



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:27 am BST

PDB ID : 2NOX  
Title : Crystal structure of tryptophan 2,3-dioxygenase from *Ralstonia metallidurans*  
Authors : Zhang, Y.; Kang, S.A.; Mukherjee, T.; Bale, S.; Crane, B.R.; Begley, T.P.; Ealick, S.E.  
Deposited on : 2006-10-26  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

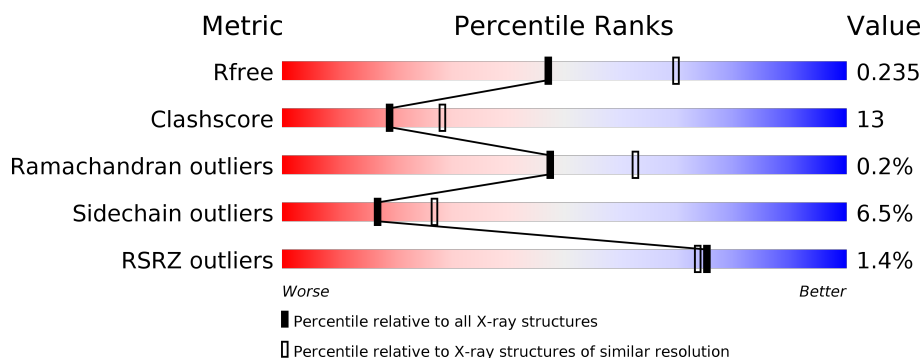
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 3907 (2.40-2.40)                                      |
| Clashscore            | 141614                      | 4398 (2.40-2.40)                                      |
| Ramachandran outliers | 138981                      | 4318 (2.40-2.40)                                      |
| Sidechain outliers    | 138945                      | 4319 (2.40-2.40)                                      |
| RSRZ outliers         | 127900                      | 3811 (2.40-2.40)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | A     | 281    | <div> <div>%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>• 7%</div> </div> </div>  |
| 1   | B     | 281    | <div> <div>2%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>• 5%</div> </div> </div> |
| 1   | C     | 281    | <div> <div>2%</div> <div> <div></div> <div>70%</div> <div>18%</div> <div>• 9%</div> </div> </div> |
| 1   | D     | 281    | <div> <div></div> <div> <div>70%</div> <div>19%</div> <div>• 8%</div> </div> </div>               |
| 1   | E     | 281    | <div> <div>%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>• 9%</div> </div> </div>  |
| 1   | F     | 281    | <div> <div>%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>• 7%</div> </div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | G     | 281    |                  |
| 1   | H     | 281    |                  |
| 1   | I     | 281    |                  |
| 1   | J     | 281    |                  |
| 1   | K     | 281    |                  |
| 1   | L     | 281    |                  |
| 1   | M     | 281    |                  |
| 1   | N     | 281    |                  |
| 1   | O     | 281    |                  |
| 1   | P     | 281    |                  |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 36423 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tryptophan 2,3-dioxygenase.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 261      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2160  | 1375 | 382 | 390 | 13 |         |         |       |
| 1   | B     | 266      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2192  | 1400 | 384 | 395 | 13 |         |         |       |
| 1   | C     | 255      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2106  | 1344 | 368 | 382 | 12 |         |         |       |
| 1   | D     | 259      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2133  | 1360 | 376 | 385 | 12 |         |         |       |
| 1   | E     | 256      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2126  | 1356 | 376 | 382 | 12 |         |         |       |
| 1   | F     | 260      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2152  | 1371 | 380 | 388 | 13 |         |         |       |
| 1   | G     | 259      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2137  | 1362 | 376 | 387 | 12 |         |         |       |
| 1   | H     | 259      | Total | C    | N   | O   | S  | 0       | 2       | 0     |
|     |       |          | 2147  | 1368 | 380 | 387 | 12 |         |         |       |
| 1   | I     | 259      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2133  | 1360 | 376 | 385 | 12 |         |         |       |
| 1   | J     | 257      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2126  | 1356 | 374 | 384 | 12 |         |         |       |
| 1   | K     | 255      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2119  | 1352 | 372 | 383 | 12 |         |         |       |
| 1   | L     | 260      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2141  | 1364 | 377 | 388 | 12 |         |         |       |
| 1   | M     | 255      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2111  | 1349 | 370 | 380 | 12 |         |         |       |
| 1   | N     | 260      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 2150  | 1370 | 379 | 389 | 12 |         |         |       |
| 1   | O     | 257      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2126  | 1356 | 374 | 384 | 12 |         |         |       |
| 1   | P     | 259      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2133  | 1360 | 376 | 385 | 12 |         |         |       |

- # HEM

| Mol | Chain | Residues | Atoms       |         |         |        | ZeroOcc | AltConf |   |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|---|
| 2   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 2   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |



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| Mol | Chain | Residues | Atoms |    |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|---------|
| 2   | M     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | N     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | O     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |
| 2   | P     | 1        | Total | C  | Fe | N | O | 0       | 0       |
|     |       |          | 43    | 34 | 1  | 4 | 4 |         |         |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3   | A     | 130      | Total | O   | 0       | 0       |
|     |       |          | 130   | 130 |         |         |
| 3   | B     | 126      | Total | O   | 0       | 0       |
|     |       |          | 126   | 126 |         |         |
| 3   | C     | 107      | Total | O   | 0       | 0       |
|     |       |          | 107   | 107 |         |         |
| 3   | D     | 158      | Total | O   | 0       | 0       |
|     |       |          | 158   | 158 |         |         |
| 3   | E     | 107      | Total | O   | 0       | 0       |
|     |       |          | 107   | 107 |         |         |
| 3   | F     | 72       | Total | O   | 0       | 0       |
|     |       |          | 72    | 72  |         |         |
| 3   | G     | 56       | Total | O   | 0       | 0       |
|     |       |          | 56    | 56  |         |         |
| 3   | H     | 114      | Total | O   | 0       | 0       |
|     |       |          | 114   | 114 |         |         |
| 3   | I     | 85       | Total | O   | 0       | 0       |
|     |       |          | 85    | 85  |         |         |
| 3   | J     | 82       | Total | O   | 0       | 0       |
|     |       |          | 82    | 82  |         |         |
| 3   | K     | 74       | Total | O   | 0       | 0       |
|     |       |          | 74    | 74  |         |         |
| 3   | L     | 81       | Total | O   | 0       | 0       |
|     |       |          | 81    | 81  |         |         |
| 3   | M     | 116      | Total | O   | 0       | 0       |
|     |       |          | 116   | 116 |         |         |
| 3   | N     | 66       | Total | O   | 0       | 0       |
|     |       |          | 66    | 66  |         |         |
| 3   | O     | 61       | Total | O   | 0       | 0       |
|     |       |          | 61    | 61  |         |         |

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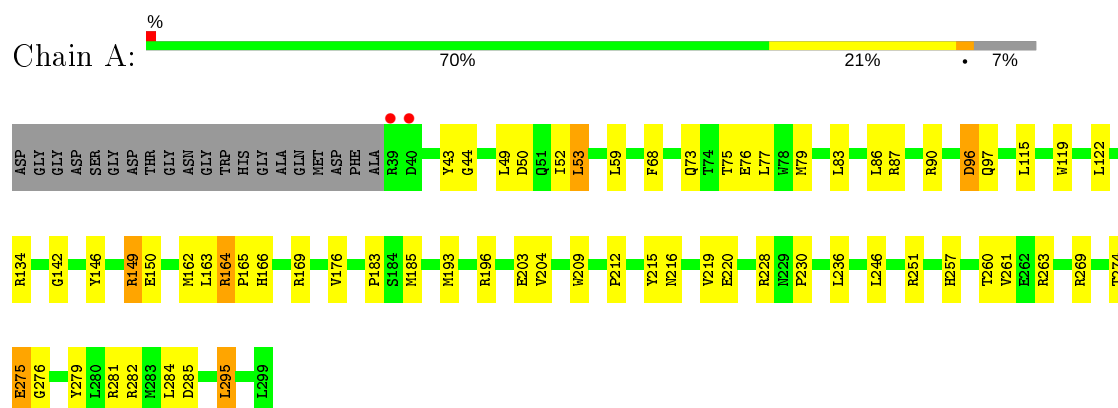
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3   | P     | 108      | Total<br>108 | O<br>108 | 0       | 0       |

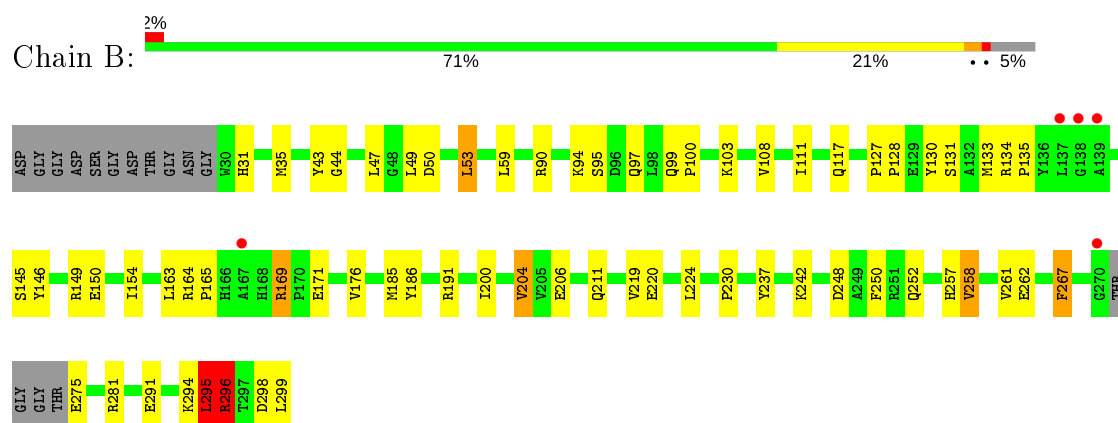
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

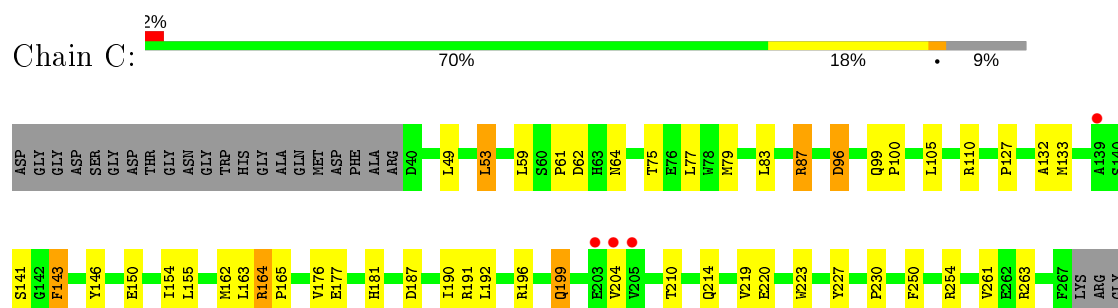
#### • Molecule 1: Tryptophan 2,3-dioxygenase



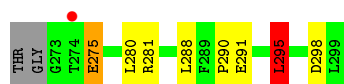
#### • Molecule 1: Tryptophan 2,3-dioxygenase



#### • Molecule 1: Tryptophan 2,3-dioxygenase

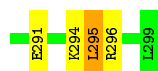






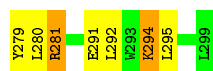
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain D: 70% 19% 8%



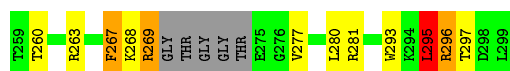
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain E: 71% 18% 9%



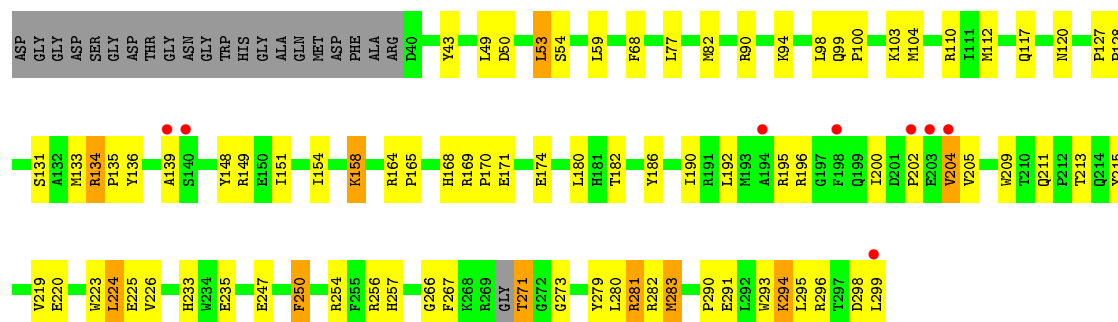
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain F: 66% 23% 7%



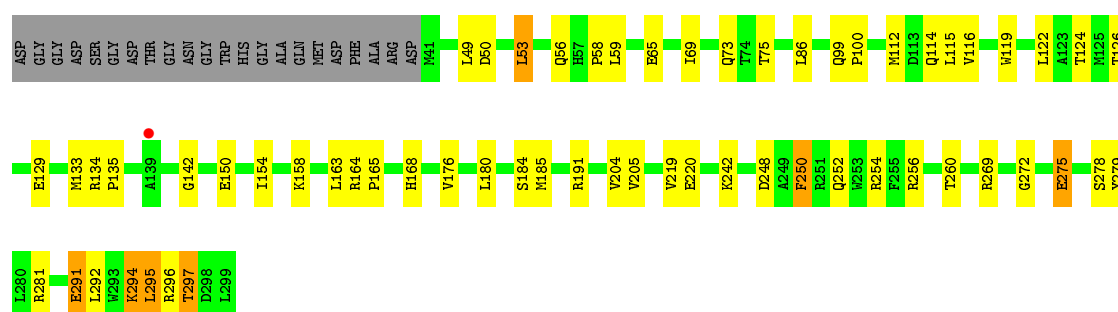
- Molecule 1: Tryptophan 2,3-dioxygenase

Chain G: 3% 62% 27% 8%



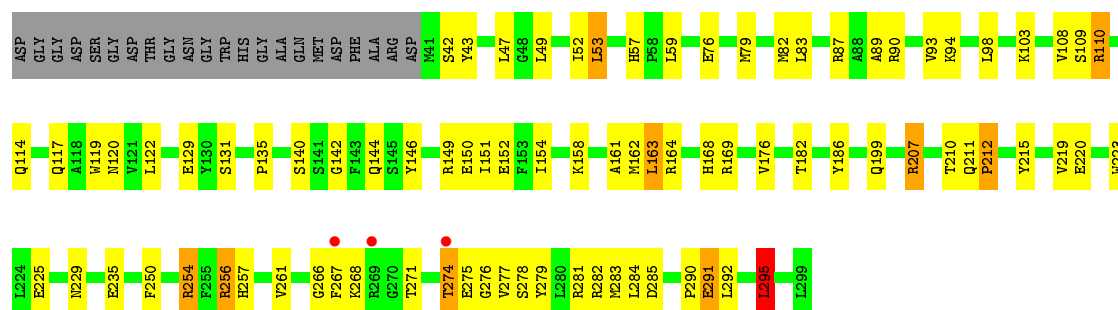
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain H: 70% 19% 8%



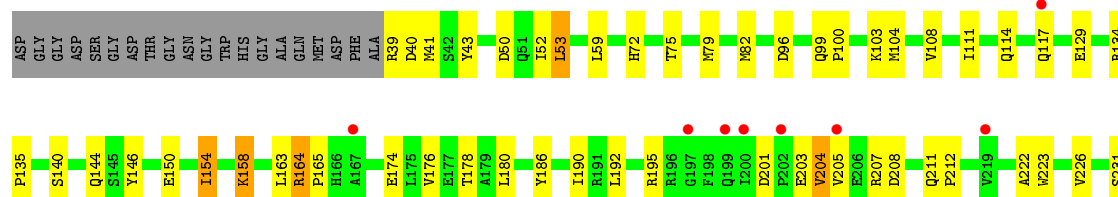
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain I: 62% 27% 8%



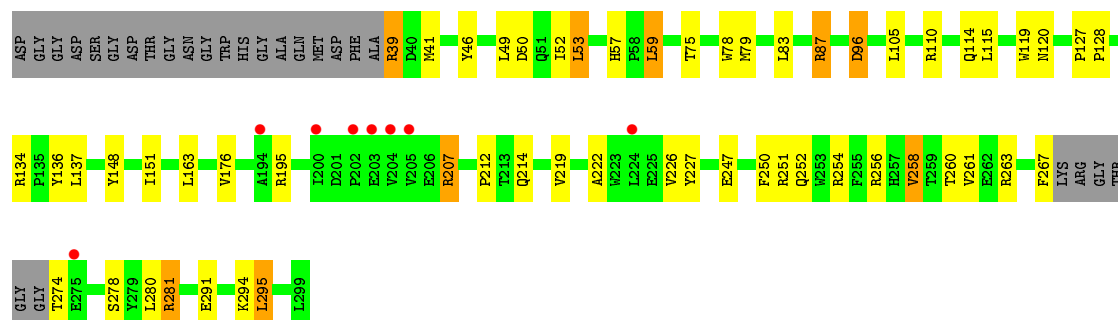
• Molecule 1: Tryptophan 2,3-dioxygenase

Chain J: 67% 22% 9%

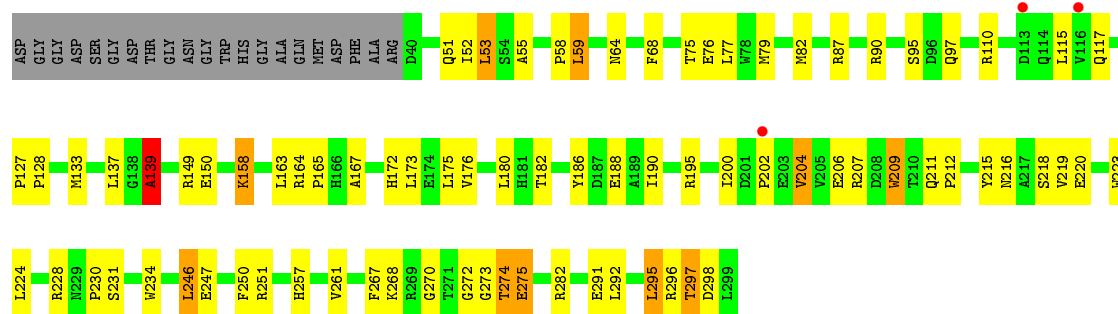




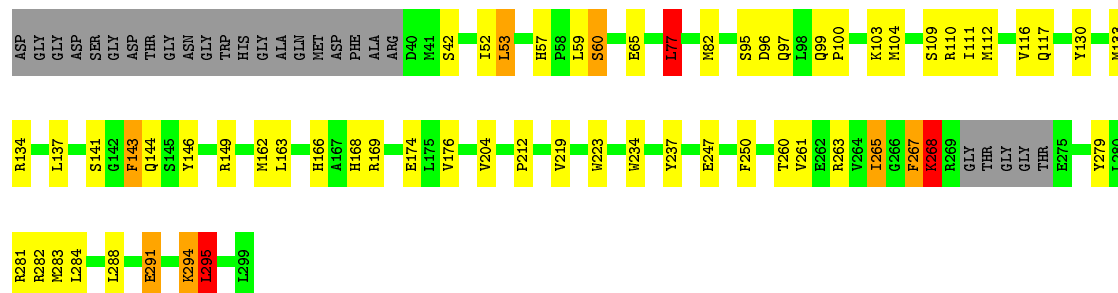
- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase

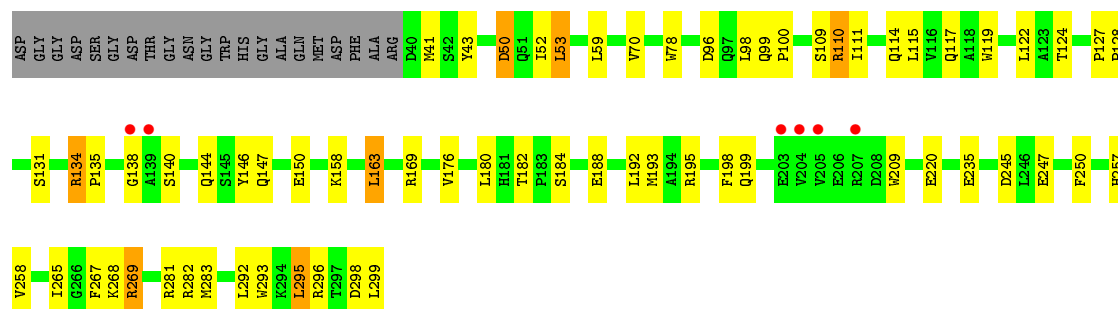


- Molecule 1: Tryptophan 2,3-dioxygenase

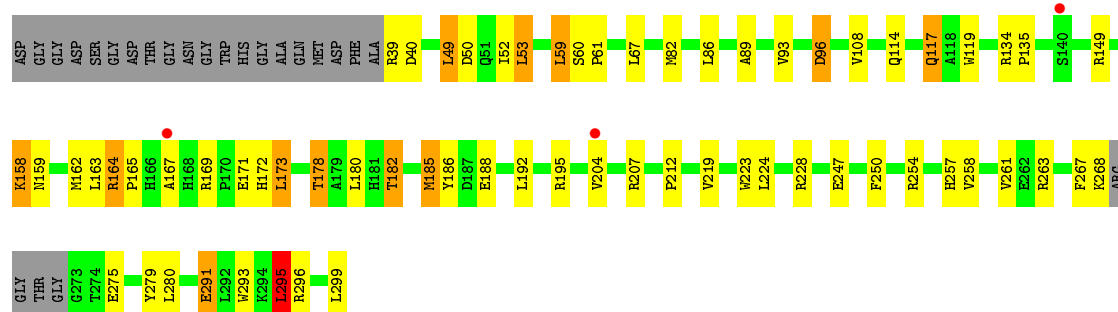


- Molecule 1: Tryptophan 2,3-dioxygenase

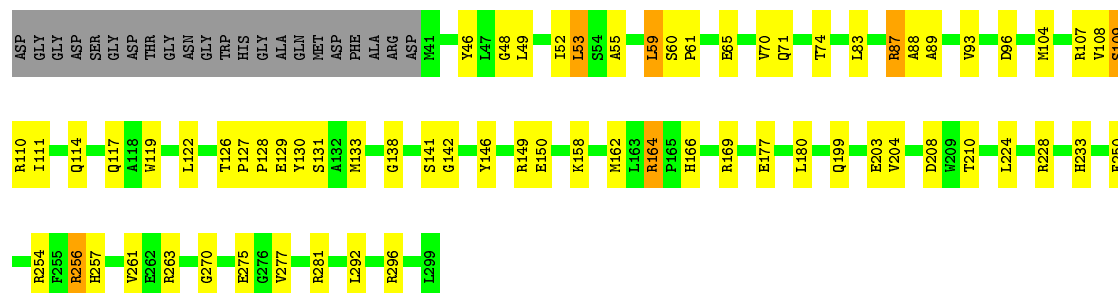




• Molecule 1: Tryptophan 2,3-dioxygenase



• Molecule 1: Tryptophan 2,3-dioxygenase



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 72.54Å 132.12Å 139.95Å<br>66.97° 85.06° 89.89°              | Depositor        |
| Resolution (Å)  | 50.12 – 2.40<br>50.09 – 2.22                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.5 (50.12-2.40)<br>86.1 (50.09-2.22)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.07  | Depositor        |
| $R_{sym}$   | 0.07  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.46 (at 2.22Å)   | Xtriage          |
| Refinement program  | REFMAC 5.2.0019   | Depositor        |
| R, $R_{free}$   | 0.210 , 0.270<br>0.163 , 0.235                              | Depositor<br>DCC |
| $R_{free}$ test set   | 11190 reflections (4.98%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 38.1  | Xtriage          |
| Anisotropy  | 0.109   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 51.3   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.96  | EDS              |
| Total number of atoms   | 36423   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 45.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.68         | 0/2217      | 0.80        | 3/3004 (0.1%)   |
| 1   | B     | 0.64         | 0/2252      | 0.78        | 5/3053 (0.2%)   |
| 1   | C     | 0.65         | 0/2162      | 0.76        | 2/2932 (0.1%)   |
| 1   | D     | 0.68         | 0/2190      | 0.80        | 1/2969 (0.0%)   |
| 1   | E     | 0.61         | 0/2182      | 0.68        | 1/2956 (0.0%)   |
| 1   | F     | 0.58         | 0/2208      | 0.71        | 1/2991 (0.0%)   |
| 1   | G     | 0.57         | 0/2193      | 0.66        | 0/2972          |
| 1   | H     | 0.60         | 0/2207      | 0.73        | 1/2992 (0.0%)   |
| 1   | I     | 0.57         | 0/2190      | 0.69        | 1/2969 (0.0%)   |
| 1   | J     | 0.54         | 0/2182      | 0.69        | 1/2957 (0.0%)   |
| 1   | K     | 0.51         | 0/2178      | 0.68        | 0/2953          |
| 1   | L     | 0.54         | 0/2198      | 0.68        | 0/2980          |
| 1   | M     | 0.64         | 0/2167      | 0.75        | 2/2938 (0.1%)   |
| 1   | N     | 0.54         | 0/2207      | 0.67        | 0/2991          |
| 1   | O     | 0.57         | 0/2182      | 0.68        | 1/2957 (0.0%)   |
| 1   | P     | 0.61         | 0/2190      | 0.73        | 2/2969 (0.1%)   |
| All | All   | 0.60         | 0/35105     | 0.72        | 21/47583 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | L     | 0                   | 1                   |

There are no bond length outliers.

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | D     | 295 | LEU  | CA-CB-CG  | 9.07  | 136.17      | 115.30   |
| 1   | M     | 295 | LEU  | CA-CB-CG  | 8.72  | 135.36      | 115.30   |
| 1   | B     | 296 | ARG  | NE-CZ-NH2 | -8.70 | 115.95      | 120.30   |
| 1   | H     | 295 | LEU  | CA-CB-CG  | 7.93  | 133.53      | 115.30   |
| 1   | B     | 296 | ARG  | NE-CZ-NH1 | 7.75  | 124.17      | 120.30   |
| 1   | I     | 295 | LEU  | CA-CB-CG  | 7.15  | 131.74      | 115.30   |
| 1   | A     | 295 | LEU  | CA-CB-CG  | 7.13  | 131.69      | 115.30   |
| 1   | F     | 295 | LEU  | CA-CB-CG  | 7.05  | 131.51      | 115.30   |
| 1   | P     | 256 | ARG  | NE-CZ-NH2 | -6.17 | 117.22      | 120.30   |
| 1   | C     | 295 | LEU  | CA-CB-CG  | 6.16  | 129.46      | 115.30   |
| 1   | B     | 295 | LEU  | CA-CB-CG  | 6.12  | 129.39      | 115.30   |
| 1   | A     | 90  | ARG  | NE-CZ-NH2 | -6.12 | 117.24      | 120.30   |
| 1   | B     | 258 | VAL  | CB-CA-C   | -6.02 | 99.97       | 111.40   |
| 1   | P     | 263 | ARG  | NE-CZ-NH2 | -5.72 | 117.44      | 120.30   |
| 1   | O     | 295 | LEU  | CA-CB-CG  | 5.55  | 128.08      | 115.30   |
| 1   | M     | 77  | LEU  | CA-CB-CG  | 5.51  | 127.98      | 115.30   |
| 1   | J     | 295 | LEU  | CA-CB-CG  | 5.30  | 127.49      | 115.30   |
| 1   | B     | 149 | ARG  | NE-CZ-NH2 | -5.25 | 117.67      | 120.30   |
| 1   | C     | 87  | ARG  | NE-CZ-NH2 | -5.23 | 117.69      | 120.30   |
| 1   | E     | 245 | ASP  | CB-CA-C   | -5.12 | 100.17      | 110.40   |
| 1   | A     | 263 | ARG  | NE-CZ-NH2 | -5.01 | 117.79      | 120.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | L     | 139 | ALA  | Peptide |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 2160  | 0        | 2108     | 65      | 0            |
| 1   | B     | 2192  | 0        | 2117     | 50      | 0            |
| 1   | C     | 2106  | 0        | 2047     | 51      | 0            |
| 1   | D     | 2133  | 0        | 2083     | 49      | 0            |
| 1   | E     | 2126  | 0        | 2076     | 51      | 0            |
| 1   | F     | 2152  | 0        | 2096     | 64      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | G     | 2137  | 0        | 2083     | 75      | 0            |
| 1   | H     | 2147  | 0        | 2101     | 34      | 0            |
| 1   | I     | 2133  | 0        | 2083     | 87      | 0            |
| 1   | J     | 2126  | 0        | 2073     | 56      | 0            |
| 1   | K     | 2119  | 0        | 2065     | 53      | 0            |
| 1   | L     | 2141  | 0        | 2087     | 78      | 0            |
| 1   | M     | 2111  | 0        | 2051     | 46      | 0            |
| 1   | N     | 2150  | 0        | 2099     | 60      | 0            |
| 1   | O     | 2126  | 0        | 2073     | 58      | 0            |
| 1   | P     | 2133  | 0        | 2083     | 62      | 0            |
| 2   | A     | 43    | 0        | 30       | 6       | 0            |
| 2   | B     | 43    | 0        | 30       | 0       | 0            |
| 2   | C     | 43    | 0        | 30       | 2       | 0            |
| 2   | D     | 43    | 0        | 30       | 2       | 0            |
| 2   | E     | 43    | 0        | 30       | 7       | 0            |
| 2   | F     | 43    | 0        | 30       | 3       | 0            |
| 2   | G     | 43    | 0        | 30       | 3       | 0            |
| 2   | H     | 43    | 0        | 30       | 2       | 0            |
| 2   | I     | 43    | 0        | 30       | 9       | 0            |
| 2   | J     | 43    | 0        | 30       | 1       | 0            |
| 2   | K     | 43    | 0        | 30       | 4       | 0            |
| 2   | L     | 43    | 0        | 30       | 5       | 0            |
| 2   | M     | 43    | 0        | 30       | 2       | 0            |
| 2   | N     | 43    | 0        | 30       | 1       | 0            |
| 2   | O     | 43    | 0        | 30       | 4       | 0            |
| 2   | P     | 43    | 0        | 30       | 7       | 0            |
| 3   | A     | 130   | 0        | 0        | 10      | 0            |
| 3   | B     | 126   | 0        | 0        | 6       | 0            |
| 3   | C     | 107   | 0        | 0        | 7       | 0            |
| 3   | D     | 158   | 0        | 0        | 4       | 0            |
| 3   | E     | 107   | 0        | 0        | 4       | 0            |
| 3   | F     | 72    | 0        | 0        | 6       | 0            |
| 3   | G     | 56    | 0        | 0        | 8       | 0            |
| 3   | H     | 114   | 0        | 0        | 3       | 0            |
| 3   | I     | 85    | 0        | 0        | 8       | 0            |
| 3   | J     | 82    | 0        | 0        | 6       | 0            |
| 3   | K     | 74    | 0        | 0        | 7       | 0            |
| 3   | L     | 81    | 0        | 0        | 10      | 0            |
| 3   | M     | 116   | 0        | 0        | 5       | 0            |
| 3   | N     | 66    | 0        | 0        | 1       | 0            |
| 3   | O     | 61    | 0        | 0        | 4       | 0            |
| 3   | P     | 108   | 0        | 0        | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| All | All   | 36423 | 0        | 33805    | 893     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (893) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:109:SER:HB3  | 1:N:110:ARG:NH1  | 1.56                     | 1.17              |
| 1:G:283:MET:HA   | 1:G:283:MET:HE2  | 1.18                     | 1.15              |
| 1:P:65:GLU:HG3   | 1:P:133:MET:CE   | 1.77                     | 1.15              |
| 1:G:82:MET:HE2   | 1:G:112:MET:HG2  | 1.31                     | 1.11              |
| 1:C:219:VAL:HG12 | 1:C:291:GLU:HG3  | 1.31                     | 1.09              |
| 1:E:281:ARG:HG2  | 1:E:281:ARG:HH11 | 1.05                     | 1.09              |
| 1:C:199:GLN:HG3  | 1:C:199:GLN:O    | 1.52                     | 1.07              |
| 1:P:65:GLU:HG3   | 1:P:133:MET:HE3  | 1.06                     | 1.06              |
| 1:P:88:ALA:HB3   | 1:P:104:MET:CE   | 1.88                     | 1.04              |
| 1:I:207:ARG:HH11 | 1:I:207:ARG:HG3  | 1.19                     | 1.01              |
| 1:N:109:SER:CB   | 1:N:110:ARG:NH1  | 2.25                     | 0.99              |
| 1:N:109:SER:HB3  | 1:N:110:ARG:HH12 | 1.16                     | 0.97              |
| 1:A:274:THR:HG22 | 1:A:276:GLY:H    | 1.30                     | 0.96              |
| 1:I:164:ARG:HD2  | 3:I:583:HOH:O    | 1.63                     | 0.96              |
| 1:G:283:MET:HA   | 1:G:283:MET:CE   | 1.96                     | 0.94              |
| 1:I:274:THR:HG22 | 1:I:276:GLY:H    | 1.29                     | 0.94              |
| 1:G:82:MET:CE    | 1:G:112:MET:HG2  | 1.96                     | 0.94              |
| 1:B:219:VAL:HG12 | 1:B:291:GLU:HG3  | 1.52                     | 0.92              |
| 1:P:88:ALA:CB    | 1:P:104:MET:CE   | 2.47                     | 0.92              |
| 1:J:96:ASP:HB2   | 3:J:534:HOH:O    | 1.68                     | 0.92              |
| 1:C:219:VAL:CG1  | 1:C:291:GLU:HG3  | 1.99                     | 0.91              |
| 1:K:278:SER:HB2  | 3:K:513:HOH:O    | 1.70                     | 0.91              |
| 1:F:109:SER:HB2  | 3:F:543:HOH:O    | 1.68                     | 0.91              |
| 1:C:181:HIS:HE1  | 3:C:584:HOH:O    | 1.52                     | 0.91              |
| 1:K:57:HIS:HD2   | 3:K:570:HOH:O    | 1.52                     | 0.90              |
| 1:O:169:ARG:HD2  | 1:O:171:GLU:OE2  | 1.70                     | 0.90              |
| 1:M:60:SER:HB3   | 1:M:65:GLU:OE1   | 1.72                     | 0.90              |
| 1:P:88:ALA:HB3   | 1:P:104:MET:HE1  | 1.51                     | 0.90              |
| 1:K:83:LEU:O     | 1:K:87:ARG:HG3   | 1.72                     | 0.89              |
| 1:E:281:ARG:HG2  | 1:E:281:ARG:NH1  | 1.82                     | 0.88              |
| 1:N:269:ARG:HB3  | 1:N:269:ARG:NH1  | 1.88                     | 0.88              |
| 1:G:82:MET:HE2   | 1:G:112:MET:CG   | 2.05                     | 0.87              |
| 1:G:158:LYS:HG3  | 1:G:180:LEU:HD12 | 1.57                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:219:VAL:HG12 | 1:I:291:GLU:HG3  | 1.55                     | 0.86              |
| 1:I:274:THR:CG2  | 1:I:276:GLY:H    | 1.89                     | 0.86              |
| 1:L:87:ARG:NH2   | 1:L:150:GLU:OE2  | 2.10                     | 0.85              |
| 1:C:96:ASP:HB2   | 3:C:549:HOH:O    | 1.75                     | 0.85              |
| 1:D:219:VAL:HG12 | 1:D:291:GLU:HG3  | 1.59                     | 0.84              |
| 1:L:275:GLU:HB2  | 2:L:500:HEM:O1A  | 1.75                     | 0.84              |
| 1:I:207:ARG:HH11 | 1:I:207:ARG:CG   | 1.88                     | 0.84              |
| 1:I:274:THR:HB   | 2:I:500:HEM:O1A  | 1.77                     | 0.84              |
| 1:N:138:GLY:C    | 1:N:140:SER:H    | 1.79                     | 0.84              |
| 1:P:164:ARG:HG3  | 1:P:164:ARG:HH11 | 1.43                     | 0.84              |
| 1:N:122:LEU:HD21 | 2:N:500:HEM:HAB  | 1.60                     | 0.83              |
| 1:J:163:LEU:HD22 | 1:J:176:VAL:HG12 | 1.60                     | 0.83              |
| 1:K:295:LEU:C    | 1:K:295:LEU:HD23 | 2.00                     | 0.82              |
| 1:P:88:ALA:CB    | 1:P:104:MET:HE3  | 2.08                     | 0.82              |
| 1:P:65:GLU:CG    | 1:P:133:MET:HE3  | 2.02                     | 0.82              |
| 1:O:254:ARG:O    | 1:O:258:VAL:HG23 | 1.79                     | 0.81              |
| 1:C:177:GLU:HG2  | 3:C:520:HOH:O    | 1.80                     | 0.81              |
| 1:O:158:LYS:HG3  | 1:O:180:LEU:HD12 | 1.62                     | 0.81              |
| 1:C:163:LEU:HD22 | 1:C:176:VAL:HG12 | 1.61                     | 0.80              |
| 1:G:134:ARG:HG3  | 1:G:135:PRO:HD3  | 1.62                     | 0.80              |
| 1:N:299:LEU:OXT  | 1:N:299:LEU:HG   | 1.80                     | 0.80              |
| 1:L:51:GLN:HG3   | 3:L:530:HOH:O    | 1.82                     | 0.79              |
| 1:O:89:ALA:HB3   | 1:O:185:MET:CE   | 2.12                     | 0.79              |
| 1:C:110:ARG:HD3  | 3:C:582:HOH:O    | 1.82                     | 0.79              |
| 1:E:79:MET:HE2   | 1:E:151:ILE:HD12 | 1.64                     | 0.79              |
| 1:F:127:PRO:HG3  | 1:G:296:ARG:CD   | 2.13                     | 0.79              |
| 1:G:50:ASP:HB2   | 3:G:524:HOH:O    | 1.83                     | 0.78              |
| 1:P:88:ALA:HB1   | 1:P:104:MET:HE3  | 1.63                     | 0.78              |
| 1:K:207:ARG:HG3  | 1:K:207:ARG:HH11 | 1.49                     | 0.78              |
| 1:F:127:PRO:HG3  | 1:G:296:ARG:NE   | 1.99                     | 0.77              |
| 1:J:52:ILE:HG22  | 1:J:53:LEU:HD13  | 1.67                     | 0.77              |
| 1:G:139:ALA:HA   | 3:G:545:HOH:O    | 1.85                     | 0.76              |
| 1:L:295:LEU:HD23 | 1:L:296:ARG:N    | 2.01                     | 0.76              |
| 1:J:150:GLU:O    | 1:J:154:ILE:HG12 | 1.86                     | 0.76              |
| 1:B:171:GLU:HG2  | 3:B:553:HOH:O    | 1.85                     | 0.76              |
| 1:L:206:GLU:HG2  | 3:L:544:HOH:O    | 1.86                     | 0.76              |
| 1:B:150:GLU:O    | 1:B:154:ILE:HG13 | 1.86                     | 0.76              |
| 2:E:500:HEM:HBB2 | 2:E:500:HEM:HMB2 | 1.67                     | 0.76              |
| 1:P:88:ALA:CB    | 1:P:104:MET:HE1  | 2.11                     | 0.75              |
| 2:I:500:HEM:HMB2 | 2:I:500:HEM:HBB2 | 1.69                     | 0.75              |
| 1:I:82:MET:HG3   | 1:I:108:VAL:HG13 | 1.67                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:79:MET:CE    | 1:E:151:ILE:HD12 | 2.16                     | 0.75              |
| 1:D:146:TYR:O    | 1:D:150:GLU:HG3  | 1.85                     | 0.74              |
| 1:M:219:VAL:HG12 | 1:M:291:GLU:HG3  | 1.68                     | 0.74              |
| 1:L:295:LEU:HD23 | 1:L:295:LEU:C    | 2.07                     | 0.74              |
| 1:P:166:HIS:HD2  | 3:P:579:HOH:O    | 1.71                     | 0.74              |
| 1:I:122:LEU:HD21 | 2:I:500:HEM:HAB  | 1.70                     | 0.74              |
| 1:H:150:GLU:O    | 1:H:154:ILE:HG13 | 1.87                     | 0.73              |
| 2:P:500:HEM:HBB2 | 2:P:500:HEM:HMB2 | 1.68                     | 0.73              |
| 1:M:53:LEU:HD21  | 1:N:147:GLN:NE2  | 2.03                     | 0.73              |
| 1:I:219:VAL:CG1  | 1:I:291:GLU:HG3  | 2.17                     | 0.73              |
| 1:I:274:THR:HG22 | 1:I:276:GLY:N    | 2.04                     | 0.73              |
| 1:O:149:ARG:NH1  | 3:O:529:HOH:O    | 2.21                     | 0.72              |
| 1:A:274:THR:HG21 | 1:A:279:TYR:CG   | 2.24                     | 0.72              |
| 1:A:96:ASP:OD1   | 1:A:196:ARG:NH2  | 2.17                     | 0.72              |
| 1:J:158:LYS:HG3  | 1:J:180:LEU:HD12 | 1.69                     | 0.72              |
| 1:K:96:ASP:OD2   | 1:K:195:ARG:NH2  | 2.22                     | 0.72              |
| 1:L:257:HIS:O    | 1:L:261:VAL:HG23 | 1.89                     | 0.72              |
| 1:A:86:LEU:HD22  | 1:A:185:MET:HE1  | 1.71                     | 0.72              |
| 1:K:295:LEU:O    | 1:K:295:LEU:HD23 | 1.89                     | 0.71              |
| 3:A:507:HOH:O    | 1:D:256:ARG:HD2  | 1.90                     | 0.71              |
| 1:A:274:THR:HB   | 2:A:500:HEM:O1A  | 1.91                     | 0.71              |
| 1:E:267:PHE:HE2  | 1:E:281:ARG:HE   | 1.36                     | 0.71              |
| 1:I:211:GLN:O    | 1:I:212:PRO:O    | 2.08                     | 0.71              |
| 1:J:277:VAL:O    | 1:J:281:ARG:HG3  | 1.91                     | 0.71              |
| 2:I:500:HEM:CMB  | 2:I:500:HEM:HBB2 | 2.21                     | 0.71              |
| 1:D:192:LEU:O    | 1:D:192:LEU:HD12 | 1.92                     | 0.70              |
| 1:F:267:PHE:HD2  | 1:F:268:LYS:H    | 1.37                     | 0.70              |
| 1:G:134:ARG:HG3  | 1:G:135:PRO:CD   | 2.20                     | 0.70              |
| 1:J:258:VAL:HG13 | 1:J:280:LEU:HB3  | 1.74                     | 0.70              |
| 1:E:150:GLU:O    | 1:E:154:ILE:HG13 | 1.91                     | 0.70              |
| 1:G:219:VAL:HG12 | 1:G:291:GLU:HG3  | 1.74                     | 0.70              |
| 3:M:510:HOH:O    | 1:P:256:ARG:HD2  | 1.92                     | 0.70              |
| 1:G:82:MET:HE1   | 1:G:112:MET:SD   | 2.31                     | 0.70              |
| 1:P:149:ARG:HD2  | 1:P:162:MET:HB3  | 1.73                     | 0.70              |
| 1:C:164:ARG:HG3  | 1:C:164:ARG:HH11 | 1.56                     | 0.69              |
| 1:P:52:ILE:HG22  | 1:P:53:LEU:HD13  | 1.73                     | 0.69              |
| 1:J:192:LEU:HD12 | 1:J:195:ARG:NH2  | 2.06                     | 0.69              |
| 1:B:95:SER:OG    | 1:B:97:GLN:HG3   | 1.92                     | 0.69              |
| 1:G:117:GLN:HG2  | 1:H:114:GLN:OE1  | 1.92                     | 0.69              |
| 2:E:500:HEM:HBB2 | 2:E:500:HEM:CMB  | 2.22                     | 0.69              |
| 1:J:250:PHE:O    | 1:J:254:ARG:HG3  | 1.92                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:42:SER:HB2   | 1:N:144:GLN:OE1  | 1.91                     | 0.69              |
| 1:G:169:ARG:HH21 | 1:G:171:GLU:HG3  | 1.57                     | 0.69              |
| 1:C:290:PRO:HG3  | 3:C:580:HOH:O    | 1.91                     | 0.69              |
| 1:N:269:ARG:HB3  | 1:N:269:ARG:HH11 | 1.56                     | 0.69              |
| 1:N:295:LEU:HD23 | 1:N:295:LEU:C    | 2.13                     | 0.69              |
| 1:G:219:VAL:CG1  | 1:G:291:GLU:HG3  | 2.23                     | 0.69              |
| 2:H:500:HEM:HBB2 | 2:H:500:HEM:HMB2 | 1.75                     | 0.69              |
| 1:A:274:THR:CG2  | 1:A:279:TYR:CB   | 2.71                     | 0.68              |
| 1:N:138:GLY:C    | 1:N:140:SER:N    | 2.43                     | 0.68              |
| 1:D:89:ALA:HB3   | 1:D:185:MET:CE   | 2.22                     | 0.68              |
| 1:L:224:LEU:O    | 1:L:228:ARG:HG3  | 1.93                     | 0.68              |
| 1:D:275:GLU:HB2  | 2:D:500:HEM:O1A  | 1.94                     | 0.68              |
| 1:K:219:VAL:HG12 | 1:K:291:GLU:HG3  | 1.76                     | 0.68              |
| 1:J:146:TYR:O    | 1:J:150:GLU:HG3  | 1.94                     | 0.67              |
| 1:C:181:HIS:CE1  | 3:C:584:HOH:O    | 2.33                     | 0.67              |
| 1:L:275:GLU:HB2  | 2:L:500:HEM:CGA  | 2.24                     | 0.67              |
| 1:I:120:ASN:OD1  | 1:I:256:ARG:NH2  | 2.20                     | 0.67              |
| 1:B:275:GLU:HG3  | 3:B:615:HOH:O    | 1.93                     | 0.67              |
| 1:A:274:THR:HG21 | 1:A:279:TYR:CD2  | 2.30                     | 0.67              |
| 1:J:163:LEU:CD2  | 1:J:176:VAL:HG12 | 2.25                     | 0.67              |
| 1:A:274:THR:HG21 | 1:A:279:TYR:CB   | 2.25                     | 0.67              |
| 1:P:65:GLU:CG    | 1:P:133:MET:CE   | 2.65                     | 0.67              |
| 1:B:219:VAL:CG1  | 1:B:291:GLU:HG3  | 2.23                     | 0.67              |
| 1:F:82:MET:HG3   | 1:F:108:VAL:HG13 | 1.77                     | 0.67              |
| 1:B:134:ARG:N    | 1:B:135:PRO:HD2  | 2.11                     | 0.66              |
| 1:D:133:MET:HE2  | 1:D:137:LEU:HD11 | 1.77                     | 0.66              |
| 1:L:58:PRO:HD2   | 3:L:581:HOH:O    | 1.94                     | 0.66              |
| 1:M:267:PHE:CE1  | 1:M:281:ARG:NH1  | 2.64                     | 0.66              |
| 1:N:295:LEU:CD2  | 1:N:295:LEU:C    | 2.64                     | 0.66              |
| 1:G:82:MET:CE    | 1:G:112:MET:CG   | 2.69                     | 0.66              |
| 1:E:75:THR:O     | 1:E:79:MET:HG3   | 1.94                     | 0.66              |
| 1:F:168:HIS:CD2  | 1:F:169:ARG:HG2  | 2.31                     | 0.66              |
| 1:A:52:ILE:HG22  | 1:A:53:LEU:HD13  | 1.78                     | 0.66              |
| 1:A:282:ARG:HH21 | 1:B:31:HIS:CD2   | 2.14                     | 0.66              |
| 1:I:199:GLN:HG3  | 3:I:552:HOH:O    | 1.96                     | 0.66              |
| 1:K:79:MET:CE    | 1:K:151:ILE:HD12 | 2.25                     | 0.66              |
| 1:A:274:THR:CG2  | 1:A:275:GLU:N    | 2.58                     | 0.66              |
| 1:K:79:MET:HE3   | 1:K:151:ILE:HD12 | 1.77                     | 0.65              |
| 1:I:163:LEU:HD22 | 1:I:176:VAL:HG12 | 1.78                     | 0.65              |
| 1:P:52:ILE:HG22  | 1:P:53:LEU:CD1   | 2.26                     | 0.65              |
| 1:P:250:PHE:CE1  | 1:P:254:ARG:NH2  | 2.64                     | 0.65              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:49:LEU:O     | 1:F:53:LEU:HB2   | 1.96                     | 0.65              |
| 1:M:219:VAL:HG12 | 1:M:291:GLU:CG   | 2.27                     | 0.65              |
| 1:A:274:THR:HG22 | 1:A:275:GLU:N    | 2.10                     | 0.65              |
| 1:P:199:GLN:HG3  | 3:P:571:HOH:O    | 1.97                     | 0.65              |
| 1:B:220:GLU:HG2  | 1:B:224:LEU:HD12 | 1.78                     | 0.64              |
| 1:G:82:MET:CE    | 1:G:112:MET:SD   | 2.85                     | 0.64              |
| 1:G:90:ARG:O     | 1:G:94:LYS:HG2   | 1.95                     | 0.64              |
| 1:F:257:HIS:HE1  | 2:F:500:HEM:C4D  | 2.15                     | 0.64              |
| 1:H:250:PHE:O    | 1:H:254:ARG:HG3  | 1.97                     | 0.64              |
| 1:K:87:ARG:HD2   | 3:K:569:HOH:O    | 1.96                     | 0.64              |
| 1:K:295:LEU:C    | 1:K:295:LEU:CD2  | 2.65                     | 0.64              |
| 1:L:247:GLU:O    | 1:L:251:ARG:HG3  | 1.97                     | 0.64              |
| 1:E:134:ARG:HA   | 1:E:137:LEU:HD22 | 1.77                     | 0.64              |
| 1:E:295:LEU:HD12 | 1:E:295:LEU:C    | 2.17                     | 0.64              |
| 1:M:267:PHE:HE1  | 1:M:281:ARG:NH1  | 1.96                     | 0.64              |
| 1:O:82:MET:HG3   | 1:O:108:VAL:HG13 | 1.79                     | 0.64              |
| 1:N:109:SER:CB   | 1:N:110:ARG:HH11 | 2.09                     | 0.64              |
| 1:B:164:ARG:HB3  | 1:B:165:PRO:HD3  | 1.80                     | 0.64              |
| 1:I:186:TYR:OH   | 1:I:291:GLU:HG2  | 1.97                     | 0.64              |
| 1:A:68:PHE:HE1   | 2:A:500:HEM:HAB  | 1.63                     | 0.64              |
| 1:J:295:LEU:C    | 1:J:295:LEU:HD23 | 2.18                     | 0.64              |
| 1:D:126:THR:OG1  | 1:D:129:GLU:HG3  | 1.98                     | 0.63              |
| 1:K:52:ILE:HD11  | 1:L:55:ALA:HB3   | 1.80                     | 0.63              |
| 1:J:231:SER:HB2  | 3:J:540:HOH:O    | 1.97                     | 0.63              |
| 1:M:166:HIS:HD2  | 3:M:582:HOH:O    | 1.81                     | 0.63              |
| 1:N:138:GLY:HA3  | 1:N:140:SER:OG   | 1.97                     | 0.63              |
| 1:H:272:GLY:HA3  | 1:I:57:HIS:CD2   | 2.33                     | 0.63              |
| 2:L:500:HEM:HBC2 | 2:L:500:HEM:HHD  | 1.79                     | 0.63              |
| 1:A:146:TYR:HE2  | 3:A:597:HOH:O    | 1.80                     | 0.63              |
| 1:K:207:ARG:CG   | 1:K:207:ARG:HH11 | 2.11                     | 0.63              |
| 1:P:166:HIS:HE1  | 3:P:558:HOH:O    | 1.81                     | 0.63              |
| 1:O:178:THR:O    | 1:O:182:THR:OG1  | 2.17                     | 0.62              |
| 1:O:219:VAL:HG12 | 1:O:291:GLU:HG3  | 1.81                     | 0.62              |
| 1:G:100:PRO:O    | 1:G:104:MET:HG3  | 1.98                     | 0.62              |
| 1:L:273:GLY:HA3  | 1:N:41:MET:HE1   | 1.81                     | 0.62              |
| 1:A:68:PHE:CE1   | 2:A:500:HEM:HAB  | 2.33                     | 0.62              |
| 1:G:281:ARG:NH2  | 3:G:520:HOH:O    | 2.33                     | 0.62              |
| 1:L:200:ILE:HA   | 1:L:218:SER:OG   | 1.98                     | 0.62              |
| 1:L:207:ARG:HG2  | 1:L:209:TRP:CZ3  | 2.35                     | 0.62              |
| 1:B:248:ASP:O    | 1:B:252:GLN:HG3  | 1.99                     | 0.62              |
| 1:E:168:HIS:HA   | 1:F:35:MET:HA    | 1.82                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:87:ARG:HD2   | 3:F:562:HOH:O    | 1.99                     | 0.62              |
| 1:O:257:HIS:O    | 1:O:261:VAL:HG23 | 2.00                     | 0.62              |
| 1:L:82:MET:HE1   | 1:L:115:LEU:HD12 | 1.82                     | 0.62              |
| 1:C:295:LEU:HD23 | 1:C:295:LEU:O    | 2.00                     | 0.62              |
| 1:B:49:LEU:O     | 1:B:53:LEU:HB2   | 2.00                     | 0.62              |
| 1:E:99:GLN:HB2   | 1:E:100:PRO:HD3  | 1.82                     | 0.61              |
| 1:M:141:SER:OG   | 1:M:143:PHE:HB2  | 2.00                     | 0.61              |
| 1:M:149:ARG:CZ   | 1:M:162:MET:CE   | 2.78                     | 0.61              |
| 1:P:292:LEU:O    | 1:P:296:ARG:NH1  | 2.32                     | 0.61              |
| 1:C:164:ARG:CG   | 1:C:164:ARG:HH11 | 2.14                     | 0.61              |
| 1:M:219:VAL:CG1  | 1:M:291:GLU:HG3  | 2.29                     | 0.61              |
| 1:L:219:VAL:HG12 | 1:L:291:GLU:HG3  | 1.81                     | 0.61              |
| 1:F:164:ARG:N    | 1:F:165:PRO:HD2  | 2.16                     | 0.61              |
| 1:L:220:GLU:OE2  | 1:L:298:ASP:OD2  | 2.18                     | 0.61              |
| 1:N:109:SER:CB   | 1:N:110:ARG:HH12 | 1.95                     | 0.61              |
| 1:A:163:LEU:HD22 | 1:A:176:VAL:HG12 | 1.81                     | 0.61              |
| 1:C:295:LEU:C    | 1:C:295:LEU:HD23 | 2.21                     | 0.60              |
| 1:H:158:LYS:HG3  | 1:H:180:LEU:HD12 | 1.83                     | 0.60              |
| 1:J:75:THR:O     | 1:J:79:MET:HG3   | 2.01                     | 0.60              |
| 1:J:39:ARG:HA    | 3:J:541:HOH:O    | 2.01                     | 0.60              |
| 1:P:49:LEU:O     | 1:P:53:LEU:HB2   | 2.01                     | 0.60              |
| 1:F:150:GLU:O    | 1:F:154:ILE:HG13 | 2.01                     | 0.60              |
| 1:J:186:TYR:OH   | 1:J:291:GLU:HG2  | 2.01                     | 0.60              |
| 1:H:134:ARG:HG2  | 1:H:135:PRO:HD3  | 1.83                     | 0.60              |
| 2:K:500:HEM:HHD  | 2:K:500:HEM:HBC2 | 1.83                     | 0.60              |
| 1:M:149:ARG:CZ   | 1:M:162:MET:HE3  | 2.31                     | 0.60              |
| 1:C:146:TYR:O    | 1:C:150:GLU:HG3  | 2.01                     | 0.60              |
| 1:C:275:GLU:N    | 1:C:275:GLU:OE2  | 2.35                     | 0.60              |
| 1:O:119:TRP:CH2  | 1:O:257:HIS:HD2  | 2.20                     | 0.60              |
| 1:E:219:VAL:CG1  | 1:E:291:GLU:HG3  | 2.32                     | 0.60              |
| 1:F:83:LEU:O     | 1:F:87:ARG:HG3   | 2.02                     | 0.60              |
| 1:K:163:LEU:HD22 | 1:K:176:VAL:HG12 | 1.84                     | 0.60              |
| 1:L:90:ARG:HB3   | 3:L:534:HOH:O    | 2.01                     | 0.60              |
| 1:N:269:ARG:CB   | 1:N:269:ARG:HH11 | 2.15                     | 0.60              |
| 1:J:222:ALA:O    | 1:J:226:VAL:HG23 | 2.02                     | 0.60              |
| 1:K:258:VAL:HG13 | 1:K:280:LEU:CB   | 2.32                     | 0.60              |
| 1:B:146:TYR:O    | 1:B:150:GLU:HG3  | 2.01                     | 0.60              |
| 1:C:150:GLU:O    | 1:C:154:ILE:HG13 | 2.02                     | 0.60              |
| 1:D:274:THR:HG21 | 3:E:550:HOH:O    | 2.01                     | 0.60              |
| 1:O:114:GLN:OE1  | 1:P:117:GLN:HG2  | 2.02                     | 0.60              |
| 1:C:77:LEU:HD12  | 1:D:77:LEU:HD12  | 1.84                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:79:MET:HE1   | 1:K:148:TYR:HD1  | 1.67                     | 0.59              |
| 1:L:270:GLY:HA3  | 1:N:50:ASP:HB2   | 1.84                     | 0.59              |
| 1:P:122:LEU:HD21 | 2:P:500:HEM:HAB  | 1.84                     | 0.59              |
| 1:P:126:THR:OG1  | 1:P:129:GLU:HG3  | 2.01                     | 0.59              |
| 1:F:127:PRO:HG3  | 1:G:296:ARG:HD2  | 1.84                     | 0.59              |
| 2:P:500:HEM:HBB2 | 2:P:500:HEM:CMB  | 2.31                     | 0.59              |
| 1:P:89:ALA:O     | 1:P:93:VAL:HG23  | 2.03                     | 0.59              |
| 1:N:109:SER:HB2  | 1:N:110:ARG:HH11 | 1.67                     | 0.59              |
| 1:A:261:VAL:HG22 | 2:A:500:HEM:C1B  | 2.37                     | 0.59              |
| 1:G:120:ASN:OD1  | 1:G:256:ARG:NH2  | 2.26                     | 0.59              |
| 1:G:151:ILE:O    | 1:G:154:ILE:HG22 | 2.02                     | 0.59              |
| 1:I:89:ALA:O     | 1:I:93:VAL:HG23  | 2.03                     | 0.59              |
| 1:L:186:TYR:O    | 1:L:190:ILE:HG13 | 2.02                     | 0.59              |
| 1:C:141:SER:OG   | 1:C:143:PHE:HB2  | 2.02                     | 0.59              |
| 1:D:219:VAL:CG1  | 1:D:291:GLU:HG3  | 2.29                     | 0.59              |
| 1:K:75:THR:O     | 1:K:79:MET:HG3   | 2.03                     | 0.58              |
| 1:D:89:ALA:HB3   | 1:D:185:MET:HE1  | 1.85                     | 0.58              |
| 1:J:295:LEU:HD23 | 1:J:295:LEU:O    | 2.03                     | 0.58              |
| 1:O:49:LEU:O     | 1:O:53:LEU:HB2   | 2.01                     | 0.58              |
| 1:E:183:PRO:HG2  | 3:E:502:HOH:O    | 2.03                     | 0.58              |
| 1:B:99:GLN:HB2   | 1:B:100:PRO:HD3  | 1.84                     | 0.58              |
| 2:O:500:HEM:HBB2 | 2:O:500:HEM:CMB  | 2.34                     | 0.58              |
| 1:E:100:PRO:O    | 1:E:104:MET:HG3  | 2.04                     | 0.58              |
| 1:K:214:GLN:HG2  | 3:K:553:HOH:O    | 2.04                     | 0.58              |
| 1:K:119:TRP:CD1  | 1:K:256:ARG:HG2  | 2.39                     | 0.58              |
| 1:C:49:LEU:O     | 1:C:53:LEU:HB2   | 2.03                     | 0.58              |
| 1:J:190:ILE:HG21 | 1:J:204:VAL:CG1  | 2.34                     | 0.58              |
| 1:L:163:LEU:HD23 | 1:L:176:VAL:HG12 | 1.85                     | 0.58              |
| 1:A:282:ARG:HH21 | 1:B:31:HIS:HD2   | 1.52                     | 0.58              |
| 1:D:141:SER:OG   | 1:D:143:PHE:HB2  | 2.04                     | 0.58              |
| 1:O:295:LEU:HD23 | 1:O:295:LEU:C    | 2.24                     | 0.58              |
| 1:I:52:ILE:HG22  | 1:I:53:LEU:HD13  | 1.85                     | 0.58              |
| 1:P:166:HIS:CE1  | 3:P:558:HOH:O    | 2.55                     | 0.58              |
| 1:A:212:PRO:HB2  | 3:A:586:HOH:O    | 2.04                     | 0.57              |
| 1:L:274:THR:HG22 | 1:L:275:GLU:OE2  | 2.04                     | 0.57              |
| 1:N:163:LEU:HD22 | 1:N:176:VAL:HG12 | 1.85                     | 0.57              |
| 1:D:103:LYS:HG2  | 3:D:520:HOH:O    | 2.04                     | 0.57              |
| 1:E:79:MET:CE    | 1:E:151:ILE:CD1  | 2.82                     | 0.57              |
| 1:E:143:PHE:HE2  | 1:E:279:TYR:HH   | 1.53                     | 0.57              |
| 1:G:99:GLN:HB2   | 1:G:100:PRO:HD3  | 1.86                     | 0.57              |
| 1:G:283:MET:CE   | 1:G:283:MET:CA   | 2.77                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:I:109:SER:HB3   | 1:I:110:ARG:HH21 | 1.68                     | 0.57              |
| 1:I:43:TYR:HB3    | 1:J:144:GLN:HB2  | 1.86                     | 0.57              |
| 1:K:222:ALA:O     | 1:K:226:VAL:HG23 | 2.04                     | 0.57              |
| 1:N:158[A]:LYS:NZ | 1:N:209:TRP:O    | 2.37                     | 0.57              |
| 1:B:296:ARG:HD3   | 1:C:127:PRO:HG3  | 1.86                     | 0.57              |
| 1:L:167:ALA:HA    | 1:L:173:LEU:HD22 | 1.86                     | 0.57              |
| 1:O:224:LEU:O     | 1:O:228:ARG:HG3  | 2.05                     | 0.57              |
| 1:L:95:SER:HB3    | 1:L:97:GLN:HG3   | 1.86                     | 0.57              |
| 1:N:292:LEU:HA    | 1:N:295:LEU:HD13 | 1.87                     | 0.57              |
| 1:E:219:VAL:HG12  | 1:E:291:GLU:HG3  | 1.87                     | 0.57              |
| 1:J:258:VAL:HG13  | 1:J:280:LEU:CB   | 2.35                     | 0.57              |
| 1:P:250:PHE:CD1   | 1:P:254:ARG:NH2  | 2.72                     | 0.57              |
| 1:K:258:VAL:HG13  | 1:K:280:LEU:HB3  | 1.87                     | 0.57              |
| 1:K:50:ASP:HB2    | 3:K:563:HOH:O    | 2.05                     | 0.57              |
| 1:A:216:ASN:OD1   | 1:A:219:VAL:HG23 | 2.04                     | 0.57              |
| 1:D:192:LEU:C     | 1:D:192:LEU:HD12 | 2.26                     | 0.57              |
| 1:F:146:TYR:O     | 1:F:150:GLU:HG3  | 2.05                     | 0.57              |
| 1:H:248:ASP:O     | 1:H:252:GLN:HG3  | 2.05                     | 0.57              |
| 1:O:188:GLU:OE2   | 3:O:516:HOH:O    | 2.17                     | 0.56              |
| 1:I:82:MET:CG     | 1:I:108:VAL:HG13 | 2.35                     | 0.56              |
| 1:I:140:SER:O     | 1:I:271:THR:OG1  | 2.22                     | 0.56              |
| 1:L:268:LYS:HG3   | 3:L:573:HOH:O    | 2.05                     | 0.56              |
| 1:L:282:ARG:HD2   | 1:N:41:MET:HE3   | 1.85                     | 0.56              |
| 1:O:279:TYR:HD2   | 1:O:280:LEU:HD23 | 1.70                     | 0.56              |
| 1:O:52:ILE:HD11   | 1:P:55:ALA:HB3   | 1.87                     | 0.56              |
| 1:O:50:ASP:OD1    | 1:P:169:ARG:NH2  | 2.38                     | 0.56              |
| 1:G:127:PRO:HB2   | 1:G:128:PRO:HD3  | 1.87                     | 0.56              |
| 1:J:267:PHE:CE1   | 1:J:281:ARG:HD2  | 2.41                     | 0.56              |
| 1:D:90:ARG:HB2    | 1:D:185:MET:HG3  | 1.87                     | 0.56              |
| 1:P:146:TYR:O     | 1:P:150:GLU:HG3  | 2.05                     | 0.56              |
| 1:B:163:LEU:HD23  | 1:B:176:VAL:HG12 | 1.88                     | 0.56              |
| 1:J:207:ARG:HG3   | 1:J:208:ASP:N    | 2.21                     | 0.56              |
| 1:G:186:TYR:OH    | 1:G:291:GLU:HG2  | 2.06                     | 0.55              |
| 1:J:201:ASP:HB3   | 1:J:203:GLU:HG2  | 1.88                     | 0.55              |
| 1:F:216:ASN:OD1   | 1:F:218:SER:HB3  | 2.05                     | 0.55              |
| 1:I:207:ARG:CG    | 1:I:207:ARG:NH1  | 2.57                     | 0.55              |
| 2:O:500:HEM:HBB2  | 2:O:500:HEM:HMB2 | 1.88                     | 0.55              |
| 1:G:68:PHE:CB     | 1:G:133:MET:HE1  | 2.36                     | 0.55              |
| 1:H:191:ARG:HG2   | 1:H:205:VAL:HG13 | 1.88                     | 0.55              |
| 1:I:207:ARG:HG3   | 1:I:207:ARG:NH1  | 2.01                     | 0.55              |
| 1:F:267:PHE:HD2   | 1:F:268:LYS:N    | 2.04                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:192:LEU:HD12 | 1:J:195:ARG:HH21 | 1.71                     | 0.55              |
| 1:O:89:ALA:HB3   | 1:O:185:MET:HE2  | 1.86                     | 0.55              |
| 2:G:500:HEM:HHD  | 2:G:500:HEM:HBC2 | 1.89                     | 0.55              |
| 1:I:168:HIS:CE1  | 1:I:169:ARG:HG2  | 2.41                     | 0.55              |
| 1:I:279:TYR:CE1  | 1:I:283:MET:CE   | 2.90                     | 0.55              |
| 2:L:500:HEM:CBC  | 2:L:500:HEM:HHD  | 2.36                     | 0.55              |
| 1:H:49:LEU:O     | 1:H:53:LEU:HB2   | 2.07                     | 0.55              |
| 1:O:167:ALA:HA   | 1:O:173:LEU:HD22 | 1.89                     | 0.55              |
| 1:N:109:SER:HB2  | 1:N:110:ARG:NH1  | 2.17                     | 0.55              |
| 1:E:79:MET:HE3   | 1:E:151:ILE:CD1  | 2.37                     | 0.55              |
| 1:I:290:PRO:HG3  | 3:I:577:HOH:O    | 2.06                     | 0.55              |
| 1:A:146:TYR:HD2  | 3:A:595:HOH:O    | 1.90                     | 0.54              |
| 1:C:192:LEU:O    | 1:C:196:ARG:HG3  | 2.06                     | 0.54              |
| 1:E:256:ARG:HD2  | 3:H:502:HOH:O    | 2.06                     | 0.54              |
| 1:N:293:TRP:CZ3  | 1:O:263:ARG:HB3  | 2.42                     | 0.54              |
| 1:M:282:ARG:NH2  | 3:M:536:HOH:O    | 2.40                     | 0.54              |
| 1:D:200:ILE:HG22 | 1:D:205:VAL:HG23 | 1.88                     | 0.54              |
| 1:I:149:ARG:CZ   | 1:I:162:MET:CE   | 2.85                     | 0.54              |
| 1:I:266:GLY:HA3  | 1:L:297:THR:HG22 | 1.90                     | 0.54              |
| 1:I:149:ARG:CZ   | 1:I:162:MET:HE3  | 2.37                     | 0.54              |
| 1:A:274:THR:CG2  | 1:A:279:TYR:HB2  | 2.38                     | 0.54              |
| 1:I:211:GLN:C    | 1:I:212:PRO:O    | 2.44                     | 0.54              |
| 1:L:219:VAL:CG1  | 1:L:291:GLU:HG3  | 2.38                     | 0.54              |
| 1:G:59:LEU:HD23  | 1:G:136:TYR:O    | 2.07                     | 0.54              |
| 1:L:295:LEU:CD2  | 1:L:296:ARG:N    | 2.70                     | 0.54              |
| 1:G:223:TRP:HB3  | 1:G:295:LEU:HD12 | 1.90                     | 0.54              |
| 1:I:250:PHE:O    | 1:I:254:ARG:CD   | 2.56                     | 0.54              |
| 1:K:261:VAL:HG22 | 2:K:500:HEM:C2B  | 2.43                     | 0.54              |
| 1:M:247:GLU:HG3  | 1:M:288:LEU:HD12 | 1.90                     | 0.54              |
| 1:N:131:SER:HB2  | 1:O:299:LEU:HD23 | 1.90                     | 0.54              |
| 1:F:172:HIS:O    | 1:F:176:VAL:HG23 | 2.08                     | 0.53              |
| 1:G:254:ARG:NH1  | 3:G:537:HOH:O    | 2.41                     | 0.53              |
| 1:H:126:THR:OG1  | 1:H:129:GLU:HG3  | 2.07                     | 0.53              |
| 1:A:275:GLU:HB2  | 3:A:572:HOH:O    | 2.06                     | 0.53              |
| 1:I:254:ARG:HB2  | 3:I:521:HOH:O    | 2.07                     | 0.53              |
| 1:N:192:LEU:HD13 | 1:N:195:ARG:NH2  | 2.23                     | 0.53              |
| 1:B:262:GLU:OE1  | 1:B:281:ARG:NH2  | 2.40                     | 0.53              |
| 1:I:122:LEU:HD21 | 2:I:500:HEM:CAB  | 2.35                     | 0.53              |
| 1:C:275:GLU:OE2  | 1:C:275:GLU:CA   | 2.57                     | 0.53              |
| 1:K:114:GLN:OE1  | 1:L:117:GLN:HG2  | 2.08                     | 0.53              |
| 1:M:267:PHE:HE1  | 1:M:281:ARG:HH11 | 1.54                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:119:TRP:CH2  | 1:A:257:HIS:HD2  | 2.27                     | 0.53              |
| 1:C:295:LEU:C    | 1:C:295:LEU:CD2  | 2.77                     | 0.53              |
| 1:G:148:TYR:CE1  | 1:G:250:PHE:HZ   | 2.26                     | 0.53              |
| 1:L:291:GLU:O    | 1:L:295:LEU:HB3  | 2.09                     | 0.53              |
| 1:O:159:ASN:OD1  | 1:O:162:MET:HG2  | 2.09                     | 0.53              |
| 1:M:99:GLN:HB2   | 1:M:100:PRO:HD3  | 1.91                     | 0.53              |
| 1:G:279:TYR:O    | 1:G:282:ARG:HB2  | 2.08                     | 0.53              |
| 1:E:266:GLY:HA3  | 1:H:297:THR:HG22 | 1.90                     | 0.53              |
| 1:O:223:TRP:HB3  | 1:O:295:LEU:HD12 | 1.91                     | 0.53              |
| 1:D:272:GLY:HA3  | 3:D:589:HOH:O    | 2.08                     | 0.53              |
| 1:F:110:ARG:CD   | 3:F:534:HOH:O    | 2.56                     | 0.52              |
| 1:P:83:LEU:HD21  | 1:P:150:GLU:HB2  | 1.92                     | 0.52              |
| 1:D:150:GLU:O    | 1:D:154:ILE:HG13 | 2.09                     | 0.52              |
| 1:K:127:PRO:N    | 1:K:128:PRO:HD2  | 2.24                     | 0.52              |
| 1:K:39:ARG:HH11  | 1:K:39:ARG:HA    | 1.73                     | 0.52              |
| 1:L:195:ARG:NH1  | 3:L:548:HOH:O    | 2.42                     | 0.52              |
| 1:O:186:TYR:OH   | 1:O:291:GLU:HG2  | 2.10                     | 0.52              |
| 1:C:75:THR:O     | 1:C:79:MET:HG3   | 2.09                     | 0.52              |
| 1:I:76:GLU:HA    | 1:I:79:MET:HE2   | 1.90                     | 0.52              |
| 1:F:158:LYS:HG3  | 1:F:180:LEU:HD12 | 1.91                     | 0.52              |
| 1:I:267:PHE:H    | 1:L:297:THR:CG2  | 2.23                     | 0.52              |
| 1:P:164:ARG:NH1  | 1:P:164:ARG:HG3  | 2.19                     | 0.52              |
| 1:E:163:LEU:HD23 | 1:E:176:VAL:HG12 | 1.92                     | 0.52              |
| 1:L:75:THR:HG23  | 1:L:115:LEU:HD22 | 1.91                     | 0.52              |
| 1:N:146:TYR:O    | 1:N:150:GLU:HG3  | 2.09                     | 0.52              |
| 1:L:273:GLY:HA3  | 1:N:41:MET:CE    | 2.39                     | 0.52              |
| 1:B:296:ARG:HD3  | 1:C:127:PRO:CG   | 2.40                     | 0.52              |
| 1:F:127:PRO:N    | 1:F:128:PRO:HD2  | 2.25                     | 0.52              |
| 2:H:500:HEM:CMB  | 2:H:500:HEM:HBB2 | 2.39                     | 0.52              |
| 1:I:114:GLN:OE1  | 1:J:117:GLN:HG2  | 2.10                     | 0.52              |
| 1:J:163:LEU:HD22 | 1:J:176:VAL:CG1  | 2.35                     | 0.52              |
| 1:F:254:ARG:HD2  | 3:F:506:HOH:O    | 2.10                     | 0.52              |
| 1:H:99:GLN:HB2   | 1:H:100:PRO:HD3  | 1.91                     | 0.52              |
| 1:I:163:LEU:CD2  | 1:I:176:VAL:HG12 | 2.40                     | 0.52              |
| 1:L:64:ASN:HA    | 3:L:529:HOH:O    | 2.09                     | 0.52              |
| 1:L:295:LEU:CD2  | 1:L:295:LEU:C    | 2.77                     | 0.51              |
| 1:O:169:ARG:HH21 | 1:O:172:HIS:CE1  | 2.28                     | 0.51              |
| 1:K:261:VAL:HG22 | 2:K:500:HEM:C1B  | 2.44                     | 0.51              |
| 1:N:292:LEU:O    | 1:N:296:ARG:NH1  | 2.41                     | 0.51              |
| 1:N:269:ARG:HB3  | 1:N:269:ARG:CZ   | 2.40                     | 0.51              |
| 1:H:275:GLU:HG2  | 3:H:595:HOH:O    | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:90:ARG:O     | 1:I:94:LYS:HG3   | 2.10                     | 0.51              |
| 1:J:82:MET:HG3   | 1:J:111:ILE:HG21 | 1.92                     | 0.51              |
| 1:P:65:GLU:HA    | 1:P:133:MET:HE1  | 1.93                     | 0.51              |
| 1:E:261:VAL:HG22 | 2:E:500:HEM:C1B  | 2.45                     | 0.51              |
| 1:E:267:PHE:CE2  | 1:E:281:ARG:NE   | 2.77                     | 0.51              |
| 1:A:146:TYR:O    | 1:A:150:GLU:HG3  | 2.11                     | 0.51              |
| 1:I:275:GLU:HB3  | 1:I:278:SER:OG   | 2.10                     | 0.51              |
| 1:C:99:GLN:HB2   | 1:C:100:PRO:HD3  | 1.92                     | 0.51              |
| 1:H:168:HIS:H    | 1:H:168:HIS:CD2  | 2.29                     | 0.51              |
| 1:I:223:TRP:CD2  | 1:I:292:LEU:HD21 | 2.46                     | 0.51              |
| 1:M:261:VAL:HG22 | 2:M:500:HEM:C1B  | 2.46                     | 0.51              |
| 1:M:281:ARG:O    | 1:M:284:LEU:HB2  | 2.10                     | 0.51              |
| 1:E:215:TYR:CE1  | 1:E:294:LYS:HD3  | 2.46                     | 0.51              |
| 1:G:226:VAL:HG13 | 1:G:233:HIS:HB2  | 1.93                     | 0.51              |
| 1:M:168:HIS:CE1  | 1:M:169:ARG:HG2  | 2.47                     | 0.51              |
| 1:N:99:GLN:HB2   | 1:N:100:PRO:HD3  | 1.92                     | 0.51              |
| 1:F:152:GLU:OE2  | 1:F:254:ARG:NH1  | 2.41                     | 0.50              |
| 1:G:158:LYS:CG   | 1:G:180:LEU:HD12 | 2.36                     | 0.50              |
| 1:L:188:GLU:HA   | 1:L:188:GLU:OE2  | 2.12                     | 0.50              |
| 1:N:119:TRP:CH2  | 1:N:257:HIS:HD2  | 2.29                     | 0.50              |
| 1:O:89:ALA:CB    | 1:O:185:MET:HE2  | 2.40                     | 0.50              |
| 1:P:119:TRP:CH2  | 1:P:257:HIS:CD2  | 3.00                     | 0.50              |
| 1:D:269:ARG:NH1  | 1:F:45:ASP:OD1   | 2.45                     | 0.50              |
| 1:N:295:LEU:HD23 | 1:N:295:LEU:O    | 2.10                     | 0.50              |
| 1:O:163:LEU:HD22 | 1:O:173:LEU:CD1  | 2.41                     | 0.50              |
| 1:C:164:ARG:HB2  | 1:C:164:ARG:CZ   | 2.41                     | 0.50              |
| 1:F:200:ILE:HG22 | 1:F:204:VAL:HG23 | 1.92                     | 0.50              |
| 1:F:258:VAL:HG21 | 1:F:281:ARG:HG2  | 1.93                     | 0.50              |
| 1:I:279:TYR:CE1  | 1:I:283:MET:HE3  | 2.45                     | 0.50              |
| 1:G:257:HIS:HE1  | 2:G:500:HEM:C4D  | 2.29                     | 0.50              |
| 1:H:65:GLU:HG3   | 1:H:133:MET:CE   | 2.41                     | 0.50              |
| 1:I:49:LEU:HB3   | 1:I:53:LEU:HD22  | 1.94                     | 0.50              |
| 1:M:261:VAL:HG22 | 2:M:500:HEM:C2B  | 2.47                     | 0.50              |
| 1:F:163:LEU:CD2  | 1:F:176:VAL:HG12 | 2.41                     | 0.50              |
| 1:G:131:SER:HA   | 1:G:134:ARG:HG2  | 1.93                     | 0.50              |
| 1:I:250:PHE:O    | 1:I:254:ARG:HD2  | 2.11                     | 0.50              |
| 1:O:247:GLU:OE1  | 1:O:293:TRP:NE1  | 2.40                     | 0.50              |
| 1:P:149:ARG:HD2  | 1:P:162:MET:CB   | 2.42                     | 0.50              |
| 1:P:119:TRP:CH2  | 1:P:257:HIS:HD2  | 2.30                     | 0.50              |
| 1:G:134:ARG:N    | 1:G:135:PRO:HD2  | 2.27                     | 0.50              |
| 1:N:247:GLU:CD   | 1:N:293:TRP:HE1  | 2.14                     | 0.49              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:N:119:TRP:CH2    | 1:N:257:HIS:CD2  | 3.00                     | 0.49              |
| 1:B:267:PHE:CE1    | 1:B:281:ARG:CD   | 2.95                     | 0.49              |
| 1:D:274:THR:HG22   | 1:D:275:GLU:OE2  | 2.13                     | 0.49              |
| 1:F:174:GLU:HG2    | 1:F:175:LEU:N    | 2.27                     | 0.49              |
| 1:A:165:PRO:HA     | 1:B:35:MET:O     | 2.13                     | 0.49              |
| 1:F:161:ALA:O      | 1:F:164:ARG:HG2  | 2.12                     | 0.49              |
| 1:F:158:LYS:HG2    | 1:F:209:TRP:O    | 2.12                     | 0.49              |
| 1:A:282:ARG:HG2    | 3:A:623:HOH:O    | 2.12                     | 0.49              |
| 1:D:163:LEU:HD23   | 1:D:176:VAL:HG12 | 1.95                     | 0.49              |
| 1:G:202:PRO:HD2    | 3:G:540:HOH:O    | 2.13                     | 0.49              |
| 1:E:143:PHE:HE2    | 1:E:279:TYR:CZ   | 2.31                     | 0.49              |
| 1:G:247:GLU:OE1    | 1:G:293:TRP:NE1  | 2.45                     | 0.49              |
| 1:K:120:ASN:OD1    | 1:K:256:ARG:NH1  | 2.31                     | 0.49              |
| 1:G:68:PHE:HB3     | 1:G:133:MET:HE1  | 1.94                     | 0.49              |
| 1:F:153:PHE:O      | 1:F:158:LYS:HE3  | 2.13                     | 0.49              |
| 1:K:134:ARG:HA     | 1:K:137:LEU:HG   | 1.95                     | 0.49              |
| 1:A:269:ARG:NH1    | 1:A:275:GLU:OE2  | 2.46                     | 0.49              |
| 1:A:76:GLU:HA      | 1:A:79:MET:HE2   | 1.94                     | 0.49              |
| 1:E:119:TRP:CH2    | 1:E:257:HIS:CD2  | 3.01                     | 0.49              |
| 1:K:247:GLU:O      | 1:K:251:ARG:HG3  | 2.12                     | 0.49              |
| 1:O:158:LYS:O      | 1:O:212:PRO:HG3  | 2.12                     | 0.49              |
| 1:A:284:LEU:HD23   | 1:A:284:LEU:HA   | 1.38                     | 0.48              |
| 1:C:83:LEU:O       | 1:C:87:ARG:HG3   | 2.13                     | 0.48              |
| 2:I:500:HEM:HBC2   | 2:I:500:HEM:HHD  | 1.95                     | 0.48              |
| 1:K:49:LEU:O       | 1:K:53:LEU:HB2   | 2.13                     | 0.48              |
| 1:L:272:GLY:HA3    | 1:M:57:HIS:CD2   | 2.48                     | 0.48              |
| 1:C:223:TRP:HB3    | 1:C:295:LEU:HD12 | 1.95                     | 0.48              |
| 1:N:158[A]:LYS:HD2 | 1:N:180:LEU:HD12 | 1.94                     | 0.48              |
| 1:B:257:HIS:O      | 1:B:261:VAL:HG23 | 2.13                     | 0.48              |
| 1:B:99:GLN:HB3     | 1:D:234:TRP:NE1  | 2.28                     | 0.48              |
| 1:L:202:PRO:HD2    | 3:L:547:HOH:O    | 2.13                     | 0.48              |
| 1:O:171:GLU:CD     | 1:O:171:GLU:H    | 2.16                     | 0.48              |
| 1:P:158:LYS:HD2    | 1:P:180:LEU:HD12 | 1.94                     | 0.48              |
| 1:A:282:ARG:NH2    | 1:B:31:HIS:HD2   | 2.11                     | 0.48              |
| 1:C:227:TYR:O      | 1:C:230:PRO:HD3  | 2.14                     | 0.48              |
| 1:E:267:PHE:CZ     | 1:E:281:ARG:HD2  | 2.47                     | 0.48              |
| 1:L:190:ILE:HG21   | 1:L:204:VAL:HG13 | 1.95                     | 0.48              |
| 1:M:219:VAL:CG1    | 1:M:291:GLU:CG   | 2.89                     | 0.48              |
| 1:O:39:ARG:O       | 1:P:138:GLY:HA3  | 2.13                     | 0.48              |
| 2:E:500:HEM:CBB    | 2:E:500:HEM:HMB2 | 2.41                     | 0.48              |
| 1:J:39:ARG:NH1     | 3:J:556:HOH:O    | 2.46                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:57:HIS:CD2   | 3:K:570:HOH:O    | 2.41                     | 0.48              |
| 1:L:76:GLU:HA    | 1:L:79:MET:HE2   | 1.96                     | 0.48              |
| 1:O:89:ALA:HB3   | 1:O:185:MET:HE1  | 1.92                     | 0.48              |
| 1:P:88:ALA:HB1   | 1:P:104:MET:CE   | 2.29                     | 0.48              |
| 1:G:54:SER:HA    | 3:G:551:HOH:O    | 2.14                     | 0.48              |
| 1:N:188:GLU:OE2  | 1:N:188:GLU:HA   | 2.14                     | 0.48              |
| 1:G:223:TRP:HB3  | 1:G:295:LEU:CD1  | 2.44                     | 0.48              |
| 1:E:295:LEU:HD12 | 1:E:295:LEU:O    | 2.12                     | 0.48              |
| 1:E:69:ILE:O     | 1:E:73:GLN:HG3   | 2.14                     | 0.48              |
| 1:I:49:LEU:O     | 1:I:53:LEU:HB2   | 2.13                     | 0.48              |
| 1:O:195:ARG:NH2  | 3:O:516:HOH:O    | 2.47                     | 0.48              |
| 1:O:117:GLN:HB3  | 1:P:114:GLN:OE1  | 2.13                     | 0.48              |
| 1:C:220:GLU:OE2  | 1:C:298:ASP:OD2  | 2.32                     | 0.48              |
| 1:E:261:VAL:HG22 | 2:E:500:HEM:C2B  | 2.49                     | 0.48              |
| 1:H:122:LEU:HD23 | 1:H:260:THR:HG21 | 1.96                     | 0.48              |
| 1:I:120:ASN:CG   | 1:I:256:ARG:HH22 | 2.14                     | 0.48              |
| 1:O:86:LEU:O     | 1:O:185:MET:HE3  | 2.14                     | 0.48              |
| 2:I:500:HEM:HMB2 | 2:I:500:HEM:CBB  | 2.40                     | 0.47              |
| 1:L:68:PHE:HB2   | 1:L:133:MET:HE1  | 1.96                     | 0.47              |
| 1:C:62:ASP:OD1   | 1:C:64:ASN:HB2   | 2.14                     | 0.47              |
| 1:D:171:GLU:HG2  | 3:D:600:HOH:O    | 2.14                     | 0.47              |
| 1:I:117:GLN:HB2  | 3:I:547:HOH:O    | 2.13                     | 0.47              |
| 1:I:142:GLY:HA3  | 2:I:500:HEM:C1D  | 2.48                     | 0.47              |
| 1:L:158:LYS:NZ   | 1:L:182:THR:O    | 2.33                     | 0.47              |
| 1:L:246:LEU:HD13 | 3:L:579:HOH:O    | 2.14                     | 0.47              |
| 1:O:223:TRP:HB3  | 1:O:295:LEU:CD1  | 2.44                     | 0.47              |
| 1:P:48:GLY:HA2   | 3:P:568:HOH:O    | 2.14                     | 0.47              |
| 1:E:281:ARG:NH1  | 1:E:281:ARG:CG   | 2.62                     | 0.47              |
| 1:I:279:TYR:CE1  | 1:I:283:MET:HE2  | 2.48                     | 0.47              |
| 1:M:96:ASP:HB3   | 3:M:594:HOH:O    | 2.13                     | 0.47              |
| 1:O:275:GLU:HA   | 1:O:279:TYR:HB2  | 1.96                     | 0.47              |
| 1:L:158:LYS:HG3  | 1:L:180:LEU:HD12 | 1.96                     | 0.47              |
| 1:F:215:TYR:CD2  | 1:F:215:TYR:C    | 2.87                     | 0.47              |
| 1:K:39:ARG:O     | 1:L:139:ALA:HB2  | 2.14                     | 0.47              |
| 1:I:267:PHE:H    | 1:L:297:THR:HG22 | 1.80                     | 0.47              |
| 1:P:224:LEU:O    | 1:P:228:ARG:HG3  | 2.15                     | 0.47              |
| 1:A:169:ARG:HD3  | 3:B:580:HOH:O    | 2.14                     | 0.47              |
| 1:B:186:TYR:OH   | 1:B:291:GLU:HG2  | 2.15                     | 0.47              |
| 1:D:134:ARG:HB3  | 1:D:135:PRO:HD3  | 1.97                     | 0.47              |
| 1:K:258:VAL:HG13 | 1:K:280:LEU:HB2  | 1.96                     | 0.47              |
| 1:L:127:PRO:HB2  | 1:L:128:PRO:CD   | 2.45                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:149:ARG:CZ   | 1:M:162:MET:HE2  | 2.44                     | 0.47              |
| 1:C:164:ARG:NH1  | 1:C:164:ARG:CG   | 2.76                     | 0.47              |
| 1:D:78:TRP:HB2   | 1:D:115:LEU:HD21 | 1.96                     | 0.47              |
| 1:N:293:TRP:O    | 1:N:296:ARG:HB2  | 2.14                     | 0.47              |
| 1:P:70:VAL:O     | 1:P:74:THR:HG23  | 2.15                     | 0.47              |
| 1:A:274:THR:CG2  | 1:A:279:TYR:HB3  | 2.44                     | 0.47              |
| 1:G:103:LYS:NZ   | 3:G:534:HOH:O    | 2.40                     | 0.47              |
| 1:G:170:PRO:O    | 1:G:174:GLU:HB2  | 2.15                     | 0.47              |
| 1:I:149:ARG:NH2  | 1:I:162:MET:HE2  | 2.30                     | 0.47              |
| 1:J:203:GLU:HB3  | 3:J:544:HOH:O    | 2.15                     | 0.47              |
| 1:J:292:LEU:O    | 1:J:296:ARG:NH1  | 2.46                     | 0.47              |
| 1:O:96:ASP:HB2   | 3:O:507:HOH:O    | 2.14                     | 0.47              |
| 1:D:215:TYR:OH   | 1:D:220:GLU:OE1  | 2.21                     | 0.47              |
| 1:N:52:ILE:HG22  | 1:N:53:LEU:HD13  | 1.96                     | 0.47              |
| 1:O:67:LEU:O     | 1:O:67:LEU:HD12  | 2.14                     | 0.47              |
| 1:M:260:THR:O    | 1:M:263:ARG:HB2  | 2.15                     | 0.47              |
| 1:N:182:THR:HG22 | 3:N:532:HOH:O    | 2.15                     | 0.47              |
| 1:O:119:TRP:CH2  | 1:O:257:HIS:CD2  | 3.01                     | 0.47              |
| 1:L:274:THR:HB   | 1:M:57:HIS:HB3   | 1.97                     | 0.46              |
| 1:C:164:ARG:NH1  | 1:C:164:ARG:HB2  | 2.30                     | 0.46              |
| 1:D:133:MET:CE   | 1:D:137:LEU:HD11 | 2.42                     | 0.46              |
| 1:G:220:GLU:OE2  | 1:G:298:ASP:OD2  | 2.32                     | 0.46              |
| 1:O:134:ARG:N    | 1:O:135:PRO:HD2  | 2.30                     | 0.46              |
| 1:A:86:LEU:CD2   | 1:A:185:MET:HE1  | 2.43                     | 0.46              |
| 1:B:295:LEU:C    | 1:B:295:LEU:CD2  | 2.84                     | 0.46              |
| 1:H:112:MET:O    | 1:H:116:VAL:HG23 | 2.16                     | 0.46              |
| 2:D:500:HEM:HHD  | 2:D:500:HEM:HBC2 | 1.96                     | 0.46              |
| 1:F:267:PHE:CZ   | 1:F:281:ARG:HD2  | 2.51                     | 0.46              |
| 1:G:49:LEU:O     | 1:G:53:LEU:HB2   | 2.15                     | 0.46              |
| 1:M:212:PRO:HB3  | 3:M:588:HOH:O    | 2.15                     | 0.46              |
| 1:O:134:ARG:HB3  | 1:O:135:PRO:CD   | 2.45                     | 0.46              |
| 1:P:277:VAL:O    | 1:P:281:ARG:HG3  | 2.15                     | 0.46              |
| 1:B:130:TYR:CE1  | 1:B:134:ARG:HG3  | 2.50                     | 0.46              |
| 1:E:141:SER:HA   | 3:E:554:HOH:O    | 2.15                     | 0.46              |
| 1:D:241:GLU:OE2  | 1:D:296:ARG:NH2  | 2.39                     | 0.46              |
| 1:E:280:LEU:HD11 | 2:E:500:HEM:C2A  | 2.51                     | 0.46              |
| 1:F:200:ILE:HA   | 1:F:218:SER:OG   | 2.14                     | 0.46              |
| 1:F:296:ARG:HD3  | 1:G:127:PRO:HG3  | 1.98                     | 0.46              |
| 1:I:149:ARG:HD3  | 1:I:149:ARG:HA   | 1.72                     | 0.46              |
| 1:L:52:ILE:HG22  | 1:L:53:LEU:HD13  | 1.98                     | 0.46              |
| 1:L:82:MET:HE1   | 1:L:115:LEU:CD1  | 2.45                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:40:ASP:O     | 1:O:40:ASP:CG    | 2.53                     | 0.46              |
| 1:P:59:LEU:HA    | 1:P:59:LEU:HD12  | 1.68                     | 0.46              |
| 1:E:120:ASN:OD1  | 1:E:256:ARG:NH2  | 2.35                     | 0.46              |
| 1:G:294:LYS:NZ   | 1:G:294:LYS:HB3  | 2.29                     | 0.46              |
| 1:I:168:HIS:CD2  | 3:I:551:HOH:O    | 2.69                     | 0.46              |
| 1:M:100:PRO:O    | 1:M:104:MET:HG3  | 2.15                     | 0.46              |
| 1:A:183:PRO:HG3  | 1:A:209:TRP:CE2  | 2.51                     | 0.46              |
| 1:J:207:ARG:CG   | 1:J:208:ASP:N    | 2.77                     | 0.46              |
| 1:A:274:THR:HG21 | 1:A:279:TYR:HB3  | 1.96                     | 0.46              |
| 1:B:103:LYS:HG2  | 3:B:533:HOH:O    | 2.16                     | 0.46              |
| 1:F:164:ARG:HB2  | 1:F:165:PRO:HD3  | 1.96                     | 0.46              |
| 1:I:129:GLU:OE2  | 1:J:103:LYS:NZ   | 2.37                     | 0.46              |
| 1:I:42:SER:HB2   | 1:J:144:GLN:OE1  | 2.16                     | 0.46              |
| 1:J:295:LEU:CD2  | 1:J:295:LEU:C    | 2.84                     | 0.46              |
| 1:D:93:VAL:HG13  | 1:D:192:LEU:HD23 | 1.97                     | 0.46              |
| 1:I:149:ARG:NH2  | 1:I:162:MET:CE   | 2.79                     | 0.46              |
| 1:J:104:MET:O    | 1:J:108:VAL:HG23 | 2.15                     | 0.46              |
| 1:J:134:ARG:N    | 1:J:135:PRO:CD   | 2.78                     | 0.46              |
| 2:K:500:HEM:HBB2 | 2:K:500:HEM:CMB  | 2.46                     | 0.46              |
| 2:O:500:HEM:HHD  | 2:O:500:HEM:HBC2 | 1.97                     | 0.46              |
| 1:B:127:PRO:N    | 1:B:128:PRO:HD2  | 2.30                     | 0.45              |
| 1:G:192:LEU:HD13 | 1:G:195:ARG:NH2  | 2.31                     | 0.45              |
| 1:I:215:TYR:OH   | 1:I:220:GLU:OE1  | 2.22                     | 0.45              |
| 1:L:223:TRP:HB3  | 1:L:295:LEU:HD12 | 1.97                     | 0.45              |
| 1:N:193:MET:O    | 1:N:198:PHE:HD1  | 1.98                     | 0.45              |
| 1:A:149:ARG:HD3  | 1:A:149:ARG:HA   | 1.59                     | 0.45              |
| 1:B:191:ARG:NH2  | 1:B:206:GLU:OE2  | 2.49                     | 0.45              |
| 1:E:261:VAL:HG12 | 1:E:277:VAL:CG2  | 2.46                     | 0.45              |
| 1:G:190:ILE:HG21 | 1:G:204:VAL:HG13 | 1.98                     | 0.45              |
| 1:J:247:GLU:O    | 1:J:251:ARG:HG3  | 2.16                     | 0.45              |
| 1:K:41:MET:O     | 1:L:139:ALA:HB3  | 2.16                     | 0.45              |
| 1:L:186:TYR:OH   | 1:L:291:GLU:HG2  | 2.17                     | 0.45              |
| 1:A:43:TYR:CE1   | 1:B:145:SER:HB2  | 2.51                     | 0.45              |
| 1:B:267:PHE:HE1  | 1:B:281:ARG:CD   | 2.29                     | 0.45              |
| 1:F:127:PRO:CD   | 1:F:128:PRO:HD2  | 2.46                     | 0.45              |
| 1:L:158:LYS:CG   | 1:L:180:LEU:HD12 | 2.47                     | 0.45              |
| 1:I:161:ALA:O    | 1:I:164:ARG:HG3  | 2.16                     | 0.45              |
| 1:J:257:HIS:HE1  | 2:J:500:HEM:C4D  | 2.34                     | 0.45              |
| 1:O:169:ARG:CD   | 1:O:171:GLU:OE2  | 2.55                     | 0.45              |
| 1:A:236:LEU:HA   | 1:A:236:LEU:HD23 | 1.87                     | 0.45              |
| 1:F:142:GLY:C    | 1:F:144:GLN:H    | 2.20                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:198:PHE:HA   | 3:F:552:HOH:O    | 2.17                     | 0.45              |
| 1:F:277:VAL:O    | 1:F:281:ARG:HG3  | 2.16                     | 0.45              |
| 1:G:148:TYR:CE1  | 1:G:250:PHE:CZ   | 3.04                     | 0.45              |
| 1:N:192:LEU:HD12 | 1:N:192:LEU:O    | 2.16                     | 0.45              |
| 1:P:83:LEU:O     | 1:P:87:ARG:HG3   | 2.17                     | 0.45              |
| 1:C:261:VAL:HG22 | 2:C:500:HEM:C1B  | 2.52                     | 0.45              |
| 1:E:119:TRP:CH2  | 1:E:257:HIS:HD2  | 2.35                     | 0.45              |
| 1:G:149:ARG:HA   | 1:G:149:ARG:HD3  | 1.70                     | 0.45              |
| 1:H:163:LEU:HD22 | 1:H:176:VAL:HG12 | 1.98                     | 0.45              |
| 1:L:292:LEU:HA   | 1:L:292:LEU:HD23 | 1.68                     | 0.45              |
| 1:A:274:THR:CG2  | 1:A:275:GLU:H    | 2.30                     | 0.45              |
| 1:E:260:THR:HA   | 1:E:263:ARG:HG2  | 1.99                     | 0.45              |
| 1:G:209:TRP:C    | 1:G:211:GLN:H    | 2.19                     | 0.45              |
| 1:G:77:LEU:HA    | 1:G:77:LEU:HD23  | 1.58                     | 0.45              |
| 1:J:201:ASP:O    | 1:J:205:VAL:HG23 | 2.17                     | 0.45              |
| 1:J:211:GLN:NE2  | 1:J:212:PRO:HD2  | 2.32                     | 0.45              |
| 1:K:79:MET:CE    | 1:K:148:TYR:HA   | 2.47                     | 0.45              |
| 1:B:90:ARG:HB2   | 1:B:185:MET:HE2  | 1.99                     | 0.45              |
| 1:B:186:TYR:HH   | 1:B:291:GLU:HG2  | 1.82                     | 0.45              |
| 1:D:260:THR:HA   | 1:D:263:ARG:HG2  | 1.99                     | 0.45              |
| 1:E:248:ASP:C    | 1:E:248:ASP:OD1  | 2.56                     | 0.45              |
| 1:F:78:TRP:HB2   | 1:F:115:LEU:HD21 | 1.99                     | 0.45              |
| 1:M:234:TRP:O    | 1:M:237:TYR:HB3  | 2.17                     | 0.45              |
| 1:P:164:ARG:CG   | 1:P:164:ARG:HH11 | 2.20                     | 0.45              |
| 1:D:59:LEU:HB3   | 1:D:136:TYR:HB3  | 1.98                     | 0.45              |
| 1:F:104:MET:O    | 1:F:108:VAL:HG23 | 2.17                     | 0.45              |
| 1:I:250:PHE:O    | 1:I:254:ARG:HD3  | 2.16                     | 0.45              |
| 1:M:52:ILE:HG22  | 1:M:53:LEU:HD13  | 1.98                     | 0.45              |
| 1:P:142:GLY:HA3  | 2:P:500:HEM:C2D  | 2.52                     | 0.45              |
| 1:B:230:PRO:HB3  | 1:B:237:TYR:CD2  | 2.53                     | 0.44              |
| 1:L:295:LEU:HD22 | 1:L:296:ARG:HD2  | 1.99                     | 0.44              |
| 1:A:122:LEU:HD21 | 2:A:500:HEM:CBB  | 2.48                     | 0.44              |
| 1:G:98:LEU:HD12  | 1:G:235:GLU:OE1  | 2.18                     | 0.44              |
| 1:J:226:VAL:HG13 | 1:J:233:HIS:HB2  | 1.98                     | 0.44              |
| 1:O:60:SER:CB    | 1:O:61:PRO:CD    | 2.95                     | 0.44              |
| 1:P:261:VAL:HG22 | 2:P:500:HEM:C1B  | 2.52                     | 0.44              |
| 1:B:296:ARG:HG2  | 1:B:296:ARG:H    | 1.68                     | 0.44              |
| 1:L:110:ARG:HA   | 1:L:110:ARG:HD3  | 1.84                     | 0.44              |
| 1:M:279:TYR:O    | 1:M:283:MET:HG2  | 2.17                     | 0.44              |
| 1:N:268:LYS:HB3  | 1:N:268:LYS:HE2  | 1.80                     | 0.44              |
| 1:O:149:ARG:HD2  | 1:O:162:MET:HB3  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:F:120:ASN:OD1    | 1:F:256:ARG:NH2  | 2.40                     | 0.44              |
| 1:F:200:ILE:CG2    | 1:F:204:VAL:HG23 | 2.47                     | 0.44              |
| 1:N:134:ARG:HB3    | 1:N:135:PRO:HD3  | 1.99                     | 0.44              |
| 1:A:146:TYR:HB3    | 1:A:166:HIS:CE1  | 2.52                     | 0.44              |
| 1:A:274:THR:HG23   | 1:A:279:TYR:HB2  | 1.97                     | 0.44              |
| 1:C:199:GLN:O      | 1:C:199:GLN:CG   | 2.42                     | 0.44              |
| 1:I:87:ARG:HD2     | 3:I:584:HOH:O    | 2.16                     | 0.44              |
| 1:L:82:MET:CE      | 1:L:115:LEU:CD1  | 2.95                     | 0.44              |
| 1:M:82:MET:HG3     | 1:M:111:ILE:HG21 | 1.99                     | 0.44              |
| 1:E:49:LEU:O       | 1:E:53:LEU:HB2   | 2.18                     | 0.44              |
| 1:F:85:GLU:OE2     | 1:F:107:ARG:NH1  | 2.43                     | 0.44              |
| 1:K:39:ARG:HH11    | 1:K:39:ARG:CA    | 2.31                     | 0.44              |
| 1:M:223:TRP:HB3    | 1:M:295:LEU:HD12 | 1.99                     | 0.44              |
| 1:O:280:LEU:HD21   | 2:O:500:HEM:HAA2 | 2.00                     | 0.44              |
| 1:P:107:ARG:O      | 1:P:111:ILE:HG13 | 2.16                     | 0.44              |
| 1:F:293:TRP:O      | 1:F:296:ARG:HG2  | 2.18                     | 0.44              |
| 1:H:56:GLN:O       | 1:H:58:PRO:HD3   | 2.17                     | 0.44              |
| 1:N:220:GLU:OE2    | 1:N:298:ASP:OD2  | 2.36                     | 0.44              |
| 1:O:223:TRP:CB     | 1:O:295:LEU:HD12 | 2.48                     | 0.44              |
| 1:D:270:GLY:HA2    | 1:F:45:ASP:HA    | 1.99                     | 0.44              |
| 1:P:122:LEU:HD21   | 2:P:500:HEM:CAB  | 2.48                     | 0.44              |
| 1:D:134:ARG:N      | 1:D:135:PRO:HD2  | 2.32                     | 0.44              |
| 1:F:134:ARG:N      | 1:F:135:PRO:CD   | 2.81                     | 0.44              |
| 1:M:163:LEU:CD2    | 1:M:176:VAL:HG12 | 2.48                     | 0.44              |
| 1:N:78:TRP:HB2     | 1:N:115:LEU:HD21 | 2.00                     | 0.44              |
| 1:O:117:GLN:HB3    | 1:O:117:GLN:HE21 | 1.71                     | 0.44              |
| 1:A:149:ARG:NE     | 1:A:162:MET:HE2  | 2.34                     | 0.43              |
| 1:C:190:ILE:HG21   | 1:C:204:VAL:HG13 | 2.00                     | 0.43              |
| 1:I:163:LEU:HD22   | 1:I:176:VAL:CG1  | 2.46                     | 0.43              |
| 1:I:274:THR:HG23   | 1:I:275:GLU:N    | 2.32                     | 0.43              |
| 1:I:268:LYS:HD2    | 1:L:297:THR:HA   | 1.99                     | 0.43              |
| 1:M:168:HIS:ND1    | 1:M:169:ARG:HG2  | 2.33                     | 0.43              |
| 1:D:186:TYR:OH     | 1:D:291:GLU:HG2  | 2.18                     | 0.43              |
| 1:I:131:SER:O      | 1:I:135:PRO:HD3  | 2.18                     | 0.43              |
| 1:I:47:LEU:HD13    | 1:J:72:HIS:HB3   | 2.00                     | 0.43              |
| 1:L:164:ARG:N      | 1:L:165:PRO:CD   | 2.81                     | 0.43              |
| 1:O:279:TYR:CD2    | 1:O:280:LEU:HD23 | 2.53                     | 0.43              |
| 1:E:224:LEU:HD22   | 1:E:228:ARG:CZ   | 2.48                     | 0.43              |
| 2:I:500:HEM:CMB    | 2:I:500:HEM:CBB  | 2.95                     | 0.43              |
| 1:D:97:GLN:O       | 1:D:100:PRO:HD2  | 2.18                     | 0.43              |
| 1:H:164[B]:ARG:HB3 | 1:H:165:PRO:HD3  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:75:THR:HG23  | 1:H:115:LEU:HD22 | 2.00                     | 0.43              |
| 1:M:144:GLN:HB2  | 1:N:43:TYR:HB3   | 1.99                     | 0.43              |
| 1:O:167:ALA:HA   | 1:O:173:LEU:CD2  | 2.48                     | 0.43              |
| 1:P:71:GLN:HG2   | 2:P:500:HEM:CMC  | 2.48                     | 0.43              |
| 1:A:142:GLY:HA2  | 1:B:43:TYR:CE2   | 2.54                     | 0.43              |
| 1:B:44:GLY:O     | 1:P:270:GLY:HA2  | 2.18                     | 0.43              |
| 1:I:281:ARG:O    | 1:I:284:LEU:HB2  | 2.19                     | 0.43              |
| 1:L:127:PRO:HB2  | 1:L:128:PRO:HD3  | 2.01                     | 0.43              |
| 1:L:216:ASN:OD1  | 1:L:218:SER:HB3  | 2.18                     | 0.43              |
| 1:D:224:LEU:O    | 1:D:228:ARG:HG3  | 2.19                     | 0.43              |
| 1:G:205:VAL:HG12 | 1:G:205:VAL:O    | 2.18                     | 0.43              |
| 1:I:211:GLN:O    | 1:I:212:PRO:C    | 2.56                     | 0.43              |
| 1:I:292:LEU:O    | 1:I:295:LEU:HD13 | 2.19                     | 0.43              |
| 1:K:79:MET:HE2   | 1:K:148:TYR:HA   | 2.01                     | 0.43              |
| 1:A:203:GLU:HG2  | 3:A:573:HOH:O    | 2.18                     | 0.43              |
| 1:D:143:PHE:HE2  | 1:D:279:TYR:CZ   | 2.37                     | 0.43              |
| 1:F:269:ARG:HE   | 1:F:269:ARG:HB2  | 1.61                     | 0.43              |
| 2:G:500:HEM:HHD  | 2:G:500:HEM:CBC  | 2.49                     | 0.43              |
| 1:H:219:VAL:HB   | 1:H:291:GLU:HG3  | 1.99                     | 0.43              |
| 1:I:266:GLY:O    | 1:I:277:VAL:HG21 | 2.19                     | 0.43              |
| 1:M:163:LEU:HD22 | 1:M:176:VAL:HG12 | 2.01                     | 0.43              |
| 1:N:258:VAL:HG21 | 1:N:281:ARG:HG3  | 2.01                     | 0.43              |
| 1:O:169:ARG:HH21 | 1:O:172:HIS:HE1  | 1.65                     | 0.43              |
| 1:A:119:TRP:CH2  | 1:A:257:HIS:CD2  | 3.05                     | 0.43              |
| 1:A:77:LEU:HD23  | 1:A:77:LEU:HA    | 1.88                     | 0.43              |
| 1:C:280:LEU:HA   | 1:C:280:LEU:HD23 | 1.69                     | 0.43              |
| 1:E:141:SER:OG   | 1:E:143:PHE:HB2  | 2.18                     | 0.43              |
| 1:I:151:ILE:O    | 1:I:154:ILE:HG22 | 2.18                     | 0.43              |
| 1:I:168:HIS:HD2  | 3:I:551:HOH:O    | 2.01                     | 0.43              |
| 1:K:105:LEU:HA   | 1:K:105:LEU:HD23 | 1.90                     | 0.43              |
| 1:K:79:MET:HE2   | 1:K:151:ILE:HD12 | 2.00                     | 0.43              |
| 1:A:122:LEU:HD23 | 1:A:260:THR:HG21 | 2.00                     | 0.43              |
| 1:A:164:ARG:C    | 1:A:166:HIS:H    | 2.22                     | 0.43              |
| 1:A:282:ARG:O    | 1:A:285:ASP:HB2  | 2.19                     | 0.43              |
| 1:C:288:LEU:C    | 1:C:290:PRO:HD3  | 2.39                     | 0.43              |
| 1:A:134:ARG:NH2  | 1:A:269:ARG:O    | 2.51                     | 0.43              |
| 1:D:134:ARG:HB3  | 1:D:135:PRO:CD   | 2.49                     | 0.43              |
| 1:D:272:GLY:HA3  | 1:E:57:HIS:CD2   | 2.54                     | 0.43              |
| 1:I:257:HIS:O    | 1:I:261:VAL:HG23 | 2.18                     | 0.43              |
| 1:P:130:TYR:O    | 1:P:133:MET:HG2  | 2.18                     | 0.43              |
| 1:A:164:ARG:C    | 1:A:166:HIS:N    | 2.72                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:49:LEU:O     | 1:A:53:LEU:HB2   | 2.19                     | 0.42              |
| 1:E:280:LEU:HD11 | 2:E:500:HEM:C3A  | 2.54                     | 0.42              |
| 1:F:141:SER:O    | 1:F:144:GLN:HB2  | 2.18                     | 0.42              |
| 1:G:192:LEU:HD13 | 1:G:195:ARG:HH21 | 1.84                     | 0.42              |
| 1:I:149:ARG:CZ   | 1:I:162:MET:HE2  | 2.48                     | 0.42              |
| 1:J:41:MET:HA    | 3:J:538:HOH:O    | 2.18                     | 0.42              |
| 2:L:500:HEM:CHD  | 2:L:500:HEM:HBC2 | 2.47                     | 0.42              |
| 1:A:83:LEU:O     | 1:A:87:ARG:HG3   | 2.19                     | 0.42              |
| 1:A:50:ASP:OD1   | 1:B:169:ARG:NH2  | 2.52                     | 0.42              |
| 1:D:89:ALA:CB    | 1:D:185:MET:HE2  | 2.49                     | 0.42              |
| 1:E:43:TYR:HA    | 1:F:140:SER:HB2  | 2.00                     | 0.42              |
| 1:G:280:LEU:HD23 | 1:G:280:LEU:HA   | 1.85                     | 0.42              |
| 1:M:95:SER:O     | 1:M:97:GLN:HG3   | 2.19                     | 0.42              |
| 1:P:109:SER:HB3  | 1:P:110:ARG:NH2  | 2.34                     | 0.42              |
| 1:B:94:LYS:NZ    | 3:B:526:HOH:O    | 2.46                     | 0.42              |
| 1:G:164:ARG:N    | 1:G:165:PRO:HD2  | 2.34                     | 0.42              |
| 1:I:146:TYR:O    | 1:I:150:GLU:HG3  | 2.18                     | 0.42              |
| 1:K:227:TYR:CD2  | 1:K:295:LEU:HD11 | 2.54                     | 0.42              |
| 1:E:215:TYR:OH   | 1:E:220:GLU:OE1  | 2.28                     | 0.42              |
| 1:F:83:LEU:HD23  | 1:F:83:LEU:HA    | 1.72                     | 0.42              |
| 1:G:110:ARG:HH11 | 1:G:110:ARG:HG2  | 1.84                     | 0.42              |
| 1:F:162:MET:HE2  | 3:F:501:HOH:O    | 2.19                     | 0.42              |
| 1:H:292:LEU:O    | 1:H:296:ARG:NH1  | 2.51                     | 0.42              |
| 1:P:127:PRO:HB2  | 1:P:128:PRO:HD3  | 2.01                     | 0.42              |
| 1:C:162:MET:O    | 1:C:165:PRO:HD2  | 2.20                     | 0.42              |
| 1:F:164:ARG:N    | 1:F:165:PRO:CD   | 2.83                     | 0.42              |
| 1:G:224:LEU:HD21 | 1:G:299:LEU:HA   | 2.01                     | 0.42              |
| 3:A:588:HOH:O    | 1:M:294:LYS:HE2  | 2.20                     | 0.42              |
| 1:A:115:LEU:HD23 | 1:A:115:LEU:HA   | 1.63                     | 0.42              |
| 1:C:132:ALA:HB1  | 3:C:587:HOH:O    | 2.18                     | 0.42              |
| 1:D:59:LEU:HD23  | 1:D:136:TYR:O    | 2.18                     | 0.42              |
| 1:G:168:HIS:CD2  | 1:G:168:HIS:H    | 2.38                     | 0.42              |
| 1:F:297:THR:HG23 | 1:G:266:GLY:HA3  | 2.00                     | 0.42              |
| 1:G:103:LYS:NZ   | 1:H:124:THR:O    | 2.43                     | 0.42              |
| 1:H:275:GLU:N    | 1:H:279:TYR:HB2  | 2.34                     | 0.42              |
| 1:I:144:GLN:HB2  | 1:J:43:TYR:HB3   | 2.02                     | 0.42              |
| 1:K:252:GLN:O    | 1:K:256:ARG:HB2  | 2.18                     | 0.42              |
| 1:K:278:SER:CB   | 3:K:513:HOH:O    | 2.48                     | 0.42              |
| 1:K:78:TRP:HB2   | 1:K:115:LEU:HD21 | 2.00                     | 0.42              |
| 1:A:251:ARG:HG2  | 3:A:525:HOH:O    | 2.19                     | 0.42              |
| 1:G:200:ILE:HG22 | 1:G:204:VAL:HG12 | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:290:PRO:HD2  | 1:G:291:GLU:OE1  | 2.20                     | 0.42              |
| 1:I:98:LEU:HD12  | 1:I:235:GLU:HB3  | 2.02                     | 0.42              |
| 1:K:59:LEU:HD23  | 1:K:136:TYR:O    | 2.20                     | 0.42              |
| 1:N:163:LEU:HD22 | 1:N:176:VAL:CG1  | 2.48                     | 0.42              |
| 1:N:269:ARG:CB   | 1:N:269:ARG:NH1  | 2.69                     | 0.42              |
| 1:A:68:PHE:HE1   | 2:A:500:HEM:CAB  | 2.31                     | 0.42              |
| 1:J:164:ARG:HG2  | 1:J:165:PRO:HD3  | 2.02                     | 0.42              |
| 1:N:111:ILE:O    | 1:N:114:GLN:HB2  | 2.20                     | 0.42              |
| 1:O:89:ALA:CB    | 1:O:185:MET:CE   | 2.89                     | 0.42              |
| 1:B:220:GLU:OE2  | 1:B:298:ASP:OD2  | 2.38                     | 0.42              |
| 1:F:69:ILE:O     | 1:F:73:GLN:HG3   | 2.20                     | 0.42              |
| 1:I:110:ARG:HH12 | 1:K:110:ARG:CZ   | 2.33                     | 0.42              |
| 1:I:149:ARG:NH1  | 1:I:152:GLU:OE2  | 2.52                     | 0.42              |
| 1:I:158:LYS:NZ   | 1:I:182:THR:O    | 2.29                     | 0.42              |
| 1:A:75:THR:O     | 1:A:79:MET:HG3   | 2.20                     | 0.41              |
| 1:B:90:ARG:HD2   | 3:B:556:HOH:O    | 2.19                     | 0.41              |
| 1:D:170:PRO:HB2  | 3:D:600:HOH:O    | 2.20                     | 0.41              |
| 1:D:186:TYR:HH   | 1:D:291:GLU:HG2  | 1.84                     | 0.41              |
| 3:A:507:HOH:O    | 1:D:256:ARG:CD   | 2.60                     | 0.41              |
| 1:G:215:TYR:OH   | 1:G:220:GLU:OE1  | 2.23                     | 0.41              |
| 1:I:282:ARG:O    | 1:I:285:ASP:HB2  | 2.20                     | 0.41              |
| 1:I:103:LYS:NZ   | 1:J:129:GLU:OE2  | 2.52                     | 0.41              |
| 1:J:99:GLN:HB2   | 1:J:100:PRO:HD3  | 2.02                     | 0.41              |
| 1:J:99:GLN:HB3   | 1:L:234:TRP:NE1  | 2.35                     | 0.41              |
| 1:K:267:PHE:HE1  | 1:K:281:ARG:HE   | 1.66                     | 0.41              |
| 1:M:65:GLU:HG3   | 1:M:133:MET:HE1  | 2.02                     | 0.41              |
| 1:P:162:MET:HA   | 1:P:162:MET:HE3  | 2.01                     | 0.41              |
| 1:C:155:LEU:HD23 | 1:C:155:LEU:HA   | 1.90                     | 0.41              |
| 1:G:192:LEU:O    | 1:G:196:ARG:HG3  | 2.20                     | 0.41              |
| 1:I:292:LEU:HA   | 1:I:295:LEU:CD1  | 2.50                     | 0.41              |
| 1:I:292:LEU:HA   | 1:I:295:LEU:HD12 | 2.02                     | 0.41              |
| 1:M:146:TYR:HB3  | 1:M:166:HIS:CD2  | 2.54                     | 0.41              |
| 1:D:274:THR:HB   | 1:E:57:HIS:HB3   | 2.01                     | 0.41              |
| 1:F:223:TRP:HB3  | 1:F:295:LEU:HD12 | 2.02                     | 0.41              |
| 1:H:220:GLU:HB2  | 1:H:291:GLU:HB2  | 2.03                     | 0.41              |
| 1:H:269:ARG:HH22 | 1:J:39:ARG:HH21  | 1.68                     | 0.41              |
| 1:K:219:VAL:CG1  | 1:K:291:GLU:HG3  | 2.49                     | 0.41              |
| 1:L:82:MET:HE2   | 1:L:82:MET:HB2   | 1.74                     | 0.41              |
| 1:O:60:SER:HB2   | 1:O:61:PRO:HD2   | 2.01                     | 0.41              |
| 1:A:44:GLY:HA2   | 1:A:49:LEU:HD12  | 2.02                     | 0.41              |
| 1:C:163:LEU:CD2  | 1:C:176:VAL:HG12 | 2.42                     | 0.41              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:H:69:ILE:O       | 1:H:73:GLN:HG3   | 2.21                     | 0.41              |
| 1:L:295:LEU:CD2    | 1:L:296:ARG:HD2  | 2.50                     | 0.41              |
| 1:K:46:TYR:CE1     | 1:L:59:LEU:HD22  | 2.55                     | 0.41              |
| 1:N:158[B]:LYS:HE3 | 1:N:184:SER:HB3  | 2.02                     | 0.41              |
| 1:J:192:LEU:O      | 1:J:192:LEU:HG   | 2.20                     | 0.41              |
| 1:N:127:PRO:N      | 1:N:128:PRO:HD2  | 2.35                     | 0.41              |
| 1:C:105:LEU:HA     | 1:C:105:LEU:HD23 | 1.76                     | 0.41              |
| 1:F:164:ARG:HB2    | 1:F:165:PRO:CD   | 2.51                     | 0.41              |
| 1:G:219:VAL:HG11   | 1:G:291:GLU:HG3  | 2.00                     | 0.41              |
| 1:J:154:ILE:HG12   | 1:J:154:ILE:H    | 1.77                     | 0.41              |
| 1:L:158:LYS:HD3    | 3:L:516:HOH:O    | 2.20                     | 0.41              |
| 1:L:215:TYR:HE1    | 1:L:220:GLU:OE1  | 2.04                     | 0.41              |
| 1:M:112:MET:O      | 1:M:116:VAL:HG23 | 2.21                     | 0.41              |
| 1:P:104:MET:O      | 1:P:108:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:73:GLN:NE2     | 1:B:47:LEU:O     | 2.43                     | 0.41              |
| 1:F:257:HIS:CE1    | 2:F:500:HEM:C4D  | 3.01                     | 0.41              |
| 1:H:294:LYS:HE2    | 3:H:604:HOH:O    | 2.21                     | 0.41              |
| 1:K:260:THR:HA     | 1:K:263:ARG:HG2  | 2.03                     | 0.41              |
| 1:L:149:ARG:HD3    | 1:L:149:ARG:HA   | 1.69                     | 0.41              |
| 1:M:103:LYS:NZ     | 1:N:124:THR:O    | 2.54                     | 0.41              |
| 1:N:98:LEU:HD12    | 1:N:235:GLU:OE1  | 2.20                     | 0.41              |
| 1:P:60:SER:HB2     | 1:P:61:PRO:HD2   | 2.03                     | 0.41              |
| 1:A:185:MET:HB2    | 1:A:185:MET:HE2  | 1.93                     | 0.41              |
| 1:B:295:LEU:HD22   | 1:B:295:LEU:C    | 2.41                     | 0.41              |
| 1:D:268:LYS:HG3    | 1:D:271:THR:HG21 | 2.02                     | 0.41              |
| 1:E:168:HIS:H      | 1:E:168:HIS:CD2  | 2.39                     | 0.41              |
| 1:E:188:GLU:OE2    | 1:E:188:GLU:HA   | 2.21                     | 0.41              |
| 1:F:280:LEU:HD21   | 2:F:500:HEM:CHA  | 2.51                     | 0.41              |
| 1:H:119:TRP:CD1    | 1:H:256:ARG:HB3  | 2.56                     | 0.41              |
| 1:I:119:TRP:CH2    | 1:I:257:HIS:CD2  | 3.09                     | 0.41              |
| 1:I:83:LEU:HD23    | 1:I:83:LEU:HA    | 1.77                     | 0.41              |
| 1:L:53:LEU:HD12    | 1:L:53:LEU:HA    | 1.90                     | 0.41              |
| 1:A:215:TYR:OH     | 1:A:220:GLU:OE1  | 2.28                     | 0.41              |
| 1:C:133:MET:HB2    | 1:C:133:MET:HE2  | 1.79                     | 0.41              |
| 1:C:261:VAL:HG22   | 2:C:500:HEM:C2B  | 2.55                     | 0.41              |
| 1:E:292:LEU:HA     | 1:E:295:LEU:HD23 | 2.03                     | 0.41              |
| 1:H:134:ARG:N      | 1:H:135:PRO:HD2  | 2.36                     | 0.41              |
| 1:M:268:LYS:H      | 1:M:268:LYS:HG2  | 1.55                     | 0.41              |
| 1:B:200:ILE:HG22   | 1:B:204:VAL:HG12 | 2.03                     | 0.41              |
| 1:F:152:GLU:CD     | 1:F:254:ARG:HH12 | 2.24                     | 0.41              |
| 1:G:295:LEU:HD22   | 1:G:296:ARG:HH11 | 1.84                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:86:LEU:O     | 1:H:185:MET:CE   | 2.69                     | 0.41              |
| 1:P:208:ASP:OD1  | 1:P:210:THR:HB   | 2.21                     | 0.41              |
| 1:B:108:VAL:HA   | 1:B:111:ILE:HD12 | 2.03                     | 0.40              |
| 1:B:134:ARG:N    | 1:B:135:PRO:CD   | 2.83                     | 0.40              |
| 1:C:187:ASP:O    | 1:C:191:ARG:HG3  | 2.21                     | 0.40              |
| 1:D:86:LEU:O     | 1:D:185:MET:HE3  | 2.21                     | 0.40              |
| 1:I:110:ARG:HE   | 1:I:110:ARG:N    | 2.19                     | 0.40              |
| 1:J:111:ILE:O    | 1:J:114:GLN:HB2  | 2.21                     | 0.40              |
| 1:L:228:ARG:C    | 1:L:230:PRO:HD3  | 2.42                     | 0.40              |
| 1:O:93:VAL:O     | 1:O:192:LEU:HD13 | 2.21                     | 0.40              |
| 1:J:186:TYR:OH   | 1:J:291:GLU:CG   | 2.69                     | 0.40              |
| 1:J:186:TYR:O    | 1:J:190:ILE:HG13 | 2.20                     | 0.40              |
| 1:M:130:TYR:CE1  | 1:M:265:ILE:HG22 | 2.56                     | 0.40              |
| 1:N:169:ARG:HB3  | 1:N:169:ARG:HE   | 1.77                     | 0.40              |
| 1:A:228:ARG:C    | 1:A:230:PRO:HD3  | 2.42                     | 0.40              |
| 1:B:296:ARG:HD2  | 1:C:263:ARG:O    | 2.22                     | 0.40              |
| 1:C:291:GLU:O    | 1:C:295:LEU:HB3  | 2.22                     | 0.40              |
| 1:E:261:VAL:HG12 | 1:E:277:VAL:HG22 | 2.03                     | 0.40              |
| 1:H:220:GLU:HB2  | 1:H:291:GLU:CB   | 2.51                     | 0.40              |
| 1:J:223:TRP:HB3  | 1:J:295:LEU:HD12 | 2.04                     | 0.40              |
| 1:K:79:MET:HE1   | 1:K:148:TYR:CD1  | 2.52                     | 0.40              |
| 1:L:133:MET:HG3  | 1:L:137:LEU:HD11 | 2.02                     | 0.40              |
| 1:L:211:GLN:HG3  | 1:L:212:PRO:CD   | 2.51                     | 0.40              |
| 1:O:164:ARG:N    | 1:O:165:PRO:CD   | 2.85                     | 0.40              |
| 1:P:65:GLU:CG    | 1:P:133:MET:HE1  | 2.49                     | 0.40              |
| 1:B:224:LEU:HG   | 1:B:295:LEU:HB2  | 2.04                     | 0.40              |
| 1:F:142:GLY:C    | 1:F:144:GLN:N    | 2.74                     | 0.40              |
| 1:G:43:TYR:CE2   | 1:H:142:GLY:HA2  | 2.56                     | 0.40              |
| 1:L:77:LEU:HD23  | 1:L:77:LEU:HA    | 1.87                     | 0.40              |
| 1:M:77:LEU:HD23  | 1:N:70:VAL:HG22  | 2.03                     | 0.40              |
| 1:B:299:LEU:HD22 | 1:C:127:PRO:HB2  | 2.02                     | 0.40              |
| 1:D:191:ARG:HG2  | 1:D:205:VAL:HG13 | 2.03                     | 0.40              |
| 1:E:242:LYS:HD2  | 3:E:563:HOH:O    | 2.21                     | 0.40              |
| 1:F:260:THR:HA   | 1:F:263:ARG:HG2  | 2.04                     | 0.40              |
| 1:F:267:PHE:CD2  | 1:F:268:LYS:N    | 2.86                     | 0.40              |
| 1:G:271:THR:HG23 | 3:G:554:HOH:O    | 2.22                     | 0.40              |
| 1:K:207:ARG:NH1  | 1:K:207:ARG:CG   | 2.78                     | 0.40              |
| 1:L:172:HIS:HA   | 1:L:175:LEU:HD12 | 2.02                     | 0.40              |
| 1:N:282:ARG:HG3  | 1:N:283:MET:CE   | 2.51                     | 0.40              |
| 1:O:59:LEU:HD22  | 1:P:46:TYR:HD1   | 1.86                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 260/281 (92%)   | 254 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 1   | B     | 262/281 (93%)   | 254 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 1   | C     | 251/281 (89%)   | 244 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 1   | D     | 257/281 (92%)   | 248 (96%)  | 8 (3%)   | 1 (0%)   | 34          | 48  |
| 1   | E     | 252/281 (90%)   | 241 (96%)  | 9 (4%)   | 2 (1%)   | 19          | 29  |
| 1   | F     | 256/281 (91%)   | 249 (97%)  | 6 (2%)   | 1 (0%)   | 34          | 48  |
| 1   | G     | 255/281 (91%)   | 242 (95%)  | 12 (5%)  | 1 (0%)   | 34          | 48  |
| 1   | H     | 259/281 (92%)   | 254 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | I     | 257/281 (92%)   | 249 (97%)  | 7 (3%)   | 1 (0%)   | 34          | 48  |
| 1   | J     | 253/281 (90%)   | 244 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 1   | K     | 252/281 (90%)   | 246 (98%)  | 5 (2%)   | 1 (0%)   | 34          | 48  |
| 1   | L     | 258/281 (92%)   | 250 (97%)  | 6 (2%)   | 2 (1%)   | 19          | 29  |
| 1   | M     | 252/281 (90%)   | 244 (97%)  | 7 (3%)   | 1 (0%)   | 34          | 48  |
| 1   | N     | 259/281 (92%)   | 250 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 1   | O     | 253/281 (90%)   | 238 (94%)  | 15 (6%)  | 0        | 100         | 100 |
| 1   | P     | 257/281 (92%)   | 249 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| All | All   | 4093/4496 (91%) | 3956 (97%) | 127 (3%) | 10 (0%)  | 47          | 62  |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 140 | SER  |
| 1   | E     | 268 | LYS  |
| 1   | I     | 212 | PRO  |
| 1   | M     | 268 | LYS  |
| 1   | E     | 141 | SER  |
| 1   | L     | 139 | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 140 | SER  |
| 1   | L     | 209 | TRP  |
| 1   | K     | 212 | PRO  |
| 1   | G     | 273 | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 229/240 (95%)   | 217 (95%)  | 12 (5%)  | 23          | 38 |
| 1   | B     | 230/240 (96%)   | 214 (93%)  | 16 (7%)  | 15          | 24 |
| 1   | C     | 224/240 (93%)   | 210 (94%)  | 14 (6%)  | 18          | 28 |
| 1   | D     | 226/240 (94%)   | 211 (93%)  | 15 (7%)  | 16          | 26 |
| 1   | E     | 226/240 (94%)   | 212 (94%)  | 14 (6%)  | 18          | 29 |
| 1   | F     | 228/240 (95%)   | 213 (93%)  | 15 (7%)  | 16          | 26 |
| 1   | G     | 227/240 (95%)   | 213 (94%)  | 14 (6%)  | 18          | 29 |
| 1   | H     | 228/240 (95%)   | 214 (94%)  | 14 (6%)  | 18          | 30 |
| 1   | I     | 226/240 (94%)   | 213 (94%)  | 13 (6%)  | 20          | 32 |
| 1   | J     | 226/240 (94%)   | 209 (92%)  | 17 (8%)  | 13          | 21 |
| 1   | K     | 226/240 (94%)   | 213 (94%)  | 13 (6%)  | 20          | 32 |
| 1   | L     | 227/240 (95%)   | 215 (95%)  | 12 (5%)  | 22          | 37 |
| 1   | M     | 223/240 (93%)   | 204 (92%)  | 19 (8%)  | 10          | 16 |
| 1   | N     | 228/240 (95%)   | 213 (93%)  | 15 (7%)  | 16          | 26 |
| 1   | O     | 226/240 (94%)   | 207 (92%)  | 19 (8%)  | 11          | 16 |
| 1   | P     | 226/240 (94%)   | 213 (94%)  | 13 (6%)  | 20          | 32 |
| All | All   | 3626/3840 (94%) | 3391 (94%) | 235 (6%) | 17          | 27 |

All (235) residues with a non-rotameric sidechain are listed below:



| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 53  | LEU  |
| 1   | A     | 59  | LEU  |
| 1   | A     | 96  | ASP  |
| 1   | A     | 97  | GLN  |
| 1   | A     | 149 | ARG  |
| 1   | A     | 164 | ARG  |
| 1   | A     | 193 | MET  |
| 1   | A     | 204 | VAL  |
| 1   | A     | 246 | LEU  |
| 1   | A     | 275 | GLU  |
| 1   | A     | 281 | ARG  |
| 1   | A     | 295 | LEU  |
| 1   | B     | 50  | ASP  |
| 1   | B     | 53  | LEU  |
| 1   | B     | 59  | LEU  |
| 1   | B     | 117 | GLN  |
| 1   | B     | 131 | SER  |
| 1   | B     | 133 | MET  |
| 1   | B     | 169 | ARG  |
| 1   | B     | 204 | VAL  |
| 1   | B     | 211 | GLN  |
| 1   | B     | 242 | LYS  |
| 1   | B     | 250 | PHE  |
| 1   | B     | 258 | VAL  |
| 1   | B     | 267 | PHE  |
| 1   | B     | 294 | LYS  |
| 1   | B     | 295 | LEU  |
| 1   | B     | 296 | ARG  |
| 1   | C     | 53  | LEU  |
| 1   | C     | 59  | LEU  |
| 1   | C     | 61  | PRO  |
| 1   | C     | 96  | ASP  |
| 1   | C     | 143 | PHE  |
| 1   | C     | 164 | ARG  |
| 1   | C     | 199 | GLN  |
| 1   | C     | 210 | THR  |
| 1   | C     | 214 | GLN  |
| 1   | C     | 250 | PHE  |
| 1   | C     | 254 | ARG  |
| 1   | C     | 275 | GLU  |
| 1   | C     | 281 | ARG  |
| 1   | C     | 295 | LEU  |
| 1   | D     | 53  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 59  | LEU  |
| 1   | D     | 82  | MET  |
| 1   | D     | 125 | MET  |
| 1   | D     | 143 | PHE  |
| 1   | D     | 185 | MET  |
| 1   | D     | 192 | LEU  |
| 1   | D     | 200 | ILE  |
| 1   | D     | 250 | PHE  |
| 1   | D     | 267 | PHE  |
| 1   | D     | 268 | LYS  |
| 1   | D     | 274 | THR  |
| 1   | D     | 278 | SER  |
| 1   | D     | 294 | LYS  |
| 1   | D     | 295 | LEU  |
| 1   | E     | 53  | LEU  |
| 1   | E     | 59  | LEU  |
| 1   | E     | 94  | LYS  |
| 1   | E     | 96  | ASP  |
| 1   | E     | 137 | LEU  |
| 1   | E     | 143 | PHE  |
| 1   | E     | 199 | GLN  |
| 1   | E     | 204 | VAL  |
| 1   | E     | 231 | SER  |
| 1   | E     | 250 | PHE  |
| 1   | E     | 267 | PHE  |
| 1   | E     | 275 | GLU  |
| 1   | E     | 281 | ARG  |
| 1   | E     | 294 | LYS  |
| 1   | F     | 40  | ASP  |
| 1   | F     | 53  | LEU  |
| 1   | F     | 59  | LEU  |
| 1   | F     | 109 | SER  |
| 1   | F     | 158 | LYS  |
| 1   | F     | 203 | GLU  |
| 1   | F     | 204 | VAL  |
| 1   | F     | 231 | SER  |
| 1   | F     | 246 | LEU  |
| 1   | F     | 250 | PHE  |
| 1   | F     | 254 | ARG  |
| 1   | F     | 267 | PHE  |
| 1   | F     | 269 | ARG  |
| 1   | F     | 295 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 296 | ARG  |
| 1   | G     | 53  | LEU  |
| 1   | G     | 134 | ARG  |
| 1   | G     | 158 | LYS  |
| 1   | G     | 182 | THR  |
| 1   | G     | 204 | VAL  |
| 1   | G     | 213 | THR  |
| 1   | G     | 224 | LEU  |
| 1   | G     | 225 | GLU  |
| 1   | G     | 250 | PHE  |
| 1   | G     | 267 | PHE  |
| 1   | G     | 271 | THR  |
| 1   | G     | 281 | ARG  |
| 1   | G     | 283 | MET  |
| 1   | G     | 294 | LYS  |
| 1   | H     | 50  | ASP  |
| 1   | H     | 53  | LEU  |
| 1   | H     | 59  | LEU  |
| 1   | H     | 184 | SER  |
| 1   | H     | 204 | VAL  |
| 1   | H     | 242 | LYS  |
| 1   | H     | 250 | PHE  |
| 1   | H     | 275 | GLU  |
| 1   | H     | 278 | SER  |
| 1   | H     | 281 | ARG  |
| 1   | H     | 291 | GLU  |
| 1   | H     | 294 | LYS  |
| 1   | H     | 295 | LEU  |
| 1   | H     | 297 | THR  |
| 1   | I     | 53  | LEU  |
| 1   | I     | 59  | LEU  |
| 1   | I     | 110 | ARG  |
| 1   | I     | 163 | LEU  |
| 1   | I     | 207 | ARG  |
| 1   | I     | 210 | THR  |
| 1   | I     | 225 | GLU  |
| 1   | I     | 229 | ASN  |
| 1   | I     | 254 | ARG  |
| 1   | I     | 256 | ARG  |
| 1   | I     | 274 | THR  |
| 1   | I     | 291 | GLU  |
| 1   | I     | 295 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 40  | ASP  |
| 1   | J     | 50  | ASP  |
| 1   | J     | 53  | LEU  |
| 1   | J     | 59  | LEU  |
| 1   | J     | 140 | SER  |
| 1   | J     | 154 | ILE  |
| 1   | J     | 158 | LYS  |
| 1   | J     | 164 | ARG  |
| 1   | J     | 174 | GLU  |
| 1   | J     | 178 | THR  |
| 1   | J     | 204 | VAL  |
| 1   | J     | 246 | LEU  |
| 1   | J     | 250 | PHE  |
| 1   | J     | 258 | VAL  |
| 1   | J     | 265 | ILE  |
| 1   | J     | 291 | GLU  |
| 1   | J     | 295 | LEU  |
| 1   | K     | 39  | ARG  |
| 1   | K     | 53  | LEU  |
| 1   | K     | 59  | LEU  |
| 1   | K     | 87  | ARG  |
| 1   | K     | 96  | ASP  |
| 1   | K     | 207 | ARG  |
| 1   | K     | 250 | PHE  |
| 1   | K     | 254 | ARG  |
| 1   | K     | 258 | VAL  |
| 1   | K     | 274 | THR  |
| 1   | K     | 281 | ARG  |
| 1   | K     | 294 | LYS  |
| 1   | K     | 295 | LEU  |
| 1   | L     | 53  | LEU  |
| 1   | L     | 59  | LEU  |
| 1   | L     | 158 | LYS  |
| 1   | L     | 204 | VAL  |
| 1   | L     | 231 | SER  |
| 1   | L     | 246 | LEU  |
| 1   | L     | 250 | PHE  |
| 1   | L     | 267 | PHE  |
| 1   | L     | 274 | THR  |
| 1   | L     | 275 | GLU  |
| 1   | L     | 295 | LEU  |
| 1   | L     | 297 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 53  | LEU  |
| 1   | M     | 59  | LEU  |
| 1   | M     | 60  | SER  |
| 1   | M     | 77  | LEU  |
| 1   | M     | 109 | SER  |
| 1   | M     | 110 | ARG  |
| 1   | M     | 117 | GLN  |
| 1   | M     | 134 | ARG  |
| 1   | M     | 137 | LEU  |
| 1   | M     | 143 | PHE  |
| 1   | M     | 174 | GLU  |
| 1   | M     | 204 | VAL  |
| 1   | M     | 250 | PHE  |
| 1   | M     | 265 | ILE  |
| 1   | M     | 267 | PHE  |
| 1   | M     | 268 | LYS  |
| 1   | M     | 291 | GLU  |
| 1   | M     | 294 | LYS  |
| 1   | M     | 295 | LEU  |
| 1   | N     | 50  | ASP  |
| 1   | N     | 53  | LEU  |
| 1   | N     | 59  | LEU  |
| 1   | N     | 96  | ASP  |
| 1   | N     | 110 | ARG  |
| 1   | N     | 117 | GLN  |
| 1   | N     | 134 | ARG  |
| 1   | N     | 163 | LEU  |
| 1   | N     | 199 | GLN  |
| 1   | N     | 245 | ASP  |
| 1   | N     | 250 | PHE  |
| 1   | N     | 265 | ILE  |
| 1   | N     | 267 | PHE  |
| 1   | N     | 269 | ARG  |
| 1   | N     | 295 | LEU  |
| 1   | O     | 49  | LEU  |
| 1   | O     | 53  | LEU  |
| 1   | O     | 59  | LEU  |
| 1   | O     | 96  | ASP  |
| 1   | O     | 117 | GLN  |
| 1   | O     | 158 | LYS  |
| 1   | O     | 164 | ARG  |
| 1   | O     | 173 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 178 | THR  |
| 1   | O     | 182 | THR  |
| 1   | O     | 185 | MET  |
| 1   | O     | 204 | VAL  |
| 1   | O     | 207 | ARG  |
| 1   | O     | 250 | PHE  |
| 1   | O     | 267 | PHE  |
| 1   | O     | 268 | LYS  |
| 1   | O     | 291 | GLU  |
| 1   | O     | 295 | LEU  |
| 1   | O     | 296 | ARG  |
| 1   | P     | 53  | LEU  |
| 1   | P     | 59  | LEU  |
| 1   | P     | 87  | ARG  |
| 1   | P     | 96  | ASP  |
| 1   | P     | 109 | SER  |
| 1   | P     | 131 | SER  |
| 1   | P     | 141 | SER  |
| 1   | P     | 164 | ARG  |
| 1   | P     | 177 | GLU  |
| 1   | P     | 203 | GLU  |
| 1   | P     | 204 | VAL  |
| 1   | P     | 233 | HIS  |
| 1   | P     | 275 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 168 | HIS  |
| 1   | A     | 252 | GLN  |
| 1   | B     | 31  | HIS  |
| 1   | B     | 34  | GLN  |
| 1   | C     | 214 | GLN  |
| 1   | C     | 252 | GLN  |
| 1   | D     | 252 | GLN  |
| 1   | E     | 172 | HIS  |
| 1   | E     | 211 | GLN  |
| 1   | E     | 252 | GLN  |
| 1   | G     | 166 | HIS  |
| 1   | G     | 181 | HIS  |
| 1   | J     | 51  | GLN  |
| 1   | J     | 211 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 144 | GLN  |
| 1   | K     | 252 | GLN  |
| 1   | L     | 51  | GLN  |
| 1   | L     | 114 | GLN  |
| 1   | M     | 252 | GLN  |
| 1   | N     | 181 | HIS  |
| 1   | O     | 172 | HIS  |
| 1   | O     | 181 | HIS  |
| 1   | P     | 233 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | HEM  | I     | 500 | 1    | 27,50,50     | 2.19 | 7 (25%)     | 17,82,82    | 1.70 | 5 (29%)     |
| 2   | HEM  | J     | 500 | 1    | 27,50,50     | 2.37 | 6 (22%)     | 17,82,82    | 1.68 | 3 (17%)     |
| 2   | HEM  | O     | 500 | 1    | 27,50,50     | 2.10 | 6 (22%)     | 17,82,82    | 1.80 | 3 (17%)     |
| 2   | HEM  | H     | 500 | 1    | 27,50,50     | 2.16 | 7 (25%)     | 17,82,82    | 2.46 | 6 (35%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | HEM  | M     | 500 | 1    | 27,50,50     | 2.15 | 8 (29%)  | 17,82,82    | 2.27 | 6 (35%)  |
| 2   | HEM  | N     | 500 | 1    | 27,50,50     | 2.16 | 6 (22%)  | 17,82,82    | 1.54 | 5 (29%)  |
| 2   | HEM  | P     | 500 | 1,3  | 27,50,50     | 2.22 | 8 (29%)  | 17,82,82    | 1.86 | 3 (17%)  |
| 2   | HEM  | D     | 500 | 1,3  | 27,50,50     | 2.22 | 7 (25%)  | 17,82,82    | 1.78 | 4 (23%)  |
| 2   | HEM  | C     | 500 | 1    | 27,50,50     | 2.24 | 7 (25%)  | 17,82,82    | 1.77 | 3 (17%)  |
| 2   | HEM  | L     | 500 | 1    | 27,50,50     | 2.11 | 8 (29%)  | 17,82,82    | 2.23 | 6 (35%)  |
| 2   | HEM  | A     | 500 | 1,3  | 27,50,50     | 2.15 | 7 (25%)  | 17,82,82    | 2.23 | 3 (17%)  |
| 2   | HEM  | B     | 500 | 1    | 27,50,50     | 2.27 | 9 (33%)  | 17,82,82    | 1.84 | 6 (35%)  |
| 2   | HEM  | G     | 500 | 1    | 27,50,50     | 2.23 | 7 (25%)  | 17,82,82    | 1.55 | 5 (29%)  |
| 2   | HEM  | E     | 500 | 1,3  | 27,50,50     | 2.12 | 7 (25%)  | 17,82,82    | 2.19 | 8 (47%)  |
| 2   | HEM  | F     | 500 | 1    | 27,50,50     | 2.17 | 5 (18%)  | 17,82,82    | 1.93 | 3 (17%)  |
| 2   | HEM  | K     | 500 | 1    | 27,50,50     | 2.21 | 7 (25%)  | 17,82,82    | 1.45 | 2 (11%)  |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings |
|-----|------|-------|-----|------|---------|-----------|-------|
| 2   | HEM  | I     | 500 | 1    | -       | 0/6/54/54 | -     |
| 2   | HEM  | J     | 500 | 1    | -       | 2/6/54/54 | -     |
| 2   | HEM  | O     | 500 | 1    | -       | 0/6/54/54 | -     |
| 2   | HEM  | H     | 500 | 1    | -       | 0/6/54/54 | -     |
| 2   | HEM  | M     | 500 | 1    | -       | 0/6/54/54 | -     |
| 2   | HEM  | N     | 500 | 1    | -       | 0/6/54/54 | -     |
| 2   | HEM  | P     | 500 | 1,3  | -       | 0/6/54/54 | -     |
| 2   | HEM  | D     | 500 | 1,3  | -       | 0/6/54/54 | -     |
| 2   | HEM  | C     | 500 | 1    | -       | 0/6/54/54 | -     |
| 2   | HEM  | L     | 500 | 1    | -       | 0/6/54/54 | -     |
| 2   | HEM  | A     | 500 | 1,3  | -       | 0/6/54/54 | -     |
| 2   | HEM  | B     | 500 | 1    | -       | 0/6/54/54 | -     |
| 2   | HEM  | G     | 500 | 1    | -       | 0/6/54/54 | -     |
| 2   | HEM  | E     | 500 | 1,3  | -       | 0/6/54/54 | -     |
| 2   | HEM  | F     | 500 | 1    | -       | 0/6/54/54 | -     |
| 2   | HEM  | K     | 500 | 1    | -       | 0/6/54/54 | -     |

All (112) bond length outliers are listed below:



| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | B     | 500 | HEM  | C3D-C2D | 5.77  | 1.54        | 1.37     |
| 2   | G     | 500 | HEM  | C3D-C2D | 5.66  | 1.54        | 1.37     |
| 2   | I     | 500 | HEM  | C3D-C2D | 5.62  | 1.54        | 1.37     |
| 2   | J     | 500 | HEM  | C3B-C2B | -5.60 | 1.32        | 1.40     |
| 2   | C     | 500 | HEM  | C3D-C2D | 5.56  | 1.54        | 1.37     |
| 2   | J     | 500 | HEM  | C3D-C2D | 5.54  | 1.54        | 1.37     |
| 2   | D     | 500 | HEM  | C3D-C2D | 5.48  | 1.53        | 1.37     |
| 2   | F     | 500 | HEM  | C3D-C2D | 5.46  | 1.53        | 1.37     |
| 2   | O     | 500 | HEM  | C3D-C2D | 5.37  | 1.53        | 1.37     |
| 2   | N     | 500 | HEM  | C3D-C2D | 5.32  | 1.53        | 1.37     |
| 2   | H     | 500 | HEM  | C3D-C2D | 5.31  | 1.53        | 1.37     |
| 2   | M     | 500 | HEM  | C3D-C2D | 5.28  | 1.53        | 1.37     |
| 2   | E     | 500 | HEM  | C3D-C2D | 5.25  | 1.53        | 1.37     |
| 2   | J     | 500 | HEM  | C3C-C2C | -5.21 | 1.33        | 1.40     |
| 2   | F     | 500 | HEM  | C3C-C2C | -5.19 | 1.33        | 1.40     |
| 2   | A     | 500 | HEM  | C3D-C2D | 5.12  | 1.52        | 1.37     |
| 2   | K     | 500 | HEM  | C3D-C2D | 5.12  | 1.52        | 1.37     |
| 2   | B     | 500 | HEM  | C3C-C2C | -5.06 | 1.33        | 1.40     |
| 2   | L     | 500 | HEM  | C3D-C2D | 5.01  | 1.52        | 1.37     |
| 2   | A     | 500 | HEM  | C3B-C2B | -4.99 | 1.33        | 1.40     |
| 2   | K     | 500 | HEM  | C3C-C2C | -4.94 | 1.33        | 1.40     |
| 2   | P     | 500 | HEM  | C3C-C2C | -4.92 | 1.33        | 1.40     |
| 2   | H     | 500 | HEM  | C3C-C2C | -4.78 | 1.33        | 1.40     |
| 2   | P     | 500 | HEM  | C3D-C2D | 4.77  | 1.51        | 1.37     |
| 2   | I     | 500 | HEM  | C3B-C2B | -4.63 | 1.33        | 1.40     |
| 2   | C     | 500 | HEM  | C3C-C2C | -4.55 | 1.34        | 1.40     |
| 2   | K     | 500 | HEM  | C3B-C2B | -4.54 | 1.34        | 1.40     |
| 2   | F     | 500 | HEM  | C3B-C2B | -4.46 | 1.34        | 1.40     |
| 2   | E     | 500 | HEM  | C3B-C2B | -4.40 | 1.34        | 1.40     |
| 2   | D     | 500 | HEM  | C3B-C2B | -4.39 | 1.34        | 1.40     |
| 2   | G     | 500 | HEM  | C3B-C2B | -4.34 | 1.34        | 1.40     |
| 2   | D     | 500 | HEM  | C3C-C2C | -4.32 | 1.34        | 1.40     |
| 2   | N     | 500 | HEM  | C3C-C2C | -4.28 | 1.34        | 1.40     |
| 2   | C     | 500 | HEM  | C3B-C2B | -4.26 | 1.34        | 1.40     |
| 2   | L     | 500 | HEM  | C3B-C2B | -4.15 | 1.34        | 1.40     |
| 2   | B     | 500 | HEM  | C3B-C2B | -4.08 | 1.34        | 1.40     |
| 2   | L     | 500 | HEM  | C3B-CAB | 4.07  | 1.56        | 1.47     |
| 2   | A     | 500 | HEM  | C3C-CAC | 4.03  | 1.56        | 1.47     |
| 2   | M     | 500 | HEM  | C3C-C2C | -4.01 | 1.34        | 1.40     |
| 2   | D     | 500 | HEM  | C3B-CAB | 4.00  | 1.56        | 1.47     |
| 2   | O     | 500 | HEM  | C3C-C2C | -3.99 | 1.34        | 1.40     |
| 2   | N     | 500 | HEM  | C3B-C2B | -3.97 | 1.34        | 1.40     |
| 2   | M     | 500 | HEM  | C3B-C2B | -3.94 | 1.34        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | O     | 500 | HEM  | C3B-C2B | -3.93 | 1.34        | 1.40     |
| 2   | P     | 500 | HEM  | C3B-C2B | -3.91 | 1.34        | 1.40     |
| 2   | N     | 500 | HEM  | C3C-CAC | 3.91  | 1.55        | 1.47     |
| 2   | E     | 500 | HEM  | C3C-CAC | 3.87  | 1.55        | 1.47     |
| 2   | G     | 500 | HEM  | C3B-CAB | 3.87  | 1.55        | 1.47     |
| 2   | J     | 500 | HEM  | C3B-CAB | 3.86  | 1.55        | 1.47     |
| 2   | G     | 500 | HEM  | C3C-CAC | 3.84  | 1.55        | 1.47     |
| 2   | C     | 500 | HEM  | C3B-CAB | 3.84  | 1.55        | 1.47     |
| 2   | A     | 500 | HEM  | C3C-C2C | -3.80 | 1.35        | 1.40     |
| 2   | P     | 500 | HEM  | C3C-CAC | 3.78  | 1.55        | 1.47     |
| 2   | N     | 500 | HEM  | C3B-CAB | 3.76  | 1.55        | 1.47     |
| 2   | O     | 500 | HEM  | C3C-CAC | 3.70  | 1.55        | 1.47     |
| 2   | C     | 500 | HEM  | C3C-CAC | 3.66  | 1.55        | 1.47     |
| 2   | I     | 500 | HEM  | C3C-CAC | 3.64  | 1.55        | 1.47     |
| 2   | M     | 500 | HEM  | C3C-CAC | 3.64  | 1.55        | 1.47     |
| 2   | M     | 500 | HEM  | C3B-CAB | 3.62  | 1.55        | 1.47     |
| 2   | H     | 500 | HEM  | C3B-C2B | -3.60 | 1.35        | 1.40     |
| 2   | A     | 500 | HEM  | C3B-CAB | 3.58  | 1.55        | 1.47     |
| 2   | I     | 500 | HEM  | C3C-C2C | -3.56 | 1.35        | 1.40     |
| 2   | F     | 500 | HEM  | C3B-CAB | 3.55  | 1.55        | 1.47     |
| 2   | G     | 500 | HEM  | C3C-C2C | -3.52 | 1.35        | 1.40     |
| 2   | H     | 500 | HEM  | C3C-CAC | 3.48  | 1.54        | 1.47     |
| 2   | E     | 500 | HEM  | C3B-CAB | 3.44  | 1.54        | 1.47     |
| 2   | P     | 500 | HEM  | CAA-C2A | 3.38  | 1.57        | 1.52     |
| 2   | D     | 500 | HEM  | C3C-CAC | 3.33  | 1.54        | 1.47     |
| 2   | L     | 500 | HEM  | C3C-C2C | -3.32 | 1.35        | 1.40     |
| 2   | H     | 500 | HEM  | C3B-CAB | 3.32  | 1.54        | 1.47     |
| 2   | B     | 500 | HEM  | C3B-CAB | 3.30  | 1.54        | 1.47     |
| 2   | K     | 500 | HEM  | C3C-CAC | 3.25  | 1.54        | 1.47     |
| 2   | O     | 500 | HEM  | C3B-CAB | 3.19  | 1.54        | 1.47     |
| 2   | B     | 500 | HEM  | C3C-CAC | 3.17  | 1.54        | 1.47     |
| 2   | E     | 500 | HEM  | C3C-C2C | -3.16 | 1.36        | 1.40     |
| 2   | P     | 500 | HEM  | C3B-CAB | 3.16  | 1.54        | 1.47     |
| 2   | I     | 500 | HEM  | C3B-CAB | 3.10  | 1.54        | 1.47     |
| 2   | F     | 500 | HEM  | C3C-CAC | 3.08  | 1.54        | 1.47     |
| 2   | J     | 500 | HEM  | C3C-CAC | 3.08  | 1.54        | 1.47     |
| 2   | K     | 500 | HEM  | C3B-CAB | 3.00  | 1.54        | 1.47     |
| 2   | K     | 500 | HEM  | CAA-C2A | 2.86  | 1.56        | 1.52     |
| 2   | E     | 500 | HEM  | CAA-C2A | 2.86  | 1.56        | 1.52     |
| 2   | I     | 500 | HEM  | C1D-ND  | 2.80  | 1.41        | 1.36     |
| 2   | L     | 500 | HEM  | C3C-CAC | 2.79  | 1.53        | 1.47     |
| 2   | G     | 500 | HEM  | CAA-C2A | 2.79  | 1.56        | 1.52     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2   | C     | 500 | HEM  | CAA-C2A | 2.74 | 1.56        | 1.52     |
| 2   | B     | 500 | HEM  | CAA-C2A | 2.60 | 1.55        | 1.52     |
| 2   | L     | 500 | HEM  | CAA-C2A | 2.59 | 1.55        | 1.52     |
| 2   | H     | 500 | HEM  | CAA-C2A | 2.56 | 1.55        | 1.52     |
| 2   | J     | 500 | HEM  | C1D-ND  | 2.49 | 1.41        | 1.36     |
| 2   | I     | 500 | HEM  | CAA-C2A | 2.39 | 1.55        | 1.52     |
| 2   | G     | 500 | HEM  | C1D-ND  | 2.33 | 1.41        | 1.36     |
| 2   | D     | 500 | HEM  | C4A-NA  | 2.31 | 1.40        | 1.36     |
| 2   | N     | 500 | HEM  | CAA-C2A | 2.29 | 1.55        | 1.52     |
| 2   | B     | 500 | HEM  | CMD-C2D | 2.23 | 1.56        | 1.51     |
| 2   | C     | 500 | HEM  | C1D-ND  | 2.21 | 1.40        | 1.36     |
| 2   | K     | 500 | HEM  | C4B-NB  | 2.17 | 1.40        | 1.36     |
| 2   | L     | 500 | HEM  | C1B-C2B | 2.17 | 1.47        | 1.42     |
| 2   | M     | 500 | HEM  | CAA-C2A | 2.16 | 1.55        | 1.52     |
| 2   | P     | 500 | HEM  | C4B-NB  | 2.16 | 1.40        | 1.36     |
| 2   | M     | 500 | HEM  | CMA-C3A | 2.13 | 1.56        | 1.51     |
| 2   | B     | 500 | HEM  | C1D-ND  | 2.12 | 1.40        | 1.36     |
| 2   | L     | 500 | HEM  | C1D-ND  | 2.10 | 1.40        | 1.36     |
| 2   | A     | 500 | HEM  | C4A-NA  | 2.08 | 1.40        | 1.36     |
| 2   | B     | 500 | HEM  | CAD-C3D | 2.08 | 1.55        | 1.52     |
| 2   | O     | 500 | HEM  | CAA-C2A | 2.07 | 1.55        | 1.52     |
| 2   | M     | 500 | HEM  | C4A-NA  | 2.06 | 1.40        | 1.36     |
| 2   | A     | 500 | HEM  | CAA-C2A | 2.05 | 1.55        | 1.52     |
| 2   | D     | 500 | HEM  | C1B-C2B | 2.04 | 1.47        | 1.42     |
| 2   | H     | 500 | HEM  | C1B-C2B | 2.03 | 1.47        | 1.42     |
| 2   | E     | 500 | HEM  | CMB-C2B | 2.01 | 1.56        | 1.51     |
| 2   | P     | 500 | HEM  | C1B-C2B | 2.01 | 1.47        | 1.42     |

All (71) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | A     | 500 | HEM  | CBD-CAD-C3D | -6.64 | 100.24      | 112.48   |
| 2   | M     | 500 | HEM  | CBD-CAD-C3D | -6.20 | 101.05      | 112.48   |
| 2   | H     | 500 | HEM  | CBD-CAD-C3D | -6.08 | 101.28      | 112.48   |
| 2   | P     | 500 | HEM  | CBD-CAD-C3D | -5.52 | 102.30      | 112.48   |
| 2   | C     | 500 | HEM  | CBD-CAD-C3D | -4.94 | 103.38      | 112.48   |
| 2   | F     | 500 | HEM  | CBD-CAD-C3D | -4.80 | 103.64      | 112.48   |
| 2   | O     | 500 | HEM  | CBD-CAD-C3D | -4.70 | 103.81      | 112.48   |
| 2   | H     | 500 | HEM  | CMA-C3A-C4A | -4.65 | 121.32      | 128.46   |
| 2   | B     | 500 | HEM  | CBD-CAD-C3D | -4.44 | 104.30      | 112.48   |
| 2   | A     | 500 | HEM  | CAA-CBA-CGA | -4.36 | 105.36      | 112.67   |
| 2   | L     | 500 | HEM  | CAA-CBA-CGA | -4.26 | 105.52      | 112.67   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 500 | HEM  | CAA-CBA-CGA | -4.08 | 105.82      | 112.67   |
| 2   | L     | 500 | HEM  | CBD-CAD-C3D | -3.98 | 105.15      | 112.48   |
| 2   | I     | 500 | HEM  | CMA-C3A-C4A | -3.96 | 122.38      | 128.46   |
| 2   | J     | 500 | HEM  | CMA-C3A-C4A | -3.95 | 122.39      | 128.46   |
| 2   | H     | 500 | HEM  | CAD-CBD-CGD | 3.82  | 119.08      | 112.67   |
| 2   | E     | 500 | HEM  | CMA-C3A-C4A | -3.61 | 122.91      | 128.46   |
| 2   | L     | 500 | HEM  | CMA-C3A-C4A | -3.54 | 123.03      | 128.46   |
| 2   | D     | 500 | HEM  | CMD-C2D-C1D | -3.46 | 123.15      | 128.46   |
| 2   | N     | 500 | HEM  | CMA-C3A-C4A | -3.39 | 123.25      | 128.46   |
| 2   | E     | 500 | HEM  | CAD-CBD-CGD | -3.29 | 107.14      | 112.67   |
| 2   | K     | 500 | HEM  | CMA-C3A-C4A | -3.26 | 123.45      | 128.46   |
| 2   | E     | 500 | HEM  | CBD-CAD-C3D | -3.24 | 106.51      | 112.48   |
| 2   | E     | 500 | HEM  | CMD-C2D-C3D | 3.22  | 131.01      | 124.94   |
| 2   | E     | 500 | HEM  | CMD-C2D-C1D | -3.18 | 123.58      | 128.46   |
| 2   | D     | 500 | HEM  | CBD-CAD-C3D | -3.17 | 106.64      | 112.48   |
| 2   | P     | 500 | HEM  | CMA-C3A-C4A | -3.11 | 123.68      | 128.46   |
| 2   | E     | 500 | HEM  | C4A-C3A-C2A | 3.08  | 109.14      | 107.00   |
| 2   | D     | 500 | HEM  | CMD-C2D-C3D | 2.97  | 130.54      | 124.94   |
| 2   | L     | 500 | HEM  | C1D-C2D-C3D | -2.86 | 105.01      | 107.00   |
| 2   | P     | 500 | HEM  | C4A-C3A-C2A | 2.82  | 108.96      | 107.00   |
| 2   | M     | 500 | HEM  | CMA-C3A-C4A | -2.82 | 124.14      | 128.46   |
| 2   | I     | 500 | HEM  | CMA-C3A-C2A | 2.80  | 130.23      | 124.94   |
| 2   | H     | 500 | HEM  | C4A-C3A-C2A | 2.74  | 108.90      | 107.00   |
| 2   | B     | 500 | HEM  | C4C-C3C-C2C | 2.74  | 108.81      | 106.90   |
| 2   | G     | 500 | HEM  | CBD-CAD-C3D | -2.73 | 107.45      | 112.48   |
| 2   | J     | 500 | HEM  | CBD-CAD-C3D | -2.63 | 107.62      | 112.48   |
| 2   | C     | 500 | HEM  | CAD-CBD-CGD | 2.62  | 117.07      | 112.67   |
| 2   | D     | 500 | HEM  | C4A-C3A-C2A | 2.62  | 108.82      | 107.00   |
| 2   | M     | 500 | HEM  | CMD-C2D-C1D | -2.58 | 124.50      | 128.46   |
| 2   | M     | 500 | HEM  | CMC-C2C-C3C | 2.57  | 129.49      | 124.68   |
| 2   | G     | 500 | HEM  | C4A-C3A-C2A | 2.57  | 108.78      | 107.00   |
| 2   | H     | 500 | HEM  | CMA-C3A-C2A | 2.56  | 129.78      | 124.94   |
| 2   | L     | 500 | HEM  | C4A-C3A-C2A | 2.55  | 108.77      | 107.00   |
| 2   | B     | 500 | HEM  | C4A-C3A-C2A | 2.53  | 108.75      | 107.00   |
| 2   | L     | 500 | HEM  | CMC-C2C-C3C | 2.50  | 129.36      | 124.68   |
| 2   | J     | 500 | HEM  | CMA-C3A-C2A | 2.49  | 129.64      | 124.94   |
| 2   | M     | 500 | HEM  | CMD-C2D-C3D | 2.48  | 129.62      | 124.94   |
| 2   | H     | 500 | HEM  | CAA-CBA-CGA | -2.38 | 108.67      | 112.67   |
| 2   | I     | 500 | HEM  | CBD-CAD-C3D | -2.35 | 108.14      | 112.48   |
| 2   | F     | 500 | HEM  | CMA-C3A-C4A | -2.32 | 124.90      | 128.46   |
| 2   | O     | 500 | HEM  | CBA-CAA-C2A | -2.30 | 108.24      | 112.49   |
| 2   | E     | 500 | HEM  | C1D-C2D-C3D | -2.30 | 105.39      | 107.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | B     | 500 | HEM  | CAD-CBD-CGD | 2.27  | 116.48      | 112.67   |
| 2   | I     | 500 | HEM  | CMC-C2C-C3C | 2.23  | 128.86      | 124.68   |
| 2   | O     | 500 | HEM  | C1D-C2D-C3D | -2.21 | 105.46      | 107.00   |
| 2   | N     | 500 | HEM  | CMA-C3A-C2A | 2.19  | 129.08      | 124.94   |
| 2   | C     | 500 | HEM  | CMA-C3A-C4A | -2.19 | 125.09      | 128.46   |
| 2   | N     | 500 | HEM  | C1D-C2D-C3D | -2.19 | 105.47      | 107.00   |
| 2   | K     | 500 | HEM  | CAA-CBA-CGA | -2.16 | 109.04      | 112.67   |
| 2   | M     | 500 | HEM  | CAA-CBA-CGA | -2.15 | 109.07      | 112.67   |
| 2   | B     | 500 | HEM  | CMA-C3A-C4A | -2.14 | 125.17      | 128.46   |
| 2   | E     | 500 | HEM  | CMC-C2C-C3C | 2.14  | 128.68      | 124.68   |
| 2   | N     | 500 | HEM  | CBA-CAA-C2A | -2.13 | 108.55      | 112.49   |
| 2   | N     | 500 | HEM  | CBD-CAD-C3D | -2.13 | 108.55      | 112.48   |
| 2   | G     | 500 | HEM  | C1D-C2D-C3D | -2.10 | 105.53      | 107.00   |
| 2   | G     | 500 | HEM  | C3C-C4C-NC  | -2.08 | 107.02      | 110.94   |
| 2   | B     | 500 | HEM  | C3C-C4C-NC  | -2.07 | 107.04      | 110.94   |
| 2   | A     | 500 | HEM  | CMC-C2C-C3C | 2.06  | 128.54      | 124.68   |
| 2   | I     | 500 | HEM  | CBA-CAA-C2A | -2.03 | 108.74      | 112.49   |
| 2   | G     | 500 | HEM  | CMA-C3A-C4A | -2.02 | 125.35      | 128.46   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | J     | 500 | HEM  | C2D-C3D-CAD-CBD |
| 2   | J     | 500 | HEM  | C4D-C3D-CAD-CBD |

There are no ring outliers.

15 monomers are involved in 58 short contacts:

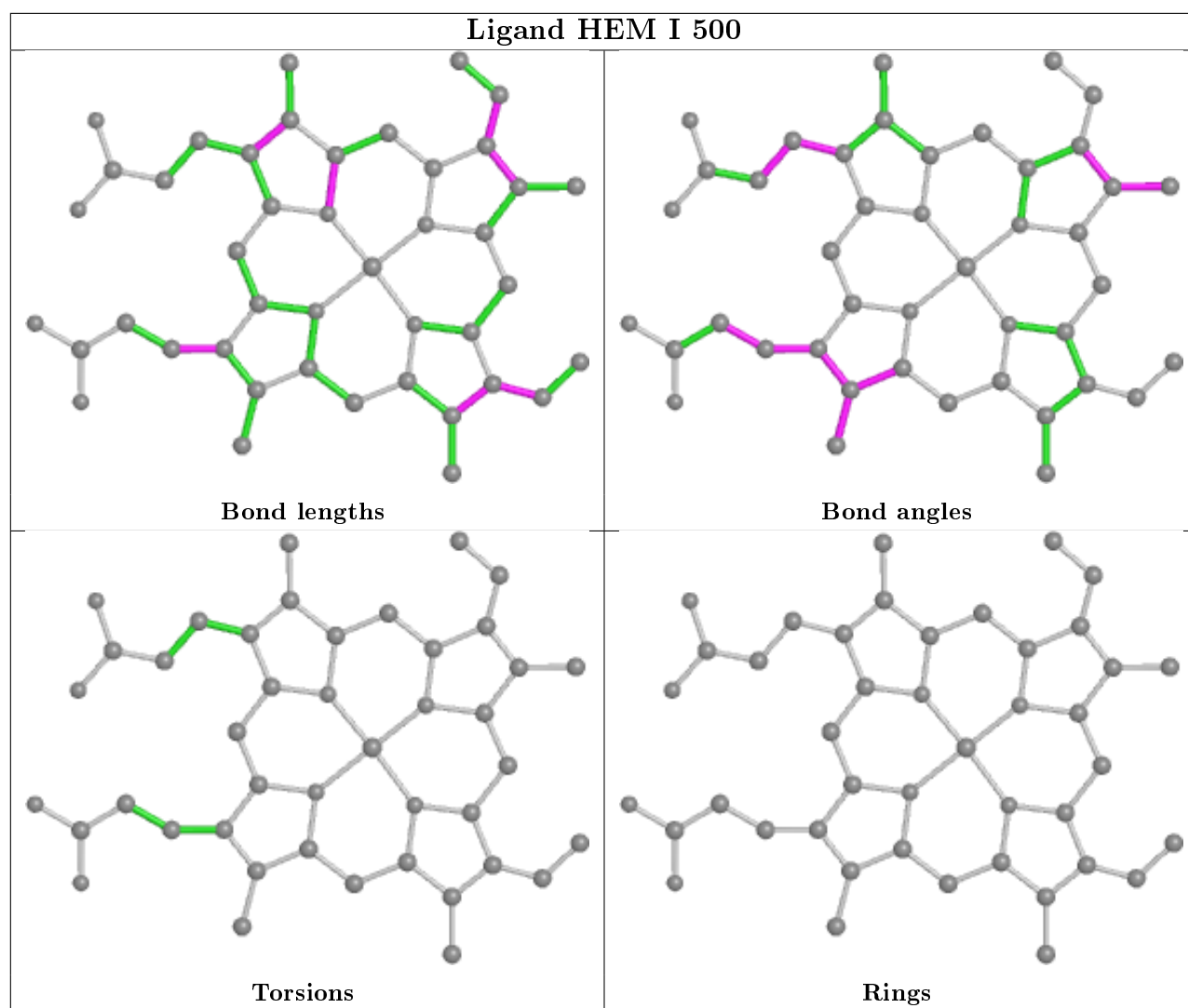
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | I     | 500 | HEM  | 9       | 0            |
| 2   | J     | 500 | HEM  | 1       | 0            |
| 2   | O     | 500 | HEM  | 4       | 0            |
| 2   | H     | 500 | HEM  | 2       | 0            |
| 2   | M     | 500 | HEM  | 2       | 0            |
| 2   | N     | 500 | HEM  | 1       | 0            |
| 2   | P     | 500 | HEM  | 7       | 0            |
| 2   | D     | 500 | HEM  | 2       | 0            |
| 2   | C     | 500 | HEM  | 2       | 0            |
| 2   | L     | 500 | HEM  | 5       | 0            |
| 2   | A     | 500 | HEM  | 6       | 0            |

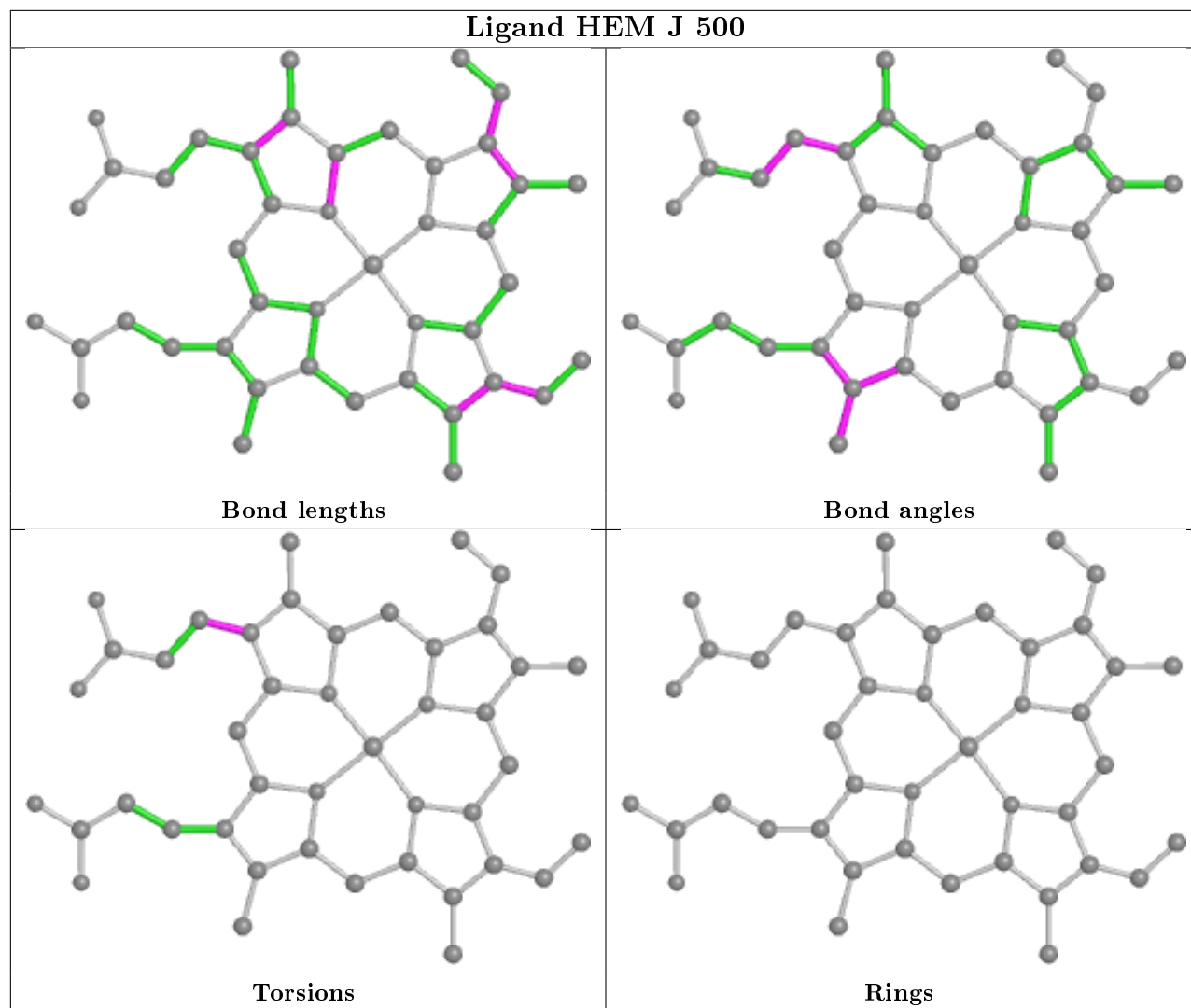
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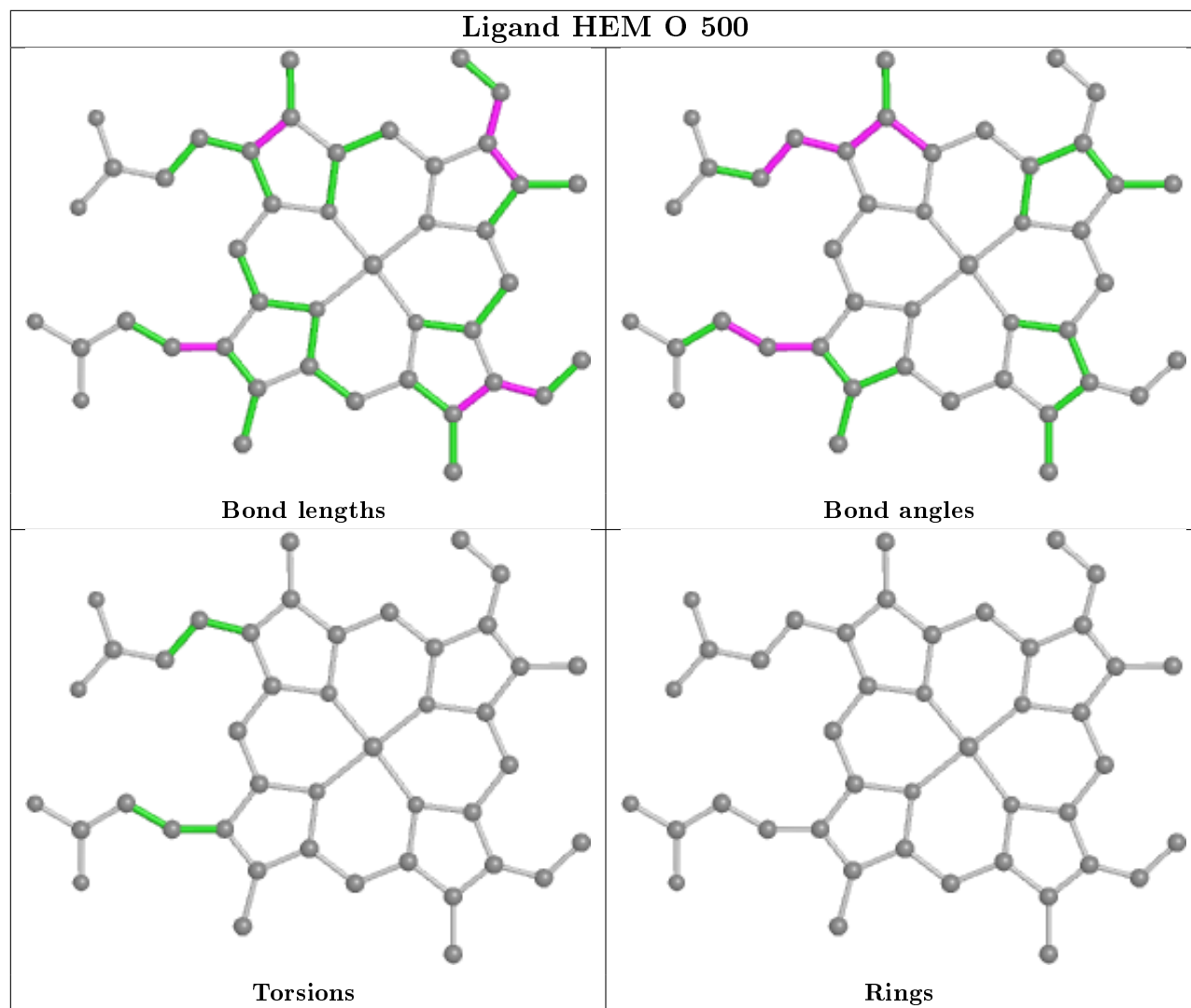
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2   | G     | 500 | HEM  | 3       | 0            |
| 2   | E     | 500 | HEM  | 7       | 0            |
| 2   | F     | 500 | HEM  | 3       | 0            |
| 2   | K     | 500 | HEM  | 4       | 0            |

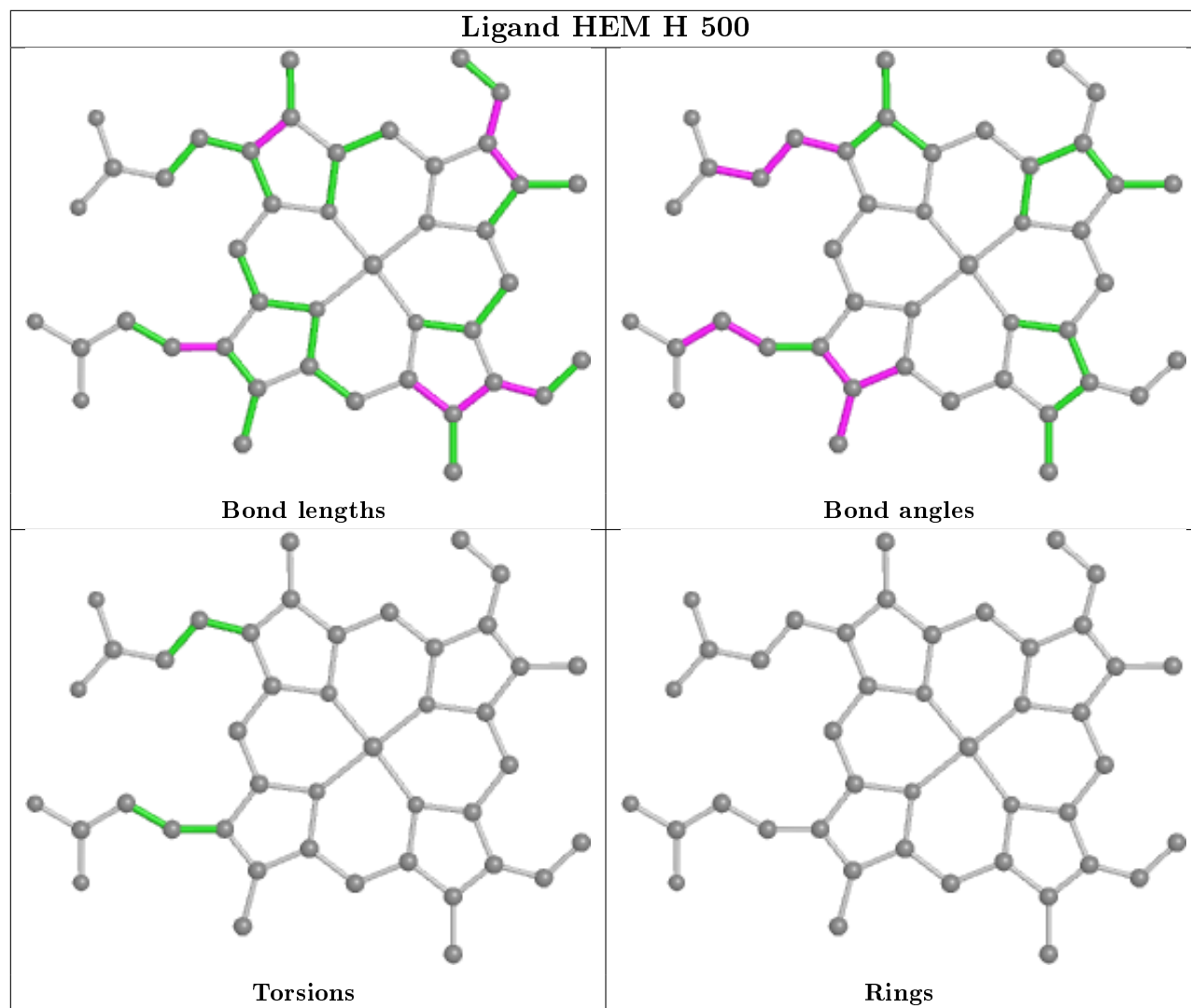
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

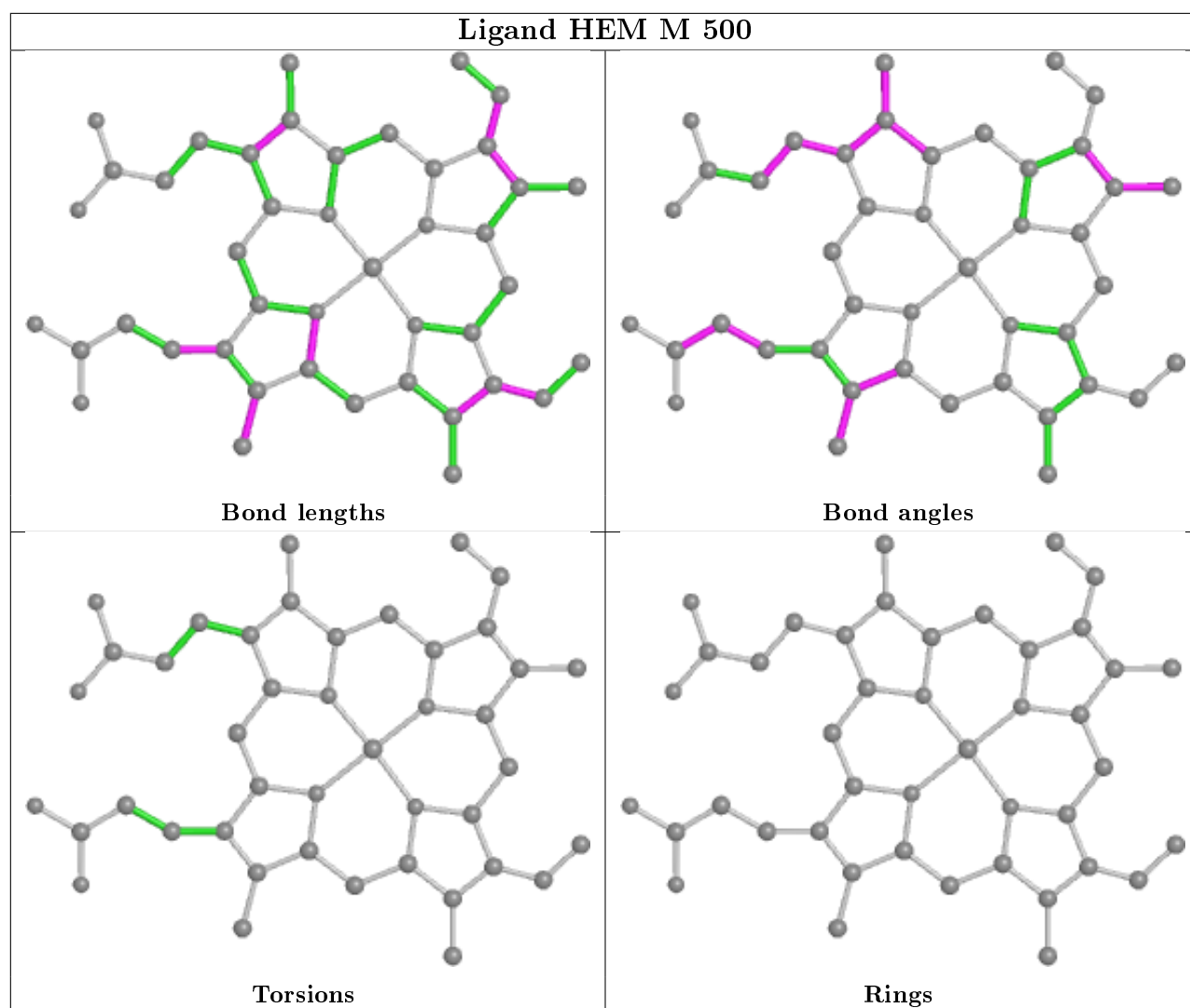


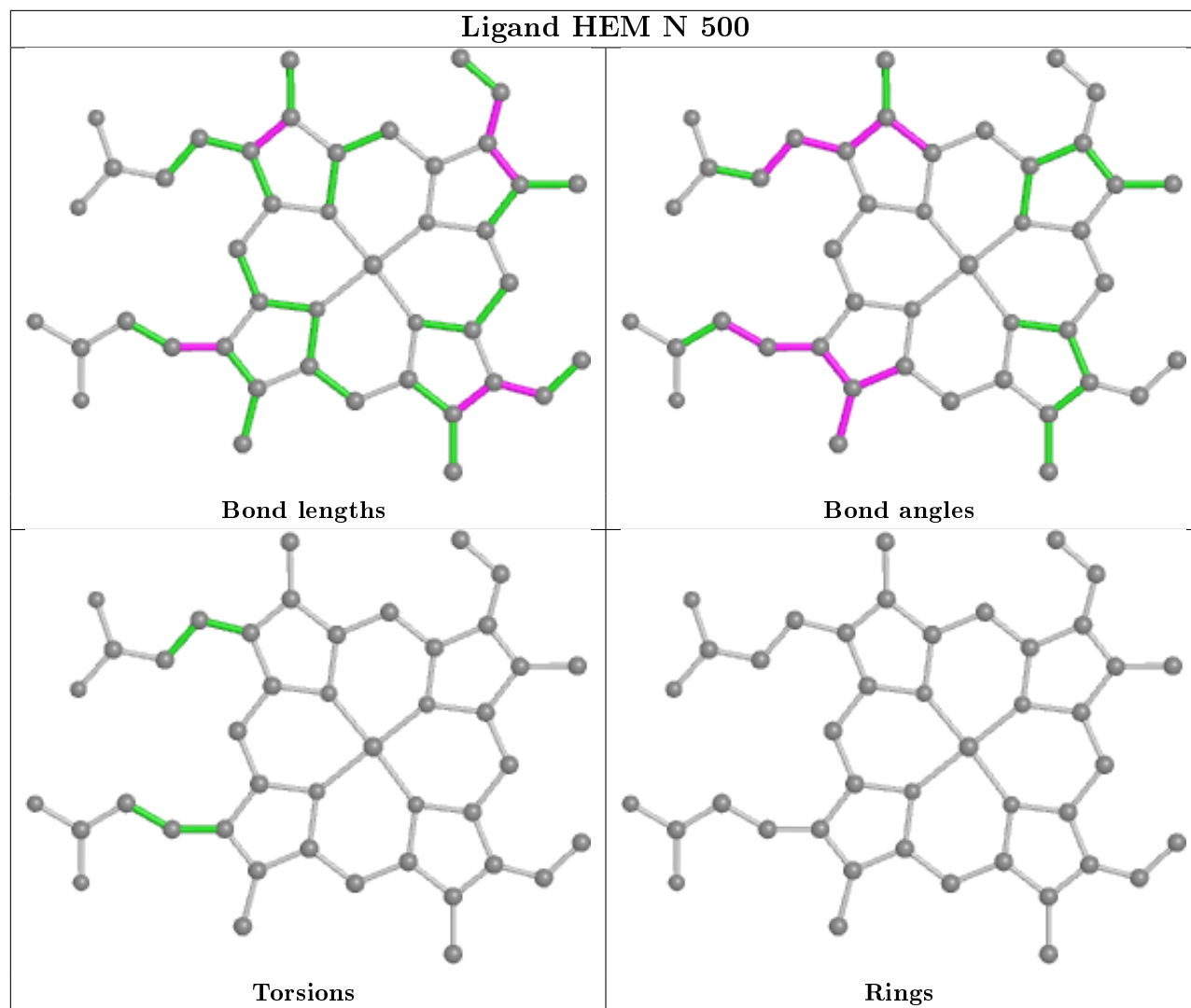


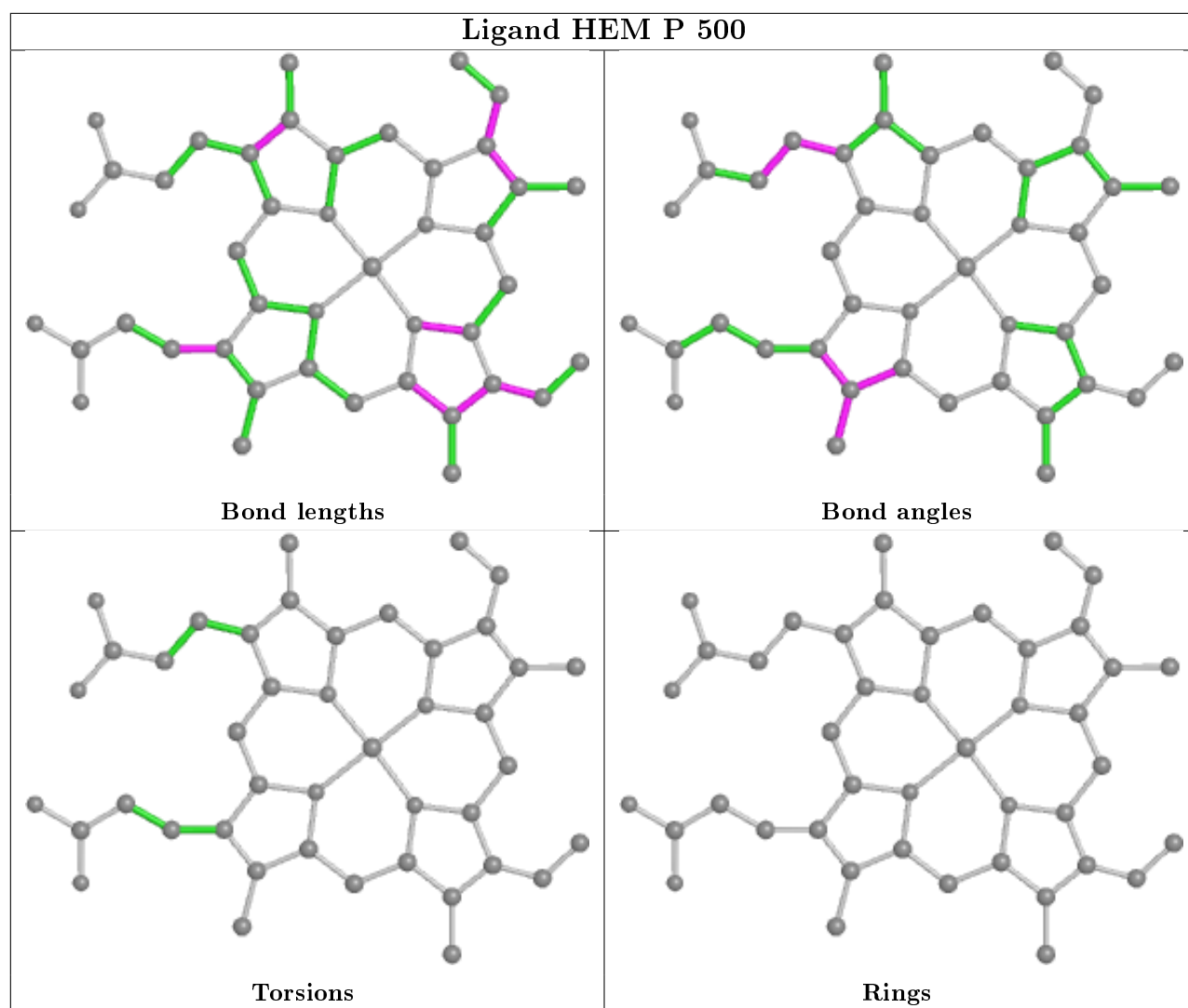


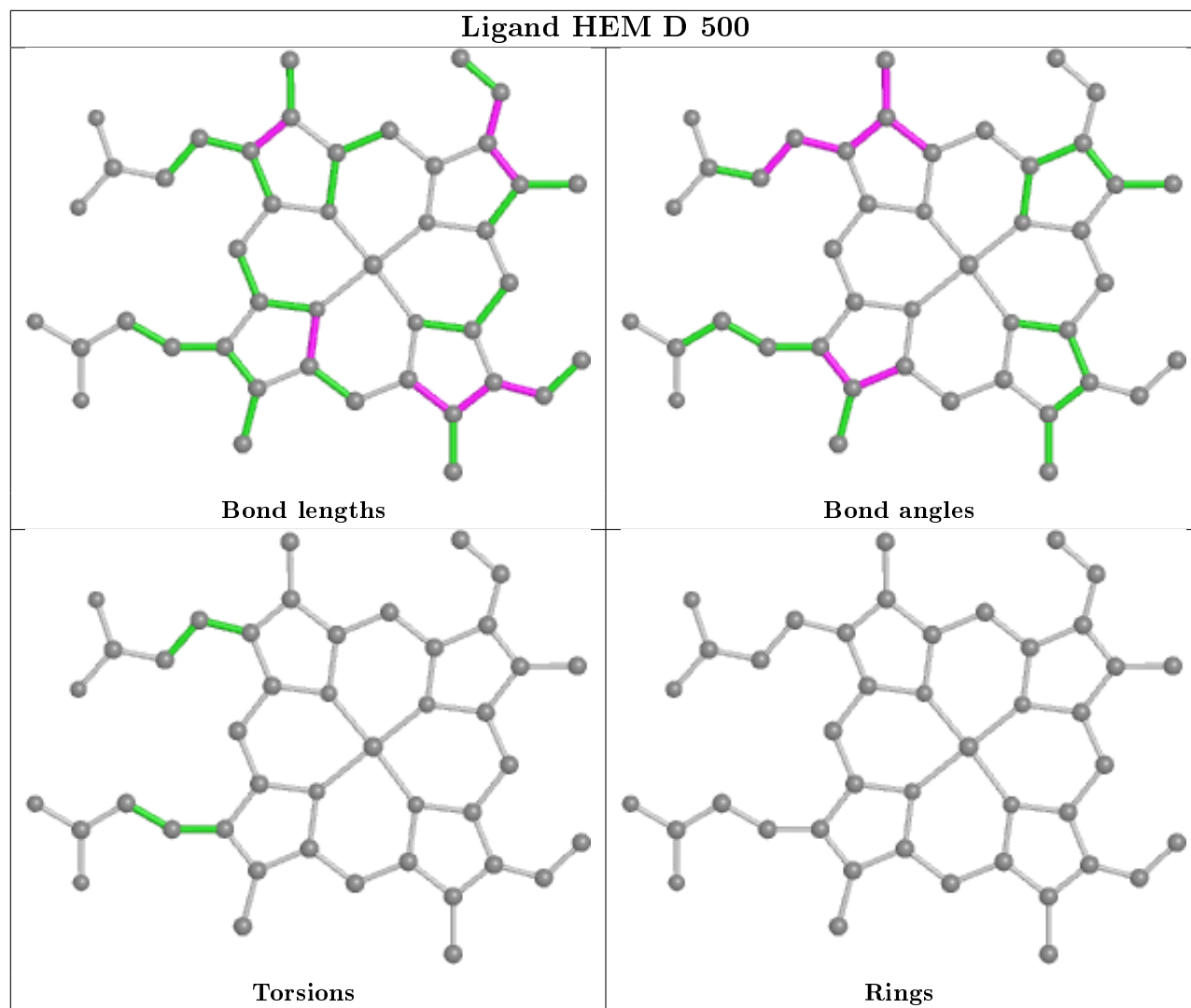


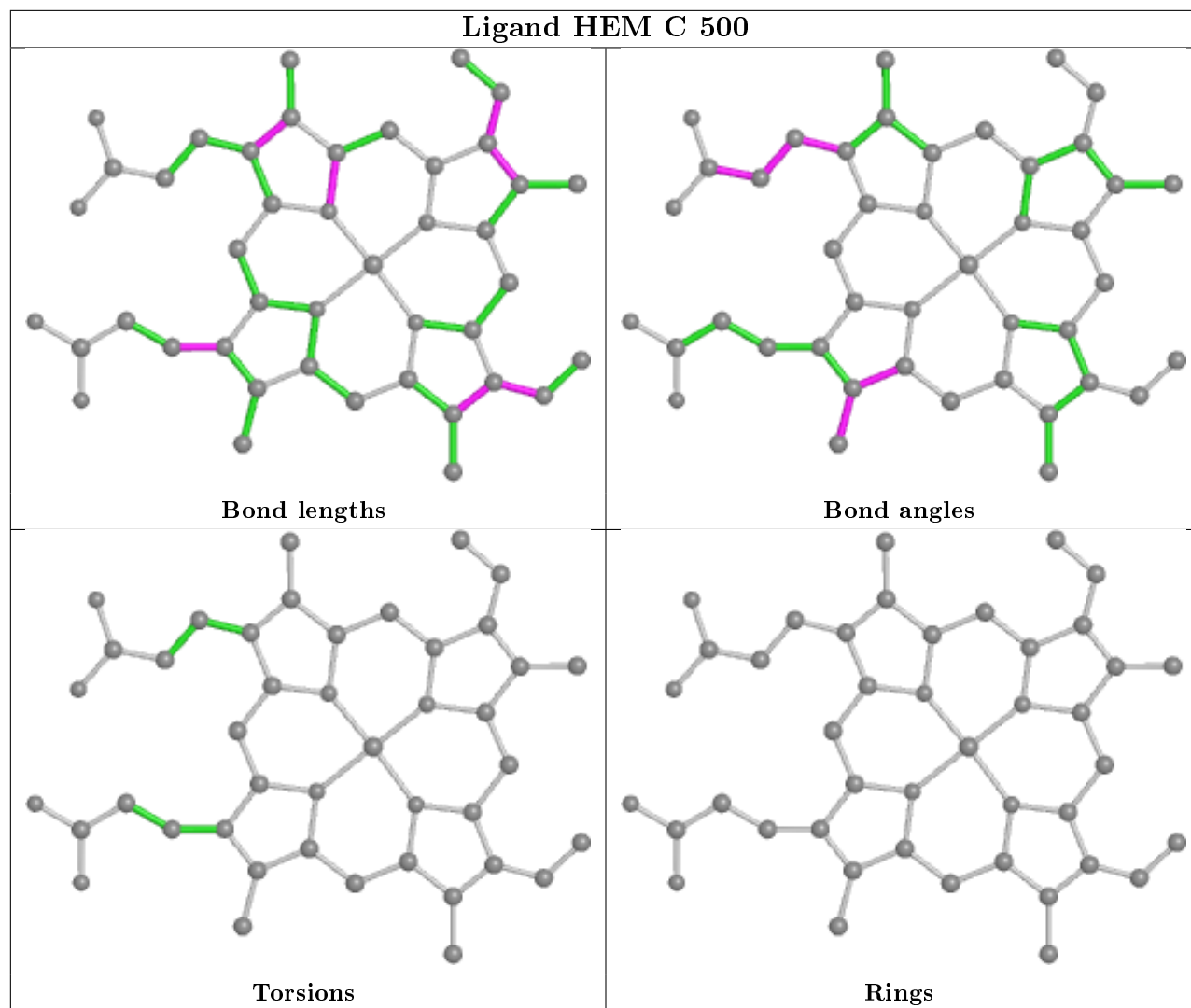


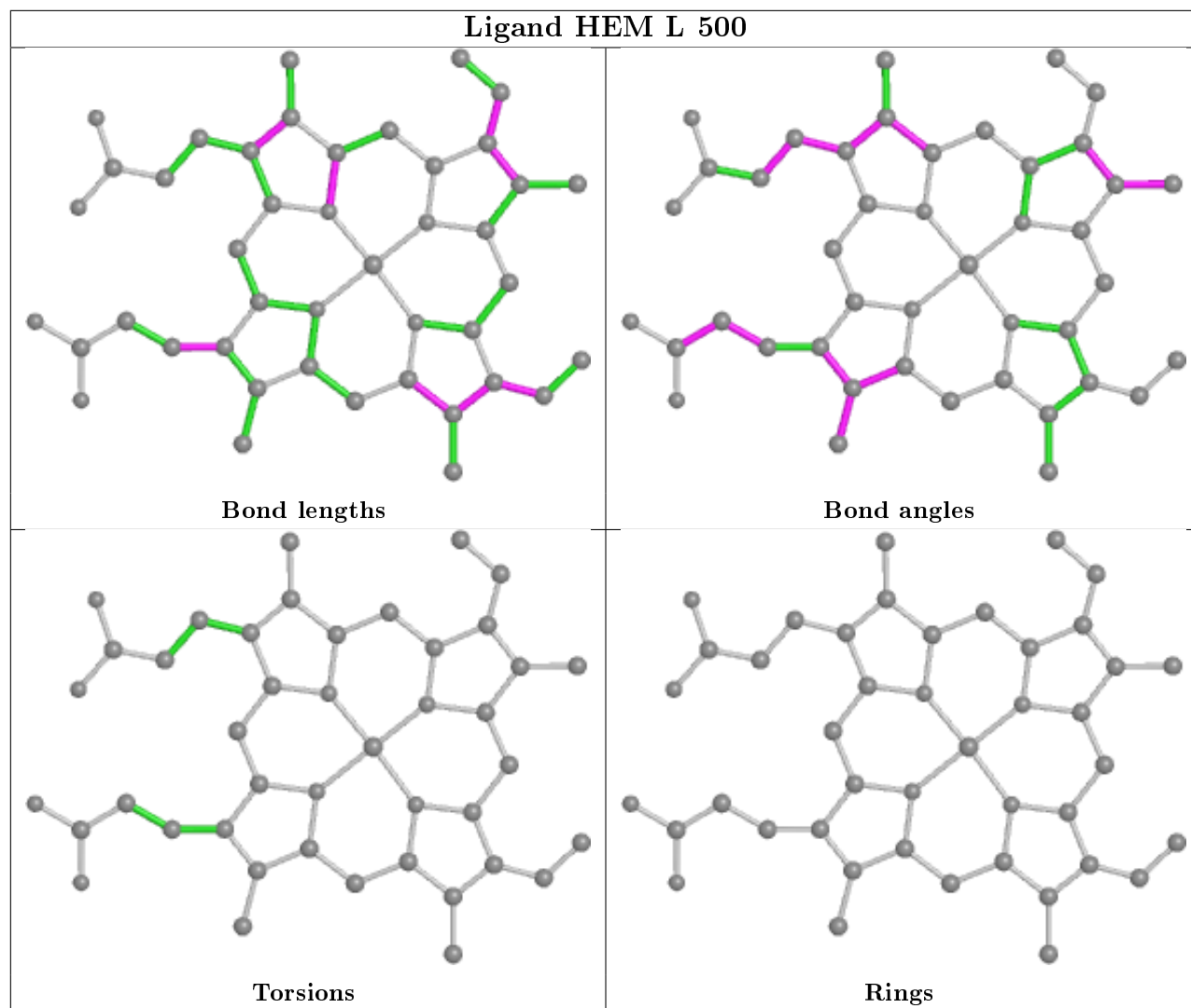




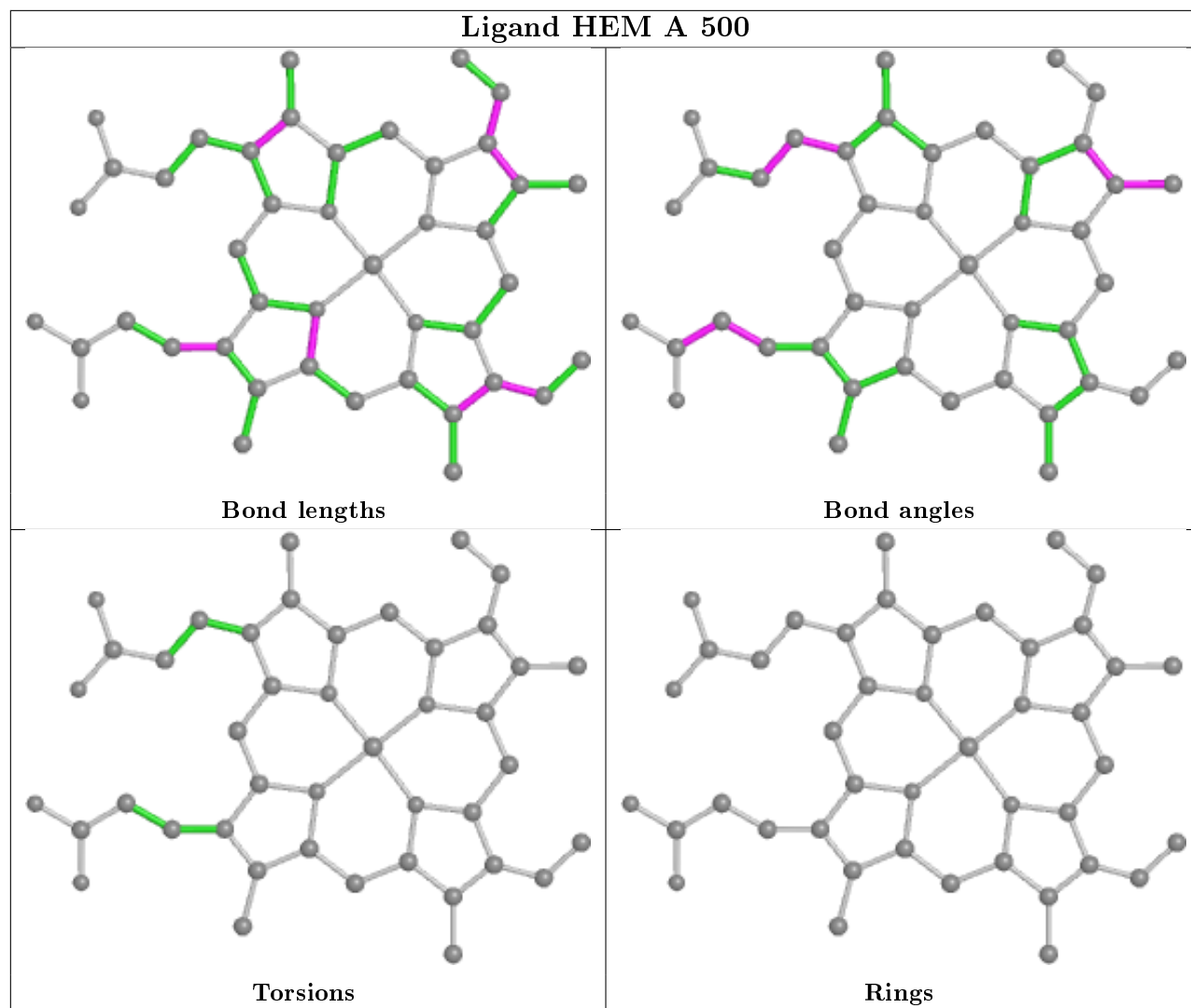


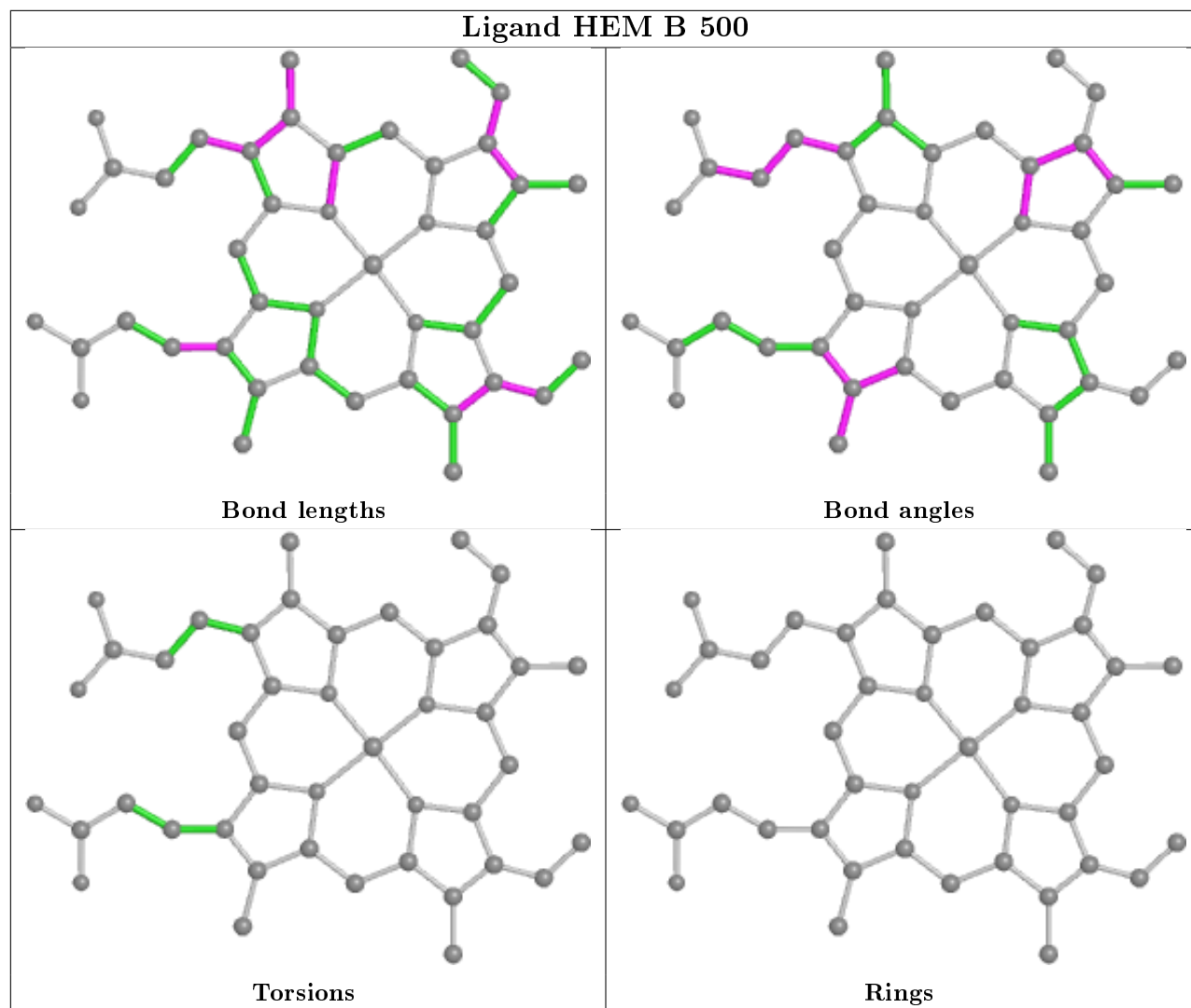


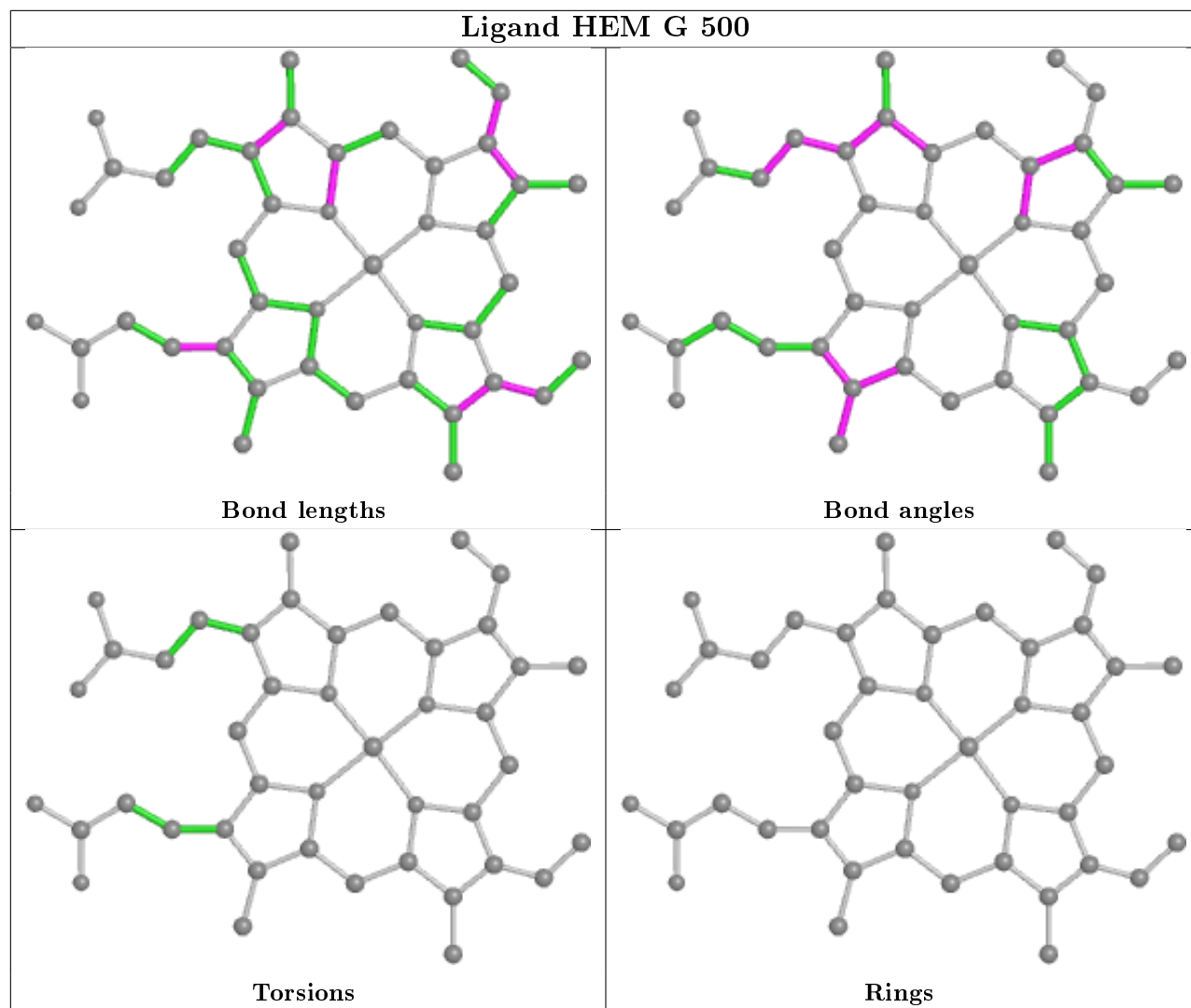


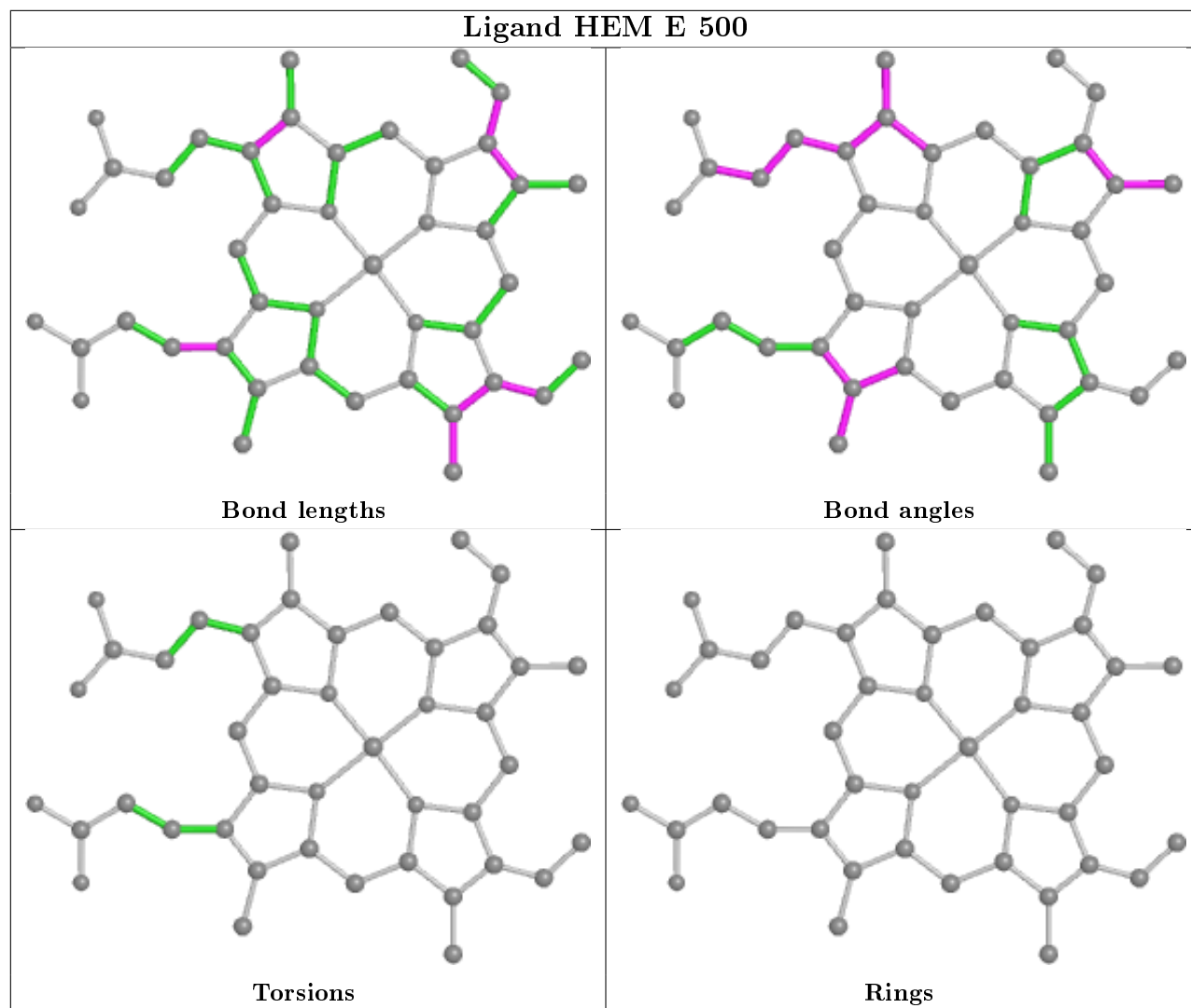


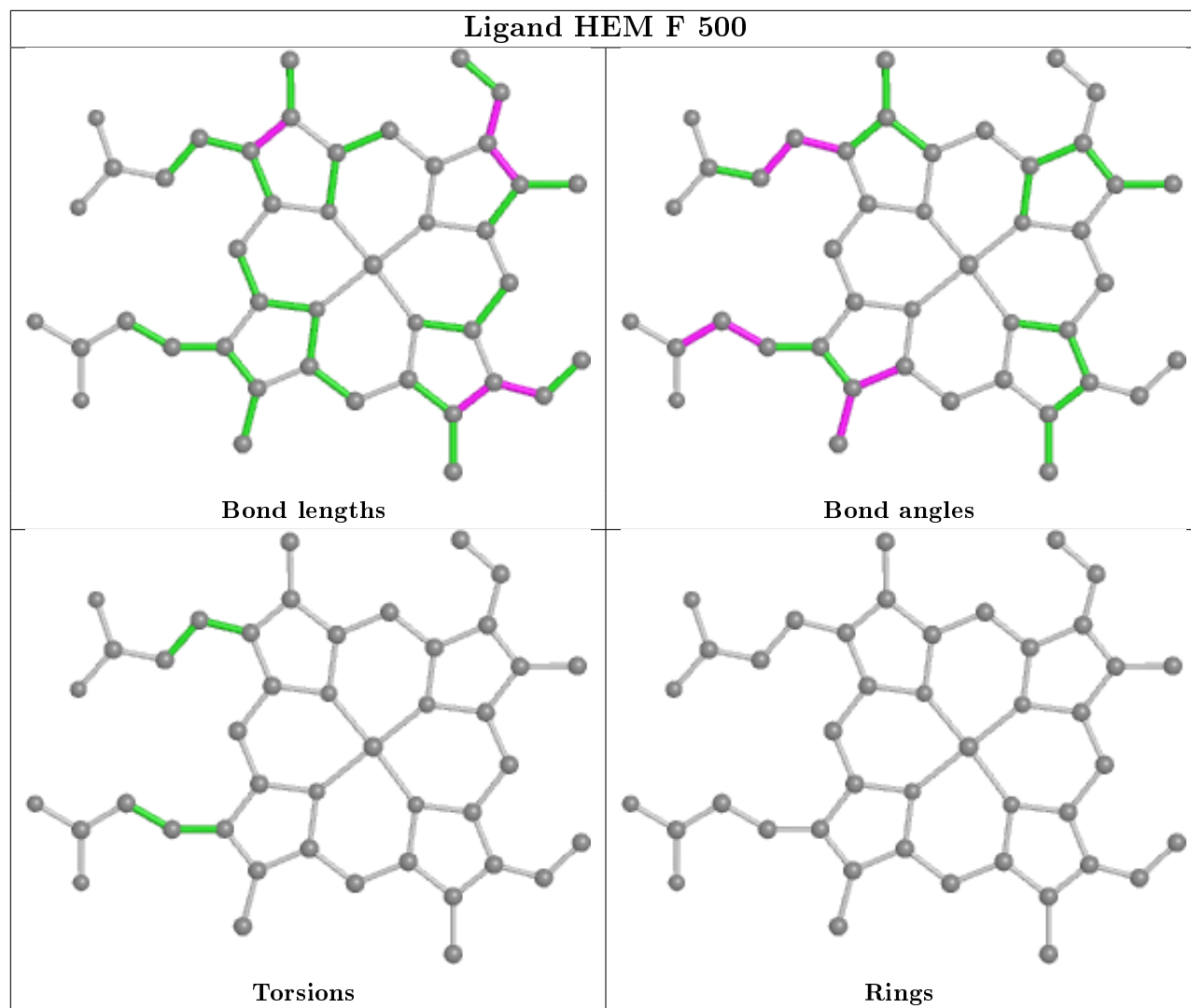


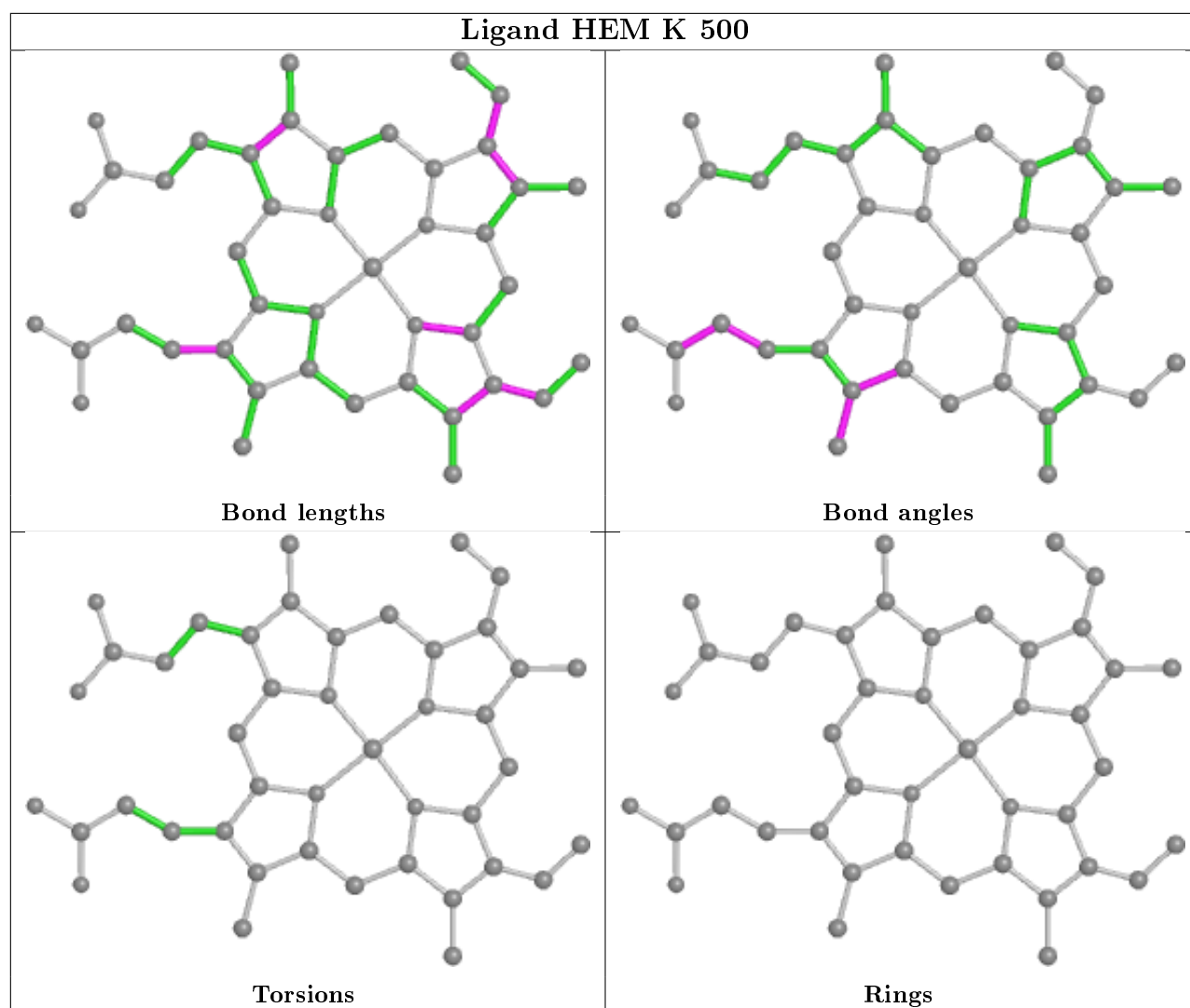












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 261/281 (92%)   | -0.42  | 2 (0%) 86 84  | 27, 41, 65, 121       | 0     |
| 1   | B     | 266/281 (94%)   | -0.34  | 5 (1%) 66 64  | 30, 43, 70, 102       | 0     |
| 1   | C     | 255/281 (90%)   | -0.33  | 5 (1%) 65 63  | 29, 43, 70, 101       | 0     |
| 1   | D     | 259/281 (92%)   | -0.45  | 0 100 100     | 27, 40, 64, 92        | 0     |
| 1   | E     | 256/281 (91%)   | -0.49  | 2 (0%) 86 84  | 26, 42, 70, 120       | 0     |
| 1   | F     | 260/281 (92%)   | -0.34  | 2 (0%) 86 84  | 29, 44, 80, 106       | 0     |
| 1   | G     | 259/281 (92%)   | -0.21  | 8 (3%) 49 47  | 29, 45, 76, 106       | 0     |
| 1   | H     | 259/281 (92%)   | -0.47  | 1 (0%) 92 91  | 27, 41, 63, 92        | 0     |
| 1   | I     | 259/281 (92%)   | -0.36  | 3 (1%) 79 77  | 29, 44, 68, 83        | 0     |
| 1   | J     | 257/281 (91%)   | -0.10  | 10 (3%) 39 38 | 28, 43, 71, 109       | 0     |
| 1   | K     | 255/281 (90%)   | -0.05  | 8 (3%) 49 47  | 28, 41, 66, 99        | 0     |
| 1   | L     | 260/281 (92%)   | -0.33  | 3 (1%) 79 77  | 28, 43, 66, 91        | 0     |
| 1   | M     | 255/281 (90%)   | -0.47  | 0 100 100     | 27, 42, 70, 97        | 0     |
| 1   | N     | 260/281 (92%)   | -0.16  | 6 (2%) 60 58  | 29, 44, 74, 105       | 0     |
| 1   | O     | 257/281 (91%)   | -0.22  | 3 (1%) 79 77  | 28, 44, 74, 116       | 0     |
| 1   | P     | 259/281 (92%)   | -0.48  | 0 100 100     | 27, 43, 65, 93        | 0     |
| All | All   | 4137/4496 (92%) | -0.33  | 58 (1%) 75 73 | 26, 43, 70, 121       | 0     |

All (58) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | N     | 139 | ALA  | 4.5  |
| 1   | B     | 270 | GLY  | 4.4  |
| 1   | B     | 139 | ALA  | 4.2  |
| 1   | A     | 39  | ARG  | 3.8  |
| 1   | K     | 275 | GLU  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 139 | ALA  | 3.6  |
| 1   | J     | 200 | ILE  | 3.5  |
| 1   | N     | 205 | VAL  | 3.5  |
| 1   | F     | 205 | VAL  | 3.4  |
| 1   | C     | 274 | THR  | 3.2  |
| 1   | I     | 274 | THR  | 3.1  |
| 1   | J     | 202 | PRO  | 3.0  |
| 1   | J     | 199 | GLN  | 3.0  |
| 1   | O     | 204 | VAL  | 2.9  |
| 1   | K     | 205 | VAL  | 2.9  |
| 1   | E     | 269 | ARG  | 2.8  |
| 1   | E     | 40  | ASP  | 2.7  |
| 1   | G     | 299 | LEU  | 2.7  |
| 1   | H     | 139 | ALA  | 2.7  |
| 1   | K     | 204 | VAL  | 2.7  |
| 1   | G     | 202 | PRO  | 2.7  |
| 1   | B     | 167 | ALA  | 2.6  |
| 1   | K     | 194 | ALA  | 2.6  |
| 1   | J     | 219 | VAL  | 2.6  |
| 1   | A     | 40  | ASP  | 2.6  |
| 1   | J     | 167 | ALA  | 2.6  |
| 1   | B     | 137 | LEU  | 2.6  |
| 1   | G     | 140 | SER  | 2.6  |
| 1   | K     | 224 | LEU  | 2.5  |
| 1   | C     | 139 | ALA  | 2.5  |
| 1   | G     | 204 | VAL  | 2.5  |
| 1   | N     | 204 | VAL  | 2.4  |
| 1   | N     | 138 | GLY  | 2.4  |
| 1   | I     | 267 | PHE  | 2.4  |
| 1   | N     | 207 | ARG  | 2.4  |
| 1   | C     | 205 | VAL  | 2.4  |
| 1   | L     | 116 | VAL  | 2.4  |
| 1   | O     | 167 | ALA  | 2.4  |
| 1   | I     | 269 | ARG  | 2.3  |
| 1   | K     | 200 | ILE  | 2.3  |
| 1   | K     | 202 | PRO  | 2.3  |
| 1   | O     | 140 | SER  | 2.2  |
| 1   | G     | 198 | PHE  | 2.2  |
| 1   | C     | 204 | VAL  | 2.2  |
| 1   | J     | 197 | GLY  | 2.2  |
| 1   | G     | 203 | GLU  | 2.2  |
| 1   | L     | 202 | PRO  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 206 | GLU  | 2.2  |
| 1   | J     | 205 | VAL  | 2.1  |
| 1   | L     | 113 | ASP  | 2.1  |
| 1   | C     | 203 | GLU  | 2.1  |
| 1   | K     | 203 | GLU  | 2.1  |
| 1   | N     | 203 | GLU  | 2.1  |
| 1   | J     | 117 | GLN  | 2.1  |
| 1   | J     | 273 | GLY  | 2.0  |
| 1   | G     | 194 | ALA  | 2.0  |
| 1   | B     | 138 | GLY  | 2.0  |
| 1   | J     | 298 | ASP  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | HEM  | I     | 500 | 43/43 | 0.97 | 0.10 | 24,37,57,60                | 0     |
| 2   | HEM  | J     | 500 | 43/43 | 0.97 | 0.10 | 27,42,57,67                | 0     |
| 2   | HEM  | O     | 500 | 43/43 | 0.97 | 0.11 | 48,58,68,80                | 0     |
| 2   | HEM  | G     | 500 | 43/43 | 0.97 | 0.10 | 43,52,63,70                | 0     |
| 2   | HEM  | F     | 500 | 43/43 | 0.97 | 0.11 | 39,47,58,74                | 0     |
| 2   | HEM  | N     | 500 | 43/43 | 0.98 | 0.10 | 37,56,65,74                | 0     |
| 2   | HEM  | D     | 500 | 43/43 | 0.98 | 0.10 | 18,29,37,44                | 0     |
| 2   | HEM  | C     | 500 | 43/43 | 0.98 | 0.09 | 28,42,62,68                | 0     |
| 2   | HEM  | L     | 500 | 43/43 | 0.98 | 0.10 | 20,34,53,63                | 0     |
| 2   | HEM  | A     | 500 | 43/43 | 0.98 | 0.09 | 18,28,39,57                | 0     |
| 2   | HEM  | B     | 500 | 43/43 | 0.98 | 0.10 | 32,43,56,62                | 0     |
| 2   | HEM  | H     | 500 | 43/43 | 0.98 | 0.09 | 16,29,37,43                | 0     |

*Continued on next page...*

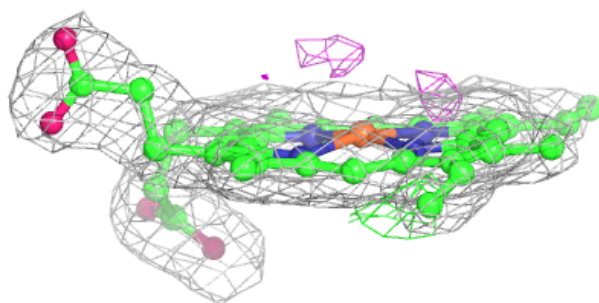
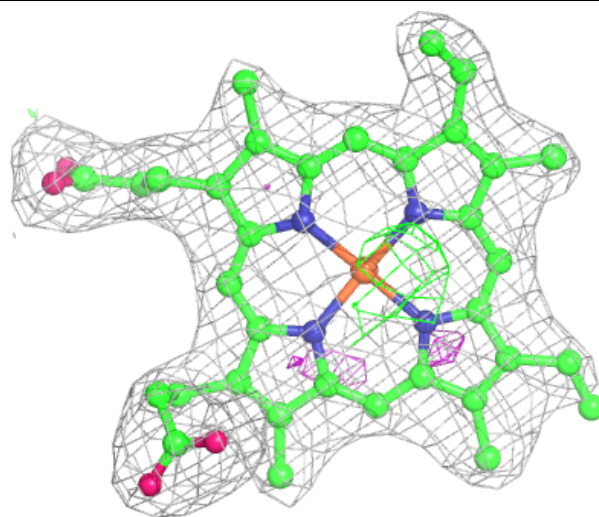
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | HEM  | E     | 500 | 43/43 | 0.98 | 0.09 | 21,32,48,58                 | 0     |
| 2   | HEM  | M     | 500 | 43/43 | 0.98 | 0.10 | 25,37,48,52                 | 0     |
| 2   | HEM  | K     | 500 | 43/43 | 0.98 | 0.10 | 28,43,61,71                 | 0     |
| 2   | HEM  | P     | 500 | 43/43 | 0.99 | 0.08 | 20,31,42,54                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

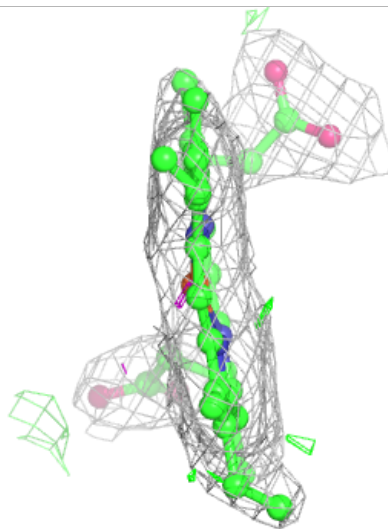
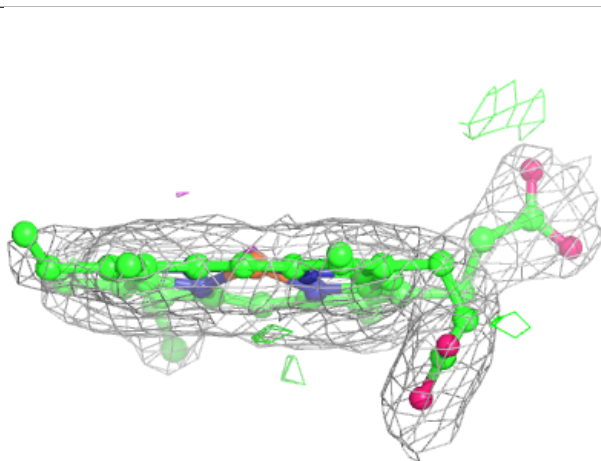
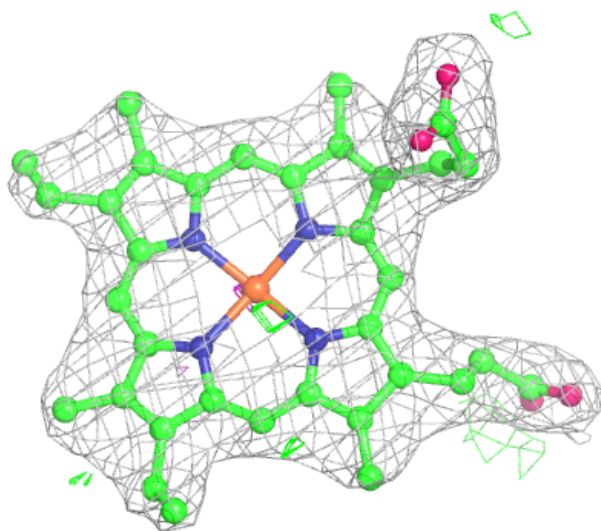
**Electron density around HEM I 500:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



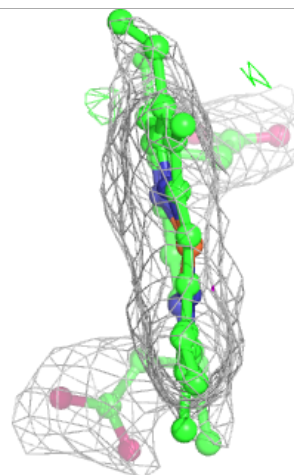
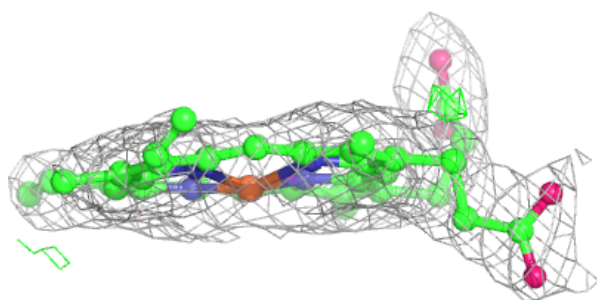
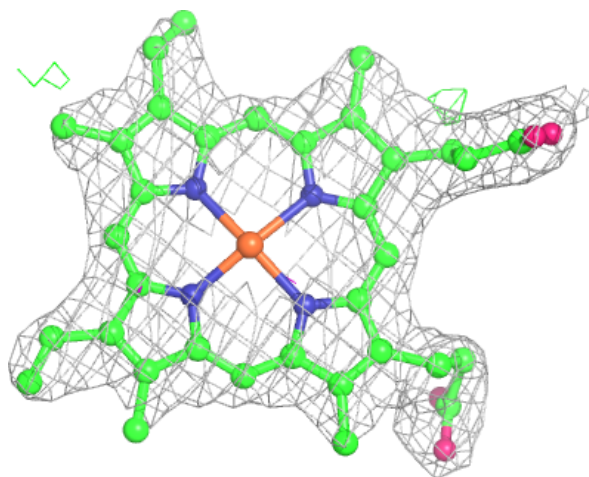
**Electron density around HEM J 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



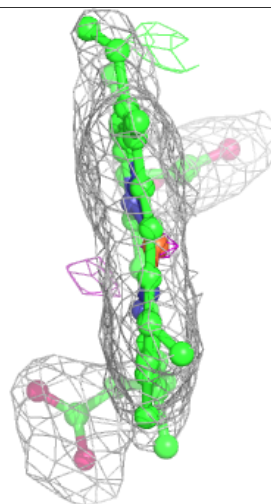
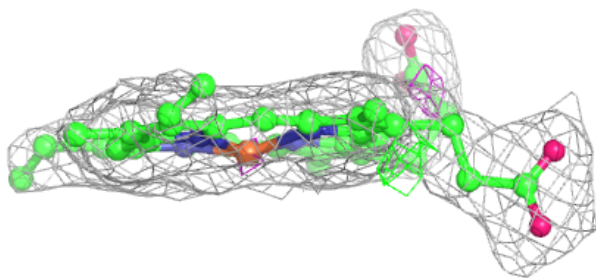
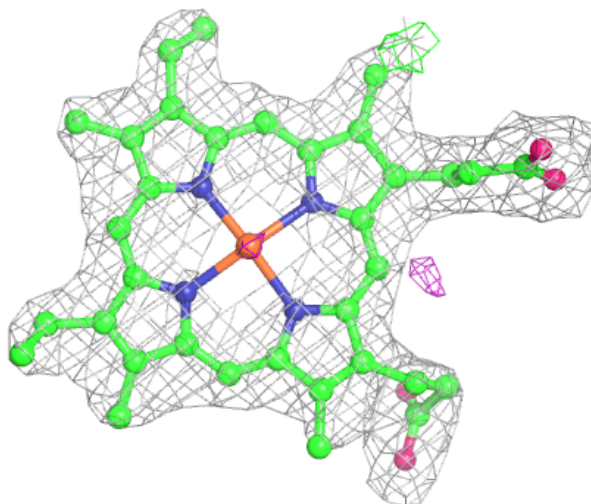
**Electron density around HEM O 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



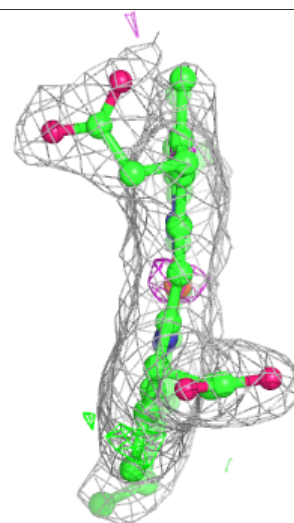
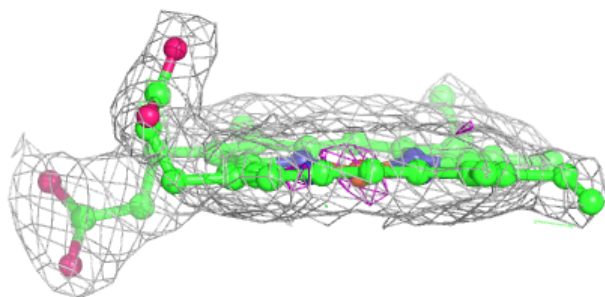
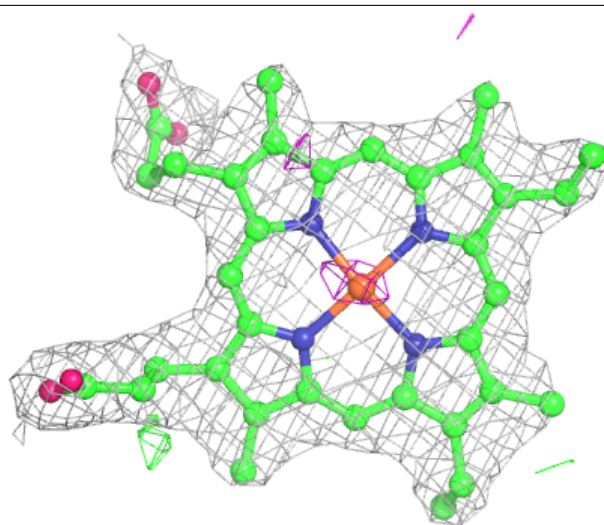
**Electron density around HEM G 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



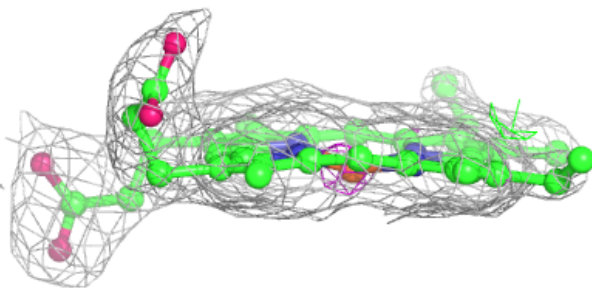
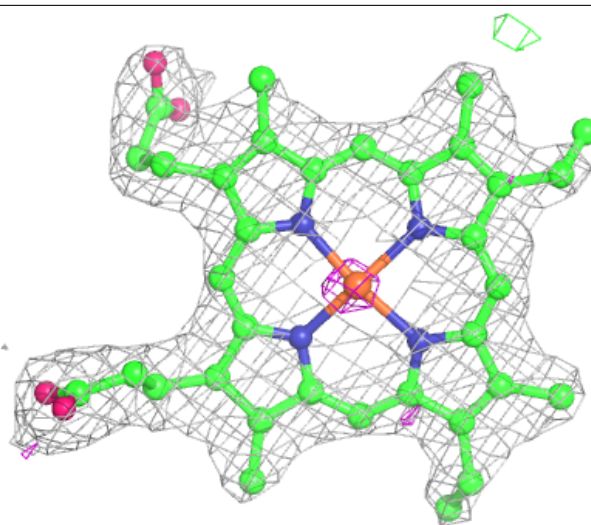
**Electron density around HEM F 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM N 500:**

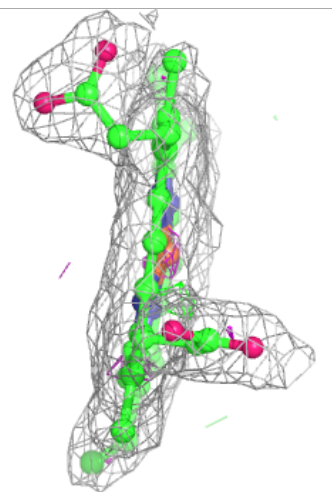
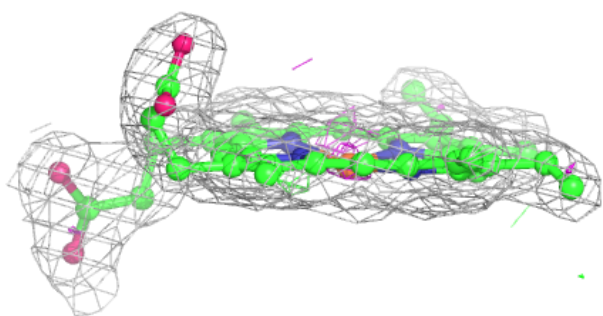
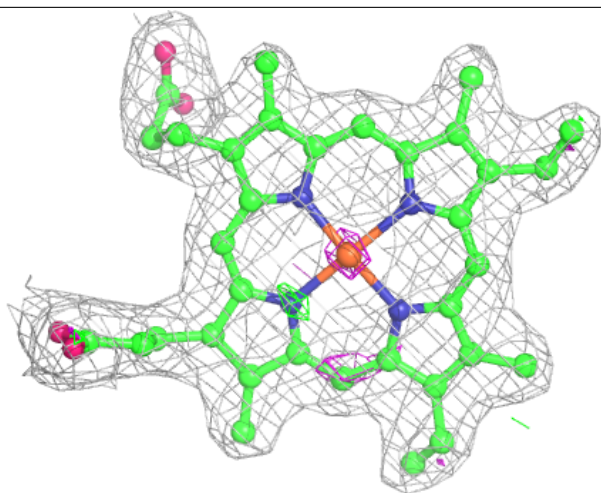
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM D 500:**

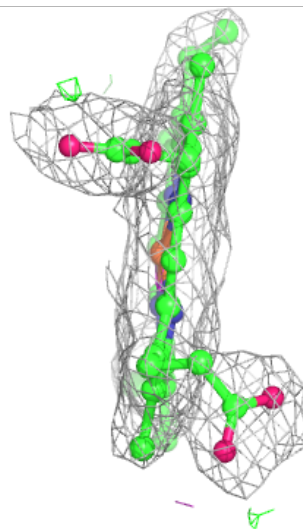
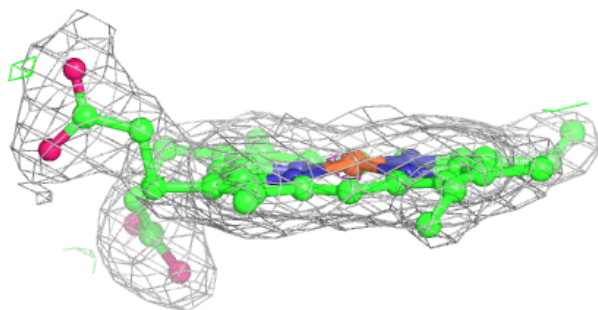
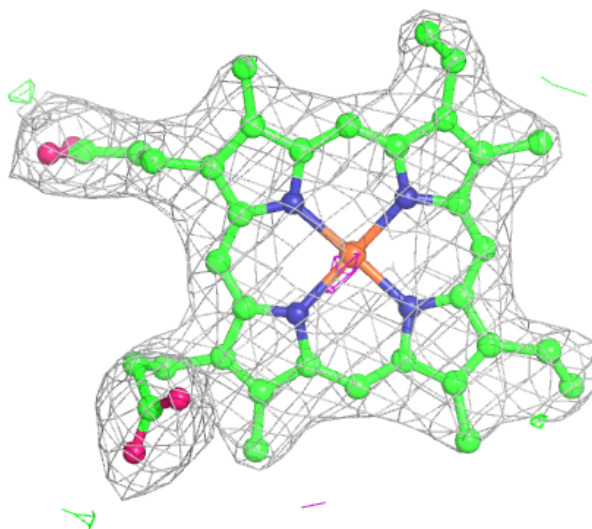
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





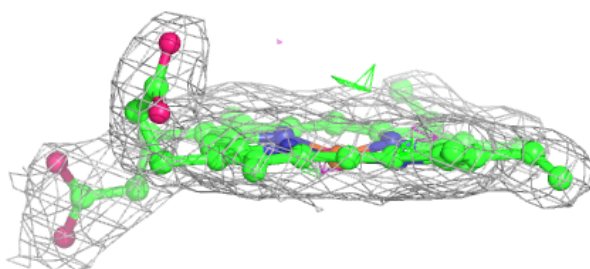
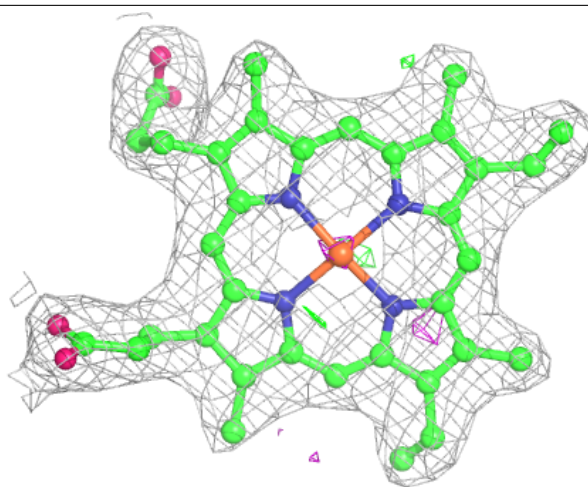
**Electron density around HEM C 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



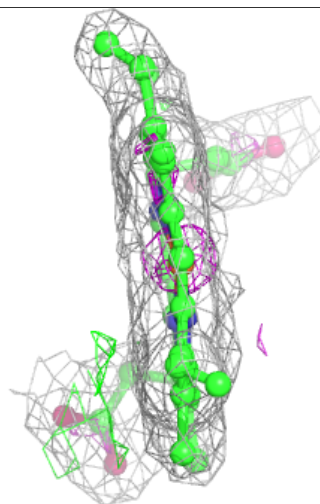
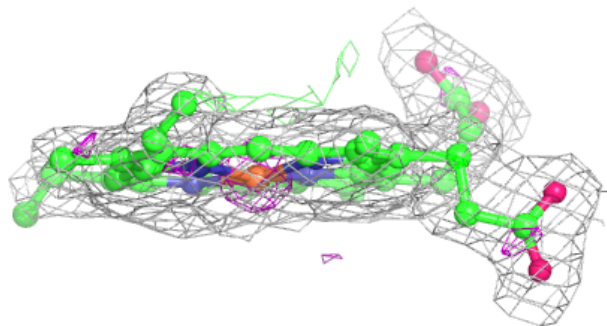
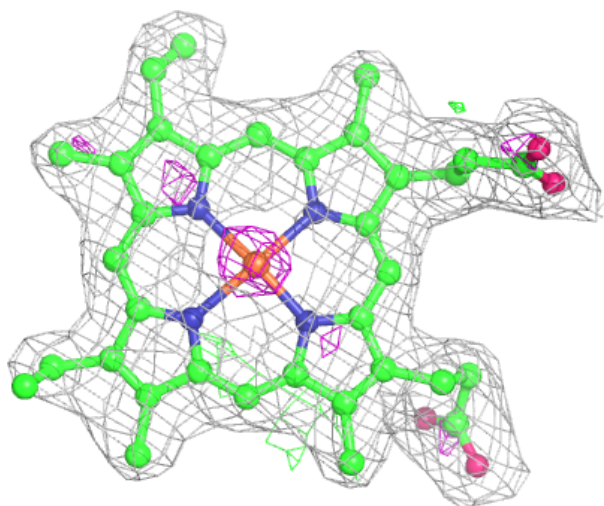
**Electron density around HEM L 500:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



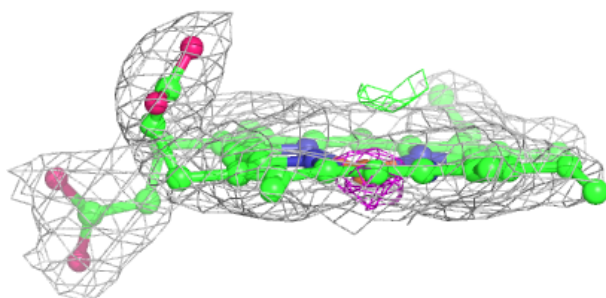
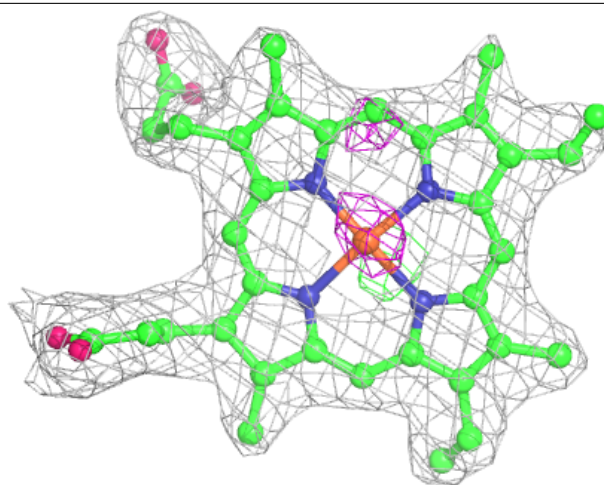
**Electron density around HEM A 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



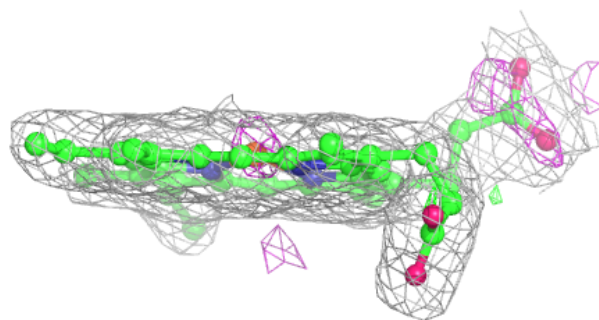
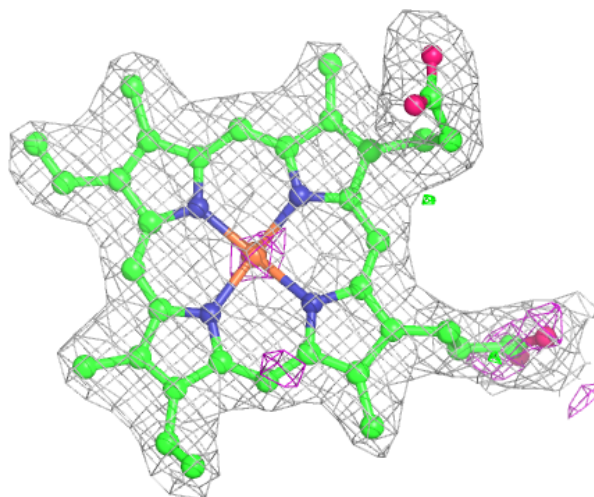
**Electron density around HEM B 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



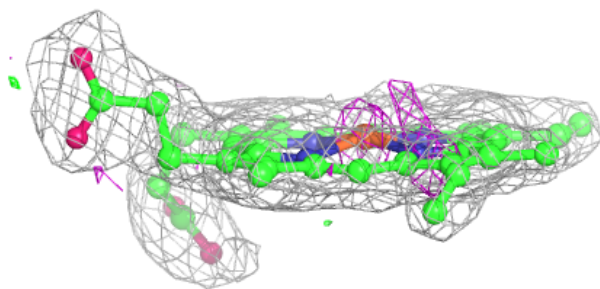
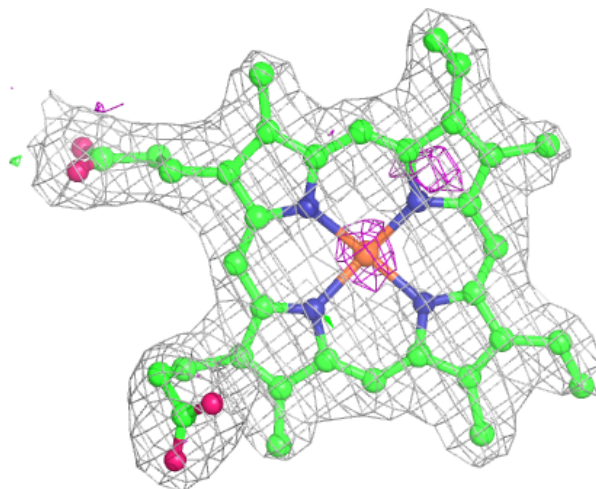
**Electron density around HEM H 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM E 500:**

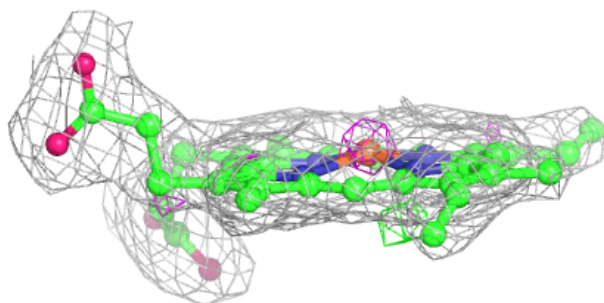
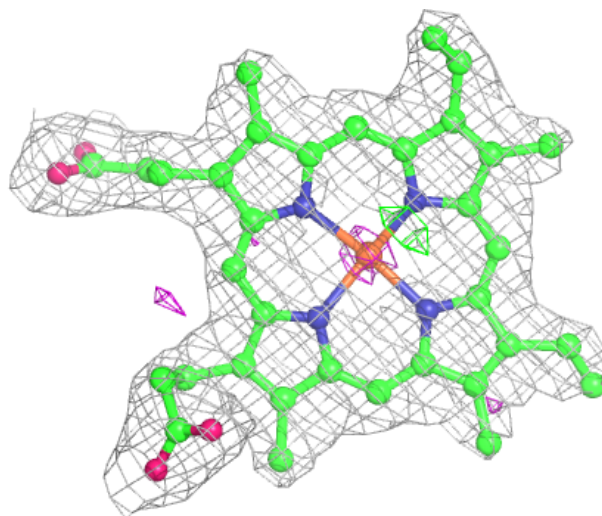
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





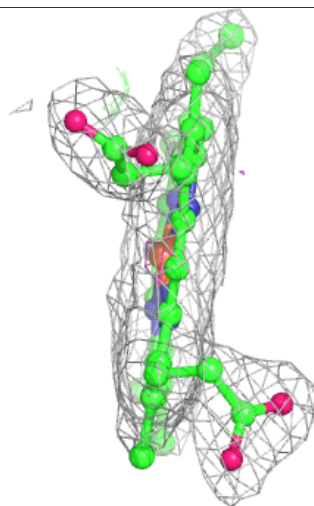
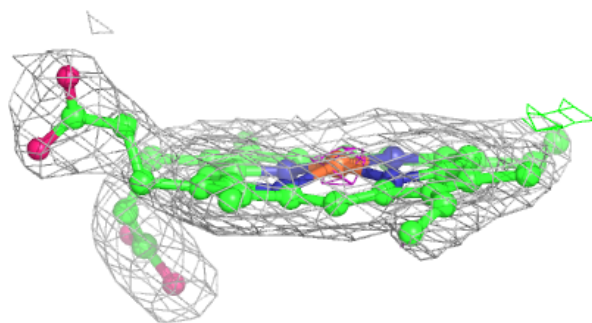
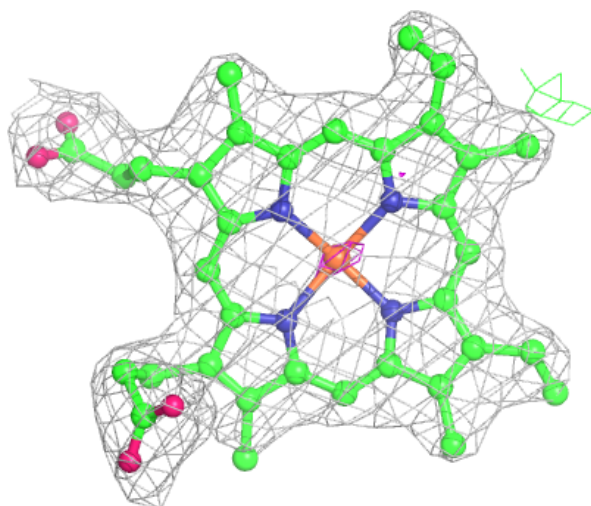
**Electron density around HEM M 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM K 500:**

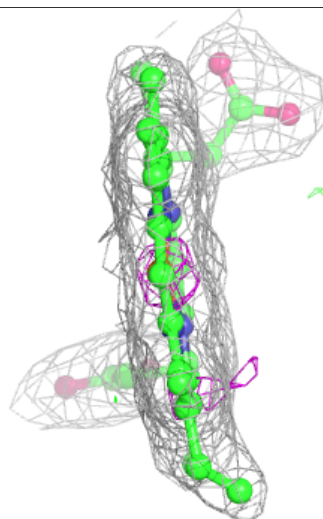
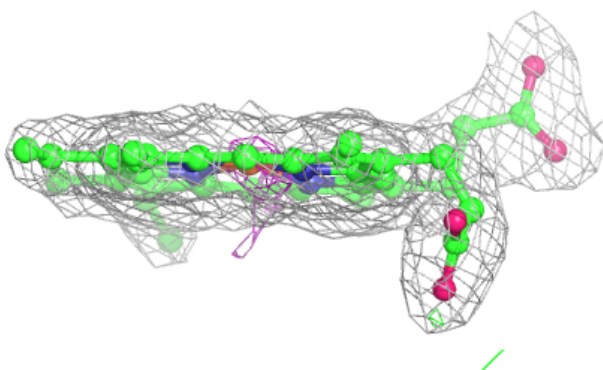
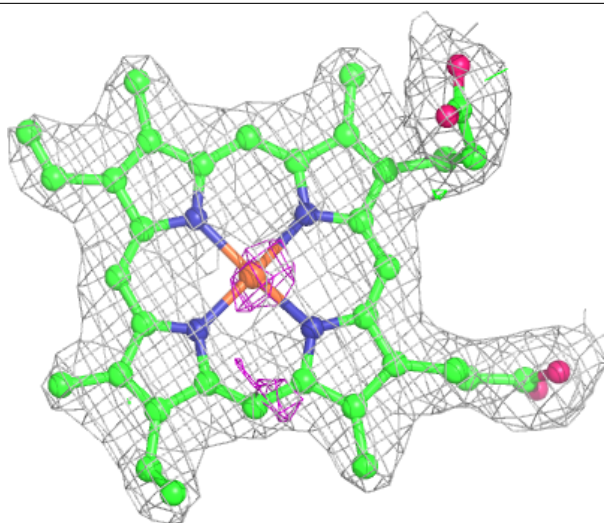
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM P 500:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.