



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2024 – 12:07 PM EST

PDB ID : 1NGK  
Title : Crystallographic Structure of Mycobacterium tuberculosis Hemoglobin O  
Authors : Milani, M.; Savard, P.-Y.; Oullet, H.; Ascenzi, P.; Guertin, M.; Bolognesi, M.  
Deposited on : 2002-12-17  
Resolution : 2.11 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                     | : | 4.02b-467  |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                       |
| Xtriage (Phenix)               | : | 1.20.1   |
| EDS                            | : | 3.0  |
| buster-report                  | : | 1.1.7 (2018)   |
| Percentile statistics          | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| CCP4                           | : | 9.0.003 (Gargrove)   |
| Density-Fitness                | : | 1.0.11   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.39   |

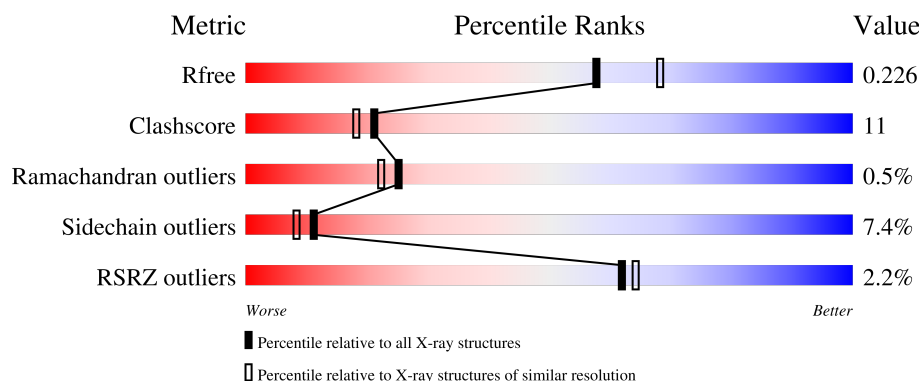
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 Å.

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




| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 164625                      | 7689 (2.14-2.10)                                      |
| Clashscore            | 180529                      | 8431 (2.14-2.10)                                      |
| Ramachandran outliers | 177936                      | 8366 (2.14-2.10)                                      |
| Sidechain outliers    | 177891                      | 8367 (2.14-2.10)                                      |
| RSRZ outliers         | 164620                      | 7689 (2.14-2.10)                                      |

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     | 128    | <div> <div>2%</div> <div>74%</div> <div>20%</div> <div>5%</div> <div>.</div> </div> |
| 1   | B     | 128    | <div> <div>4%</div> <div>75%</div> <div>23%</div> <div>..</div> </div>              |
| 1   | C     | 128    | <div> <div>3%</div> <div>76%</div> <div>19%</div> <div>...</div> </div>             |
| 1   | D     | 128    | <div> <div>3%</div> <div>78%</div> <div>18%</div> <div>...</div> </div>             |
| 1   | E     | 128    | <div> <div>4%</div> <div>71%</div> <div>23%</div> <div>...</div> </div>             |

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| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | F     | 128    |  <div> <div></div> <div>3%</div> <div>74%</div> <div>20%</div> <div>5%</div> </div> |
| 1   | G     | 128    |  <div> <div></div> <div>1%</div> <div>75%</div> <div>23%</div> <div>2%</div> </div> |
| 1   | H     | 128    |  <div> <div></div> <div>1%</div> <div>73%</div> <div>22%</div> <div>4%</div> </div> |
| 1   | I     | 128    |  <div> <div></div> <div>0%</div> <div>74%</div> <div>22%</div> <div>4%</div> </div> |
| 1   | J     | 128    |  <div> <div></div> <div>2%</div> <div>75%</div> <div>23%</div> <div>2%</div> </div> |
| 1   | K     | 128    |  <div> <div></div> <div>1%</div> <div>75%</div> <div>20%</div> <div>4%</div> </div> |
| 1   | L     | 128    |  <div> <div></div> <div>2%</div> <div>71%</div> <div>25%</div> <div>2%</div> </div> |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15104 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 Hemoglobin-like protein HbO.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | A     | 126      | Total | C   | N   | O   | S | 18      | 5       | 0     |
|     |       |          | 1078  | 675 | 194 | 204 | 5 |         |         |       |
| 1   | B     | 127      | Total | C   | N   | O   | S | 33      | 5       | 0     |
|     |       |          | 1085  | 680 | 195 | 205 | 5 |         |         |       |
| 1   | C     | 126      | Total | C   | N   | O   | S | 7       | 6       | 0     |
|     |       |          | 1087  | 680 | 195 | 207 | 5 |         |         |       |
| 1   | D     | 126      | Total | C   | N   | O   | S | 22      | 6       | 0     |
|     |       |          | 1089  | 681 | 198 | 205 | 5 |         |         |       |
| 1   | E     | 127      | Total | C   | N   | O   | S | 44      | 7       | 0     |
|     |       |          | 1106  | 692 | 202 | 207 | 5 |         |         |       |
| 1   | F     | 126      | Total | C   | N   | O   | S | 25      | 6       | 0     |
|     |       |          | 1089  | 681 | 198 | 205 | 5 |         |         |       |
| 1   | G     | 127      | Total | C   | N   | O   | S | 13      | 0       | 0     |
|     |       |          | 1045  | 656 | 190 | 194 | 5 |         |         |       |
| 1   | H     | 127      | Total | C   | N   | O   | S | 15      | 1       | 0     |
|     |       |          | 1054  | 661 | 191 | 197 | 5 |         |         |       |
| 1   | I     | 127      | Total | C   | N   | O   | S | 4       | 2       | 0     |
|     |       |          | 1066  | 668 | 197 | 196 | 5 |         |         |       |
| 1   | J     | 127      | Total | C   | N   | O   | S | 45      | 1       | 0     |
|     |       |          | 1056  | 662 | 194 | 195 | 5 |         |         |       |
| 1   | K     | 127      | Total | C   | N   | O   | S | 21      | 1       | 0     |
|     |       |          | 1056  | 662 | 194 | 195 | 5 |         |         |       |
| 1   | L     | 127      | Total | C   | N   | O   | S | 23      | 0       | 0     |
|     |       |          | 1045  | 656 | 190 | 194 | 5 |         |         |       |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



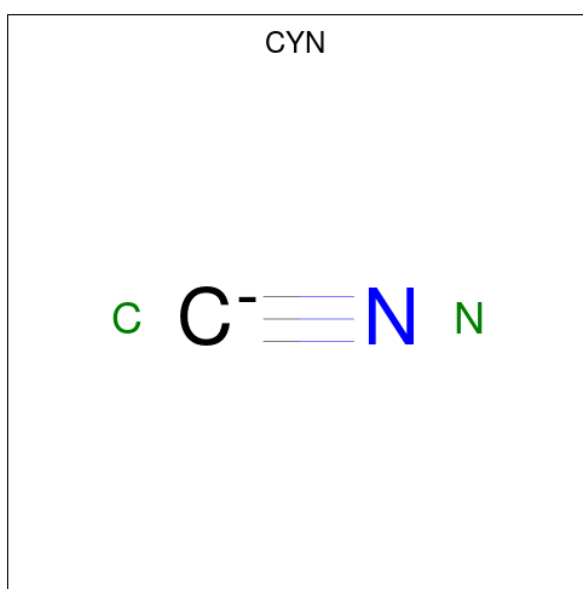
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | D     | 1        | Total | O | S | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | E     | 1        | Total | O | S | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | J     | 1        | Total | O | S | 0       | 1       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 2   | L     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 3 is CYANIDE ION (three-letter code: CYN) (formula: CN).



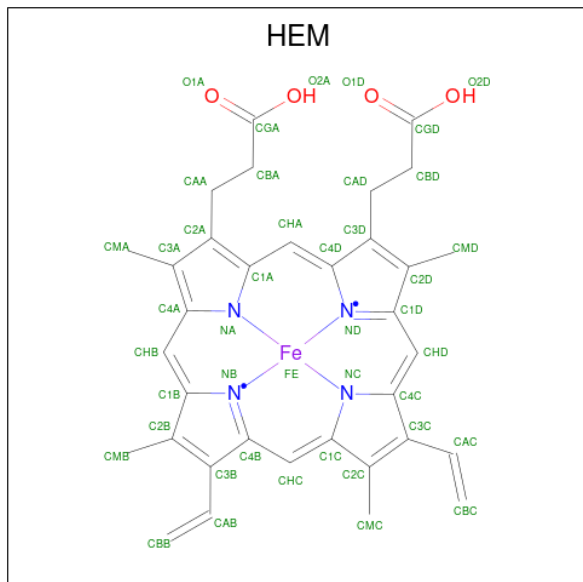
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | B     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | C     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | D     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | E     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | F     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |
| 3   | G     | 1        | Total | C | N | 0       | 0       |
|     |       |          | 2     | 1 | 1 |         |         |

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| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 3   | H     | 1        | Total<br>2 | C<br>1 | N<br>1 | 0       | 0       |
| 3   | I     | 1        | Total<br>2 | C<br>1 | N<br>1 | 0       | 0       |
| 3   | J     | 1        | Total<br>2 | C<br>1 | N<br>1 | 0       | 0       |
| 3   | K     | 1        | Total<br>2 | C<br>1 | N<br>1 | 0       | 0       |
| 3   | L     | 1        | Total<br>2 | C<br>1 | N<br>1 | 0       | 0       |

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        | ZeroOcc | AltConf |   |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|---|
| 4   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 4   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 4   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 4   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 4   | E     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |
| 4   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4  | 0       | 0 |

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

- Molecule 5 is water.

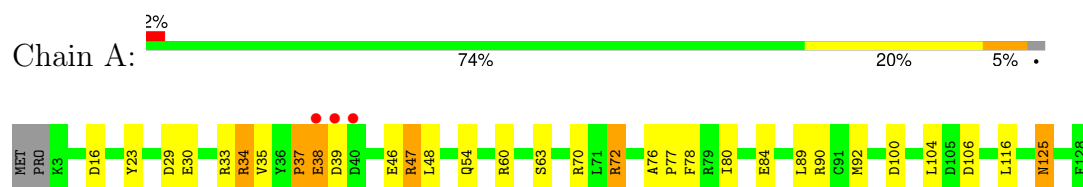
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5   | A     | 138      | Total<br>138 | O<br>138 | 0       | 0       |
| 5   | B     | 123      | Total<br>123 | O<br>123 | 0       | 0       |
| 5   | C     | 184      | Total<br>184 | O<br>184 | 0       | 0       |
| 5   | D     | 136      | Total<br>136 | O<br>136 | 0       | 0       |
| 5   | E     | 112      | Total<br>112 | O<br>112 | 0       | 0       |
| 5   | F     | 123      | Total<br>123 | O<br>123 | 0       | 0       |
| 5   | G     | 165      | Total<br>165 | O<br>165 | 0       | 0       |
| 5   | H     | 128      | Total<br>128 | O<br>128 | 0       | 0       |
| 5   | I     | 183      | Total<br>183 | O<br>183 | 0       | 0       |
| 5   | J     | 101      | Total<br>101 | O<br>101 | 0       | 0       |
| 5   | K     | 119      | Total<br>119 | O<br>119 | 0       | 0       |
| 5   | L     | 106      | Total<br>106 | O<br>106 | 0       | 0       |



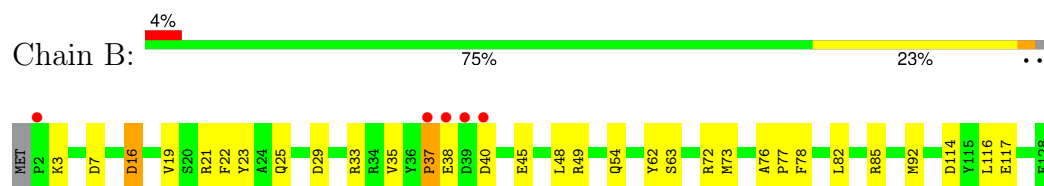
### 3 Residue-property plots [i](#)

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

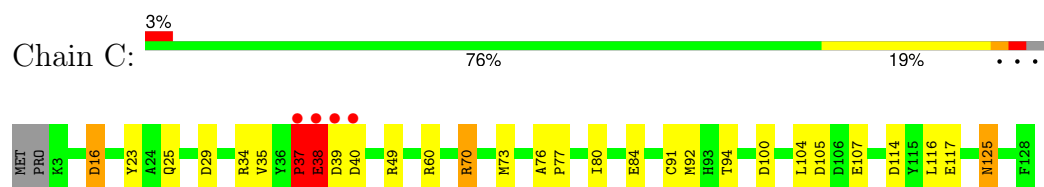
- Molecule 1: Hemoglobin-like protein HbO



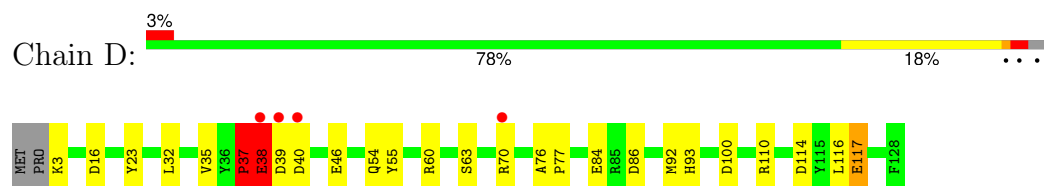
- Molecule 1: Hemoglobin-like protein HbO



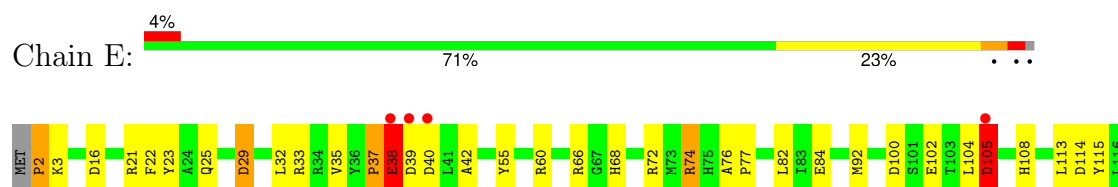
- Molecule 1: Hemoglobin-like protein HbO



- Molecule 1: Hemoglobin-like protein HbO



- Molecule 1: Hemoglobin-like protein HbO

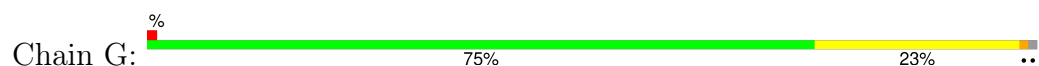




- Molecule 1: Hemoglobin-like protein HbO



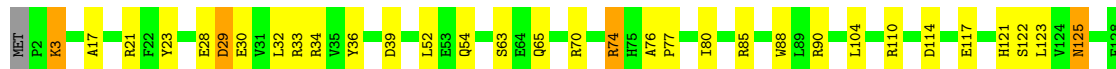
- Molecule 1: Hemoglobin-like protein HbO



- Molecule 1: Hemoglobin-like protein HbO



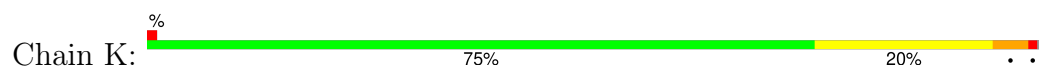
- Molecule 1: Hemoglobin-like protein HbO



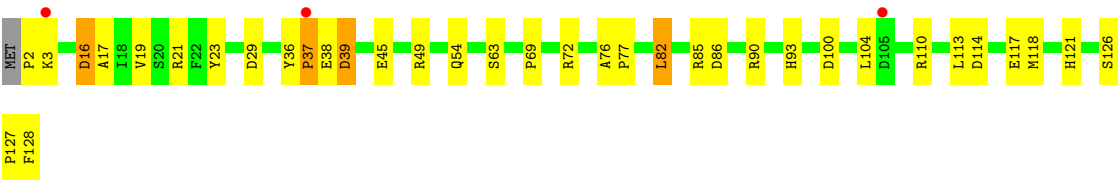
- Molecule 1: Hemoglobin-like protein HbO



- Molecule 1: Hemoglobin-like protein HbO



● Molecule 1: Hemoglobin-like protein HbO



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | I 41 2 2  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 187.03Å 187.03Å 274.86Å<br>90.00° 90.00° 90.00°   | Depositor        |
| Resolution (Å)  | 50.00 – 2.11<br>50.00 – 2.11  | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.7 (50.00-2.11)<br>99.7 (50.00-2.11)  | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.69 (at 2.12Å)   | Xtriage          |
| Refinement program  | REFMAC 5.1.19   | Depositor        |
| R, $R_{free}$   | 0.186 , 0.226<br>0.185 , 0.226  | Depositor<br>DCC |
| $R_{free}$ test set   | 6934 reflections (5.02%)  | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 25.0  | Xtriage          |
| Anisotropy  | 0.059   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 51.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$   | Xtriage          |
| Estimated twinning fraction   | 0.015 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k<br>0.011 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 15104   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 26.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4, CYN

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     | 0.51         | 0/1104  | 0.97        | 10/1490 (0.7%)  |
| 1   | B     | 0.50         | 0/1112  | 0.92        | 7/1501 (0.5%)   |
| 1   | C     | 0.49         | 0/1113  | 0.89        | 11/1502 (0.7%)  |
| 1   | D     | 0.50         | 0/1115  | 0.88        | 10/1504 (0.7%)  |
| 1   | E     | 0.46         | 0/1134  | 0.90        | 10/1531 (0.7%)  |
| 1   | F     | 0.49         | 0/1115  | 0.88        | 6/1504 (0.4%)   |
| 1   | G     | 0.47         | 0/1071  | 0.71        | 2/1445 (0.1%)   |
| 1   | H     | 0.43         | 0/1080  | 0.70        | 4/1457 (0.3%)   |
| 1   | I     | 0.49         | 0/1093  | 0.75        | 3/1474 (0.2%)   |
| 1   | J     | 0.42         | 0/1082  | 0.83        | 6/1459 (0.4%)   |
| 1   | K     | 0.48         | 0/1082  | 0.82        | 7/1459 (0.5%)   |
| 1   | L     | 0.43         | 0/1071  | 0.88        | 8/1445 (0.6%)   |
| All | All   | 0.47         | 0/13172 | 0.85        | 84/17771 (0.5%) |

There are no bond length outliers.

All (84) bond angle outliers are listed below:

| Mol | Chain | Res   | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-------|------|---------|--------|-------------|----------|
| 1   | J     | 2     | PRO  | CA-N-CD | -15.89 | 89.25       | 111.50   |
| 1   | B     | 37[A] | PRO  | CA-N-CD | -12.26 | 94.33       | 111.50   |
| 1   | B     | 37[B] | PRO  | CA-N-CD | -12.26 | 94.33       | 111.50   |
| 1   | A     | 37[A] | PRO  | CA-N-CD | -12.03 | 94.66       | 111.50   |
| 1   | A     | 37[B] | PRO  | CA-N-CD | -12.03 | 94.66       | 111.50   |
| 1   | L     | 2     | PRO  | CA-N-CD | -11.80 | 94.98       | 111.50   |
| 1   | L     | 37    | PRO  | CA-N-CD | -10.90 | 96.23       | 111.50   |
| 1   | E     | 2     | PRO  | CA-N-CD | -10.67 | 96.56       | 111.50   |
| 1   | K     | 69    | PRO  | CA-N-CD | -9.41  | 98.32       | 111.50   |
| 1   | F     | 37[A] | PRO  | CA-N-CD | -9.29  | 98.50       | 111.50   |
| 1   | F     | 37[B] | PRO  | CA-N-CD | -9.29  | 98.50       | 111.50   |
| 1   | E     | 37[A] | PRO  | CA-N-CD | -7.42  | 101.11      | 111.50   |

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| Mol | Chain | Res   | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 1   | E     | 37[B] | PRO  | CA-N-CD   | -7.42 | 101.11      | 111.50   |
| 1   | F     | 100   | ASP  | CB-CG-OD2 | 7.34  | 124.90      | 118.30   |
| 1   | A     | 100   | ASP  | CB-CG-OD2 | 7.30  | 124.87      | 118.30   |
| 1   | D     | 100   | ASP  | CB-CG-OD2 | 7.00  | 124.60      | 118.30   |
| 1   | A     | 47    | ARG  | NE-CZ-NH2 | -6.79 | 116.90      | 120.30   |
| 1   | C     | 100   | ASP  | CB-CG-OD2 | 6.68  | 124.31      | 118.30   |
| 1   | L     | 114   | ASP  | CB-CG-OD2 | 6.50  | 124.15      | 118.30   |
| 1   | B     | 114   | ASP  | CB-CG-OD2 | 6.38  | 124.05      | 118.30   |
| 1   | C     | 114   | ASP  | CB-CG-OD2 | 6.29  | 123.96      | 118.30   |
| 1   | E     | 114   | ASP  | CB-CG-OD2 | 6.28  | 123.95      | 118.30   |
| 1   | J     | 100   | ASP  | CB-CG-OD2 | 6.19  | 123.88      | 118.30   |
| 1   | A     | 38[A] | GLU  | N-CA-C    | 6.18  | 127.70      | 111.00   |
| 1   | A     | 38[B] | GLU  | N-CA-C    | 6.18  | 127.70      | 111.00   |
| 1   | L     | 100   | ASP  | CB-CG-OD2 | 6.17  | 123.85      | 118.30   |
| 1   | C     | 105   | ASP  | CB-CG-OD2 | 6.03  | 123.73      | 118.30   |
| 1   | D     | 38[A] | GLU  | N-CA-C    | 6.01  | 127.22      | 111.00   |
| 1   | D     | 38[B] | GLU  | N-CA-C    | 6.01  | 127.22      | 111.00   |
| 1   | C     | 38[A] | GLU  | N-CA-C    | 5.98  | 127.14      | 111.00   |
| 1   | C     | 38[B] | GLU  | N-CA-C    | 5.98  | 127.14      | 111.00   |
| 1   | D     | 16    | ASP  | CB-CG-OD2 | 5.96  | 123.66      | 118.30   |
| 1   | E     | 100   | ASP  | CB-CG-OD2 | 5.95  | 123.65      | 118.30   |
| 1   | H     | 39    | ASP  | CB-CG-OD2 | 5.94  | 123.65      | 118.30   |
| 1   | K     | 39    | ASP  | CB-CG-OD2 | 5.93  | 123.64      | 118.30   |
| 1   | B     | 7     | ASP  | CB-CG-OD2 | 5.91  | 123.61      | 118.30   |
| 1   | C     | 37[A] | PRO  | CA-N-CD   | -5.90 | 103.23      | 111.50   |
| 1   | C     | 37[B] | PRO  | CA-N-CD   | -5.90 | 103.23      | 111.50   |
| 1   | D     | 37[A] | PRO  | CA-N-CD   | -5.87 | 103.28      | 111.50   |
| 1   | D     | 37[B] | PRO  | CA-N-CD   | -5.87 | 103.28      | 111.50   |
| 1   | F     | 16    | ASP  | CB-CG-OD2 | 5.84  | 123.56      | 118.30   |
| 1   | L     | 16    | ASP  | CB-CG-OD2 | 5.83  | 123.54      | 118.30   |
| 1   | F     | 38[A] | GLU  | N-CA-C    | 5.81  | 126.68      | 111.00   |
| 1   | F     | 38[B] | GLU  | N-CA-C    | 5.81  | 126.68      | 111.00   |
| 1   | D     | 114   | ASP  | CB-CG-OD2 | 5.72  | 123.45      | 118.30   |
| 1   | K     | 29    | ASP  | CB-CG-OD2 | 5.69  | 123.42      | 118.30   |
| 1   | E     | 105   | ASP  | CB-CG-OD2 | 5.61  | 123.35      | 118.30   |
| 1   | I     | 114   | ASP  | CB-CG-OD2 | 5.59  | 123.33      | 118.30   |
| 1   | C     | 16    | ASP  | CB-CG-OD2 | 5.59  | 123.33      | 118.30   |
| 1   | D     | 40[A] | ASP  | CB-CG-OD2 | 5.56  | 123.31      | 118.30   |
| 1   | D     | 40[B] | ASP  | CB-CG-OD2 | 5.56  | 123.31      | 118.30   |
| 1   | G     | 39    | ASP  | CB-CG-OD2 | 5.54  | 123.29      | 118.30   |
| 1   | K     | 16    | ASP  | CB-CG-OD2 | 5.53  | 123.28      | 118.30   |
| 1   | C     | 40[A] | ASP  | CB-CG-OD2 | 5.52  | 123.27      | 118.30   |

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| Mol | Chain | Res   | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-----------|-------|-------------|----------|
| 1   | C     | 40[B] | ASP  | CB-CG-OD2 | 5.52  | 123.27      | 118.30   |
| 1   | J     | 39    | ASP  | CB-CG-OD2 | 5.52  | 123.27      | 118.30   |
| 1   | J     | 105   | ASP  | CB-CG-OD2 | 5.52  | 123.27      | 118.30   |
| 1   | K     | 100   | ASP  | CB-CG-OD2 | 5.51  | 123.26      | 118.30   |
| 1   | I     | 39    | ASP  | CB-CG-OD2 | 5.42  | 123.17      | 118.30   |
| 1   | D     | 86    | ASP  | CB-CG-OD2 | 5.41  | 123.16      | 118.30   |
| 1   | L     | 29    | ASP  | CB-CG-OD2 | 5.29  | 123.06      | 118.30   |
| 1   | E     | 16    | ASP  | CB-CG-OD2 | 5.29  | 123.06      | 118.30   |
| 1   | J     | 16    | ASP  | CB-CG-OD2 | 5.29  | 123.06      | 118.30   |
| 1   | B     | 16    | ASP  | CB-CG-OD2 | 5.27  | 123.05      | 118.30   |
| 1   | L     | 39    | ASP  | CB-CG-OD2 | 5.25  | 123.03      | 118.30   |
| 1   | H     | 16    | ASP  | CB-CG-OD2 | 5.25  | 123.03      | 118.30   |
| 1   | H     | 100   | ASP  | CB-CG-OD2 | 5.24  | 123.01      | 118.30   |
| 1   | E     | 38[A] | GLU  | N-CA-C    | 5.23  | 125.12      | 111.00   |
| 1   | E     | 38[B] | GLU  | N-CA-C    | 5.23  | 125.12      | 111.00   |
| 1   | L     | 86    | ASP  | CB-CG-OD2 | 5.23  | 123.01      | 118.30   |
| 1   | K     | 105   | ASP  | CB-CG-OD2 | 5.22  | 123.00      | 118.30   |
| 1   | C     | 29    | ASP  | CB-CG-OD2 | 5.21  | 122.98      | 118.30   |
| 1   | E     | 29    | ASP  | CB-CG-OD2 | 5.19  | 122.97      | 118.30   |
| 1   | A     | 16    | ASP  | CB-CG-OD2 | 5.19  | 122.97      | 118.30   |
| 1   | I     | 29    | ASP  | CB-CG-OD2 | 5.18  | 122.96      | 118.30   |
| 1   | A     | 106   | ASP  | CB-CG-OD2 | 5.16  | 122.94      | 118.30   |
| 1   | J     | 29    | ASP  | CB-CG-OD2 | 5.11  | 122.90      | 118.30   |
| 1   | G     | 16    | ASP  | CB-CG-OD2 | 5.10  | 122.89      | 118.30   |
| 1   | B     | 38[A] | GLU  | N-CA-C    | 5.09  | 124.75      | 111.00   |
| 1   | B     | 38[B] | GLU  | N-CA-C    | 5.09  | 124.75      | 111.00   |
| 1   | H     | 7     | ASP  | CB-CG-OD2 | 5.09  | 122.88      | 118.30   |
| 1   | A     | 29    | ASP  | CB-CG-OD2 | 5.03  | 122.82      | 118.30   |
| 1   | A     | 90    | ARG  | NE-CZ-NH2 | -5.02 | 117.79      | 120.30   |
| 1   | K     | 40    | ASP  | CB-CG-OD2 | 5.02  | 122.82      | 118.30   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1078  | 0        | 1021     | 23      | 0            |
| 1   | B     | 1085  | 0        | 1029     | 18      | 0            |
| 1   | C     | 1087  | 0        | 1026     | 23      | 0            |
| 1   | D     | 1089  | 0        | 1033     | 19      | 0            |
| 1   | E     | 1106  | 0        | 1048     | 24      | 0            |
| 1   | F     | 1089  | 0        | 1033     | 22      | 0            |
| 1   | G     | 1045  | 0        | 999      | 22      | 0            |
| 1   | H     | 1054  | 0        | 1004     | 27      | 0            |
| 1   | I     | 1066  | 0        | 1017     | 26      | 0            |
| 1   | J     | 1056  | 0        | 1011     | 27      | 0            |
| 1   | K     | 1056  | 0        | 1011     | 21      | 0            |
| 1   | L     | 1045  | 0        | 999      | 24      | 0            |
| 2   | A     | 25    | 0        | 0        | 1       | 0            |
| 2   | B     | 10    | 0        | 0        | 1       | 0            |
| 2   | C     | 10    | 0        | 0        | 0       | 0            |
| 2   | D     | 5     | 0        | 0        | 0       | 0            |
| 2   | E     | 10    | 0        | 0        | 1       | 0            |
| 2   | G     | 10    | 0        | 0        | 0       | 0            |
| 2   | I     | 5     | 0        | 0        | 0       | 0            |
| 2   | J     | 10    | 0        | 0        | 1       | 0            |
| 2   | L     | 5     | 0        | 0        | 0       | 0            |
| 3   | A     | 2     | 0        | 0        | 0       | 0            |
| 3   | B     | 2     | 0        | 0        | 0       | 0            |
| 3   | C     | 2     | 0        | 0        | 0       | 0            |
| 3   | D     | 2     | 0        | 0        | 0       | 0            |
| 3   | E     | 2     | 0        | 0        | 0       | 0            |
| 3   | F     | 2     | 0        | 0        | 0       | 0            |
| 3   | G     | 2     | 0        | 0        | 0       | 0            |
| 3   | H     | 2     | 0        | 0        | 0       | 0            |
| 3   | I     | 2     | 0        | 0        | 0       | 0            |
| 3   | J     | 2     | 0        | 0        | 0       | 0            |
| 3   | K     | 2     | 0        | 0        | 1       | 0            |
| 3   | L     | 2     | 0        | 0        | 0       | 0            |
| 4   | A     | 43    | 0        | 30       | 2       | 0            |
| 4   | B     | 43    | 0        | 30       | 1       | 0            |
| 4   | C     | 43    | 0        | 30       | 3       | 0            |
| 4   | D     | 43    | 0        | 30       | 2       | 0            |
| 4   | E     | 43    | 0        | 30       | 3       | 0            |
| 4   | F     | 43    | 0        | 30       | 2       | 0            |
| 4   | G     | 43    | 0        | 30       | 2       | 0            |
| 4   | H     | 43    | 0        | 30       | 3       | 0            |
| 4   | I     | 43    | 0        | 30       | 1       | 0            |
| 4   | J     | 43    | 0        | 30       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | K     | 43    | 0        | 30       | 3       | 0            |
| 4   | L     | 43    | 0        | 30       | 1       | 0            |
| 5   | A     | 138   | 0        | 0        | 3       | 0            |
| 5   | B     | 123   | 0        | 0        | 4       | 0            |
| 5   | C     | 184   | 0        | 0        | 4       | 0            |
| 5   | D     | 136   | 0        | 0        | 3       | 0            |
| 5   | E     | 112   | 0        | 0        | 2       | 0            |
| 5   | F     | 123   | 0        | 0        | 6       | 0            |
| 5   | G     | 165   | 0        | 0        | 2       | 0            |
| 5   | H     | 128   | 0        | 0        | 7       | 0            |
| 5   | I     | 183   | 0        | 0        | 7       | 0            |
| 5   | J     | 101   | 0        | 0        | 3       | 0            |
| 5   | K     | 119   | 0        | 0        | 6       | 0            |
| 5   | L     | 106   | 0        | 0        | 4       | 0            |
| All | All   | 15104 | 0        | 12591    | 275     | 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 11.

All (275) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:25:GLN:HG2    | 5:C:2078:HOH:O   | 1.48                     | 1.13              |
| 1:C:70:ARG:HH11   | 1:C:70:ARG:HG2   | 1.08                     | 1.09              |
| 1:E:60:ARG:HD3    | 1:J:90:ARG:CZ    | 1.83                     | 1.09              |
| 1:H:70:ARG:HD2    | 5:H:846:HOH:O    | 1.53                     | 1.06              |
| 1:K:117:GLU:HG2   | 5:K:906:HOH:O    | 1.62                     | 1.00              |
| 1:G:44:ALA:HA     | 1:G:47:ARG:HH12  | 1.26                     | 0.99              |
| 1:I:23:TYR:OH     | 1:I:36:TYR:HE2   | 1.46                     | 0.97              |
| 1:B:40[B]:ASP:OD1 | 5:B:2132:HOH:O   | 1.81                     | 0.97              |
| 1:D:60:ARG:HD3    | 1:L:90:ARG:CZ    | 1.94                     | 0.96              |
| 1:I:23:TYR:OH     | 1:I:36:TYR:CE2   | 2.17                     | 0.96              |
| 1:H:72:ARG:HD3    | 5:H:897:HOH:O    | 1.62                     | 0.96              |
| 1:E:60:ARG:HD3    | 1:J:90:ARG:NH1   | 1.79                     | 0.95              |
| 1:C:70:ARG:HG2    | 1:C:70:ARG:NH1   | 1.83                     | 0.92              |
| 1:H:80:ILE:H      | 1:H:125:ASN:HD21 | 1.16                     | 0.92              |
| 1:A:34:ARG:HH11   | 1:A:34:ARG:CG    | 1.86                     | 0.88              |
| 1:H:74:ARG:HG2    | 4:H:700:HEM:HBD2 | 1.53                     | 0.88              |
| 1:L:72:ARG:HD3    | 5:L:2032:HOH:O   | 1.74                     | 0.87              |
| 1:E:21:ARG:NH1    | 1:E:25:GLN:HE21  | 1.73                     | 0.86              |
| 1:E:21:ARG:HH12   | 1:E:25:GLN:HE21  | 1.18                     | 0.85              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:80:ILE:H     | 1:A:125:ASN:HD21 | 1.24                     | 0.84              |
| 1:I:74:ARG:HD2   | 5:I:2054:HOH:O   | 1.78                     | 0.84              |
| 1:C:80:ILE:H     | 1:C:125:ASN:HD21 | 1.24                     | 0.84              |
| 1:G:23:TYR:OH    | 1:G:36:TYR:CE2   | 2.30                     | 0.84              |
| 1:D:110:ARG:HG3  | 1:D:110:ARG:HH11 | 1.44                     | 0.83              |
| 1:L:54:GLN:HE22  | 1:L:63:SER:H     | 1.25                     | 0.83              |
| 1:J:23:TYR:HH    | 1:J:36:TYR:HE2   | 0.84                     | 0.83              |
| 1:I:54:GLN:HE22  | 1:I:63:SER:H     | 1.24                     | 0.83              |
| 1:G:47:ARG:HH11  | 1:G:47:ARG:HB2   | 1.44                     | 0.82              |
| 1:A:34:ARG:HH11  | 1:A:34:ARG:HG2   | 1.45                     | 0.82              |
| 1:H:54:GLN:HE22  | 1:H:63:SER:H     | 1.28                     | 0.81              |
| 1:H:80:ILE:H     | 1:H:125:ASN:ND2  | 1.80                     | 0.80              |
| 1:I:80:ILE:H     | 1:I:125:ASN:HD21 | 1.26                     | 0.80              |
| 1:J:23:TYR:OH    | 1:J:36:TYR:HE2   | 1.64                     | 0.80              |
| 1:F:61:THR:HG21  | 5:F:881:HOH:O    | 1.81                     | 0.79              |
| 1:G:23:TYR:OH    | 1:G:36:TYR:HE2   | 1.65                     | 0.79              |
| 4:K:700:HEM:HMC1 | 4:K:700:HEM:HBC2 | 1.64                     | 0.78              |
| 1:H:23:TYR:OH    | 1:H:36:TYR:CE2   | 2.37                     | 0.78              |
| 4:J:700:HEM:HMC1 | 4:J:700:HEM:HBC2 | 1.66                     | 0.77              |
| 1:H:23:TYR:OH    | 1:H:36:TYR:HE2   | 1.67                     | 0.77              |
| 1:D:54:GLN:HE22  | 1:D:63:SER:H     | 1.30                     | 0.77              |
| 1:A:54:GLN:HE22  | 1:A:63:SER:H     | 1.31                     | 0.76              |
| 4:I:700:HEM:HMC1 | 4:I:700:HEM:HBC2 | 1.69                     | 0.75              |
| 4:E:700:HEM:HMC1 | 4:E:700:HEM:HBC2 | 1.69                     | 0.75              |
| 1:C:25:GLN:HE22  | 1:C:94:THR:HB    | 1.52                     | 0.74              |
| 1:L:23:TYR:OH    | 1:L:36:TYR:HE2   | 1.70                     | 0.74              |
| 1:K:23:TYR:OH    | 1:K:36:TYR:CE2   | 2.40                     | 0.73              |
| 1:E:60:ARG:HG3   | 2:E:2003:SO4:O2  | 1.88                     | 0.73              |
| 1:I:80:ILE:H     | 1:I:125:ASN:ND2  | 1.86                     | 0.73              |
| 1:L:23:TYR:HH    | 1:L:36:TYR:HE2   | 1.32                     | 0.73              |
| 1:K:23:TYR:OH    | 1:K:36:TYR:HE2   | 1.72                     | 0.73              |
| 4:C:700:HEM:HMC1 | 4:C:700:HEM:HBC2 | 1.71                     | 0.72              |
| 1:G:29:ASP:O     | 1:G:33:ARG:HG2   | 1.89                     | 0.72              |
| 1:C:25:GLN:NE2   | 5:C:2078:HOH:O   | 2.21                     | 0.72              |
| 1:B:54:GLN:HE22  | 1:B:63:SER:H     | 1.37                     | 0.72              |
| 1:C:70:ARG:HH11  | 1:C:70:ARG:CG    | 1.96                     | 0.71              |
| 1:K:90:ARG:O     | 1:K:94:THR:HG23  | 1.90                     | 0.71              |
| 1:A:34:ARG:HG2   | 1:A:34:ARG:NH1   | 2.03                     | 0.70              |
| 1:A:30:GLU:O     | 1:A:34:ARG:HG3   | 1.92                     | 0.69              |
| 1:K:74:ARG:HG2   | 4:K:700:HEM:HBD2 | 1.73                     | 0.69              |
| 1:L:93:HIS:HE1   | 1:L:117:GLU:OE1  | 1.75                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:A:80:ILE:H      | 1:A:125:ASN:ND2    | 1.91                     | 0.69              |
| 1:L:23:TYR:OH     | 1:L:36:TYR:CE2     | 2.44                     | 0.69              |
| 1:C:80:ILE:H      | 1:C:125:ASN:ND2    | 1.90                     | 0.69              |
| 1:E:29:ASP:O      | 1:E:33:ARG:HG2     | 1.93                     | 0.69              |
| 1:A:72:ARG:HD2    | 5:A:2131:HOH:O     | 1.93                     | 0.68              |
| 1:C:125:ASN:C     | 1:C:125:ASN:HD22   | 1.96                     | 0.68              |
| 5:A:2138:HOH:O    | 1:G:30:GLU:HB2     | 1.94                     | 0.68              |
| 1:G:47:ARG:NH1    | 5:G:2065:HOH:O     | 2.29                     | 0.67              |
| 1:I:34:ARG:NH1    | 5:I:2038:HOH:O     | 2.27                     | 0.66              |
| 4:L:700:HEM:HMC1  | 4:L:700:HEM:HBC2   | 1.78                     | 0.65              |
| 1:D:60:ARG:HD3    | 1:L:90:ARG:NH2     | 2.11                     | 0.65              |
| 1:H:74:ARG:HG2    | 4:H:700:HEM:CBD    | 2.27                     | 0.65              |
| 1:C:35:VAL:HG11   | 1:C:84:GLU:HG2     | 1.78                     | 0.64              |
| 1:F:118:MET:HG3   | 1:F:119:ALA:N      | 2.12                     | 0.64              |
| 4:A:700:HEM:HBC2  | 4:A:700:HEM:HMC1   | 1.80                     | 0.64              |
| 1:F:60:ARG:HH21   | 1:K:90:ARG:HD2     | 1.62                     | 0.64              |
| 1:D:35:VAL:HG21   | 1:D:84:GLU:HG2     | 1.80                     | 0.64              |
| 1:I:23:TYR:HH     | 1:I:36:TYR:HE2     | 0.72                     | 0.64              |
| 1:J:23:TYR:OH     | 1:J:36:TYR:CE2     | 2.42                     | 0.64              |
| 1:K:88:TRP:HE1    | 3:K:800:CYN:C      | 2.11                     | 0.63              |
| 1:F:60:ARG:NH2    | 1:K:90:ARG:HD2     | 2.13                     | 0.63              |
| 1:E:60:ARG:CD     | 1:J:90:ARG:CZ      | 2.71                     | 0.63              |
| 4:C:700:HEM:HBC2  | 4:C:700:HEM:CMC    | 2.29                     | 0.62              |
| 1:I:54:GLN:NE2    | 1:I:63:SER:H       | 1.95                     | 0.62              |
| 1:I:125:ASN:C     | 1:I:125:ASN:HD22   | 2.03                     | 0.62              |
| 1:G:90:ARG:NH1    | 5:G:2126:HOH:O     | 2.23                     | 0.62              |
| 1:A:46:GLU:HG3    | 5:A:2064:HOH:O     | 2.00                     | 0.62              |
| 1:G:44:ALA:HA     | 1:G:47:ARG:NH1     | 2.08                     | 0.61              |
| 1:J:46:GLU:O      | 1:J:50:MET:HG3     | 1.99                     | 0.61              |
| 1:F:102:GLU:HB2   | 5:F:869:HOH:O      | 1.99                     | 0.61              |
| 4:D:700:HEM:HMC1  | 4:D:700:HEM:HBC2   | 1.83                     | 0.61              |
| 1:C:25:GLN:CG     | 5:C:2078:HOH:O     | 2.23                     | 0.60              |
| 1:F:113:LEU:O     | 1:F:117:GLU:HG3    | 2.01                     | 0.60              |
| 1:I:54:GLN:HE22   | 1:I:63:SER:N       | 1.98                     | 0.60              |
| 1:A:60:ARG:HD3    | 1:G:90:ARG:CZ      | 2.32                     | 0.60              |
| 1:D:70[B]:ARG:HD3 | 5:D:2038:HOH:O     | 2.02                     | 0.60              |
| 1:D:110:ARG:HG3   | 1:D:110:ARG:NH1    | 2.15                     | 0.60              |
| 1:D:37[B]:PRO:O   | 1:D:39[B]:ASP:N    | 2.35                     | 0.60              |
| 1:F:35:VAL:HG21   | 1:F:84:GLU:HG2     | 1.84                     | 0.59              |
| 1:I:117:GLU:O     | 1:I:121[A]:HIS:CD2 | 2.55                     | 0.59              |
| 1:I:85:ARG:HD2    | 1:I:121[A]:HIS:CD2 | 2.38                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:54:GLN:NE2    | 1:L:63:SER:H      | 1.98                     | 0.59              |
| 2:B:2017:SO4:O2   | 1:J:79:ARG:NH2    | 2.33                     | 0.58              |
| 1:E:60:ARG:HH11   | 1:J:90:ARG:NE     | 2.01                     | 0.58              |
| 1:A:35:VAL:HG21   | 1:A:84:GLU:HG2    | 1.86                     | 0.58              |
| 1:K:94:THR:HG22   | 5:K:860:HOH:O     | 2.03                     | 0.58              |
| 4:E:700:HEM:HBC2  | 4:E:700:HEM:CMC   | 2.33                     | 0.58              |
| 1:H:107[A]:GLU:CG | 5:H:898:HOH:O     | 2.52                     | 0.57              |
| 1:A:125:ASN:C     | 1:A:125:ASN:HD22  | 2.07                     | 0.57              |
| 1:C:60:ARG:NH1    | 1:I:90:ARG:HD2    | 2.18                     | 0.57              |
| 1:C:37[B]:PRO:O   | 1:C:39[B]:ASP:N   | 2.38                     | 0.57              |
| 1:E:35:VAL:HG21   | 1:E:84:GLU:HG2    | 1.87                     | 0.56              |
| 1:I:3:LYS:HE3     | 5:I:2022:HOH:O    | 2.04                     | 0.56              |
| 1:H:118:MET:SD    | 1:H:118:MET:C     | 2.85                     | 0.55              |
| 1:D:37[A]:PRO:HB2 | 5:D:2055:HOH:O    | 2.07                     | 0.54              |
| 1:G:46:GLU:HG3    | 1:G:49:ARG:NH2    | 2.21                     | 0.54              |
| 1:G:79:ARG:HH21   | 1:G:127:PRO:HD2   | 1.72                     | 0.54              |
| 4:F:700:HEM:HBC2  | 4:F:700:HEM:HMC1  | 1.88                     | 0.54              |
| 1:E:21:ARG:NH1    | 1:E:25:GLN:NE2    | 2.50                     | 0.54              |
| 1:I:23:TYR:CZ     | 1:I:36:TYR:CE2    | 2.96                     | 0.54              |
| 1:H:85:ARG:HH11   | 1:H:121:HIS:HD2   | 1.54                     | 0.54              |
| 1:B:76:ALA:N      | 1:B:77:PRO:CD     | 2.72                     | 0.53              |
| 1:E:76:ALA:N      | 1:E:77:PRO:CD     | 2.71                     | 0.53              |
| 1:G:32:LEU:HD11   | 1:G:88:TRP:HA     | 1.91                     | 0.53              |
| 1:F:38[A]:GLU:O   | 1:F:39[A]:ASP:OD1 | 2.26                     | 0.53              |
| 1:F:73:MET:HG3    | 1:J:65:GLN:HE22   | 1.72                     | 0.53              |
| 1:D:38[A]:GLU:O   | 1:D:39[A]:ASP:OD1 | 2.26                     | 0.53              |
| 1:B:22:PHE:O      | 1:B:25:GLN:HB2    | 2.09                     | 0.53              |
| 1:B:35:VAL:HG13   | 1:B:78:PHE:HB3    | 1.90                     | 0.53              |
| 4:D:700:HEM:HBC2  | 4:D:700:HEM:CMC   | 2.39                     | 0.52              |
| 1:G:47:ARG:HH11   | 1:G:47:ARG:CB     | 2.19                     | 0.52              |
| 1:K:74:ARG:HG2    | 4:K:700:HEM:CBD   | 2.39                     | 0.52              |
| 1:L:85:ARG:HH11   | 1:L:121:HIS:HD2   | 1.57                     | 0.52              |
| 1:B:73:MET:HG3    | 1:I:65:GLN:HE22   | 1.74                     | 0.52              |
| 1:K:29:ASP:O      | 1:K:33:ARG:HG2    | 2.09                     | 0.52              |
| 1:L:76:ALA:N      | 1:L:77:PRO:CD     | 2.72                     | 0.52              |
| 1:A:34:ARG:HH11   | 1:A:34:ARG:HG3    | 1.69                     | 0.52              |
| 1:F:60:ARG:HH21   | 1:K:90:ARG:CD     | 2.22                     | 0.52              |
| 4:H:700:HEM:HMC1  | 4:H:700:HEM:HBC2  | 1.90                     | 0.52              |
| 1:I:63:SER:HB3    | 5:I:2186:HOH:O    | 2.10                     | 0.52              |
| 1:L:93:HIS:CE1    | 1:L:117:GLU:OE1   | 2.62                     | 0.52              |
| 1:L:85:ARG:HH11   | 1:L:121:HIS:CD2   | 2.28                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:E:38[A]:GLU:O    | 1:E:39[A]:ASP:OD1 | 2.28                     | 0.51              |
| 1:G:76:ALA:N       | 1:G:77:PRO:CD     | 2.74                     | 0.51              |
| 1:H:63:SER:HB2     | 5:H:891:HOH:O     | 2.09                     | 0.51              |
| 1:H:107[A]:GLU:HG2 | 5:H:898:HOH:O     | 2.08                     | 0.51              |
| 1:A:92:MET:HG3     | 1:A:116:LEU:HD13  | 1.92                     | 0.51              |
| 1:B:21:ARG:NH1     | 1:B:25:GLN:HG2    | 2.26                     | 0.51              |
| 1:F:76:ALA:N       | 1:F:77:PRO:CD     | 2.72                     | 0.51              |
| 1:B:92:MET:CG      | 1:B:116:LEU:HD13  | 2.41                     | 0.51              |
| 4:F:700:HEM:HBC2   | 4:F:700:HEM:CMC   | 2.40                     | 0.51              |
| 1:H:54:GLN:NE2     | 1:H:63:SER:H      | 2.02                     | 0.51              |
| 1:K:3:LYS:HD3      | 1:K:8:ALA:HA      | 1.93                     | 0.51              |
| 1:B:29:ASP:O       | 1:B:33:ARG:HG2    | 2.11                     | 0.51              |
| 1:J:109:ARG:HD3    | 5:J:2063:HOH:O    | 2.11                     | 0.51              |
| 1:E:60:ARG:HD3     | 1:J:90:ARG:NH2    | 2.24                     | 0.51              |
| 1:E:102:GLU:HB2    | 5:E:1258:HOH:O    | 2.11                     | 0.51              |
| 1:E:68[B]:HIS:CE1  | 1:J:84:GLU:OE1    | 2.64                     | 0.50              |
| 1:H:85:ARG:HH11    | 1:H:121:HIS:CD2   | 2.28                     | 0.50              |
| 1:I:70:ARG:NH2     | 5:I:2188:HOH:O    | 2.43                     | 0.50              |
| 1:C:125:ASN:ND2    | 1:C:125:ASN:C     | 2.64                     | 0.50              |
| 1:K:30:GLU:CD      | 1:K:30:GLU:H      | 2.15                     | 0.50              |
| 1:K:70[B]:ARG:HD3  | 5:K:859:HOH:O     | 2.11                     | 0.50              |
| 1:L:16:ASP:HB2     | 5:L:2045:HOH:O    | 2.11                     | 0.50              |
| 1:K:72:ARG:NH1     | 5:K:807:HOH:O     | 2.27                     | 0.49              |
| 1:C:38[A]:GLU:O    | 1:C:39[A]:ASP:OD1 | 2.29                     | 0.49              |
| 1:D:55:TYR:CZ      | 1:L:82:LEU:HD22   | 2.47                     | 0.49              |
| 1:L:38:GLU:OE2     | 1:L:39:ASP:HB3    | 2.12                     | 0.49              |
| 1:H:2:PRO:HB3      | 1:H:8:ALA:HA      | 1.94                     | 0.49              |
| 1:A:76:ALA:N       | 1:A:77:PRO:CD     | 2.75                     | 0.49              |
| 1:B:82:LEU:HD22    | 1:B:85:ARG:NH2    | 2.28                     | 0.49              |
| 1:D:110:ARG:HH11   | 1:D:110:ARG:CG    | 2.21                     | 0.49              |
| 1:C:16:ASP:HA      | 1:C:49:ARG:HD3    | 1.95                     | 0.48              |
| 1:C:92:MET:CG      | 1:C:116:LEU:HD13  | 2.43                     | 0.48              |
| 1:F:61:THR:HB      | 5:F:805:HOH:O     | 2.12                     | 0.48              |
| 1:H:76:ALA:N       | 1:H:77:PRO:CD     | 2.76                     | 0.48              |
| 1:J:71:LEU:HB3     | 1:J:123:LEU:HD21  | 1.96                     | 0.48              |
| 1:H:90:ARG:CZ      | 5:H:802:HOH:O     | 2.61                     | 0.48              |
| 1:F:35:VAL:HG21    | 1:F:84:GLU:CG     | 2.42                     | 0.48              |
| 1:H:101:SER:HA     | 1:H:104:LEU:O     | 2.14                     | 0.48              |
| 4:B:700:HEM:HMC1   | 4:B:700:HEM:HBC2  | 1.97                     | 0.47              |
| 1:L:17:ALA:O       | 1:L:21:ARG:HD2    | 2.13                     | 0.47              |
| 1:F:70[A]:ARG:HD3  | 5:F:898:HOH:O     | 2.12                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:L:49:ARG:NH2    | 5:L:2068:HOH:O    | 2.46                     | 0.47              |
| 1:J:23:TYR:HE1    | 1:J:36:TYR:CD2    | 2.32                     | 0.47              |
| 1:B:16:ASP:HA     | 1:B:49:ARG:HD3    | 1.96                     | 0.47              |
| 1:E:105:ASP:HB3   | 1:E:108:HIS:H     | 1.79                     | 0.47              |
| 1:H:125:ASN:C     | 1:H:125:ASN:HD22  | 2.17                     | 0.47              |
| 1:K:63:SER:HB3    | 5:K:857:HOH:O     | 2.14                     | 0.47              |
| 1:L:54:GLN:HE22   | 1:L:63:SER:N      | 2.05                     | 0.47              |
| 1:C:92:MET:HG3    | 1:C:116:LEU:HD13  | 1.96                     | 0.47              |
| 1:I:122:SER:C     | 5:I:2187:HOH:O    | 2.53                     | 0.47              |
| 1:I:74:ARG:NH2    | 2:J:2018:SO4:O3   | 2.48                     | 0.47              |
| 1:B:40[B]:ASP:HA  | 5:B:2132:HOH:O    | 2.15                     | 0.47              |
| 1:D:93:HIS:NE2    | 1:D:117:GLU:OE1   | 2.47                     | 0.47              |
| 1:K:76:ALA:N      | 1:K:77:PRO:CD     | 2.77                     | 0.46              |
| 1:B:72:ARG:HB3    | 5:B:2104:HOH:O    | 2.14                     | 0.46              |
| 1:E:40[A]:ASP:OD1 | 1:E:42:ALA:CB     | 2.64                     | 0.46              |
| 1:E:66:ARG:NH2    | 1:E:74:ARG:HH21   | 2.14                     | 0.46              |
| 1:E:60:ARG:NH1    | 1:J:90:ARG:NH2    | 2.64                     | 0.46              |
| 1:F:79:ARG:NH2    | 5:I:2187:HOH:O    | 2.49                     | 0.46              |
| 1:G:17:ALA:O      | 1:G:21:ARG:HD2    | 2.15                     | 0.46              |
| 1:D:76:ALA:N      | 1:D:77:PRO:CD     | 2.79                     | 0.46              |
| 1:H:19:VAL:HG12   | 1:H:45:GLU:HG3    | 1.98                     | 0.46              |
| 1:J:92:MET:HG3    | 1:J:116:LEU:HD13  | 1.98                     | 0.46              |
| 4:A:700:HEM:HBC2  | 4:A:700:HEM:CMC   | 2.46                     | 0.46              |
| 1:C:107:GLU:HG3   | 5:C:2049:HOH:O    | 2.15                     | 0.46              |
| 4:J:700:HEM:HHC   | 4:J:700:HEM:HBB2  | 1.98                     | 0.46              |
| 1:J:23:TYR:CZ     | 1:J:36:TYR:CE2    | 3.04                     | 0.45              |
| 1:J:49:ARG:NH1    | 5:J:2093:HOH:O    | 2.49                     | 0.45              |
| 1:E:55:TYR:CZ     | 1:E:115:TYR:CE2   | 3.04                     | 0.45              |
| 1:J:76:ALA:N      | 1:J:77:PRO:CD     | 2.79                     | 0.45              |
| 1:J:105:ASP:O     | 1:J:109:ARG:HB2   | 2.17                     | 0.45              |
| 1:L:126:SER:OG    | 1:L:127:PRO:HD2   | 2.16                     | 0.45              |
| 4:E:700:HEM:HAD1  | 5:E:227:HOH:O     | 2.17                     | 0.45              |
| 1:H:2:PRO:CB      | 1:H:8:ALA:HA      | 2.47                     | 0.45              |
| 1:C:60:ARG:NH1    | 1:I:90:ARG:CD     | 2.78                     | 0.45              |
| 1:C:73:MET:HG3    | 1:G:65:GLN:HE22   | 1.81                     | 0.45              |
| 1:F:70[B]:ARG:HD2 | 5:J:2030:HOH:O    | 2.16                     | 0.44              |
| 4:J:700:HEM:HBC2  | 4:J:700:HEM:CMC   | 2.43                     | 0.44              |
| 1:K:34:ARG:NH1    | 5:K:904:HOH:O     | 2.49                     | 0.44              |
| 1:A:38[A]:GLU:O   | 1:A:39[A]:ASP:OD1 | 2.35                     | 0.44              |
| 1:G:120:ALA:HA    | 4:G:700:HEM:HMC1  | 1.99                     | 0.44              |
| 1:F:70[B]:ARG:NE  | 5:F:909:HOH:O     | 2.51                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:I:32:LEU:HD11    | 1:I:88:TRP:HA      | 2.00                     | 0.44              |
| 1:F:41[A]:LEU:HD23 | 5:F:877:HOH:O      | 2.16                     | 0.44              |
| 1:H:54:GLN:HE22    | 1:H:63:SER:N       | 2.05                     | 0.44              |
| 1:D:54:GLN:NE2     | 1:D:63:SER:H       | 2.06                     | 0.43              |
| 1:G:23:TYR:CZ      | 1:G:36:TYR:CE2     | 3.06                     | 0.43              |
| 1:D:110:ARG:NH1    | 1:D:110:ARG:CG     | 2.80                     | 0.43              |
| 1:E:60:ARG:HH11    | 1:J:90:ARG:CZ      | 2.30                     | 0.43              |
| 1:F:36:TYR:HB3     | 1:F:41[A]:LEU:HD21 | 2.00                     | 0.43              |
| 1:L:19:VAL:HG12    | 1:L:45:GLU:HG3     | 2.00                     | 0.43              |
| 1:C:76:ALA:N       | 1:C:77:PRO:CD      | 2.81                     | 0.43              |
| 1:D:92:MET:CG      | 1:D:116:LEU:HD13   | 2.49                     | 0.43              |
| 1:E:40[A]:ASP:OD1  | 1:E:42:ALA:HB2     | 2.19                     | 0.43              |
| 1:F:26:VAL:HG22    | 1:F:32:LEU:HD13    | 2.00                     | 0.43              |
| 1:K:105:ASP:HB2    | 1:K:108:HIS:CD2    | 2.53                     | 0.43              |
| 1:J:92:MET:CG      | 1:J:116:LEU:HD13   | 2.48                     | 0.43              |
| 1:B:19:VAL:HG12    | 1:B:45:GLU:HG3     | 2.00                     | 0.43              |
| 1:C:25:GLN:NE2     | 1:C:91:CYS:HA      | 2.34                     | 0.43              |
| 1:E:68[B]:HIS:HE1  | 1:J:84:GLU:OE1     | 2.00                     | 0.43              |
| 1:H:72:ARG:NH2     | 1:H:124:VAL:O      | 2.52                     | 0.42              |
| 1:B:82:LEU:HG      | 5:B:2024:HOH:O     | 2.19                     | 0.42              |
| 4:G:700:HEM:CMC    | 4:G:700:HEM:HBC2   | 2.50                     | 0.42              |
| 1:J:23:TYR:CE1     | 1:J:36:TYR:CE2     | 3.07                     | 0.42              |
| 1:A:35:VAL:CG1     | 1:A:78:PHE:HB3     | 2.50                     | 0.42              |
| 1:G:47:ARG:HB2     | 1:G:47:ARG:NH1     | 2.23                     | 0.42              |
| 1:I:17:ALA:O       | 1:I:21:ARG:HD3     | 2.20                     | 0.42              |
| 1:L:72:ARG:CD      | 5:L:2032:HOH:O     | 2.52                     | 0.41              |
| 4:C:700:HEM:HMC1   | 4:C:700:HEM:CBC    | 2.46                     | 0.41              |
| 1:G:118:MET:SD     | 1:G:118:MET:C      | 2.99                     | 0.41              |
| 1:B:54:GLN:NE2     | 1:B:62:TYR:HB3     | 2.36                     | 0.41              |
| 1:A:125:ASN:ND2    | 1:A:125:ASN:C      | 2.73                     | 0.41              |
| 1:I:76:ALA:N       | 1:I:77:PRO:CD      | 2.83                     | 0.41              |
| 1:F:16:ASP:HA      | 1:F:49:ARG:HD3     | 2.02                     | 0.41              |
| 1:E:22:PHE:CD1     | 1:E:92:MET:HE2     | 2.55                     | 0.41              |
| 1:A:34:ARG:CG      | 1:A:34:ARG:NH1     | 2.55                     | 0.41              |
| 1:A:92:MET:CG      | 1:A:116:LEU:HD13   | 2.51                     | 0.41              |
| 1:H:23:TYR:CZ      | 1:H:36:TYR:CE2     | 3.08                     | 0.41              |
| 1:A:33:ARG:HG2     | 1:A:33:ARG:HH11    | 1.86                     | 0.41              |
| 1:D:55:TYR:CE1     | 1:L:82:LEU:HD22    | 2.56                     | 0.41              |
| 1:J:62:TYR:CE1     | 1:J:66:ARG:HG3     | 2.55                     | 0.41              |
| 1:F:19:VAL:HG21    | 1:F:49:ARG:HA      | 2.01                     | 0.41              |
| 1:H:32:LEU:HD21    | 1:H:88:TRP:HA      | 2.02                     | 0.40              |

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| Atom-1          | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|--------------------|--------------------------|-------------------|
| 1:A:47:ARG:NH2  | 2:A:2011[A]:SO4:O2 | 2.45                     | 0.40              |
| 1:B:92:MET:HG3  | 1:B:116:LEU:HD13   | 2.01                     | 0.40              |
| 1:G:19:VAL:HG12 | 1:G:45:GLU:HG3     | 2.03                     | 0.40              |
| 1:K:118:MET:C   | 1:K:118:MET:SD     | 2.99                     | 0.40              |
| 1:A:70:ARG:HG3  | 5:H:911:HOH:O      | 2.22                     | 0.40              |
| 1:J:19:VAL:HG21 | 1:J:49:ARG:HA      | 2.01                     | 0.40              |
| 1:L:19:VAL:HG12 | 1:L:45:GLU:CG      | 2.52                     | 0.40              |
| 1:B:92:MET:HG2  | 1:B:116:LEU:HD13   | 2.04                     | 0.40              |
| 1:D:46:GLU:HG3  | 5:D:2110:HOH:O     | 2.21                     | 0.40              |
| 1:I:29:ASP:O    | 1:I:33:ARG:HG2     | 2.22                     | 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     | 129/128 (101%) | 126 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | B     | 130/128 (102%) | 122 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 1   | C     | 130/128 (102%) | 123 (95%) | 5 (4%)  | 2 (2%)   | 8           | 4   |
| 1   | D     | 130/128 (102%) | 121 (93%) | 7 (5%)  | 2 (2%)   | 8           | 4   |
| 1   | E     | 132/128 (103%) | 125 (95%) | 4 (3%)  | 3 (2%)   | 5           | 2   |
| 1   | F     | 130/128 (102%) | 125 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 1   | G     | 125/128 (98%)  | 123 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | H     | 126/128 (98%)  | 124 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | I     | 127/128 (99%)  | 125 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | J     | 126/128 (98%)  | 124 (98%) | 1 (1%)  | 1 (1%)   | 16          | 12  |
| 1   | K     | 126/128 (98%)  | 123 (98%) | 1 (1%)  | 2 (2%)   | 8           | 4   |
| 1   | L     | 125/128 (98%)  | 122 (98%) | 3 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|------------------|------------|---------|----------|-------------|----|
| All | All   | 1536/1536 (100%) | 1483 (96%) | 43 (3%) | 10 (1%)  | 25          | 15 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | D     | 38[A] | GLU  |
| 1   | D     | 38[B] | GLU  |
| 1   | K     | 105   | ASP  |
| 1   | C     | 38[A] | GLU  |
| 1   | C     | 38[B] | GLU  |
| 1   | E     | 38[A] | GLU  |
| 1   | E     | 38[B] | GLU  |
| 1   | K     | 3     | LYS  |
| 1   | E     | 105   | ASP  |
| 1   | J     | 105   | ASP  |

### 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     | 112/109 (103%) | 103 (92%) | 9 (8%)   | 10          | 7  |
| 1   | B     | 113/109 (104%) | 107 (95%) | 6 (5%)   | 19          | 17 |
| 1   | C     | 113/109 (104%) | 104 (92%) | 9 (8%)   | 10          | 7  |
| 1   | D     | 113/109 (104%) | 107 (95%) | 6 (5%)   | 19          | 17 |
| 1   | E     | 115/109 (106%) | 102 (89%) | 13 (11%) | 4           | 2  |
| 1   | F     | 113/109 (104%) | 102 (90%) | 11 (10%) | 6           | 4  |
| 1   | G     | 108/109 (99%)  | 101 (94%) | 7 (6%)   | 14          | 11 |
| 1   | H     | 109/109 (100%) | 100 (92%) | 9 (8%)   | 9           | 6  |
| 1   | I     | 110/109 (101%) | 101 (92%) | 9 (8%)   | 9           | 6  |
| 1   | J     | 109/109 (100%) | 101 (93%) | 8 (7%)   | 11          | 9  |
| 1   | K     | 109/109 (100%) | 101 (93%) | 8 (7%)   | 11          | 9  |
| 1   | L     | 108/109 (99%)  | 99 (92%)  | 9 (8%)   | 9           | 6  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |
|-----|-------|------------------|------------|----------|-------------|
| All | All   | 1332/1308 (102%) | 1228 (92%) | 104 (8%) | 11 7        |

All (104) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 23     | TYR  |
| 1   | A     | 34     | ARG  |
| 1   | A     | 37[A]  | PRO  |
| 1   | A     | 37[B]  | PRO  |
| 1   | A     | 48     | LEU  |
| 1   | A     | 72     | ARG  |
| 1   | A     | 89     | LEU  |
| 1   | A     | 104    | LEU  |
| 1   | A     | 125    | ASN  |
| 1   | B     | 3      | LYS  |
| 1   | B     | 23     | TYR  |
| 1   | B     | 37[A]  | PRO  |
| 1   | B     | 37[B]  | PRO  |
| 1   | B     | 48     | LEU  |
| 1   | B     | 117    | GLU  |
| 1   | C     | 23     | TYR  |
| 1   | C     | 34     | ARG  |
| 1   | C     | 37[A]  | PRO  |
| 1   | C     | 37[B]  | PRO  |
| 1   | C     | 70     | ARG  |
| 1   | C     | 104    | LEU  |
| 1   | C     | 117[A] | GLU  |
| 1   | C     | 117[B] | GLU  |
| 1   | C     | 125    | ASN  |
| 1   | D     | 3      | LYS  |
| 1   | D     | 23     | TYR  |
| 1   | D     | 32     | LEU  |
| 1   | D     | 37[A]  | PRO  |
| 1   | D     | 37[B]  | PRO  |
| 1   | D     | 117    | GLU  |
| 1   | E     | 2      | PRO  |
| 1   | E     | 3      | LYS  |
| 1   | E     | 23     | TYR  |
| 1   | E     | 32     | LEU  |
| 1   | E     | 37[A]  | PRO  |
| 1   | E     | 37[B]  | PRO  |
| 1   | E     | 72     | ARG  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | E     | 74    | ARG  |
| 1   | E     | 82    | LEU  |
| 1   | E     | 104   | LEU  |
| 1   | E     | 105   | ASP  |
| 1   | E     | 113   | LEU  |
| 1   | E     | 117   | GLU  |
| 1   | F     | 23    | TYR  |
| 1   | F     | 34    | ARG  |
| 1   | F     | 37[A] | PRO  |
| 1   | F     | 37[B] | PRO  |
| 1   | F     | 48    | LEU  |
| 1   | F     | 61    | THR  |
| 1   | F     | 82    | LEU  |
| 1   | F     | 89    | LEU  |
| 1   | F     | 104   | LEU  |
| 1   | F     | 113   | LEU  |
| 1   | F     | 118   | MET  |
| 1   | G     | 3     | LYS  |
| 1   | G     | 34    | ARG  |
| 1   | G     | 47    | ARG  |
| 1   | G     | 82    | LEU  |
| 1   | G     | 104   | LEU  |
| 1   | G     | 113   | LEU  |
| 1   | G     | 117   | GLU  |
| 1   | H     | 3     | LYS  |
| 1   | H     | 32    | LEU  |
| 1   | H     | 72    | ARG  |
| 1   | H     | 74    | ARG  |
| 1   | H     | 82    | LEU  |
| 1   | H     | 90    | ARG  |
| 1   | H     | 113   | LEU  |
| 1   | H     | 125   | ASN  |
| 1   | H     | 128   | PHE  |
| 1   | I     | 3     | LYS  |
| 1   | I     | 28    | GLU  |
| 1   | I     | 30    | GLU  |
| 1   | I     | 52    | LEU  |
| 1   | I     | 74    | ARG  |
| 1   | I     | 104   | LEU  |
| 1   | I     | 110   | ARG  |
| 1   | I     | 123   | LEU  |
| 1   | I     | 125   | ASN  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | J     | 3     | LYS  |
| 1   | J     | 60    | ARG  |
| 1   | J     | 71    | LEU  |
| 1   | J     | 72[A] | ARG  |
| 1   | J     | 72[B] | ARG  |
| 1   | J     | 104   | LEU  |
| 1   | J     | 113   | LEU  |
| 1   | J     | 128   | PHE  |
| 1   | K     | 30    | GLU  |
| 1   | K     | 32    | LEU  |
| 1   | K     | 69    | PRO  |
| 1   | K     | 74    | ARG  |
| 1   | K     | 82    | LEU  |
| 1   | K     | 104   | LEU  |
| 1   | K     | 113   | LEU  |
| 1   | K     | 128   | PHE  |
| 1   | L     | 3     | LYS  |
| 1   | L     | 37    | PRO  |
| 1   | L     | 69    | PRO  |
| 1   | L     | 82    | LEU  |
| 1   | L     | 104   | LEU  |
| 1   | L     | 110   | ARG  |
| 1   | L     | 113   | LEU  |
| 1   | L     | 118   | MET  |
| 1   | L     | 128   | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 54  | GLN  |
| 1   | A     | 93  | HIS  |
| 1   | A     | 125 | ASN  |
| 1   | B     | 54  | GLN  |
| 1   | C     | 25  | GLN  |
| 1   | C     | 125 | ASN  |
| 1   | D     | 54  | GLN  |
| 1   | D     | 65  | GLN  |
| 1   | D     | 68  | HIS  |
| 1   | D     | 121 | HIS  |
| 1   | E     | 25  | GLN  |
| 1   | E     | 65  | GLN  |
| 1   | E     | 93  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 65  | GLN  |
| 1   | G     | 65  | GLN  |
| 1   | G     | 68  | HIS  |
| 1   | H     | 25  | GLN  |
| 1   | H     | 54  | GLN  |
| 1   | H     | 121 | HIS  |
| 1   | H     | 125 | ASN  |
| 1   | I     | 54  | GLN  |
| 1   | I     | 65  | GLN  |
| 1   | I     | 125 | ASN  |
| 1   | J     | 65  | GLN  |
| 1   | J     | 93  | HIS  |
| 1   | K     | 108 | HIS  |
| 1   | L     | 54  | GLN  |
| 1   | L     | 93  | HIS  |
| 1   | L     | 121 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

42 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 |
| 3   | CYN  | L     | 800     | 4    | 1,1,1        | 0.32 | 0        | -           |      |          |
| 3   | CYN  | D     | 800     | 4    | 1,1,1        | 0.29 | 0        | -           |      |          |
| 4   | HEM  | C     | 700     | 1,3  | 42,50,50     | 1.90 | 7 (16%)  | 46,82,82    | 1.69 | 9 (19%)  |
| 3   | CYN  | F     | 800     | 4    | 1,1,1        | 0.30 | 0        | -           |      |          |
| 3   | CYN  | A     | 800     | 4    | 1,1,1        | 0.35 | 0        | -           |      |          |
| 4   | HEM  | A     | 700     | 1,3  | 42,50,50     | 1.81 | 6 (14%)  | 46,82,82    | 1.78 | 11 (23%) |
| 2   | SO4  | E     | 2006[A] | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.13 | 0        |
| 2   | SO4  | A     | 2004    | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.16 | 0        |
| 3   | CYN  | B     | 800     | 4    | 1,1,1        | 0.35 | 0        | -           |      |          |
| 2   | SO4  | C     | 2013    | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.06 | 0        |
| 3   | CYN  | E     | 800     | 4    | 1,1,1        | 0.29 | 0        | -           |      |          |
| 3   | CYN  | I     | 800     | 4    | 1,1,1        | 0.30 | 0        | -           |      |          |
| 4   | HEM  | B     | 700     | 1,3  | 42,50,50     | 1.86 | 5 (11%)  | 46,82,82    | 1.71 | 7 (15%)  |
| 2   | SO4  | D     | 2010[A] | -    | 4,4,4        | 0.28 | 0        | 6,6,6       | 0.18 | 0        |
| 2   | SO4  | E     | 2003    | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.11 | 0        |
| 4   | HEM  | L     | 700     | 1,3  | 42,50,50     | 1.90 | 6 (14%)  | 46,82,82    | 1.66 | 8 (17%)  |
| 4   | HEM  | G     | 700     | 1,3  | 42,50,50     | 2.05 | 7 (16%)  | 46,82,82    | 1.49 | 5 (10%)  |
| 3   | CYN  | G     | 800     | 4    | 1,1,1        | 0.29 | 0        | -           |      |          |
| 2   | SO4  | G     | 2002    | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.17 | 0        |
| 2   | SO4  | J     | 2018    | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.12 | 0        |
| 2   | SO4  | J     | 2008[A] | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.12 | 0        |
| 4   | HEM  | E     | 700     | 1,3  | 42,50,50     | 1.87 | 7 (16%)  | 46,82,82    | 1.67 | 9 (19%)  |
| 4   | HEM  | D     | 700     | 1,3  | 42,50,50     | 1.86 | 6 (14%)  | 46,82,82    | 1.64 | 6 (13%)  |
| 3   | CYN  | C     | 800     | 4    | 1,1,1        | 0.30 | 0        | -           |      |          |
| 3   | CYN  | H     | 800     | 4    | 1,1,1        | 0.32 | 0        | -           |      |          |
| 4   | HEM  | F     | 700     | 1,3  | 42,50,50     | 1.86 | 6 (14%)  | 46,82,82    | 1.65 | 9 (19%)  |
| 2   | SO4  | B     | 2017    | -    | 4,4,4        | 0.21 | 0        | 6,6,6       | 0.17 | 0        |
| 2   | SO4  | L     | 2005    | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.14 | 0        |
| 4   | HEM  | H     | 700     | 1,3  | 42,50,50     | 1.90 | 7 (16%)  | 46,82,82    | 1.59 | 8 (17%)  |
| 4   | HEM  | K     | 700     | 1,3  | 42,50,50     | 1.89 | 6 (14%)  | 46,82,82    | 1.55 | 5 (10%)  |
| 2   | SO4  | A     | 2016    | -    | 4,4,4        | 0.24 | 0        | 6,6,6       | 0.11 | 0        |
| 2   | SO4  | B     | 2007[A] | -    | 4,4,4        | 0.22 | 0        | 6,6,6       | 0.29 | 0        |
| 2   | SO4  | I     | 2015    | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.21 | 0        |
| 2   | SO4  | G     | 2001    | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.09 | 0        |
| 2   | SO4  | A     | 2012    | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.28 | 0        |
| 3   | CYN  | K     | 800     | 4    | 1,1,1        | 0.28 | 0        | -           |      |          |
| 2   | SO4  | A     | 2014    | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.14 | 0        |
| 2   | SO4  | C     | 2009[A] | -    | 4,4,4        | 0.19 | 0        | 6,6,6       | 0.22 | 0        |
| 4   | HEM  | I     | 700     | 1,3  | 42,50,50     | 1.88 | 9 (21%)  | 46,82,82    | 1.51 | 6 (13%)  |
| 4   | HEM  | J     | 700     | 1,3  | 42,50,50     | 1.91 | 7 (16%)  | 46,82,82    | 1.67 | 10 (21%) |

| Mol | Type | Chain | Res     | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|---------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |         |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | SO4  | A     | 2011[A] | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.13 | 0        |
| 3   | CYN  | J     | 800     | 4    | 1,1,1        | 0.33 | 0        | -           |      |          |

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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 4   | HEM  | L     | 700 | 1,3  | -       | 5/12/54/54 | -     |
| 4   | HEM  | E     | 700 | 1,3  | -       | 6/12/54/54 | -     |
| 4   | HEM  | D     | 700 | 1,3  | -       | 4/12/54/54 | -     |
| 4   | HEM  | C     | 700 | 1,3  | -       | 6/12/54/54 | -     |
| 4   | HEM  | F     | 700 | 1,3  | -       | 6/12/54/54 | -     |
| 4   | HEM  | G     | 700 | 1,3  | -       | 4/12/54/54 | -     |
| 4   | HEM  | I     | 700 | 1,3  | -       | 5/12/54/54 | -     |
| 4   | HEM  | J     | 700 | 1,3  | -       | 5/12/54/54 | -     |
| 4   | HEM  | H     | 700 | 1,3  | -       | 5/12/54/54 | -     |
| 4   | HEM  | K     | 700 | 1,3  | -       | 7/12/54/54 | -     |
| 4   | HEM  | A     | 700 | 1,3  | -       | 4/12/54/54 | -     |
| 4   | HEM  | B     | 700 | 1,3  | -       | 4/12/54/54 | -     |

All (79) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | G     | 700 | HEM  | C3D-C2D | 7.92  | 1.53        | 1.36     |
| 4   | K     | 700 | HEM  | C3D-C2D | 7.72  | 1.53        | 1.36     |
| 4   | I     | 700 | HEM  | C3D-C2D | 7.61  | 1.53        | 1.36     |
| 4   | J     | 700 | HEM  | C3D-C2D | 7.59  | 1.53        | 1.36     |
| 4   | C     | 700 | HEM  | C3D-C2D | 7.56  | 1.53        | 1.36     |
| 4   | B     | 700 | HEM  | C3D-C2D | 7.54  | 1.53        | 1.36     |
| 4   | H     | 700 | HEM  | C3D-C2D | 7.39  | 1.52        | 1.36     |
| 4   | F     | 700 | HEM  | C3D-C2D | 7.38  | 1.52        | 1.36     |
| 4   | L     | 700 | HEM  | C3D-C2D | 7.36  | 1.52        | 1.36     |
| 4   | A     | 700 | HEM  | C3D-C2D | 7.33  | 1.52        | 1.36     |
| 4   | E     | 700 | HEM  | C3D-C2D | 7.21  | 1.52        | 1.36     |
| 4   | D     | 700 | HEM  | C3D-C2D | 7.13  | 1.52        | 1.36     |
| 4   | G     | 700 | HEM  | C3C-C2C | -5.13 | 1.33        | 1.40     |
| 4   | L     | 700 | HEM  | C3C-C2C | -4.95 | 1.33        | 1.40     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4   | C     | 700 | HEM  | C3C-C2C | -4.84 | 1.33        | 1.40     |
| 4   | D     | 700 | HEM  | C3C-C2C | -4.72 | 1.34        | 1.40     |
| 4   | K     | 700 | HEM  | C3C-C2C | -4.33 | 1.34        | 1.40     |
| 4   | F     | 700 | HEM  | C3C-C2C | -4.26 | 1.34        | 1.40     |
| 4   | H     | 700 | HEM  | C3C-C2C | -4.20 | 1.34        | 1.40     |
| 4   | E     | 700 | HEM  | C3C-C2C | -4.17 | 1.34        | 1.40     |
| 4   | B     | 700 | HEM  | C3C-C2C | -4.05 | 1.34        | 1.40     |
| 4   | I     | 700 | HEM  | C3C-C2C | -3.96 | 1.35        | 1.40     |
| 4   | J     | 700 | HEM  | C3C-C2C | -3.82 | 1.35        | 1.40     |
| 4   | A     | 700 | HEM  | C3C-C2C | -3.77 | 1.35        | 1.40     |
| 4   | B     | 700 | HEM  | C3C-CAC | 3.73  | 1.56        | 1.47     |
| 4   | H     | 700 | HEM  | C3C-CAC | 3.53  | 1.55        | 1.47     |
| 4   | F     | 700 | HEM  | C3C-CAC | 3.49  | 1.55        | 1.47     |
| 4   | J     | 700 | HEM  | C3C-CAC | 3.49  | 1.55        | 1.47     |
| 4   | C     | 700 | HEM  | C3C-CAC | 3.36  | 1.55        | 1.47     |
| 4   | D     | 700 | HEM  | C3C-CAC | 3.36  | 1.55        | 1.47     |
| 4   | A     | 700 | HEM  | C3C-CAC | 3.31  | 1.55        | 1.47     |
| 4   | E     | 700 | HEM  | C3C-CAC | 3.30  | 1.55        | 1.47     |
| 4   | K     | 700 | HEM  | C3C-CAC | 3.28  | 1.55        | 1.47     |
| 4   | G     | 700 | HEM  | C3C-CAC | 3.28  | 1.55        | 1.47     |
| 4   | I     | 700 | HEM  | C3C-CAC | 3.23  | 1.54        | 1.47     |
| 4   | L     | 700 | HEM  | C3C-CAC | 3.19  | 1.54        | 1.47     |
| 4   | G     | 700 | HEM  | C3C-C4C | 3.17  | 1.46        | 1.41     |
| 4   | J     | 700 | HEM  | CAB-C3B | 3.01  | 1.55        | 1.47     |
| 4   | G     | 700 | HEM  | CAB-C3B | 2.91  | 1.55        | 1.47     |
| 4   | H     | 700 | HEM  | C3C-C4C | 2.86  | 1.45        | 1.41     |
| 4   | C     | 700 | HEM  | CAB-C3B | 2.86  | 1.55        | 1.47     |
| 4   | D     | 700 | HEM  | CAB-C3B | 2.83  | 1.54        | 1.47     |
| 4   | L     | 700 | HEM  | C3C-C4C | 2.83  | 1.45        | 1.41     |
| 4   | E     | 700 | HEM  | FE-ND   | 2.80  | 2.13        | 1.98     |
| 4   | K     | 700 | HEM  | CAB-C3B | 2.79  | 1.54        | 1.47     |
| 4   | H     | 700 | HEM  | CAB-C3B | 2.73  | 1.54        | 1.47     |
| 4   | L     | 700 | HEM  | CAB-C3B | 2.64  | 1.54        | 1.47     |
| 4   | E     | 700 | HEM  | CAB-C3B | 2.63  | 1.54        | 1.47     |
| 4   | J     | 700 | HEM  | C3C-C4C | 2.63  | 1.45        | 1.41     |
| 4   | E     | 700 | HEM  | C3C-C4C | 2.60  | 1.45        | 1.41     |
| 4   | B     | 700 | HEM  | C3C-C4C | 2.60  | 1.45        | 1.41     |
| 4   | H     | 700 | HEM  | CMB-C2B | 2.60  | 1.56        | 1.50     |
| 4   | G     | 700 | HEM  | CMB-C2B | 2.57  | 1.56        | 1.50     |
| 4   | B     | 700 | HEM  | CAB-C3B | 2.54  | 1.54        | 1.47     |
| 4   | I     | 700 | HEM  | CAB-C3B | 2.54  | 1.54        | 1.47     |
| 4   | C     | 700 | HEM  | CMB-C2B | 2.51  | 1.55        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4   | I     | 700 | HEM  | C3C-C4C | 2.48 | 1.45        | 1.41     |
| 4   | G     | 700 | HEM  | CMD-C2D | 2.39 | 1.55        | 1.50     |
| 4   | F     | 700 | HEM  | CAB-C3B | 2.35 | 1.53        | 1.47     |
| 4   | I     | 700 | HEM  | CMB-C2B | 2.29 | 1.55        | 1.50     |
| 4   | D     | 700 | HEM  | CMB-C2B | 2.29 | 1.55        | 1.50     |
| 4   | J     | 700 | HEM  | CMD-C2D | 2.28 | 1.55        | 1.50     |
| 4   | A     | 700 | HEM  | CMD-C2D | 2.26 | 1.55        | 1.50     |
| 4   | A     | 700 | HEM  | CMB-C2B | 2.23 | 1.55        | 1.50     |
| 4   | K     | 700 | HEM  | CMB-C2B | 2.20 | 1.55        | 1.50     |
| 4   | L     | 700 | HEM  | CMD-C2D | 2.18 | 1.55        | 1.50     |
| 4   | A     | 700 | HEM  | CAB-C3B | 2.18 | 1.53        | 1.47     |
| 4   | K     | 700 | HEM  | CMD-C2D | 2.17 | 1.55        | 1.50     |
| 4   | C     | 700 | HEM  | C3C-C4C | 2.17 | 1.44        | 1.41     |
| 4   | I     | 700 | HEM  | FE-ND   | 2.16 | 2.10        | 1.98     |
| 4   | F     | 700 | HEM  | CMB-C2B | 2.12 | 1.55        | 1.50     |
| 4   | I     | 700 | HEM  | CMA-C3A | 2.12 | 1.55        | 1.51     |
| 4   | E     | 700 | HEM  | CMB-C2B | 2.10 | 1.55        | 1.50     |
| 4   | F     | 700 | HEM  | CMD-C2D | 2.09 | 1.55        | 1.50     |
| 4   | D     | 700 | HEM  | CMD-C2D | 2.09 | 1.55        | 1.50     |
| 4   | H     | 700 | HEM  | CMD-C2D | 2.08 | 1.55        | 1.50     |
| 4   | I     | 700 | HEM  | CMD-C2D | 2.04 | 1.55        | 1.50     |
| 4   | J     | 700 | HEM  | FE-NB   | 2.01 | 2.09        | 1.98     |
| 4   | C     | 700 | HEM  | CMD-C2D | 2.00 | 1.54        | 1.50     |

All (93) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | B     | 700 | HEM  | C4D-ND-C1D  | 5.37  | 111.56      | 105.21   |
| 4   | J     | 700 | HEM  | C4D-ND-C1D  | 5.34  | 111.53      | 105.21   |
| 4   | C     | 700 | HEM  | C4D-ND-C1D  | 5.19  | 111.36      | 105.21   |
| 4   | I     | 700 | HEM  | C4D-ND-C1D  | 5.17  | 111.33      | 105.21   |
| 4   | L     | 700 | HEM  | C4D-ND-C1D  | 5.01  | 111.14      | 105.21   |
| 4   | G     | 700 | HEM  | C4D-ND-C1D  | 4.97  | 111.09      | 105.21   |
| 4   | C     | 700 | HEM  | CBA-CAA-C2A | -4.95 | 104.22      | 112.54   |
| 4   | E     | 700 | HEM  | C4D-ND-C1D  | 4.93  | 111.05      | 105.21   |
| 4   | A     | 700 | HEM  | C4D-ND-C1D  | 4.89  | 111.00      | 105.21   |
| 4   | H     | 700 | HEM  | C4D-ND-C1D  | 4.87  | 110.98      | 105.21   |
| 4   | A     | 700 | HEM  | CBA-CAA-C2A | -4.83 | 104.41      | 112.54   |
| 4   | F     | 700 | HEM  | C4D-ND-C1D  | 4.80  | 110.89      | 105.21   |
| 4   | D     | 700 | HEM  | C4D-ND-C1D  | 4.68  | 110.75      | 105.21   |
| 4   | D     | 700 | HEM  | CBA-CAA-C2A | -4.66 | 104.70      | 112.54   |
| 4   | E     | 700 | HEM  | CBA-CAA-C2A | -4.59 | 104.82      | 112.54   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | B     | 700 | HEM  | CBA-CAA-C2A | -4.54 | 104.91      | 112.54   |
| 4   | K     | 700 | HEM  | C4D-ND-C1D  | 4.46  | 110.48      | 105.21   |
| 4   | F     | 700 | HEM  | CBA-CAA-C2A | -4.14 | 105.57      | 112.54   |
| 4   | K     | 700 | HEM  | CBA-CAA-C2A | -4.05 | 105.73      | 112.54   |
| 4   | L     | 700 | HEM  | CBA-CAA-C2A | -3.99 | 105.83      | 112.54   |
| 4   | G     | 700 | HEM  | C4C-CHD-C1D | 3.77  | 127.53      | 122.56   |
| 4   | H     | 700 | HEM  | C4C-CHD-C1D | 3.54  | 127.23      | 122.56   |
| 4   | J     | 700 | HEM  | CBA-CAA-C2A | -3.52 | 106.63      | 112.54   |
| 4   | G     | 700 | HEM  | CAA-CBA-CGA | -3.49 | 104.42      | 113.83   |
| 4   | A     | 700 | HEM  | C3B-C4B-NB  | -3.26 | 107.13      | 109.47   |
| 4   | L     | 700 | HEM  | C4C-CHD-C1D | 3.11  | 126.66      | 122.56   |
| 4   | H     | 700 | HEM  | CBA-CAA-C2A | -3.11 | 107.32      | 112.54   |
| 4   | K     | 700 | HEM  | CAA-CBA-CGA | -2.88 | 106.08      | 113.83   |
| 4   | I     | 700 | HEM  | CBA-CAA-C2A | -2.87 | 107.72      | 112.54   |
| 4   | C     | 700 | HEM  | C4C-CHD-C1D | 2.82  | 126.28      | 122.56   |
| 4   | J     | 700 | HEM  | CMA-C3A-C4A | -2.81 | 124.34      | 128.46   |
| 4   | C     | 700 | HEM  | CMA-C3A-C4A | -2.79 | 124.38      | 128.46   |
| 4   | J     | 700 | HEM  | C4C-CHD-C1D | 2.78  | 126.23      | 122.56   |
| 4   | J     | 700 | HEM  | C4B-CHC-C1C | 2.77  | 126.21      | 122.56   |
| 4   | B     | 700 | HEM  | CMA-C3A-C4A | -2.68 | 124.53      | 128.46   |
| 4   | A     | 700 | HEM  | C4B-CHC-C1C | 2.67  | 126.08      | 122.56   |
| 4   | I     | 700 | HEM  | C4C-CHD-C1D | 2.64  | 126.05      | 122.56   |
| 4   | L     | 700 | HEM  | C4B-CHC-C1C | 2.64  | 126.04      | 122.56   |
| 4   | K     | 700 | HEM  | C4C-CHD-C1D | 2.63  | 126.02      | 122.56   |
| 4   | E     | 700 | HEM  | C4C-CHD-C1D | 2.62  | 126.02      | 122.56   |
| 4   | F     | 700 | HEM  | C3B-C4B-NB  | -2.60 | 107.60      | 109.47   |
| 4   | B     | 700 | HEM  | C4C-CHD-C1D | 2.58  | 125.96      | 122.56   |
| 4   | F     | 700 | HEM  | C1D-C2D-C3D | -2.57 | 104.27      | 106.98   |
| 4   | E     | 700 | HEM  | C4B-CHC-C1C | 2.56  | 125.94      | 122.56   |
| 4   | A     | 700 | HEM  | CMD-C2D-C1D | 2.54  | 129.00      | 125.03   |
| 4   | C     | 700 | HEM  | CAD-CBD-CGD | -2.54 | 106.93      | 113.67   |
| 4   | I     | 700 | HEM  | CAD-CBD-CGD | -2.52 | 106.97      | 113.67   |
| 4   | E     | 700 | HEM  | C1B-NB-C4B  | 2.52  | 108.19      | 105.21   |
| 4   | D     | 700 | HEM  | C4C-CHD-C1D | 2.49  | 125.84      | 122.56   |
| 4   | H     | 700 | HEM  | C4B-CHC-C1C | 2.49  | 125.84      | 122.56   |
| 4   | E     | 700 | HEM  | C3B-C4B-NB  | -2.49 | 107.68      | 109.47   |
| 4   | B     | 700 | HEM  | CAD-C3D-C4D | 2.46  | 128.99      | 124.70   |
| 4   | A     | 700 | HEM  | CMA-C3A-C4A | -2.46 | 124.85      | 128.46   |
| 4   | L     | 700 | HEM  | O1A-CGA-CBA | -2.45 | 115.31      | 123.09   |
| 4   | D     | 700 | HEM  | CAD-C3D-C4D | 2.44  | 128.96      | 124.70   |
| 4   | I     | 700 | HEM  | O1A-CGA-CBA | -2.43 | 115.38      | 123.09   |
| 4   | J     | 700 | HEM  | O1A-CGA-CBA | -2.41 | 115.43      | 123.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4   | L     | 700 | HEM  | CBD-CAD-C3D | -2.41 | 105.87      | 112.53   |
| 4   | A     | 700 | HEM  | C1B-NB-C4B  | 2.41  | 108.06      | 105.21   |
| 4   | H     | 700 | HEM  | O1A-CGA-CBA | -2.40 | 115.47      | 123.09   |
| 4   | E     | 700 | HEM  | CAD-CBD-CGD | -2.38 | 107.34      | 113.67   |
| 4   | A     | 700 | HEM  | CAD-CBD-CGD | -2.38 | 107.36      | 113.67   |
| 4   | H     | 700 | HEM  | CAD-CBD-CGD | -2.34 | 107.45      | 113.67   |
| 4   | F     | 700 | HEM  | CAD-CBD-CGD | -2.33 | 107.48      | 113.67   |
| 4   | F     | 700 | HEM  | C4B-CHC-C1C | 2.32  | 125.61      | 122.56   |
| 4   | D     | 700 | HEM  | CAD-CBD-CGD | -2.29 | 107.58      | 113.67   |
| 4   | H     | 700 | HEM  | CMD-C2D-C1D | 2.27  | 128.58      | 125.03   |
| 4   | C     | 700 | HEM  | CBD-CAD-C3D | -2.25 | 106.30      | 112.53   |
| 4   | B     | 700 | HEM  | C4B-CHC-C1C | 2.23  | 125.50      | 122.56   |
| 4   | E     | 700 | HEM  | CAD-C3D-C4D | 2.20  | 128.54      | 124.70   |
| 4   | F     | 700 | HEM  | CMA-C3A-C4A | -2.20 | 125.23      | 128.46   |
| 4   | G     | 700 | HEM  | C3B-C2B-C1B | 2.20  | 108.06      | 106.41   |
| 4   | F     | 700 | HEM  | C1B-NB-C4B  | 2.18  | 107.78      | 105.21   |
| 4   | C     | 700 | HEM  | C1D-C2D-C3D | -2.16 | 104.71      | 106.98   |
| 4   | D     | 700 | HEM  | C1D-C2D-C3D | -2.15 | 104.72      | 106.98   |
| 4   | K     | 700 | HEM  | O1A-CGA-CBA | -2.13 | 116.33      | 123.09   |
| 4   | A     | 700 | HEM  | C1D-C2D-C3D | -2.12 | 104.75      | 106.98   |
| 4   | A     | 700 | HEM  | CHA-C4D-ND  | 2.12  | 127.00      | 124.37   |
| 4   | J     | 700 | HEM  | C1D-C2D-C3D | -2.11 | 104.76      | 106.98   |
| 4   | B     | 700 | HEM  | CHD-C1D-ND  | 2.10  | 126.70      | 124.44   |
| 4   | F     | 700 | HEM  | CBD-CAD-C3D | -2.09 | 106.76      | 112.53   |
| 4   | J     | 700 | HEM  | C1B-NB-C4B  | 2.06  | 107.64      | 105.21   |
| 4   | E     | 700 | HEM  | CMA-C3A-C4A | -2.06 | 125.44      | 128.46   |
| 4   | A     | 700 | HEM  | CAD-C3D-C4D | 2.06  | 128.28      | 124.70   |
| 4   | J     | 700 | HEM  | C3B-C2B-C1B | 2.05  | 107.95      | 106.41   |
| 4   | H     | 700 | HEM  | CBB-CAB-C3B | -2.04 | 117.32      | 127.53   |
| 4   | C     | 700 | HEM  | CBB-CAB-C3B | -2.04 | 117.34      | 127.53   |
| 4   | I     | 700 | HEM  | CBD-CAD-C3D | -2.04 | 106.90      | 112.53   |
| 4   | G     | 700 | HEM  | C2C-C3C-C4C | 2.03  | 108.31      | 106.90   |
| 4   | L     | 700 | HEM  | C3B-C2B-C1B | 2.02  | 107.92      | 106.41   |
| 4   | L     | 700 | HEM  | CAA-CBA-CGA | -2.02 | 108.40      | 113.83   |
| 4   | J     | 700 | HEM  | CAA-CBA-CGA | -2.01 | 108.42      | 113.83   |
| 4   | C     | 700 | HEM  | C4B-CHC-C1C | 2.00  | 125.20      | 122.56   |

There are no chirality outliers.

All (61) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | H     | 700 | HEM  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | I     | 700 | HEM  | C2A-CAA-CBA-CGA |
| 4   | J     | 700 | HEM  | C2A-CAA-CBA-CGA |
| 4   | E     | 700 | HEM  | C2B-C3B-CAB-CBB |
| 4   | K     | 700 | HEM  | C2A-CAA-CBA-CGA |
| 4   | C     | 700 | HEM  | C2B-C3B-CAB-CBB |
| 4   | F     | 700 | HEM  | C2B-C3B-CAB-CBB |
| 4   | K     | 700 | HEM  | C2B-C3B-CAB-CBB |
| 4   | C     | 700 | HEM  | C4B-C3B-CAB-CBB |
| 4   | E     | 700 | HEM  | C4B-C3B-CAB-CBB |
| 4   | F     | 700 | HEM  | C4B-C3B-CAB-CBB |
| 4   | K     | 700 | HEM  | C4B-C3B-CAB-CBB |
| 4   | L     | 700 | HEM  | C2A-CAA-CBA-CGA |
| 4   | C     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | C     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | E     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | A     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | D     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | I     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | J     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | K     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | A     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | F     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | D     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | F     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | E     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | B     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | C     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | F     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | H     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | B     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | D     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | F     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | L     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | L     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | G     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | H     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | J     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | E     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | K     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | A     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | J     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | B     | 700 | HEM  | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 4   | C     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | E     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | J     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | B     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | D     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | I     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | A     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | G     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | G     | 700 | HEM  | CAD-CBD-CGD-O1D |
| 4   | I     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | G     | 700 | HEM  | CAD-CBD-CGD-O2D |
| 4   | H     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | H     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | I     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | K     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | L     | 700 | HEM  | CAA-CBA-CGA-O1A |
| 4   | L     | 700 | HEM  | CAA-CBA-CGA-O2A |
| 4   | K     | 700 | HEM  | CAA-CBA-CGA-O2A |

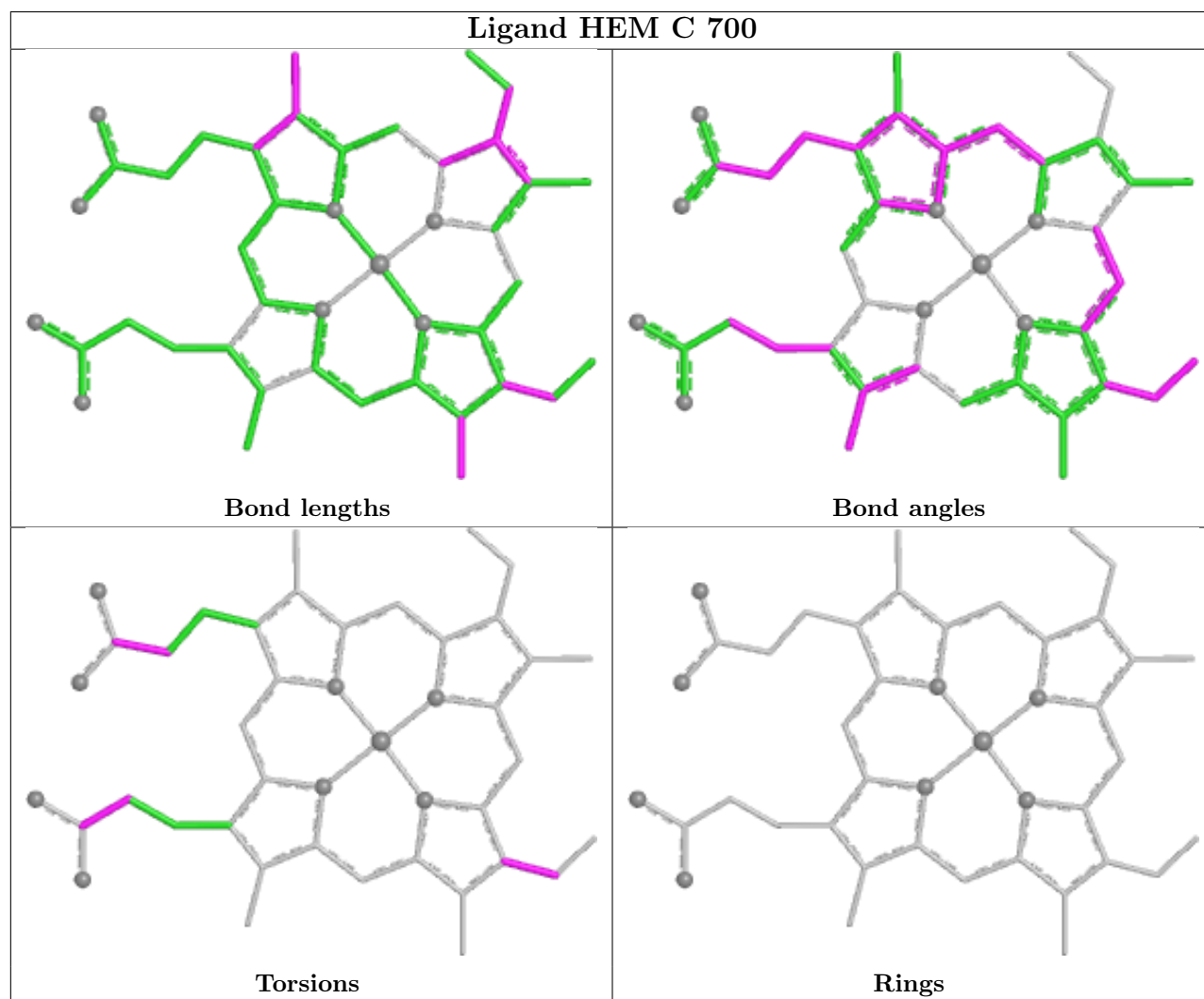
There are no ring outliers.

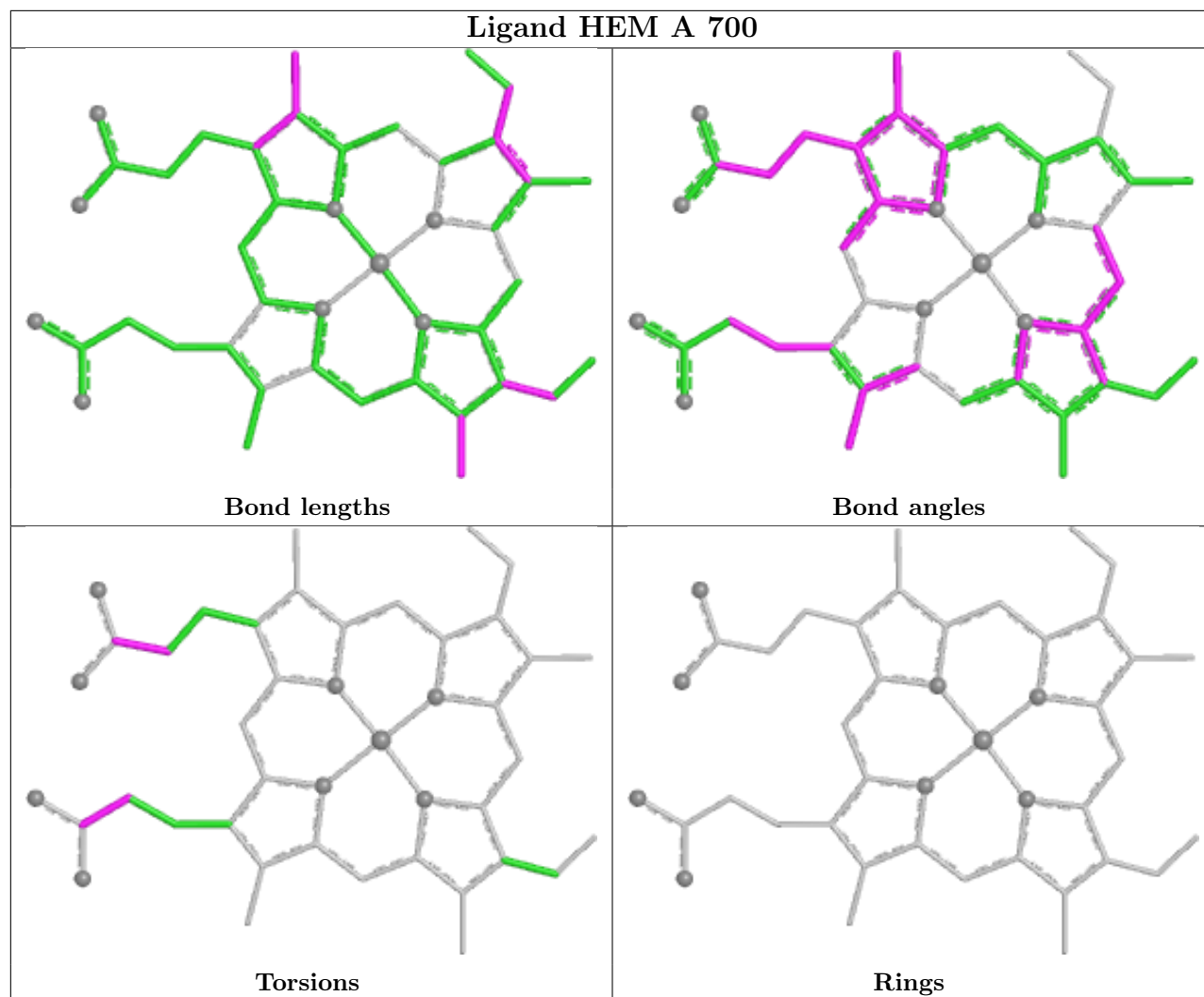
17 monomers are involved in 31 short contacts:

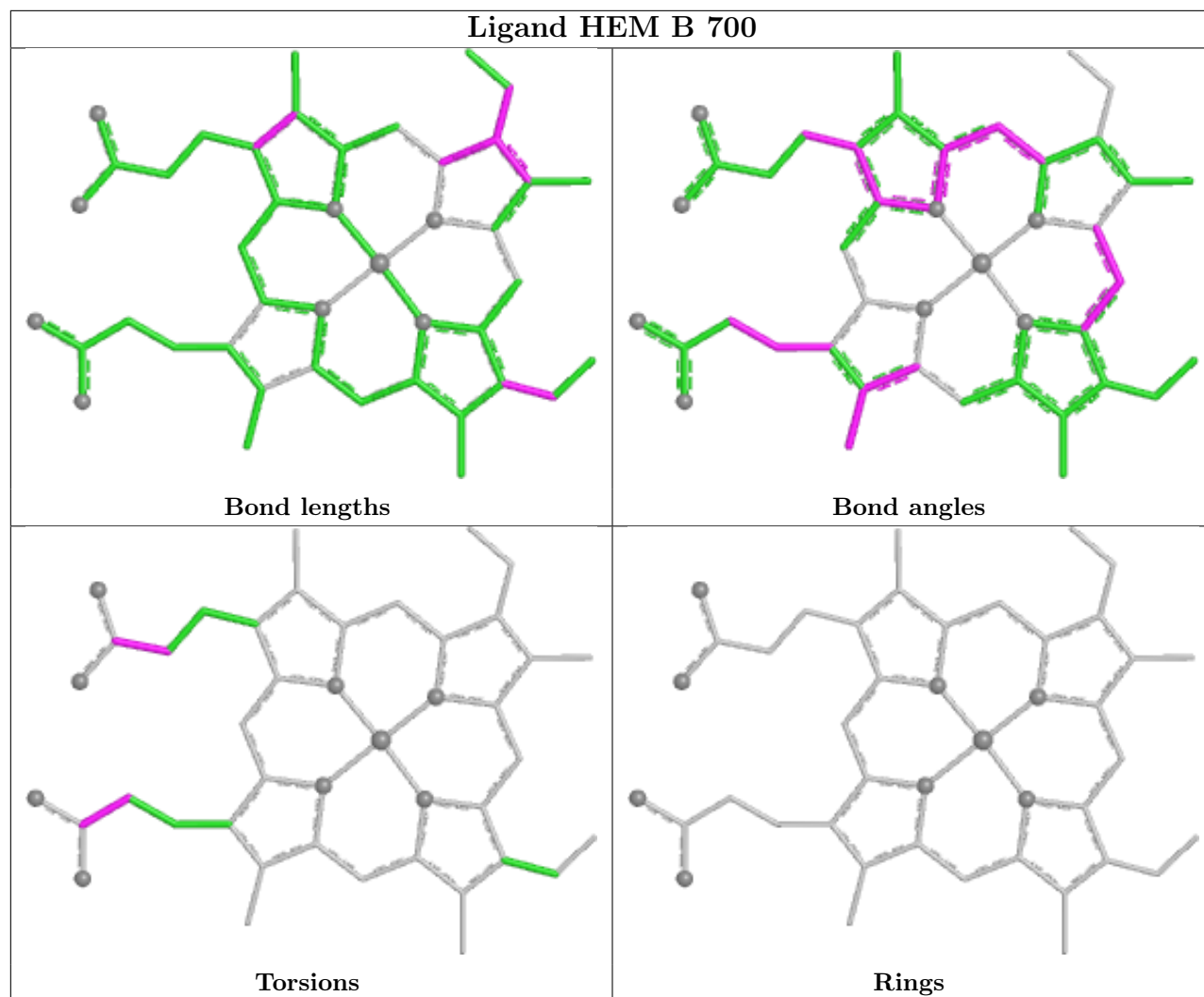
| Mol | Chain | Res     | Type | Clashes | Symm-Clashes |
|-----|-------|---------|------|---------|--------------|
| 4   | C     | 700     | HEM  | 3       | 0            |
| 4   | A     | 700     | HEM  | 2       | 0            |
| 4   | B     | 700     | HEM  | 1       | 0            |
| 2   | E     | 2003    | SO4  | 1       | 0            |
| 4   | L     | 700     | HEM  | 1       | 0            |
| 4   | G     | 700     | HEM  | 2       | 0            |
| 2   | J     | 2018    | SO4  | 1       | 0            |
| 4   | E     | 700     | HEM  | 3       | 0            |
| 4   | D     | 700     | HEM  | 2       | 0            |
| 4   | F     | 700     | HEM  | 2       | 0            |
| 2   | B     | 2017    | SO4  | 1       | 0            |
| 4   | H     | 700     | HEM  | 3       | 0            |
| 4   | K     | 700     | HEM  | 3       | 0            |
| 3   | K     | 800     | CYN  | 1       | 0            |
| 4   | I     | 700     | HEM  | 1       | 0            |
| 4   | J     | 700     | HEM  | 3       | 0            |
| 2   | A     | 2011[A] | SO4  | 1       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

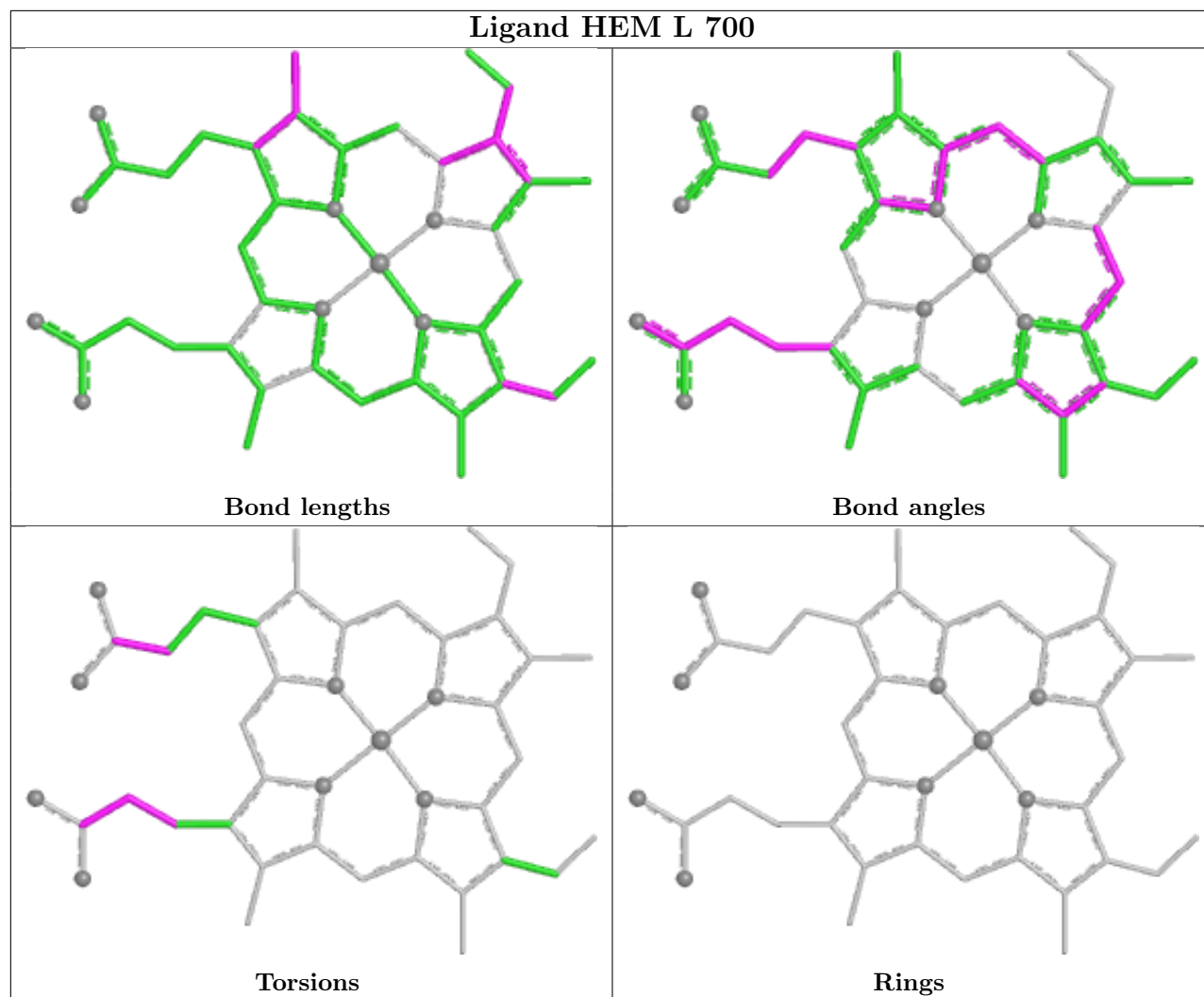
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

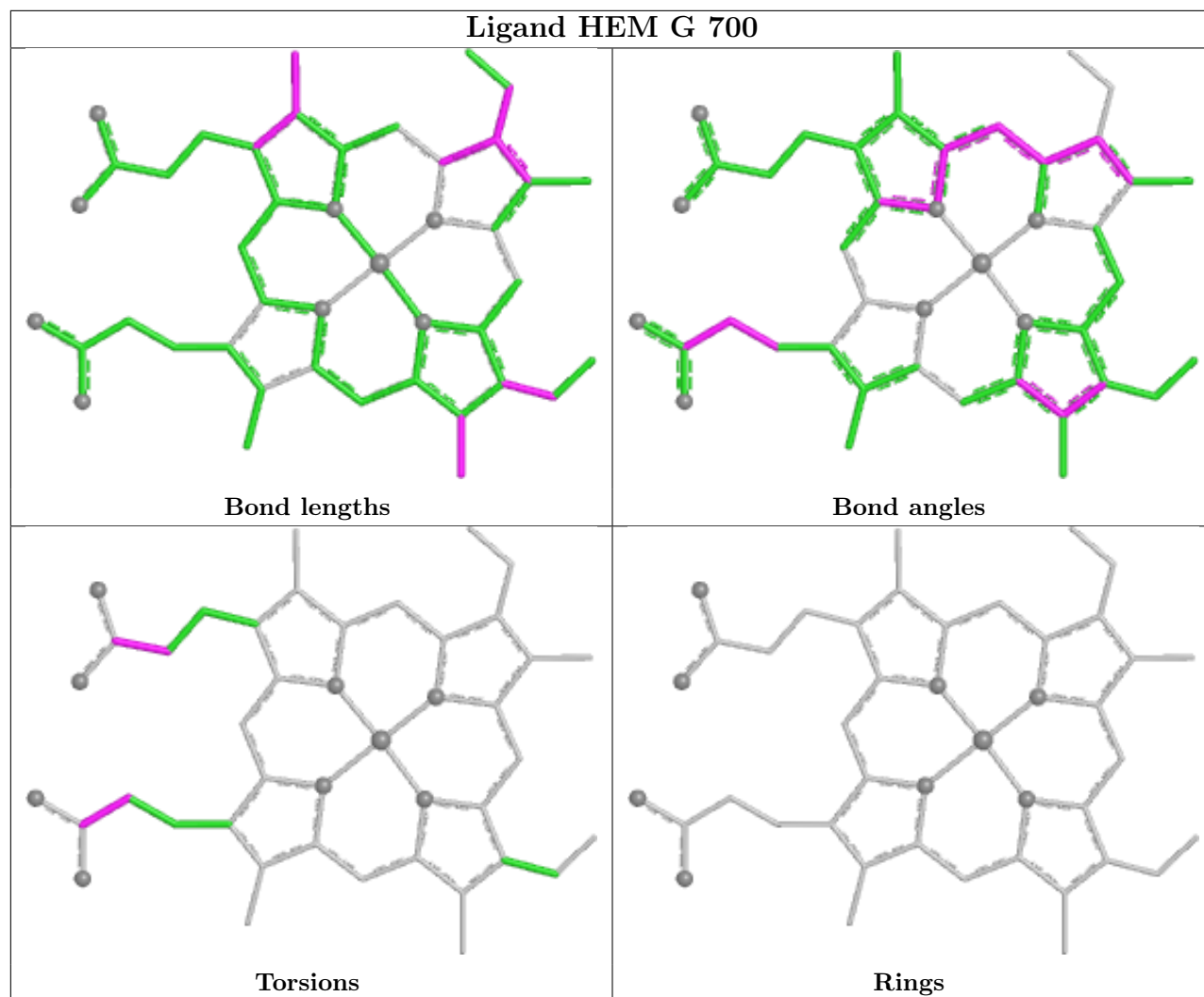


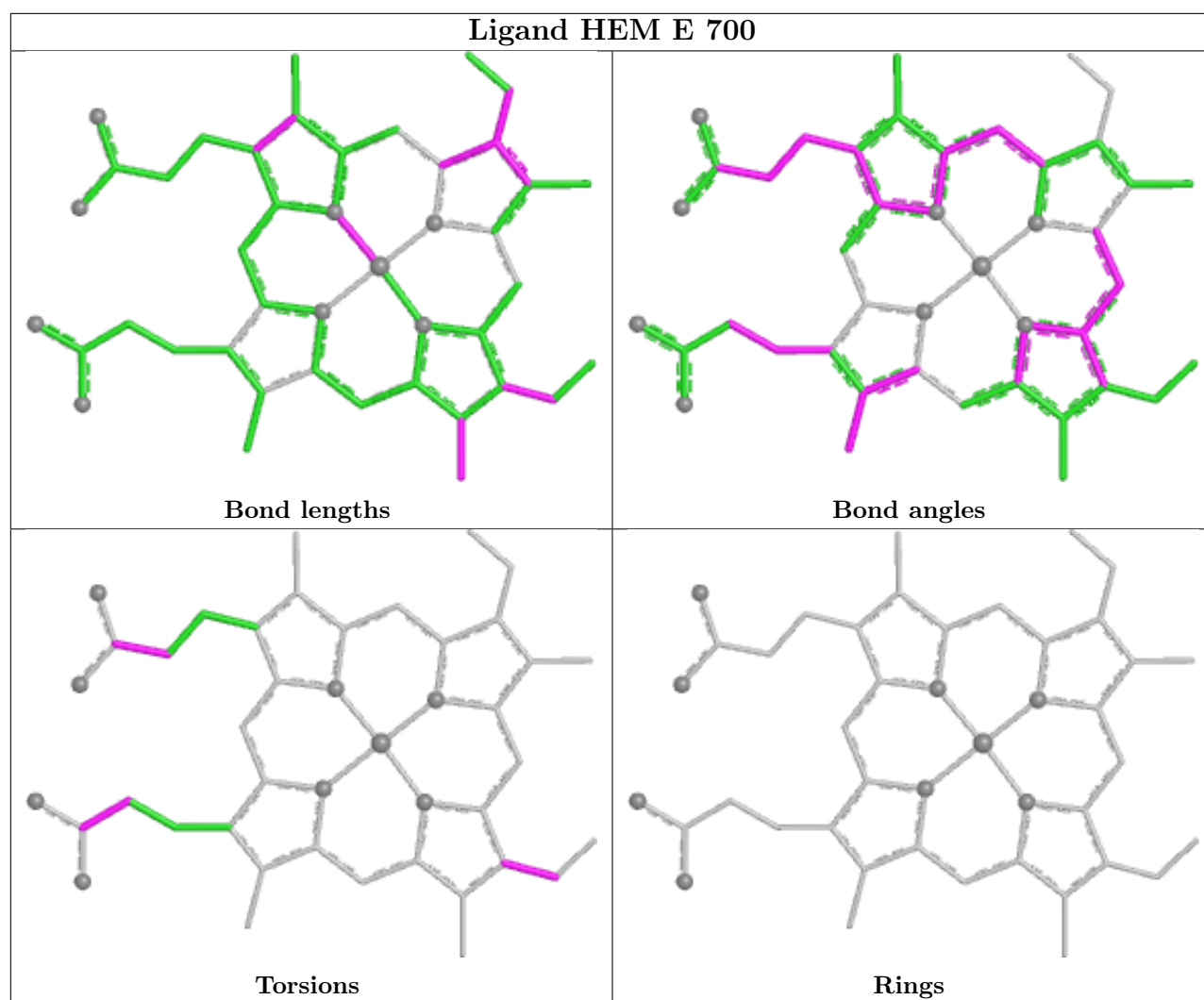


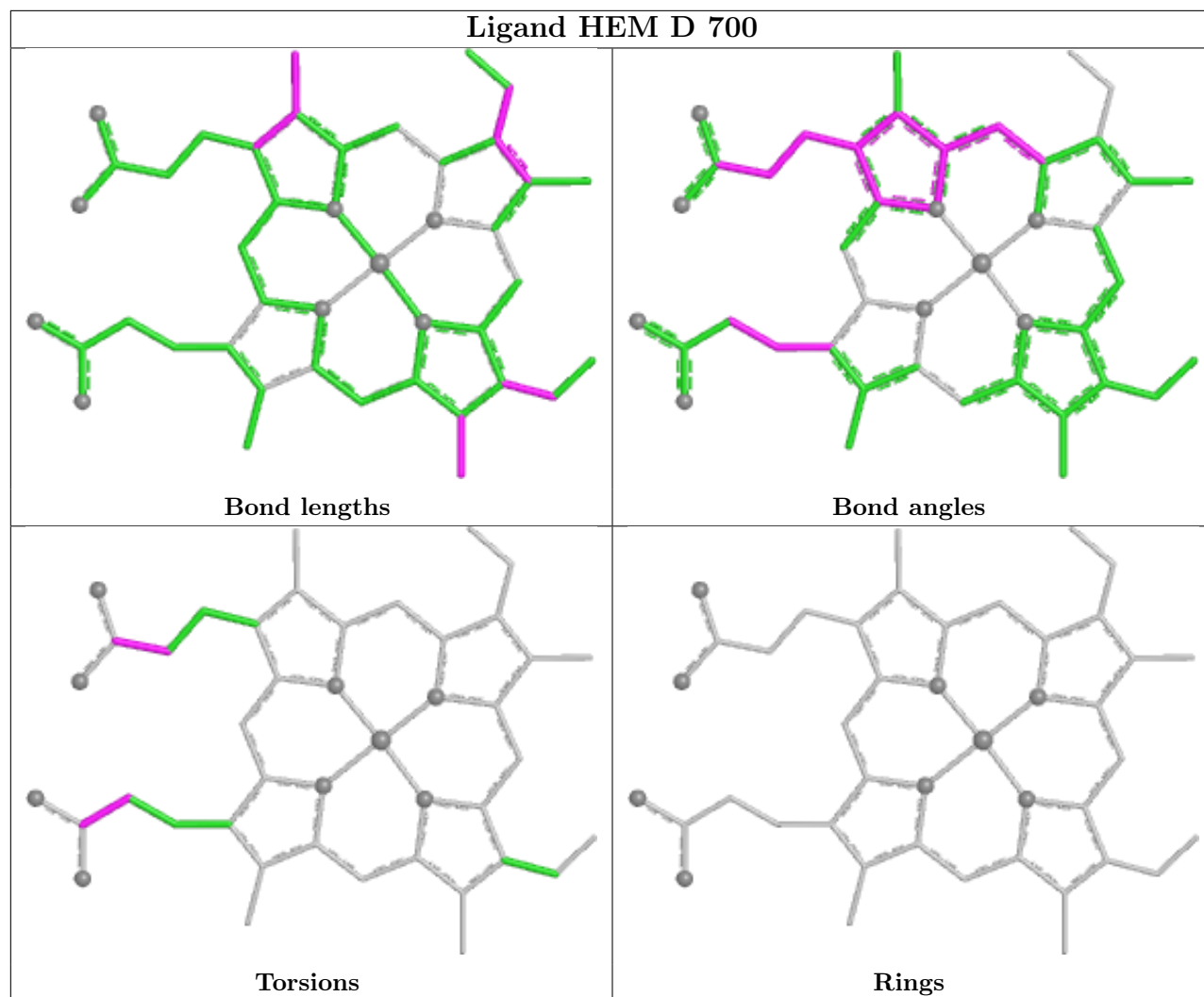


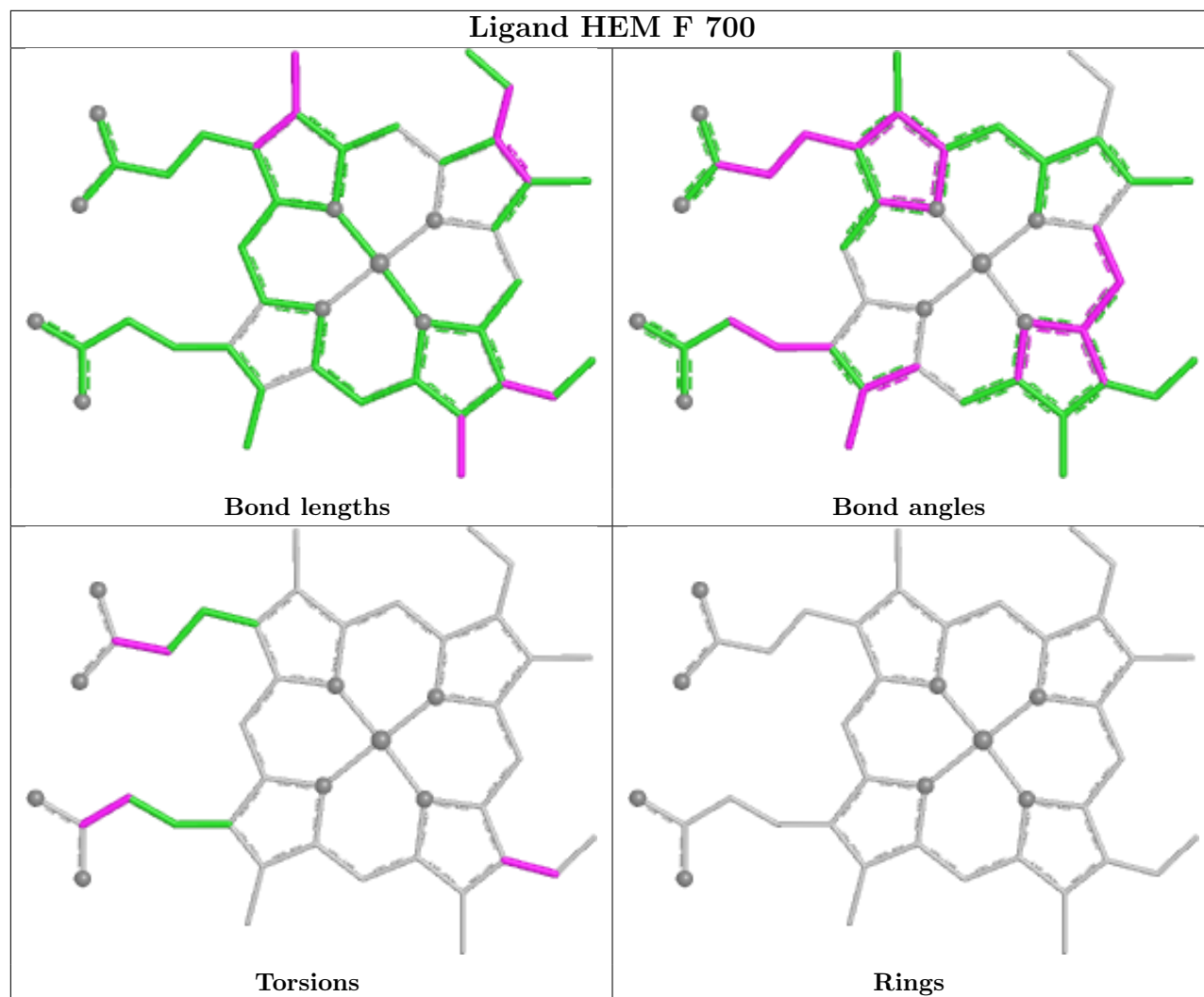


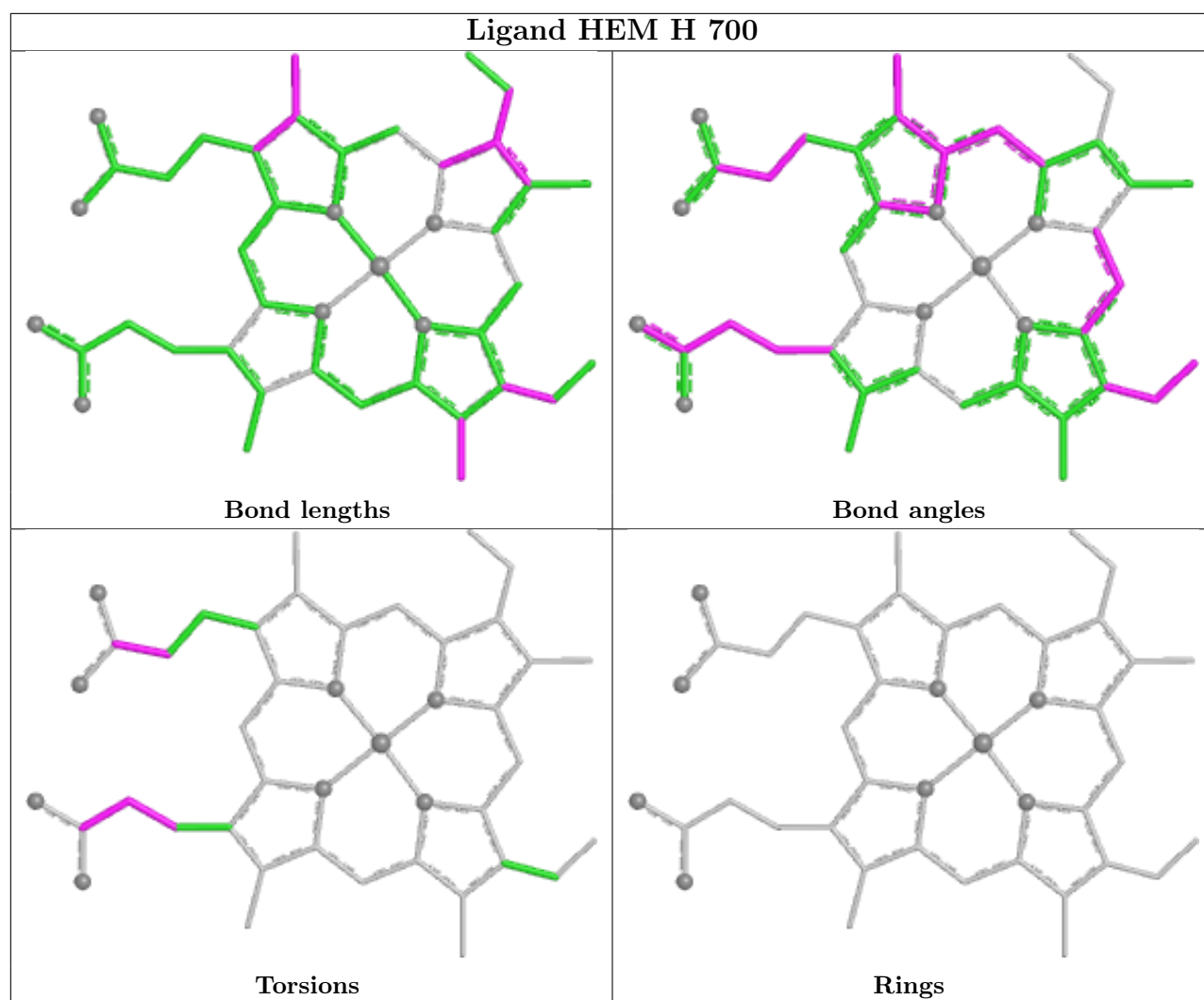


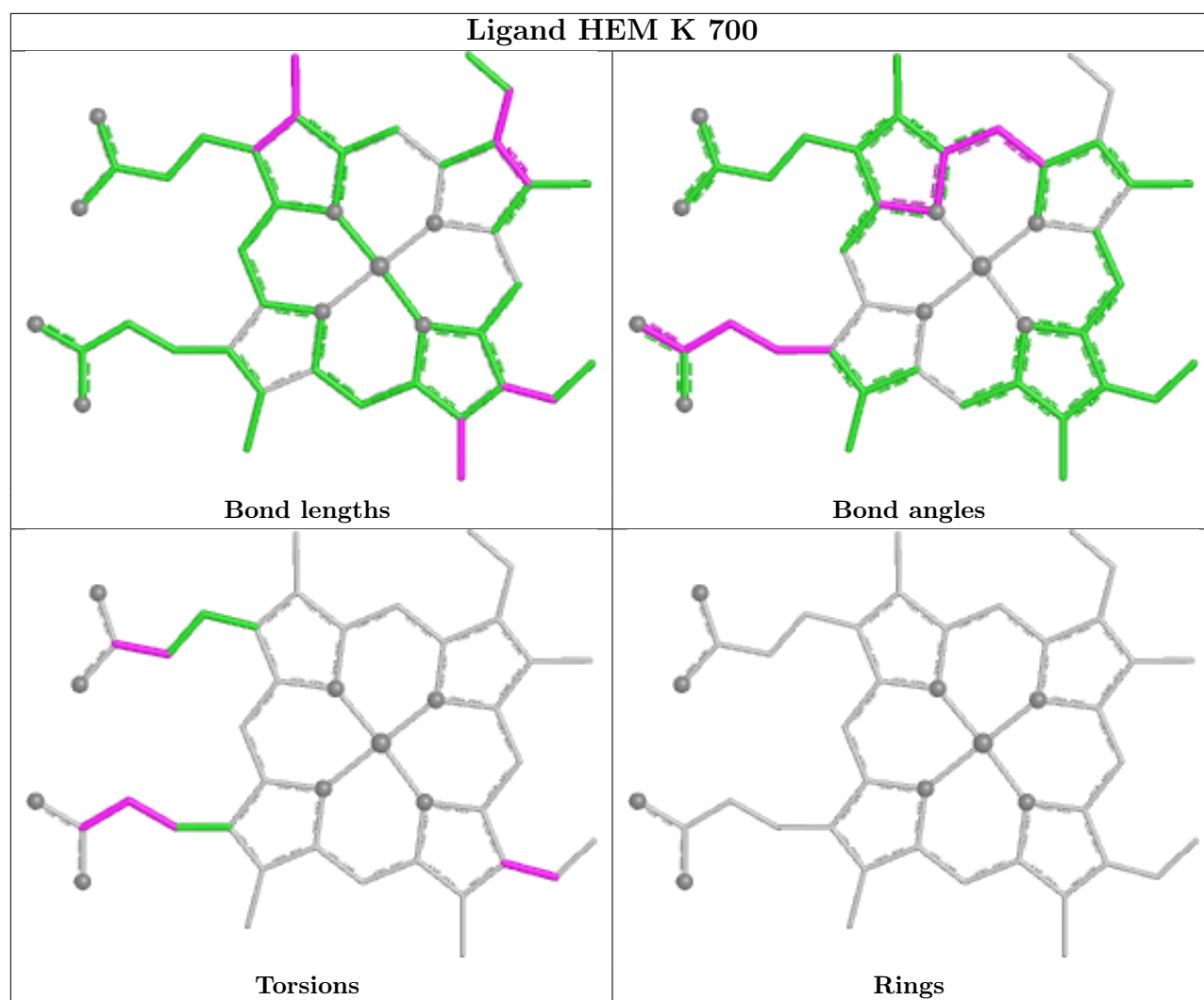




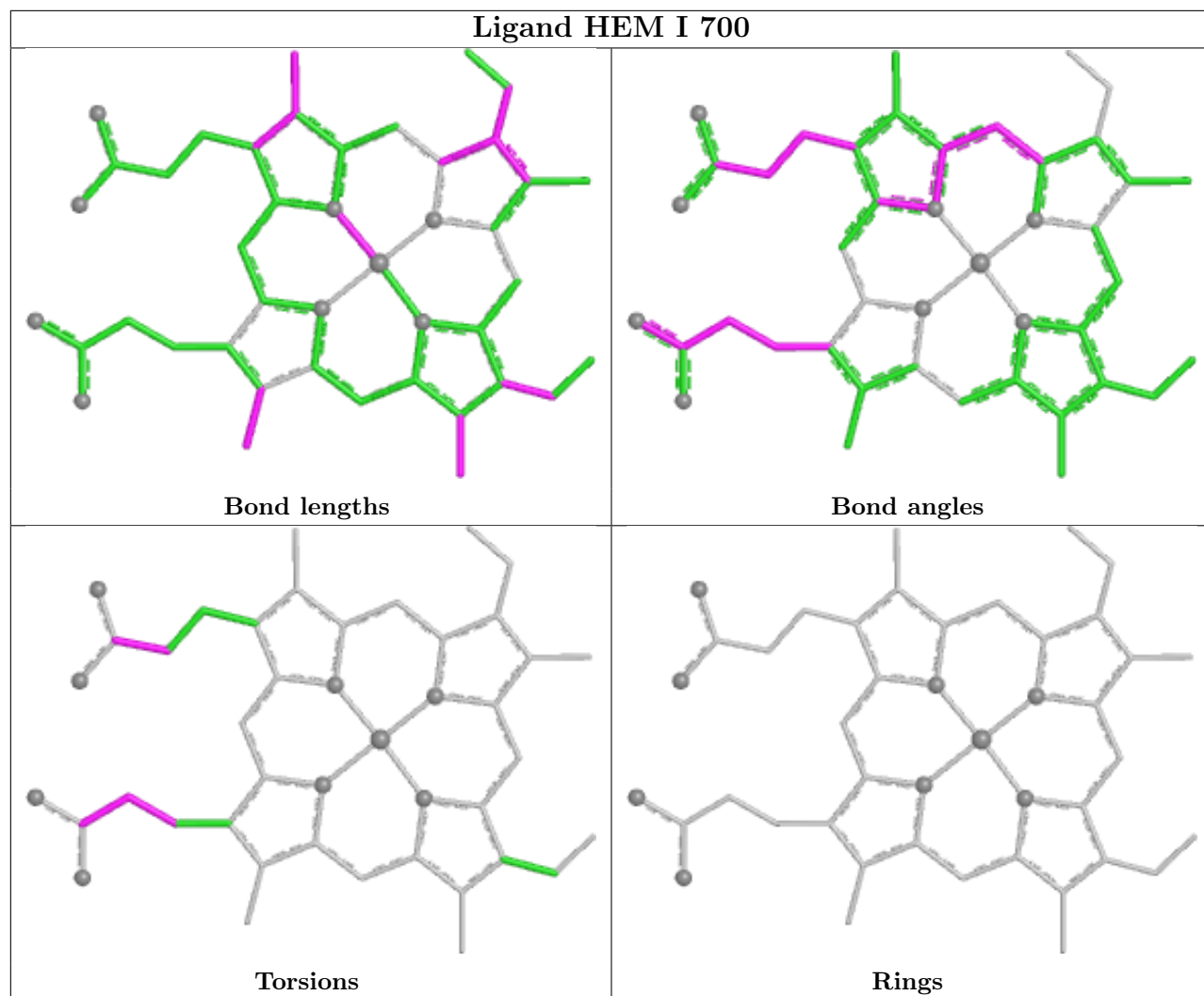




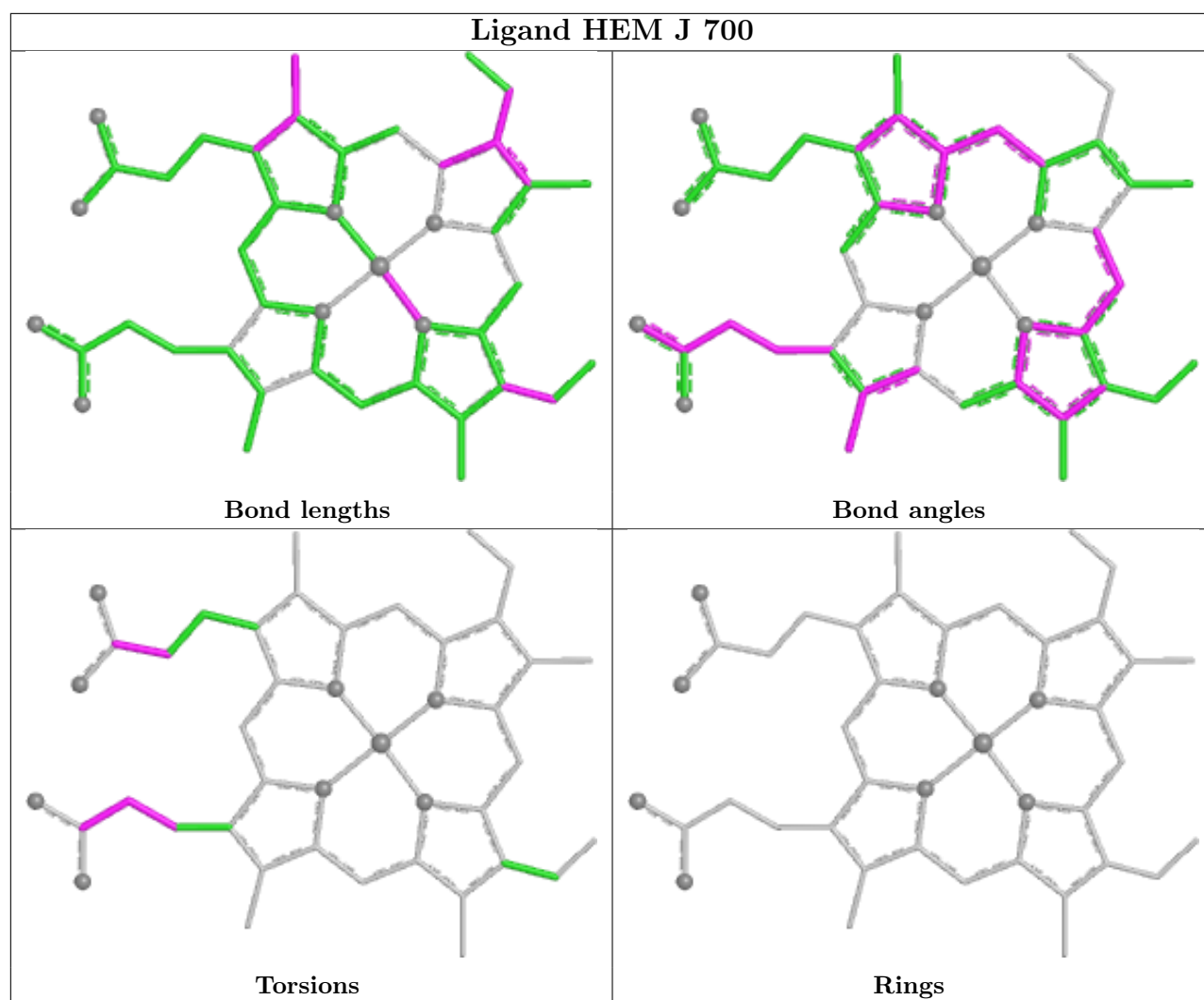




## Ligand HEM I 700







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9    |
|-----|-------|-----------------|--------|---------------|-----------------------|----------|
| 1   | A     | 126/128 (98%)   | -0.46  | 3 (2%) 59 62  | 10, 19, 31, 44        | 9 (7%)   |
| 1   | B     | 127/128 (99%)   | -0.28  | 5 (3%) 44 46  | 8, 21, 32, 59         | 12 (9%)  |
| 1   | C     | 126/128 (98%)   | -0.52  | 4 (3%) 50 53  | 8, 16, 29, 40         | 8 (6%)   |
| 1   | D     | 126/128 (98%)   | -0.36  | 4 (3%) 50 53  | 10, 19, 31, 43        | 12 (9%)  |
| 1   | E     | 126/128 (98%)   | -0.06  | 5 (3%) 43 45  | 10, 25, 37, 46        | 14 (11%) |
| 1   | F     | 126/128 (98%)   | -0.21  | 4 (3%) 50 53  | 11, 20, 33, 40        | 12 (9%)  |
| 1   | G     | 127/128 (99%)   | -0.39  | 1 (0%) 82 84  | 8, 20, 35, 46         | 3 (2%)   |
| 1   | H     | 127/128 (99%)   | -0.17  | 1 (0%) 82 84  | 14, 25, 38, 46        | 5 (3%)   |
| 1   | I     | 127/128 (99%)   | -0.46  | 0 100 100     | 8, 21, 33, 38         | 3 (2%)   |
| 1   | J     | 126/128 (98%)   | 0.04   | 2 (1%) 70 72  | 14, 31, 43, 49        | 10 (7%)  |
| 1   | K     | 127/128 (99%)   | -0.20  | 1 (0%) 82 84  | 9, 26, 38, 49         | 7 (5%)   |
| 1   | L     | 126/128 (98%)   | 0.01   | 3 (2%) 59 62  | 17, 30, 43, 53        | 5 (3%)   |
| All | All   | 1517/1536 (98%) | -0.25  | 33 (2%) 62 64 | 8, 23, 38, 59         | 100 (6%) |

All (33) RSRZ outliers are listed below:

| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | B     | 38[A] | GLU  | 8.3  |
| 1   | B     | 2     | PRO  | 6.0  |
| 1   | F     | 39[A] | ASP  | 5.8  |
| 1   | F     | 38[A] | GLU  | 5.7  |
| 1   | H     | 2     | PRO  | 5.2  |
| 1   | C     | 38[A] | GLU  | 4.9  |
| 1   | A     | 38[A] | GLU  | 4.4  |
| 1   | B     | 39[A] | ASP  | 4.4  |
| 1   | F     | 40[A] | ASP  | 3.9  |
| 1   | D     | 40[A] | ASP  | 3.9  |
| 1   | B     | 40[A] | ASP  | 3.8  |

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| Mol | Chain | Res   | Type | RSRZ |
|-----|-------|-------|------|------|
| 1   | D     | 38[A] | GLU  | 3.8  |
| 1   | E     | 38[A] | GLU  | 3.8  |
| 1   | D     | 39[A] | ASP  | 3.7  |
| 1   | C     | 40[A] | ASP  | 3.4  |
| 1   | E     | 39[A] | ASP  | 3.1  |
| 1   | K     | 105   | ASP  | 3.1  |
| 1   | L     | 105   | ASP  | 3.1  |
| 1   | A     | 39[A] | ASP  | 3.0  |
| 1   | A     | 40[A] | ASP  | 2.8  |
| 1   | B     | 37[A] | PRO  | 2.8  |
| 1   | E     | 40[A] | ASP  | 2.7  |
| 1   | G     | 34    | ARG  | 2.6  |
| 1   | L     | 37    | PRO  | 2.6  |
| 1   | E     | 105   | ASP  | 2.6  |
| 1   | C     | 37[A] | PRO  | 2.4  |
| 1   | J     | 33    | ARG  | 2.3  |
| 1   | F     | 70[A] | ARG  | 2.3  |
| 1   | J     | 3     | LYS  | 2.3  |
| 1   | L     | 3     | LYS  | 2.3  |
| 1   | D     | 70[A] | ARG  | 2.3  |
| 1   | C     | 39[A] | ASP  | 2.2  |
| 1   | E     | 128   | PHE  | 2.1  |

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|----------------------------|-------|
| 2   | SO4  | J     | 2018 | 5/5   | 0.57 | 0.18 | 97,97,98,98                | 0     |

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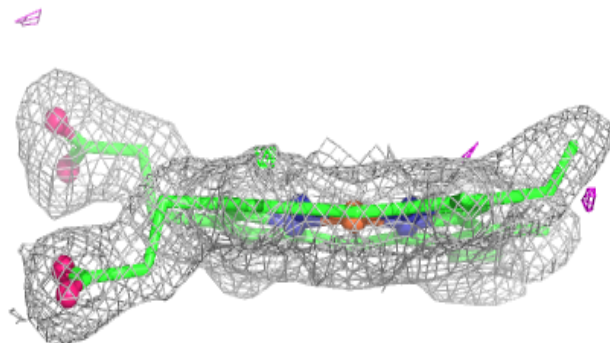
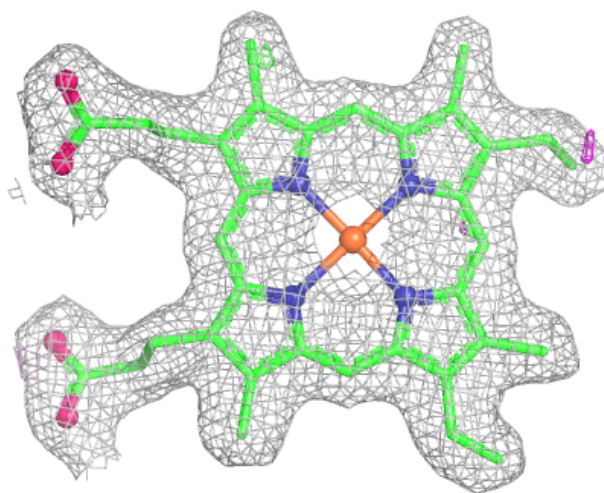
| Mol | Type | Chain | Res     | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|-----------------------------|-------|
| 2   | SO4  | B     | 2017    | 5/5   | 0.67 | 0.17 | 92,93,93,93                 | 0     |
| 2   | SO4  | A     | 2016    | 5/5   | 0.70 | 0.15 | 94,94,95,95                 | 0     |
| 2   | SO4  | E     | 2003    | 5/5   | 0.75 | 0.15 | 79,80,81,82                 | 0     |
| 2   | SO4  | I     | 2015    | 5/5   | 0.76 | 0.14 | 69,70,71,72                 | 0     |
| 2   | SO4  | G     | 2001    | 5/5   | 0.77 | 0.10 | 94,95,95,95                 | 0     |
| 2   | SO4  | G     | 2002    | 5/5   | 0.78 | 0.13 | 84,85,85,85                 | 0     |
| 2   | SO4  | A     | 2004    | 5/5   | 0.78 | 0.15 | 85,85,85,85                 | 0     |
| 2   | SO4  | A     | 2012    | 5/5   | 0.78 | 0.17 | 67,67,69,69                 | 0     |
| 2   | SO4  | L     | 2005    | 5/5   | 0.79 | 0.13 | 78,79,79,80                 | 0     |
| 2   | SO4  | E     | 2006[A] | 5/5   | 0.80 | 0.20 | 47,48,49,49                 | 5     |
| 2   | SO4  | C     | 2013    | 5/5   | 0.80 | 0.10 | 80,80,80,81                 | 0     |
| 2   | SO4  | A     | 2011[A] | 5/5   | 0.80 | 0.21 | 42,43,44,44                 | 5     |
| 2   | SO4  | A     | 2014    | 5/5   | 0.87 | 0.09 | 66,66,66,67                 | 0     |
| 2   | SO4  | D     | 2010[A] | 5/5   | 0.90 | 0.11 | 26,26,28,28                 | 5     |
| 2   | SO4  | J     | 2008[A] | 5/5   | 0.91 | 0.15 | 29,29,30,30                 | 5     |
| 2   | SO4  | B     | 2007[A] | 5/5   | 0.92 | 0.10 | 20,20,22,22                 | 5     |
| 2   | SO4  | C     | 2009[A] | 5/5   | 0.96 | 0.08 | 10,13,15,17                 | 5     |
| 3   | CYN  | K     | 800     | 2/2   | 0.97 | 0.06 | 17,17,17,24                 | 0     |
| 3   | CYN  | L     | 800     | 2/2   | 0.97 | 0.05 | 21,21,21,22                 | 0     |
| 3   | CYN  | H     | 800     | 2/2   | 0.98 | 0.06 | 14,14,14,16                 | 0     |
| 3   | CYN  | B     | 800     | 2/2   | 0.98 | 0.07 | 16,16,16,19                 | 0     |
| 3   | CYN  | E     | 800     | 2/2   | 0.98 | 0.06 | 19,19,19,22                 | 0     |
| 4   | HEM  | E     | 700     | 43/43 | 0.98 | 0.06 | 14,19,26,28                 | 0     |
| 4   | HEM  | I     | 700     | 43/43 | 0.98 | 0.06 | 10,14,22,29                 | 0     |
| 4   | HEM  | J     | 700     | 43/43 | 0.98 | 0.07 | 16,20,30,36                 | 0     |
| 4   | HEM  | K     | 700     | 43/43 | 0.98 | 0.06 | 13,17,27,34                 | 0     |
| 4   | HEM  | L     | 700     | 43/43 | 0.98 | 0.06 | 14,19,26,30                 | 0     |
| 3   | CYN  | D     | 800     | 2/2   | 0.99 | 0.04 | 14,14,14,14                 | 0     |
| 3   | CYN  | A     | 800     | 2/2   | 0.99 | 0.05 | 11,11,11,14                 | 0     |
| 4   | HEM  | A     | 700     | 43/43 | 0.99 | 0.05 | 10,14,21,22                 | 0     |
| 4   | HEM  | B     | 700     | 43/43 | 0.99 | 0.04 | 11,16,20,24                 | 0     |
| 4   | HEM  | C     | 700     | 43/43 | 0.99 | 0.04 | 7,11,18,20                  | 0     |
| 4   | HEM  | D     | 700     | 43/43 | 0.99 | 0.05 | 11,15,22,24                 | 0     |
| 3   | CYN  | F     | 800     | 2/2   | 0.99 | 0.07 | 17,17,17,21                 | 0     |
| 4   | HEM  | F     | 700     | 43/43 | 0.99 | 0.05 | 13,15,23,26                 | 0     |
| 4   | HEM  | G     | 700     | 43/43 | 0.99 | 0.06 | 11,16,29,38                 | 0     |
| 4   | HEM  | H     | 700     | 43/43 | 0.99 | 0.05 | 13,17,22,29                 | 0     |
| 3   | CYN  | G     | 800     | 2/2   | 0.99 | 0.04 | 20,20,20,23                 | 0     |
| 3   | CYN  | C     | 800     | 2/2   | 0.99 | 0.05 | 8,8,8,10                    | 0     |
| 3   | CYN  | I     | 800     | 2/2   | 0.99 | 0.05 | 16,16,16,22                 | 0     |
| 3   | CYN  | J     | 800     | 2/2   | 0.99 | 0.03 | 16,16,16,20                 | 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.

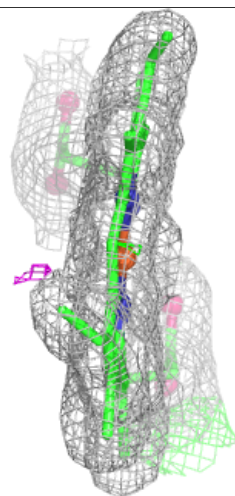
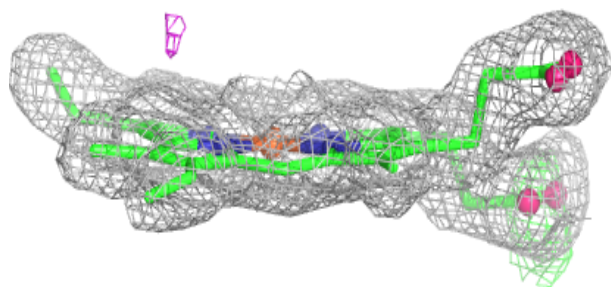
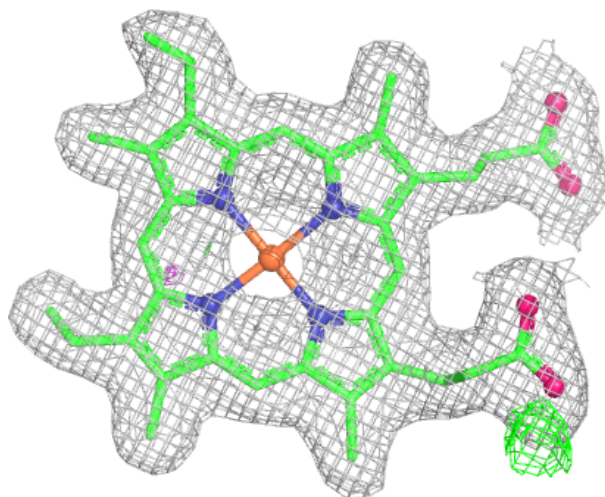
**Electron density around HEM E 700:**

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



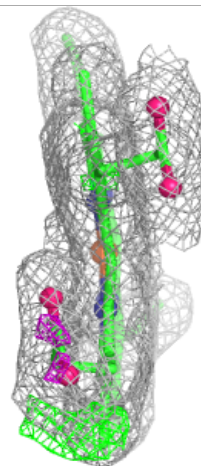
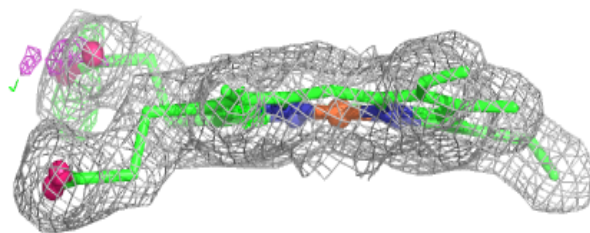
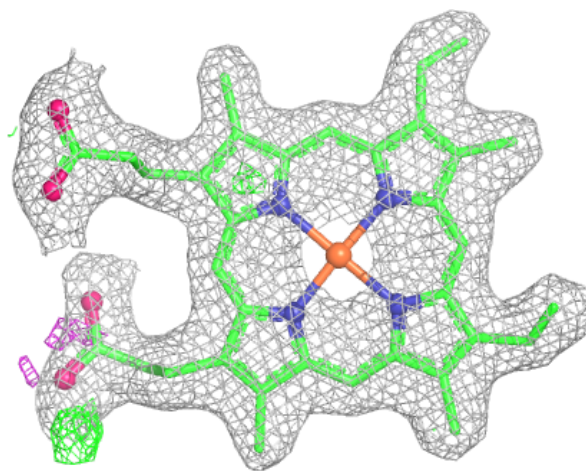
**Electron density around HEM I 700:**

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



**Electron density around HEM J 700:**

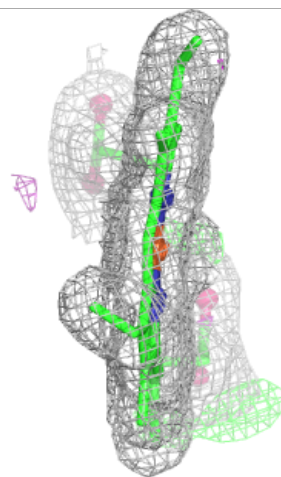
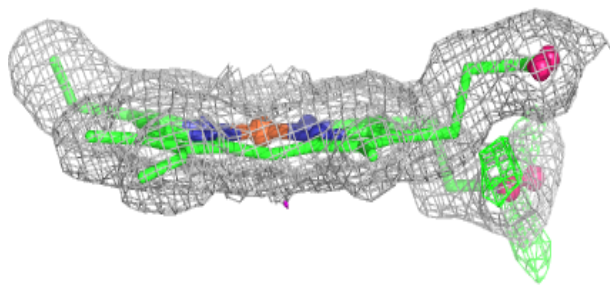
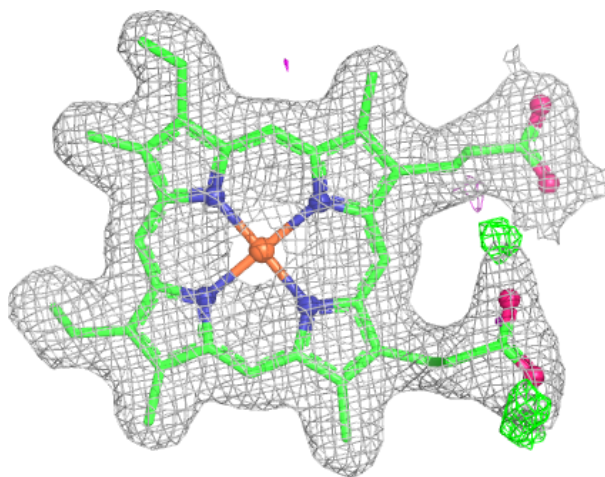
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM K 700:**

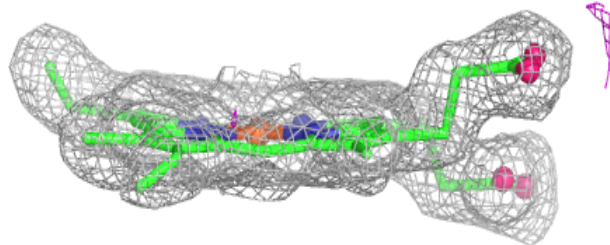
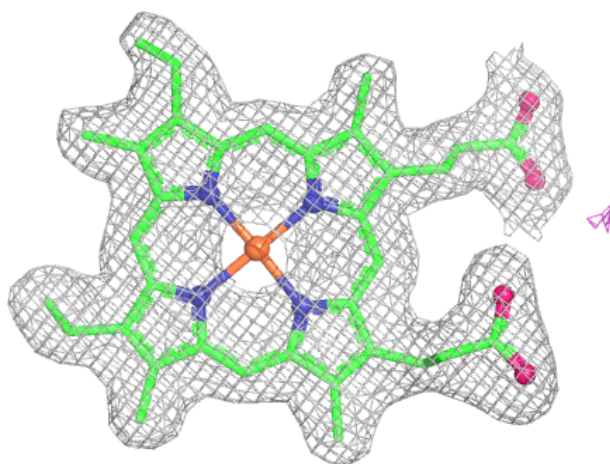
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





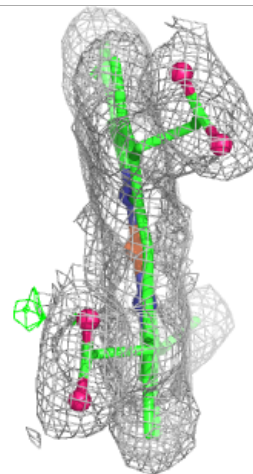
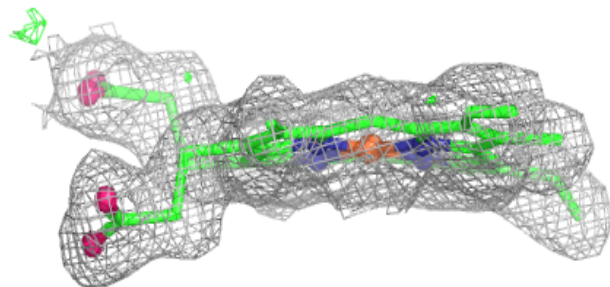
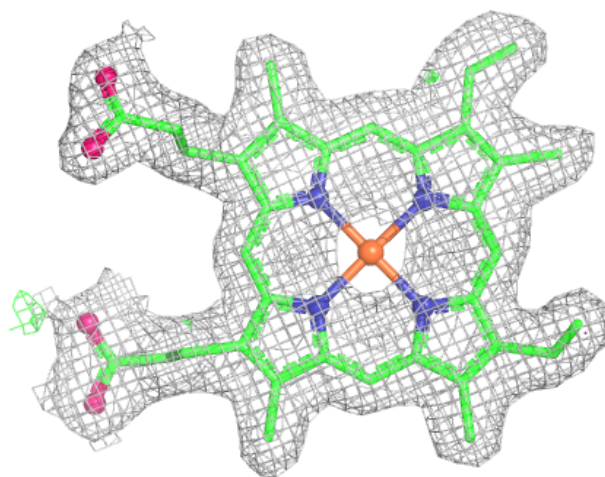
**Electron density around HEM L 700:**

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



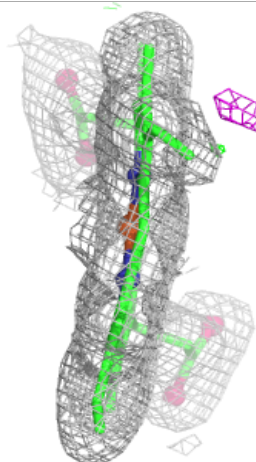
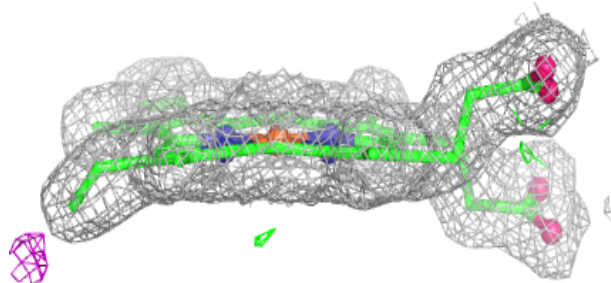
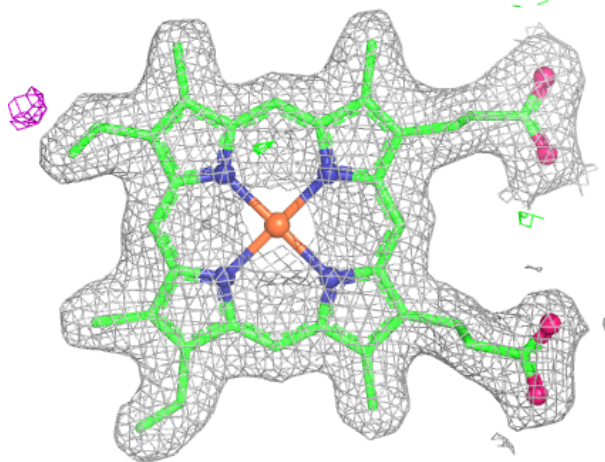
**Electron density around HEM A 700:**

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



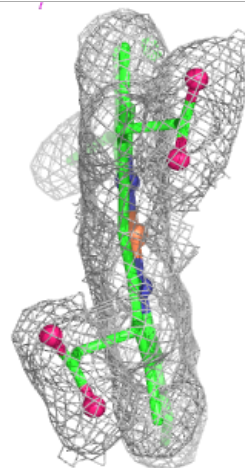
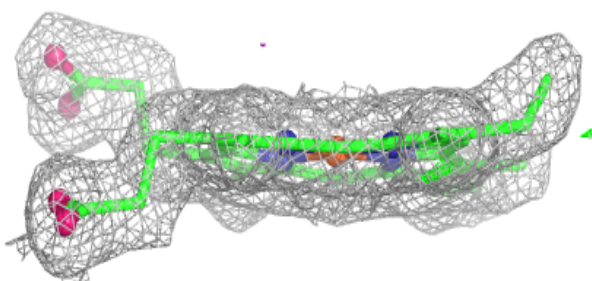
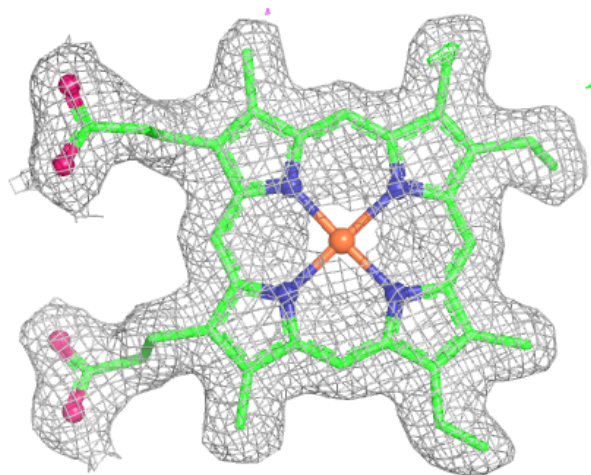
**Electron density around HEM B 700:**

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



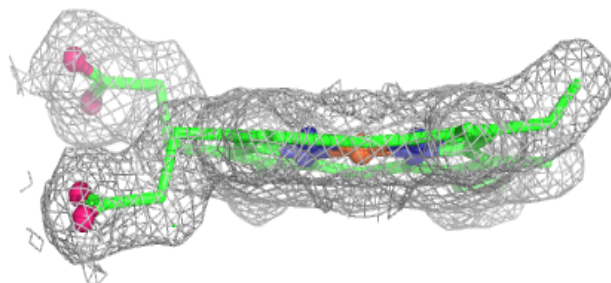
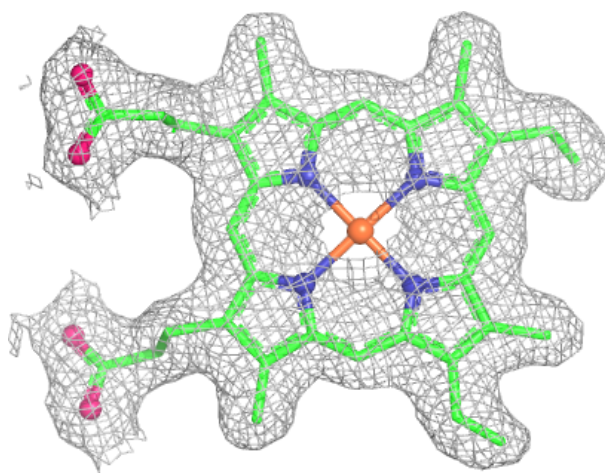
**Electron density around HEM C 700:**

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



**Electron density around HEM D 700:**

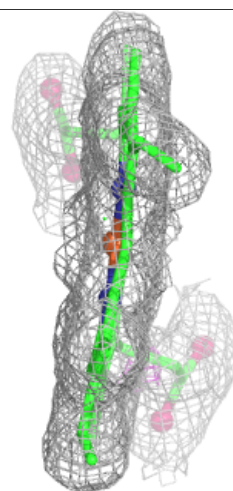
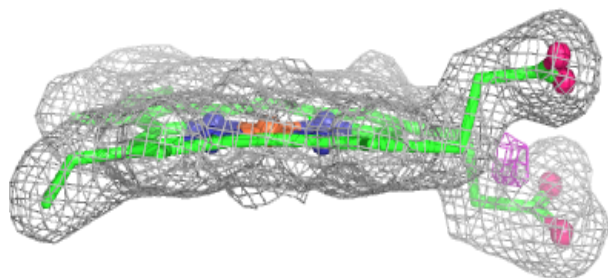
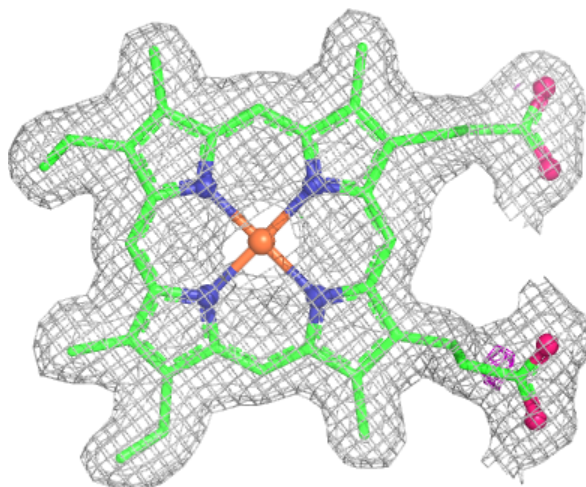
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





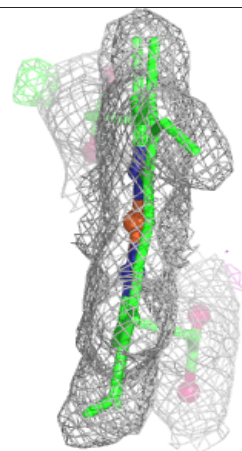
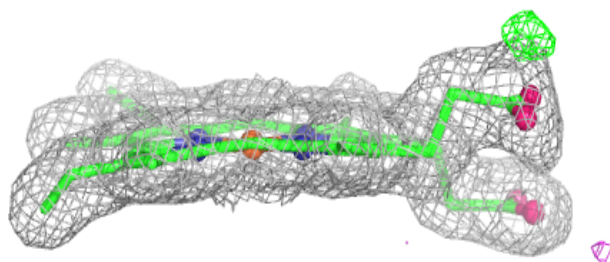
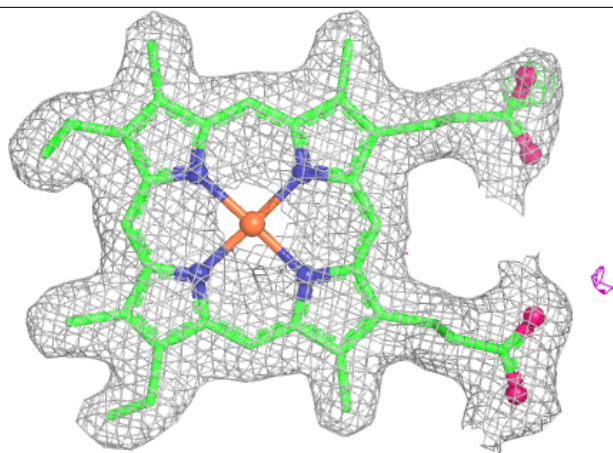
**Electron density around HEM F 700:**

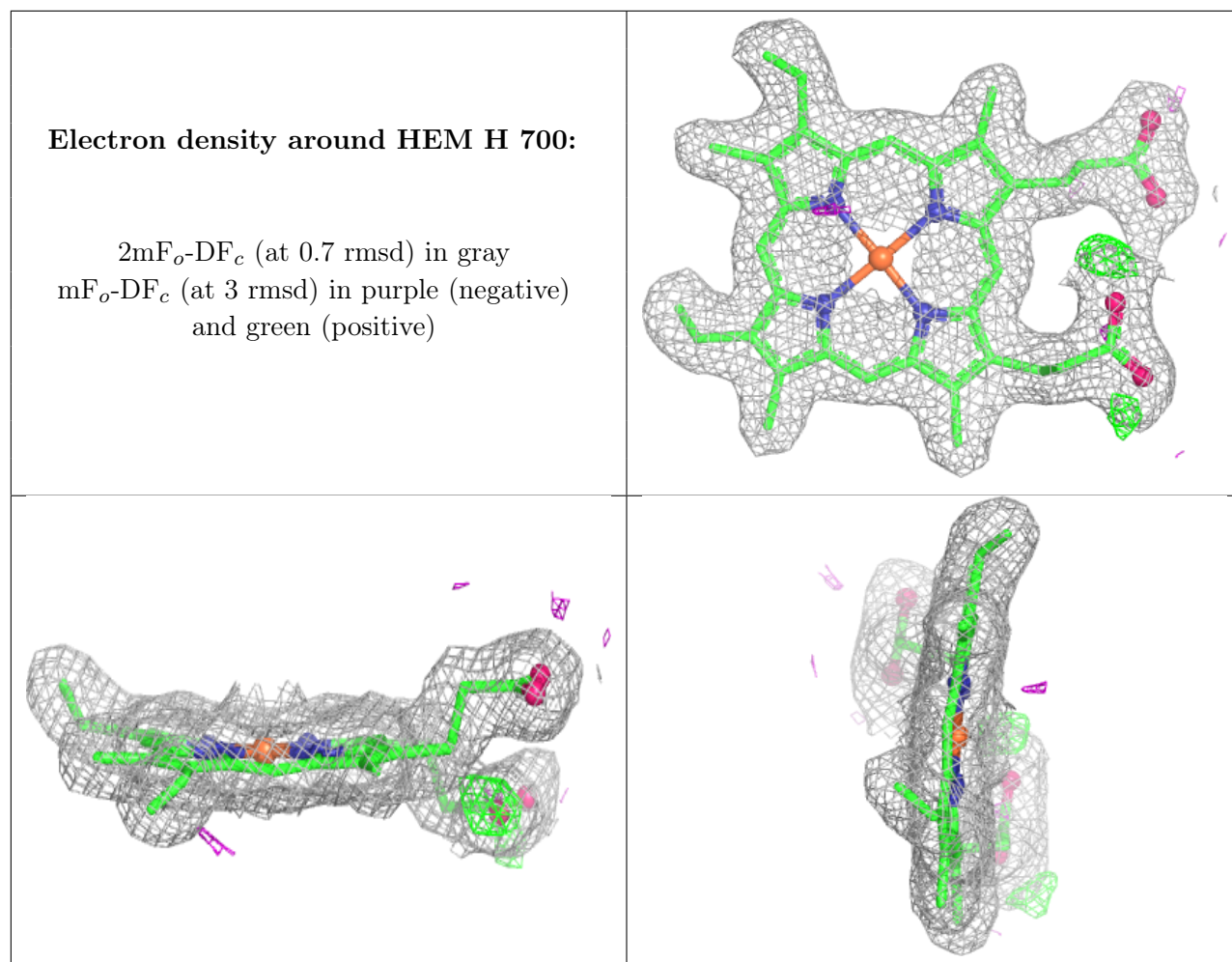
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM G 700:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.