---|
| strbnd | 412 | 408 | 406 | 0 | 0 |
| strbnd | 413 | 415 | 420 | 0 | 0 |
| strbnd | 415 | 409 | 406 | 20.4528 | 20.4528 |
| strbnd | 415 | 409 | 406 | 20.4528 | 20.4528 |
| strbnd | 415 | 413 | 409 | 20.4528 | 20.4528 |
| strbnd | 416 | 411 | 415 | 20.4528 | 20.4528 |
| strbnd | 408 | 411 | 415 | 20.4528 | 20.4528 |
| strbnd | 448 | 422 | 420 | 34.2002 | 34.2002 |
| strbnd | 449 | 424 | 428 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 428 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
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| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
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| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
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| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
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| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
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| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
| strbnd | 449 | 424 | 426 | 20.4528 | 20.4528 |
strbnd 432 401 405 5.7126 5.7126
strbnd 402 401 405 5.7126 5.7126
strbnd 401 405 435 25.9516 25.9516
strbnd 431 402 401 5.7126 5.7126
strbnd 432 401 432 5.7126 5.7126
strbnd 402 401 432 5.7126 5.7126
strbnd 431 402 431 5.7126 5.7126
strbnd 429 402 431 5.7126 5.7126
strbnd 434 404 429 5.7126 5.7126
strbnd 434 404 434 5.7126 5.7126
opbend 410 407 0 0 42.40
opbend 443 420 0 0 140.30
opbend 448 422 0 0 140.30
opbend 446 425 0 0 140.30
opbend 438 410 0 0 140.30
opbend 415 420 0 0 42.40
opbend 403 406 0 0 12.90
opbend 422 425 0 0 42.40
opbend 422 420 0 0 14.40
opbend 419 425 0 0 14.40
opbend 414 419 0 0 18.00
opbend 414 418 0 0 18.00
opbend 420 415 0 0 14.40
opbend 406 408 0 0 14.40
opbend 419 414 0 0 10.80
opbend 418 414 0 0 10.80
opbend 413 409 0 0 34.0822
opbend 409 413 0 0 34.0822
opbend 437 409 0 0 72.8135
opbend 415 413 0 0 84.8861
opbend 413 415 0 0 84.8861
opbend 440 413 0 0 72.8135
opbend 411 415 0 0 100.1116
opbend 415 411 0 0 100.1116
opbend 418 427 0 0 47.0937
opbend 427 418 0 0 47.0937
opbend 423 427 0 0 14.9839
opbend 427 423 0 0 14.9839
opbend 428 423 0 0 84.8861
opbend 423 428 0 0 84.8861
opbend 450 423 0 0 72.8135
opbend 424 428 0 0 84.8861
opbend 428 424 0 0 84.8861
opbend 447 428 0 0 72.8135
opbend 426 424 0 0 84.8861
opbend 424 426 0 0 84.8861
opbend 449 424 0 0 72.8135
opbend 418 426 0 0 39.6142
opbend 426 418 0 0 39.6142
opbend 445 426 0 0 72.8135
opbend 416 411 0 0 95.117
opbend 411 416 0 0 95.117
opbend 408 411 0 0 47.0937
opbend 411 408 0 0 47.0937
opbend 421 416 0 0 84.8861
opbend 416 421 0 0 84.8861
opbend 441 416 0 0 72.8135
opbend 417 421 0 0 84.8861
opbend 421 417 0 0 84.8861
opbend 444 421 0 0 72.8135
opbend 412 417 0 0 84.8861
opbend 417 412 0 0 84.8861
opbend 442 417 0 0 72.8135
opbend 408 412 0 0 47.0937
opbend 412 408 0 0 47.0937
opbend 439 412 0 0 72.8135
opbend 436 407 0 0 16.5045
opbend 405 407 0 0 92.7841
opbend 407 405 0 0 92.7841
opbend 435 405 0 0 26.8945
opbend 401 405 0 0 16.5457
opbend 406 409 0 0 14.39
opbend 409 406 0 0 3.6
opbend 420 422 0 0 14.39
opbend 425 419 0 0 14.39
opbend 425 422 0 0 14.39
opbend 430 419 0 0 14.39
opbend 414 410 0 0 14.39
opbend 410 414 0 0 3.6
opbend 430 427 0 0 14.39
opbend 407 410 0 0 14.39
opbend 408 406 0 0 3.6
torsion 425 422 420 415 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 448 422 420 415 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 420 422 425 419 12.504 0.0 1 -9.345 180.0 2 2.432 0.0 3
torsion 414 419 425 422 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 430 419 425 422 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 443 420 422 425 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 418 414 419 425 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 410 414 419 425 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 427 430 419 425 0.854 0.0 1 -0.374 180.0 2 0.108 0.0 3
torsion 448 422 419 0.0 1 0 180.0 2 0.108 0.0 3
torsion 438 410 414 419 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 407 410 414 419 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 418 427 430 419 0.854 0.0 1 -0.374 180.0 2 0.108 0.0 3
torsion 423 427 430 419 0.854 0.0 1 -0.374 180.0 2 0.108 0.0 3
torsion 410 414 418 427 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 414 419 430 427 0.854 0.0 1 -0.374 180.0 2 0.108 0.0 3
torsion 430 427 418 426 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 410 414 418 426 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 438 410 414 418 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 407 410 414 418 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 430 419 414 410 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 446 425 419 414 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 430 427 418 414 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 436 407 410 414 0.747 0.0 1 -0.991 180.0 2 -1.637 0.0 3
torsion 405 407 410 414 1.838 0.0 1 -0.988 180.0 2 0.608 0.0 3
torsion 446 425 419 430 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 448 422 420 443 0.000 0.0 1 0.000 180.0 2 0.299 0.0 3
torsion 405 401 402 429 -2.572 0.0 1 2.571 180.0 2 -2.571 0.0 3
torsion 401 402 429 404 -1.165 0.0 1 -0.066 180.0 2 0.911 0.0 3
torsion 434 404 429 402 0 0.0 1 0 180.0 2 0.108 0.0 3
torsion 430 427 423 428 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 430 427 423 450 0.55 0.0 1 6.187 180.0 2 -0.55 0.0 3
torsion 403 406 409 413 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 433 403 406 409 0.072 0.0 1 -0.012 180.0 2 0.563 0.0 3
torsion 437 409 406 403 0.121 0.0 1 -0.648 180.0 2 0.199 0.0 3
torsion 436 407 410 438 0 0.0 1 0 180.0 2 0.108 0.0 3
torsion 405 407 410 438 0 0.0 1 0 180.0 2 0.108 0.0 3
torsion 433 403 406 408 0 0.0 1 0 180.0 2 0.108 0.0 3
torsion 403 406 408 412 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 401 405 407 410 -1.000 0.0 1 4.2833333333333333 180.0 2 2.050 0.0 3
torsion 435 405 407 410 0.000 0.0 1 3.4833333333333334 180.0 2 0.800 0.0 3
torsion 436 407 405 401 1.000 0.0 1 9.1 180.0 2 -2.250 0.0 3
torsion 435 405 407 436 0.000 0.0 1 1.6193333333333333 180.0 2 -0.357 0.0 3
torsion 406 409 413 415 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 414 418 427 423 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 414 418 426 424 -0.67 0.0 1 6.287 180.0 2 0.0 0.3
torsion 440 413 409 437 0.000 0.0 1 10.922 180.0 2 0.000 0.0 3
torsion 406 409 413 440 0.55 0.0 1 6.187 180.0 2 -0.55 0.0 3
torsion 414 418 426 445 0.55 0.0 1 6.187 180.0 2 -0.55 0.0 3
torsion 419 414 418 427 -0.67 0.0 1 6.287 180.0 2 0 0.0 3
 torsion 419 414 418 426 -0.67 0.0 1 6.287 180.0 2 0 0.0 3
 torsion 424 426 418 427 -0.67 0.0 1 6.287 180.0 2 0 0.0 3
 torsion 418 427 423 428 -0.67 0.0 1 6.287 180.0 2 0 0.0 3
 torsion 418 426 424 428 -0.67 0.0 1 6.287 180.0 2 0 0.0 3
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 torsion 449 424 426 418 0.55 0.0 1 6.187 180.0 2 -0.55 0.0 3
 torsion 449 424 428 447 0.000 0.0 1 7.072 180.0 2 0.000 0.0 3
 torsion 445 426 424 449 0.000 0.0 1 7.072 180.0 2 0.000 0.0 3
 torsion 444 421 416 441 0.000 0.0 1 7.072 180.0 2 0.000 0.0 3
 torsion 442 417 421 444 0.000 0.0 1 7.072 180.0 2 0.000 0.0 3
 torsion 439 412 417 442 0.000 0.0 1 7.072 180.0 2 0.000 0.0 3
 torsion 406 408 412 439 0.55 0.0 1 6.187 180.0 2 -0.55 0.0 3
 torsion 415 411 416 441 0.250 0.0 1 5.534 180.0 2 -0.550 0.0 3
 torsion 427 418 426 445 0.55 0.0 1 6.187 180.0 2 -0.55 0.0 3
 torsion 423 428 424 449 0.250 0.0 1 5.534 180.0 2 -0.550 0.0 3
 torsion 428 424 426 445 0.250 0.0 1 5.534 180.0 2 -0.550 0.0 3
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 torsion 417 412 408 406 -0.67 0.0 1 6.287 180.0 2 0 0.0 3
 torsion 421 416 411 415 -0.670 0.0 1 4.304 180.0 2 0.000 0.0 3
 torsion 412 408 411 415 -0.670 0.0 1 4.304 180.0 2 0.000 0.0 3
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torsion 412 417 421 416 -0.670 0.0 1 4.304 180.0 2 0.000 0.0 3
torsion 417 412 408 411 -0.670 0.0 1 4.304 180.0 2 0.000 0.0 3
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torsion 413 415 409 437 -0.670 0.0 1 4.304 180.0 2 0.000 0.0 3
torsion 408 411 416 420 0.000 0.0 1 0.000 180.0 2 0.341 0.0 3
torsion 409 413 415 420 0.000 0.0 1 0.000 180.0 2 0.341 0.0 3
SOLUTE 437 2.9059 2.602 2.5726
SOLUTE 440 2.574 2.758 2.9054
SOLUTE 443 2.574 2.758 2.9054
SOLUTE 448 2.574 2.758 2.9054
SOLUTE 446 2.574 2.758 2.9054
SOLUTE 450 2.574 2.758 2.9054
SOLUTE 447 2.574 2.758 2.9054
SOLUTE 449 2.574 2.758 2.9054
SOLUTE 445 2.574 2.758 2.9054
SOLUTE 438 2.574 2.758 2.9054
SOLUTE 441 2.574 2.758 2.9054
SOLUTE 444 2.574 2.758 2.9054
SOLUTE 442 2.574 2.758 2.9054
SOLUTE 439 2.574 2.758 2.9054
SOLUTE 432 3.0556 2.996 4.032
SOLUTE 434 2.6533 3.392 2.9044
SOLUTE 435 3.6491 3.404 2.9894
| SOLUTE | Value 1 | Value 2 | Value 3 |
|--------|---------|---------|---------|
| 431    | 3.9912  | 4.144   | 3.8925  |
| 433    | 3.143   | 3.374   | 4.144   |
| 409    | 3.8286  | 3.893   | 4.5084  |
| 419    | 3.8286  | 3.893   | 4.5084  |
| 418    | 3.8585  | 3.766   | 3.8448  |
| 408    | 3.8286  | 3.893   | 4.5084  |
| 413    | 3.8286  | 3.893   | 4.5084  |
| 415    | 3.8286  | 3.893   | 4.5084  |
| 427    | 3.8585  | 3.766   | 3.8448  |
| 423    | 3.8286  | 3.893   | 4.5084  |
| 426    | 3.8286  | 3.893   | 4.5084  |
| 411    | 3.8286  | 3.893   | 4.5084  |
| 416    | 3.8286  | 3.893   | 4.5084  |
| 412    | 3.8286  | 3.893   | 4.5084  |
| 407    | 2.9301  | 4.506   | 4.2118  |
| 428    | 3.8286  | 3.893   | 4.5084  |
| 424    | 3.8286  | 3.893   | 4.5084  |
| 421    | 3.8286  | 3.893   | 4.5084  |
| 417    | 3.8286  | 3.893   | 4.5084  |
| 420    | 2.9301  | 4.506   | 4.2118  |
| 422    | 2.9301  | 4.506   | 4.2118  |
| 425    | 2.9301  | 4.506   | 4.2118  |
| 410    | 2.9301  | 4.506   | 4.2118  |
| 403    | 3.5062  | 3.309   | 4.536   |
| 404    | 3.5062  | 3.309   | 4.536   |
| 401    | 3.3025  | 2.854   | 4.9016  |
| 402    | 3.3025  | 2.854   | 4.9016  |
| 406    | 3.4243  | 3.491   | 4.2676  |
| 414    | 3.4243  | 3.491   | 4.2676  |
| 405    | 2.8836  | 2.99    | 3.218   |
| 436    | 2.9835  | 3.356   | 2.9616  |
| 429    | 3.1684  | 3.134   | 3.0999  |
| 430    | 4.4346  | 4.194   | 4.5431  |
| polarize | 403   | 1.6196  | 0.3900 433 |
| polarize | 409   | 2.0645  | 0.3900 413 406 437 |
| polarize | 413   | 2.0645  | 0.3900 409 415 440 |
| polarize | 415   | 2.0645  | 0.3900 413 411 |
| polarize | 420   | 1.4150  | 0.3900 443 |
| polarize | 422   | 2.0645  | 0.3900 448 |
| polarize | 425   | 1.4150  | 0.3900 446 |
| polarize | 419   | 2.0645  | 0.3900 414 430 |
| polarize | 427   | 2.0645  | 0.3900 423 418 430 |
| polarize | 423   | 2.0645  | 0.3900 427 428 450 |
| polarize | 428   | 2.0645  | 0.3900 423 424 447 |
| Orders | Polarization | Multipole  | Electric Fields | Magnetic Fields |
|--------|--------------|------------|----------------|----------------|
| 403    | 406          | 408        | -0.07427       |                |
|        |              |            | -0.04534       | 0.00000        | 0.43601        |
|        |              |            | -0.47165       |                |
|        |              |            | 0.00000        | -0.43942       |                |
|        |              |            | -0.07611       | 0.00000        | 0.91107        |
| Multipole | 409 | 437 | 406 | 0.24552 |
|-----------|-----|-----|-----|---------|
|           |     |     |     | 0.21240 |
|           |     |     |     | 0.01602 |
|           |     |     |     | 0.00000 |
|           |     |     |     | -0.14121 |
| Multipole | 413 | 440 | 415 | -0.09886 |
|           |     |     |     | 0.00874 |
|           |     |     |     | 0.26031 |
|           |     |     |     | 0.00000 |
|           |     |     |     | -0.18674 |
|           |     |     |     | 0.01602 |
|           |     |     |     | 0.00000 |
| Multipole | 415 | 411 | 420 | 0.12227 |
|           |     |     |     | 0.31099 |
|           |     |     |     | 0.28419 |
|           |     |     |     | 0.00000 |
|           |     |     |     | 0.31541 |
| Multipole | 420 | 443 | 422 | -0.10008 |
|           |     |     |     | -0.11973 |
|           |     |     |     | -0.22853 |
|           |     |     |     | 0.00000 |
|           |     |     |     | 0.18618 |
|           |     |     |     | -0.11052 |
| Multipole | 422 | 448 | 425 | -0.12184 |
|           |     |     |     | 0.14300 |
|           |     |     |     | -0.04906 |
|           |     |     |     | 0.00000 |
|           |     |     |     | 0.15625 |
| Multipole | 425 | 446 | 419 | 0.07128 |
|           |     |     |     | -0.00760 |
|           |     |     |     | 0.01113 |
|           |     |     |     | 0.00000 |
|           |     |     |     | -0.13075 |
| Multipole | 419 | 430 | 414 | -0.33573 |
|           |     |     |     | 0.05734 |
|           |     |     |     | 0.41520 |
|           |     |     |     | 0.00000 |
|           |     |     |     | -0.11749 |
| Multipole | 427 | 430 | 418 | -0.19537 |
|           |     |     |     | -0.00958 |
|           |     |     |     | 0.01733 |
|           |     |     |     | 0.00000 |
|           |     |     |     | -0.2430 |
| Multipole | 423 | 450 | 428 | -0.08001 |
|           |     |     |     | -0.22464 |
|           |     |     |     | 0.01803 |
|           |     |     |     | 0.00000 |

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| Multipole  | 428  | 447  | 424  | -0.05903 | 0.00000 | -0.09007 |
|-----------|------|------|------|----------|---------|----------|
|           | 0.00857 |      |      | 0.01491  | 0.00000 | 0.22064  |
|           | 0.26540 |      |      | 0.00000  | -0.03842 |         |
|           | -0.00073 | 0.00000 | -0.22698 |         |         |          |
| Multipole | 424  | 449  | 426  | 0.28987  |         |          |
|           | -0.05892 | 0.00000 | -0.49393 |         |         |          |
|           | -0.93825 |      |      | 0.00000  | -0.83585 |         |
|           | 0.14921  | 0.00000 | 1.77410  |         |         |          |
| Multipole | 426  | 445  | 418  | -0.09442 |         |          |
|           | 0.09308  | 0.00000 | 0.14249  |         |         |          |
|           | 0.04240  |      |      | 0.00000  | 0.10295  |         |
|           | -0.01357 | 0.00000 | -0.14535 |         |         |          |
| Multipole | 418  | 414  | 426  | -0.03625 |         |          |
|           | -0.05872 | 0.00000 | 0.24976  |         |         |          |
|           | -0.31397 |      |      | 0.00000  | 0.0966   |         |
|           | 0.09209  | 0.00000 | 0.30431  |         |         |          |
| Multipole | 410  | 407  | 438  | -0.03108 |         |          |
|           | -0.21460 | 0.00000 | -0.03980 |         |         |          |
|           | -0.18766 |      |      | 0.00000  | 0.14409  |         |
|           | 0.57826  | 0.00000 | 0.04357  |         |         |          |
| Multipole | 411  | 408  | 416  | -0.04598 |         |          |
|           | 0.16201  | 0.00000 | 0.03346  |         |         |          |
|           | -0.52308 |      |      | 0.00000  | 0.61501  |         |
|           | -0.07957 | 0.00000 | -0.09193 |         |         |          |
| Multipole | 416  | 441  | 421  | -0.16937 |         |          |
|           | 0.03187  | 0.00000 | 0.21548  |         |         |          |
|           | -0.02480 |      |      | 0.00000  | 0.11593  |         |
|           | -0.22898 | 0.00000 | -0.09113 |         |         |          |
| Multipole | 421  | 444  | 417  | 0.21376  |         |          |
|           | 0.04445  | 0.00000 | -0.21321 |         |         |          |
|           | -0.51415 |      |      | 0.00000  | -0.48991 |         |
|           | -0.06162 | 0.00000 | 1.00406  |         |         |          |
| Multipole | 417  | 442  | 412  | 0.00021  |         |          |
|           | -0.08919 | 0.00000 | 0.18633  |         |         |          |
|           | 0.24288  |      |      |           |         |          |
| Multipole | 412 439 408 | 408 406 412 | 406 408 409 | 414 410 418 | 430 427 419 | 433 403 406 | 437 409 406 | 440 413 415 | 443 420 422 |
|-----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
|          | 0.00000     | -0.02997    | 0.00945     | 0.00000     | -0.21291    | 0.22323     | 0.00000     | -0.10153    | 0.00000     |
|          | -0.10153    | 0.05821     | 0.00000     | 0.08079     | 0.25705     | 0.02471     | 0.00000     | 0.37522     | 0.00000     |
|          | -0.16896    | 0.22323     | 0.02258     | 0.00000     | -0.08079    | 0.02471     | 0.00000     | 0.10499     | 0.00000     |
|          | 0.00000     | -0.16896    | -0.055282   | 0.00000     | 0.25705     | 0.02471     | -0.05282    | 0.92804     | 0.00000     |
|          | 0.00945     | 0.00000     | -0.85046    | 0.00000     | 0.03353     | 0.00242     | -0.85046    | 0.92804     | 0.00000     |
|          | 0.00000     | 1.15091     | 0.00000     | 0.01137     | 0.00000     | 0.00000     | 0.01137     | 0.00000     | 0.00000     |
|          | 0.00000     | 0.11832     | 0.00000     | 0.00000     | 0.06821     | 0.00000     | 0.00000     | 0.00000     | 0.00000     |
|          | 0.00000     | -0.59208    | -0.055282   | 0.92804     | 0.25705     | 0.02471     | -0.59208    | 0.92804     | 0.25705     |
|          | 1.15091     | 0.00000     | 0.52446     | 0.00000     | 0.03353     | 0.00242     | -0.59208    | 0.92804     | 0.03353     |
|          | 0.00000     | 0.00000     | 0.52446     | 0.00000     | 0.03353     | 0.00242     | 0.00000     | 0.00000     | 0.00000     |
|          | 0.00000     | -0.59208    | -0.85046    | 0.00000     | 0.03353     | 0.00242     | -0.59208    | 0.92804     | 0.03353     |
|          | 0.00000     | -0.85046    | 0.52446     | 0.00000     | 0.03353     | 0.00242     | 0.52446     | 0.92804     | 0.52446     |
|          | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     |
|          | 0.00000     | -2.03975    | 2.03975     | 0.00000     | 0.00000     | 0.00000     | -2.03975    | 0.00000     | 0.00000     |
|          | -0.03780    | 0.00000     | -0.03780    | 0.00000     | 0.00000     | 0.00000     | -0.03780    | 0.00000     | 0.00000     |
|          | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     |
|          | 0.04693     | 0.00000     | 0.04693     | 0.00000     | 0.00000     | 0.00000     | 0.04693     | 0.00000     | 0.04693     |
|          | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     |
|          | -0.02665    | 0.00000     | -0.02665    | 0.00000     | 0.00000     | 0.00000     | -0.02665    | 0.00000     | -0.02665    |
|          | 0.08796     | 0.00000     | -0.17056    | 0.00000     | 0.00000     | 0.00000     | -0.17056    | 0.00000     | -0.17056    |
| multipole | 448 422 425 | 446 425 419 | 450 423 428 | 447 428 424 | 449 424 426 | 445 426 418 | 438 410 407 | 441 416 421 | 444 421 417 |
|-----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
|           | 0.26868     | 0.10890     | 0.04281     | 0.05488     | 0.05260     | 0.08142     | 0.09344     | 0.03410     | 0.05126     |
|           | 0.00000     | 0.01340     | 0.02419     | -0.02454    | -0.00230    | -0.03458    | -0.02141    | 0.07648     | 0.00000     |
|           | -0.10024    | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     | 0.00000     |
|           | -0.16844    | -0.07678    | -0.14897    | -0.10892    | 0.03004     | -0.15042    | -0.13402    | -0.17264    | -0.04110    |
|           |             |             |             |             |             |             |             |             |             |
|           |             |             |             |             |             |             |             |             |             |
| Multipole | 442 417 412 | 439 412 408 | 407 405 436 | 436 407 405 | 405 401 435 | 435 405 401 | 401 402 405 | 432 401 402 |
|-----------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
|           | -0.04429    | 0.00000     | -0.03261    | 0.01535     | 0.00000     | -0.08229    | -0.04372    | 0.00000     | 0.06694     |
|           | 0.01592     | 0.00000     | -0.12772    | 0.03687     | 0.00000     | -0.01513    | 0.00734     | 0.00000     | -0.02174    |
|           | 0.00000     | -0.1592     | 0.00798     | 0.18894     | 0.00000     | -0.05680    | -0.06533    | 0.00000     | -0.13214    |
|           | -0.04429    | 0.00000     | -0.12772    | 0.03687     | 0.00000     | -0.01513    | 0.00734     | 0.00000     | -0.02174    |
|           | 0.01592     | 0.00000     | -0.12772    | 0.03687     | 0.00000     | -0.01513    | 0.00734     | 0.00000     | -0.02174    |
|           | 0.00000     | -0.1592     | 0.00798     | 0.18894     | 0.00000     | -0.05680    | -0.06533    | 0.00000     | -0.13214    |
|           | -0.04429    | 0.00000     | -0.12772    | 0.03687     | 0.00000     | -0.01513    | 0.00734     | 0.00000     | -0.02174    |
|           | 0.01592     | 0.00000     | -0.12772    | 0.03687     | 0.00000     | -0.01513    | 0.00734     | 0.00000     | -0.02174    |
|           | 0.00000     | -0.1592     | 0.00798     | 0.18894     | 0.00000     | -0.05680    | -0.06533    | 0.00000     | -0.13214    |
|           | -0.04429    | 0.00000     | -0.12772    | 0.03687     | 0.00000     | -0.01513    | 0.00734     | 0.00000     | -0.02174    |
| Multipole   | Numbers | Coefficients |
|------------|---------|--------------|
| 402 429 401 |         | 0.18260      |
|            |         | 0.35324      |
|            |         | 0.06113      |
|            |         | 0.00000      |
|            |         | 0.00000      |
|            |         | 0.00000      |
|            |         | -0.31230     |
|            |         | 0.16991      |
| 431 402 429 |         | 0.00261      |
|            |         | -0.01926     |
|            |         | 0.06983      |
|            |         | 0.00000      |
|            |         | 0.00216      |
| 429 404 402 |         | -0.31988     |
|            |         | 0.29821      |
|            |         | 0.14167      |
|            |         | 0.00000      |
|            |         | -0.93403     |
| 404 -434 -434 |         | 0.07601      |
|            |         | 0.00270      |
|            |         | -0.44750     |
|            |         | 0.00000      |
|            |         | -0.44027     |
| 434 404 429 |         | 0.04188      |
|            |         | 0.05369      |
|            |         | -0.01856     |
|            |         | 0.00000      |
|            |         | -0.01890     |
|            |         | 0.03864      |