



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 1X9F / pdb\_00001x9f  
Title : Hemoglobin Dodecamer from Lumbricus Erythrocrurin  
Authors : Strand, K.; Knapp, J.E.; Bhayravbhatla, B.; Royer Jr., W.E.  
Deposited on : 2004-08-20  
Resolution : 2.60 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

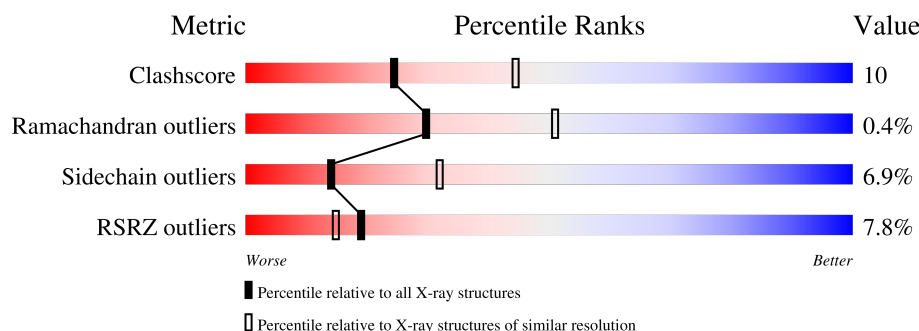
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 4347 (2.60-2.60)                                      |
| Ramachandran outliers | 187476                      | 4277 (2.60-2.60)                                      |
| Sidechain outliers    | 187428                      | 4277 (2.60-2.60)                                      |
| RSRZ outliers         | 180081                      | 4008 (2.60-2.60)                                      |

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 of 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     | 151    | <div> <div>11%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>5%</div> <div>.</div> </div> </div> |
| 1   | E     | 151    | <div> <div>10%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>5%</div> <div>.</div> </div> </div> |
| 1   | I     | 151    | <div> <div>11%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>5%</div> <div>.</div> </div> </div> |
| 2   | B     | 145    | <div> <div>6%</div> <div> <div></div> <div>83%</div> <div>17%</div> <div>.</div> </div> </div>                |
| 2   | F     | 145    | <div> <div>7%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>                |
| 2   | J     | 145    | <div> <div>8%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>                |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | C     | 153    |                  |
| 3   | G     | 153    |                  |
| 3   | K     | 153    |                  |
| 4   | D     | 140    |                  |
| 4   | H     | 140    |                  |
| 4   | L     | 140    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 6   | CMO  | D     | 1164 | -         | -        | X       | -                |
| 6   | CMO  | E     | 2161 | -         | -        | -       | X                |
| 6   | CMO  | F     | 2162 | -         | -        | X       | -                |
| 6   | CMO  | H     | 2164 | -         | -        | X       | -                |
| 6   | CMO  | J     | 3162 | -         | -        | X       | -                |
| 6   | CMO  | L     | 3164 | -         | -        | X       | -                |

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14847 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 Globin IV, extracellular.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1209  | 769 | 222 | 214 | 4 |         |         |       |
| 1   | E     | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1209  | 769 | 222 | 214 | 4 |         |         |       |
| 1   | I     | 147      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1209  | 769 | 222 | 214 | 4 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 78      | LYS      | ASP    | conflict | UNP P13579 |
| E     | 78      | LYS      | ASP    | conflict | UNP P13579 |
| I     | 78      | LYS      | ASP    | conflict | UNP P13579 |

- Molecule 2 is a protein called Globin II, extracellular.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | B     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1148  | 720 | 212 | 213 | 3 |         |         |       |
| 2   | F     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1148  | 720 | 212 | 213 | 3 |         |         |       |
| 2   | J     | 145      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1148  | 720 | 212 | 213 | 3 |         |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 66      | ASP      | GLU    | conflict | UNP P02218 |
| F     | 66      | ASP      | GLU    | conflict | UNP P02218 |
| J     | 66      | ASP      | GLU    | conflict | UNP P02218 |

- Molecule 3 is a protein called Globin III, extracellular.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3   | C     | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1190  | 758 | 212 | 217 | 3 |         |         |       |
| 3   | G     | 149      | Total | C   | N   | O   | S | 5       | 0       | 0     |
|     |       |          | 1190  | 758 | 212 | 217 | 3 |         |         |       |
| 3   | K     | 149      | Total | C   | N   | O   | S | 5       | 0       | 0     |
|     |       |          | 1190  | 758 | 212 | 217 | 3 |         |         |       |

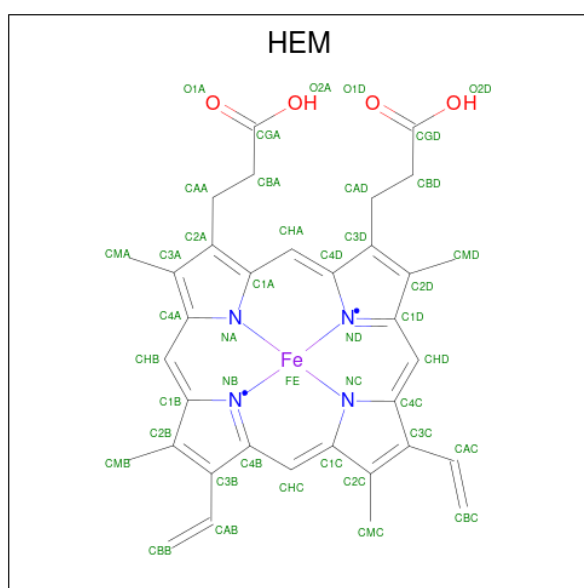
There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 49      | GLU      | ASP    | conflict | UNP P11069 |
| G     | 49      | GLU      | ASP    | conflict | UNP P11069 |
| K     | 49      | GLU      | ASP    | conflict | UNP P11069 |

- Molecule 4 is a protein called hemoglobin chain d1.

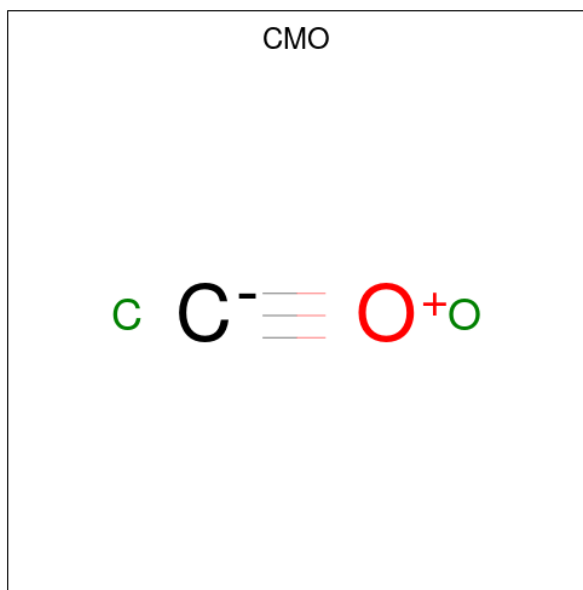
| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 725 | 198 | 202 | 4 |         |         |       |
| 4   | H     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 725 | 198 | 202 | 4 |         |         |       |
| 4   | L     | 140      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 725 | 198 | 202 | 4 |         |         |       |

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



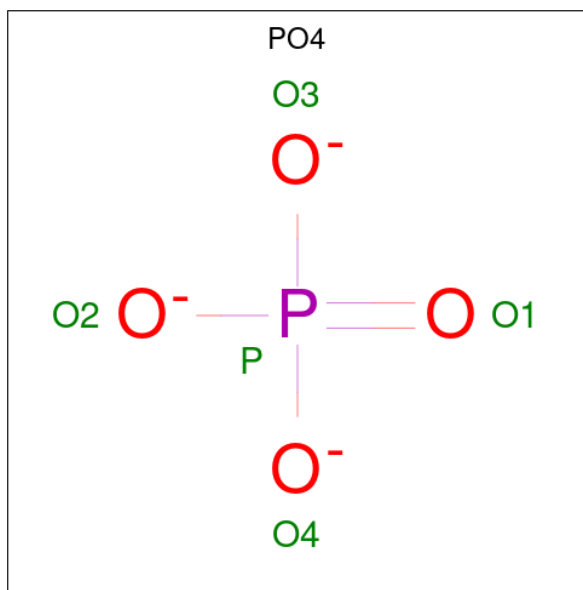
| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 5   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | G     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | I     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | J     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |
| 5   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 0       |

- Molecule 6 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6   | A     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | B     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | C     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | D     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | E     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | F     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | G     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | H     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | I     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | J     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | K     | 1        | Total C O<br>2 1 1 | 0       | 0       |
| 6   | L     | 1        | Total C O<br>2 1 1 | 0       | 0       |

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7   | C     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 7   | G     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 7   | K     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

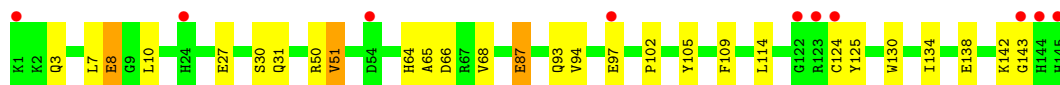
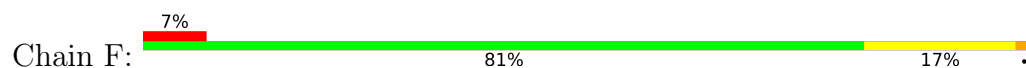
- Molecule 8 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 8   | A     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 8   | B     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 8   | C     | 28       | Total | O  | 0       | 0       |
|     |       |          | 28    | 28 |         |         |
| 8   | D     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 8   | E     | 21       | Total | O  | 0       | 0       |
|     |       |          | 21    | 21 |         |         |
| 8   | F     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 8   | G     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 8   | H     | 22       | Total | O  | 0       | 0       |
|     |       |          | 22    | 22 |         |         |
| 8   | I     | 31       | Total | O  | 0       | 0       |
|     |       |          | 31    | 31 |         |         |
| 8   | J     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 8   | K     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 8   | L     | 20       | Total | O  | 0       | 0       |
|     |       |          | 20    | 20 |         |         |

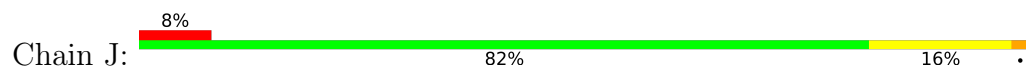




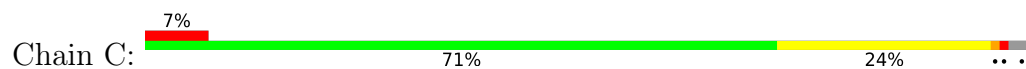
- Molecule 2: Globin II, extracellular



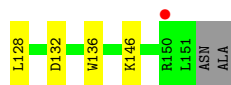
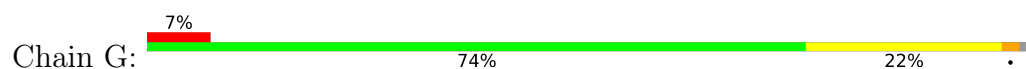
- Molecule 2: Globin II, extracellular



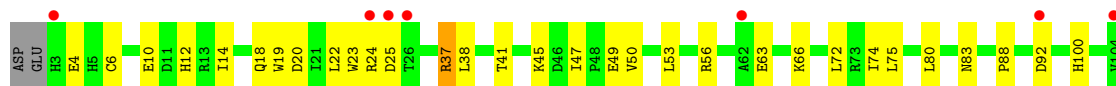
- Molecule 3: Globin III, extracellular



- Molecule 3: Globin III, extracellular

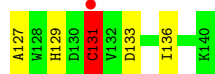
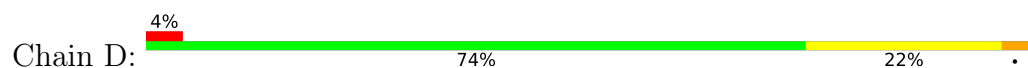


- Molecule 3: Globin III, extracellular

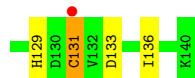
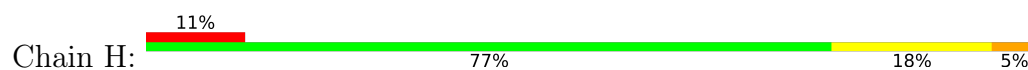




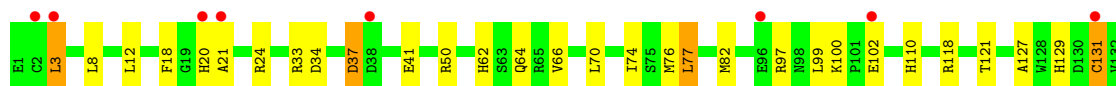
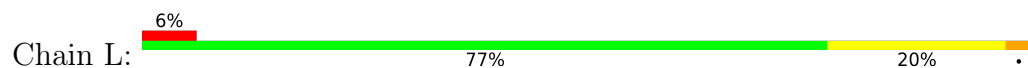
- Molecule 4: hemoglobin chain d1



- Molecule 4: hemoglobin chain d1



- Molecule 4: hemoglobin chain d1



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 139.22Å 172.07Å 202.89Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 105.41 – 2.60<br>105.41 – 2.60                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.7 (105.41-2.60)<br>88.7 (105.41-2.60)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 5.10 (at 2.62Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2, CNS                                             | Depositor        |
| R, $R_{free}$                                                           | 0.213 , 0.246<br>0.213 , (Not available)                    | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 34.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.402                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.36 , 36.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.92                                                        | EDS              |
| Total number of atoms                                                   | 14847                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 34.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CMO, PO4

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     | 0.57         | 2/1237 (0.2%)  | 0.96        | 1/1670 (0.1%)   |
| 1   | E     | 0.54         | 2/1237 (0.2%)  | 0.96        | 5/1670 (0.3%)   |
| 1   | I     | 0.54         | 2/1237 (0.2%)  | 0.94        | 2/1670 (0.1%)   |
| 2   | B     | 0.46         | 0/1176         | 0.90        | 0/1587          |
| 2   | F     | 0.44         | 0/1176         | 0.90        | 0/1587          |
| 2   | J     | 0.42         | 0/1176         | 0.90        | 0/1587          |
| 3   | C     | 0.58         | 2/1214 (0.2%)  | 1.09        | 5/1638 (0.3%)   |
| 3   | G     | 0.45         | 0/1215         | 0.95        | 0/1641          |
| 3   | K     | 0.45         | 0/1215         | 0.92        | 1/1641 (0.1%)   |
| 4   | D     | 0.45         | 0/1159         | 0.91        | 2/1568 (0.1%)   |
| 4   | H     | 0.46         | 0/1159         | 0.93        | 2/1568 (0.1%)   |
| 4   | L     | 0.43         | 0/1159         | 0.93        | 0/1568          |
| All | All   | 0.49         | 8/14360 (0.1%) | 0.94        | 18/19395 (0.1%) |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | C     | 3   | HIS  | CB-CG | 9.57 | 1.63        | 1.50     |
| 1   | E     | 32  | VAL  | N-CA  | 7.92 | 1.55        | 1.46     |
| 3   | C     | 3   | HIS  | CA-CB | 7.29 | 1.68        | 1.53     |
| 1   | A     | 31  | ARG  | C-O   | 6.94 | 1.32        | 1.24     |
| 1   | I     | 31  | ARG  | C-O   | 6.89 | 1.32        | 1.24     |
| 1   | I     | 32  | VAL  | N-CA  | 5.31 | 1.52        | 1.46     |
| 1   | E     | 31  | ARG  | C-O   | 5.23 | 1.30        | 1.24     |
| 1   | A     | 32  | VAL  | N-CA  | 5.10 | 1.52        | 1.46     |

All (18) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | C     | 3   | HIS  | CA-CB-CG | 17.88 | 131.68      | 113.80   |

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| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 3   | C     | 3   | HIS  | N-CA-C  | -16.09 | 65.95       | 111.00   |
| 3   | C     | 3   | HIS  | N-CA-CB | 5.85   | 120.45      | 110.50   |
| 3   | K     | 88  | PRO  | N-CA-C  | 5.58   | 117.51      | 110.70   |
| 1   | E     | 57  | LYS  | N-CA-C  | 5.57   | 119.31      | 111.52   |
| 1   | A     | 63  | SER  | N-CA-C  | 5.44   | 119.17      | 112.54   |
| 1   | E     | 32  | VAL  | N-CA-C  | 5.39   | 116.02      | 110.36   |
| 4   | D     | 20  | HIS  | N-CA-C  | 5.33   | 116.17      | 108.34   |
| 4   | D     | 131 | CYS  | N-CA-C  | 5.25   | 116.69      | 111.07   |
| 1   | E     | 63  | SER  | N-CA-C  | 5.21   | 117.87      | 111.82   |
| 1   | I     | 31  | ARG  | CA-C-N  | -5.21  | 114.00      | 120.56   |
| 1   | I     | 31  | ARG  | C-N-CA  | -5.21  | 114.00      | 120.56   |
| 1   | E     | 31  | ARG  | CA-C-N  | -5.17  | 113.93      | 120.60   |
| 1   | E     | 31  | ARG  | C-N-CA  | -5.17  | 113.93      | 120.60   |
| 4   | H     | 131 | CYS  | N-CA-C  | 5.12   | 117.27      | 111.02   |
| 4   | H     | 20  | HIS  | N-CA-C  | 5.08   | 115.80      | 108.34   |
| 3   | C     | 88  | PRO  | N-CA-C  | 5.06   | 116.88      | 110.70   |
| 3   | C     | 3   | HIS  | CB-CA-C | 5.02   | 119.64      | 110.10   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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     | 1209  | 0        | 1194     | 33      | 0            |
| 1   | E     | 1209  | 0        | 1195     | 32      | 0            |
| 1   | I     | 1209  | 0        | 1194     | 29      | 0            |
| 2   | B     | 1148  | 0        | 1103     | 16      | 0            |
| 2   | F     | 1148  | 0        | 1104     | 20      | 0            |
| 2   | J     | 1148  | 0        | 1103     | 20      | 0            |
| 3   | C     | 1190  | 0        | 1195     | 30      | 0            |
| 3   | G     | 1190  | 0        | 1196     | 27      | 0            |
| 3   | K     | 1190  | 0        | 1196     | 25      | 0            |
| 4   | D     | 1129  | 0        | 1105     | 27      | 0            |
| 4   | H     | 1129  | 0        | 1105     | 23      | 0            |
| 4   | L     | 1129  | 0        | 1105     | 25      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | A     | 43    | 0        | 30       | 1       | 0            |
| 5   | B     | 43    | 0        | 30       | 0       | 0            |
| 5   | C     | 43    | 0        | 30       | 5       | 0            |
| 5   | D     | 43    | 0        | 30       | 4       | 0            |
| 5   | E     | 43    | 0        | 30       | 1       | 0            |
| 5   | F     | 43    | 0        | 30       | 1       | 0            |
| 5   | G     | 43    | 0        | 30       | 3       | 0            |
| 5   | H     | 43    | 0        | 30       | 3       | 0            |
| 5   | I     | 43    | 0        | 30       | 1       | 0            |
| 5   | J     | 43    | 0        | 30       | 0       | 0            |
| 5   | K     | 43    | 0        | 30       | 5       | 0            |
| 5   | L     | 43    | 0        | 30       | 3       | 0            |
| 6   | A     | 2     | 0        | 0        | 0       | 0            |
| 6   | B     | 2     | 0        | 0        | 1       | 0            |
| 6   | C     | 2     | 0        | 0        | 0       | 0            |
| 6   | D     | 2     | 0        | 0        | 2       | 0            |
| 6   | E     | 2     | 0        | 0        | 0       | 0            |
| 6   | F     | 2     | 0        | 0        | 2       | 0            |
| 6   | G     | 2     | 0        | 0        | 0       | 0            |
| 6   | H     | 2     | 0        | 0        | 2       | 0            |
| 6   | I     | 2     | 0        | 0        | 1       | 0            |
| 6   | J     | 2     | 0        | 0        | 3       | 0            |
| 6   | K     | 2     | 0        | 0        | 0       | 0            |
| 6   | L     | 2     | 0        | 0        | 2       | 0            |
| 7   | C     | 5     | 0        | 0        | 0       | 0            |
| 7   | G     | 5     | 0        | 0        | 1       | 0            |
| 7   | K     | 5     | 0        | 0        | 0       | 0            |
| 8   | A     | 26    | 0        | 0        | 0       | 0            |
| 8   | B     | 31    | 0        | 0        | 0       | 0            |
| 8   | C     | 28    | 0        | 0        | 3       | 0            |
| 8   | D     | 18    | 0        | 0        | 0       | 0            |
| 8   | E     | 21    | 0        | 0        | 1       | 0            |
| 8   | F     | 23    | 0        | 0        | 0       | 0            |
| 8   | G     | 26    | 0        | 0        | 0       | 0            |
| 8   | H     | 22    | 0        | 0        | 0       | 0            |
| 8   | I     | 31    | 0        | 0        | 0       | 0            |
| 8   | J     | 13    | 0        | 0        | 1       | 0            |
| 8   | K     | 5     | 0        | 0        | 0       | 0            |
| 8   | L     | 20    | 0        | 0        | 1       | 0            |
| All | All   | 14847 | 0        | 14155    | 283     | 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 10.

All (283) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:C:3:HIS:ND1    | 3:C:4:GLU:HG2    | 1.76                     | 0.99              |
| 4:H:50:ARG:HG2   | 4:H:50:ARG:HH11  | 1.33                     | 0.90              |
| 1:A:110:GLU:HG3  | 1:A:113:ARG:HH22 | 1.34                     | 0.90              |
| 3:K:108:VAL:HG13 | 5:K:160:HEM:HBC2 | 1.57                     | 0.85              |
| 3:G:18:GLN:HE21  | 3:G:136:TRP:HE1  | 1.26                     | 0.83              |
| 1:A:110:GLU:HG3  | 1:A:113:ARG:NH2  | 1.94                     | 0.82              |
| 5:H:160:HEM:HHD  | 5:H:160:HEM:HBC2 | 1.61                     | 0.81              |
| 1:A:19:TRP:HE1   | 1:A:78:LYS:HD3   | 1.46                     | 0.80              |
| 3:C:108:VAL:HG13 | 5:C:160:HEM:HBC2 | 1.61                     | 0.80              |
| 3:K:18:GLN:HE21  | 3:K:136:TRP:HE1  | 1.29                     | 0.79              |
| 3:C:18:GLN:HE21  | 3:C:136:TRP:HE1  | 1.29                     | 0.77              |
| 4:D:118:ARG:HH11 | 4:D:118:ARG:HG2  | 1.51                     | 0.76              |
| 4:L:118:ARG:HG2  | 4:L:118:ARG:HH11 | 1.51                     | 0.75              |
| 1:I:19:TRP:HE1   | 1:I:78:LYS:HD3   | 1.51                     | 0.75              |
| 4:D:50:ARG:HG2   | 4:D:50:ARG:HH11  | 1.52                     | 0.74              |
| 1:E:5:ASP:N      | 8:E:2170:HOH:O   | 2.21                     | 0.73              |
| 4:L:129:HIS:O    | 4:L:133:ASP:HB2  | 1.88                     | 0.73              |
| 1:I:78:LYS:HE3   | 4:L:24:ARG:HH22  | 1.55                     | 0.72              |
| 2:F:51:VAL:HG21  | 2:F:64:HIS:HB2   | 1.71                     | 0.71              |
| 4:D:129:HIS:O    | 4:D:133:ASP:HB2  | 1.90                     | 0.71              |
| 4:H:20:HIS:O     | 4:H:24:ARG:HG3   | 1.91                     | 0.71              |
| 4:H:129:HIS:O    | 4:H:133:ASP:HB2  | 1.90                     | 0.71              |
| 3:C:50:VAL:HA    | 3:C:53:LEU:HD12  | 1.72                     | 0.71              |
| 1:I:28:THR:HG21  | 1:I:71:VAL:HG21  | 1.74                     | 0.70              |
| 3:K:22:LEU:HG    | 3:K:128:LEU:HD21 | 1.74                     | 0.69              |
| 1:E:78:LYS:HD2   | 1:E:82:ASN:ND2   | 2.08                     | 0.69              |
| 1:A:28:THR:HG21  | 1:A:71:VAL:HG21  | 1.76                     | 0.68              |
| 3:K:18:GLN:HE22  | 3:K:132:ASP:H    | 1.42                     | 0.67              |
| 3:C:3:HIS:N      | 8:C:1185:HOH:O   | 2.28                     | 0.67              |
| 3:G:37:ARG:HG3   | 3:G:37:ARG:HH11  | 1.60                     | 0.67              |
| 1:E:19:TRP:HE1   | 1:E:78:LYS:HD3   | 1.59                     | 0.66              |
| 2:J:3:GLN:O      | 2:J:8:GLU:HG3    | 1.95                     | 0.66              |
| 3:K:10:GLU:O     | 3:K:14:ILE:HG12  | 1.95                     | 0.66              |
| 4:L:66:VAL:HG22  | 6:L:3164:CMO:C   | 2.26                     | 0.66              |
| 4:L:76:MET:HE2   | 4:L:82:MET:HE2   | 1.77                     | 0.66              |
| 2:B:34:TRP:CZ2   | 6:B:1162:CMO:O   | 2.49                     | 0.65              |
| 5:D:160:HEM:HBC2 | 5:D:160:HEM:HHD  | 1.78                     | 0.64              |
| 1:I:109:LYS:HG3  | 1:I:151:PRO:HD3  | 1.79                     | 0.64              |
| 3:G:22:LEU:HG    | 3:G:128:LEU:HD21 | 1.80                     | 0.64              |
| 4:D:76:MET:HE2   | 4:D:82:MET:HE2   | 1.80                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:G:37:ARG:HG3   | 3:G:37:ARG:NH1   | 2.14                     | 0.63              |
| 1:E:79:LEU:HD22  | 1:E:83:LEU:HD22  | 1.81                     | 0.62              |
| 1:A:79:LEU:HD22  | 1:A:83:LEU:HD22  | 1.80                     | 0.62              |
| 1:E:18:ILE:HG21  | 1:E:130:PHE:HE1  | 1.64                     | 0.62              |
| 4:H:33:ARG:O     | 4:H:37:ASP:HB2   | 2.00                     | 0.61              |
| 1:A:23:TRP:CH2   | 1:A:31:ARG:HD3   | 2.36                     | 0.61              |
| 3:C:22:LEU:HG    | 3:C:128:LEU:HD21 | 1.83                     | 0.61              |
| 2:B:3:GLN:O      | 2:B:8:GLU:HG3    | 2.01                     | 0.60              |
| 4:D:20:HIS:O     | 4:D:24:ARG:HG3   | 2.02                     | 0.60              |
| 3:G:108:VAL:HG13 | 5:G:160:HEM:HBC2 | 1.83                     | 0.60              |
| 4:H:50:ARG:HG2   | 4:H:50:ARG:NH1   | 2.09                     | 0.60              |
| 1:E:129:CYS:HG   | 2:F:124:CYS:HG   | 1.50                     | 0.59              |
| 1:I:78:LYS:HD2   | 1:I:82:ASN:ND2   | 2.17                     | 0.59              |
| 3:C:24:ARG:HE    | 3:C:24:ARG:HA    | 1.68                     | 0.59              |
| 3:C:18:GLN:NE2   | 3:C:136:TRP:HE1  | 2.00                     | 0.58              |
| 1:I:23:TRP:CH2   | 1:I:31:ARG:HD3   | 2.38                     | 0.58              |
| 3:G:18:GLN:NE2   | 3:G:136:TRP:HE1  | 2.00                     | 0.58              |
| 2:J:143:GLY:HA2  | 8:J:3170:HOH:O   | 2.04                     | 0.58              |
| 1:E:18:ILE:HG21  | 1:E:130:PHE:CE1  | 2.38                     | 0.57              |
| 3:G:18:GLN:HE22  | 3:G:132:ASP:H    | 1.53                     | 0.57              |
| 4:L:100:LYS:H    | 4:L:100:LYS:HD2  | 1.70                     | 0.57              |
| 1:E:25:SER:HA    | 3:G:25:ASP:HB2   | 1.87                     | 0.56              |
| 1:A:24:SER:O     | 1:A:25:SER:O     | 2.24                     | 0.56              |
| 1:A:25:SER:HA    | 3:C:25:ASP:HB2   | 1.86                     | 0.56              |
| 1:I:79:LEU:HD22  | 1:I:83:LEU:HD22  | 1.87                     | 0.56              |
| 2:J:66:ASP:HB3   | 3:K:80:LEU:CD1   | 2.35                     | 0.56              |
| 3:G:127:VAL:HB   | 4:H:8:LEU:HD12   | 1.87                     | 0.56              |
| 1:E:18:ILE:HG23  | 1:E:127:LEU:HD11 | 1.88                     | 0.56              |
| 2:J:51:VAL:HG21  | 2:J:64:HIS:HB2   | 1.87                     | 0.56              |
| 4:D:107:PHE:CE2  | 5:D:160:HEM:HBB1 | 2.40                     | 0.55              |
| 3:G:108:VAL:HG22 | 5:G:160:HEM:HBC2 | 1.89                     | 0.55              |
| 1:I:79:LEU:HD21  | 4:L:64:GLN:HB3   | 1.88                     | 0.55              |
| 4:L:20:HIS:O     | 4:L:24:ARG:HG3   | 2.07                     | 0.55              |
| 3:K:18:GLN:NE2   | 3:K:136:TRP:HE1  | 2.02                     | 0.55              |
| 4:H:76:MET:HE2   | 4:H:82:MET:HE2   | 1.88                     | 0.54              |
| 2:J:87:GLU:HG2   | 3:K:66:LYS:HA    | 1.90                     | 0.54              |
| 1:A:123:LEU:N    | 1:A:124:PRO:HD2  | 2.22                     | 0.54              |
| 2:B:51:VAL:HG21  | 2:B:64:HIS:HB2   | 1.89                     | 0.54              |
| 3:C:144:LEU:HD21 | 5:C:160:HEM:HBB1 | 1.88                     | 0.54              |
| 4:D:118:ARG:HG2  | 4:D:118:ARG:NH1  | 2.20                     | 0.54              |
| 1:E:79:LEU:HD21  | 4:H:64:GLN:HB3   | 1.89                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:D:66:VAL:HG22  | 6:D:1164:CMO:C   | 2.37                     | 0.54              |
| 4:D:99:LEU:HD22  | 5:D:160:HEM:CBC  | 2.38                     | 0.54              |
| 1:E:28:THR:HG21  | 1:E:71:VAL:HG21  | 1.90                     | 0.54              |
| 3:K:22:LEU:HG    | 3:K:128:LEU:CD2  | 2.38                     | 0.54              |
| 2:F:68:VAL:HG22  | 6:F:2162:CMO:C   | 2.37                     | 0.53              |
| 2:F:114:LEU:HD11 | 2:F:130:TRP:HB3  | 1.90                     | 0.53              |
| 1:I:18:ILE:HG21  | 1:I:130:PHE:CE1  | 2.43                     | 0.53              |
| 2:F:87:GLU:OE2   | 3:G:66:LYS:HE3   | 2.09                     | 0.53              |
| 2:B:66:ASP:HB3   | 3:C:80:LEU:CD1   | 2.39                     | 0.53              |
| 3:K:144:LEU:CD2  | 5:K:160:HEM:HBB1 | 2.38                     | 0.53              |
| 1:A:79:LEU:HD21  | 4:D:64:GLN:HB3   | 1.91                     | 0.53              |
| 1:E:120:ALA:HB2  | 1:E:136:ASN:HD21 | 1.73                     | 0.53              |
| 1:E:131:ASN:C    | 1:E:131:ASN:HD22 | 2.17                     | 0.53              |
| 5:L:160:HEM:HBC2 | 5:L:160:HEM:HHD  | 1.91                     | 0.53              |
| 1:E:24:SER:O     | 1:E:25:SER:O     | 2.27                     | 0.52              |
| 3:K:24:ARG:HE    | 3:K:24:ARG:HA    | 1.74                     | 0.52              |
| 4:L:62:HIS:O     | 4:L:66:VAL:HG23  | 2.09                     | 0.52              |
| 4:L:74:ILE:HA    | 4:L:77:LEU:HD22  | 1.90                     | 0.52              |
| 4:L:118:ARG:HG2  | 4:L:118:ARG:NH1  | 2.22                     | 0.52              |
| 4:H:20:HIS:O     | 4:H:24:ARG:CG    | 2.57                     | 0.52              |
| 4:H:62:HIS:NE2   | 6:H:2164:CMO:O   | 2.42                     | 0.52              |
| 1:I:123:LEU:N    | 1:I:124:PRO:HD2  | 2.25                     | 0.52              |
| 2:J:102:PRO:HD2  | 2:J:105:TYR:CD1  | 2.44                     | 0.52              |
| 2:F:3:GLN:O      | 2:F:8:GLU:HG3    | 2.09                     | 0.52              |
| 3:K:100:HIS:CE1  | 3:K:150:ARG:CZ   | 2.93                     | 0.52              |
| 4:L:99:LEU:HD22  | 5:L:160:HEM:CBC  | 2.40                     | 0.52              |
| 4:H:62:HIS:O     | 4:H:66:VAL:HG23  | 2.10                     | 0.52              |
| 1:I:110:GLU:HG3  | 1:I:113:ARG:NH2  | 2.25                     | 0.51              |
| 3:C:100:HIS:CE1  | 3:C:150:ARG:CZ   | 2.94                     | 0.51              |
| 2:B:145:HIS:H    | 2:B:145:HIS:CD2  | 2.27                     | 0.51              |
| 4:D:66:VAL:CG2   | 6:D:1164:CMO:C   | 2.88                     | 0.51              |
| 1:E:123:LEU:N    | 1:E:124:PRO:HD2  | 2.26                     | 0.51              |
| 1:E:98:ALA:O     | 1:E:102:ILE:HG13 | 2.11                     | 0.50              |
| 3:G:47:ILE:HG22  | 3:G:49:GLU:HG2   | 1.92                     | 0.50              |
| 2:B:109:PHE:CE1  | 2:B:113:ILE:HD11 | 2.46                     | 0.50              |
| 1:A:150:LEU:N    | 1:A:151:PRO:HD2  | 2.27                     | 0.50              |
| 4:L:33:ARG:O     | 4:L:37:ASP:HB2   | 2.13                     | 0.49              |
| 4:H:107:PHE:CE2  | 5:H:160:HEM:HBB1 | 2.47                     | 0.49              |
| 1:E:109:LYS:NZ   | 1:E:151:PRO:HD3  | 2.27                     | 0.49              |
| 3:K:144:LEU:HD23 | 5:K:160:HEM:HBB1 | 1.94                     | 0.49              |
| 4:L:66:VAL:CG2   | 6:L:3164:CMO:C   | 2.91                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:J:109:PHE:CE1  | 2:J:113:ILE:HD11 | 2.47                     | 0.49              |
| 3:K:108:VAL:CG1  | 5:K:160:HEM:HBC2 | 2.38                     | 0.49              |
| 3:C:47:ILE:HG22  | 3:C:49:GLU:HG2   | 1.94                     | 0.49              |
| 4:D:7:SER:O      | 4:D:11:LYS:HG3   | 2.12                     | 0.49              |
| 2:B:74:ILE:HG23  | 3:C:72:LEU:HD13  | 1.93                     | 0.49              |
| 3:C:10:GLU:O     | 3:C:14:ILE:HG12  | 2.13                     | 0.49              |
| 3:C:18:GLN:HE22  | 3:C:132:ASP:H    | 1.59                     | 0.49              |
| 2:J:68:VAL:HG22  | 6:J:3162:CMO:C   | 2.43                     | 0.49              |
| 2:F:68:VAL:CG2   | 6:F:2162:CMO:C   | 2.91                     | 0.48              |
| 3:G:124:LEU:N    | 3:G:125:PRO:HD2  | 2.27                     | 0.48              |
| 1:A:83:LEU:HD11  | 4:D:64:GLN:HG3   | 1.95                     | 0.48              |
| 2:B:93:GLN:HE21  | 2:B:143:GLY:HA3  | 1.78                     | 0.48              |
| 1:I:83:LEU:HD11  | 4:L:64:GLN:HG3   | 1.95                     | 0.48              |
| 2:F:64:HIS:O     | 2:F:68:VAL:HG23  | 2.11                     | 0.48              |
| 1:A:107:VAL:HG13 | 5:A:160:HEM:HAC  | 1.95                     | 0.48              |
| 3:C:144:LEU:CD2  | 5:C:160:HEM:HBB1 | 2.44                     | 0.48              |
| 1:A:131:ASN:C    | 1:A:131:ASN:HD22 | 2.22                     | 0.48              |
| 4:D:96:GLU:HA    | 4:D:96:GLU:OE1   | 2.14                     | 0.48              |
| 4:D:50:ARG:HD3   | 4:D:58:GLU:OE1   | 2.14                     | 0.48              |
| 1:E:19:TRP:NE1   | 1:E:78:LYS:HD3   | 2.28                     | 0.48              |
| 2:F:93:GLN:HE21  | 2:F:143:GLY:HA3  | 1.78                     | 0.48              |
| 3:G:8:SER:N      | 3:G:11:ASP:HB2   | 2.28                     | 0.48              |
| 3:K:47:ILE:HG22  | 3:K:49:GLU:HG2   | 1.95                     | 0.48              |
| 2:B:5:GLY:H      | 2:B:8:GLU:CG     | 2.26                     | 0.48              |
| 4:L:99:LEU:HD22  | 5:L:160:HEM:HBC2 | 1.94                     | 0.48              |
| 4:D:18:PHE:CZ    | 4:D:24:ARG:HD3   | 2.49                     | 0.47              |
| 4:D:33:ARG:O     | 4:D:37:ASP:HB2   | 2.14                     | 0.47              |
| 4:H:74:ILE:HA    | 4:H:77:LEU:HD22  | 1.94                     | 0.47              |
| 2:B:64:HIS:O     | 2:B:68:VAL:HG23  | 2.13                     | 0.47              |
| 3:G:10:GLU:O     | 3:G:14:ILE:HG12  | 2.14                     | 0.47              |
| 3:G:37:ARG:HH11  | 3:G:37:ARG:CG    | 2.26                     | 0.47              |
| 1:I:78:LYS:HE3   | 4:L:24:ARG:NH2   | 2.27                     | 0.47              |
| 2:J:93:GLN:HE21  | 2:J:143:GLY:HA3  | 1.79                     | 0.47              |
| 4:L:100:LYS:HB3  | 4:L:102:GLU:CD   | 2.39                     | 0.47              |
| 1:I:18:ILE:HG21  | 1:I:130:PHE:HE1  | 1.77                     | 0.47              |
| 1:E:23:TRP:CH2   | 1:E:31:ARG:HD3   | 2.49                     | 0.47              |
| 3:G:22:LEU:HG    | 3:G:128:LEU:CD2  | 2.43                     | 0.47              |
| 1:A:22:VAL:HG23  | 1:A:23:TRP:N     | 2.29                     | 0.47              |
| 2:J:22:SER:HB2   | 3:K:83:ASN:OD1   | 2.15                     | 0.47              |
| 4:D:99:LEU:HD22  | 5:D:160:HEM:HBC2 | 1.96                     | 0.47              |
| 2:F:50:ARG:NH1   | 7:G:154:PO4:O2   | 2.47                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:94:VAL:HA    | 2:F:97:GLU:HG2   | 1.97                     | 0.47              |
| 1:I:28:THR:CG2   | 1:I:71:VAL:HG21  | 2.44                     | 0.47              |
| 3:G:108:VAL:HG13 | 5:G:160:HEM:CBC  | 2.45                     | 0.47              |
| 3:K:50:VAL:HA    | 3:K:53:LEU:HD12  | 1.97                     | 0.47              |
| 4:L:50:ARG:NE    | 8:L:3168:HOH:O   | 2.48                     | 0.47              |
| 2:B:106:PHE:CE1  | 2:B:142:LYS:HG2  | 2.50                     | 0.46              |
| 1:I:120:ALA:HB2  | 1:I:136:ASN:HD21 | 1.80                     | 0.46              |
| 3:K:37:ARG:HH22  | 3:K:63:GLU:HB3   | 1.80                     | 0.46              |
| 2:B:87:GLU:HG2   | 3:C:66:LYS:HA    | 1.97                     | 0.46              |
| 3:C:22:LEU:HG    | 3:C:128:LEU:CD2  | 2.46                     | 0.46              |
| 1:E:107:VAL:HG13 | 5:E:160:HEM:HAC  | 1.97                     | 0.46              |
| 1:I:69:HIS:O     | 1:I:73:VAL:HG23  | 2.15                     | 0.46              |
| 2:J:68:VAL:CG2   | 6:J:3162:CMO:C   | 2.94                     | 0.46              |
| 3:C:127:VAL:HB   | 4:D:8:LEU:HD12   | 1.98                     | 0.46              |
| 1:E:57:LYS:HD2   | 1:E:65:GLU:HG3   | 1.98                     | 0.46              |
| 2:F:30:SER:HB3   | 2:F:65:ALA:HB1   | 1.96                     | 0.46              |
| 1:I:73:VAL:HG22  | 6:I:3161:CMO:C   | 2.45                     | 0.46              |
| 1:A:78:LYS:HD2   | 1:A:82:ASN:ND2   | 2.30                     | 0.46              |
| 1:E:147:ALA:HA   | 1:E:150:LEU:HD12 | 1.98                     | 0.46              |
| 4:H:18:PHE:CE1   | 4:H:24:ARG:HG2   | 2.50                     | 0.46              |
| 4:H:34:ASP:HB3   | 4:H:110:HIS:CD2  | 2.51                     | 0.46              |
| 3:K:108:VAL:HG13 | 5:K:160:HEM:CBC  | 2.38                     | 0.46              |
| 4:D:74:ILE:HA    | 4:D:77:LEU:HD22  | 1.98                     | 0.45              |
| 4:L:3:LEU:HD23   | 4:L:3:LEU:H      | 1.80                     | 0.45              |
| 1:I:150:LEU:N    | 1:I:151:PRO:HD2  | 2.32                     | 0.45              |
| 1:A:18:ILE:HG21  | 1:A:130:PHE:HE1  | 1.82                     | 0.45              |
| 2:F:27:GLU:O     | 2:F:31:GLN:HG3   | 2.17                     | 0.45              |
| 1:I:58:ILE:HG23  | 1:I:66:PHE:CE1   | 2.51                     | 0.45              |
| 4:D:127:ALA:O    | 4:D:131:CYS:HB2  | 2.17                     | 0.45              |
| 4:H:66:VAL:HG22  | 6:H:2164:CMO:C   | 2.46                     | 0.45              |
| 2:J:64:HIS:O     | 2:J:68:VAL:HG23  | 2.17                     | 0.45              |
| 1:A:150:LEU:N    | 1:A:151:PRO:CD   | 2.80                     | 0.44              |
| 3:C:10:GLU:HB2   | 1:I:10:GLU:CD    | 2.42                     | 0.44              |
| 1:E:58:ILE:HG23  | 1:E:66:PHE:CE1   | 2.52                     | 0.44              |
| 1:A:78:LYS:HE3   | 4:D:24:ARG:HH22  | 1.81                     | 0.44              |
| 3:C:63:GLU:CD    | 3:C:63:GLU:H     | 2.24                     | 0.44              |
| 1:E:29:ASP:OD2   | 3:G:30:LYS:HE3   | 2.17                     | 0.44              |
| 3:G:4:GLU:CD     | 3:G:4:GLU:H      | 2.25                     | 0.44              |
| 1:E:22:VAL:CG1   | 1:E:127:LEU:HD22 | 2.47                     | 0.44              |
| 4:H:50:ARG:NH1   | 4:H:50:ARG:CG    | 2.78                     | 0.44              |
| 2:J:50:ARG:HG2   | 2:J:50:ARG:O     | 2.17                     | 0.44              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:E:150:LEU:N   | 1:E:151:PRO:CD   | 2.81                     | 0.44              |
| 1:I:22:VAL:HG12 | 1:I:127:LEU:HD22 | 1.99                     | 0.44              |
| 1:I:34:ILE:O    | 1:I:38:VAL:HG23  | 2.17                     | 0.44              |
| 2:J:74:ILE:HG23 | 3:K:72:LEU:HD13  | 1.98                     | 0.44              |
| 1:A:10:GLU:CD   | 3:G:10:GLU:HB2   | 2.43                     | 0.44              |
| 1:A:60:GLU:HB2  | 1:A:63:SER:HB3   | 1.98                     | 0.44              |
| 4:L:18:PHE:CZ   | 4:L:24:ARG:HD3   | 2.52                     | 0.44              |
| 1:A:109:LYS:HZ3 | 1:A:151:PRO:HG3  | 1.83                     | 0.44              |
| 4:H:97:ARG:O    | 4:H:99:LEU:N     | 2.51                     | 0.43              |
| 1:I:34:ILE:HG12 | 1:I:126:VAL:HG11 | 1.99                     | 0.43              |
| 1:I:57:LYS:HD2  | 1:I:65:GLU:HG3   | 1.99                     | 0.43              |
| 1:E:27:PHE:CD2  | 3:G:30:LYS:HG2   | 2.54                     | 0.43              |
| 1:A:150:LEU:O   | 1:A:151:PRO:O    | 2.37                     | 0.43              |
| 5:C:160:HEM:HHC | 5:C:160:HEM:HAB  | 1.94                     | 0.43              |
| 4:D:34:ASP:HB3  | 4:D:110:HIS:CD2  | 2.54                     | 0.43              |
| 1:E:69:HIS:O    | 1:E:73:VAL:HG23  | 2.19                     | 0.43              |
| 2:J:5:GLY:H     | 2:J:8:GLU:CG     | 2.31                     | 0.43              |
| 3:K:56:ARG:HD2  | 3:K:56:ARG:O     | 2.18                     | 0.43              |
| 1:E:129:CYS:SG  | 2:F:124:CYS:SG   | 3.12                     | 0.43              |
| 2:J:118:ALA:HB2 | 2:J:125:TYR:CZ   | 2.54                     | 0.43              |
| 4:D:44:ALA:N    | 4:D:45:PRO:HD2   | 2.33                     | 0.43              |
| 1:E:78:LYS:HD2  | 1:E:82:ASN:HD22  | 1.79                     | 0.43              |
| 2:J:87:GLU:OE2  | 3:K:66:LYS:HE3   | 2.19                     | 0.43              |
| 1:A:31:ARG:HD2  | 1:A:71:VAL:HG13  | 2.01                     | 0.42              |
| 2:B:96:HIS:HA   | 2:B:99:ARG:HD2   | 2.00                     | 0.42              |
| 4:H:118:ARG:HG2 | 4:H:118:ARG:HH11 | 1.84                     | 0.42              |
| 1:A:19:TRP:CE3  | 1:A:22:VAL:HG21  | 2.54                     | 0.42              |
| 1:A:69:HIS:O    | 1:A:73:VAL:HG23  | 2.19                     | 0.42              |
| 1:I:25:SER:HB2  | 3:K:25:ASP:OD1   | 2.19                     | 0.42              |
| 3:C:13:ARG:HH12 | 3:C:17:LYS:NZ    | 2.17                     | 0.42              |
| 2:F:93:GLN:HE21 | 2:F:143:GLY:CA   | 2.32                     | 0.42              |
| 3:C:22:LEU:HD23 | 3:C:22:LEU:HA    | 1.94                     | 0.42              |
| 4:H:100:LYS:H   | 4:H:100:LYS:HD2  | 1.85                     | 0.42              |
| 1:I:150:LEU:HA  | 1:I:150:LEU:HD23 | 1.78                     | 0.42              |
| 5:I:160:HEM:HHC | 5:I:160:HEM:HAB  | 1.96                     | 0.42              |
| 2:J:51:VAL:O    | 2:J:51:VAL:HG13  | 2.19                     | 0.42              |
| 2:B:50:ARG:O    | 2:B:50:ARG:HG2   | 2.20                     | 0.42              |
| 3:C:37:ARG:NH1  | 3:C:37:ARG:HG3   | 2.34                     | 0.42              |
| 3:C:56:ARG:NH1  | 8:C:1190:HOH:O   | 2.52                     | 0.42              |
| 1:E:131:ASN:C   | 1:E:131:ASN:ND2  | 2.78                     | 0.42              |
| 2:F:130:TRP:O   | 2:F:134:ILE:HG12 | 2.20                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 2:J:34:TRP:CZ2  | 6:J:3162:CMO:O   | 2.73                     | 0.42              |
| 3:K:19:TRP:CZ2  | 3:K:23:TRP:HZ2   | 2.38                     | 0.42              |
| 4:D:20:HIS:O    | 4:D:24:ARG:CG    | 2.67                     | 0.42              |
| 1:A:110:GLU:CG  | 1:A:113:ARG:NH2  | 2.77                     | 0.42              |
| 3:C:124:LEU:N   | 3:C:125:PRO:HD2  | 2.35                     | 0.42              |
| 1:I:23:TRP:CD1  | 1:I:78:LYS:HE2   | 2.55                     | 0.42              |
| 3:C:56:ARG:NH2  | 5:C:160:HEM:O2D  | 2.52                     | 0.41              |
| 2:F:102:PRO:HD2 | 2:F:105:TYR:CD1  | 2.55                     | 0.41              |
| 3:K:12:HIS:CD2  | 3:K:12:HIS:C     | 2.98                     | 0.41              |
| 2:F:109:PHE:CE1 | 5:F:160:HEM:HAB  | 2.55                     | 0.41              |
| 1:A:23:TRP:HZ3  | 1:A:74:ALA:HB1   | 1.85                     | 0.41              |
| 1:A:28:THR:CG2  | 1:A:71:VAL:HG21  | 2.47                     | 0.41              |
| 4:H:18:PHE:CZ   | 4:H:24:ARG:HD3   | 2.56                     | 0.41              |
| 4:H:99:LEU:HD22 | 5:H:160:HEM:CBC  | 2.50                     | 0.41              |
| 1:I:18:ILE:HG23 | 1:I:127:LEU:HD11 | 2.02                     | 0.41              |
| 4:L:127:ALA:O   | 4:L:131:CYS:HB2  | 2.20                     | 0.41              |
| 4:D:100:LYS:HD3 | 4:D:103:PHE:CZ   | 2.56                     | 0.41              |
| 1:E:7:CYS:HB2   | 1:E:138:CYS:HA   | 2.03                     | 0.41              |
| 3:G:19:TRP:CZ2  | 3:G:23:TRP:HZ2   | 2.39                     | 0.41              |
| 3:G:74:ILE:HD11 | 3:G:116:PHE:CZ   | 2.56                     | 0.41              |
| 1:A:57:LYS:HD2  | 1:A:65:GLU:HG3   | 2.03                     | 0.41              |
| 1:A:104:ARG:HA  | 1:A:104:ARG:HD3  | 1.87                     | 0.41              |
| 2:B:27:GLU:O    | 2:B:31:GLN:HG3   | 2.21                     | 0.41              |
| 4:L:34:ASP:HB3  | 4:L:110:HIS:CD2  | 2.55                     | 0.41              |
| 4:L:77:LEU:HG   | 4:L:131:CYS:SG   | 2.61                     | 0.41              |
| 1:A:57:LYS:CD   | 1:A:65:GLU:HG3   | 2.51                     | 0.40              |
| 3:C:56:ARG:HD2  | 3:C:56:ARG:O     | 2.20                     | 0.40              |
| 2:F:66:ASP:HB3  | 3:G:80:LEU:CD1   | 2.51                     | 0.40              |
| 2:F:138:GLU:O   | 2:F:142:LYS:HG3  | 2.21                     | 0.40              |
| 2:B:145:HIS:H   | 2:B:145:HIS:HD2  | 1.70                     | 0.40              |
| 1:A:120:ALA:HB2 | 1:A:136:ASN:HD21 | 1.86                     | 0.40              |
| 3:G:47:ILE:HA   | 3:G:48:PRO:HD2   | 1.84                     | 0.40              |
| 4:L:97:ARG:O    | 4:L:99:LEU:N     | 2.51                     | 0.40              |
| 3:C:3:HIS:N     | 8:C:1186:HOH:O   | 2.53                     | 0.40              |
| 4:H:18:PHE:CD1  | 4:H:24:ARG:HG2   | 2.57                     | 0.40              |
| 4:D:77:LEU:HG   | 4:D:131:CYS:SG   | 2.61                     | 0.40              |
| 3:G:24:ARG:HA   | 3:G:24:ARG:HE    | 1.87                     | 0.40              |
| 2:J:130:TRP:O   | 2:J:134:ILE:HG12 | 2.21                     | 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     | 145/151 (96%)   | 138 (95%)  | 6 (4%)  | 1 (1%)   | 18          | 38  |
| 1   | E     | 145/151 (96%)   | 136 (94%)  | 8 (6%)  | 1 (1%)   | 18          | 38  |
| 1   | I     | 145/151 (96%)   | 139 (96%)  | 5 (3%)  | 1 (1%)   | 18          | 38  |
| 2   | B     | 143/145 (99%)   | 140 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 2   | F     | 143/145 (99%)   | 140 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 2   | J     | 143/145 (99%)   | 137 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 3   | C     | 146/153 (95%)   | 141 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 3   | G     | 147/153 (96%)   | 141 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 3   | K     | 147/153 (96%)   | 140 (95%)  | 7 (5%)  | 0        | 100         | 100 |
| 4   | D     | 138/140 (99%)   | 134 (97%)  | 3 (2%)  | 1 (1%)   | 18          | 38  |
| 4   | H     | 138/140 (99%)   | 135 (98%)  | 1 (1%)  | 2 (1%)   | 9           | 19  |
| 4   | L     | 138/140 (99%)   | 132 (96%)  | 5 (4%)  | 1 (1%)   | 18          | 38  |
| All | All   | 1718/1767 (97%) | 1653 (96%) | 58 (3%) | 7 (0%)   | 30          | 51  |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 25  | SER  |
| 4   | D     | 21  | ALA  |
| 1   | E     | 25  | SER  |
| 4   | H     | 21  | ALA  |
| 1   | I     | 25  | SER  |
| 4   | L     | 21  | ALA  |
| 4   | H     | 98  | ASN  |

### 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     | 131/134 (98%)   | 125 (95%)  | 6 (5%)   | 24          | 49 |
| 1   | E     | 131/134 (98%)   | 125 (95%)  | 6 (5%)   | 24          | 49 |
| 1   | I     | 131/134 (98%)   | 124 (95%)  | 7 (5%)   | 20          | 43 |
| 2   | B     | 117/117 (100%)  | 113 (97%)  | 4 (3%)   | 32          | 60 |
| 2   | F     | 117/117 (100%)  | 111 (95%)  | 6 (5%)   | 21          | 45 |
| 2   | J     | 117/117 (100%)  | 110 (94%)  | 7 (6%)   | 17          | 37 |
| 3   | C     | 128/131 (98%)   | 116 (91%)  | 12 (9%)  | 8           | 18 |
| 3   | G     | 128/131 (98%)   | 116 (91%)  | 12 (9%)  | 8           | 18 |
| 3   | K     | 128/131 (98%)   | 116 (91%)  | 12 (9%)  | 8           | 18 |
| 4   | D     | 121/121 (100%)  | 112 (93%)  | 9 (7%)   | 13          | 29 |
| 4   | H     | 121/121 (100%)  | 109 (90%)  | 12 (10%) | 7           | 16 |
| 4   | L     | 121/121 (100%)  | 111 (92%)  | 10 (8%)  | 10          | 23 |
| All | All   | 1491/1509 (99%) | 1388 (93%) | 103 (7%) | 14          | 32 |

All (103) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 28  | THR  |
| 1   | A     | 58  | ILE  |
| 1   | A     | 65  | GLU  |
| 1   | A     | 79  | LEU  |
| 1   | A     | 83  | LEU  |
| 1   | A     | 94  | LEU  |
| 2   | B     | 7   | LEU  |
| 2   | B     | 8   | GLU  |
| 2   | B     | 10  | LEU  |
| 2   | B     | 125 | TYR  |
| 3   | C     | 3   | HIS  |
| 3   | C     | 6   | CYS  |
| 3   | C     | 20  | ASP  |
| 3   | C     | 24  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 37  | ARG  |
| 3   | C     | 38  | LEU  |
| 3   | C     | 41  | THR  |
| 3   | C     | 45  | LYS  |
| 3   | C     | 75  | LEU  |
| 3   | C     | 92  | ASP  |
| 3   | C     | 115 | LYS  |
| 3   | C     | 146 | LYS  |
| 4   | D     | 8   | LEU  |
| 4   | D     | 12  | LEU  |
| 4   | D     | 37  | ASP  |
| 4   | D     | 41  | GLU  |
| 4   | D     | 70  | LEU  |
| 4   | D     | 77  | LEU  |
| 4   | D     | 121 | THR  |
| 4   | D     | 131 | CYS  |
| 4   | D     | 136 | ILE  |
| 1   | E     | 28  | THR  |
| 1   | E     | 58  | ILE  |
| 1   | E     | 65  | GLU  |
| 1   | E     | 79  | LEU  |
| 1   | E     | 83  | LEU  |
| 1   | E     | 94  | LEU  |
| 2   | F     | 7   | LEU  |
| 2   | F     | 8   | GLU  |
| 2   | F     | 10  | LEU  |
| 2   | F     | 51  | VAL  |
| 2   | F     | 87  | GLU  |
| 2   | F     | 125 | TYR  |
| 3   | G     | 4   | GLU  |
| 3   | G     | 6   | CYS  |
| 3   | G     | 20  | ASP  |
| 3   | G     | 37  | ARG  |
| 3   | G     | 38  | LEU  |
| 3   | G     | 41  | THR  |
| 3   | G     | 45  | LYS  |
| 3   | G     | 74  | ILE  |
| 3   | G     | 75  | LEU  |
| 3   | G     | 92  | ASP  |
| 3   | G     | 115 | LYS  |
| 3   | G     | 146 | LYS  |
| 4   | H     | 8   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | H     | 12  | LEU  |
| 4   | H     | 29  | LEU  |
| 4   | H     | 37  | ASP  |
| 4   | H     | 41  | GLU  |
| 4   | H     | 50  | ARG  |
| 4   | H     | 70  | LEU  |
| 4   | H     | 77  | LEU  |
| 4   | H     | 100 | LYS  |
| 4   | H     | 121 | THR  |
| 4   | H     | 131 | CYS  |
| 4   | H     | 136 | ILE  |
| 1   | I     | 28  | THR  |
| 1   | I     | 58  | ILE  |
| 1   | I     | 65  | GLU  |
| 1   | I     | 79  | LEU  |
| 1   | I     | 83  | LEU  |
| 1   | I     | 94  | LEU  |
| 1   | I     | 115 | ILE  |
| 2   | J     | 7   | LEU  |
| 2   | J     | 8   | GLU  |
| 2   | J     | 10  | LEU  |
| 2   | J     | 18  | ARG  |
| 2   | J     | 87  | GLU  |
| 2   | J     | 125 | TYR  |
| 2   | J     | 135 | ASP  |
| 3   | K     | 4   | GLU  |
| 3   | K     | 6   | CYS  |
| 3   | K     | 20  | ASP  |
| 3   | K     | 37  | ARG  |
| 3   | K     | 38  | LEU  |
| 3   | K     | 41  | THR  |
| 3   | K     | 45  | LYS  |
| 3   | K     | 74  | ILE  |
| 3   | K     | 75  | LEU  |
| 3   | K     | 92  | ASP  |
| 3   | K     | 115 | LYS  |
| 3   | K     | 146 | LYS  |
| 4   | L     | 3   | LEU  |
| 4   | L     | 8   | LEU  |
| 4   | L     | 12  | LEU  |
| 4   | L     | 37  | ASP  |
| 4   | L     | 41  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | L     | 70  | LEU  |
| 4   | L     | 77  | LEU  |
| 4   | L     | 121 | THR  |
| 4   | L     | 131 | CYS  |
| 4   | L     | 136 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 82  | ASN  |
| 1   | A     | 100 | GLN  |
| 1   | A     | 125 | GLN  |
| 1   | A     | 131 | ASN  |
| 1   | A     | 136 | ASN  |
| 2   | B     | 52  | HIS  |
| 2   | B     | 93  | GLN  |
| 2   | B     | 145 | HIS  |
| 3   | C     | 18  | GLN  |
| 3   | C     | 51  | ASN  |
| 3   | C     | 100 | HIS  |
| 3   | C     | 101 | GLN  |
| 3   | C     | 109 | GLN  |
| 4   | D     | 134 | GLN  |
| 1   | E     | 82  | ASN  |
| 1   | E     | 96  | HIS  |
| 1   | E     | 125 | GLN  |
| 1   | E     | 131 | ASN  |
| 1   | E     | 136 | ASN  |
| 2   | F     | 31  | GLN  |
| 2   | F     | 52  | HIS  |
| 2   | F     | 93  | GLN  |
| 2   | F     | 145 | HIS  |
| 3   | G     | 18  | GLN  |
| 3   | G     | 100 | HIS  |
| 3   | G     | 109 | GLN  |
| 4   | H     | 110 | HIS  |
| 4   | H     | 134 | GLN  |
| 1   | I     | 125 | GLN  |
| 1   | I     | 131 | ASN  |
| 1   | I     | 136 | ASN  |
| 2   | J     | 40  | GLN  |
| 2   | J     | 52  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | J     | 93  | GLN  |
| 2   | J     | 95  | GLN  |
| 2   | J     | 145 | HIS  |
| 3   | K     | 12  | HIS  |
| 3   | K     | 18  | GLN  |
| 3   | K     | 100 | HIS  |
| 3   | K     | 109 | GLN  |
| 4   | L     | 110 | HIS  |
| 4   | L     | 134 | GLN  |

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

27 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 | $\# Z  > 2$ |
| 6   | CMO  | A     | 1161 | 5    | 0,1,1        | -    | -           | -           |      |             |
| 6   | CMO  | I     | 3161 | 5    | 0,1,1        | -    | -           | -           |      |             |
| 6   | CMO  | K     | 3163 | 5    | 0,1,1        | -    | -           | -           |      |             |
| 5   | HEM  | I     | 160  | 1,6  | 50,50,50     | 2.51 | 22 (44%)    | 67,82,82    | 2.85 | 29 (43%)    |
| 7   | PO4  | K     | 154  | -    | 4,4,4        | 0.82 | 0           | 6,6,6       | 0.50 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 5   | HEM  | H     | 160  | 4,6  | 50,50,50     | 2.43 | 22 (44%) | 67,82,82    | 2.90 | 30 (44%) |
| 6   | CMO  | F     | 2162 | 5    | 0,1,1        | -    | -        | -           |      |          |
| 6   | CMO  | B     | 1162 | 5    | 0,1,1        | -    | -        | -           |      |          |
| 6   | CMO  | E     | 2161 | 5    | 0,1,1        | -    | -        | -           |      |          |
| 5   | HEM  | E     | 160  | 1,6  | 50,50,50     | 2.46 | 23 (46%) | 67,82,82    | 2.97 | 28 (41%) |
| 6   | CMO  | C     | 1163 | 5    | 0,1,1        | -    | -        | -           |      |          |
| 6   | CMO  | L     | 3164 | 5    | 0,1,1        | -    | -        | -           |      |          |
| 7   | PO4  | C     | 154  | -    | 4,4,4        | 0.85 | 0        | 6,6,6       | 0.58 | 0        |
| 5   | HEM  | J     | 160  | 6,2  | 50,50,50     | 2.41 | 21 (42%) | 67,82,82    | 2.92 | 30 (44%) |
| 5   | HEM  | B     | 160  | 6,2  | 50,50,50     | 2.45 | 24 (48%) | 67,82,82    | 2.73 | 28 (41%) |
| 6   | CMO  | D     | 1164 | 5    | 0,1,1        | -    | -        | -           |      |          |
| 7   | PO4  | G     | 154  | -    | 4,4,4        | 0.83 | 0        | 6,6,6       | 0.48 | 0        |
| 5   | HEM  | A     | 160  | 1,6  | 50,50,50     | 2.49 | 22 (44%) | 67,82,82    | 2.88 | 30 (44%) |
| 6   | CMO  | G     | 2163 | 5    | 0,1,1        | -    | -        | -           |      |          |
| 5   | HEM  | L     | 160  | 4,6  | 50,50,50     | 2.46 | 23 (46%) | 67,82,82    | 2.77 | 30 (44%) |
| 5   | HEM  | K     | 160  | 6,3  | 50,50,50     | 2.48 | 23 (46%) | 67,82,82    | 2.72 | 28 (41%) |
| 6   | CMO  | J     | 3162 | 5    | 0,1,1        | -    | -        | -           |      |          |
| 6   | CMO  | H     | 2164 | 5    | 0,1,1        | -    | -        | -           |      |          |
| 5   | HEM  | G     | 160  | 6,3  | 50,50,50     | 2.46 | 23 (46%) | 67,82,82    | 2.67 | 27 (40%) |
| 5   | HEM  | C     | 160  | 6,3  | 50,50,50     | 2.49 | 25 (50%) | 67,82,82    | 2.74 | 27 (40%) |
| 5   | HEM  | F     | 160  | 6,2  | 50,50,50     | 2.44 | 22 (44%) | 67,82,82    | 2.82 | 28 (41%) |
| 5   | HEM  | D     | 160  | 4,6  | 50,50,50     | 2.50 | 25 (50%) | 67,82,82    | 2.90 | 31 (46%) |

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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 5   | HEM  | J     | 160 | 6,2  | -       | 6/14/54/54 | -     |
| 5   | HEM  | L     | 160 | 4,6  | -       | 6/14/54/54 | -     |
| 5   | HEM  | E     | 160 | 1,6  | -       | 8/14/54/54 | -     |
| 5   | HEM  | B     | 160 | 6,2  | -       | 6/14/54/54 | -     |
| 5   | HEM  | K     | 160 | 6,3  | -       | 6/14/54/54 | -     |
| 5   | HEM  | G     | 160 | 6,3  | -       | 4/14/54/54 | -     |
| 5   | HEM  | C     | 160 | 6,3  | -       | 6/14/54/54 | -     |
| 5   | HEM  | A     | 160 | 1,6  | -       | 6/14/54/54 | -     |
| 5   | HEM  | D     | 160 | 4,6  | -       | 6/14/54/54 | -     |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 5   | HEM  | F     | 160 | 6,2  | -       | 8/14/54/54 | -     |
| 5   | HEM  | I     | 160 | 1,6  | -       | 6/14/54/54 | -     |
| 5   | HEM  | H     | 160 | 4,6  | -       | 7/14/54/54 | -     |

All (275) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | D     | 160 | HEM  | CAB-C3B | -5.48 | 1.32        | 1.47     |
| 5   | H     | 160 | HEM  | CHD-C4C | 5.39  | 1.49        | 1.38     |
| 5   | I     | 160 | HEM  | CAB-C3B | -5.35 | 1.33        | 1.47     |
| 5   | L     | 160 | HEM  | CAB-C3B | -5.34 | 1.33        | 1.47     |
| 5   | D     | 160 | HEM  | CHD-C4C | 5.29  | 1.48        | 1.38     |
| 5   | E     | 160 | HEM  | CAB-C3B | -5.25 | 1.33        | 1.47     |
| 5   | A     | 160 | HEM  | CAB-C3B | -5.25 | 1.33        | 1.47     |
| 5   | H     | 160 | HEM  | CAB-C3B | -5.25 | 1.33        | 1.47     |
| 5   | J     | 160 | HEM  | CHD-C4C | 5.23  | 1.48        | 1.38     |
| 5   | F     | 160 | HEM  | CAB-C3B | -5.20 | 1.33        | 1.47     |
| 5   | E     | 160 | HEM  | CHD-C4C | 5.15  | 1.48        | 1.38     |
| 5   | E     | 160 | HEM  | CHC-C1C | 5.14  | 1.48        | 1.38     |
| 5   | B     | 160 | HEM  | CAB-C3B | -5.13 | 1.33        | 1.47     |
| 5   | J     | 160 | HEM  | CHC-C1C | 5.13  | 1.48        | 1.38     |
| 5   | B     | 160 | HEM  | CHD-C4C | 5.12  | 1.48        | 1.38     |
| 5   | I     | 160 | HEM  | CHC-C1C | 5.07  | 1.48        | 1.38     |
| 5   | K     | 160 | HEM  | CHC-C1C | 5.03  | 1.48        | 1.38     |
| 5   | G     | 160 | HEM  | CAB-C3B | -4.99 | 1.34        | 1.47     |
| 5   | K     | 160 | HEM  | CAB-C3B | -4.99 | 1.34        | 1.47     |
| 5   | C     | 160 | HEM  | CAB-C3B | -4.98 | 1.34        | 1.47     |
| 5   | L     | 160 | HEM  | CHD-C4C | 4.97  | 1.48        | 1.38     |
| 5   | F     | 160 | HEM  | CHD-C4C | 4.94  | 1.48        | 1.38     |
| 5   | K     | 160 | HEM  | CHA-C4D | 4.91  | 1.48        | 1.38     |
| 5   | K     | 160 | HEM  | CHD-C4C | 4.90  | 1.48        | 1.38     |
| 5   | F     | 160 | HEM  | CHC-C1C | 4.89  | 1.48        | 1.38     |
| 5   | I     | 160 | HEM  | CHA-C4D | 4.86  | 1.48        | 1.38     |
| 5   | A     | 160 | HEM  | CHD-C4C | 4.84  | 1.47        | 1.38     |
| 5   | G     | 160 | HEM  | CHC-C1C | 4.83  | 1.47        | 1.38     |
| 5   | J     | 160 | HEM  | CAB-C3B | -4.82 | 1.34        | 1.47     |
| 5   | A     | 160 | HEM  | CHA-C4D | 4.82  | 1.48        | 1.38     |
| 5   | C     | 160 | HEM  | CHC-C1C | 4.78  | 1.47        | 1.38     |
| 5   | G     | 160 | HEM  | CHA-C4D | 4.76  | 1.48        | 1.38     |
| 5   | C     | 160 | HEM  | CHD-C4C | 4.75  | 1.47        | 1.38     |
| 5   | I     | 160 | HEM  | CHD-C4C | 4.75  | 1.47        | 1.38     |
| 5   | A     | 160 | HEM  | CHC-C1C | 4.74  | 1.47        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 160 | HEM  | CHA-C4D | 4.74  | 1.48        | 1.38     |
| 5   | D     | 160 | HEM  | CHC-C1C | 4.66  | 1.47        | 1.38     |
| 5   | G     | 160 | HEM  | CHD-C4C | 4.63  | 1.47        | 1.38     |
| 5   | C     | 160 | HEM  | C3C-C4C | -4.56 | 1.38        | 1.46     |
| 5   | F     | 160 | HEM  | CHA-C4D | 4.53  | 1.47        | 1.38     |
| 5   | B     | 160 | HEM  | CHC-C1C | 4.51  | 1.47        | 1.38     |
| 5   | E     | 160 | HEM  | CHA-C4D | 4.48  | 1.47        | 1.38     |
| 5   | L     | 160 | HEM  | CHC-C1C | 4.46  | 1.47        | 1.38     |
| 5   | A     | 160 | HEM  | C3C-C4C | -4.45 | 1.38        | 1.46     |
| 5   | H     | 160 | HEM  | CHC-C1C | 4.44  | 1.47        | 1.38     |
| 5   | I     | 160 | HEM  | C3C-C4C | -4.40 | 1.38        | 1.46     |
| 5   | B     | 160 | HEM  | CHA-C4D | 4.38  | 1.47        | 1.38     |
| 5   | J     | 160 | HEM  | CHA-C4D | 4.35  | 1.47        | 1.38     |
| 5   | H     | 160 | HEM  | CHA-C4D | 4.26  | 1.47        | 1.38     |
| 5   | H     | 160 | HEM  | CHD-C1D | 4.19  | 1.48        | 1.39     |
| 5   | J     | 160 | HEM  | CHD-C1D | 4.16  | 1.48        | 1.39     |
| 5   | E     | 160 | HEM  | C3C-C4C | -4.16 | 1.38        | 1.46     |
| 5   | E     | 160 | HEM  | CHD-C1D | 4.15  | 1.48        | 1.39     |
| 5   | E     | 160 | HEM  | CHC-C4B | 4.10  | 1.48        | 1.39     |
| 5   | I     | 160 | HEM  | CHA-C1A | 4.09  | 1.48        | 1.39     |
| 5   | L     | 160 | HEM  | CHA-C4D | 4.09  | 1.46        | 1.38     |
| 5   | L     | 160 | HEM  | CHB-C1B | 4.08  | 1.46        | 1.38     |
| 5   | K     | 160 | HEM  | CHA-C1A | 4.07  | 1.48        | 1.39     |
| 5   | L     | 160 | HEM  | CHD-C1D | 4.07  | 1.48        | 1.39     |
| 5   | D     | 160 | HEM  | CHD-C1D | 4.05  | 1.48        | 1.39     |
| 5   | B     | 160 | HEM  | CHD-C1D | 4.02  | 1.48        | 1.39     |
| 5   | F     | 160 | HEM  | CHB-C1B | 4.02  | 1.46        | 1.38     |
| 5   | K     | 160 | HEM  | C3C-C4C | -4.01 | 1.39        | 1.46     |
| 5   | D     | 160 | HEM  | C3B-C4B | -4.00 | 1.37        | 1.44     |
| 5   | A     | 160 | HEM  | C3B-C4B | -4.00 | 1.37        | 1.44     |
| 5   | D     | 160 | HEM  | CHA-C4D | 3.99  | 1.46        | 1.38     |
| 5   | B     | 160 | HEM  | CHB-C1B | 3.98  | 1.46        | 1.38     |
| 5   | D     | 160 | HEM  | CHB-C1B | 3.96  | 1.46        | 1.38     |
| 5   | C     | 160 | HEM  | CHB-C1B | 3.95  | 1.46        | 1.38     |
| 5   | H     | 160 | HEM  | C3B-C4B | -3.94 | 1.37        | 1.44     |
| 5   | J     | 160 | HEM  | CHB-C1B | 3.94  | 1.46        | 1.38     |
| 5   | A     | 160 | HEM  | CHD-C1D | 3.93  | 1.48        | 1.39     |
| 5   | F     | 160 | HEM  | CHD-C1D | 3.87  | 1.48        | 1.39     |
| 5   | L     | 160 | HEM  | C3B-C4B | -3.87 | 1.37        | 1.44     |
| 5   | C     | 160 | HEM  | CHA-C1A | 3.87  | 1.48        | 1.39     |
| 5   | A     | 160 | HEM  | CHA-C1A | 3.86  | 1.48        | 1.39     |
| 5   | G     | 160 | HEM  | CHA-C1A | 3.85  | 1.48        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | K     | 160 | HEM  | CHD-C1D | 3.83  | 1.47        | 1.39     |
| 5   | E     | 160 | HEM  | CHB-C1B | 3.82  | 1.46        | 1.38     |
| 5   | I     | 160 | HEM  | CHB-C1B | 3.82  | 1.46        | 1.38     |
| 5   | K     | 160 | HEM  | CHB-C1B | 3.81  | 1.46        | 1.38     |
| 5   | G     | 160 | HEM  | C3C-C4C | -3.79 | 1.39        | 1.46     |
| 5   | G     | 160 | HEM  | CHC-C4B | 3.78  | 1.47        | 1.39     |
| 5   | I     | 160 | HEM  | CHC-C4B | 3.76  | 1.47        | 1.39     |
| 5   | K     | 160 | HEM  | CHC-C4B | 3.76  | 1.47        | 1.39     |
| 5   | G     | 160 | HEM  | CHD-C1D | 3.72  | 1.47        | 1.39     |
| 5   | H     | 160 | HEM  | C3C-C4C | -3.70 | 1.39        | 1.46     |
| 5   | F     | 160 | HEM  | C3C-C4C | -3.68 | 1.39        | 1.46     |
| 5   | I     | 160 | HEM  | CHD-C1D | 3.67  | 1.47        | 1.39     |
| 5   | F     | 160 | HEM  | C3B-C4B | -3.67 | 1.37        | 1.44     |
| 5   | C     | 160 | HEM  | CHD-C1D | 3.66  | 1.47        | 1.39     |
| 5   | B     | 160 | HEM  | CHA-C1A | 3.64  | 1.47        | 1.39     |
| 5   | H     | 160 | HEM  | CHB-C1B | 3.64  | 1.45        | 1.38     |
| 5   | A     | 160 | HEM  | CHB-C1B | 3.62  | 1.45        | 1.38     |
| 5   | J     | 160 | HEM  | CHA-C1A | 3.62  | 1.47        | 1.39     |
| 5   | G     | 160 | HEM  | CHB-C1B | 3.61  | 1.45        | 1.38     |
| 5   | A     | 160 | HEM  | CHC-C4B | 3.60  | 1.47        | 1.39     |
| 5   | E     | 160 | HEM  | CHA-C1A | 3.58  | 1.47        | 1.39     |
| 5   | F     | 160 | HEM  | CHA-C1A | 3.56  | 1.47        | 1.39     |
| 5   | D     | 160 | HEM  | C3C-C4C | -3.55 | 1.39        | 1.46     |
| 5   | E     | 160 | HEM  | C3B-C4B | -3.54 | 1.38        | 1.44     |
| 5   | I     | 160 | HEM  | C3B-C4B | -3.53 | 1.38        | 1.44     |
| 5   | F     | 160 | HEM  | CHC-C4B | 3.52  | 1.47        | 1.39     |
| 5   | B     | 160 | HEM  | C3B-C4B | -3.50 | 1.38        | 1.44     |
| 5   | C     | 160 | HEM  | CHC-C4B | 3.49  | 1.47        | 1.39     |
| 5   | G     | 160 | HEM  | C3B-C4B | -3.47 | 1.38        | 1.44     |
| 5   | J     | 160 | HEM  | CHC-C4B | 3.46  | 1.47        | 1.39     |
| 5   | C     | 160 | HEM  | C3B-C4B | -3.44 | 1.38        | 1.44     |
| 5   | B     | 160 | HEM  | C1C-C2C | -3.43 | 1.38        | 1.45     |
| 5   | J     | 160 | HEM  | C3C-C4C | -3.39 | 1.40        | 1.46     |
| 5   | K     | 160 | HEM  | C3B-C4B | -3.38 | 1.38        | 1.44     |
| 5   | B     | 160 | HEM  | C3C-C4C | -3.38 | 1.40        | 1.46     |
| 5   | D     | 160 | HEM  | CHC-C4B | 3.38  | 1.46        | 1.39     |
| 5   | D     | 160 | HEM  | C1C-C2C | -3.37 | 1.38        | 1.45     |
| 5   | L     | 160 | HEM  | CHC-C4B | 3.36  | 1.46        | 1.39     |
| 5   | H     | 160 | HEM  | CHA-C1A | 3.33  | 1.46        | 1.39     |
| 5   | H     | 160 | HEM  | CHC-C4B | 3.30  | 1.46        | 1.39     |
| 5   | K     | 160 | HEM  | C2A-C3A | 3.27  | 1.47        | 1.38     |
| 5   | J     | 160 | HEM  | CHB-C4A | 3.24  | 1.46        | 1.39     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | C     | 160 | HEM  | CHB-C4A | 3.23  | 1.46        | 1.39     |
| 5   | L     | 160 | HEM  | CHA-C1A | 3.23  | 1.46        | 1.39     |
| 5   | B     | 160 | HEM  | CHC-C4B | 3.22  | 1.46        | 1.39     |
| 5   | C     | 160 | HEM  | C1C-C2C | -3.22 | 1.39        | 1.45     |
| 5   | L     | 160 | HEM  | C3C-C4C | -3.21 | 1.40        | 1.46     |
| 5   | F     | 160 | HEM  | CHB-C4A | 3.19  | 1.46        | 1.39     |
| 5   | L     | 160 | HEM  | C1C-C2C | -3.16 | 1.39        | 1.45     |
| 5   | H     | 160 | HEM  | C1C-C2C | -3.15 | 1.39        | 1.45     |
| 5   | D     | 160 | HEM  | CHB-C4A | 3.14  | 1.46        | 1.39     |
| 5   | L     | 160 | HEM  | C4D-ND  | -3.14 | 1.34        | 1.40     |
| 5   | I     | 160 | HEM  | C2A-C3A | 3.12  | 1.47        | 1.38     |
| 5   | C     | 160 | HEM  | C2A-C3A | 3.12  | 1.47        | 1.38     |
| 5   | E     | 160 | HEM  | CHB-C4A | 3.10  | 1.46        | 1.39     |
| 5   | B     | 160 | HEM  | C1B-C2B | -3.09 | 1.38        | 1.44     |
| 5   | L     | 160 | HEM  | CHB-C4A | 3.08  | 1.46        | 1.39     |
| 5   | I     | 160 | HEM  | C4D-ND  | -3.08 | 1.34        | 1.40     |
| 5   | D     | 160 | HEM  | CHA-C1A | 3.08  | 1.46        | 1.39     |
| 5   | D     | 160 | HEM  | C4D-ND  | -3.06 | 1.34        | 1.40     |
| 5   | F     | 160 | HEM  | C4D-ND  | -3.06 | 1.34        | 1.40     |
| 5   | G     | 160 | HEM  | C2A-C3A | 3.05  | 1.46        | 1.38     |
| 5   | G     | 160 | HEM  | C4D-ND  | -3.04 | 1.35        | 1.40     |
| 5   | I     | 160 | HEM  | C1C-C2C | -3.03 | 1.39        | 1.45     |
| 5   | K     | 160 | HEM  | CHB-C4A | 3.03  | 1.46        | 1.39     |
| 5   | B     | 160 | HEM  | C2A-C3A | 3.03  | 1.46        | 1.38     |
| 5   | L     | 160 | HEM  | C2A-C3A | 3.03  | 1.46        | 1.38     |
| 5   | B     | 160 | HEM  | CHB-C4A | 3.01  | 1.46        | 1.39     |
| 5   | L     | 160 | HEM  | C1B-C2B | -3.01 | 1.38        | 1.44     |
| 5   | D     | 160 | HEM  | C1A-C2A | -2.99 | 1.38        | 1.44     |
| 5   | J     | 160 | HEM  | C2A-C3A | 2.97  | 1.46        | 1.38     |
| 5   | A     | 160 | HEM  | CHB-C4A | 2.95  | 1.46        | 1.39     |
| 5   | D     | 160 | HEM  | C2A-C3A | 2.95  | 1.46        | 1.38     |
| 5   | G     | 160 | HEM  | C1C-C2C | -2.94 | 1.39        | 1.45     |
| 5   | A     | 160 | HEM  | C4D-ND  | -2.94 | 1.35        | 1.40     |
| 5   | J     | 160 | HEM  | FE-NB   | 2.94  | 2.03        | 1.94     |
| 5   | E     | 160 | HEM  | C2A-C3A | 2.93  | 1.46        | 1.38     |
| 5   | I     | 160 | HEM  | CHB-C4A | 2.93  | 1.46        | 1.39     |
| 5   | A     | 160 | HEM  | C1C-C2C | -2.92 | 1.39        | 1.45     |
| 5   | F     | 160 | HEM  | C2A-C3A | 2.91  | 1.46        | 1.38     |
| 5   | A     | 160 | HEM  | C2A-C3A | 2.91  | 1.46        | 1.38     |
| 5   | H     | 160 | HEM  | C4D-ND  | -2.91 | 1.35        | 1.40     |
| 5   | J     | 160 | HEM  | C1C-C2C | -2.91 | 1.39        | 1.45     |
| 5   | H     | 160 | HEM  | C2A-C3A | 2.90  | 1.46        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | H     | 160 | HEM  | CHB-C4A | 2.89  | 1.45        | 1.39     |
| 5   | C     | 160 | HEM  | FE-NB   | 2.89  | 2.03        | 1.94     |
| 5   | F     | 160 | HEM  | C1B-C2B | -2.89 | 1.38        | 1.44     |
| 5   | K     | 160 | HEM  | FE-NB   | 2.88  | 2.03        | 1.94     |
| 5   | K     | 160 | HEM  | FE-ND   | 2.88  | 2.03        | 1.94     |
| 5   | K     | 160 | HEM  | C1C-C2C | -2.87 | 1.39        | 1.45     |
| 5   | J     | 160 | HEM  | FE-ND   | 2.87  | 2.03        | 1.94     |
| 5   | E     | 160 | HEM  | FE-ND   | 2.86  | 2.03        | 1.94     |
| 5   | I     | 160 | HEM  | FE-NB   | 2.86  | 2.03        | 1.94     |
| 5   | B     | 160 | HEM  | C4D-ND  | -2.86 | 1.35        | 1.40     |
| 5   | J     | 160 | HEM  | C3B-C4B | -2.85 | 1.39        | 1.44     |
| 5   | C     | 160 | HEM  | FE-ND   | 2.85  | 2.03        | 1.94     |
| 5   | G     | 160 | HEM  | CHB-C4A | 2.84  | 1.45        | 1.39     |
| 5   | E     | 160 | HEM  | FE-NB   | 2.84  | 2.03        | 1.94     |
| 5   | A     | 160 | HEM  | FE-NB   | 2.83  | 2.03        | 1.94     |
| 5   | I     | 160 | HEM  | FE-ND   | 2.81  | 2.03        | 1.94     |
| 5   | B     | 160 | HEM  | FE-NB   | 2.80  | 2.03        | 1.94     |
| 5   | H     | 160 | HEM  | FE-NB   | 2.80  | 2.03        | 1.94     |
| 5   | H     | 160 | HEM  | FE-ND   | 2.79  | 2.03        | 1.94     |
| 5   | B     | 160 | HEM  | FE-ND   | 2.77  | 2.03        | 1.94     |
| 5   | D     | 160 | HEM  | C1B-C2B | -2.77 | 1.38        | 1.44     |
| 5   | A     | 160 | HEM  | FE-ND   | 2.77  | 2.03        | 1.94     |
| 5   | F     | 160 | HEM  | FE-NB   | 2.76  | 2.03        | 1.94     |
| 5   | D     | 160 | HEM  | FE-ND   | 2.76  | 2.03        | 1.94     |
| 5   | G     | 160 | HEM  | FE-NB   | 2.73  | 2.03        | 1.94     |
| 5   | D     | 160 | HEM  | FE-NB   | 2.73  | 2.03        | 1.94     |
| 5   | L     | 160 | HEM  | FE-NB   | 2.72  | 2.03        | 1.94     |
| 5   | F     | 160 | HEM  | FE-ND   | 2.72  | 2.03        | 1.94     |
| 5   | G     | 160 | HEM  | C1B-C2B | -2.72 | 1.39        | 1.44     |
| 5   | E     | 160 | HEM  | FE-NC   | 2.70  | 2.04        | 1.95     |
| 5   | I     | 160 | HEM  | C1B-C2B | -2.69 | 1.39        | 1.44     |
| 5   | G     | 160 | HEM  | FE-ND   | 2.69  | 2.03        | 1.94     |
| 5   | K     | 160 | HEM  | C1B-C2B | -2.69 | 1.39        | 1.44     |
| 5   | F     | 160 | HEM  | FE-NA   | 2.68  | 2.04        | 1.95     |
| 5   | L     | 160 | HEM  | C1A-C2A | -2.64 | 1.39        | 1.44     |
| 5   | J     | 160 | HEM  | C4D-ND  | -2.64 | 1.35        | 1.40     |
| 5   | F     | 160 | HEM  | C1C-C2C | -2.64 | 1.40        | 1.45     |
| 5   | K     | 160 | HEM  | C4D-ND  | -2.63 | 1.35        | 1.40     |
| 5   | I     | 160 | HEM  | FE-NA   | 2.62  | 2.03        | 1.95     |
| 5   | L     | 160 | HEM  | FE-NA   | 2.62  | 2.03        | 1.95     |
| 5   | L     | 160 | HEM  | FE-ND   | 2.62  | 2.03        | 1.94     |
| 5   | G     | 160 | HEM  | FE-NC   | 2.61  | 2.03        | 1.95     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | J     | 160 | HEM  | FE-NA   | 2.61  | 2.03        | 1.95     |
| 5   | B     | 160 | HEM  | FE-NA   | 2.61  | 2.03        | 1.95     |
| 5   | G     | 160 | HEM  | C1D-C2D | -2.61 | 1.39        | 1.44     |
| 5   | F     | 160 | HEM  | FE-NC   | 2.61  | 2.03        | 1.95     |
| 5   | K     | 160 | HEM  | FE-NA   | 2.60  | 2.03        | 1.95     |
| 5   | K     | 160 | HEM  | FE-NC   | 2.59  | 2.03        | 1.95     |
| 5   | B     | 160 | HEM  | FE-NC   | 2.57  | 2.03        | 1.95     |
| 5   | C     | 160 | HEM  | C4D-ND  | -2.57 | 1.35        | 1.40     |
| 5   | D     | 160 | HEM  | FE-NA   | 2.56  | 2.03        | 1.95     |
| 5   | J     | 160 | HEM  | FE-NC   | 2.55  | 2.03        | 1.95     |
| 5   | G     | 160 | HEM  | FE-NA   | 2.55  | 2.03        | 1.95     |
| 5   | E     | 160 | HEM  | FE-NA   | 2.55  | 2.03        | 1.95     |
| 5   | L     | 160 | HEM  | FE-NC   | 2.54  | 2.03        | 1.95     |
| 5   | A     | 160 | HEM  | FE-NC   | 2.53  | 2.03        | 1.95     |
| 5   | H     | 160 | HEM  | FE-NA   | 2.52  | 2.03        | 1.95     |
| 5   | H     | 160 | HEM  | FE-NC   | 2.52  | 2.03        | 1.95     |
| 5   | I     | 160 | HEM  | FE-NC   | 2.51  | 2.03        | 1.95     |
| 5   | H     | 160 | HEM  | C1B-C2B | -2.51 | 1.39        | 1.44     |
| 5   | C     | 160 | HEM  | FE-NA   | 2.51  | 2.03        | 1.95     |
| 5   | C     | 160 | HEM  | C1B-C2B | -2.50 | 1.39        | 1.44     |
| 5   | A     | 160 | HEM  | C1B-C2B | -2.50 | 1.39        | 1.44     |
| 5   | A     | 160 | HEM  | FE-NA   | 2.50  | 2.03        | 1.95     |
| 5   | E     | 160 | HEM  | C4D-ND  | -2.49 | 1.35        | 1.40     |
| 5   | C     | 160 | HEM  | FE-NC   | 2.49  | 2.03        | 1.95     |
| 5   | C     | 160 | HEM  | C4C-NC  | -2.48 | 1.34        | 1.39     |
| 5   | E     | 160 | HEM  | C1A-C2A | -2.45 | 1.39        | 1.44     |
| 5   | D     | 160 | HEM  | FE-NC   | 2.44  | 2.03        | 1.95     |
| 5   | E     | 160 | HEM  | C1B-C2B | -2.44 | 1.39        | 1.44     |
| 5   | B     | 160 | HEM  | C1A-C2A | -2.44 | 1.39        | 1.44     |
| 5   | I     | 160 | HEM  | C1D-C2D | -2.41 | 1.39        | 1.44     |
| 5   | B     | 160 | HEM  | C1B-NB  | -2.40 | 1.36        | 1.40     |
| 5   | C     | 160 | HEM  | C1A-C2A | -2.39 | 1.39        | 1.44     |
| 5   | J     | 160 | HEM  | C1B-C2B | -2.38 | 1.39        | 1.44     |
| 5   | A     | 160 | HEM  | C1D-C2D | -2.36 | 1.39        | 1.44     |
| 5   | H     | 160 | HEM  | C4A-NA  | -2.36 | 1.35        | 1.39     |
| 5   | D     | 160 | HEM  | CBC-CAC | 2.35  | 1.41        | 1.30     |
| 5   | F     | 160 | HEM  | C1D-C2D | -2.35 | 1.39        | 1.44     |
| 5   | L     | 160 | HEM  | C1D-C2D | -2.35 | 1.39        | 1.44     |
| 5   | C     | 160 | HEM  | C1D-C2D | -2.34 | 1.39        | 1.44     |
| 5   | B     | 160 | HEM  | C1D-C2D | -2.33 | 1.39        | 1.44     |
| 5   | H     | 160 | HEM  | C1A-C2A | -2.32 | 1.40        | 1.44     |
| 5   | K     | 160 | HEM  | C1D-C2D | -2.31 | 1.39        | 1.44     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | G     | 160 | HEM  | C1A-C2A | -2.29 | 1.40        | 1.44     |
| 5   | L     | 160 | HEM  | C4A-C3A | 2.29  | 1.48        | 1.43     |
| 5   | K     | 160 | HEM  | C4D-C3D | 2.29  | 1.48        | 1.45     |
| 5   | E     | 160 | HEM  | C1C-C2C | -2.29 | 1.40        | 1.45     |
| 5   | J     | 160 | HEM  | C1A-C2A | -2.29 | 1.40        | 1.44     |
| 5   | G     | 160 | HEM  | C1B-NB  | -2.25 | 1.36        | 1.40     |
| 5   | A     | 160 | HEM  | C1A-C2A | -2.22 | 1.40        | 1.44     |
| 5   | K     | 160 | HEM  | C1A-C2A | -2.21 | 1.40        | 1.44     |
| 5   | J     | 160 | HEM  | C1D-C2D | -2.18 | 1.40        | 1.44     |
| 5   | B     | 160 | HEM  | C4A-C3A | 2.16  | 1.48        | 1.43     |
| 5   | L     | 160 | HEM  | C1B-NB  | -2.15 | 1.36        | 1.40     |
| 5   | F     | 160 | HEM  | C1A-C2A | -2.15 | 1.40        | 1.44     |
| 5   | D     | 160 | HEM  | C4A-C3A | 2.15  | 1.48        | 1.43     |
| 5   | C     | 160 | HEM  | C4D-C3D | 2.14  | 1.48        | 1.45     |
| 5   | C     | 160 | HEM  | C4A-NA  | -2.12 | 1.35        | 1.39     |
| 5   | E     | 160 | HEM  | C4A-NA  | -2.11 | 1.35        | 1.39     |
| 5   | E     | 160 | HEM  | C4D-C3D | 2.08  | 1.48        | 1.45     |
| 5   | A     | 160 | HEM  | C4A-NA  | -2.07 | 1.35        | 1.39     |
| 5   | H     | 160 | HEM  | C1B-NB  | -2.06 | 1.36        | 1.40     |
| 5   | K     | 160 | HEM  | C4A-C3A | 2.06  | 1.48        | 1.43     |
| 5   | D     | 160 | HEM  | C1D-C2D | -2.06 | 1.40        | 1.44     |
| 5   | C     | 160 | HEM  | CBC-CAC | 2.05  | 1.40        | 1.30     |
| 5   | D     | 160 | HEM  | C1A-NA  | -2.04 | 1.35        | 1.39     |
| 5   | I     | 160 | HEM  | C1A-C2A | -2.04 | 1.40        | 1.44     |
| 5   | F     | 160 | HEM  | C4A-C3A | 2.04  | 1.47        | 1.43     |
| 5   | B     | 160 | HEM  | C4A-NA  | -2.03 | 1.35        | 1.39     |
| 5   | D     | 160 | HEM  | C1B-NB  | -2.03 | 1.36        | 1.40     |
| 5   | G     | 160 | HEM  | C4A-NA  | -2.03 | 1.35        | 1.39     |
| 5   | I     | 160 | HEM  | C4D-C3D | 2.02  | 1.48        | 1.45     |
| 5   | E     | 160 | HEM  | C1D-C2D | -2.02 | 1.40        | 1.44     |

All (346) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | J     | 160 | HEM  | CBB-CAB-C3B | 9.96  | 177.31      | 127.53   |
| 5   | E     | 160 | HEM  | CBB-CAB-C3B | 9.94  | 177.18      | 127.53   |
| 5   | B     | 160 | HEM  | CBB-CAB-C3B | 9.50  | 174.98      | 127.53   |
| 5   | F     | 160 | HEM  | CBB-CAB-C3B | 9.44  | 174.67      | 127.53   |
| 5   | A     | 160 | HEM  | C3B-C2B-C1B | -9.38 | 99.36       | 106.41   |
| 5   | E     | 160 | HEM  | C3B-C2B-C1B | -9.38 | 99.37       | 106.41   |
| 5   | A     | 160 | HEM  | CBB-CAB-C3B | 9.10  | 172.97      | 127.53   |
| 5   | H     | 160 | HEM  | C3B-C2B-C1B | -8.88 | 99.74       | 106.41   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | D     | 160 | HEM  | CBB-CAB-C3B | 8.63  | 170.66      | 127.53   |
| 5   | I     | 160 | HEM  | C3B-C2B-C1B | -8.63 | 99.93       | 106.41   |
| 5   | G     | 160 | HEM  | C3B-C2B-C1B | -8.23 | 100.23      | 106.41   |
| 5   | I     | 160 | HEM  | CBB-CAB-C3B | 8.21  | 168.54      | 127.53   |
| 5   | F     | 160 | HEM  | C3B-C2B-C1B | -8.08 | 100.34      | 106.41   |
| 5   | J     | 160 | HEM  | C3B-C2B-C1B | -7.99 | 100.41      | 106.41   |
| 5   | D     | 160 | HEM  | C3B-C2B-C1B | -7.98 | 100.42      | 106.41   |
| 5   | C     | 160 | HEM  | C3B-C2B-C1B | -7.97 | 100.43      | 106.41   |
| 5   | K     | 160 | HEM  | C3B-C2B-C1B | -7.96 | 100.43      | 106.41   |
| 5   | H     | 160 | HEM  | CBB-CAB-C3B | 7.72  | 166.11      | 127.53   |
| 5   | L     | 160 | HEM  | C3B-C2B-C1B | -7.66 | 100.66      | 106.41   |
| 5   | K     | 160 | HEM  | CBB-CAB-C3B | 7.65  | 165.77      | 127.53   |
| 5   | L     | 160 | HEM  | C2A-C1A-NA  | 7.62  | 118.61      | 110.15   |
| 5   | C     | 160 | HEM  | CBB-CAB-C3B | 7.37  | 164.35      | 127.53   |
| 5   | D     | 160 | HEM  | C2A-C1A-NA  | 7.32  | 118.28      | 110.15   |
| 5   | J     | 160 | HEM  | C2B-C1B-NB  | 7.07  | 117.96      | 109.84   |
| 5   | L     | 160 | HEM  | CBB-CAB-C3B | 6.86  | 161.81      | 127.53   |
| 5   | B     | 160 | HEM  | C2A-C1A-NA  | 6.68  | 117.56      | 110.15   |
| 5   | B     | 160 | HEM  | C3B-C2B-C1B | -6.67 | 101.41      | 106.41   |
| 5   | H     | 160 | HEM  | C2A-C1A-NA  | 6.60  | 117.47      | 110.15   |
| 5   | C     | 160 | HEM  | C2B-C1B-NB  | 6.59  | 117.41      | 109.84   |
| 5   | E     | 160 | HEM  | C2A-C1A-NA  | 6.55  | 117.42      | 110.15   |
| 5   | I     | 160 | HEM  | C2B-C1B-NB  | 6.51  | 117.33      | 109.84   |
| 5   | F     | 160 | HEM  | C2A-C1A-NA  | 6.49  | 117.35      | 110.15   |
| 5   | G     | 160 | HEM  | CBB-CAB-C3B | 6.46  | 159.81      | 127.53   |
| 5   | C     | 160 | HEM  | C2D-C1D-ND  | 6.45  | 117.36      | 109.90   |
| 5   | E     | 160 | HEM  | C2B-C1B-NB  | 6.45  | 117.25      | 109.84   |
| 5   | I     | 160 | HEM  | C2D-C1D-ND  | 6.42  | 117.33      | 109.90   |
| 5   | A     | 160 | HEM  | C2B-C1B-NB  | 6.39  | 117.18      | 109.84   |
| 5   | K     | 160 | HEM  | C2B-C1B-NB  | 6.37  | 117.17      | 109.84   |
| 5   | J     | 160 | HEM  | C2A-C1A-NA  | 6.37  | 117.22      | 110.15   |
| 5   | H     | 160 | HEM  | C2B-C1B-NB  | 6.35  | 117.14      | 109.84   |
| 5   | G     | 160 | HEM  | C2B-C1B-NB  | 6.32  | 117.11      | 109.84   |
| 5   | K     | 160 | HEM  | C2A-C1A-NA  | 6.27  | 117.10      | 110.15   |
| 5   | F     | 160 | HEM  | C2B-C1B-NB  | 6.07  | 116.81      | 109.84   |
| 5   | K     | 160 | HEM  | C2D-C1D-ND  | 6.05  | 116.89      | 109.90   |
| 5   | G     | 160 | HEM  | C2A-C1A-NA  | 5.95  | 116.76      | 110.15   |
| 5   | I     | 160 | HEM  | C2A-C1A-NA  | 5.94  | 116.75      | 110.15   |
| 5   | C     | 160 | HEM  | C2A-C1A-NA  | 5.84  | 116.63      | 110.15   |
| 5   | J     | 160 | HEM  | C2D-C1D-ND  | 5.75  | 116.55      | 109.90   |
| 5   | A     | 160 | HEM  | C2D-C1D-ND  | 5.69  | 116.48      | 109.90   |
| 5   | D     | 160 | HEM  | C2B-C1B-NB  | 5.67  | 116.36      | 109.84   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | E     | 160 | HEM  | C2D-C1D-ND  | 5.64  | 116.42      | 109.90   |
| 5   | B     | 160 | HEM  | C2D-C1D-ND  | 5.59  | 116.37      | 109.90   |
| 5   | D     | 160 | HEM  | C2D-C1D-ND  | 5.56  | 116.33      | 109.90   |
| 5   | K     | 160 | HEM  | C4A-C3A-C2A | -5.55 | 100.46      | 106.82   |
| 5   | G     | 160 | HEM  | C4A-C3A-C2A | -5.55 | 100.46      | 106.82   |
| 5   | A     | 160 | HEM  | C2A-C1A-NA  | 5.54  | 116.30      | 110.15   |
| 5   | I     | 160 | HEM  | C4A-C3A-C2A | -5.54 | 100.47      | 106.82   |
| 5   | G     | 160 | HEM  | C2D-C1D-ND  | 5.54  | 116.31      | 109.90   |
| 5   | L     | 160 | HEM  | C2B-C1B-NB  | 5.50  | 116.16      | 109.84   |
| 5   | B     | 160 | HEM  | C2B-C1B-NB  | 5.49  | 116.15      | 109.84   |
| 5   | F     | 160 | HEM  | C2D-C1D-ND  | 5.45  | 116.20      | 109.90   |
| 5   | A     | 160 | HEM  | C4A-C3A-C2A | -5.29 | 100.76      | 106.82   |
| 5   | D     | 160 | HEM  | C4A-C3A-C2A | -5.24 | 100.81      | 106.82   |
| 5   | H     | 160 | HEM  | C2D-C1D-ND  | 5.22  | 115.94      | 109.90   |
| 5   | F     | 160 | HEM  | C4A-C3A-C2A | -5.20 | 100.87      | 106.82   |
| 5   | H     | 160 | HEM  | C4A-C3A-C2A | -5.04 | 101.04      | 106.82   |
| 5   | L     | 160 | HEM  | C4A-C3A-C2A | -5.03 | 101.06      | 106.82   |
| 5   | L     | 160 | HEM  | C2D-C1D-ND  | 5.03  | 115.71      | 109.90   |
| 5   | C     | 160 | HEM  | C4A-C3A-C2A | -4.95 | 101.14      | 106.82   |
| 5   | B     | 160 | HEM  | C4A-C3A-C2A | -4.86 | 101.25      | 106.82   |
| 5   | E     | 160 | HEM  | C4B-C3B-C2B | 4.80  | 111.69      | 107.28   |
| 5   | J     | 160 | HEM  | C4A-C3A-C2A | -4.77 | 101.35      | 106.82   |
| 5   | C     | 160 | HEM  | C3C-C2C-C1C | -4.76 | 102.54      | 107.05   |
| 5   | J     | 160 | HEM  | C1B-NB-C4B  | -4.76 | 99.57       | 105.21   |
| 5   | L     | 160 | HEM  | C3C-C2C-C1C | -4.73 | 102.57      | 107.05   |
| 5   | A     | 160 | HEM  | C4B-C3B-C2B | 4.71  | 111.61      | 107.28   |
| 5   | B     | 160 | HEM  | C3C-C2C-C1C | -4.66 | 102.64      | 107.05   |
| 5   | D     | 160 | HEM  | C3C-C2C-C1C | -4.61 | 102.69      | 107.05   |
| 5   | E     | 160 | HEM  | C3C-C2C-C1C | -4.57 | 102.72      | 107.05   |
| 5   | A     | 160 | HEM  | C3C-C2C-C1C | -4.57 | 102.72      | 107.05   |
| 5   | E     | 160 | HEM  | C4A-C3A-C2A | -4.47 | 101.70      | 106.82   |
| 5   | H     | 160 | HEM  | C3C-C2C-C1C | -4.38 | 102.90      | 107.05   |
| 5   | C     | 160 | HEM  | C1B-NB-C4B  | -4.35 | 100.06      | 105.21   |
| 5   | H     | 160 | HEM  | CMB-C2B-C1B | 4.32  | 131.78      | 125.03   |
| 5   | H     | 160 | HEM  | C4B-C3B-C2B | 4.28  | 111.21      | 107.28   |
| 5   | G     | 160 | HEM  | C3C-C2C-C1C | -4.20 | 103.07      | 107.05   |
| 5   | A     | 160 | HEM  | CMB-C2B-C1B | 4.20  | 131.60      | 125.03   |
| 5   | I     | 160 | HEM  | C4B-C3B-C2B | 4.14  | 111.08      | 107.28   |
| 5   | I     | 160 | HEM  | C3C-C2C-C1C | -4.14 | 103.13      | 107.05   |
| 5   | F     | 160 | HEM  | C3C-C2C-C1C | -4.12 | 103.15      | 107.05   |
| 5   | D     | 160 | HEM  | C4B-C3B-C2B | 4.09  | 111.04      | 107.28   |
| 5   | J     | 160 | HEM  | C3C-C2C-C1C | -4.02 | 103.24      | 107.05   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | L     | 160 | HEM  | C4B-C3B-C2B | 3.98  | 110.94      | 107.28   |
| 5   | A     | 160 | HEM  | C1B-NB-C4B  | -3.95 | 100.53      | 105.21   |
| 5   | I     | 160 | HEM  | C1B-NB-C4B  | -3.94 | 100.54      | 105.21   |
| 5   | K     | 160 | HEM  | C1B-NB-C4B  | -3.93 | 100.56      | 105.21   |
| 5   | C     | 160 | HEM  | C4D-ND-C1D  | -3.91 | 100.57      | 105.21   |
| 5   | D     | 160 | HEM  | C3D-C4D-ND  | 3.91  | 114.46      | 110.17   |
| 5   | F     | 160 | HEM  | C4B-C3B-C2B | 3.90  | 110.86      | 107.28   |
| 5   | H     | 160 | HEM  | C1B-NB-C4B  | -3.89 | 100.60      | 105.21   |
| 5   | G     | 160 | HEM  | C3A-C4A-NA  | 3.87  | 116.34      | 110.14   |
| 5   | I     | 160 | HEM  | C3A-C4A-NA  | 3.87  | 116.34      | 110.14   |
| 5   | J     | 160 | HEM  | C3B-C4B-NB  | 3.87  | 112.25      | 109.47   |
| 5   | K     | 160 | HEM  | C3A-C4A-NA  | 3.85  | 116.32      | 110.14   |
| 5   | H     | 160 | HEM  | C3A-C4A-NA  | 3.85  | 116.31      | 110.14   |
| 5   | I     | 160 | HEM  | C4D-ND-C1D  | -3.80 | 100.71      | 105.21   |
| 5   | H     | 160 | HEM  | CAA-CBA-CGA | -3.78 | 103.63      | 113.67   |
| 5   | K     | 160 | HEM  | C3C-C2C-C1C | -3.77 | 103.47      | 107.05   |
| 5   | F     | 160 | HEM  | C3A-C4A-NA  | 3.77  | 116.18      | 110.14   |
| 5   | J     | 160 | HEM  | CAA-CBA-CGA | -3.74 | 103.73      | 113.67   |
| 5   | G     | 160 | HEM  | C4B-C3B-C2B | 3.70  | 110.68      | 107.28   |
| 5   | A     | 160 | HEM  | C3A-C4A-NA  | 3.70  | 116.08      | 110.14   |
| 5   | J     | 160 | HEM  | C4D-ND-C1D  | -3.69 | 100.84      | 105.21   |
| 5   | E     | 160 | HEM  | C1B-NB-C4B  | -3.69 | 100.84      | 105.21   |
| 5   | B     | 160 | HEM  | C2C-C1C-NC  | 3.68  | 116.45      | 109.64   |
| 5   | J     | 160 | HEM  | C3D-C4D-ND  | 3.67  | 114.20      | 110.17   |
| 5   | I     | 160 | HEM  | CAA-CBA-CGA | -3.66 | 103.95      | 113.67   |
| 5   | D     | 160 | HEM  | CAA-CBA-CGA | -3.66 | 103.95      | 113.67   |
| 5   | D     | 160 | HEM  | C4D-ND-C1D  | -3.65 | 100.89      | 105.21   |
| 5   | F     | 160 | HEM  | CAA-CBA-CGA | -3.61 | 104.10      | 113.67   |
| 5   | L     | 160 | HEM  | C3A-C4A-NA  | 3.60  | 115.91      | 110.14   |
| 5   | E     | 160 | HEM  | C4D-ND-C1D  | -3.59 | 100.95      | 105.21   |
| 5   | E     | 160 | HEM  | CMB-C2B-C1B | 3.59  | 130.64      | 125.03   |
| 5   | H     | 160 | HEM  | CHD-C1D-ND  | -3.58 | 120.57      | 124.42   |
| 5   | E     | 160 | HEM  | CHC-C1C-NC  | -3.57 | 120.56      | 124.45   |
| 5   | B     | 160 | HEM  | C3A-C4A-NA  | 3.56  | 115.85      | 110.14   |
| 5   | F     | 160 | HEM  | C1B-NB-C4B  | -3.53 | 101.03      | 105.21   |
| 5   | I     | 160 | HEM  | CMB-C2B-C1B | 3.52  | 130.54      | 125.03   |
| 5   | G     | 160 | HEM  | C1B-NB-C4B  | -3.52 | 101.04      | 105.21   |
| 5   | D     | 160 | HEM  | CMB-C2B-C1B | 3.51  | 130.53      | 125.03   |
| 5   | E     | 160 | HEM  | CAA-CBA-CGA | -3.51 | 104.35      | 113.67   |
| 5   | E     | 160 | HEM  | C3A-C4A-NA  | 3.51  | 115.77      | 110.14   |
| 5   | L     | 160 | HEM  | CAA-CBA-CGA | -3.50 | 104.39      | 113.67   |
| 5   | H     | 160 | HEM  | C3D-C4D-ND  | 3.49  | 114.00      | 110.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | L     | 160 | HEM  | C2C-C1C-NC  | 3.47  | 116.06      | 109.64   |
| 5   | B     | 160 | HEM  | C4D-ND-C1D  | -3.46 | 101.11      | 105.21   |
| 5   | D     | 160 | HEM  | C3A-C4A-NA  | 3.43  | 115.64      | 110.14   |
| 5   | C     | 160 | HEM  | CMB-C2B-C1B | 3.43  | 130.39      | 125.03   |
| 5   | K     | 160 | HEM  | C4B-C3B-C2B | 3.41  | 110.42      | 107.28   |
| 5   | K     | 160 | HEM  | C4D-ND-C1D  | -3.41 | 101.17      | 105.21   |
| 5   | J     | 160 | HEM  | C3A-C4A-NA  | 3.40  | 115.60      | 110.14   |
| 5   | D     | 160 | HEM  | CHD-C1D-ND  | -3.40 | 120.77      | 124.42   |
| 5   | L     | 160 | HEM  | CMB-C2B-C1B | 3.39  | 130.32      | 125.03   |
| 5   | L     | 160 | HEM  | C4A-NA-C1A  | -3.37 | 100.33      | 105.82   |
| 5   | F     | 160 | HEM  | C3D-C4D-ND  | 3.36  | 113.86      | 110.17   |
| 5   | F     | 160 | HEM  | C4C-NC-C1C  | -3.35 | 100.35      | 105.82   |
| 5   | G     | 160 | HEM  | C2C-C1C-NC  | 3.35  | 115.83      | 109.64   |
| 5   | H     | 160 | HEM  | C4D-ND-C1D  | -3.34 | 101.26      | 105.21   |
| 5   | F     | 160 | HEM  | C2C-C1C-NC  | 3.33  | 115.80      | 109.64   |
| 5   | E     | 160 | HEM  | C3D-C4D-ND  | 3.32  | 113.82      | 110.17   |
| 5   | G     | 160 | HEM  | CMB-C2B-C1B | 3.32  | 130.23      | 125.03   |
| 5   | A     | 160 | HEM  | CAA-CBA-CGA | -3.31 | 104.89      | 113.67   |
| 5   | J     | 160 | HEM  | CMB-C2B-C1B | 3.30  | 130.19      | 125.03   |
| 5   | G     | 160 | HEM  | C4C-NC-C1C  | -3.30 | 100.45      | 105.82   |
| 5   | C     | 160 | HEM  | C3A-C4A-NA  | 3.29  | 115.42      | 110.14   |
| 5   | C     | 160 | HEM  | C3B-C4B-NB  | 3.27  | 111.82      | 109.47   |
| 5   | D     | 160 | HEM  | CMA-C3A-C4A | 3.24  | 130.35      | 125.42   |
| 5   | D     | 160 | HEM  | C1B-NB-C4B  | -3.24 | 101.37      | 105.21   |
| 5   | C     | 160 | HEM  | C4B-C3B-C2B | 3.23  | 110.25      | 107.28   |
| 5   | I     | 160 | HEM  | CAD-CBD-CGD | -3.22 | 105.12      | 113.67   |
| 5   | B     | 160 | HEM  | C3D-C4D-ND  | 3.21  | 113.69      | 110.17   |
| 5   | F     | 160 | HEM  | C4D-ND-C1D  | -3.19 | 101.42      | 105.21   |
| 5   | F     | 160 | HEM  | CMB-C2B-C1B | 3.17  | 129.99      | 125.03   |
| 5   | A     | 160 | HEM  | C4D-ND-C1D  | -3.16 | 101.46      | 105.21   |
| 5   | I     | 160 | HEM  | C3D-C4D-ND  | 3.16  | 113.64      | 110.17   |
| 5   | J     | 160 | HEM  | C2C-C1C-NC  | 3.15  | 115.47      | 109.64   |
| 5   | A     | 160 | HEM  | C2C-C1C-NC  | 3.14  | 115.44      | 109.64   |
| 5   | C     | 160 | HEM  | C3D-C4D-ND  | 3.14  | 113.61      | 110.17   |
| 5   | F     | 160 | HEM  | C4A-NA-C1A  | -3.12 | 100.73      | 105.82   |
| 5   | L     | 160 | HEM  | CAD-CBD-CGD | -3.11 | 105.41      | 113.67   |
| 5   | E     | 160 | HEM  | C2C-C1C-NC  | 3.11  | 115.38      | 109.64   |
| 5   | D     | 160 | HEM  | C4A-NA-C1A  | -3.10 | 100.77      | 105.82   |
| 5   | K     | 160 | HEM  | CMB-C2B-C1B | 3.09  | 129.87      | 125.03   |
| 5   | D     | 160 | HEM  | C2C-C1C-NC  | 3.09  | 115.35      | 109.64   |
| 5   | D     | 160 | HEM  | CAD-CBD-CGD | -3.09 | 105.47      | 113.67   |
| 5   | L     | 160 | HEM  | C3D-C4D-ND  | 3.08  | 113.55      | 110.17   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | E     | 160 | HEM  | C4C-NC-C1C  | -3.08 | 100.80      | 105.82   |
| 5   | H     | 160 | HEM  | C4A-NA-C1A  | -3.06 | 100.83      | 105.82   |
| 5   | A     | 160 | HEM  | CHB-C4A-C3A | -3.05 | 118.57      | 127.43   |
| 5   | B     | 160 | HEM  | C4A-NA-C1A  | -3.05 | 100.85      | 105.82   |
| 5   | B     | 160 | HEM  | C4C-NC-C1C  | -3.04 | 100.86      | 105.82   |
| 5   | B     | 160 | HEM  | C4B-C3B-C2B | 3.02  | 110.06      | 107.28   |
| 5   | B     | 160 | HEM  | CAA-CBA-CGA | -3.01 | 105.69      | 113.67   |
| 5   | H     | 160 | HEM  | C2C-C1C-NC  | 3.01  | 115.20      | 109.64   |
| 5   | D     | 160 | HEM  | CAC-C3C-C4C | 3.00  | 131.99      | 124.82   |
| 5   | L     | 160 | HEM  | CAC-C3C-C4C | 3.00  | 131.98      | 124.82   |
| 5   | B     | 160 | HEM  | C1B-NB-C4B  | -3.00 | 101.66      | 105.21   |
| 5   | E     | 160 | HEM  | CHB-C4A-C3A | -2.98 | 118.78      | 127.43   |
| 5   | C     | 160 | HEM  | CHD-C1D-ND  | -2.97 | 121.22      | 124.42   |
| 5   | I     | 160 | HEM  | C2C-C1C-NC  | 2.96  | 115.11      | 109.64   |
| 5   | K     | 160 | HEM  | C4A-NA-C1A  | -2.96 | 101.00      | 105.82   |
| 5   | C     | 160 | HEM  | C2C-C1C-NC  | 2.94  | 115.08      | 109.64   |
| 5   | L     | 160 | HEM  | CHA-C1A-C2A | -2.94 | 118.86      | 125.30   |
| 5   | K     | 160 | HEM  | C2C-C1C-NC  | 2.94  | 115.08      | 109.64   |
| 5   | H     | 160 | HEM  | CMC-C2C-C1C | 2.93  | 129.89      | 124.73   |
| 5   | L     | 160 | HEM  | C1B-NB-C4B  | -2.92 | 101.74      | 105.21   |
| 5   | L     | 160 | HEM  | CMA-C3A-C4A | 2.92  | 129.87      | 125.42   |
| 5   | E     | 160 | HEM  | C4A-NA-C1A  | -2.92 | 101.06      | 105.82   |
| 5   | A     | 160 | HEM  | C4C-NC-C1C  | -2.92 | 101.07      | 105.82   |
| 5   | D     | 160 | HEM  | CHA-C1A-C2A | -2.91 | 118.94      | 125.30   |
| 5   | H     | 160 | HEM  | CAD-CBD-CGD | -2.90 | 105.97      | 113.67   |
| 5   | B     | 160 | HEM  | CMB-C2B-C1B | 2.89  | 129.55      | 125.03   |
| 5   | K     | 160 | HEM  | C4C-NC-C1C  | -2.89 | 101.11      | 105.82   |
| 5   | A     | 160 | HEM  | CAD-CBD-CGD | -2.88 | 106.03      | 113.67   |
| 5   | J     | 160 | HEM  | C4D-C3D-C2D | -2.86 | 102.72      | 106.89   |
| 5   | G     | 160 | HEM  | C4D-ND-C1D  | -2.86 | 101.82      | 105.21   |
| 5   | L     | 160 | HEM  | C4D-ND-C1D  | -2.85 | 101.83      | 105.21   |
| 5   | F     | 160 | HEM  | CMA-C3A-C4A | 2.85  | 129.75      | 125.42   |
| 5   | I     | 160 | HEM  | C4C-NC-C1C  | -2.82 | 101.22      | 105.82   |
| 5   | L     | 160 | HEM  | CMC-C2C-C1C | 2.82  | 129.70      | 124.73   |
| 5   | J     | 160 | HEM  | C4C-NC-C1C  | -2.82 | 101.22      | 105.82   |
| 5   | L     | 160 | HEM  | C4C-NC-C1C  | -2.81 | 101.23      | 105.82   |
| 5   | D     | 160 | HEM  | CAC-C3C-C2C | -2.80 | 119.31      | 128.43   |
| 5   | G     | 160 | HEM  | CMA-C3A-C4A | 2.80  | 129.68      | 125.42   |
| 5   | B     | 160 | HEM  | CMA-C3A-C4A | 2.80  | 129.68      | 125.42   |
| 5   | L     | 160 | HEM  | CHD-C4C-NC  | -2.79 | 121.42      | 124.45   |
| 5   | B     | 160 | HEM  | CAB-C3B-C2B | -2.79 | 119.36      | 128.43   |
| 5   | D     | 160 | HEM  | C4D-C3D-C2D | -2.79 | 102.83      | 106.89   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | J     | 160 | HEM  | C4A-NA-C1A  | -2.78 | 101.28      | 105.82   |
| 5   | G     | 160 | HEM  | C4A-NA-C1A  | -2.78 | 101.29      | 105.82   |
| 5   | I     | 160 | HEM  | C4A-NA-C1A  | -2.77 | 101.30      | 105.82   |
| 5   | L     | 160 | HEM  | CAB-C3B-C2B | -2.76 | 119.44      | 128.43   |
| 5   | E     | 160 | HEM  | CMC-C2C-C1C | 2.76  | 129.59      | 124.73   |
| 5   | J     | 160 | HEM  | C4B-C3B-C2B | 2.76  | 109.81      | 107.28   |
| 5   | K     | 160 | HEM  | C3B-C4B-NB  | 2.72  | 111.42      | 109.47   |
| 5   | H     | 160 | HEM  | CHB-C4A-C3A | -2.71 | 119.55      | 127.43   |
| 5   | B     | 160 | HEM  | CHC-C1C-C2C | -2.71 | 119.84      | 125.49   |
| 5   | D     | 160 | HEM  | CMC-C2C-C1C | 2.71  | 129.49      | 124.73   |
| 5   | H     | 160 | HEM  | CAA-C2A-C1A | 2.70  | 130.21      | 124.94   |
| 5   | C     | 160 | HEM  | CAD-CBD-CGD | -2.68 | 106.57      | 113.67   |
| 5   | E     | 160 | HEM  | CHD-C1D-ND  | -2.67 | 121.55      | 124.42   |
| 5   | F     | 160 | HEM  | C4D-C3D-C2D | -2.67 | 103.01      | 106.89   |
| 5   | L     | 160 | HEM  | C4D-C3D-C2D | -2.67 | 103.01      | 106.89   |
| 5   | K     | 160 | HEM  | C3D-C4D-ND  | 2.65  | 113.08      | 110.17   |
| 5   | A     | 160 | HEM  | C3D-C4D-ND  | 2.63  | 113.05      | 110.17   |
| 5   | K     | 160 | HEM  | CHB-C4A-C3A | -2.62 | 119.82      | 127.43   |
| 5   | I     | 160 | HEM  | CHB-C4A-C3A | -2.62 | 119.83      | 127.43   |
| 5   | K     | 160 | HEM  | CMA-C3A-C4A | 2.60  | 129.38      | 125.42   |
| 5   | L     | 160 | HEM  | CAC-C3C-C2C | -2.60 | 119.97      | 128.43   |
| 5   | D     | 160 | HEM  | CAB-C3B-C2B | -2.59 | 120.00      | 128.43   |
| 5   | B     | 160 | HEM  | CAD-CBD-CGD | -2.59 | 106.80      | 113.67   |
| 5   | C     | 160 | HEM  | C4C-NC-C1C  | -2.59 | 101.61      | 105.82   |
| 5   | I     | 160 | HEM  | CHD-C1D-C2D | -2.57 | 120.96      | 125.03   |
| 5   | J     | 160 | HEM  | CMA-C3A-C4A | 2.55  | 129.30      | 125.42   |
| 5   | H     | 160 | HEM  | C3B-C4B-NB  | 2.55  | 111.30      | 109.47   |
| 5   | A     | 160 | HEM  | C4A-NA-C1A  | -2.55 | 101.67      | 105.82   |
| 5   | G     | 160 | HEM  | CHB-C4A-C3A | -2.54 | 120.07      | 127.43   |
| 5   | A     | 160 | HEM  | CMC-C2C-C1C | 2.53  | 129.19      | 124.73   |
| 5   | I     | 160 | HEM  | CHD-C1D-ND  | -2.53 | 121.70      | 124.42   |
| 5   | I     | 160 | HEM  | CMA-C3A-C4A | 2.53  | 129.27      | 125.42   |
| 5   | D     | 160 | HEM  | CHD-C4C-NC  | -2.53 | 121.70      | 124.45   |
| 5   | F     | 160 | HEM  | CHB-C4A-C3A | -2.52 | 120.10      | 127.43   |
| 5   | A     | 160 | HEM  | C3B-C4B-NB  | 2.50  | 111.27      | 109.47   |
| 5   | G     | 160 | HEM  | CMC-C2C-C1C | 2.50  | 129.14      | 124.73   |
| 5   | J     | 160 | HEM  | CHB-C4A-C3A | -2.50 | 120.18      | 127.43   |
| 5   | K     | 160 | HEM  | CHB-C1B-C2B | -2.49 | 119.87      | 126.95   |
| 5   | G     | 160 | HEM  | CHD-C1D-C2D | -2.49 | 121.10      | 125.03   |
| 5   | A     | 160 | HEM  | CAA-C2A-C1A | 2.49  | 129.79      | 124.94   |
| 5   | F     | 160 | HEM  | CAA-C2A-C1A | 2.48  | 129.78      | 124.94   |
| 5   | H     | 160 | HEM  | CMA-C3A-C4A | 2.48  | 129.19      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | E     | 160 | HEM  | C4D-C3D-C2D | -2.46 | 103.31      | 106.89   |
| 5   | H     | 160 | HEM  | C4C-NC-C1C  | -2.46 | 101.81      | 105.82   |
| 5   | J     | 160 | HEM  | CHD-C4C-NC  | -2.45 | 121.78      | 124.45   |
| 5   | B     | 160 | HEM  | CHB-C1B-C2B | -2.45 | 119.98      | 126.95   |
| 5   | H     | 160 | HEM  | CAB-C3B-C2B | -2.45 | 120.47      | 128.43   |
| 5   | K     | 160 | HEM  | CAA-CBA-CGA | -2.44 | 107.19      | 113.67   |
| 5   | H     | 160 | HEM  | CHB-C1B-NB  | -2.44 | 121.35      | 124.37   |
| 5   | F     | 160 | HEM  | CHD-C4C-NC  | -2.44 | 121.80      | 124.45   |
| 5   | J     | 160 | HEM  | CHD-C1D-ND  | -2.43 | 121.81      | 124.42   |
| 5   | G     | 160 | HEM  | CHB-C1B-C2B | -2.43 | 120.04      | 126.95   |
| 5   | G     | 160 | HEM  | C3D-C4D-ND  | 2.43  | 112.83      | 110.17   |
| 5   | B     | 160 | HEM  | CHA-C1A-C2A | -2.42 | 119.99      | 125.30   |
| 5   | A     | 160 | HEM  | CHD-C1D-ND  | -2.42 | 121.81      | 124.42   |
| 5   | A     | 160 | HEM  | CMA-C3A-C4A | 2.41  | 129.09      | 125.42   |
| 5   | B     | 160 | HEM  | CHD-C4C-NC  | -2.41 | 121.83      | 124.45   |
| 5   | I     | 160 | HEM  | CHB-C1B-C2B | -2.41 | 120.10      | 126.95   |
| 5   | C     | 160 | HEM  | CAA-CBA-CGA | -2.41 | 107.28      | 113.67   |
| 5   | K     | 160 | HEM  | CHD-C1D-C2D | -2.41 | 121.23      | 125.03   |
| 5   | H     | 160 | HEM  | CAC-C3C-C4C | 2.40  | 130.56      | 124.82   |
| 5   | K     | 160 | HEM  | CAD-CBD-CGD | -2.40 | 107.30      | 113.67   |
| 5   | B     | 160 | HEM  | C4D-C3D-C2D | -2.40 | 103.40      | 106.89   |
| 5   | C     | 160 | HEM  | CMA-C3A-C4A | 2.40  | 129.07      | 125.42   |
| 5   | C     | 160 | HEM  | CMC-C2C-C1C | 2.40  | 128.95      | 124.73   |
| 5   | J     | 160 | HEM  | CHB-C1B-C2B | -2.40 | 120.14      | 126.95   |
| 5   | I     | 160 | HEM  | C1D-C2D-C3D | -2.39 | 104.47      | 106.98   |
| 5   | J     | 160 | HEM  | CAB-C3B-C2B | -2.39 | 120.66      | 128.43   |
| 5   | C     | 160 | HEM  | C4A-NA-C1A  | -2.38 | 101.94      | 105.82   |
| 5   | K     | 160 | HEM  | CHD-C1D-ND  | -2.38 | 121.86      | 124.42   |
| 5   | H     | 160 | HEM  | C4D-C3D-C2D | -2.37 | 103.44      | 106.89   |
| 5   | F     | 160 | HEM  | CHB-C1B-C2B | -2.37 | 120.21      | 126.95   |
| 5   | I     | 160 | HEM  | CMC-C2C-C1C | 2.37  | 128.90      | 124.73   |
| 5   | G     | 160 | HEM  | CAA-CBA-CGA | -2.36 | 107.40      | 113.67   |
| 5   | D     | 160 | HEM  | CHC-C1C-C2C | -2.34 | 120.63      | 125.49   |
| 5   | E     | 160 | HEM  | CAD-C3D-C4D | 2.33  | 128.76      | 124.70   |
| 5   | L     | 160 | HEM  | CHB-C1B-C2B | -2.32 | 120.36      | 126.95   |
| 5   | D     | 160 | HEM  | C4C-NC-C1C  | -2.31 | 102.05      | 105.82   |
| 5   | C     | 160 | HEM  | CHD-C1D-C2D | -2.31 | 121.38      | 125.03   |
| 5   | F     | 160 | HEM  | CHD-C1D-ND  | -2.30 | 121.94      | 124.42   |
| 5   | C     | 160 | HEM  | CHB-C4A-C3A | -2.30 | 120.74      | 127.43   |
| 5   | L     | 160 | HEM  | CHD-C1D-ND  | -2.30 | 121.95      | 124.42   |
| 5   | B     | 160 | HEM  | CHD-C1D-C2D | -2.28 | 121.43      | 125.03   |
| 5   | E     | 160 | HEM  | CAA-C2A-C1A | 2.28  | 129.38      | 124.94   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 5   | G     | 160 | HEM  | CAD-CBD-CGD | -2.27 | 107.64      | 113.67   |
| 5   | J     | 160 | HEM  | CAA-C2A-C1A | 2.27  | 129.37      | 124.94   |
| 5   | C     | 160 | HEM  | C4D-C3D-C2D | -2.26 | 103.60      | 106.89   |
| 5   | I     | 160 | HEM  | C3B-C4B-NB  | 2.26  | 111.09      | 109.47   |
| 5   | H     | 160 | HEM  | CAC-C3C-C2C | -2.24 | 121.15      | 128.43   |
| 5   | C     | 160 | HEM  | CHB-C1B-C2B | -2.24 | 120.58      | 126.95   |
| 5   | J     | 160 | HEM  | CHC-C4B-NB  | -2.23 | 122.02      | 124.42   |
| 5   | K     | 160 | HEM  | CAD-C3D-C4D | 2.23  | 128.58      | 124.70   |
| 5   | E     | 160 | HEM  | CHA-C1A-C2A | -2.21 | 120.47      | 125.30   |
| 5   | E     | 160 | HEM  | CAD-CBD-CGD | -2.20 | 107.82      | 113.67   |
| 5   | G     | 160 | HEM  | CHD-C4C-NC  | -2.20 | 122.06      | 124.45   |
| 5   | D     | 160 | HEM  | CHB-C1B-C2B | -2.20 | 120.71      | 126.95   |
| 5   | E     | 160 | HEM  | CHB-C1B-C2B | -2.19 | 120.73      | 126.95   |
| 5   | I     | 160 | HEM  | CAA-C2A-C1A | 2.19  | 129.21      | 124.94   |
| 5   | I     | 160 | HEM  | CMA-C3A-C2A | 2.19  | 130.26      | 125.62   |
| 5   | K     | 160 | HEM  | CMC-C2C-C1C | 2.17  | 128.55      | 124.73   |
| 5   | L     | 160 | HEM  | CHC-C1C-C2C | -2.17 | 120.97      | 125.49   |
| 5   | A     | 160 | HEM  | CHC-C1C-NC  | -2.17 | 122.09      | 124.45   |
| 5   | J     | 160 | HEM  | CHD-C1D-C2D | -2.16 | 121.62      | 125.03   |
| 5   | H     | 160 | HEM  | CMD-C2D-C1D | 2.14  | 128.38      | 125.03   |
| 5   | K     | 160 | HEM  | CMA-C3A-C2A | 2.14  | 130.16      | 125.62   |
| 5   | L     | 160 | HEM  | CHB-C4A-C3A | -2.14 | 121.22      | 127.43   |
| 5   | A     | 160 | HEM  | CMA-C3A-C2A | 2.13  | 130.14      | 125.62   |
| 5   | B     | 160 | HEM  | CHD-C1D-ND  | -2.12 | 122.14      | 124.42   |
| 5   | A     | 160 | HEM  | CHD-C1D-C2D | -2.11 | 121.70      | 125.03   |
| 5   | D     | 160 | HEM  | CHB-C4A-C3A | -2.11 | 121.31      | 127.43   |
| 5   | G     | 160 | HEM  | CAC-C3C-C4C | 2.10  | 129.84      | 124.82   |
| 5   | A     | 160 | HEM  | C1D-C2D-C3D | -2.10 | 104.77      | 106.98   |
| 5   | G     | 160 | HEM  | C4D-C3D-C2D | -2.10 | 103.83      | 106.89   |
| 5   | A     | 160 | HEM  | CHB-C1B-C2B | -2.09 | 121.00      | 126.95   |
| 5   | E     | 160 | HEM  | CMA-C3A-C2A | 2.09  | 130.06      | 125.62   |
| 5   | A     | 160 | HEM  | CHB-C1B-NB  | -2.09 | 121.78      | 124.37   |
| 5   | I     | 160 | HEM  | C4D-C3D-C2D | -2.08 | 103.86      | 106.89   |
| 5   | F     | 160 | HEM  | CHD-C1D-C2D | -2.07 | 121.75      | 125.03   |
| 5   | F     | 160 | HEM  | C3B-C4B-NB  | 2.06  | 110.94      | 109.47   |
| 5   | B     | 160 | HEM  | CHB-C4A-C3A | -2.04 | 121.50      | 127.43   |
| 5   | G     | 160 | HEM  | C3B-C4B-NB  | 2.04  | 110.93      | 109.47   |
| 5   | J     | 160 | HEM  | CHC-C1C-C2C | -2.04 | 121.24      | 125.49   |
| 5   | K     | 160 | HEM  | C4D-C3D-C2D | -2.04 | 103.92      | 106.89   |
| 5   | F     | 160 | HEM  | CAB-C3B-C2B | -2.04 | 121.80      | 128.43   |
| 5   | C     | 160 | HEM  | C1D-C2D-C3D | -2.02 | 104.85      | 106.98   |
| 5   | D     | 160 | HEM  | C4C-C3C-C2C | 2.01  | 108.56      | 106.81   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 5   | F     | 160 | HEM  | CHC-C1C-NC | -2.01 | 122.27      | 124.45   |
| 5   | J     | 160 | HEM  | CHB-C1B-NB | -2.00 | 121.89      | 124.37   |

There are no chirality outliers.

All (75) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | A     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 5   | A     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 5   | C     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 5   | E     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 5   | E     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 5   | F     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 5   | F     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 5   | H     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 5   | H     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 5   | I     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 5   | I     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 5   | J     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 5   | L     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 5   | L     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 5   | K     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 5   | C     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 5   | F     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 5   | F     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 5   | J     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 5   | B     | 160 | HEM  | C2C-C3C-CAC-CBC |
| 5   | D     | 160 | HEM  | C2B-C3B-CAB-CBB |
| 5   | D     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 5   | H     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 5   | D     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | K     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 5   | H     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | G     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | L     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | D     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | F     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | F     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | F     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | F     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | H     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | G     | 160 | HEM  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 5   | I     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | J     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | C     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | D     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | E     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | H     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | L     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | L     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | B     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | E     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | A     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | I     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | A     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | C     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | I     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | A     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | B     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | H     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | I     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | J     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | A     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | L     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | D     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | B     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | E     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | G     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | J     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | E     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | G     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | J     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | B     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | B     | 160 | HEM  | C4C-C3C-CAC-CBC |
| 5   | E     | 160 | HEM  | C4B-C3B-CAB-CBB |
| 5   | C     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | K     | 160 | HEM  | CAA-CBA-CGA-O2A |
| 5   | K     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | K     | 160 | HEM  | CAD-CBD-CGD-O2D |
| 5   | C     | 160 | HEM  | CAD-CBD-CGD-O1D |
| 5   | K     | 160 | HEM  | CAA-CBA-CGA-O1A |
| 5   | E     | 160 | HEM  | C2B-C3B-CAB-CBB |

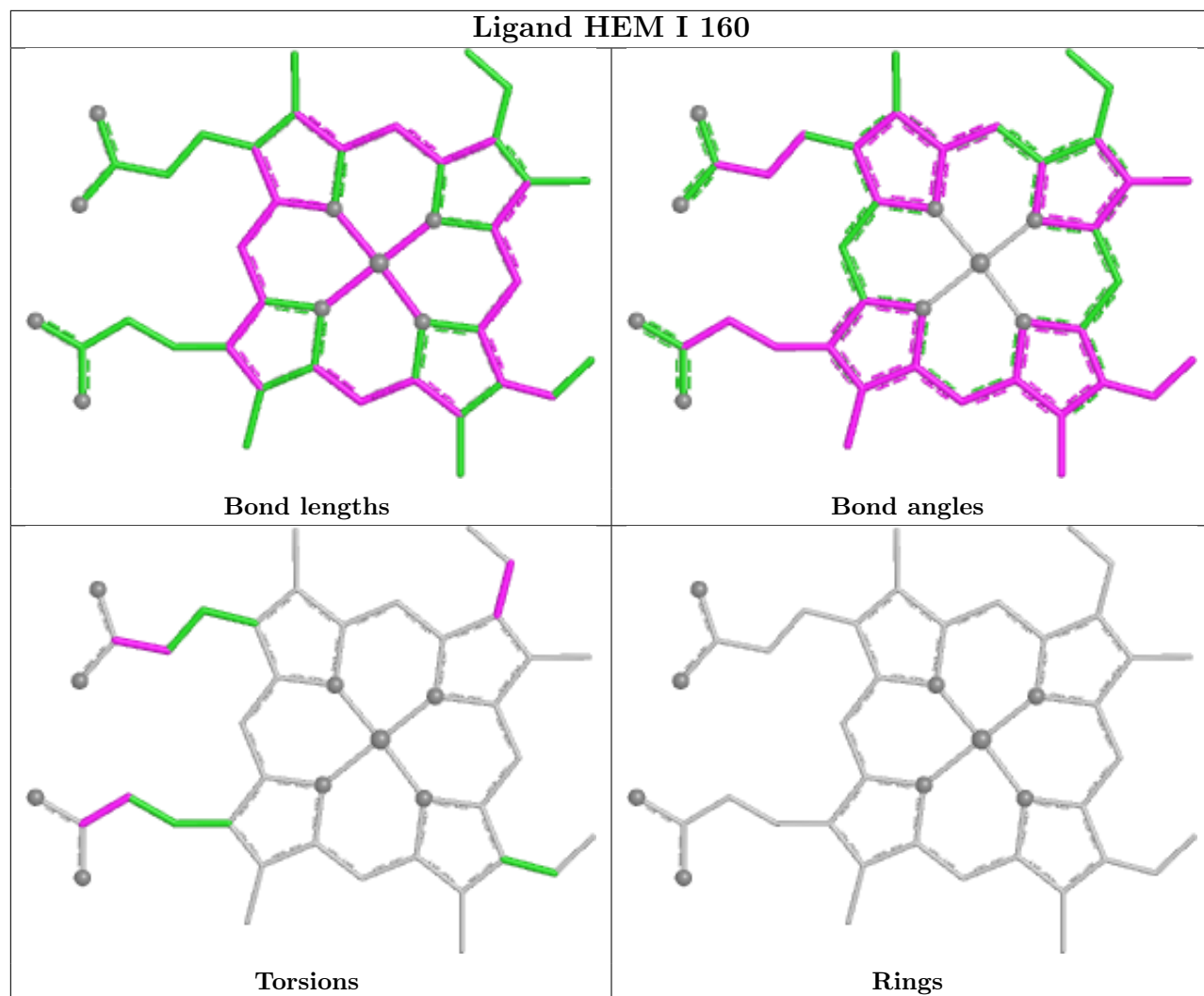
There are no ring outliers.

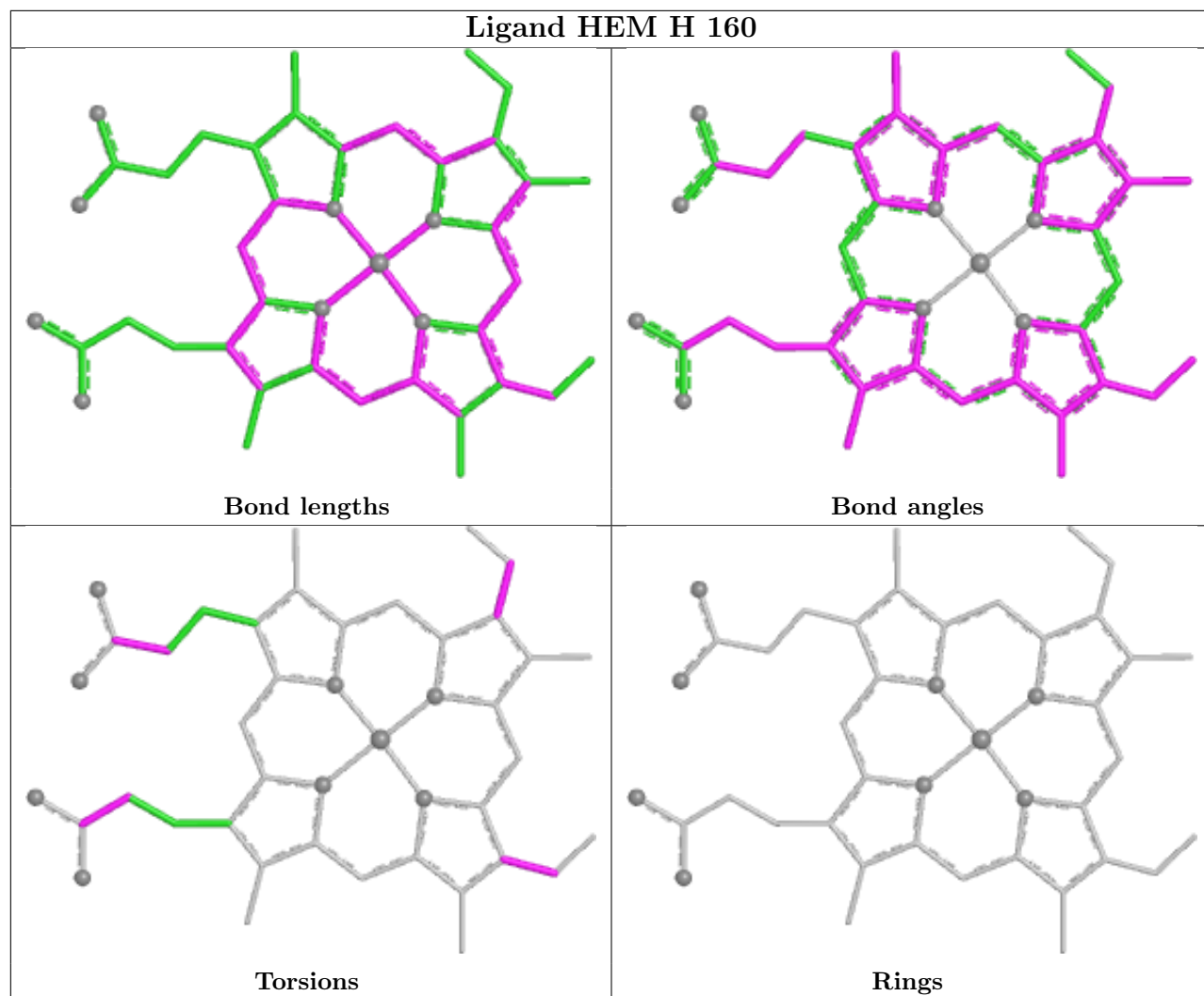
18 monomers are involved in 41 short contacts:

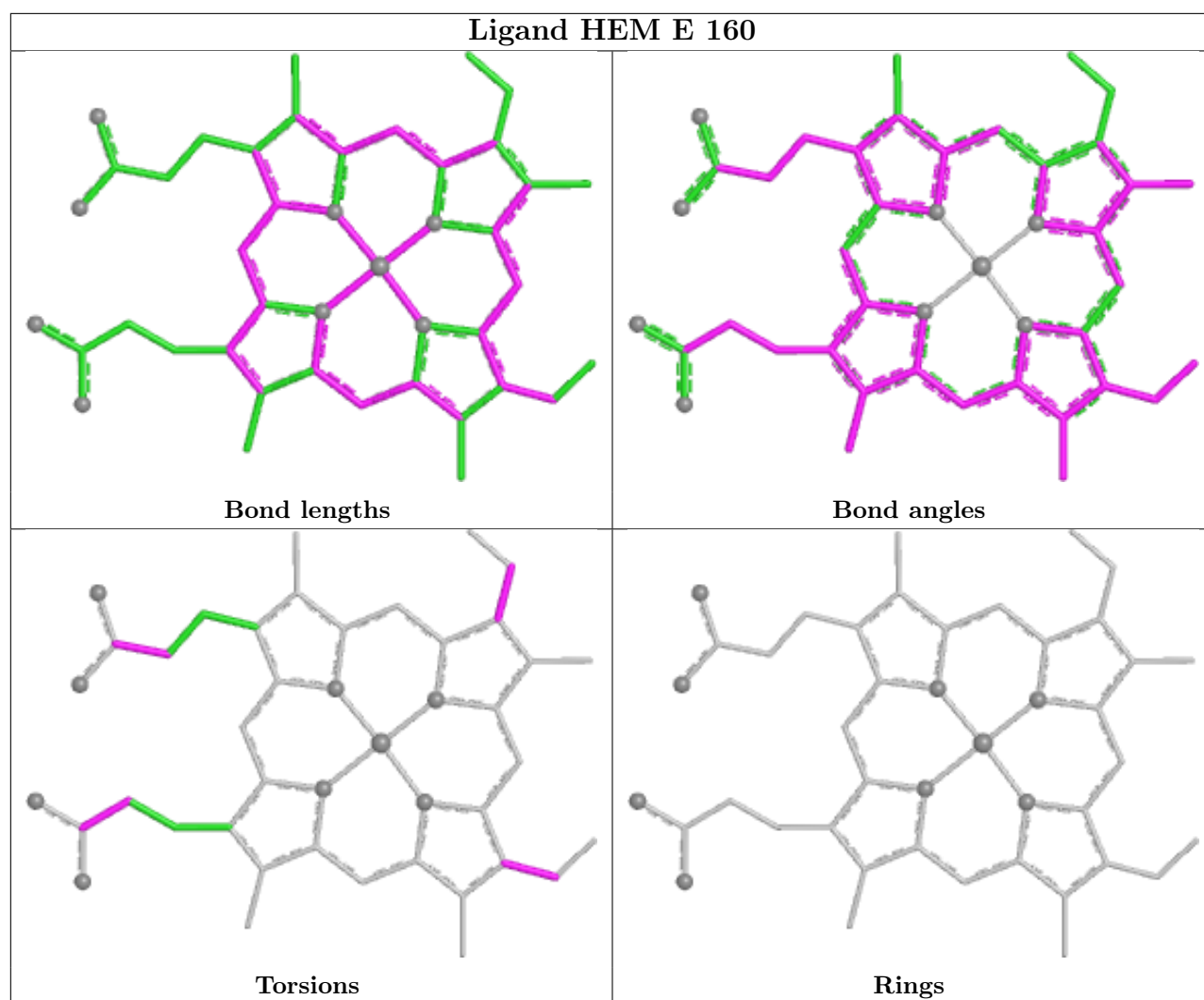
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6   | I     | 3161 | CMO  | 1       | 0            |
| 5   | I     | 160  | HEM  | 1       | 0            |
| 5   | H     | 160  | HEM  | 3       | 0            |
| 6   | F     | 2162 | CMO  | 2       | 0            |
| 6   | B     | 1162 | CMO  | 1       | 0            |
| 5   | E     | 160  | HEM  | 1       | 0            |
| 6   | L     | 3164 | CMO  | 2       | 0            |
| 6   | D     | 1164 | CMO  | 2       | 0            |
| 7   | G     | 154  | PO4  | 1       | 0            |
| 5   | A     | 160  | HEM  | 1       | 0            |
| 5   | L     | 160  | HEM  | 3       | 0            |
| 5   | K     | 160  | HEM  | 5       | 0            |
| 6   | J     | 3162 | CMO  | 3       | 0            |
| 6   | H     | 2164 | CMO  | 2       | 0            |
| 5   | G     | 160  | HEM  | 3       | 0            |
| 5   | C     | 160  | HEM  | 5       | 0            |
| 5   | F     | 160  | HEM  | 1       | 0            |
| 5   | D     | 160  | 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.

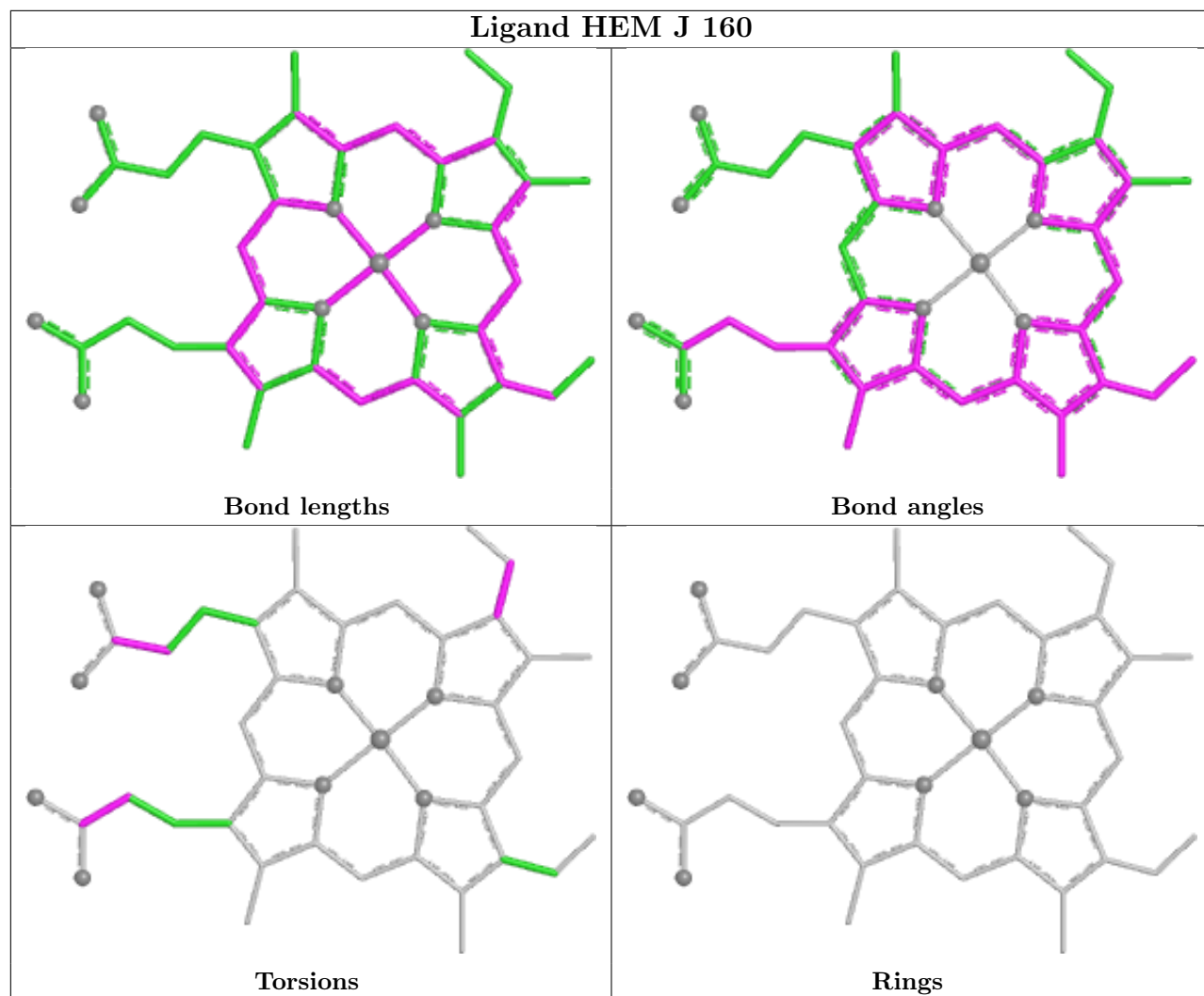
## Ligand HEM I 160

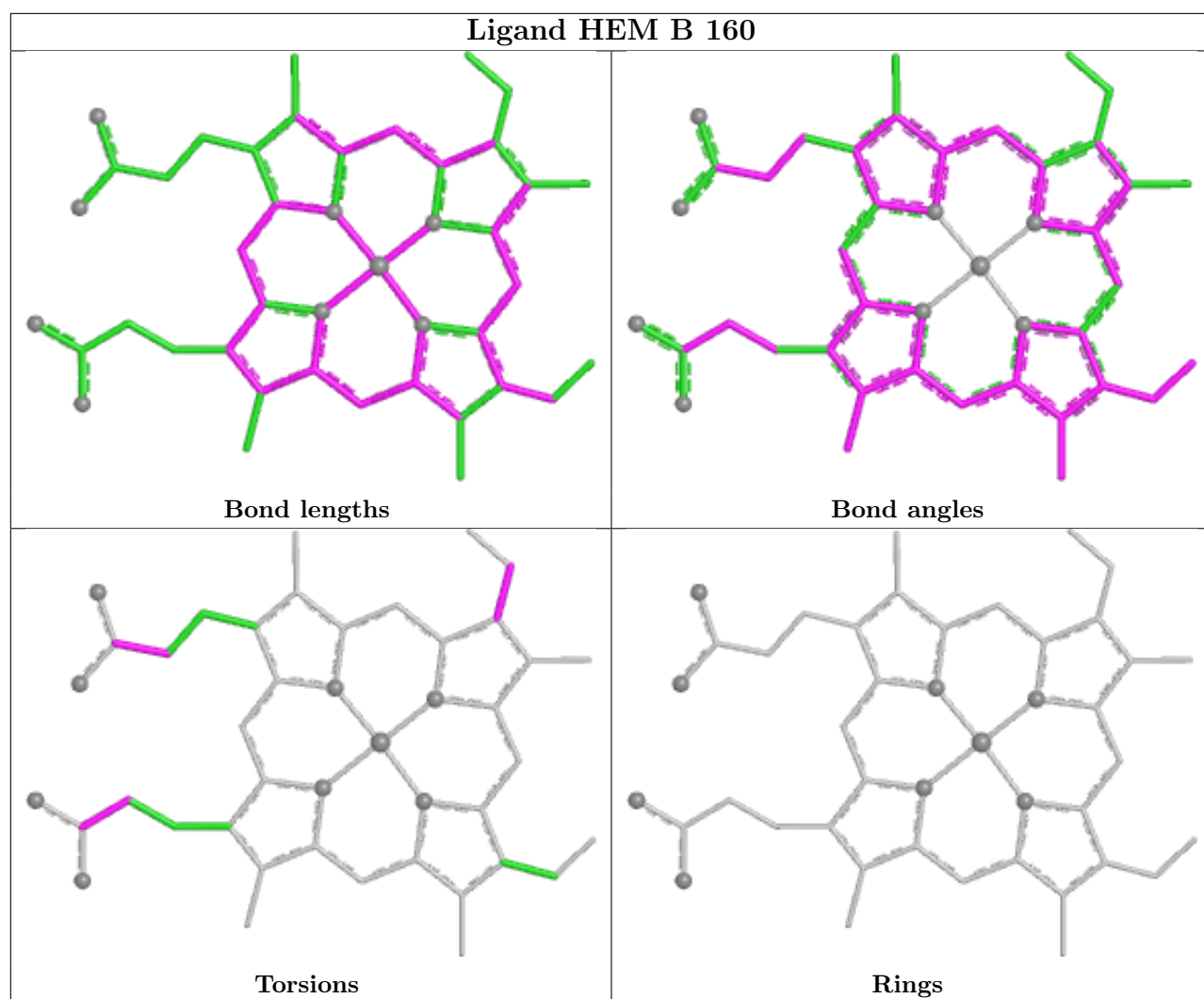


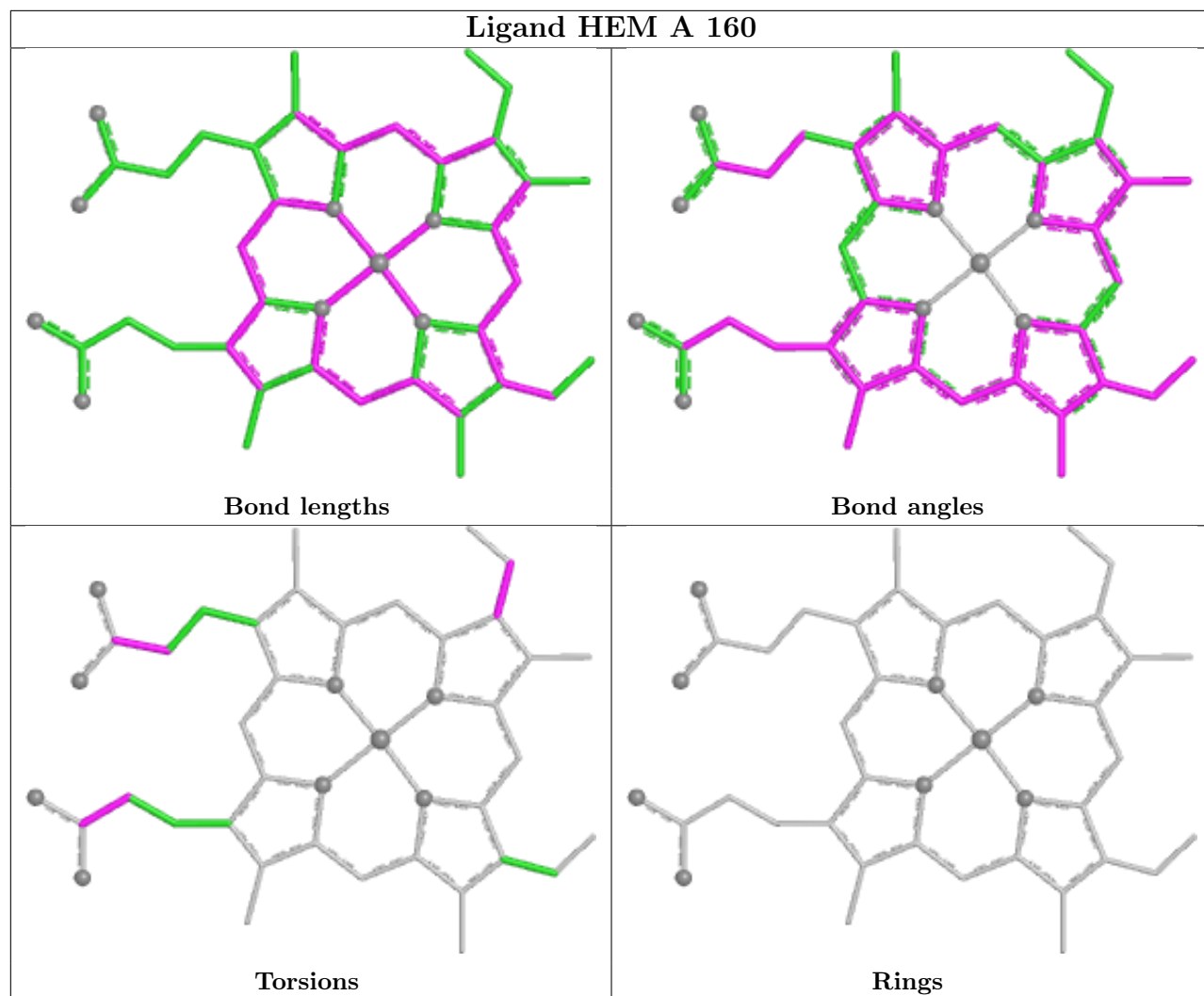


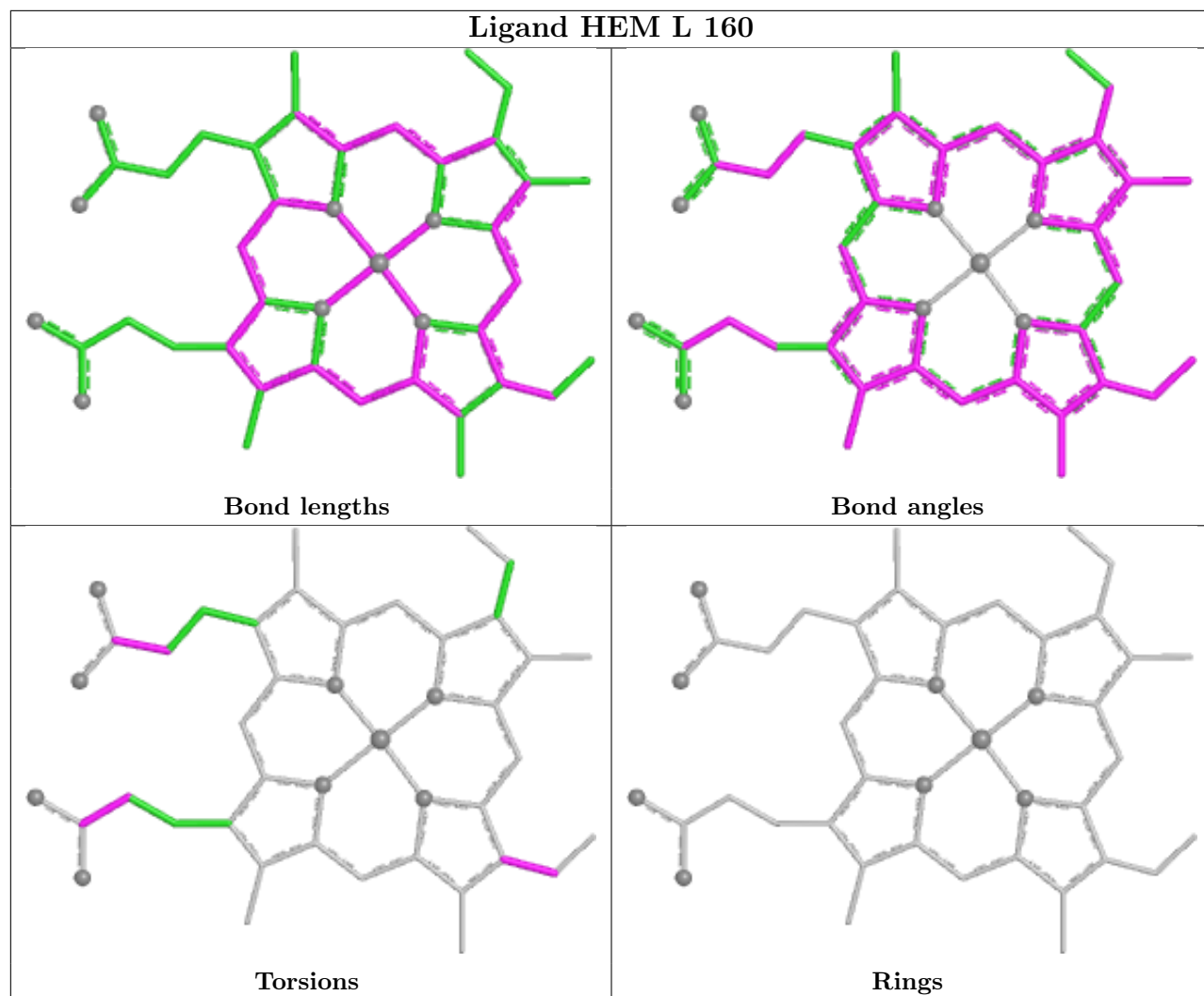


## Ligand HEM J 160

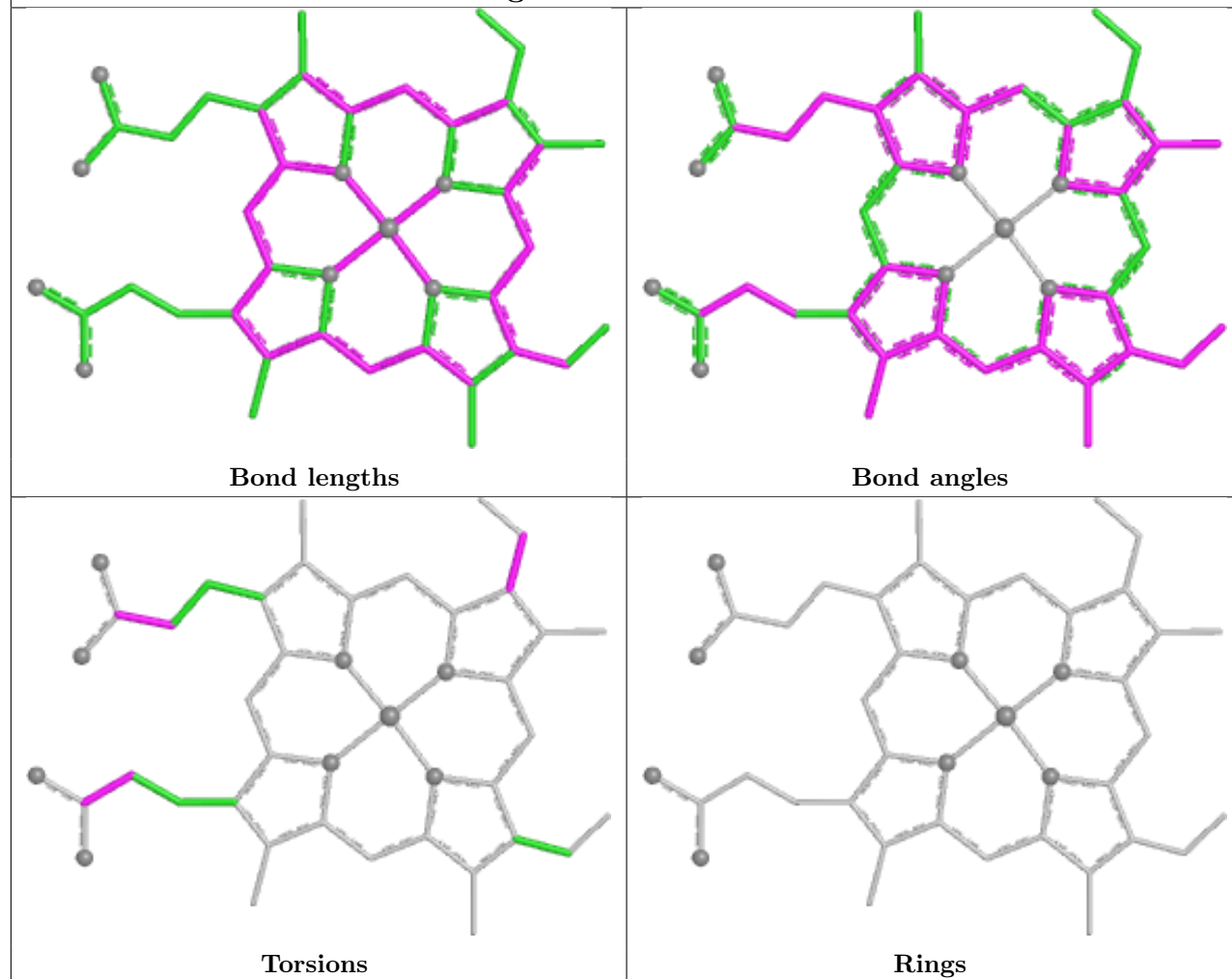


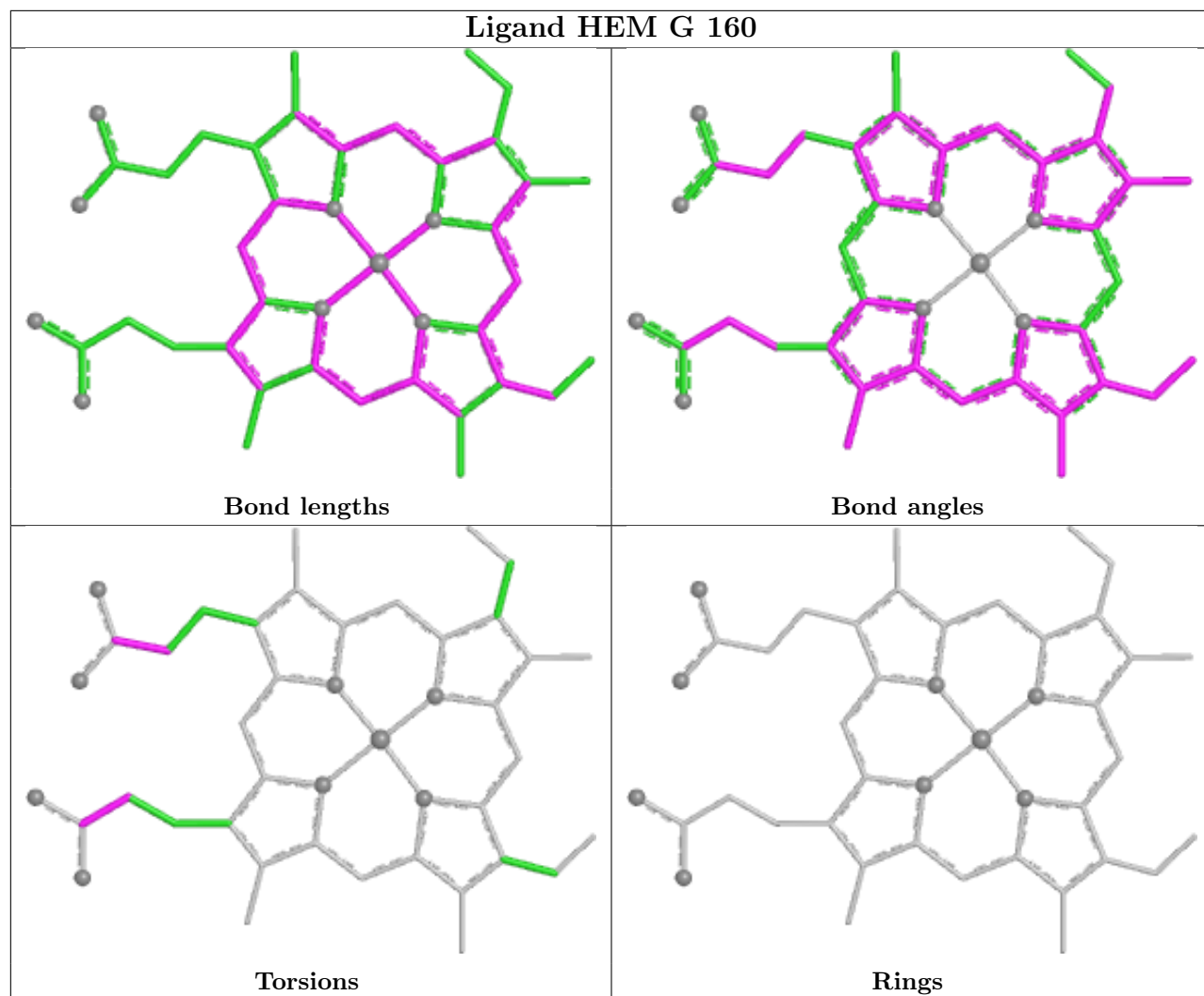


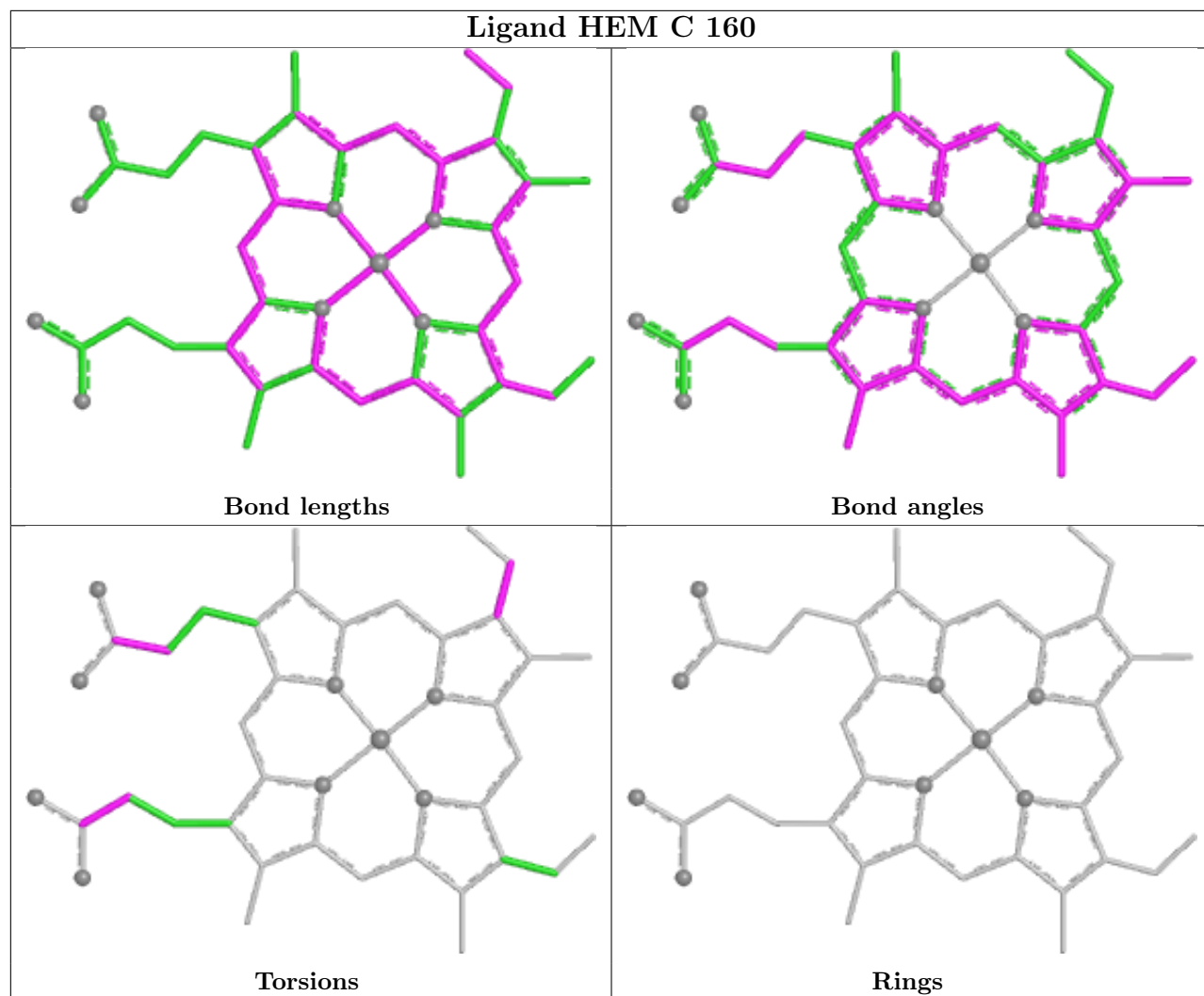


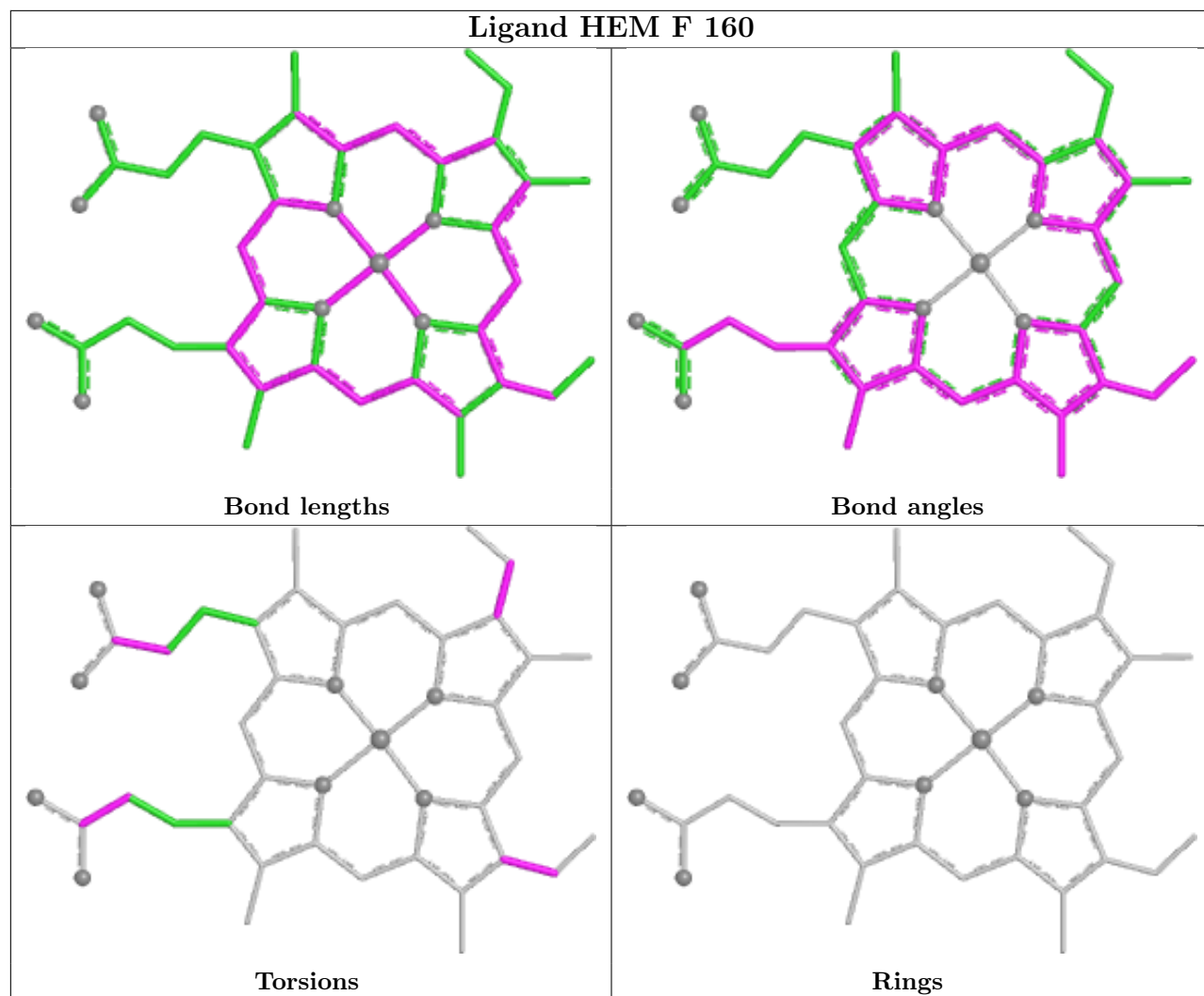


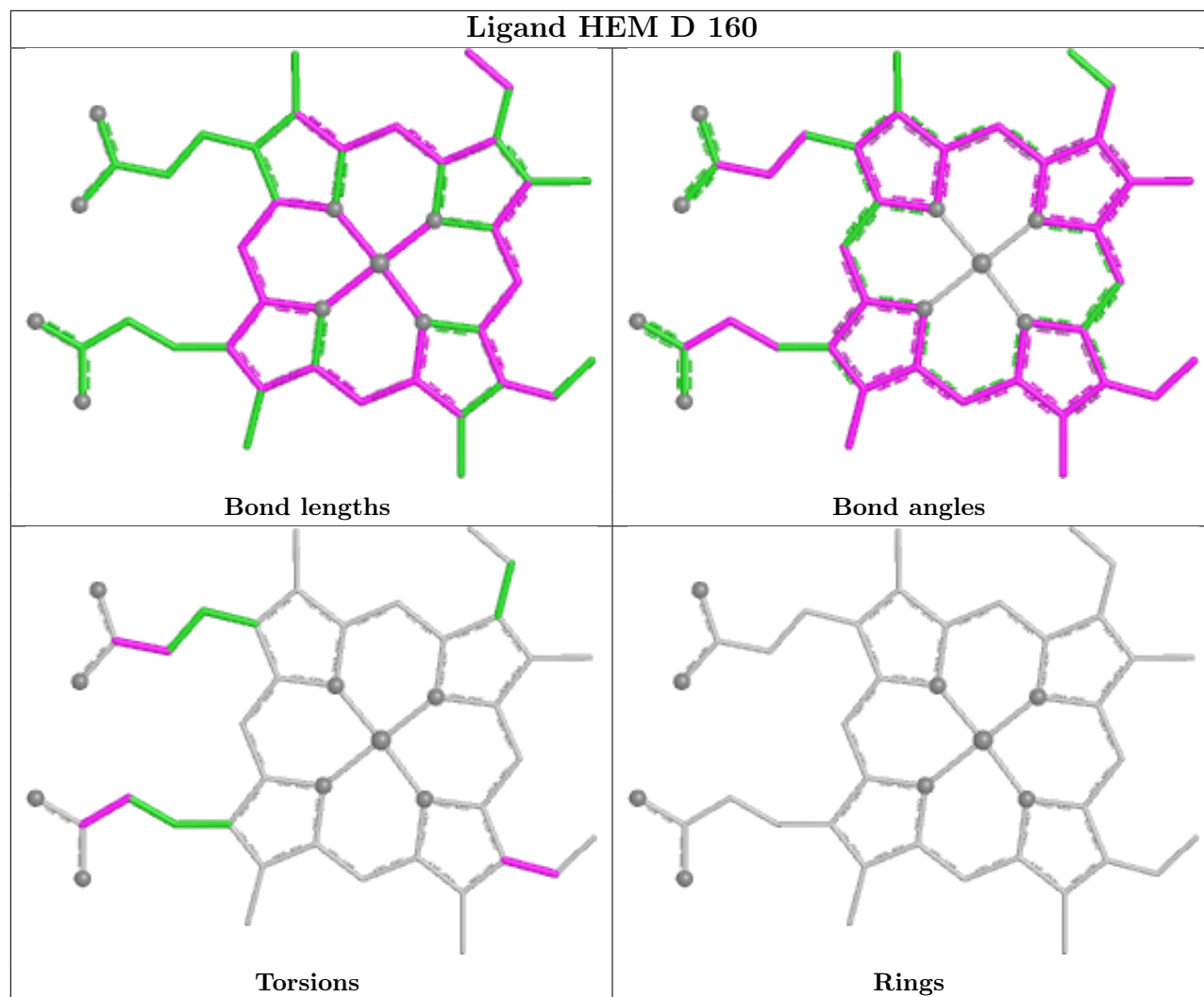
## Ligand HEM K 160











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 3   | C     | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | C     | 3:HIS     | C      | 4:GLU     | N      | 3.51         |

## 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     | 147/151 (97%)   | 0.38   | 17 (11%) 9 7   | 15, 30, 54, 65        | 0      |
| 1   | E     | 147/151 (97%)   | 0.39   | 15 (10%) 12 9  | 17, 31, 57, 72        | 0      |
| 1   | I     | 147/151 (97%)   | 0.44   | 16 (10%) 10 8  | 14, 30, 56, 65        | 0      |
| 2   | B     | 145/145 (100%)  | 0.22   | 8 (5%) 30 25   | 16, 29, 52, 87        | 0      |
| 2   | F     | 145/145 (100%)  | 0.35   | 10 (6%) 23 18  | 16, 32, 53, 89        | 0      |
| 2   | J     | 145/145 (100%)  | 0.57   | 11 (7%) 20 16  | 23, 35, 57, 89        | 0      |
| 3   | C     | 149/153 (97%)   | 0.41   | 10 (6%) 24 19  | 15, 31, 52, 74        | 0      |
| 3   | G     | 149/153 (97%)   | 0.34   | 10 (6%) 24 19  | 17, 31, 54, 69        | 1 (0%) |
| 3   | K     | 149/153 (97%)   | 0.48   | 9 (6%) 27 22   | 19, 37, 60, 75        | 1 (0%) |
| 4   | D     | 140/140 (100%)  | 0.28   | 6 (4%) 40 34   | 17, 32, 54, 77        | 0      |
| 4   | H     | 140/140 (100%)  | 0.47   | 16 (11%) 10 7  | 15, 32, 56, 78        | 0      |
| 4   | L     | 140/140 (100%)  | 0.31   | 8 (5%) 29 24   | 17, 32, 54, 76        | 0      |
| All | All   | 1743/1767 (98%) | 0.39   | 136 (7%) 19 15 | 14, 32, 57, 89        | 2 (0%) |

All (136) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3   | C     | 3   | HIS  | 6.1  |
| 4   | H     | 20  | HIS  | 6.0  |
| 2   | J     | 144 | HIS  | 5.5  |
| 2   | F     | 144 | HIS  | 5.4  |
| 3   | K     | 3   | HIS  | 5.0  |
| 3   | C     | 4   | GLU  | 5.0  |
| 2   | F     | 24  | HIS  | 4.9  |
| 4   | D     | 2   | CYS  | 4.8  |
| 4   | L     | 2   | CYS  | 4.7  |
| 1   | E     | 17  | HIS  | 4.7  |
| 1   | I     | 16  | ARG  | 4.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 23  | TRP  | 4.5  |
| 1   | A     | 17  | HIS  | 4.5  |
| 3   | G     | 3   | HIS  | 4.5  |
| 1   | E     | 24  | SER  | 4.3  |
| 1   | A     | 64  | GLY  | 4.2  |
| 4   | H     | 3   | LEU  | 4.2  |
| 1   | I     | 129 | CYS  | 4.2  |
| 1   | E     | 151 | PRO  | 4.1  |
| 4   | H     | 2   | CYS  | 3.9  |
| 2   | B     | 144 | HIS  | 3.9  |
| 3   | K     | 149 | SER  | 3.9  |
| 3   | C     | 24  | ARG  | 3.8  |
| 1   | A     | 16  | ARG  | 3.7  |
| 3   | G     | 4   | GLU  | 3.7  |
| 1   | E     | 16  | ARG  | 3.7  |
| 4   | H     | 96  | GLU  | 3.6  |
| 1   | E     | 140 | HIS  | 3.6  |
| 2   | J     | 43  | GLU  | 3.6  |
| 2   | B     | 143 | GLY  | 3.5  |
| 3   | G     | 103 | GLU  | 3.5  |
| 3   | K     | 24  | ARG  | 3.4  |
| 2   | B     | 123 | ARG  | 3.3  |
| 2   | F     | 124 | CYS  | 3.3  |
| 2   | F     | 123 | ARG  | 3.3  |
| 4   | H     | 98  | ASN  | 3.3  |
| 4   | L     | 3   | LEU  | 3.3  |
| 3   | K     | 25  | ASP  | 3.3  |
| 1   | A     | 110 | GLU  | 3.2  |
| 1   | A     | 103 | GLN  | 3.2  |
| 2   | F     | 143 | GLY  | 3.2  |
| 2   | J     | 1   | LYS  | 3.2  |
| 1   | E     | 150 | LEU  | 3.1  |
| 2   | J     | 24  | HIS  | 3.1  |
| 1   | I     | 23  | TRP  | 3.1  |
| 1   | A     | 140 | HIS  | 3.1  |
| 1   | E     | 59  | ASP  | 3.1  |
| 4   | D     | 131 | CYS  | 3.0  |
| 4   | H     | 122 | HIS  | 3.0  |
| 1   | I     | 151 | PRO  | 3.0  |
| 1   | A     | 102 | ILE  | 3.0  |
| 1   | E     | 20  | ASP  | 3.0  |
| 4   | H     | 37  | ASP  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 21  | ASP  | 2.9  |
| 1   | I     | 25  | SER  | 2.9  |
| 1   | I     | 17  | HIS  | 2.9  |
| 3   | C     | 63  | GLU  | 2.9  |
| 2   | F     | 97  | GLU  | 2.8  |
| 1   | I     | 105 | LYS  | 2.8  |
| 4   | D     | 21  | ALA  | 2.8  |
| 3   | G     | 150 | ARG  | 2.8  |
| 3   | C     | 56  | ARG  | 2.8  |
| 1   | I     | 64  | GLY  | 2.8  |
| 1   | I     | 5   | ASP  | 2.8  |
| 2   | F     | 145 | HIS  | 2.8  |
| 4   | H     | 38  | ASP  | 2.8  |
| 2   | J     | 123 | ARG  | 2.8  |
| 3   | C     | 20  | ASP  | 2.7  |
| 3   | C     | 25  | ASP  | 2.7  |
| 4   | L     | 131 | CYS  | 2.7  |
| 2   | J     | 122 | GLY  | 2.7  |
| 1   | I     | 103 | GLN  | 2.7  |
| 3   | G     | 106 | GLU  | 2.7  |
| 4   | L     | 96  | GLU  | 2.7  |
| 1   | I     | 20  | ASP  | 2.7  |
| 2   | J     | 143 | GLY  | 2.6  |
| 2   | B     | 24  | HIS  | 2.6  |
| 2   | F     | 122 | GLY  | 2.6  |
| 1   | A     | 24  | SER  | 2.6  |
| 1   | A     | 59  | ASP  | 2.6  |
| 3   | K     | 92  | ASP  | 2.6  |
| 4   | L     | 20  | HIS  | 2.6  |
| 1   | A     | 23  | TRP  | 2.5  |
| 4   | H     | 19  | GLY  | 2.5  |
| 1   | A     | 25  | SER  | 2.5  |
| 2   | J     | 49  | LYS  | 2.5  |
| 4   | D     | 3   | LEU  | 2.5  |
| 4   | D     | 100 | LYS  | 2.5  |
| 1   | I     | 140 | HIS  | 2.5  |
| 4   | H     | 18  | PHE  | 2.5  |
| 2   | J     | 145 | HIS  | 2.5  |
| 1   | A     | 22  | VAL  | 2.5  |
| 2   | B     | 98  | GLY  | 2.5  |
| 1   | E     | 22  | VAL  | 2.5  |
| 4   | D     | 98  | ASN  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | I     | 24  | SER  | 2.4  |
| 1   | A     | 151 | PRO  | 2.4  |
| 2   | B     | 1   | LYS  | 2.4  |
| 3   | K     | 26  | THR  | 2.4  |
| 1   | I     | 104 | ARG  | 2.4  |
| 4   | H     | 22  | HIS  | 2.4  |
| 1   | E     | 25  | SER  | 2.4  |
| 3   | G     | 48  | PRO  | 2.4  |
| 1   | A     | 26  | SER  | 2.4  |
| 4   | L     | 21  | ALA  | 2.4  |
| 1   | E     | 18  | ILE  | 2.3  |
| 1   | A     | 21  | ASP  | 2.3  |
| 1   | I     | 78  | LYS  | 2.3  |
| 2   | B     | 90  | ASP  | 2.3  |
| 2   | J     | 98  | GLY  | 2.3  |
| 4   | H     | 21  | ALA  | 2.3  |
| 3   | G     | 60  | GLU  | 2.3  |
| 3   | C     | 21  | ILE  | 2.3  |
| 2   | B     | 145 | HIS  | 2.3  |
| 3   | K     | 104 | VAL  | 2.3  |
| 1   | E     | 104 | ARG  | 2.2  |
| 1   | A     | 5   | ASP  | 2.2  |
| 2   | F     | 1   | LYS  | 2.2  |
| 4   | L     | 38  | ASP  | 2.2  |
| 3   | C     | 104 | VAL  | 2.2  |
| 1   | I     | 21  | ASP  | 2.1  |
| 3   | G     | 23  | TRP  | 2.1  |
| 4   | L     | 102 | GLU  | 2.1  |
| 3   | K     | 151 | LEU  | 2.1  |
| 1   | E     | 132 | VAL  | 2.1  |
| 2   | J     | 44  | SER  | 2.1  |
| 3   | G     | 24  | ARG  | 2.1  |
| 3   | G     | 49  | GLU  | 2.1  |
| 4   | H     | 17  | ALA  | 2.1  |
| 2   | F     | 54  | ASP  | 2.0  |
| 4   | H     | 97  | ARG  | 2.0  |
| 3   | K     | 62  | ALA  | 2.0  |
| 1   | A     | 18  | ILE  | 2.0  |
| 4   | H     | 131 | CYS  | 2.0  |
| 3   | C     | 106 | GLU  | 2.0  |
| 4   | H     | 44  | ALA  | 2.0  |

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

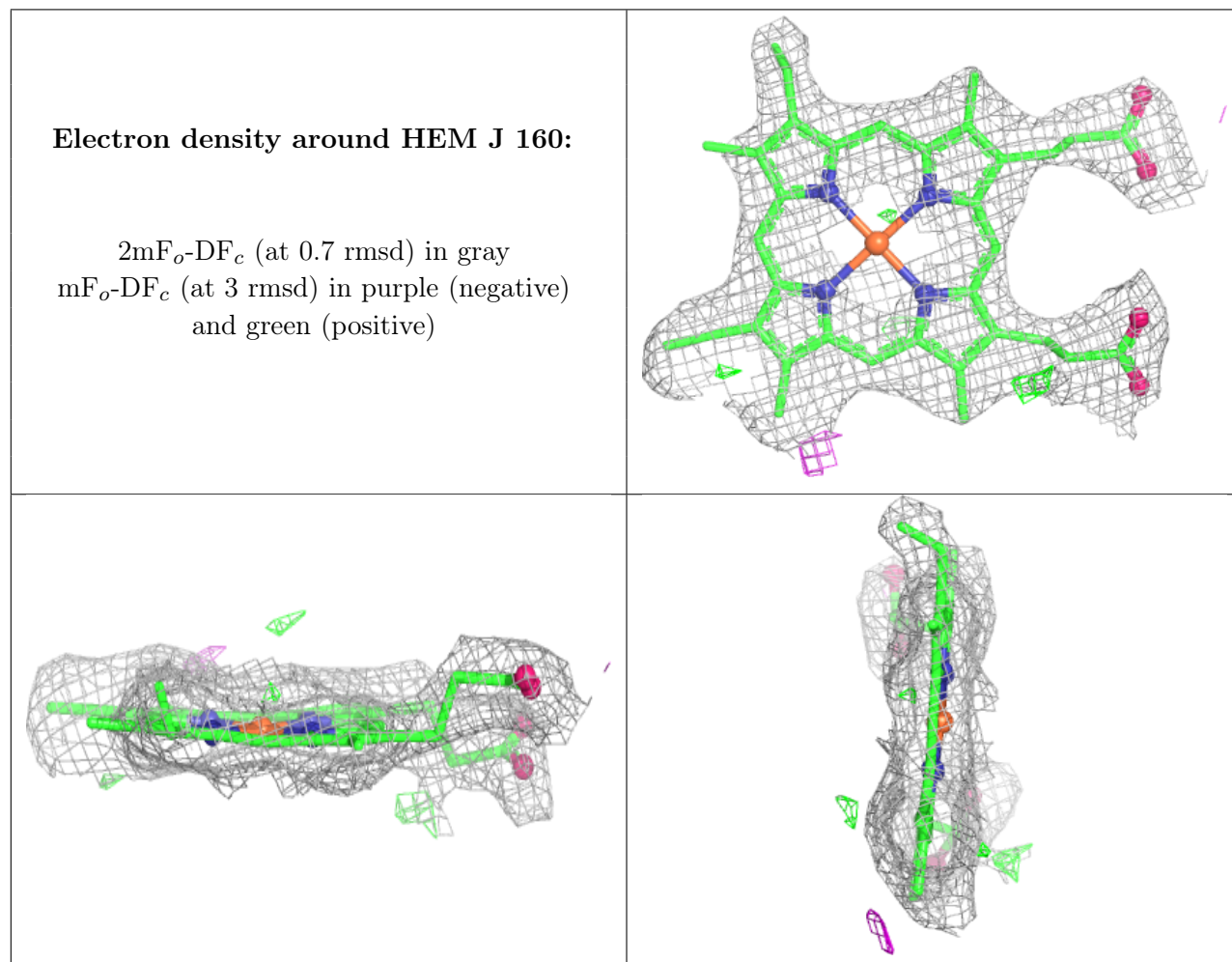
There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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.

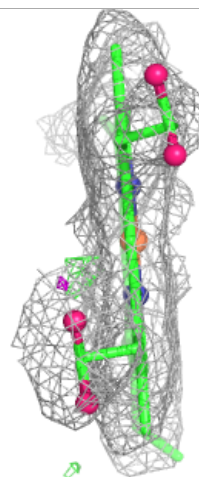
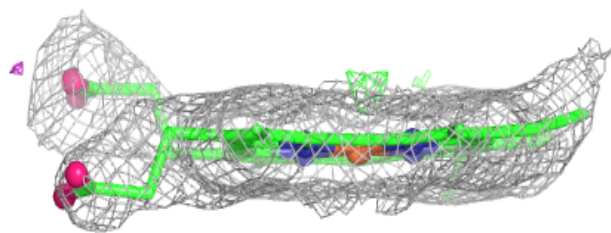
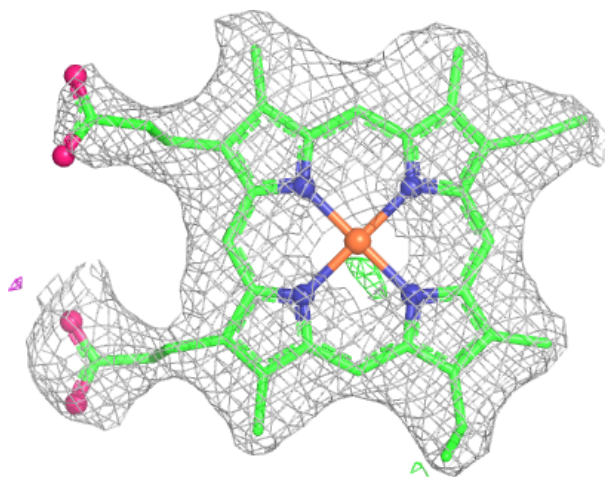
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 6   | CMO  | K     | 3163 | 2/2   | 0.70 | 0.39 | 40,40,40,43                 | 0     |
| 6   | CMO  | E     | 2161 | 2/2   | 0.76 | 0.54 | 41,41,41,43                 | 0     |
| 6   | CMO  | C     | 1163 | 2/2   | 0.83 | 0.23 | 30,30,30,37                 | 0     |
| 6   | CMO  | G     | 2163 | 2/2   | 0.84 | 0.42 | 33,33,33,38                 | 0     |
| 6   | CMO  | L     | 3164 | 2/2   | 0.85 | 0.44 | 38,38,38,44                 | 0     |
| 6   | CMO  | J     | 3162 | 2/2   | 0.86 | 0.26 | 36,36,36,38                 | 0     |
| 6   | CMO  | A     | 1161 | 2/2   | 0.86 | 0.38 | 35,35,35,35                 | 0     |
| 6   | CMO  | D     | 1164 | 2/2   | 0.86 | 0.51 | 32,32,32,37                 | 0     |
| 7   | PO4  | K     | 154  | 5/5   | 0.86 | 0.21 | 26,27,28,30                 | 0     |
| 6   | CMO  | F     | 2162 | 2/2   | 0.88 | 0.30 | 31,31,31,36                 | 0     |
| 6   | CMO  | B     | 1162 | 2/2   | 0.88 | 0.48 | 33,33,33,37                 | 0     |
| 6   | CMO  | H     | 2164 | 2/2   | 0.89 | 0.24 | 21,21,21,27                 | 0     |
| 6   | CMO  | I     | 3161 | 2/2   | 0.89 | 0.45 | 41,41,41,42                 | 0     |
| 7   | PO4  | C     | 154  | 5/5   | 0.94 | 0.15 | 23,27,28,30                 | 0     |
| 5   | HEM  | J     | 160  | 43/43 | 0.95 | 0.10 | 26,37,45,52                 | 0     |
| 5   | HEM  | K     | 160  | 43/43 | 0.95 | 0.10 | 27,35,41,46                 | 0     |
| 5   | HEM  | I     | 160  | 43/43 | 0.96 | 0.09 | 20,26,37,42                 | 0     |
| 5   | HEM  | A     | 160  | 43/43 | 0.96 | 0.09 | 19,26,34,39                 | 0     |
| 5   | HEM  | D     | 160  | 43/43 | 0.96 | 0.09 | 17,24,37,40                 | 0     |
| 5   | HEM  | L     | 160  | 43/43 | 0.96 | 0.09 | 16,24,34,42                 | 0     |
| 5   | HEM  | E     | 160  | 43/43 | 0.96 | 0.09 | 18,25,37,43                 | 0     |
| 7   | PO4  | G     | 154  | 5/5   | 0.96 | 0.21 | 23,25,27,29                 | 0     |
| 5   | HEM  | G     | 160  | 43/43 | 0.96 | 0.09 | 18,26,34,42                 | 0     |
| 5   | HEM  | H     | 160  | 43/43 | 0.97 | 0.09 | 15,21,32,38                 | 0     |
| 5   | HEM  | C     | 160  | 43/43 | 0.97 | 0.08 | 23,28,36,38                 | 0     |
| 5   | HEM  | F     | 160  | 43/43 | 0.97 | 0.09 | 22,26,32,34                 | 0     |
| 5   | HEM  | B     | 160  | 43/43 | 0.97 | 0.08 | 14,19,32,38                 | 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.



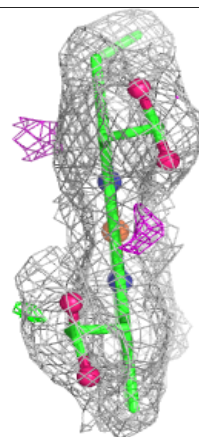
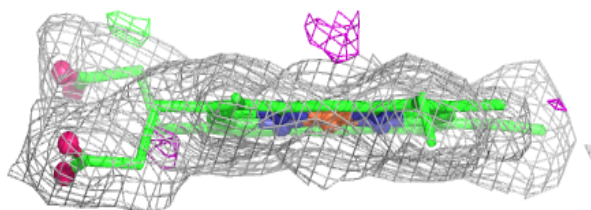
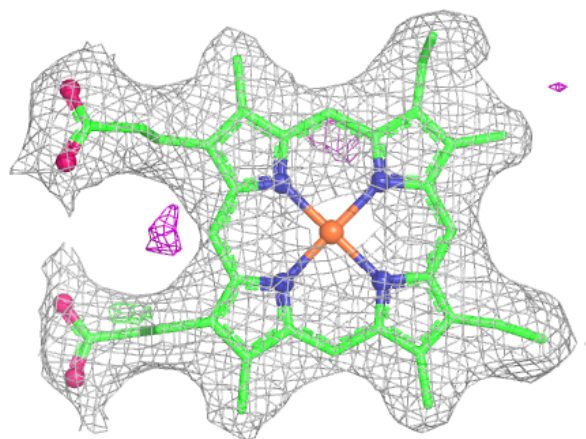
**Electron density around HEM K 160:**

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



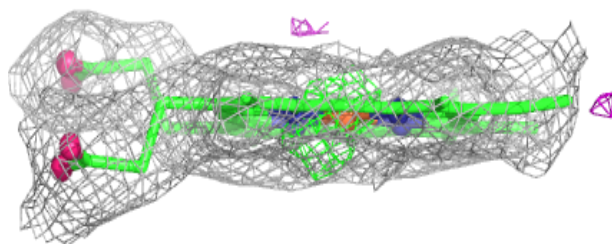
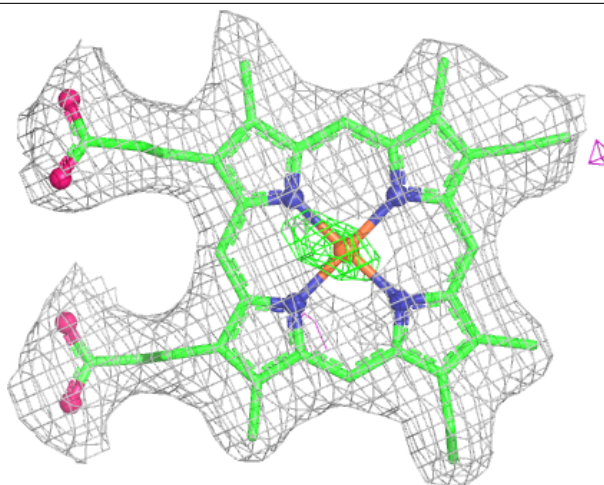
**Electron density around HEM I 160:**

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



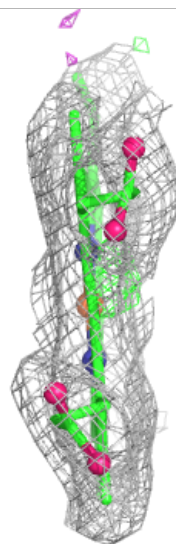
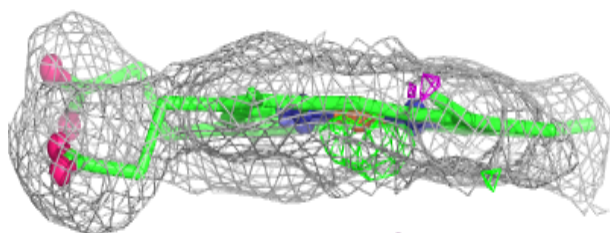
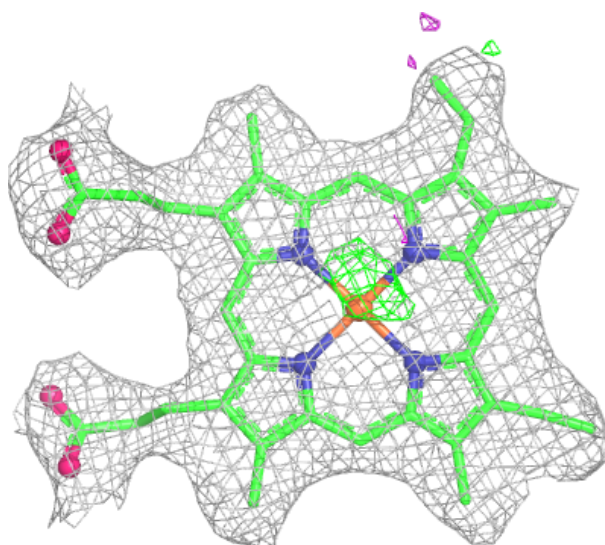
**Electron density around HEM A 160:**

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



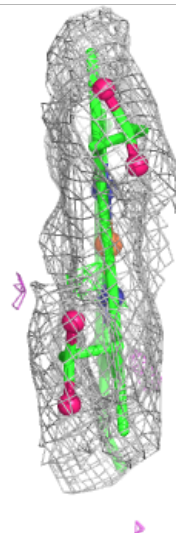
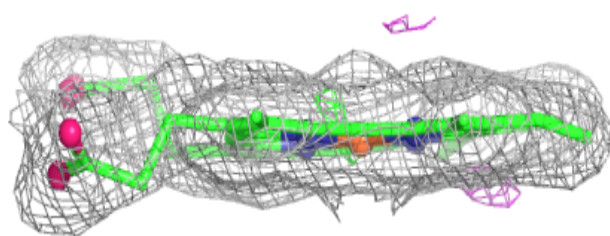
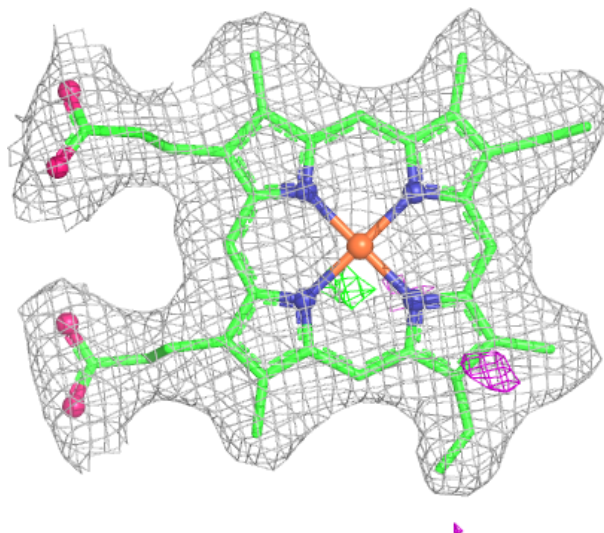
**Electron density around HEM D 160:**

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



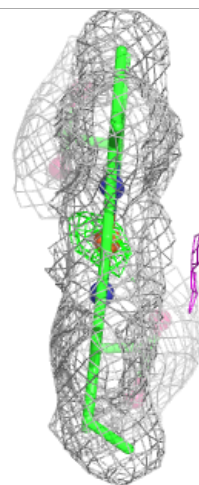
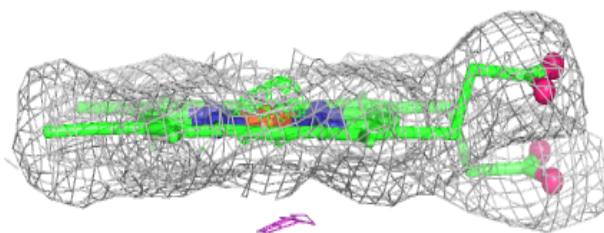
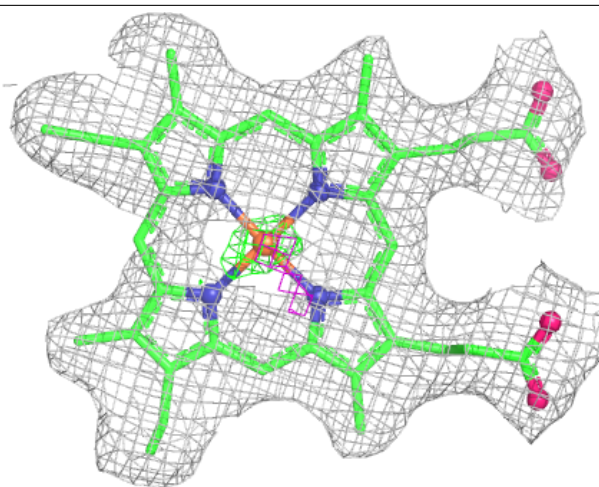
**Electron density around HEM L 160:**

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



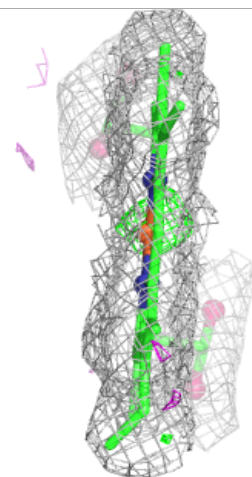
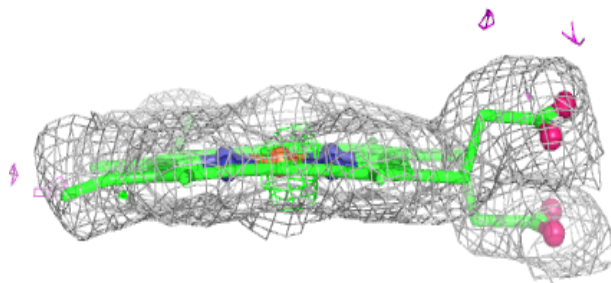
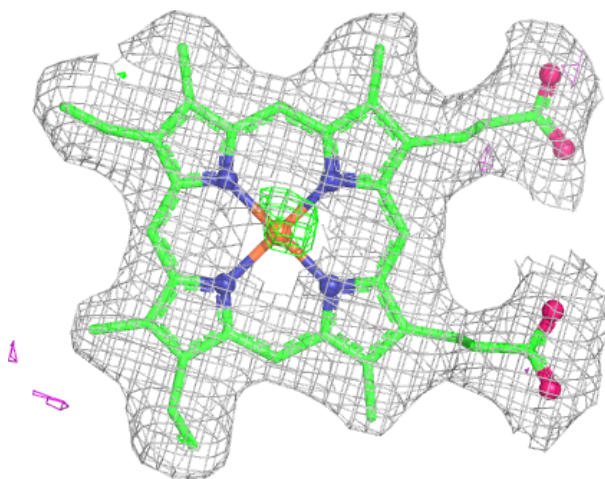
**Electron density around HEM E 160:**

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



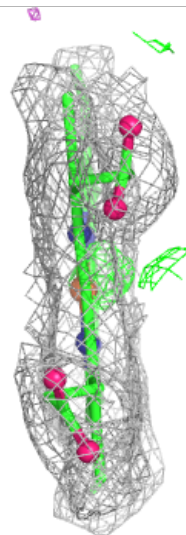
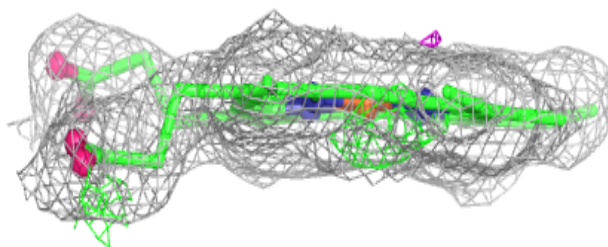
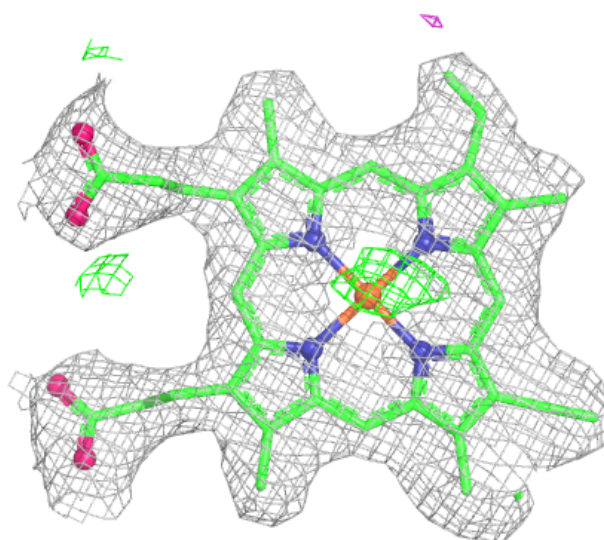
**Electron density around HEM G 160:**

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



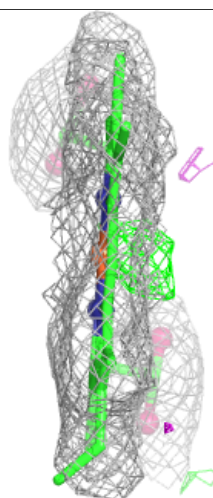
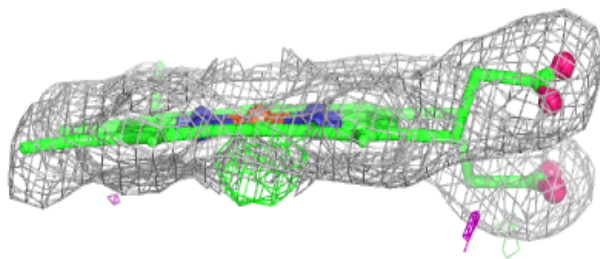
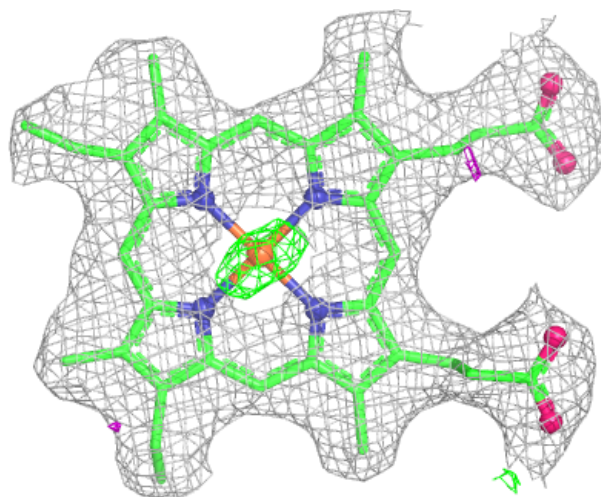
**Electron density around HEM H 160:**

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



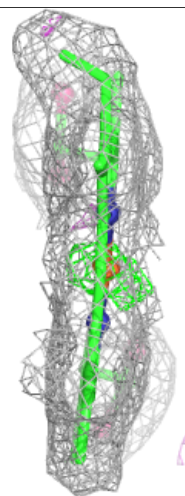
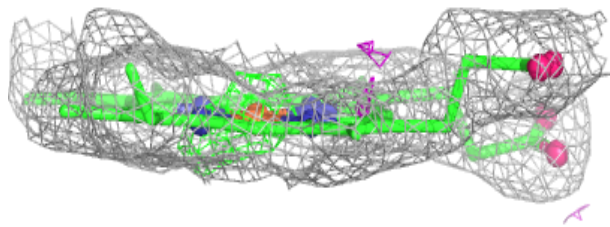
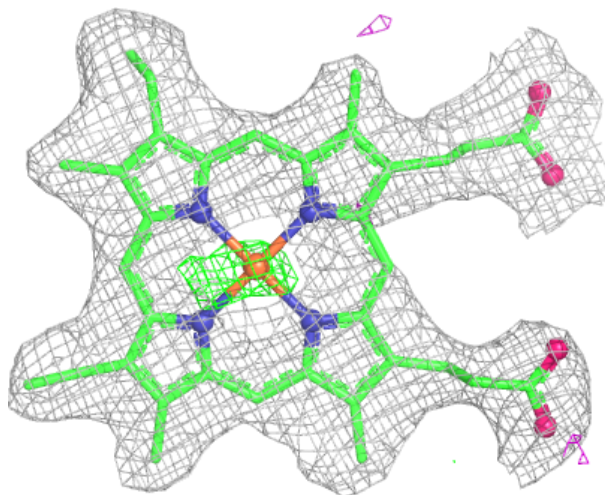
**Electron density around HEM C 160:**

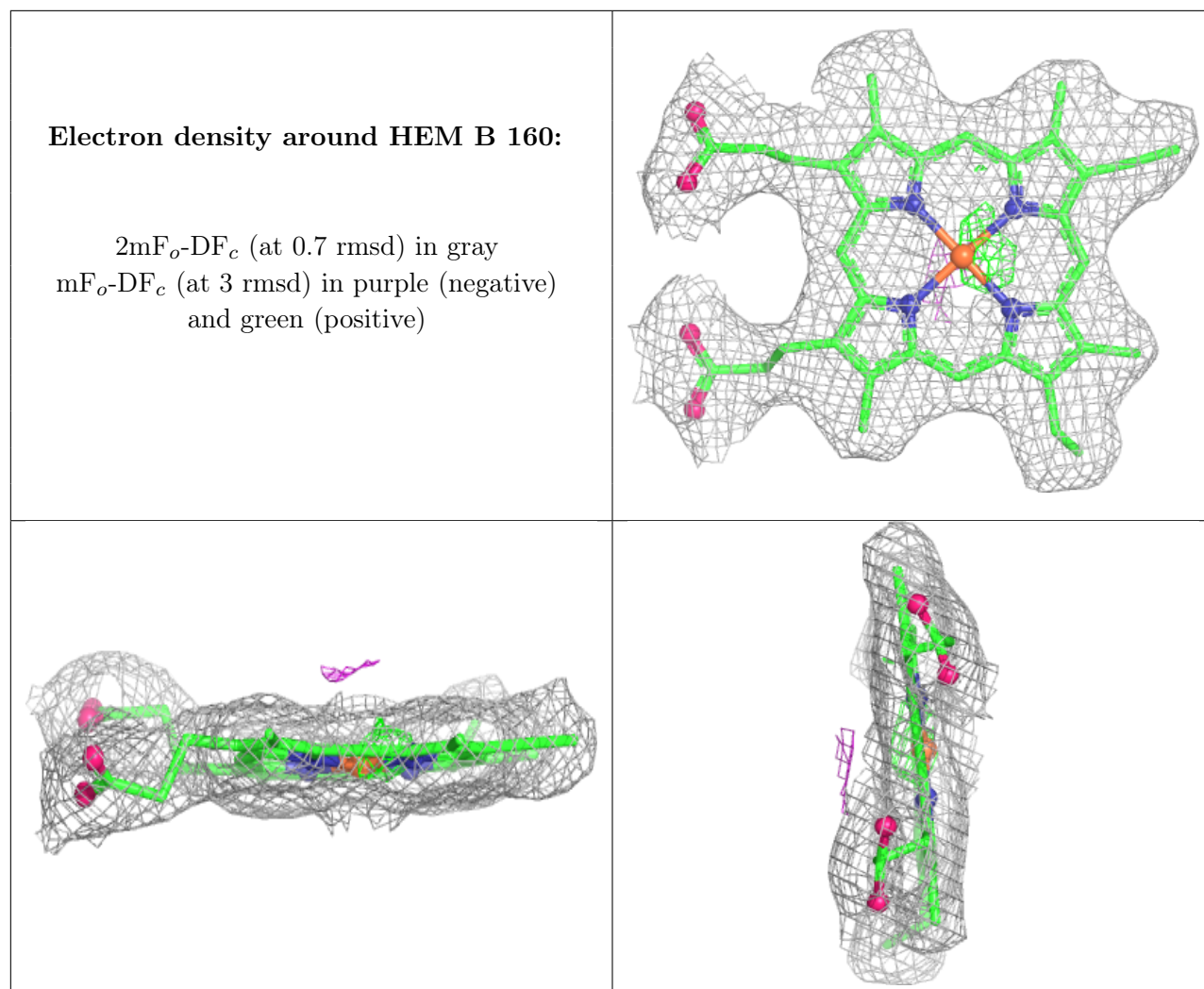
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM F 160:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.