



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:35 PM EDT

PDB ID : 4ENS / pdb\_00004ens  
Title : Structure of E530Q variant of E. coli KatE  
Authors : Loewen, P.C.; Jha, V.  
Deposited on : 2012-04-13  
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.015 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.50                                                             |

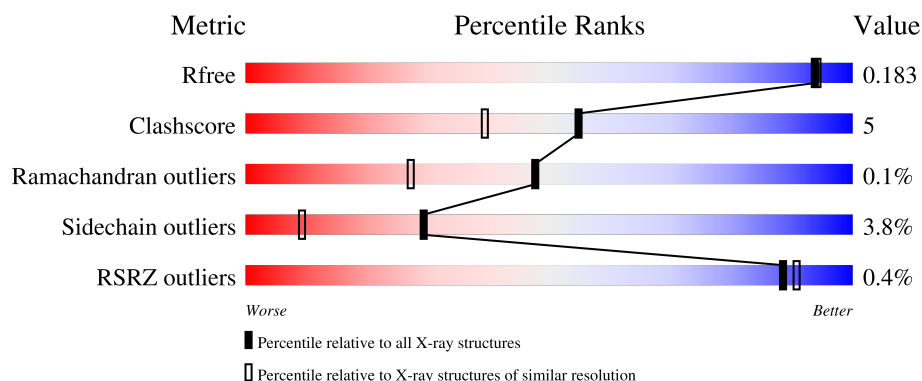
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 4673 (1.60-1.60)                                      |
| Clashscore            | 190562                      | 4931 (1.60-1.60)                                      |
| Ramachandran outliers | 187476                      | 4831 (1.60-1.60)                                      |
| Sidechain outliers    | 187428                      | 4830 (1.60-1.60)                                      |
| RSRZ outliers         | 180081                      | 4672 (1.60-1.60)                                      |

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

| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | A     | 753    |  |
| 1   | B     | 753    |  |
| 1   | C     | 753    |  |
| 1   | D     | 753    |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res    | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|--------|-----------|----------|---------|------------------|
| 2   | HDD  | A     | 801[A] | X         | -        | -       | -                |
| 2   | HDD  | B     | 801[A] | X         | -        | -       | -                |
| 2   | HDD  | C     | 801[A] | X         | -        | -       | -                |
| 2   | HDD  | D     | 801[A] | X         | -        | -       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26323 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.

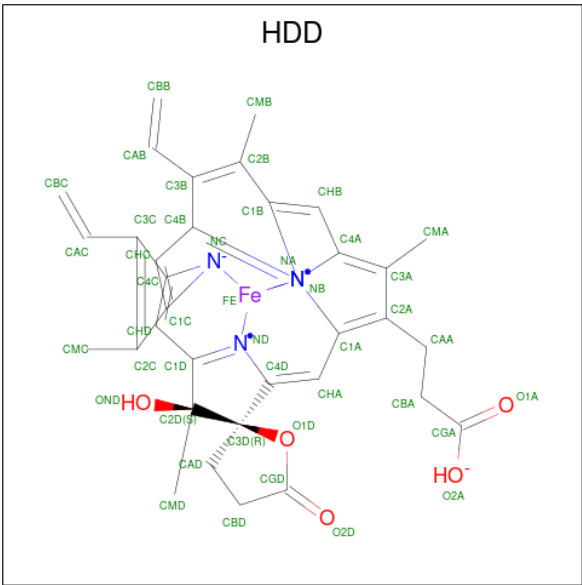
- Molecule 1 is a protein called Catalase HP11.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 726      | Total | C    | N    | O    | S  | 0       | 4       | 0     |
|     |       |          | 5755  | 3655 | 1007 | 1081 | 12 |         |         |       |
| 1   | B     | 726      | Total | C    | N    | O    | S  | 0       | 4       | 0     |
|     |       |          | 5758  | 3658 | 1008 | 1080 | 12 |         |         |       |
| 1   | C     | 726      | Total | C    | N    | O    | S  | 0       | 3       | 0     |
|     |       |          | 5756  | 3658 | 1008 | 1078 | 12 |         |         |       |
| 1   | D     | 726      | Total | C    | N    | O    | S  | 0       | 4       | 0     |
|     |       |          | 5758  | 3657 | 1008 | 1081 | 12 |         |         |       |

There are 4 discrepancies between the modelled and reference sequences:

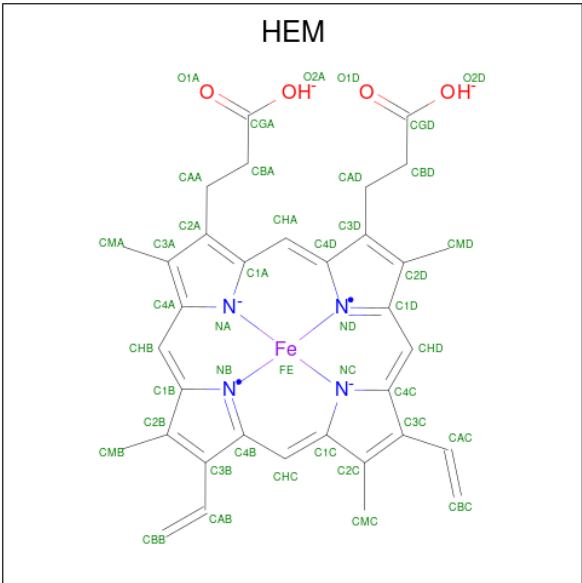
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 530     | GLN      | GLU    | engineered mutation | UNP P21179 |
| B     | 530     | GLN      | GLU    | engineered mutation | UNP P21179 |
| C     | 530     | GLN      | GLU    | engineered mutation | UNP P21179 |
| D     | 530     | GLN      | GLU    | engineered mutation | UNP P21179 |

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2   | A     | 1        | Total<br>44 | C<br>34 | Fe<br>1 | N<br>4 | O<br>5 | 0       | 1       |
| 2   | B     | 1        | Total<br>44 | C<br>34 | Fe<br>1 | N<br>4 | O<br>5 | 0       | 1       |
| 2   | C     | 1        | Total<br>44 | C<br>34 | Fe<br>1 | N<br>4 | O<br>5 | 0       | 1       |
| 2   | D     | 1        | Total<br>44 | C<br>34 | Fe<br>1 | N<br>4 | O<br>5 | 0       | 1       |

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms       |         |         |        |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 3   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 1       |
| 3   | B     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 1       |
| 3   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 1       |
| 3   | D     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       | 1       |

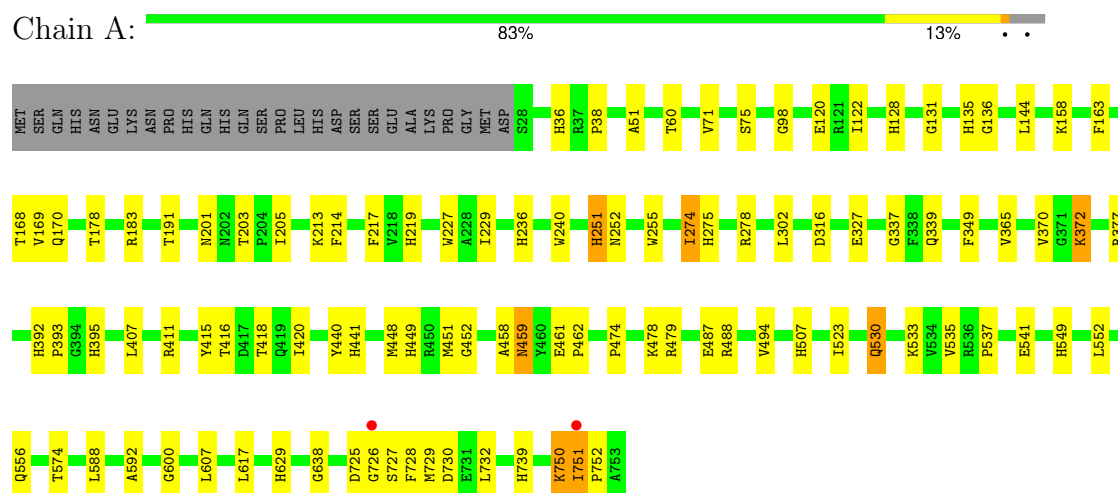
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4   | A     | 769      | Total<br>769 | O<br>769 | 0       | 0       |
| 4   | B     | 696      | Total<br>696 | O<br>696 | 0       | 0       |
| 4   | C     | 709      | Total<br>709 | O<br>709 | 0       | 0       |
| 4   | D     | 774      | Total<br>774 | O<br>774 | 0       | 0       |

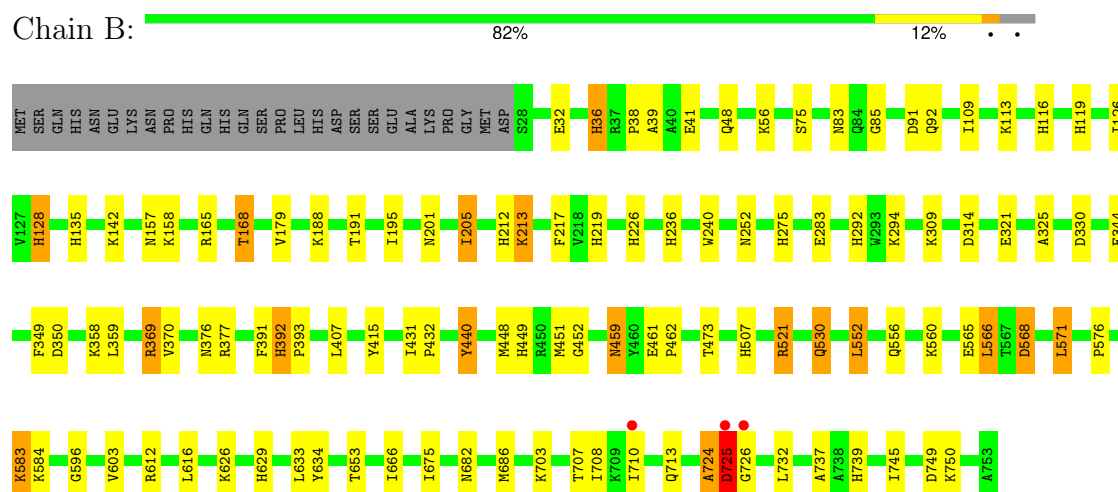
### 3 Residue-property plots

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.

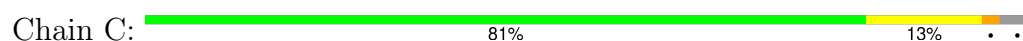
#### • Molecule 1: Catalase HP11

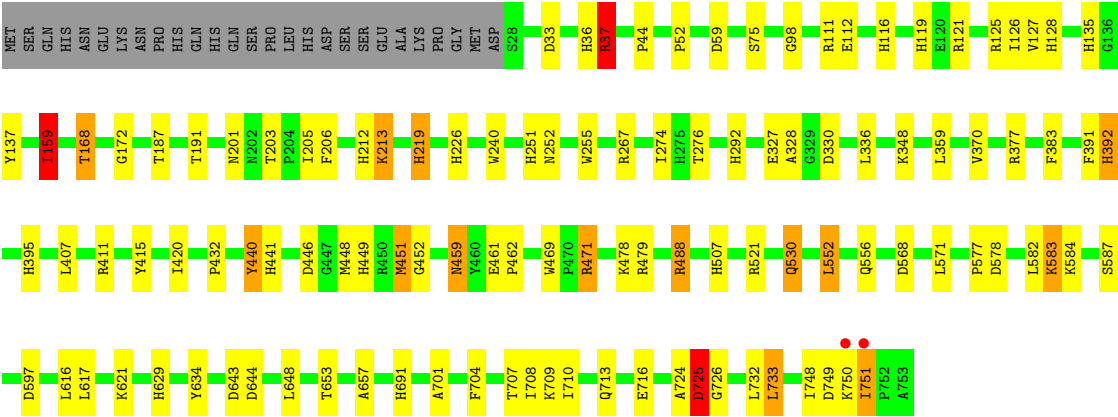


#### • Molecule 1: Catalase HP11

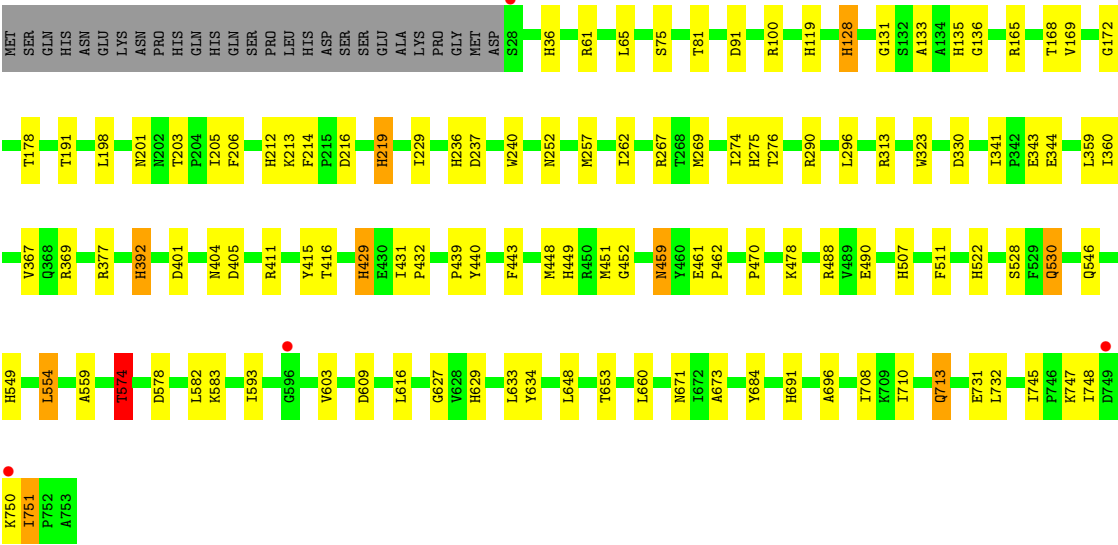
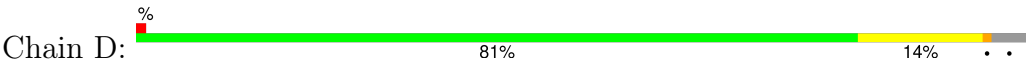


#### • Molecule 1: Catalase HP11





● Molecule 1: Catalase HP11



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 93.45Å 133.40Å 123.24Å<br>90.00° 109.18° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 32.19 – 1.60<br>32.19 – 1.60                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 91.8 (32.19-1.60)<br>91.8 (32.19-1.60)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.10                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.25 (at 1.60Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC                                                      | Depositor        |
| R, $R_{free}$                                                           | 0.151 , 0.184<br>0.149 , 0.183                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 17269 reflections (5.03%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 13.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.040                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 39.2                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                        | EDS              |
| Total number of atoms                                                   | 26323                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 16.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, HDD

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     | 1.64         | 49/5924 (0.8%)   | 1.36        | 12/8054 (0.1%)  |
| 1   | B     | 1.60         | 39/5927 (0.7%)   | 1.33        | 20/8058 (0.2%)  |
| 1   | C     | 1.57         | 41/5922 (0.7%)   | 1.34        | 23/8050 (0.3%)  |
| 1   | D     | 1.64         | 47/5927 (0.8%)   | 1.35        | 12/8058 (0.1%)  |
| All | All   | 1.61         | 176/23700 (0.7%) | 1.35        | 67/32220 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 2                   |
| All | All   | 0                   | 3                   |

All (176) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 1   | B     | 212 | HIS  | ND1-CE1 | 9.60 | 1.42        | 1.32     |
| 1   | D     | 392 | HIS  | ND1-CE1 | 9.52 | 1.42        | 1.32     |
| 1   | C     | 219 | HIS  | ND1-CE1 | 9.48 | 1.42        | 1.32     |
| 1   | A     | 275 | HIS  | ND1-CE1 | 8.38 | 1.41        | 1.32     |
| 1   | C     | 116 | HIS  | ND1-CE1 | 8.35 | 1.41        | 1.32     |
| 1   | D     | 452 | GLY  | C-O     | 8.26 | 1.32        | 1.24     |
| 1   | A     | 452 | GLY  | C-O     | 8.06 | 1.31        | 1.24     |
| 1   | A     | 629 | HIS  | ND1-CE1 | 7.51 | 1.40        | 1.32     |
| 1   | D     | 262 | ILE  | CA-C    | 7.27 | 1.60        | 1.52     |
| 1   | B     | 85  | GLY  | N-CA    | 7.24 | 1.56        | 1.45     |
| 1   | A     | 420 | ILE  | CA-CB   | 7.20 | 1.63        | 1.54     |
| 1   | D     | 216 | ASP  | N-CA    | 7.18 | 1.54        | 1.46     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 392 | HIS  | ND1-CE1 | 7.13  | 1.39        | 1.32     |
| 1   | A     | 178 | THR  | N-CA    | 6.94  | 1.53        | 1.46     |
| 1   | B     | 675 | ILE  | N-CA    | 6.86  | 1.52        | 1.46     |
| 1   | B     | 128 | HIS  | ND1-CE1 | 6.83  | 1.39        | 1.32     |
| 1   | A     | 251 | HIS  | ND1-CE1 | 6.80  | 1.39        | 1.32     |
| 1   | D     | 214 | PHE  | C-O     | -6.74 | 1.18        | 1.24     |
| 1   | D     | 511 | PHE  | C-O     | 6.64  | 1.31        | 1.24     |
| 1   | D     | 219 | HIS  | CG-CD2  | 6.62  | 1.43        | 1.35     |
| 1   | B     | 109 | ILE  | C-O     | 6.62  | 1.31        | 1.24     |
| 1   | B     | 116 | HIS  | ND1-CE1 | 6.59  | 1.39        | 1.32     |
| 1   | C     | 370 | VAL  | CA-CB   | 6.58  | 1.63        | 1.54     |
| 1   | C     | 159 | ILE  | CB-CG1  | -6.54 | 1.40        | 1.53     |
| 1   | D     | 178 | THR  | N-CA    | 6.52  | 1.54        | 1.46     |
| 1   | D     | 275 | HIS  | ND1-CE1 | 6.52  | 1.39        | 1.32     |
| 1   | B     | 219 | HIS  | ND1-CE1 | 6.45  | 1.39        | 1.32     |
| 1   | C     | 441 | HIS  | ND1-CE1 | 6.39  | 1.39        | 1.32     |
| 1   | C     | 212 | HIS  | ND1-CE1 | 6.39  | 1.39        | 1.32     |
| 1   | A     | 739 | HIS  | ND1-CE1 | 6.37  | 1.39        | 1.32     |
| 1   | A     | 122 | ILE  | CA-CB   | 6.31  | 1.62        | 1.54     |
| 1   | B     | 226 | HIS  | ND1-CE1 | 6.25  | 1.38        | 1.32     |
| 1   | D     | 128 | HIS  | ND1-CE1 | 6.25  | 1.38        | 1.32     |
| 1   | C     | 328 | ALA  | C-O     | 6.23  | 1.32        | 1.24     |
| 1   | A     | 163 | PHE  | N-CA    | 6.18  | 1.53        | 1.46     |
| 1   | C     | 36  | HIS  | CE1-NE2 | 6.16  | 1.38        | 1.32     |
| 1   | C     | 127 | VAL  | C-O     | 6.15  | 1.30        | 1.23     |
| 1   | C     | 116 | HIS  | CG-CD2  | 6.15  | 1.42        | 1.35     |
| 1   | D     | 131 | GLY  | N-CA    | 6.11  | 1.51        | 1.45     |
| 1   | C     | 292 | HIS  | CE1-NE2 | 6.11  | 1.38        | 1.32     |
| 1   | C     | 420 | ILE  | CA-CB   | 6.10  | 1.62        | 1.54     |
| 1   | D     | 367 | VAL  | C-O     | 6.10  | 1.30        | 1.24     |
| 1   | A     | 458 | ALA  | C-O     | 6.08  | 1.31        | 1.23     |
| 1   | B     | 113 | LYS  | CA-C    | 6.06  | 1.60        | 1.52     |
| 1   | D     | 198 | LEU  | C-O     | 6.06  | 1.31        | 1.23     |
| 1   | C     | 44  | PRO  | CA-C    | 6.05  | 1.57        | 1.52     |
| 1   | B     | 739 | HIS  | CG-CD2  | 6.04  | 1.42        | 1.35     |
| 1   | D     | 236 | HIS  | ND1-CE1 | 6.03  | 1.38        | 1.32     |
| 1   | B     | 219 | HIS  | CG-CD2  | 6.02  | 1.42        | 1.35     |
| 1   | B     | 119 | HIS  | ND1-CE1 | 5.99  | 1.38        | 1.32     |
| 1   | D     | 276 | THR  | C-O     | 5.98  | 1.31        | 1.24     |
| 1   | A     | 337 | GLY  | N-CA    | 5.97  | 1.51        | 1.45     |
| 1   | A     | 170 | GLN  | C-O     | -5.93 | 1.16        | 1.24     |
| 1   | D     | 627 | GLY  | N-CA    | 5.93  | 1.53        | 1.45     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 429 | HIS  | CG-ND1  | -5.92 | 1.31        | 1.38     |
| 1   | C     | 121 | ARG  | C-N     | 5.92  | 1.39        | 1.33     |
| 1   | D     | 343 | GLU  | C-O     | 5.90  | 1.31        | 1.24     |
| 1   | B     | 473 | THR  | C-N     | 5.89  | 1.38        | 1.33     |
| 1   | B     | 452 | GLY  | C-O     | 5.89  | 1.29        | 1.23     |
| 1   | C     | 276 | THR  | N-CA    | 5.89  | 1.53        | 1.46     |
| 1   | D     | 257 | MET  | C-O     | 5.88  | 1.31        | 1.24     |
| 1   | C     | 292 | HIS  | CG-CD2  | 5.88  | 1.42        | 1.35     |
| 1   | B     | 576 | PRO  | CA-C    | 5.86  | 1.57        | 1.52     |
| 1   | B     | 393 | PRO  | CA-CB   | 5.85  | 1.62        | 1.53     |
| 1   | A     | 339 | GLN  | N-CA    | 5.84  | 1.53        | 1.46     |
| 1   | A     | 135 | HIS  | CE1-NE2 | 5.81  | 1.38        | 1.32     |
| 1   | B     | 292 | HIS  | ND1-CE1 | 5.80  | 1.38        | 1.32     |
| 1   | D     | 431 | ILE  | CA-C    | 5.78  | 1.58        | 1.52     |
| 1   | A     | 377 | ARG  | CZ-NH1  | 5.78  | 1.40        | 1.32     |
| 1   | D     | 269 | MET  | N-CA    | 5.76  | 1.53        | 1.45     |
| 1   | A     | 549 | HIS  | CG-CD2  | 5.76  | 1.42        | 1.35     |
| 1   | C     | 135 | HIS  | ND1-CE1 | 5.76  | 1.38        | 1.32     |
| 1   | B     | 56  | LYS  | C-O     | 5.75  | 1.30        | 1.24     |
| 1   | B     | 376 | ASN  | N-CA    | 5.73  | 1.52        | 1.46     |
| 1   | B     | 275 | HIS  | CE1-NE2 | 5.72  | 1.38        | 1.32     |
| 1   | A     | 494 | VAL  | C-O     | 5.72  | 1.29        | 1.24     |
| 1   | D     | 236 | HIS  | CG-ND1  | -5.68 | 1.31        | 1.38     |
| 1   | D     | 219 | HIS  | ND1-CE1 | 5.67  | 1.38        | 1.32     |
| 1   | A     | 600 | GLY  | N-CA    | 5.66  | 1.53        | 1.45     |
| 1   | B     | 431 | ILE  | CA-C    | 5.66  | 1.58        | 1.53     |
| 1   | B     | 226 | HIS  | CE1-NE2 | 5.66  | 1.38        | 1.32     |
| 1   | A     | 592 | ALA  | N-CA    | 5.64  | 1.53        | 1.46     |
| 1   | A     | 588 | LEU  | N-CA    | 5.63  | 1.53        | 1.46     |
| 1   | D     | 133 | ALA  | N-CA    | 5.61  | 1.53        | 1.45     |
| 1   | D     | 439 | PRO  | N-CA    | 5.60  | 1.53        | 1.47     |
| 1   | B     | 36  | HIS  | CE1-NE2 | 5.60  | 1.38        | 1.32     |
| 1   | C     | 691 | HIS  | CE1-NE2 | 5.59  | 1.38        | 1.32     |
| 1   | B     | 165 | ARG  | CZ-NH1  | 5.55  | 1.40        | 1.32     |
| 1   | C     | 187 | THR  | N-CA    | 5.54  | 1.52        | 1.46     |
| 1   | D     | 528 | SER  | N-CA    | 5.53  | 1.53        | 1.46     |
| 1   | C     | 452 | GLY  | N-CA    | 5.53  | 1.53        | 1.45     |
| 1   | B     | 358 | LYS  | N-CA    | 5.52  | 1.52        | 1.46     |
| 1   | C     | 203 | THR  | CA-C    | 5.52  | 1.57        | 1.52     |
| 1   | B     | 391 | PHE  | C-O     | 5.50  | 1.30        | 1.23     |
| 1   | A     | 365 | VAL  | CA-C    | 5.48  | 1.58        | 1.52     |
| 1   | A     | 474 | PRO  | CA-CB   | 5.48  | 1.59        | 1.53     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 125 | ARG  | CD-NE   | 5.46  | 1.53        | 1.46     |
| 1   | C     | 59  | ASP  | C-O     | -5.46 | 1.16        | 1.24     |
| 1   | A     | 327 | GLU  | N-CA    | 5.45  | 1.53        | 1.46     |
| 1   | B     | 283 | GLU  | N-CA    | 5.43  | 1.53        | 1.46     |
| 1   | A     | 730 | ASP  | C-O     | 5.42  | 1.30        | 1.24     |
| 1   | D     | 216 | ASP  | C-O     | 5.41  | 1.30        | 1.24     |
| 1   | C     | 395 | HIS  | ND1-CE1 | 5.41  | 1.38        | 1.32     |
| 1   | A     | 255 | TRP  | CD2-CE2 | 5.40  | 1.50        | 1.41     |
| 1   | C     | 327 | GLU  | N-CA    | 5.38  | 1.53        | 1.46     |
| 1   | D     | 401 | ASP  | N-CA    | 5.38  | 1.52        | 1.46     |
| 1   | C     | 119 | HIS  | ND1-CE1 | 5.38  | 1.38        | 1.32     |
| 1   | D     | 691 | HIS  | CE1-NE2 | 5.38  | 1.38        | 1.32     |
| 1   | A     | 316 | ASP  | N-CA    | 5.37  | 1.52        | 1.46     |
| 1   | A     | 523 | ILE  | N-CA    | 5.36  | 1.52        | 1.46     |
| 1   | B     | 219 | HIS  | CE1-NE2 | 5.36  | 1.38        | 1.32     |
| 1   | B     | 188 | LYS  | CA-CB   | 5.35  | 1.60        | 1.53     |
| 1   | B     | 205 | ILE  | CA-C    | -5.34 | 1.47        | 1.52     |
| 1   | C     | 112 | GLU  | N-CA    | 5.33  | 1.52        | 1.46     |
| 1   | B     | 236 | HIS  | ND1-CE1 | 5.33  | 1.37        | 1.32     |
| 1   | A     | 60  | THR  | CA-CB   | 5.32  | 1.60        | 1.53     |
| 1   | D     | 603 | VAL  | C-O     | 5.32  | 1.29        | 1.24     |
| 1   | A     | 183 | ARG  | CD-NE   | 5.32  | 1.53        | 1.46     |
| 1   | A     | 214 | PHE  | N-CA    | 5.31  | 1.51        | 1.46     |
| 1   | A     | 418 | THR  | CA-C    | 5.31  | 1.59        | 1.52     |
| 1   | B     | 135 | HIS  | CG-ND1  | -5.31 | 1.32        | 1.38     |
| 1   | B     | 168 | THR  | N-CA    | 5.30  | 1.52        | 1.45     |
| 1   | C     | 226 | HIS  | CG-CD2  | 5.29  | 1.41        | 1.35     |
| 1   | D     | 119 | HIS  | CE1-NE2 | 5.29  | 1.37        | 1.32     |
| 1   | B     | 314 | ASP  | N-CA    | 5.28  | 1.52        | 1.46     |
| 1   | A     | 71  | VAL  | CA-CB   | 5.27  | 1.60        | 1.54     |
| 1   | D     | 81  | THR  | C-O     | 5.27  | 1.30        | 1.23     |
| 1   | A     | 131 | GLY  | N-CA    | 5.26  | 1.50        | 1.45     |
| 1   | C     | 336 | LEU  | N-CA    | 5.24  | 1.52        | 1.46     |
| 1   | C     | 135 | HIS  | CG-CD2  | 5.24  | 1.41        | 1.35     |
| 1   | D     | 237 | ASP  | N-CA    | 5.23  | 1.52        | 1.46     |
| 1   | D     | 212 | HIS  | ND1-CE1 | 5.22  | 1.37        | 1.32     |
| 1   | C     | 716 | GLU  | CA-C    | 5.22  | 1.59        | 1.52     |
| 1   | A     | 629 | HIS  | CG-CD2  | 5.20  | 1.41        | 1.35     |
| 1   | C     | 657 | ALA  | C-O     | -5.20 | 1.18        | 1.24     |
| 1   | C     | 701 | ALA  | N-CA    | 5.20  | 1.52        | 1.46     |
| 1   | A     | 607 | LEU  | N-CA    | 5.19  | 1.52        | 1.45     |
| 1   | A     | 441 | HIS  | ND1-CE1 | 5.19  | 1.37        | 1.32     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | D     | 684 | TYR  | N-CA    | 5.19  | 1.52        | 1.46     |
| 1   | D     | 203 | THR  | CA-C    | 5.19  | 1.57        | 1.52     |
| 1   | C     | 219 | HIS  | N-CA    | 5.18  | 1.52        | 1.46     |
| 1   | D     | 172 | GLY  | N-CA    | 5.18  | 1.51        | 1.45     |
| 1   | C     | 255 | TRP  | CZ2-CH2 | 5.17  | 1.47        | 1.37     |
| 1   | D     | 522 | HIS  | CG-ND1  | -5.17 | 1.32        | 1.38     |
| 1   | A     | 203 | THR  | C-N     | 5.17  | 1.37        | 1.33     |
| 1   | B     | 392 | HIS  | ND1-CE1 | 5.17  | 1.37        | 1.32     |
| 1   | B     | 142 | LYS  | N-CA    | 5.16  | 1.52        | 1.46     |
| 1   | C     | 383 | PHE  | C-O     | 5.15  | 1.30        | 1.24     |
| 1   | A     | 227 | TRP  | CD2-CE2 | 5.14  | 1.50        | 1.41     |
| 1   | A     | 727 | SER  | CA-C    | 5.14  | 1.59        | 1.52     |
| 1   | D     | 136 | GLY  | N-CA    | 5.14  | 1.51        | 1.45     |
| 1   | B     | 369 | ARG  | C-O     | 5.13  | 1.30        | 1.24     |
| 1   | C     | 587 | SER  | CA-C    | 5.13  | 1.59        | 1.52     |
| 1   | A     | 251 | HIS  | CG-CD2  | 5.13  | 1.41        | 1.35     |
| 1   | B     | 440 | TYR  | CE1-CZ  | 5.13  | 1.50        | 1.38     |
| 1   | D     | 275 | HIS  | CG-CD2  | 5.13  | 1.41        | 1.35     |
| 1   | D     | 165 | ARG  | CD-NE   | 5.12  | 1.53        | 1.46     |
| 1   | A     | 302 | LEU  | N-CA    | 5.12  | 1.52        | 1.45     |
| 1   | A     | 395 | HIS  | CE1-NE2 | 5.11  | 1.37        | 1.32     |
| 1   | A     | 274 | ILE  | N-CA    | 5.11  | 1.52        | 1.46     |
| 1   | B     | 217 | PHE  | CA-CB   | 5.09  | 1.61        | 1.53     |
| 1   | A     | 275 | HIS  | CG-CD2  | 5.08  | 1.41        | 1.35     |
| 1   | C     | 391 | PHE  | N-CA    | 5.08  | 1.51        | 1.45     |
| 1   | C     | 733 | LEU  | CA-C    | 5.06  | 1.59        | 1.52     |
| 1   | D     | 290 | ARG  | N-CA    | 5.05  | 1.52        | 1.46     |
| 1   | A     | 136 | GLY  | N-CA    | 5.04  | 1.51        | 1.45     |
| 1   | D     | 377 | ARG  | CZ-NH1  | 5.04  | 1.39        | 1.32     |
| 1   | A     | 217 | PHE  | CA-CB   | 5.04  | 1.61        | 1.53     |
| 1   | A     | 488 | ARG  | N-CA    | 5.03  | 1.52        | 1.46     |
| 1   | A     | 236 | HIS  | ND1-CE1 | 5.03  | 1.37        | 1.32     |
| 1   | D     | 323 | TRP  | NE1-CE2 | 5.03  | 1.43        | 1.37     |
| 1   | A     | 729 | MET  | N-CA    | 5.02  | 1.52        | 1.46     |
| 1   | D     | 549 | HIS  | CE1-NE2 | 5.02  | 1.37        | 1.32     |
| 1   | D     | 559 | ALA  | C-O     | -5.02 | 1.18        | 1.24     |
| 1   | C     | 172 | GLY  | N-CA    | 5.01  | 1.51        | 1.45     |
| 1   | D     | 696 | ALA  | N-CA    | 5.00  | 1.52        | 1.46     |

All (67) bond angle outliers are listed below:

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 159 | ILE  | CB-CG1-CD1 | -9.81 | 93.20       | 113.80   |
| 1   | B     | 745 | ILE  | CA-C-N     | -8.95 | 110.52      | 119.56   |
| 1   | B     | 745 | ILE  | C-N-CA     | -8.95 | 110.52      | 119.56   |
| 1   | D     | 574 | THR  | CA-C-N     | 8.48  | 125.85      | 119.66   |
| 1   | D     | 574 | THR  | C-N-CA     | 8.48  | 125.85      | 119.66   |
| 1   | A     | 574 | THR  | CA-C-N     | 8.45  | 125.83      | 119.66   |
| 1   | A     | 574 | THR  | C-N-CA     | 8.45  | 125.83      | 119.66   |
| 1   | B     | 521 | ARG  | NE-CZ-NH2  | 8.01  | 126.41      | 119.20   |
| 1   | C     | 159 | ILE  | CB-CA-C    | 7.34  | 121.96      | 110.81   |
| 1   | A     | 533 | LYS  | CG-CD-CE   | -7.17 | 94.81       | 111.30   |
| 1   | C     | 725 | ASP  | N-CA-C     | 6.70  | 125.08      | 110.80   |
| 1   | D     | 360 | ILE  | N-CA-C     | -6.65 | 100.49      | 107.60   |
| 1   | C     | 348 | LYS  | CA-CB-CG   | -6.59 | 100.92      | 114.10   |
| 1   | D     | 61  | ARG  | NE-CZ-NH2  | 6.50  | 125.06      | 119.20   |
| 1   | B     | 126 | ILE  | CB-CA-C    | -6.40 | 103.50      | 112.14   |
| 1   | D     | 377 | ARG  | NH1-CZ-NH2 | 6.34  | 127.54      | 119.30   |
| 1   | C     | 37  | ARG  | CA-C-N     | 6.29  | 126.24      | 119.76   |
| 1   | C     | 37  | ARG  | C-N-CA     | 6.29  | 126.24      | 119.76   |
| 1   | C     | 749 | ASP  | N-CA-C     | 6.27  | 118.92      | 111.71   |
| 1   | B     | 750 | LYS  | CB-CA-C    | -6.24 | 101.09      | 110.88   |
| 1   | A     | 349 | PHE  | CA-C-N     | -6.23 | 111.84      | 122.56   |
| 1   | A     | 349 | PHE  | C-N-CA     | -6.23 | 111.84      | 122.56   |
| 1   | B     | 349 | PHE  | CA-C-N     | -6.23 | 112.70      | 122.73   |
| 1   | B     | 349 | PHE  | C-N-CA     | -6.23 | 112.70      | 122.73   |
| 1   | C     | 159 | ILE  | CA-CB-CG2  | 6.05  | 120.79      | 110.50   |
| 1   | A     | 377 | ARG  | CG-CD-NE   | -5.90 | 99.02       | 112.00   |
| 1   | B     | 568 | ASP  | N-CA-C     | 5.80  | 118.34      | 111.33   |
| 1   | A     | 372 | LYS  | CD-CE-NZ   | -5.79 | 93.36       | 111.90   |
| 1   | C     | 377 | ARG  | NE-CZ-NH1  | -5.76 | 115.74      | 121.50   |
| 1   | C     | 111 | ARG  | NE-CZ-NH1  | -5.72 | 115.78      | 121.50   |
| 1   | C     | 377 | ARG  | CG-CD-NE   | -5.71 | 99.44       | 112.00   |
| 1   | D     | 745 | ILE  | CA-C-N     | -5.64 | 113.81      | 119.56   |
| 1   | D     | 745 | ILE  | C-N-CA     | -5.64 | 113.81      | 119.56   |
| 1   | C     | 471 | ARG  | NE-CZ-NH2  | -5.59 | 114.17      | 119.20   |
| 1   | C     | 451 | MET  | CA-C-N     | -5.58 | 114.62      | 120.31   |
| 1   | C     | 451 | MET  | C-N-CA     | -5.58 | 114.62      | 120.31   |
| 1   | B     | 521 | ARG  | NE-CZ-NH1  | -5.58 | 115.92      | 121.50   |
| 1   | B     | 195 | ILE  | CB-CA-C    | -5.55 | 103.89      | 111.33   |
| 1   | A     | 120 | GLU  | N-CA-C     | 5.54  | 118.25      | 111.82   |
| 1   | D     | 229 | ILE  | N-CA-CB    | -5.53 | 105.72      | 111.64   |
| 1   | D     | 431 | ILE  | N-CA-C     | -5.47 | 103.93      | 109.02   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1   | C     | 479 | ARG  | CA-C-N     | -5.46 | 115.38      | 121.83   |
| 1   | C     | 479 | ARG  | C-N-CA     | -5.46 | 115.38      | 121.83   |
| 1   | D     | 574 | THR  | CB-CA-C    | 5.44  | 118.23      | 109.41   |
| 1   | C     | 98  | GLY  | N-CA-C     | -5.43 | 105.92      | 112.48   |
| 1   | C     | 446 | ASP  | CB-CA-C    | -5.43 | 108.73      | 115.89   |
| 1   | B     | 686 | MET  | N-CA-C     | 5.42  | 116.87      | 111.07   |
| 1   | A     | 98  | GLY  | N-CA-C     | -5.36 | 105.93      | 112.68   |
| 1   | B     | 38  | PRO  | CB-CA-C    | -5.36 | 103.96      | 110.98   |
| 1   | C     | 168 | THR  | CA-C-N     | -5.32 | 117.71      | 123.08   |
| 1   | C     | 168 | THR  | C-N-CA     | -5.32 | 117.71      | 123.08   |
| 1   | C     | 488 | ARG  | N-CA-CB    | -5.28 | 102.09      | 110.06   |
| 1   | A     | 638 | GLY  | N-CA-C     | -5.28 | 104.96      | 111.45   |
| 1   | B     | 377 | ARG  | CG-CD-NE   | -5.28 | 100.39      | 112.00   |
| 1   | B     | 725 | ASP  | N-CA-C     | 5.23  | 121.94      | 110.80   |
| 1   | D     | 732 | LEU  | N-CA-C     | -5.17 | 105.72      | 111.36   |
| 1   | B     | 325 | ALA  | N-CA-C     | -5.15 | 105.67      | 111.28   |
| 1   | B     | 350 | ASP  | CB-CA-C    | 5.12  | 119.39      | 110.94   |
| 1   | C     | 126 | ILE  | CB-CA-C    | -5.12 | 105.23      | 112.14   |
| 1   | A     | 229 | ILE  | N-CA-CB    | -5.12 | 104.05      | 111.21   |
| 1   | A     | 750 | LYS  | N-CA-C     | -5.11 | 105.62      | 111.14   |
| 1   | B     | 48  | GLN  | CA-C-N     | -5.10 | 114.70      | 119.85   |
| 1   | B     | 48  | GLN  | C-N-CA     | -5.10 | 114.70      | 119.85   |
| 1   | B     | 377 | ARG  | NE-CZ-NH1  | -5.06 | 116.44      | 121.50   |
| 1   | C     | 33  | ASP  | N-CA-C     | 5.03  | 119.29      | 113.20   |
| 1   | B     | 179 | VAL  | CB-CA-C    | -5.03 | 105.82      | 111.45   |
| 1   | D     | 554 | LEU  | CD1-CG-CD2 | 5.02  | 121.84      | 110.80   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | B     | 724 | ALA  | Peptide |
| 1   | C     | 724 | ALA  | Peptide |
| 1   | C     | 725 | ASP  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 5755  | 0        | 5599     | 37      | 0            |
| 1   | B     | 5758  | 0        | 5605     | 60      | 0            |
| 1   | C     | 5756  | 0        | 5606     | 54      | 0            |
| 1   | D     | 5758  | 0        | 5602     | 62      | 0            |
| 2   | A     | 44    | 0        | 31       | 1       | 0            |
| 2   | B     | 44    | 0        | 31       | 1       | 0            |
| 2   | C     | 44    | 0        | 31       | 2       | 0            |
| 2   | D     | 44    | 0        | 31       | 4       | 0            |
| 3   | A     | 43    | 0        | 30       | 13      | 0            |
| 3   | B     | 43    | 0        | 30       | 12      | 0            |
| 3   | C     | 43    | 0        | 30       | 13      | 0            |
| 3   | D     | 43    | 0        | 30       | 8       | 0            |
| 4   | A     | 769   | 0        | 0        | 9       | 0            |
| 4   | B     | 696   | 0        | 0        | 11      | 0            |
| 4   | C     | 709   | 0        | 0        | 9       | 0            |
| 4   | D     | 774   | 0        | 0        | 16      | 0            |
| All | All   | 26323 | 0        | 22656    | 219     | 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 5.

All (219) 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:D:392:HIS:ND1     | 1:D:415:TYR:CB      | 1.69                     | 1.52              |
| 1:C:392:HIS:ND1     | 1:C:415:TYR:CB      | 1.72                     | 1.51              |
| 1:A:392:HIS:ND1     | 1:A:415:TYR:CB      | 1.75                     | 1.50              |
| 1:B:392:HIS:ND1     | 1:B:415:TYR:CB      | 1.70                     | 1.49              |
| 1:B:157:ASN:HB2     | 4:B:1578:HOH:O      | 1.28                     | 1.30              |
| 1:D:392:HIS:CE1     | 1:D:415:TYR:HB2     | 1.71                     | 1.24              |
| 1:D:449[B]:HIS:NE2  | 4:D:1534:HOH:O      | 1.66                     | 1.21              |
| 1:B:392:HIS:CE1     | 1:B:415:TYR:HB2     | 1.76                     | 1.19              |
| 1:A:392:HIS:CE1     | 1:A:415:TYR:HB2     | 1.80                     | 1.17              |
| 1:C:392:HIS:CE1     | 1:C:415:TYR:HB2     | 1.84                     | 1.13              |
| 1:C:440:TYR:CD1     | 4:C:1370:HOH:O      | 2.00                     | 1.13              |
| 1:A:392:HIS:ND1     | 1:A:415:TYR:HB2     | 0.80                     | 1.13              |
| 3:A:802[B]:HEM:HMC2 | 3:A:802[B]:HEM:HBC2 | 1.22                     | 1.13              |
| 1:B:451:MET:HE2     | 1:D:451:MET:HE2     | 1.19                     | 1.11              |
| 1:D:546:GLN:HG3     | 4:D:1590:HOH:O      | 1.50                     | 1.11              |
| 1:D:392:HIS:ND1     | 1:D:415:TYR:HB2     | 0.78                     | 1.11              |
| 1:A:451:MET:HE2     | 1:C:451:MET:HE2     | 1.22                     | 1.10              |
| 1:C:392:HIS:ND1     | 1:C:415:TYR:HB2     | 0.77                     | 1.09              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:B:392:HIS:ND1     | 1:B:415:TYR:HB2     | 0.76                     | 1.09              |
| 1:C:583[A]:LYS:H    | 1:C:583[A]:LYS:HE2  | 1.06                     | 1.06              |
| 1:C:440:TYR:HD1     | 4:C:1370:HOH:O      | 1.35                     | 1.04              |
| 1:A:541:GLU:OE2     | 4:A:1540:HOH:O      | 1.76                     | 1.01              |
| 1:B:369:ARG:HG2     | 4:B:1302:HOH:O      | 1.64                     | 0.96              |
| 1:C:392:HIS:CG      | 1:C:415:TYR:HB2     | 2.04                     | 0.93              |
| 3:C:802[B]:HEM:HBC2 | 3:C:802[B]:HEM:HMC2 | 1.52                     | 0.89              |
| 1:D:449[B]:HIS:CE1  | 4:D:1534:HOH:O      | 2.18                     | 0.84              |
| 1:D:267:ARG:HG3     | 4:D:1384:HOH:O      | 1.79                     | 0.83              |
| 1:C:578:ASP:HB2     | 1:C:582:LEU:O       | 1.77                     | 0.83              |
| 1:C:201:ASN:CG      | 3:C:802[B]:HEM:HMB2 | 2.04                     | 0.82              |
| 1:A:392:HIS:CG      | 1:A:415:TYR:HB2     | 2.07                     | 0.82              |
| 1:B:407:LEU:CD2     | 3:B:802[B]:HEM:HBB1 | 2.11                     | 0.81              |
| 1:B:708:ILE:HD12    | 1:B:710:ILE:HD11    | 1.63                     | 0.80              |
| 1:C:583[A]:LYS:H    | 1:C:583[A]:LYS:CE   | 1.91                     | 0.80              |
| 2:C:801[A]:HDD:HMB1 | 2:C:801[A]:HDD:HBB1 | 1.66                     | 0.76              |
| 3:A:802[B]:HEM:HBC2 | 3:A:802[B]:HEM:CMC  | 2.00                     | 0.75              |
| 1:D:490:GLU:OE1     | 4:D:1482:HOH:O      | 2.02                     | 0.75              |
| 2:D:801[A]:HDD:HMB1 | 2:D:801[A]:HDD:HBB1 | 1.69                     | 0.75              |
| 1:C:748:ILE:O       | 1:C:751:ILE:HG22    | 1.86                     | 0.75              |
| 1:C:440:TYR:CE1     | 4:C:1370:HOH:O      | 2.33                     | 0.74              |
| 1:D:731:GLU:OE2     | 4:D:1653:HOH:O      | 2.06                     | 0.74              |
| 1:D:546:GLN:CG      | 4:D:1590:HOH:O      | 2.19                     | 0.73              |
| 1:D:341:ILE:HG13    | 4:D:1651:HOH:O      | 1.87                     | 0.73              |
| 1:B:451:MET:CE      | 1:D:451:MET:HE2     | 2.12                     | 0.72              |
| 1:D:392:HIS:ND1     | 1:D:415:TYR:CG      | 2.58                     | 0.70              |
| 1:B:330:ASP:OD1     | 1:B:629:HIS:HE1     | 1.74                     | 0.70              |
| 1:C:201:ASN:ND2     | 3:C:802[B]:HEM:CMB  | 2.55                     | 0.70              |
| 1:C:206:PHE:CG      | 3:C:802[B]:HEM:HAB  | 2.27                     | 0.69              |
| 1:C:392:HIS:ND1     | 1:C:415:TYR:CG      | 2.59                     | 0.69              |
| 1:A:201:ASN:CG      | 3:A:802[B]:HEM:HMB2 | 2.16                     | 0.69              |
| 1:A:392:HIS:ND1     | 1:A:415:TYR:CG      | 2.60                     | 0.68              |
| 1:C:708:ILE:HG13    | 1:C:710:ILE:HG12    | 1.75                     | 0.68              |
| 1:D:201:ASN:CG      | 3:D:802[B]:HEM:HMB2 | 2.19                     | 0.68              |
| 1:B:407:LEU:HD21    | 3:B:802[B]:HEM:HBB1 | 1.74                     | 0.68              |
| 1:D:546:GLN:CD      | 4:D:1590:HOH:O      | 2.33                     | 0.67              |
| 1:C:330:ASP:OD1     | 1:C:629:HIS:HE1     | 1.78                     | 0.67              |
| 2:A:801[A]:HDD:HBB1 | 2:A:801[A]:HDD:HMB1 | 1.75                     | 0.66              |
| 1:B:157:ASN:CB      | 4:B:1578:HOH:O      | 2.07                     | 0.66              |
| 1:B:407:LEU:HD23    | 3:B:802[B]:HEM:HBB1 | 1.76                     | 0.66              |
| 1:B:392:HIS:ND1     | 1:B:415:TYR:CG      | 2.61                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:B:556:GLN:HG2     | 1:B:566:LEU:HD23    | 1.78                     | 0.64              |
| 1:A:416[B]:THR:HG22 | 4:A:1016:HOH:O      | 1.97                     | 0.64              |
| 1:B:521:ARG:HD3     | 4:B:1566:HOH:O      | 1.97                     | 0.64              |
| 2:B:801[A]:HDD:HBB1 | 2:B:801[A]:HDD:HMB1 | 1.78                     | 0.64              |
| 1:D:629:HIS:HD2     | 4:D:1267:HOH:O      | 1.81                     | 0.64              |
| 2:D:801[A]:HDD:HMC1 | 2:D:801[A]:HDD:HBC1 | 1.79                     | 0.64              |
| 1:D:206:PHE:HB2     | 3:D:802[B]:HEM:HBB1 | 1.79                     | 0.64              |
| 1:C:206:PHE:CD2     | 3:C:802[B]:HEM:HAB  | 2.33                     | 0.63              |
| 1:A:36:HIS:CD2      | 1:A:36:HIS:H        | 2.17                     | 0.62              |
| 1:B:201:ASN:CG      | 3:B:802[B]:HEM:HMB2 | 2.25                     | 0.62              |
| 1:D:574:THR:HG22    | 4:D:1313:HOH:O      | 2.00                     | 0.61              |
| 4:C:1452:HOH:O      | 1:D:488:ARG:HD2     | 2.01                     | 0.60              |
| 1:C:201:ASN:ND2     | 3:C:802[B]:HEM:HMB1 | 2.16                     | 0.60              |
| 1:D:392:HIS:ND1     | 1:D:415:TYR:HB3     | 2.02                     | 0.60              |
| 1:C:629:HIS:HD2     | 4:C:1210:HOH:O      | 1.84                     | 0.59              |
| 1:B:294:LYS:HB2     | 4:B:1189:HOH:O      | 2.01                     | 0.59              |
| 1:D:330:ASP:OD1     | 1:D:629:HIS:HE1     | 1.85                     | 0.59              |
| 1:A:240:TRP:HE1     | 1:A:530:GLN:HE21    | 1.51                     | 0.59              |
| 1:B:359:LEU:H       | 1:B:507:HIS:HD2     | 1.50                     | 0.59              |
| 1:D:448:MET:O       | 1:D:449[A]:HIS:HB2  | 2.03                     | 0.58              |
| 1:C:201:ASN:CG      | 3:C:802[B]:HEM:CMB  | 2.76                     | 0.58              |
| 1:B:552:LEU:HD22    | 1:B:556:GLN:HG3     | 1.83                     | 0.58              |
| 1:D:206:PHE:CG      | 3:D:802[B]:HEM:HAB  | 2.37                     | 0.57              |
| 1:B:521:ARG:CD      | 4:B:1566:HOH:O      | 2.52                     | 0.57              |
| 1:B:708:ILE:CD1     | 1:B:710:ILE:HD11    | 2.34                     | 0.57              |
| 1:B:725:ASP:OD1     | 1:B:725:ASP:C       | 2.46                     | 0.57              |
| 1:B:201:ASN:CG      | 3:B:802[B]:HEM:CMB  | 2.79                     | 0.56              |
| 1:D:274:ILE:HD12    | 3:D:802[B]:HEM:HMB1 | 1.88                     | 0.56              |
| 1:A:448:MET:O       | 1:A:449[B]:HIS:HB2  | 2.06                     | 0.56              |
| 1:D:359:LEU:H       | 1:D:507:HIS:HD2     | 1.53                     | 0.56              |
| 1:B:583:LYS:H       | 1:B:583:LYS:NZ      | 2.04                     | 0.56              |
| 1:A:479:ARG:NH2     | 4:A:1549:HOH:O      | 2.04                     | 0.56              |
| 1:C:201:ASN:ND2     | 3:C:802[B]:HEM:HMB2 | 2.19                     | 0.55              |
| 1:A:274:ILE:HD12    | 3:A:802[B]:HEM:HMB1 | 1.88                     | 0.55              |
| 1:D:713:GLN:O       | 1:D:713:GLN:HG2     | 2.07                     | 0.55              |
| 1:B:407:LEU:HD21    | 3:B:802[B]:HEM:CBB  | 2.36                     | 0.55              |
| 2:D:801[A]:HDD:HMC1 | 2:D:801[A]:HDD:CBC  | 2.36                     | 0.54              |
| 1:B:629:HIS:HD2     | 4:B:1157:HOH:O      | 1.89                     | 0.54              |
| 1:D:708:ILE:HG13    | 1:D:710:ILE:HG12    | 1.89                     | 0.54              |
| 1:D:206:PHE:HB2     | 3:D:802[B]:HEM:CBB  | 2.38                     | 0.54              |
| 1:D:416[B]:THR:CG2  | 4:D:1169:HOH:O      | 2.56                     | 0.53              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:B:240:TRP:HE1     | 1:B:530:GLN:HE21    | 1.57                     | 0.53              |
| 4:A:1169:HOH:O      | 1:D:100:ARG:HG3     | 2.08                     | 0.53              |
| 1:D:609:ASP:O       | 4:D:1345:HOH:O      | 2.18                     | 0.53              |
| 1:B:201:ASN:ND2     | 3:B:802[B]:HEM:HMB1 | 2.25                     | 0.52              |
| 1:D:411:ARG:HG2     | 3:D:802[B]:HEM:C2C  | 2.44                     | 0.52              |
| 1:D:478:LYS:NZ      | 4:D:1005:HOH:O      | 2.42                     | 0.52              |
| 1:A:407:LEU:CD2     | 3:A:802[B]:HEM:HBB1 | 2.39                     | 0.52              |
| 1:B:634:TYR:O       | 1:B:653:THR:HA      | 2.08                     | 0.52              |
| 4:B:1339:HOH:O      | 1:D:449[A]:HIS:HE1  | 1.92                     | 0.52              |
| 1:B:36:HIS:H        | 1:B:36:HIS:HD1      | 1.58                     | 0.52              |
| 1:B:392:HIS:ND1     | 1:B:415:TYR:HB3     | 2.06                     | 0.52              |
| 1:A:407:LEU:HD23    | 3:A:802[B]:HEM:HBB1 | 1.92                     | 0.52              |
| 1:C:621:LYS:HE3     | 4:C:1595:HOH:O      | 2.09                     | 0.52              |
| 1:B:407:LEU:CD2     | 3:B:802[B]:HEM:CBB  | 2.86                     | 0.52              |
| 1:B:682:ASN:HB3     | 1:B:707:THR:HG21    | 1.92                     | 0.52              |
| 4:B:1139:HOH:O      | 1:D:449[B]:HIS:HD2  | 1.93                     | 0.52              |
| 1:C:411:ARG:HG2     | 3:C:802[B]:HEM:C2C  | 2.45                     | 0.52              |
| 4:A:1344:HOH:O      | 1:C:449[B]:HIS:HE1  | 1.93                     | 0.51              |
| 1:B:461:GLU:HA      | 1:B:462:PRO:C       | 2.34                     | 0.51              |
| 1:B:583:LYS:O       | 1:B:584:LYS:HB3     | 2.10                     | 0.51              |
| 4:A:1047:HOH:O      | 1:C:52:PRO:HG3      | 2.09                     | 0.51              |
| 1:D:748:ILE:O       | 1:D:751:ILE:HG22    | 2.10                     | 0.51              |
| 1:B:521:ARG:NE      | 4:B:1566:HOH:O      | 2.43                     | 0.51              |
| 1:D:671:ASN:HD21    | 1:D:673:ALA:HB3     | 1.76                     | 0.50              |
| 1:D:416[B]:THR:HG22 | 4:D:1169:HOH:O      | 2.11                     | 0.50              |
| 1:C:240:TRP:HE1     | 1:C:530:GLN:HE21    | 1.60                     | 0.50              |
| 1:A:201:ASN:CG      | 3:A:802[B]:HEM:CMB  | 2.85                     | 0.50              |
| 1:C:359:LEU:H       | 1:C:507:HIS:HD2     | 1.60                     | 0.50              |
| 1:A:219:HIS:HB3     | 1:B:459:ASN:ND2     | 2.28                     | 0.49              |
| 1:A:372:LYS:NZ      | 4:A:1629:HOH:O      | 2.44                     | 0.49              |
| 1:B:359:LEU:H       | 1:B:507:HIS:CD2     | 2.29                     | 0.49              |
| 3:A:802[B]:HEM:HMC2 | 3:A:802[B]:HEM:CBC  | 2.15                     | 0.49              |
| 3:B:802[B]:HEM:HMC2 | 3:B:802[B]:HEM:HBC2 | 1.96                     | 0.48              |
| 3:A:802[B]:HEM:CMC  | 3:A:802[B]:HEM:CBC  | 2.80                     | 0.48              |
| 1:C:704:PHE:O       | 1:C:707:THR:HG22    | 2.12                     | 0.48              |
| 1:C:577:PRO:HG2     | 4:C:1495:HOH:O      | 2.13                     | 0.48              |
| 1:D:240:TRP:HE1     | 1:D:530:GLN:HE21    | 1.61                     | 0.48              |
| 1:A:411:ARG:HD2     | 3:A:802[B]:HEM:HBB2 | 1.96                     | 0.48              |
| 3:B:802[B]:HEM:HBC2 | 3:B:802[B]:HEM:CMC  | 2.44                     | 0.47              |
| 1:C:597:ASP:OD2     | 4:C:1417:HOH:O      | 2.20                     | 0.47              |
| 1:C:219:HIS:HB3     | 1:D:459:ASN:ND2     | 2.30                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:D:801[A]:HDD:HBC1 | 2:D:801[A]:HDD:CMC  | 2.44                     | 0.47              |
| 1:D:461:GLU:HA      | 1:D:462:PRO:C       | 2.41                     | 0.46              |
| 3:A:802[B]:HEM:HHC  | 3:A:802[B]:HEM:CBB  | 2.44                     | 0.46              |
| 1:B:461:GLU:OE1     | 1:D:91:ASP:OD1      | 2.34                     | 0.46              |
| 1:B:724:ALA:O       | 1:B:726:GLY:N       | 2.45                     | 0.46              |
| 1:B:448:MET:O       | 1:B:449[B]:HIS:HB2  | 2.15                     | 0.46              |
| 1:C:359:LEU:H       | 1:C:507:HIS:CD2     | 2.34                     | 0.46              |
| 1:A:36:HIS:H        | 1:A:36:HIS:HD2      | 1.62                     | 0.46              |
| 3:C:802[B]:HEM:HMC2 | 3:C:802[B]:HEM:CBC  | 2.35                     | 0.46              |
| 1:A:726:GLY:HA2     | 4:A:1492:HOH:O      | 2.16                     | 0.45              |
| 1:C:37:ARG:HD3      | 4:C:1509:HOH:O      | 2.16                     | 0.45              |
| 1:D:634:TYR:O       | 1:D:653:THR:HA      | 2.15                     | 0.45              |
| 1:D:128:HIS:HA      | 1:D:168:THR:O       | 2.17                     | 0.45              |
| 1:B:201:ASN:ND2     | 3:B:802[B]:HEM:CMB  | 2.80                     | 0.45              |
| 1:B:39:ALA:HB1      | 1:B:41:GLU:HG2      | 1.98                     | 0.45              |
| 1:D:359:LEU:H       | 1:D:507:HIS:CD2     | 2.31                     | 0.45              |
| 1:A:144:LEU:HD11    | 1:A:370:VAL:HG13    | 1.97                     | 0.45              |
| 1:C:137:TYR:HB2     | 1:C:159:ILE:CD1     | 2.47                     | 0.45              |
| 1:B:92:GLN:HA       | 1:C:213:LYS:HD2     | 1.99                     | 0.44              |
| 3:A:802[B]:HEM:CBB  | 3:A:802[B]:HEM:CHC  | 2.94                     | 0.44              |
| 1:D:404:ASN:O       | 1:D:405:ASP:C       | 2.59                     | 0.44              |
| 1:A:128:HIS:HA      | 1:A:168:THR:O       | 2.18                     | 0.44              |
| 1:B:128:HIS:HA      | 1:B:168:THR:O       | 2.17                     | 0.44              |
| 1:A:128:HIS:CE1     | 1:A:169:VAL:HG22    | 2.53                     | 0.44              |
| 1:B:530:GLN:HE21    | 1:B:530:GLN:HB3     | 1.63                     | 0.44              |
| 1:B:157:ASN:CA      | 4:B:1578:HOH:O      | 2.58                     | 0.43              |
| 1:B:201:ASN:OD1     | 3:B:802[B]:HEM:HMB2 | 2.16                     | 0.43              |
| 1:A:201:ASN:ND2     | 3:A:802[B]:HEM:CMB  | 2.81                     | 0.43              |
| 1:B:603:VAL:HG11    | 1:B:666:ILE:HD12    | 2.00                     | 0.43              |
| 1:C:201:ASN:OD1     | 3:C:802[B]:HEM:HMB2 | 2.16                     | 0.43              |
| 1:D:128:HIS:CE1     | 1:D:169:VAL:HG22    | 2.53                     | 0.43              |
| 1:D:359:LEU:HD21    | 4:D:1643:HOH:O      | 2.19                     | 0.43              |
| 1:C:461:GLU:HB2     | 1:C:462:PRO:HA      | 2.01                     | 0.43              |
| 1:A:393:PRO:HD2     | 1:A:415:TYR:CD2     | 2.54                     | 0.43              |
| 1:D:201:ASN:ND2     | 3:D:802[B]:HEM:CMB  | 2.82                     | 0.43              |
| 1:B:213:LYS:HB3     | 1:B:213:LYS:HE3     | 1.82                     | 0.43              |
| 1:B:556:GLN:HG2     | 1:B:566:LEU:CD2     | 2.47                     | 0.43              |
| 1:C:448:MET:O       | 1:C:449[B]:HIS:HB2  | 2.19                     | 0.43              |
| 1:C:274:ILE:HD12    | 3:C:802[B]:HEM:HMB1 | 2.01                     | 0.43              |
| 1:A:449[B]:HIS:CG   | 1:C:449[B]:HIS:CG   | 2.36                     | 0.42              |
| 1:A:459:ASN:HD22    | 1:A:459:ASN:H       | 1.66                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:B:83:ASN:HB3      | 1:D:429:HIS:CD2     | 2.54                     | 0.42              |
| 1:A:535:VAL:O       | 1:A:537:PRO:HD3     | 2.20                     | 0.42              |
| 1:C:643:ASP:OD1     | 1:C:644:ASP:N       | 2.52                     | 0.42              |
| 1:D:206:PHE:CG      | 3:D:802[B]:HEM:CAB  | 3.02                     | 0.42              |
| 1:B:459:ASN:H       | 1:B:459:ASN:HD22    | 1.66                     | 0.42              |
| 1:C:251:HIS:CE1     | 1:C:507:HIS:HB3     | 2.54                     | 0.42              |
| 2:C:801[A]:HDD:HMD3 | 2:C:801[A]:HDD:HAD2 | 1.88                     | 0.42              |
| 1:D:65:LEU:HD21     | 1:D:135:HIS:CG      | 2.54                     | 0.42              |
| 1:D:448:MET:O       | 1:D:449[A]:HIS:CB   | 2.67                     | 0.42              |
| 1:D:578:ASP:OD1     | 1:D:583:LYS:HE3     | 2.20                     | 0.42              |
| 1:B:91:ASP:OD1      | 1:D:461:GLU:OE1     | 2.38                     | 0.41              |
| 1:B:583:LYS:H       | 1:B:583:LYS:HZ2     | 1.68                     | 0.41              |
| 1:D:36:HIS:H        | 1:D:36:HIS:HD1      | 1.67                     | 0.41              |
| 1:C:459:ASN:ND2     | 1:D:219:HIS:HB3     | 2.35                     | 0.41              |
| 1:A:251:HIS:CE1     | 1:A:507:HIS:HB3     | 2.55                     | 0.41              |
| 1:C:407:LEU:HD23    | 3:C:802[B]:HEM:HBB1 | 2.03                     | 0.41              |
| 1:C:725:ASP:HB3     | 1:C:726:GLY:H       | 1.65                     | 0.41              |
| 1:A:751:ILE:HA      | 1:A:752:PRO:HD3     | 1.73                     | 0.41              |
| 1:A:725:ASP:H       | 1:A:728:PHE:HB3     | 1.85                     | 0.41              |
| 1:D:313:ARG:HG3     | 1:D:660:LEU:HD12    | 2.03                     | 0.41              |
| 1:A:38:PRO:HG2      | 1:A:51:ALA:HB2      | 2.03                     | 0.41              |
| 1:A:461:GLU:HA      | 1:A:462:PRO:C       | 2.45                     | 0.41              |
| 1:B:552:LEU:HD21    | 1:B:571:LEU:HD12    | 2.03                     | 0.41              |
| 1:C:128:HIS:HA      | 1:C:168:THR:O       | 2.20                     | 0.41              |
| 1:C:469:TRP:CE3     | 1:C:471:ARG:HG3     | 2.56                     | 0.41              |
| 1:B:596:GLY:HA3     | 1:B:737:ALA:O       | 2.22                     | 0.40              |
| 1:C:634:TYR:O       | 1:C:653:THR:HA      | 2.21                     | 0.40              |
| 1:D:296:LEU:HD23    | 1:D:296:LEU:HA      | 1.93                     | 0.40              |
| 1:C:552:LEU:HD22    | 1:C:556:GLN:HG3     | 2.03                     | 0.40              |
| 1:A:278:ARG:HH12    | 1:A:487:GLU:CD      | 2.29                     | 0.40              |
| 1:C:267:ARG:HH11    | 1:C:267:ARG:HD2     | 1.63                     | 0.40              |
| 1:A:449[B]:HIS:HE1  | 4:A:1344:HOH:O      | 2.03                     | 0.40              |
| 1:B:83:ASN:HB3      | 1:D:429:HIS:CG      | 2.56                     | 0.40              |
| 1:B:626:LYS:HA      | 1:B:626:LYS:HD3     | 1.69                     | 0.40              |
| 1:D:443:PHE:CZ      | 1:D:470:PRO:HD2     | 2.56                     | 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     | 728/753 (97%)   | 710 (98%)  | 17 (2%) | 1 (0%)   | 48          | 27 |
| 1   | B     | 728/753 (97%)   | 714 (98%)  | 13 (2%) | 1 (0%)   | 48          | 27 |
| 1   | C     | 727/753 (96%)   | 709 (98%)  | 17 (2%) | 1 (0%)   | 48          | 27 |
| 1   | D     | 728/753 (97%)   | 715 (98%)  | 12 (2%) | 1 (0%)   | 48          | 27 |
| All | All   | 2911/3012 (97%) | 2848 (98%) | 59 (2%) | 4 (0%)   | 48          | 27 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 75  | SER  |
| 1   | B     | 75  | SER  |
| 1   | C     | 75  | SER  |
| 1   | D     | 75  | SER  |

### 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     | 615/636 (97%)   | 600 (98%)  | 15 (2%)  | 43          | 19 |
| 1   | B     | 615/636 (97%)   | 585 (95%)  | 30 (5%)  | 22          | 5  |
| 1   | C     | 614/636 (96%)   | 586 (95%)  | 28 (5%)  | 24          | 6  |
| 1   | D     | 615/636 (97%)   | 594 (97%)  | 21 (3%)  | 32          | 11 |
| All | All   | 2459/2544 (97%) | 2365 (96%) | 94 (4%)  | 29          | 9  |

All (94) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 158    | LYS  |
| 1   | A     | 191    | THR  |
| 1   | A     | 205    | ILE  |
| 1   | A     | 213    | LYS  |
| 1   | A     | 252    | ASN  |
| 1   | A     | 440    | TYR  |
| 1   | A     | 459    | ASN  |
| 1   | A     | 478    | LYS  |
| 1   | A     | 530    | GLN  |
| 1   | A     | 552    | LEU  |
| 1   | A     | 556    | GLN  |
| 1   | A     | 617    | LEU  |
| 1   | A     | 732    | LEU  |
| 1   | A     | 750    | LYS  |
| 1   | A     | 751    | ILE  |
| 1   | B     | 32     | GLU  |
| 1   | B     | 158    | LYS  |
| 1   | B     | 191    | THR  |
| 1   | B     | 205    | ILE  |
| 1   | B     | 213    | LYS  |
| 1   | B     | 252    | ASN  |
| 1   | B     | 309    | LYS  |
| 1   | B     | 321    | GLU  |
| 1   | B     | 344    | GLU  |
| 1   | B     | 370[A] | VAL  |
| 1   | B     | 370[B] | VAL  |
| 1   | B     | 432    | PRO  |
| 1   | B     | 440    | TYR  |
| 1   | B     | 459    | ASN  |
| 1   | B     | 530    | GLN  |
| 1   | B     | 552    | LEU  |
| 1   | B     | 560    | LYS  |
| 1   | B     | 565    | GLU  |
| 1   | B     | 566    | LEU  |
| 1   | B     | 568    | ASP  |
| 1   | B     | 571    | LEU  |
| 1   | B     | 583    | LYS  |
| 1   | B     | 612    | ARG  |
| 1   | B     | 616    | LEU  |
| 1   | B     | 633    | LEU  |
| 1   | B     | 703    | LYS  |
| 1   | B     | 713    | GLN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | B     | 725    | ASP  |
| 1   | B     | 732    | LEU  |
| 1   | B     | 749    | ASP  |
| 1   | C     | 37     | ARG  |
| 1   | C     | 159    | ILE  |
| 1   | C     | 191    | THR  |
| 1   | C     | 205    | ILE  |
| 1   | C     | 213    | LYS  |
| 1   | C     | 252    | ASN  |
| 1   | C     | 432    | PRO  |
| 1   | C     | 440    | TYR  |
| 1   | C     | 459    | ASN  |
| 1   | C     | 478    | LYS  |
| 1   | C     | 488    | ARG  |
| 1   | C     | 521    | ARG  |
| 1   | C     | 530    | GLN  |
| 1   | C     | 552    | LEU  |
| 1   | C     | 568    | ASP  |
| 1   | C     | 571    | LEU  |
| 1   | C     | 583[A] | LYS  |
| 1   | C     | 583[B] | LYS  |
| 1   | C     | 616    | LEU  |
| 1   | C     | 617    | LEU  |
| 1   | C     | 648    | LEU  |
| 1   | C     | 709    | LYS  |
| 1   | C     | 713    | GLN  |
| 1   | C     | 725    | ASP  |
| 1   | C     | 732    | LEU  |
| 1   | C     | 733    | LEU  |
| 1   | C     | 750    | LYS  |
| 1   | C     | 751    | ILE  |
| 1   | D     | 191    | THR  |
| 1   | D     | 205    | ILE  |
| 1   | D     | 213    | LYS  |
| 1   | D     | 252    | ASN  |
| 1   | D     | 344    | GLU  |
| 1   | D     | 369    | ARG  |
| 1   | D     | 432    | PRO  |
| 1   | D     | 440    | TYR  |
| 1   | D     | 459    | ASN  |
| 1   | D     | 530    | GLN  |
| 1   | D     | 554    | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 574 | THR  |
| 1   | D     | 582 | LEU  |
| 1   | D     | 593 | ILE  |
| 1   | D     | 616 | LEU  |
| 1   | D     | 633 | LEU  |
| 1   | D     | 648 | LEU  |
| 1   | D     | 713 | GLN  |
| 1   | D     | 747 | LYS  |
| 1   | D     | 750 | LYS  |
| 1   | D     | 751 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 36  | HIS  |
| 1   | A     | 66  | ASN  |
| 1   | A     | 201 | ASN  |
| 1   | A     | 252 | ASN  |
| 1   | A     | 459 | ASN  |
| 1   | A     | 515 | GLN  |
| 1   | A     | 530 | GLN  |
| 1   | A     | 556 | GLN  |
| 1   | A     | 713 | GLN  |
| 1   | B     | 252 | ASN  |
| 1   | B     | 459 | ASN  |
| 1   | B     | 507 | HIS  |
| 1   | B     | 530 | GLN  |
| 1   | B     | 629 | HIS  |
| 1   | B     | 713 | GLN  |
| 1   | C     | 201 | ASN  |
| 1   | C     | 252 | ASN  |
| 1   | C     | 419 | GLN  |
| 1   | C     | 459 | ASN  |
| 1   | C     | 507 | HIS  |
| 1   | C     | 530 | GLN  |
| 1   | C     | 572 | ASN  |
| 1   | C     | 629 | HIS  |
| 1   | C     | 682 | ASN  |
| 1   | C     | 713 | GLN  |
| 1   | D     | 48  | GLN  |
| 1   | D     | 252 | ASN  |
| 1   | D     | 419 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 459 | ASN  |
| 1   | D     | 507 | HIS  |
| 1   | D     | 530 | GLN  |
| 1   | D     | 556 | GLN  |
| 1   | D     | 629 | HIS  |
| 1   | D     | 671 | ASN  |

### 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](#)

8 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res    | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|--------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |        |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | HDD  | D     | 801[A] | 1,4  | 49,52,52     | 2.20 | 20 (40%)    | 62,89,89    | 3.14 | 28 (45%)    |
| 2   | HDD  | A     | 801[A] | 1,4  | 49,52,52     | 2.22 | 19 (38%)    | 62,89,89    | 3.16 | 24 (38%)    |
| 3   | HEM  | C     | 802[B] | 1    | 50,50,50     | 2.46 | 23 (46%)    | 67,82,82    | 2.91 | 32 (47%)    |
| 3   | HEM  | A     | 802[B] | 1,4  | 50,50,50     | 2.41 | 21 (42%)    | 67,82,82    | 2.71 | 30 (44%)    |
| 2   | HDD  | B     | 801[A] | 1,4  | 49,52,52     | 2.11 | 16 (32%)    | 62,89,89    | 3.25 | 23 (37%)    |
| 2   | HDD  | C     | 801[A] | 1,4  | 49,52,52     | 2.38 | 20 (40%)    | 62,89,89    | 2.37 | 23 (37%)    |

| Mol | Type | Chain | Res    | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|--------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |        |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | HEM  | B     | 802[B] | 1,4  | 50,50,50     | 2.52 | 22 (44%) | 67,82,82    | 2.77 | 33 (49%) |
| 3   | HEM  | D     | 802[B] | 1,4  | 50,50,50     | 2.59 | 21 (42%) | 67,82,82    | 2.84 | 31 (46%) |

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

| Mol | Type | Chain | Res    | Link | Chirals  | Torsions   | Rings   |
|-----|------|-------|--------|------|----------|------------|---------|
| 2   | HDD  | D     | 801[A] | 1,4  | 1/1/8/14 | 2/9/89/89  | 0/1/9/9 |
| 2   | HDD  | A     | 801[A] | 1,4  | 1/1/8/14 | 3/9/89/89  | 0/1/9/9 |
| 3   | HEM  | C     | 802[B] | 1    | -        | 4/14/54/54 | -       |
| 3   | HEM  | A     | 802[B] | 1,4  | -        | 3/14/54/54 | -       |
| 2   | HDD  | B     | 801[A] | 1,4  | 1/1/8/14 | 3/9/89/89  | 0/1/9/9 |
| 2   | HDD  | C     | 801[A] | 1,4  | 1/1/8/14 | 2/9/89/89  | 0/1/9/9 |
| 3   | HEM  | B     | 802[B] | 1,4  | -        | 2/14/54/54 | -       |
| 3   | HEM  | D     | 802[B] | 1,4  | -        | 3/14/54/54 | -       |

All (162) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | A     | 801[A] | HDD  | C1D-ND  | 6.21  | 1.39        | 1.35     |
| 2   | C     | 801[A] | HDD  | C1D-ND  | 6.08  | 1.39        | 1.35     |
| 3   | A     | 802[B] | HEM  | FE-ND   | 5.95  | 2.13        | 1.94     |
| 3   | D     | 802[B] | HEM  | FE-ND   | 5.49  | 2.11        | 1.94     |
| 3   | C     | 802[B] | HEM  | FE-ND   | 5.39  | 2.11        | 1.94     |
| 3   | C     | 802[B] | HEM  | FE-NB   | 5.26  | 2.11        | 1.94     |
| 3   | B     | 802[B] | HEM  | FE-ND   | 5.23  | 2.11        | 1.94     |
| 2   | C     | 801[A] | HDD  | CHC-C1C | 5.20  | 1.48        | 1.38     |
| 2   | B     | 801[A] | HDD  | C4C-NC  | -5.20 | 1.29        | 1.39     |
| 3   | D     | 802[B] | HEM  | FE-NB   | 5.18  | 2.10        | 1.94     |
| 3   | C     | 802[B] | HEM  | C1C-NC  | 5.10  | 1.49        | 1.39     |
| 2   | D     | 801[A] | HDD  | C1D-ND  | 5.00  | 1.38        | 1.35     |
| 3   | B     | 802[B] | HEM  | C1C-NC  | 4.93  | 1.48        | 1.39     |
| 3   | D     | 802[B] | HEM  | C1C-NC  | 4.92  | 1.48        | 1.39     |
| 3   | D     | 802[B] | HEM  | C4C-NC  | 4.91  | 1.48        | 1.39     |
| 2   | A     | 801[A] | HDD  | CHB-C1B | 4.91  | 1.48        | 1.38     |
| 2   | C     | 801[A] | HDD  | C1A-NA  | -4.81 | 1.30        | 1.39     |
| 3   | B     | 802[B] | HEM  | C1A-NA  | 4.81  | 1.48        | 1.39     |
| 3   | B     | 802[B] | HEM  | FE-NB   | 4.77  | 2.09        | 1.94     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 3   | B     | 802[B] | HEM  | C4A-NA  | 4.74  | 1.48        | 1.39     |
| 3   | A     | 802[B] | HEM  | C1C-NC  | 4.64  | 1.48        | 1.39     |
| 2   | C     | 801[A] | HDD  | FE-NC   | 4.53  | 2.10        | 1.95     |
| 2   | D     | 801[A] | HDD  | O1D-CGD | 4.53  | 1.42        | 1.35     |
| 3   | D     | 802[B] | HEM  | C1A-NA  | 4.36  | 1.47        | 1.39     |
| 2   | D     | 801[A] | HDD  | CHB-C1B | 4.34  | 1.47        | 1.38     |
| 3   | C     | 802[B] | HEM  | C4C-NC  | 4.31  | 1.47        | 1.39     |
| 3   | A     | 802[B] | HEM  | FE-NB   | 4.23  | 2.07        | 1.94     |
| 2   | C     | 801[A] | HDD  | CHB-C4A | 4.23  | 1.48        | 1.39     |
| 3   | A     | 802[B] | HEM  | C4A-NA  | 4.22  | 1.47        | 1.39     |
| 3   | A     | 802[B] | HEM  | CHA-C4D | 4.20  | 1.46        | 1.38     |
| 3   | D     | 802[B] | HEM  | C3D-C2D | 4.16  | 1.45        | 1.36     |
| 3   | B     | 802[B] | HEM  | CHA-C4D | 4.11  | 1.46        | 1.38     |
| 3   | B     | 802[B] | HEM  | CHC-C1C | 4.10  | 1.46        | 1.38     |
| 2   | B     | 801[A] | HDD  | FE-NB   | 4.09  | 2.07        | 1.94     |
| 3   | C     | 802[B] | HEM  | CHD-C4C | 4.07  | 1.46        | 1.38     |
| 3   | C     | 802[B] | HEM  | C3C-C2C | 4.07  | 1.45        | 1.37     |
| 2   | B     | 801[A] | HDD  | FE-NC   | 4.07  | 2.08        | 1.95     |
| 3   | D     | 802[B] | HEM  | CHA-C4D | 4.04  | 1.46        | 1.38     |
| 3   | D     | 802[B] | HEM  | CHD-C1D | 4.04  | 1.48        | 1.39     |
| 3   | C     | 802[B] | HEM  | CHD-C1D | 4.03  | 1.48        | 1.39     |
| 3   | A     | 802[B] | HEM  | C1A-NA  | 4.02  | 1.47        | 1.39     |
| 3   | C     | 802[B] | HEM  | CHA-C4D | 4.00  | 1.46        | 1.38     |
| 2   | B     | 801[A] | HDD  | CHB-C1B | 3.99  | 1.46        | 1.38     |
| 3   | B     | 802[B] | HEM  | C3C-C2C | 3.98  | 1.45        | 1.37     |
| 3   | A     | 802[B] | HEM  | C3C-C2C | 3.98  | 1.45        | 1.37     |
| 2   | A     | 801[A] | HDD  | OND-C2D | 3.97  | 1.50        | 1.42     |
| 3   | D     | 802[B] | HEM  | C3C-C2C | 3.94  | 1.45        | 1.37     |
| 3   | C     | 802[B] | HEM  | C3D-C2D | 3.90  | 1.45        | 1.36     |
| 3   | A     | 802[B] | HEM  | CHC-C1C | 3.89  | 1.46        | 1.38     |
| 2   | A     | 801[A] | HDD  | C4C-NC  | -3.84 | 1.32        | 1.39     |
| 3   | A     | 802[B] | HEM  | CHD-C1D | 3.81  | 1.47        | 1.39     |
| 3   | A     | 802[B] | HEM  | C3D-C2D | 3.80  | 1.45        | 1.36     |
| 3   | A     | 802[B] | HEM  | C4C-NC  | 3.73  | 1.46        | 1.39     |
| 3   | D     | 802[B] | HEM  | C4A-NA  | 3.70  | 1.46        | 1.39     |
| 3   | A     | 802[B] | HEM  | C1B-NB  | -3.66 | 1.33        | 1.40     |
| 2   | C     | 801[A] | HDD  | FE-NA   | 3.63  | 2.07        | 1.95     |
| 2   | D     | 801[A] | HDD  | CHA-C1A | 3.60  | 1.47        | 1.39     |
| 2   | C     | 801[A] | HDD  | C3C-C2C | 3.58  | 1.44        | 1.37     |
| 3   | C     | 802[B] | HEM  | CHC-C1C | 3.58  | 1.45        | 1.38     |
| 3   | D     | 802[B] | HEM  | CHA-C1A | 3.58  | 1.47        | 1.39     |
| 2   | C     | 801[A] | HDD  | FE-NB   | 3.55  | 2.05        | 1.94     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | A     | 801[A] | HDD  | FE-NC   | 3.55  | 2.06        | 1.95     |
| 2   | D     | 801[A] | HDD  | C4C-NC  | -3.55 | 1.32        | 1.39     |
| 3   | B     | 802[B] | HEM  | CHC-C4B | 3.53  | 1.47        | 1.39     |
| 3   | C     | 802[B] | HEM  | C4A-NA  | 3.48  | 1.46        | 1.39     |
| 2   | D     | 801[A] | HDD  | FE-NB   | 3.48  | 2.05        | 1.94     |
| 2   | B     | 801[A] | HDD  | FE-NA   | 3.40  | 2.06        | 1.95     |
| 3   | C     | 802[B] | HEM  | C3B-C2B | 3.37  | 1.44        | 1.37     |
| 2   | C     | 801[A] | HDD  | CHB-C1B | 3.34  | 1.45        | 1.38     |
| 2   | B     | 801[A] | HDD  | CHC-C1C | 3.34  | 1.44        | 1.38     |
| 2   | A     | 801[A] | HDD  | CHC-C1C | 3.33  | 1.44        | 1.38     |
| 3   | D     | 802[B] | HEM  | C3B-C2B | 3.33  | 1.43        | 1.37     |
| 2   | A     | 801[A] | HDD  | CHC-C4B | 3.32  | 1.46        | 1.39     |
| 3   | C     | 802[B] | HEM  | C1A-NA  | 3.32  | 1.45        | 1.39     |
| 3   | B     | 802[B] | HEM  | C1B-NB  | -3.32 | 1.34        | 1.40     |
| 2   | C     | 801[A] | HDD  | CHC-C4B | 3.31  | 1.46        | 1.39     |
| 2   | D     | 801[A] | HDD  | C1A-NA  | -3.31 | 1.33        | 1.39     |
| 3   | D     | 802[B] | HEM  | C1C-C2C | 3.30  | 1.51        | 1.45     |
| 3   | D     | 802[B] | HEM  | CHC-C4B | 3.29  | 1.46        | 1.39     |
| 2   | D     | 801[A] | HDD  | CHD-C4C | 3.28  | 1.44        | 1.38     |
| 3   | B     | 802[B] | HEM  | CHD-C4C | 3.27  | 1.44        | 1.38     |
| 2   | B     | 801[A] | HDD  | C1D-ND  | 3.25  | 1.37        | 1.35     |
| 2   | A     | 801[A] | HDD  | FE-NA   | 3.25  | 2.05        | 1.95     |
| 2   | C     | 801[A] | HDD  | C4C-NC  | -3.25 | 1.33        | 1.39     |
| 2   | D     | 801[A] | HDD  | FE-NC   | 3.24  | 2.05        | 1.95     |
| 3   | B     | 802[B] | HEM  | CHD-C1D | 3.24  | 1.46        | 1.39     |
| 2   | B     | 801[A] | HDD  | O1D-C3D | 3.19  | 1.51        | 1.46     |
| 3   | D     | 802[B] | HEM  | CHD-C4C | 3.18  | 1.44        | 1.38     |
| 2   | A     | 801[A] | HDD  | CAD-C3D | -3.15 | 1.48        | 1.53     |
| 2   | D     | 801[A] | HDD  | OND-C2D | 3.14  | 1.48        | 1.42     |
| 3   | B     | 802[B] | HEM  | C4C-NC  | 3.13  | 1.45        | 1.39     |
| 2   | B     | 801[A] | HDD  | CHD-C4C | 3.11  | 1.44        | 1.38     |
| 2   | A     | 801[A] | HDD  | CHB-C4A | 3.07  | 1.46        | 1.39     |
| 2   | B     | 801[A] | HDD  | O1D-CGD | 3.04  | 1.40        | 1.35     |
| 3   | C     | 802[B] | HEM  | C4D-ND  | -3.03 | 1.35        | 1.40     |
| 2   | B     | 801[A] | HDD  | C4A-C3A | 3.01  | 1.50        | 1.43     |
| 2   | A     | 801[A] | HDD  | O1D-C3D | 3.01  | 1.51        | 1.46     |
| 3   | B     | 802[B] | HEM  | C3D-C2D | 2.95  | 1.43        | 1.36     |
| 3   | B     | 802[B] | HEM  | C3B-C2B | 2.94  | 1.43        | 1.37     |
| 2   | B     | 801[A] | HDD  | CHB-C4A | 2.93  | 1.46        | 1.39     |
| 3   | D     | 802[B] | HEM  | CHB-C1B | 2.93  | 1.44        | 1.38     |
| 2   | B     | 801[A] | HDD  | CHA-C1A | 2.91  | 1.45        | 1.39     |
| 3   | D     | 802[B] | HEM  | C4D-ND  | -2.90 | 1.35        | 1.40     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 2   | D     | 801[A] | HDD  | C1B-C2B | 2.87  | 1.50        | 1.44     |
| 3   | B     | 802[B] | HEM  | C2A-C3A | 2.86  | 1.46        | 1.38     |
| 3   | A     | 802[B] | HEM  | C2A-C3A | 2.85  | 1.46        | 1.38     |
| 2   | D     | 801[A] | HDD  | CMC-C2C | 2.84  | 1.56        | 1.50     |
| 3   | B     | 802[B] | HEM  | C1A-C2A | 2.82  | 1.50        | 1.44     |
| 2   | C     | 801[A] | HDD  | O1A-CGA | 2.81  | 1.31        | 1.22     |
| 3   | B     | 802[B] | HEM  | C1C-C2C | 2.81  | 1.50        | 1.45     |
| 3   | C     | 802[B] | HEM  | C2A-C3A | 2.80  | 1.46        | 1.38     |
| 2   | D     | 801[A] | HDD  | FE-NA   | 2.79  | 2.04        | 1.95     |
| 3   | D     | 802[B] | HEM  | C2A-C3A | 2.76  | 1.46        | 1.38     |
| 3   | A     | 802[B] | HEM  | CHB-C1B | 2.75  | 1.44        | 1.38     |
| 3   | D     | 802[B] | HEM  | CHC-C1C | 2.74  | 1.43        | 1.38     |
| 2   | A     | 801[A] | HDD  | C3B-C2B | 2.72  | 1.42        | 1.37     |
| 2   | C     | 801[A] | HDD  | CHD-C4C | 2.68  | 1.43        | 1.38     |
| 2   | D     | 801[A] | HDD  | C1C-NC  | -2.68 | 1.34        | 1.39     |
| 3   | D     | 802[B] | HEM  | C1B-NB  | -2.65 | 1.35        | 1.40     |
| 2   | C     | 801[A] | HDD  | CHA-C1A | 2.63  | 1.45        | 1.39     |
| 2   | C     | 801[A] | HDD  | C4A-NA  | -2.63 | 1.34        | 1.39     |
| 3   | D     | 802[B] | HEM  | C1A-C2A | 2.62  | 1.49        | 1.44     |
| 3   | A     | 802[B] | HEM  | CHC-C4B | 2.60  | 1.45        | 1.39     |
| 2   | C     | 801[A] | HDD  | O1D-CGD | 2.60  | 1.39        | 1.35     |
| 2   | D     | 801[A] | HDD  | CMA-C3A | 2.59  | 1.56        | 1.50     |
| 3   | C     | 802[B] | HEM  | C1A-C2A | 2.58  | 1.49        | 1.44     |
| 2   | A     | 801[A] | HDD  | CHA-C1A | 2.58  | 1.45        | 1.39     |
| 2   | D     | 801[A] | HDD  | CMD-C2D | 2.56  | 1.56        | 1.53     |
| 3   | A     | 802[B] | HEM  | C1A-C2A | 2.50  | 1.49        | 1.44     |
| 3   | B     | 802[B] | HEM  | CHA-C1A | 2.48  | 1.45        | 1.39     |
| 2   | C     | 801[A] | HDD  | O1D-C3D | 2.48  | 1.50        | 1.46     |
| 3   | B     | 802[B] | HEM  | C4A-C3A | 2.47  | 1.48        | 1.43     |
| 3   | A     | 802[B] | HEM  | CHB-C4A | 2.46  | 1.44        | 1.39     |
| 3   | C     | 802[B] | HEM  | C4A-C3A | 2.43  | 1.48        | 1.43     |
| 3   | A     | 802[B] | HEM  | CHD-C4C | 2.42  | 1.43        | 1.38     |
| 2   | C     | 801[A] | HDD  | C1B-C2B | 2.42  | 1.49        | 1.44     |
| 3   | A     | 802[B] | HEM  | CHA-C1A | 2.39  | 1.44        | 1.39     |
| 3   | B     | 802[B] | HEM  | CHB-C1B | 2.38  | 1.43        | 1.38     |
| 2   | A     | 801[A] | HDD  | C1B-NB  | -2.34 | 1.36        | 1.40     |
| 2   | D     | 801[A] | HDD  | CHB-C4A | 2.34  | 1.44        | 1.39     |
| 2   | B     | 801[A] | HDD  | C1C-NC  | -2.32 | 1.35        | 1.39     |
| 3   | C     | 802[B] | HEM  | CHA-C1A | 2.27  | 1.44        | 1.39     |
| 3   | C     | 802[B] | HEM  | C1B-NB  | -2.23 | 1.36        | 1.40     |
| 3   | C     | 802[B] | HEM  | CHB-C4A | 2.23  | 1.44        | 1.39     |
| 2   | A     | 801[A] | HDD  | C1A-NA  | -2.20 | 1.35        | 1.39     |

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| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 3   | C     | 802[B] | HEM  | O1A-CGA | 2.18  | 1.29        | 1.22     |
| 3   | A     | 802[B] | HEM  | C3B-C2B | 2.18  | 1.41        | 1.37     |
| 2   | D     | 801[A] | HDD  | C1B-NB  | -2.14 | 1.36        | 1.40     |
| 2   | D     | 801[A] | HDD  | CBA-CAA | 2.13  | 1.59        | 1.51     |
| 2   | A     | 801[A] | HDD  | FE-NB   | 2.12  | 2.01        | 1.94     |
| 3   | A     | 802[B] | HEM  | C4D-ND  | -2.12 | 1.36        | 1.40     |
| 3   | C     | 802[B] | HEM  | CHB-C1B | 2.11  | 1.42        | 1.38     |
| 2   | A     | 801[A] | HDD  | CHD-C4C | 2.08  | 1.42        | 1.38     |
| 3   | C     | 802[B] | HEM  | CHC-C4B | 2.08  | 1.43        | 1.39     |
| 2   | A     | 801[A] | HDD  | C3C-C2C | 2.06  | 1.41        | 1.37     |
| 2   | C     | 801[A] | HDD  | C2A-C3A | 2.05  | 1.44        | 1.38     |
| 3   | B     | 802[B] | HEM  | CHB-C4A | 2.04  | 1.44        | 1.39     |
| 2   | B     | 801[A] | HDD  | C3B-C2B | 2.04  | 1.41        | 1.37     |
| 2   | A     | 801[A] | HDD  | C2A-C3A | 2.03  | 1.44        | 1.38     |
| 2   | B     | 801[A] | HDD  | C1B-NB  | -2.02 | 1.36        | 1.40     |
| 2   | C     | 801[A] | HDD  | C1B-NB  | -2.02 | 1.36        | 1.40     |
| 2   | D     | 801[A] | HDD  | C3C-C2C | 2.02  | 1.41        | 1.37     |

All (224) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|--------|-------------|----------|
| 2   | A     | 801[A] | HDD  | O1D-CGD-CBD | -10.34 | 100.74      | 110.17   |
| 2   | B     | 801[A] | HDD  | O1D-CGD-O2D | 10.04  | 129.27      | 120.81   |
| 2   | A     | 801[A] | HDD  | C3C-C2C-C1C | -9.88  | 97.70       | 107.05   |
| 2   | B     | 801[A] | HDD  | C3C-C2C-C1C | -9.63  | 97.93       | 107.05   |
| 2   | D     | 801[A] | HDD  | C3D-O1D-CGD | 9.48   | 119.98      | 111.14   |
| 2   | B     | 801[A] | HDD  | OND-C2D-CMD | -9.16  | 91.74       | 109.45   |
| 2   | A     | 801[A] | HDD  | O1D-CGD-O2D | 8.75   | 128.18      | 120.81   |
| 2   | D     | 801[A] | HDD  | O1D-CGD-O2D | 8.69   | 128.13      | 120.81   |
| 2   | D     | 801[A] | HDD  | C3C-C2C-C1C | -8.34  | 99.15       | 107.05   |
| 3   | A     | 802[B] | HEM  | C3B-C2B-C1B | -7.73  | 100.61      | 106.41   |
| 2   | B     | 801[A] | HDD  | O1D-CGD-CBD | -7.65  | 103.20      | 110.17   |
| 3   | C     | 802[B] | HEM  | C3B-C4B-NB  | 7.64   | 114.96      | 109.47   |
| 2   | A     | 801[A] | HDD  | C3D-O1D-CGD | 7.51   | 118.15      | 111.14   |
| 3   | D     | 802[B] | HEM  | C2B-C1B-NB  | 7.50   | 118.47      | 109.84   |
| 2   | C     | 801[A] | HDD  | C3C-C2C-C1C | -7.16  | 100.27      | 107.05   |
| 3   | D     | 802[B] | HEM  | C3B-C2B-C1B | -7.08  | 101.09      | 106.41   |
| 2   | B     | 801[A] | HDD  | C3D-O1D-CGD | 7.08   | 117.74      | 111.14   |
| 3   | C     | 802[B] | HEM  | C3B-C2B-C1B | -6.86  | 101.26      | 106.41   |
| 3   | B     | 802[B] | HEM  | C2B-C1B-NB  | 6.77   | 117.62      | 109.84   |
| 2   | D     | 801[A] | HDD  | C3B-C2B-C1B | -6.69  | 101.39      | 106.41   |
| 3   | D     | 802[B] | HEM  | C4C-NC-C1C  | -6.44  | 95.32       | 105.82   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 3   | B     | 802[B] | HEM  | C3B-C2B-C1B | -6.40 | 101.60      | 106.41   |
| 3   | A     | 802[B] | HEM  | C2B-C1B-NB  | 6.39  | 117.18      | 109.84   |
| 3   | A     | 802[B] | HEM  | C3D-C4D-ND  | 6.26  | 117.04      | 110.17   |
| 3   | C     | 802[B] | HEM  | C2B-C1B-NB  | 6.21  | 116.98      | 109.84   |
| 2   | D     | 801[A] | HDD  | O1D-CGD-CBD | -6.19 | 104.53      | 110.17   |
| 3   | C     | 802[B] | HEM  | C3D-C4D-ND  | 6.01  | 116.76      | 110.17   |
| 3   | B     | 802[B] | HEM  | C2D-C1D-ND  | 5.99  | 116.83      | 109.90   |
| 2   | A     | 801[A] | HDD  | C3B-C2B-C1B | -5.97 | 101.93      | 106.41   |
| 3   | D     | 802[B] | HEM  | C3B-C4B-NB  | 5.95  | 113.74      | 109.47   |
| 3   | D     | 802[B] | HEM  | C3D-C4D-ND  | 5.89  | 116.63      | 110.17   |
| 2   | C     | 801[A] | HDD  | C3B-C2B-C1B | -5.86 | 102.01      | 106.41   |
| 3   | A     | 802[B] | HEM  | C2D-C1D-ND  | 5.83  | 116.64      | 109.90   |
| 3   | B     | 802[B] | HEM  | C3C-C2C-C1C | -5.70 | 101.65      | 107.05   |
| 2   | C     | 801[A] | HDD  | O1D-CGD-O2D | 5.68  | 125.60      | 120.81   |
| 2   | C     | 801[A] | HDD  | OND-C2D-CMD | -5.64 | 98.54       | 109.45   |
| 3   | C     | 802[B] | HEM  | C2D-C1D-ND  | 5.62  | 116.39      | 109.90   |
| 2   | D     | 801[A] | HDD  | CMC-C2C-C1C | 5.50  | 134.42      | 124.73   |
| 2   | B     | 801[A] | HDD  | C3B-C2B-C1B | -5.45 | 102.32      | 106.41   |
| 3   | B     | 802[B] | HEM  | C3D-C4D-ND  | 5.34  | 116.02      | 110.17   |
| 2   | D     | 801[A] | HDD  | CBD-CAD-C3D | 5.34  | 111.59      | 103.98   |
| 3   | D     | 802[B] | HEM  | C2D-C1D-ND  | 5.20  | 115.91      | 109.90   |
| 3   | D     | 802[B] | HEM  | CMC-C2C-C1C | 5.11  | 133.72      | 124.73   |
| 3   | D     | 802[B] | HEM  | C3C-C2C-C1C | -4.99 | 102.32      | 107.05   |
| 3   | D     | 802[B] | HEM  | CHD-C4C-C3C | -4.94 | 116.87      | 125.21   |
| 3   | C     | 802[B] | HEM  | C1D-C2D-C3D | -4.94 | 101.78      | 106.98   |
| 3   | C     | 802[B] | HEM  | C3C-C2C-C1C | -4.81 | 102.50      | 107.05   |
| 2   | D     | 801[A] | HDD  | CAA-CBA-CGA | -4.71 | 101.17      | 113.67   |
| 2   | B     | 801[A] | HDD  | C4A-C3A-C2A | -4.68 | 101.45      | 106.82   |
| 2   | B     | 801[A] | HDD  | CAA-CBA-CGA | -4.64 | 101.35      | 113.67   |
| 3   | C     | 802[B] | HEM  | C2A-C1A-NA  | 4.56  | 115.21      | 110.15   |
| 3   | B     | 802[B] | HEM  | C4A-NA-C1A  | -4.55 | 98.40       | 105.82   |
| 3   | A     | 802[B] | HEM  | C3C-C2C-C1C | -4.54 | 102.75      | 107.05   |
| 3   | C     | 802[B] | HEM  | CHC-C1C-C2C | -4.52 | 116.08      | 125.49   |
| 2   | B     | 801[A] | HDD  | C3B-C4B-NB  | 4.52  | 112.71      | 109.47   |
| 3   | A     | 802[B] | HEM  | C3B-C4B-NB  | 4.44  | 112.66      | 109.47   |
| 3   | D     | 802[B] | HEM  | C2C-C1C-NC  | 4.42  | 117.82      | 109.64   |
| 2   | A     | 801[A] | HDD  | OND-C2D-CMD | -4.33 | 101.07      | 109.45   |
| 2   | C     | 801[A] | HDD  | CBD-CAD-C3D | 4.31  | 110.13      | 103.98   |
| 2   | A     | 801[A] | HDD  | C2B-C1B-NB  | 4.30  | 114.78      | 109.84   |
| 2   | A     | 801[A] | HDD  | C2C-C1C-NC  | 4.27  | 117.54      | 109.64   |
| 2   | A     | 801[A] | HDD  | CHC-C1C-C2C | -4.26 | 116.64      | 125.49   |
| 3   | C     | 802[B] | HEM  | C4C-NC-C1C  | -4.22 | 98.94       | 105.82   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 3   | B     | 802[B] | HEM  | C2A-C1A-NA  | 4.17  | 114.78      | 110.15   |
| 2   | B     | 801[A] | HDD  | C2B-C1B-NB  | 4.14  | 114.60      | 109.84   |
| 3   | A     | 802[B] | HEM  | C1D-C2D-C3D | -4.13 | 102.63      | 106.98   |
| 3   | B     | 802[B] | HEM  | C4C-NC-C1C  | -4.13 | 99.09       | 105.82   |
| 3   | B     | 802[B] | HEM  | CMC-C2C-C1C | 4.12  | 131.99      | 124.73   |
| 3   | A     | 802[B] | HEM  | C4D-ND-C1D  | -4.11 | 100.34      | 105.21   |
| 3   | D     | 802[B] | HEM  | C1D-C2D-C3D | -4.10 | 102.67      | 106.98   |
| 2   | B     | 801[A] | HDD  | CMC-C2C-C1C | 4.10  | 131.94      | 124.73   |
| 2   | A     | 801[A] | HDD  | O1D-C3D-CAD | -4.06 | 95.55       | 103.06   |
| 2   | C     | 801[A] | HDD  | CAA-CBA-CGA | -4.06 | 102.90      | 113.67   |
| 3   | C     | 802[B] | HEM  | C2C-C1C-NC  | 3.97  | 116.99      | 109.64   |
| 3   | A     | 802[B] | HEM  | C4C-NC-C1C  | -3.95 | 99.38       | 105.82   |
| 3   | B     | 802[B] | HEM  | C4D-ND-C1D  | -3.94 | 100.54      | 105.21   |
| 2   | D     | 801[A] | HDD  | OND-C2D-CMD | -3.89 | 101.93      | 109.45   |
| 3   | A     | 802[B] | HEM  | CAA-CBA-CGA | -3.88 | 103.36      | 113.67   |
| 2   | A     | 801[A] | HDD  | CMC-C2C-C1C | 3.86  | 131.52      | 124.73   |
| 2   | C     | 801[A] | HDD  | C2D-C1D-CHD | -3.77 | 117.34      | 123.28   |
| 2   | D     | 801[A] | HDD  | C1C-CHC-C4B | 3.77  | 134.04      | 126.02   |
| 3   | C     | 802[B] | HEM  | C4A-NA-C1A  | -3.73 | 99.74       | 105.82   |
| 2   | A     | 801[A] | HDD  | CAA-C2A-C1A | 3.70  | 132.17      | 124.94   |
| 3   | C     | 802[B] | HEM  | C1C-CHC-C4B | -3.69 | 118.17      | 126.02   |
| 2   | D     | 801[A] | HDD  | C2C-C1C-NC  | 3.68  | 116.44      | 109.64   |
| 2   | B     | 801[A] | HDD  | C2C-C1C-NC  | 3.65  | 116.39      | 109.64   |
| 2   | B     | 801[A] | HDD  | C4C-C3C-C2C | 3.63  | 109.96      | 106.81   |
| 3   | B     | 802[B] | HEM  | C1D-C2D-C3D | -3.62 | 103.17      | 106.98   |
| 3   | B     | 802[B] | HEM  | CHB-C1B-C2B | -3.57 | 116.81      | 126.95   |
| 3   | B     | 802[B] | HEM  | CMB-C2B-C3B | 3.56  | 137.05      | 128.43   |
| 3   | B     | 802[B] | HEM  | CHA-C4D-C3D | -3.54 | 118.71      | 125.23   |
| 3   | C     | 802[B] | HEM  | C4D-ND-C1D  | -3.53 | 101.03      | 105.21   |
| 2   | D     | 801[A] | HDD  | C2B-C1B-NB  | 3.51  | 113.88      | 109.84   |
| 2   | D     | 801[A] | HDD  | CAA-C2A-C1A | 3.49  | 131.76      | 124.94   |
| 3   | B     | 802[B] | HEM  | CBD-CAD-C3D | -3.46 | 102.97      | 112.53   |
| 2   | A     | 801[A] | HDD  | CAA-CBA-CGA | -3.46 | 104.50      | 113.67   |
| 2   | A     | 801[A] | HDD  | CHD-C4C-NC  | -3.45 | 120.69      | 124.45   |
| 3   | B     | 802[B] | HEM  | C3A-C4A-NA  | 3.45  | 115.68      | 110.14   |
| 2   | D     | 801[A] | HDD  | CHC-C4B-NB  | -3.45 | 120.71      | 124.42   |
| 3   | C     | 802[B] | HEM  | CHC-C4B-C3B | -3.43 | 118.22      | 125.07   |
| 2   | C     | 801[A] | HDD  | C2B-C1B-NB  | 3.43  | 113.79      | 109.84   |
| 3   | D     | 802[B] | HEM  | C1B-NB-C4B  | -3.43 | 101.14      | 105.21   |
| 2   | C     | 801[A] | HDD  | C2C-C1C-NC  | 3.43  | 115.98      | 109.64   |
| 3   | C     | 802[B] | HEM  | C1B-NB-C4B  | -3.43 | 101.15      | 105.21   |
| 2   | B     | 801[A] | HDD  | CBD-CAD-C3D | 3.42  | 108.85      | 103.98   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 3   | B     | 802[B] | HEM  | C2C-C1C-NC  | 3.40  | 115.93      | 109.64   |
| 3   | A     | 802[B] | HEM  | CMB-C2B-C1B | 3.40  | 130.35      | 125.03   |
| 3   | A     | 802[B] | HEM  | CHC-C1C-C2C | -3.36 | 118.49      | 125.49   |
| 3   | B     | 802[B] | HEM  | CHB-C4A-C3A | -3.35 | 117.71      | 127.43   |
| 2   | C     | 801[A] | HDD  | CMC-C2C-C1C | 3.27  | 130.49      | 124.73   |
| 2   | D     | 801[A] | HDD  | CHD-C4C-NC  | -3.26 | 120.91      | 124.45   |
| 3   | D     | 802[B] | HEM  | CHB-C1B-C2B | -3.25 | 117.70      | 126.95   |
| 3   | A     | 802[B] | HEM  | C4A-NA-C1A  | -3.25 | 100.52      | 105.82   |
| 3   | C     | 802[B] | HEM  | CBD-CAD-C3D | -3.23 | 103.60      | 112.53   |
| 3   | A     | 802[B] | HEM  | CHD-C1D-C2D | -3.22 | 119.94      | 125.03   |
| 3   | A     | 802[B] | HEM  | C2C-C1C-NC  | 3.20  | 115.56      | 109.64   |
| 3   | A     | 802[B] | HEM  | C4A-CHB-C1B | -3.19 | 118.75      | 126.25   |
| 2   | D     | 801[A] | HDD  | O1D-C3D-CAD | -3.16 | 97.21       | 103.06   |
| 3   | A     | 802[B] | HEM  | CBB-CAB-C3B | -3.16 | 111.73      | 127.53   |
| 3   | C     | 802[B] | HEM  | CHB-C1B-C2B | -3.15 | 117.99      | 126.95   |
| 3   | A     | 802[B] | HEM  | CHB-C4A-C3A | -3.15 | 118.28      | 127.43   |
| 2   | B     | 801[A] | HDD  | CMD-C2D-C3D | 3.15  | 123.39      | 115.11   |
| 3   | A     | 802[B] | HEM  | CHB-C1B-C2B | -3.06 | 118.24      | 126.95   |
| 3   | D     | 802[B] | HEM  | CAD-C3D-C2D | 3.06  | 133.60      | 127.87   |
| 2   | A     | 801[A] | HDD  | CHB-C1B-C2B | -3.05 | 118.28      | 126.95   |
| 2   | B     | 801[A] | HDD  | CHB-C1B-NB  | -3.03 | 120.62      | 124.37   |
| 3   | C     | 802[B] | HEM  | CHA-C1A-C2A | -3.02 | 118.68      | 125.30   |
| 2   | C     | 801[A] | HDD  | C4A-C3A-C2A | -3.00 | 103.38      | 106.82   |
| 3   | D     | 802[B] | HEM  | C4D-ND-C1D  | -2.99 | 101.67      | 105.21   |
| 2   | B     | 801[A] | HDD  | CAD-CBD-CGD | 2.98  | 108.91      | 104.48   |
| 3   | C     | 802[B] | HEM  | C4A-CHB-C1B | -2.96 | 119.28      | 126.25   |
| 3   | D     | 802[B] | HEM  | CHD-C1D-C2D | -2.96 | 120.36      | 125.03   |
| 3   | C     | 802[B] | HEM  | CBB-CAB-C3B | -2.95 | 112.81      | 127.53   |
| 3   | B     | 802[B] | HEM  | C3B-C4B-NB  | 2.94  | 111.58      | 109.47   |
| 3   | B     | 802[B] | HEM  | CAA-C2A-C1A | 2.94  | 130.68      | 124.94   |
| 3   | A     | 802[B] | HEM  | C2A-C1A-NA  | 2.91  | 113.38      | 110.15   |
| 2   | D     | 801[A] | HDD  | C3B-C4B-NB  | 2.88  | 111.54      | 109.47   |
| 3   | B     | 802[B] | HEM  | CHD-C1D-C2D | -2.87 | 120.49      | 125.03   |
| 3   | C     | 802[B] | HEM  | CHA-C4D-C3D | -2.83 | 120.00      | 125.23   |
| 3   | C     | 802[B] | HEM  | C3A-C4A-NA  | 2.82  | 114.67      | 110.14   |
| 3   | D     | 802[B] | HEM  | CHC-C1C-C2C | -2.82 | 119.61      | 125.49   |
| 2   | B     | 801[A] | HDD  | CMA-C3A-C2A | 2.82  | 131.60      | 125.62   |
| 3   | A     | 802[B] | HEM  | CHA-C4D-C3D | -2.80 | 120.06      | 125.23   |
| 3   | B     | 802[B] | HEM  | CHD-C4C-C3C | -2.79 | 120.51      | 125.21   |
| 2   | C     | 801[A] | HDD  | CHD-C4C-NC  | -2.79 | 121.42      | 124.45   |
| 3   | D     | 802[B] | HEM  | C4A-CHB-C1B | -2.79 | 119.70      | 126.25   |
| 3   | B     | 802[B] | HEM  | CHC-C1C-NC  | -2.77 | 121.43      | 124.45   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 3   | D     | 802[B] | HEM  | CMB-C2B-C3B | 2.77  | 135.13      | 128.43   |
| 3   | D     | 802[B] | HEM  | C4C-CHD-C1D | -2.77 | 120.14      | 126.02   |
| 3   | A     | 802[B] | HEM  | CMC-C2C-C1C | 2.76  | 129.59      | 124.73   |
| 2   | B     | 801[A] | HDD  | CBA-CAA-C2A | -2.71 | 105.04      | 112.53   |
| 3   | C     | 802[B] | HEM  | C4C-C3C-C2C | 2.70  | 109.15      | 106.81   |
| 3   | C     | 802[B] | HEM  | CHD-C1D-C2D | -2.68 | 120.79      | 125.03   |
| 3   | C     | 802[B] | HEM  | CMC-C2C-C1C | 2.66  | 129.41      | 124.73   |
| 3   | C     | 802[B] | HEM  | C4C-CHD-C1D | -2.66 | 120.37      | 126.02   |
| 2   | B     | 801[A] | HDD  | C4D-ND-C1D  | -2.66 | 102.16      | 105.27   |
| 3   | D     | 802[B] | HEM  | C4D-C3D-C2D | -2.61 | 103.09      | 106.89   |
| 3   | A     | 802[B] | HEM  | CAA-C2A-C1A | 2.60  | 130.03      | 124.94   |
| 2   | A     | 801[A] | HDD  | C4A-CHB-C1B | -2.59 | 120.16      | 126.25   |
| 3   | D     | 802[B] | HEM  | CBD-CAD-C3D | -2.59 | 105.38      | 112.53   |
| 3   | D     | 802[B] | HEM  | C1C-CHC-C4B | -2.57 | 120.56      | 126.02   |
| 3   | B     | 802[B] | HEM  | C4C-C3C-C2C | 2.53  | 109.01      | 106.81   |
| 2   | C     | 801[A] | HDD  | CMD-C2D-C3D | 2.53  | 121.78      | 115.11   |
| 3   | C     | 802[B] | HEM  | CHB-C4A-C3A | -2.53 | 120.09      | 127.43   |
| 3   | A     | 802[B] | HEM  | C4D-C3D-C2D | -2.52 | 103.22      | 106.89   |
| 2   | D     | 801[A] | HDD  | O2A-CGA-CBA | 2.52  | 121.96      | 114.00   |
| 3   | A     | 802[B] | HEM  | C1B-NB-C4B  | -2.51 | 102.24      | 105.21   |
| 3   | B     | 802[B] | HEM  | O2A-CGA-O1A | -2.51 | 116.88      | 123.33   |
| 2   | D     | 801[A] | HDD  | C4C-CHD-C1D | -2.50 | 121.96      | 125.99   |
| 2   | B     | 801[A] | HDD  | CHC-C1C-C2C | -2.50 | 120.29      | 125.49   |
| 3   | B     | 802[B] | HEM  | C4D-C3D-C2D | -2.48 | 103.28      | 106.89   |
| 3   | B     | 802[B] | HEM  | C4A-CHB-C1B | -2.48 | 120.42      | 126.25   |
| 2   | A     | 801[A] | HDD  | C4C-C3C-C2C | 2.47  | 108.95      | 106.81   |
| 3   | B     | 802[B] | HEM  | C1A-CHA-C4D | -2.46 | 120.45      | 126.25   |
| 2   | A     | 801[A] | HDD  | C2A-C1A-NA  | 2.46  | 112.89      | 110.15   |
| 2   | D     | 801[A] | HDD  | CHB-C1B-NB  | -2.44 | 121.35      | 124.37   |
| 3   | D     | 802[B] | HEM  | CAA-CBA-CGA | -2.43 | 107.21      | 113.67   |
| 2   | C     | 801[A] | HDD  | CAA-C2A-C1A | 2.43  | 129.69      | 124.94   |
| 2   | D     | 801[A] | HDD  | C4D-ND-C1D  | -2.40 | 102.45      | 105.27   |
| 2   | A     | 801[A] | HDD  | C4C-NC-C1C  | -2.39 | 101.92      | 105.82   |
| 3   | B     | 802[B] | HEM  | CAD-C3D-C2D | 2.38  | 132.32      | 127.87   |
| 3   | A     | 802[B] | HEM  | C3A-C4A-NA  | 2.37  | 113.94      | 110.14   |
| 3   | B     | 802[B] | HEM  | CMB-C2B-C1B | -2.37 | 121.33      | 125.03   |
| 3   | A     | 802[B] | HEM  | C4C-CHD-C1D | -2.35 | 121.02      | 126.02   |
| 3   | C     | 802[B] | HEM  | CAA-C2A-C1A | 2.34  | 129.51      | 124.94   |
| 2   | A     | 801[A] | HDD  | O2A-CGA-CBA | 2.33  | 121.35      | 114.00   |
| 2   | C     | 801[A] | HDD  | CBA-CAA-C2A | -2.31 | 106.16      | 112.53   |
| 2   | D     | 801[A] | HDD  | CMA-C3A-C2A | 2.29  | 130.48      | 125.62   |
| 2   | C     | 801[A] | HDD  | CHC-C1C-C2C | -2.29 | 120.72      | 125.49   |

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| Mol | Chain | Res    | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-------------|-------|-------------|----------|
| 2   | D     | 801[A] | HDD  | OND-C2D-C3D | -2.29 | 105.10      | 110.46   |
| 3   | D     | 802[B] | HEM  | CHA-C4D-C3D | -2.28 | 121.02      | 125.23   |
| 3   | C     | 802[B] | HEM  | CMD-C2D-C3D | 2.28  | 132.31      | 126.15   |
| 2   | D     | 801[A] | HDD  | CHB-C4A-C3A | -2.26 | 120.86      | 127.43   |
| 2   | A     | 801[A] | HDD  | C1A-C2A-C3A | -2.26 | 103.37      | 106.87   |
| 3   | C     | 802[B] | HEM  | CHC-C1C-NC  | 2.26  | 126.91      | 124.45   |
| 2   | C     | 801[A] | HDD  | C3D-O1D-CGD | 2.25  | 113.24      | 111.14   |
| 3   | D     | 802[B] | HEM  | C4A-NA-C1A  | -2.25 | 102.16      | 105.82   |
| 2   | D     | 801[A] | HDD  | CBA-CAA-C2A | -2.23 | 106.38      | 112.53   |
| 2   | C     | 801[A] | HDD  | O2A-CGA-CBA | 2.23  | 121.03      | 114.00   |
| 3   | A     | 802[B] | HEM  | C1C-CHC-C4B | -2.22 | 121.29      | 126.02   |
| 3   | D     | 802[B] | HEM  | O2A-CGA-CBA | 2.20  | 120.96      | 114.00   |
| 3   | D     | 802[B] | HEM  | CHB-C4A-C3A | -2.20 | 121.03      | 127.43   |
| 2   | B     | 801[A] | HDD  | CBC-CAC-C3C | -2.19 | 116.60      | 127.53   |
| 3   | B     | 802[B] | HEM  | CMD-C2D-C1D | 2.18  | 128.44      | 125.03   |
| 3   | D     | 802[B] | HEM  | CMD-C2D-C3D | 2.17  | 132.03      | 126.15   |
| 2   | D     | 801[A] | HDD  | CHC-C1C-C2C | -2.16 | 120.99      | 125.49   |
| 3   | C     | 802[B] | HEM  | C4D-C3D-C2D | -2.16 | 103.75      | 106.89   |
| 2   | D     | 801[A] | HDD  | C2D-C1D-CHD | -2.13 | 119.93      | 123.28   |
| 2   | C     | 801[A] | HDD  | C4D-ND-C1D  | -2.12 | 102.79      | 105.27   |
| 2   | A     | 801[A] | HDD  | CMA-C3A-C4A | 2.10  | 128.61      | 125.42   |
| 2   | C     | 801[A] | HDD  | CHB-C4A-C3A | -2.09 | 121.37      | 127.43   |
| 3   | A     | 802[B] | HEM  | CHB-C4A-NA  | 2.08  | 127.64      | 123.86   |
| 3   | B     | 802[B] | HEM  | CBB-CAB-C3B | -2.08 | 117.11      | 127.53   |
| 3   | D     | 802[B] | HEM  | C2A-C1A-NA  | 2.08  | 112.46      | 110.15   |
| 2   | D     | 801[A] | HDD  | C4C-NC-C1C  | -2.07 | 102.44      | 105.82   |
| 2   | A     | 801[A] | HDD  | CMD-C2D-C3D | 2.06  | 120.53      | 115.11   |
| 2   | C     | 801[A] | HDD  | CMA-C3A-C2A | 2.06  | 129.99      | 125.62   |
| 2   | A     | 801[A] | HDD  | CHB-C1B-NB  | 2.06  | 126.91      | 124.37   |
| 2   | C     | 801[A] | HDD  | C4B-C3B-C2B | 2.05  | 109.17      | 107.28   |
| 2   | C     | 801[A] | HDD  | CMB-C2B-C3B | 2.04  | 133.37      | 128.43   |
| 3   | D     | 802[B] | HEM  | CHC-C4B-C3B | -2.03 | 121.02      | 125.07   |
| 2   | B     | 801[A] | HDD  | CHB-C4A-C3A | -2.02 | 121.56      | 127.43   |
| 3   | A     | 802[B] | HEM  | C4C-C3C-C2C | 2.02  | 108.56      | 106.81   |
| 3   | B     | 802[B] | HEM  | CMA-C3A-C2A | 2.01  | 129.89      | 125.62   |

All (4) chirality outliers are listed below:

| Mol | Chain | Res    | Type | Atom |
|-----|-------|--------|------|------|
| 2   | A     | 801[A] | HDD  | NC   |
| 2   | B     | 801[A] | HDD  | NC   |
| 2   | C     | 801[A] | HDD  | NC   |

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| Mol | Chain | Res    | Type | Atom |
|-----|-------|--------|------|------|
| 2   | D     | 801[A] | HDD  | NC   |

All (22) torsion outliers are listed below:

| Mol | Chain | Res    | Type | Atoms           |
|-----|-------|--------|------|-----------------|
| 3   | C     | 802[B] | HEM  | C2B-C3B-CAB-CBB |
| 2   | A     | 801[A] | HDD  | C2C-C3C-CAC-CBC |
| 2   | B     | 801[A] | HDD  | C2C-C3C-CAC-CBC |
| 3   | C     | 802[B] | HEM  | C4B-C3B-CAB-CBB |
| 2   | B     | 801[A] | HDD  | CAA-CBA-CGA-O2A |
| 3   | A     | 802[B] | HEM  | CAA-CBA-CGA-O2A |
| 2   | A     | 801[A] | HDD  | CAA-CBA-CGA-O1A |
| 2   | B     | 801[A] | HDD  | CAA-CBA-CGA-O1A |
| 3   | C     | 802[B] | HEM  | CAA-CBA-CGA-O1A |
| 3   | C     | 802[B] | HEM  | CAA-CBA-CGA-O2A |
| 2   | C     | 801[A] | HDD  | CAA-CBA-CGA-O2A |
| 2   | D     | 801[A] | HDD  | CAA-CBA-CGA-O1A |
| 3   | D     | 802[B] | HEM  | CAA-CBA-CGA-O2A |
| 2   | A     | 801[A] | HDD  | CAA-CBA-CGA-O2A |
| 2   | C     | 801[A] | HDD  | CAA-CBA-CGA-O1A |
| 2   | D     | 801[A] | HDD  | CAA-CBA-CGA-O2A |
| 3   | D     | 802[B] | HEM  | CAA-CBA-CGA-O1A |
| 3   | B     | 802[B] | HEM  | CAA-CBA-CGA-O2A |
| 3   | A     | 802[B] | HEM  | CAA-CBA-CGA-O1A |
| 3   | B     | 802[B] | HEM  | CAA-CBA-CGA-O1A |
| 3   | A     | 802[B] | HEM  | C2B-C3B-CAB-CBB |
| 3   | D     | 802[B] | HEM  | C2B-C3B-CAB-CBB |

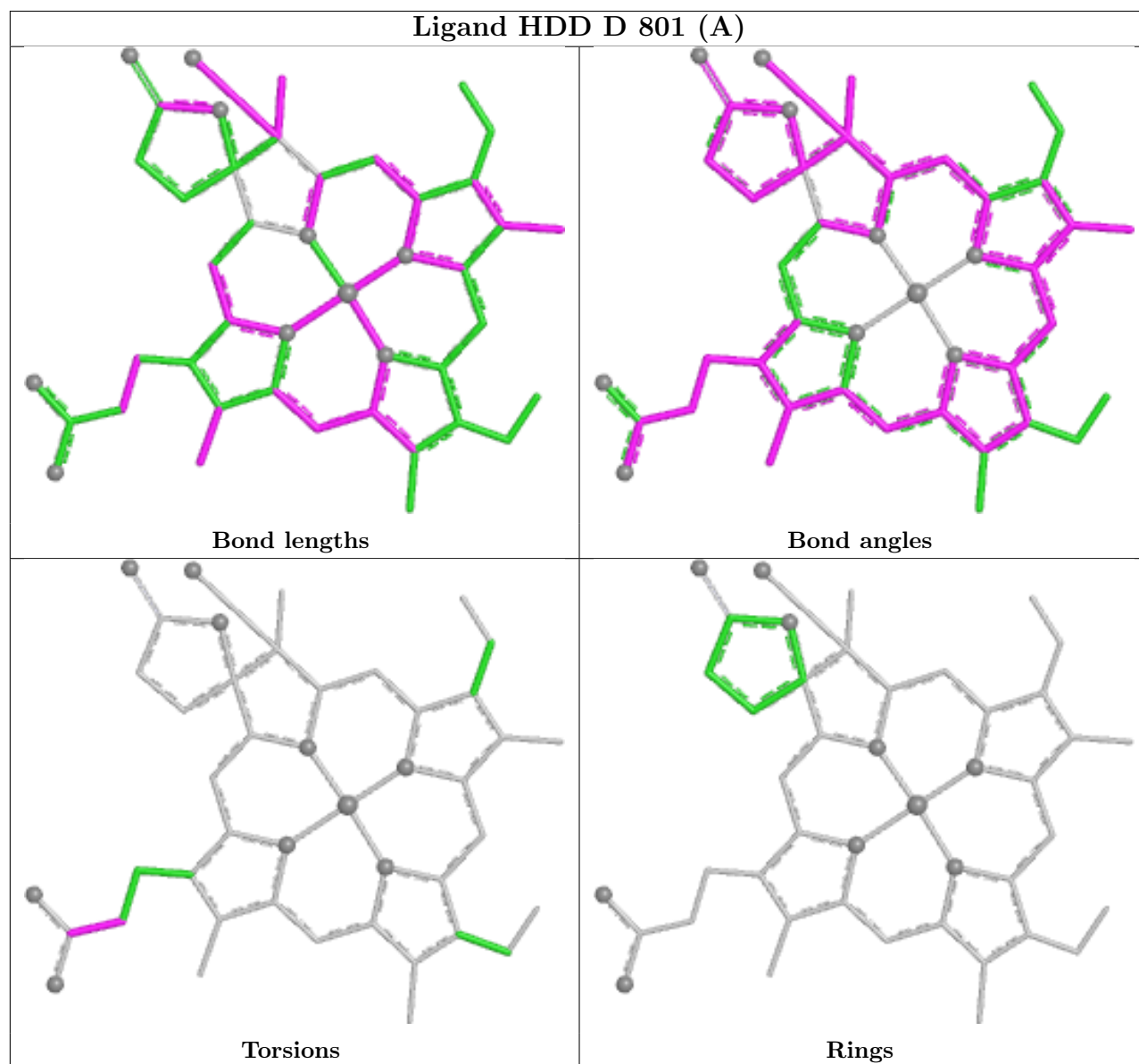
There are no ring outliers.

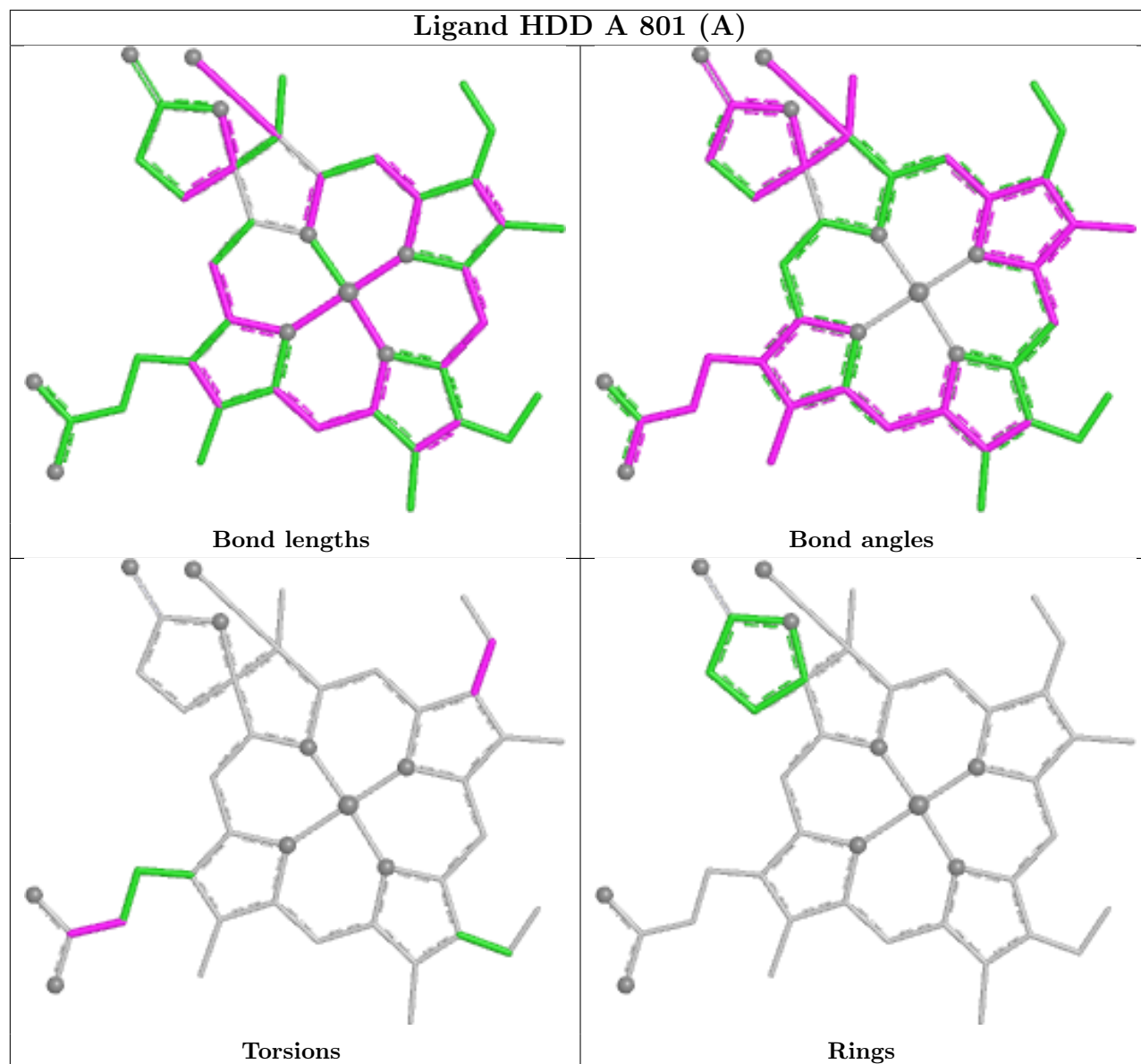
8 monomers are involved in 54 short contacts:

| Mol | Chain | Res    | Type | Clashes | Symm-Clashes |
|-----|-------|--------|------|---------|--------------|
| 2   | D     | 801[A] | HDD  | 4       | 0            |
| 2   | A     | 801[A] | HDD  | 1       | 0            |
| 3   | C     | 802[B] | HEM  | 13      | 0            |
| 3   | A     | 802[B] | HEM  | 13      | 0            |
| 2   | B     | 801[A] | HDD  | 1       | 0            |
| 2   | C     | 801[A] | HDD  | 2       | 0            |
| 3   | B     | 802[B] | HEM  | 12      | 0            |
| 3   | D     | 802[B] | HEM  | 8       | 0            |

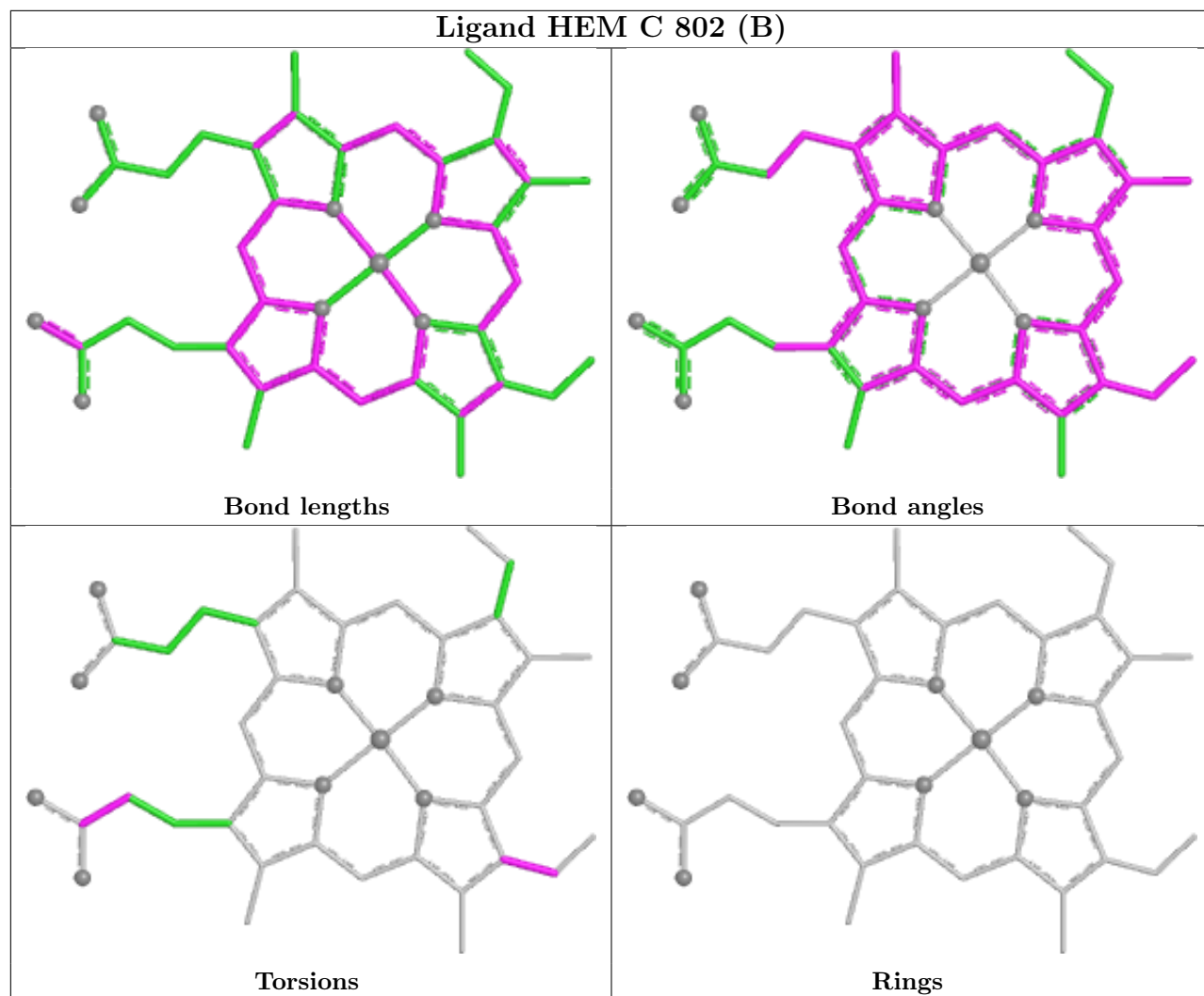
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

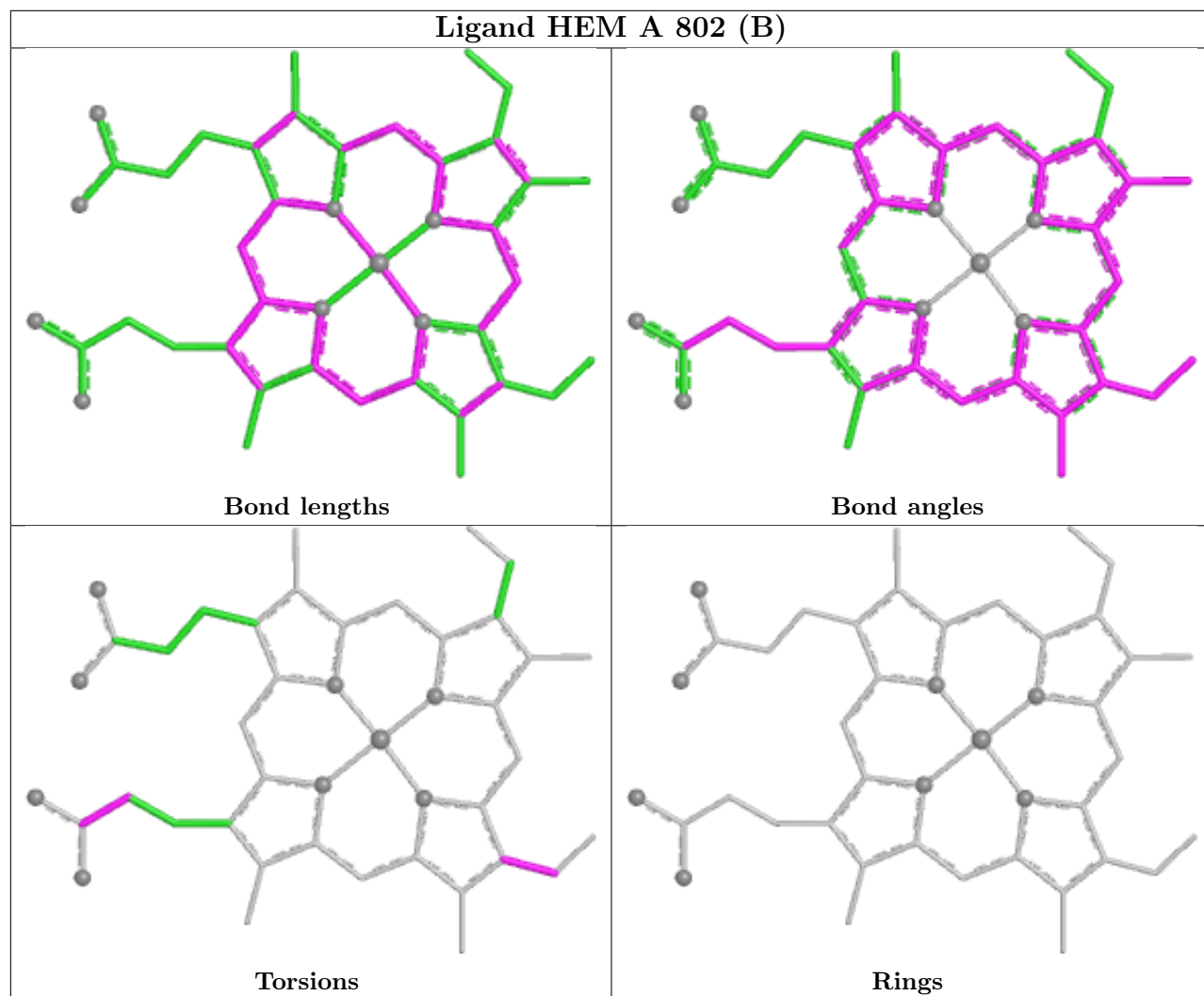


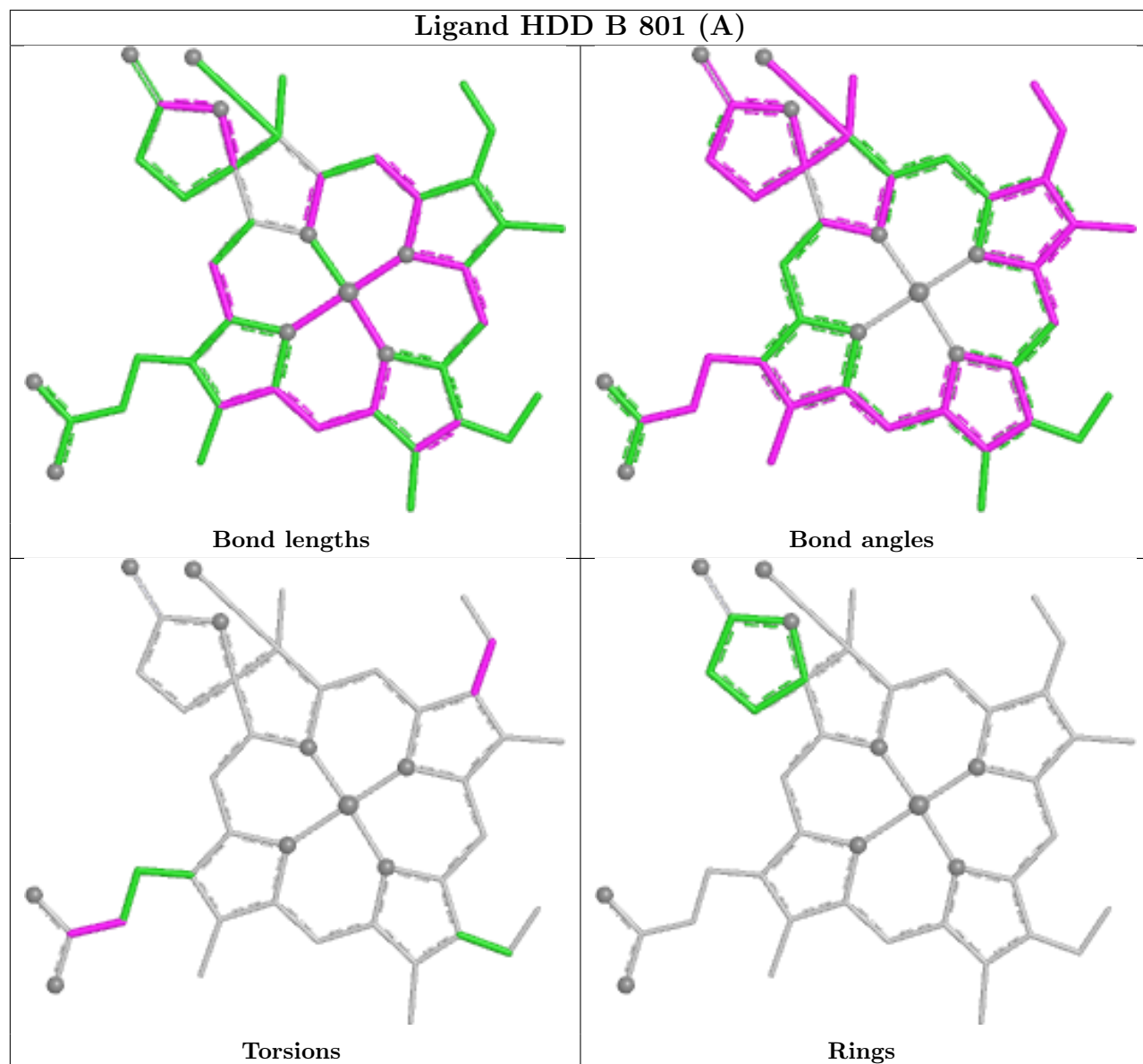


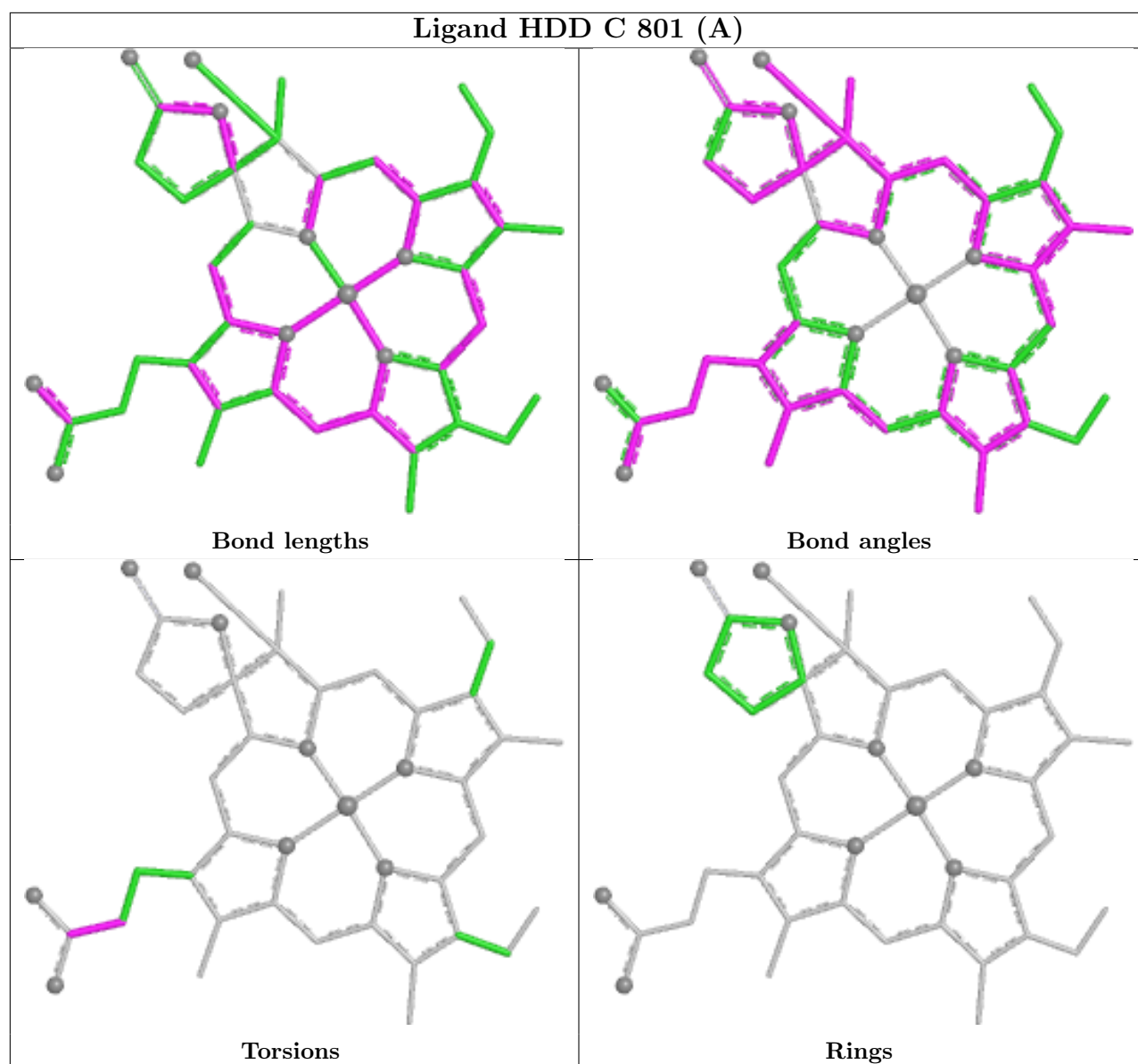
## Ligand HEM C 802 (B)



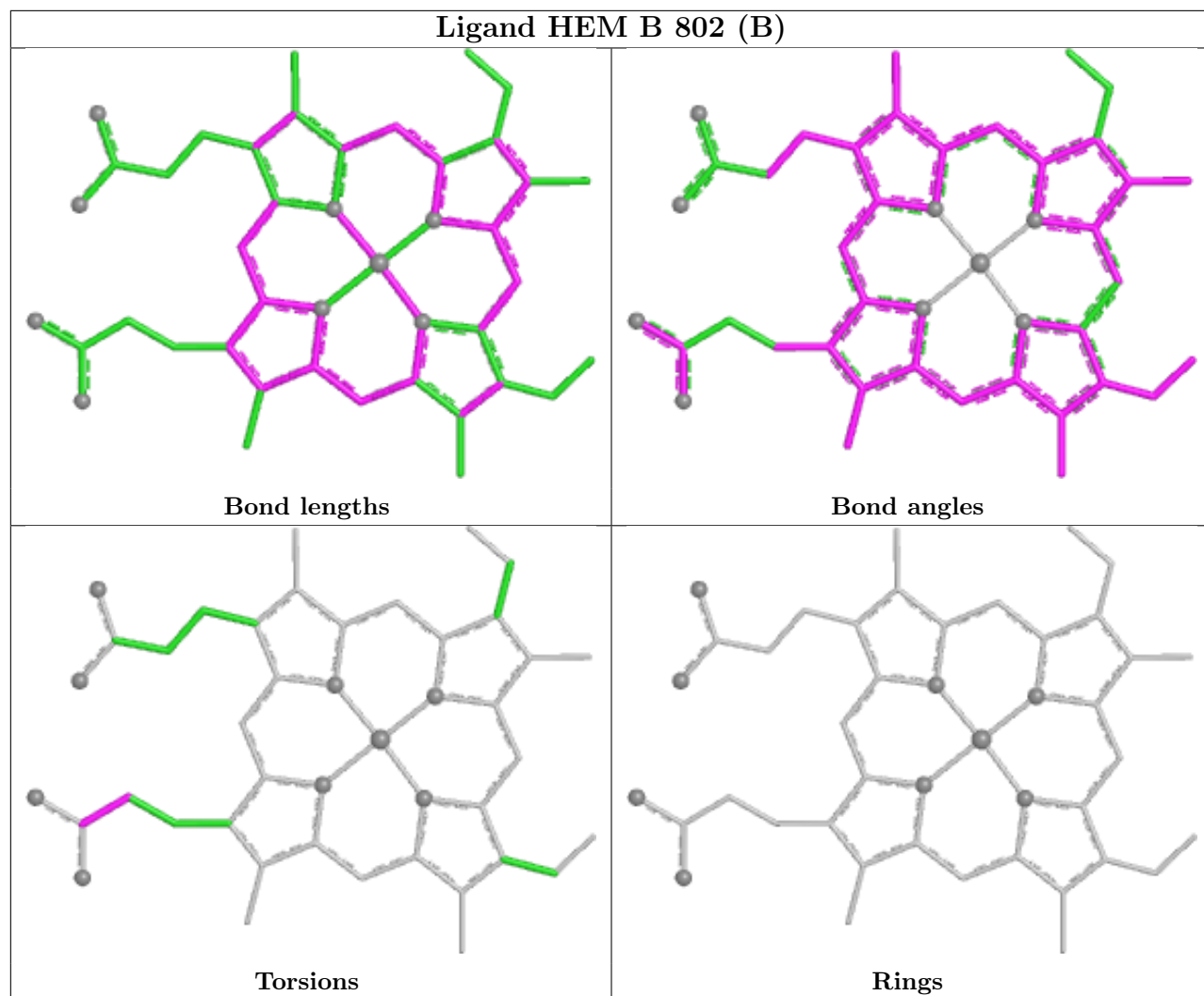
## Ligand HEM A 802 (B)

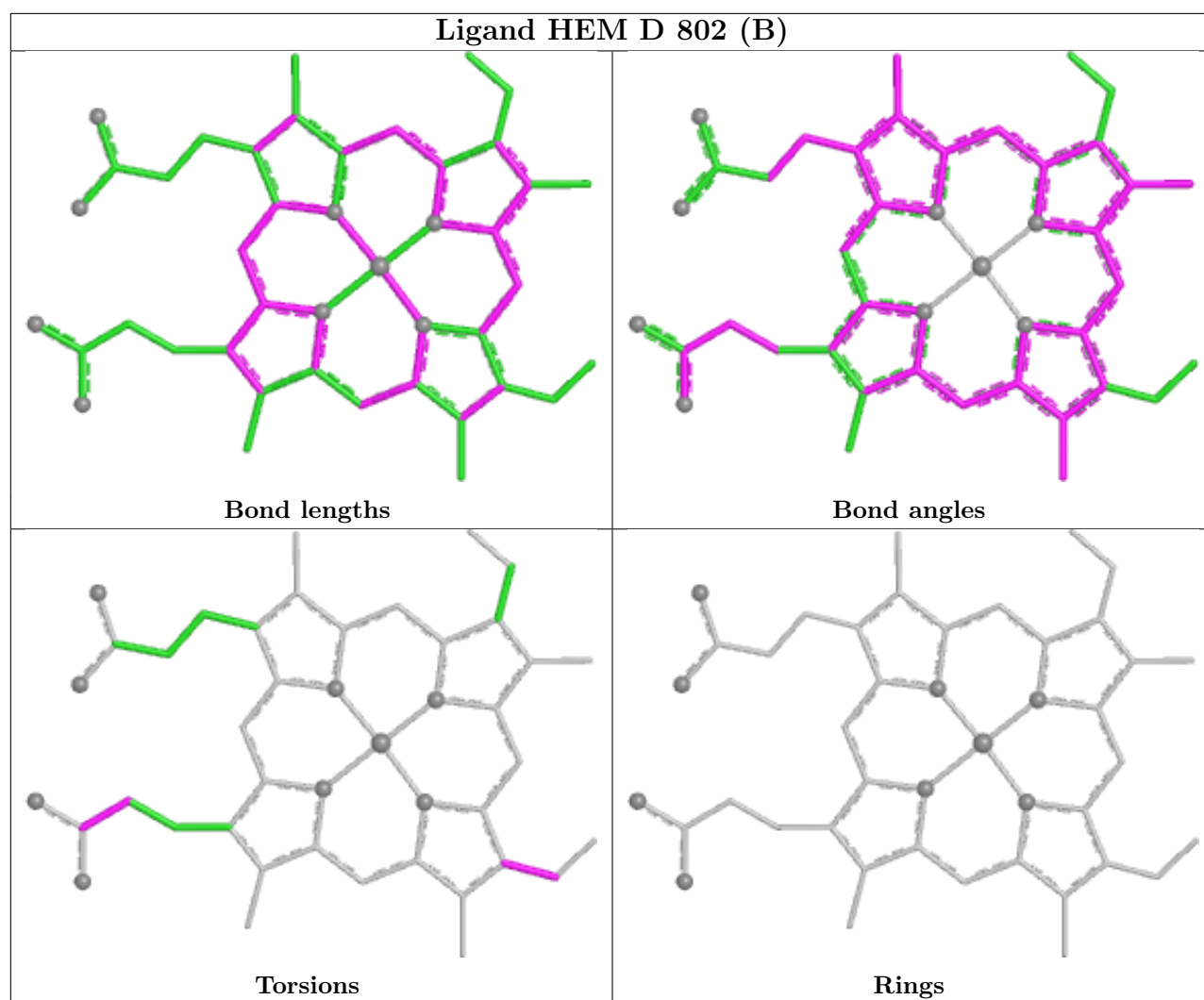






## Ligand HEM B 802 (B)





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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     | 726/753 (96%)   | -0.70  | 2 (0%) 90 91  | 6, 12, 26, 58         | 5 (0%)  |
| 1   | B     | 726/753 (96%)   | -0.55  | 3 (0%) 88 91  | 6, 13, 36, 65         | 5 (0%)  |
| 1   | C     | 726/753 (96%)   | -0.56  | 2 (0%) 90 91  | 5, 13, 36, 62         | 4 (0%)  |
| 1   | D     | 726/753 (96%)   | -0.60  | 4 (0%) 85 88  | 5, 12, 32, 62         | 5 (0%)  |
| All | All   | 2904/3012 (96%) | -0.60  | 11 (0%) 88 91 | 5, 13, 33, 65         | 19 (0%) |

All (11) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 726 | GLY  | 3.9  |
| 1   | C     | 751 | ILE  | 3.0  |
| 1   | D     | 28  | SER  | 3.0  |
| 1   | D     | 750 | LYS  | 2.8  |
| 1   | B     | 710 | ILE  | 2.7  |
| 1   | D     | 749 | ASP  | 2.7  |
| 1   | C     | 750 | LYS  | 2.6  |
| 1   | D     | 596 | GLY  | 2.3  |
| 1   | B     | 725 | ASP  | 2.3  |
| 1   | A     | 726 | GLY  | 2.2  |
| 1   | A     | 751 | ILE  | 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 oligosaccharides in this entry.

## 6.4 Ligands

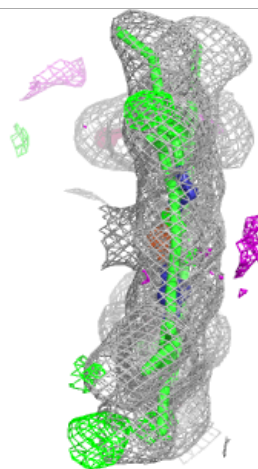
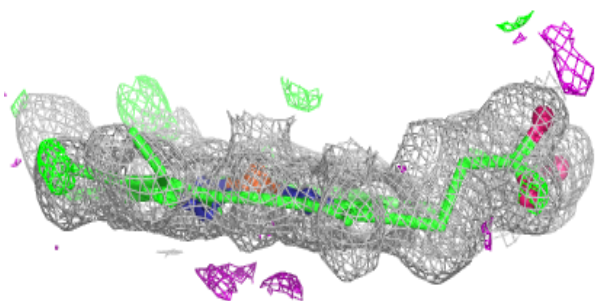
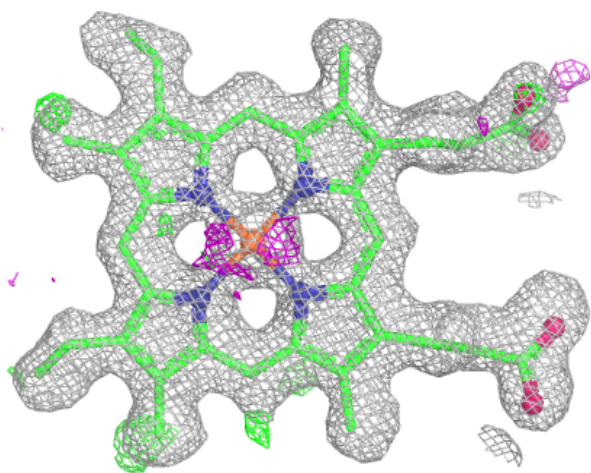
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

| Mol | Type | Chain | Res    | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|--------|-------|------|------|----------------------------|-------|
| 3   | HEM  | D     | 802[B] | 43/43 | 0.97 | 0.06 | 4,6,8,9                    | 43    |
| 2   | HDD  | B     | 801[A] | 44/44 | 0.98 | 0.05 | 6,7,14,18                  | 44    |
| 2   | HDD  | C     | 801[A] | 44/44 | 0.98 | 0.05 | 6,7,14,18                  | 44    |
| 2   | HDD  | D     | 801[A] | 44/44 | 0.98 | 0.05 | 5,7,12,16                  | 44    |
| 3   | HEM  | A     | 802[B] | 43/43 | 0.98 | 0.05 | 3,5,6,7                    | 43    |
| 3   | HEM  | B     | 802[B] | 43/43 | 0.98 | 0.05 | 4,7,8,8                    | 43    |
| 3   | HEM  | C     | 802[B] | 43/43 | 0.98 | 0.06 | 4,6,8,9                    | 43    |
| 2   | HDD  | A     | 801[A] | 44/44 | 0.98 | 0.05 | 5,6,12,15                  | 44    |

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.

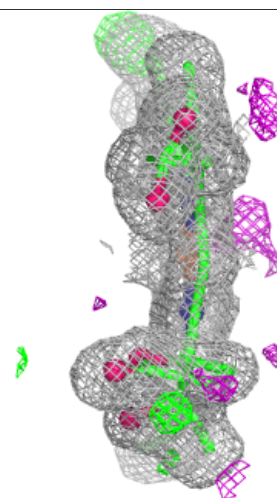
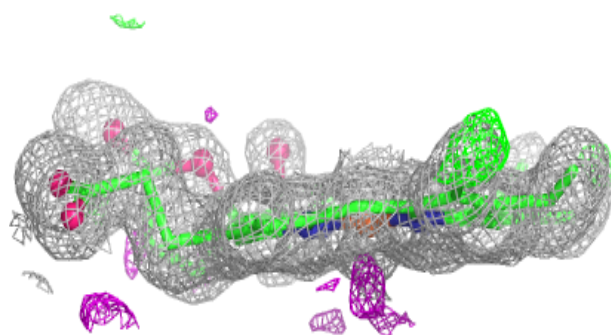
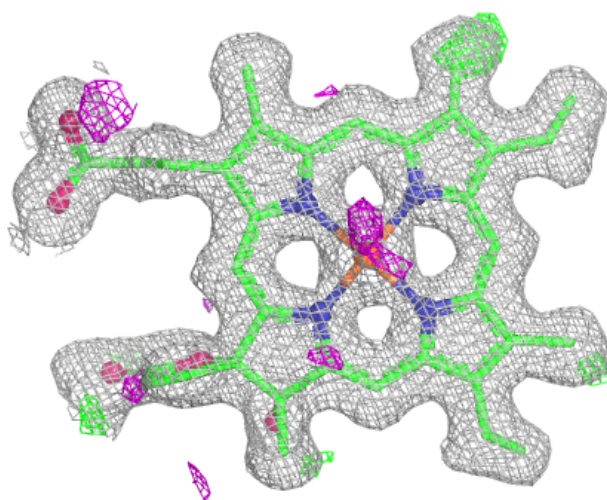
**Electron density around HEM D 802 (B):**

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



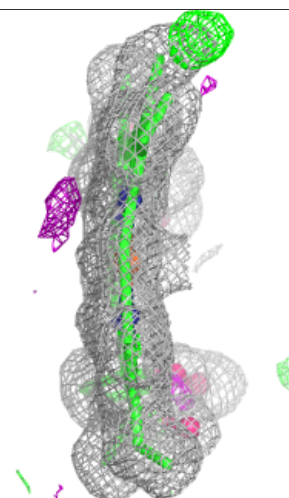
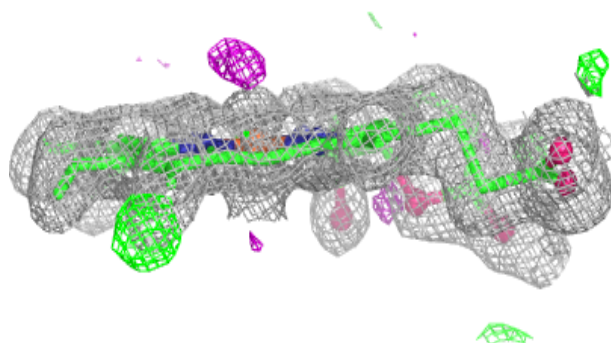
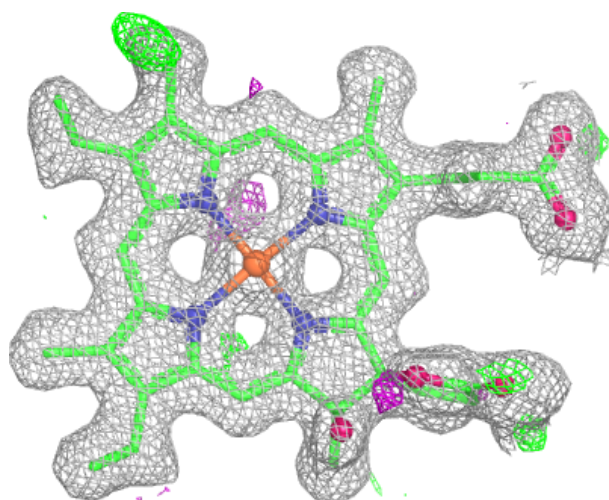
**Electron density around HDD B 801 (A):**

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



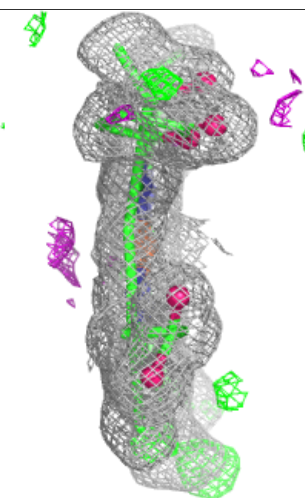
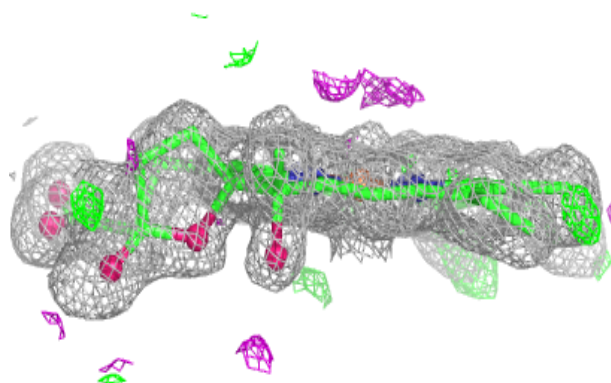
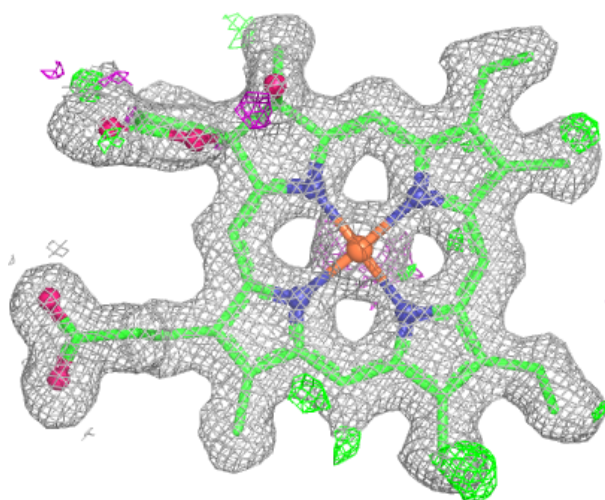
**Electron density around HDD C 801 (A):**

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



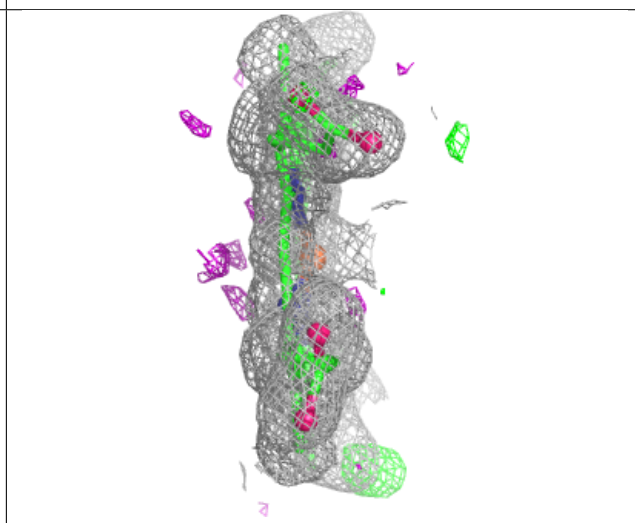
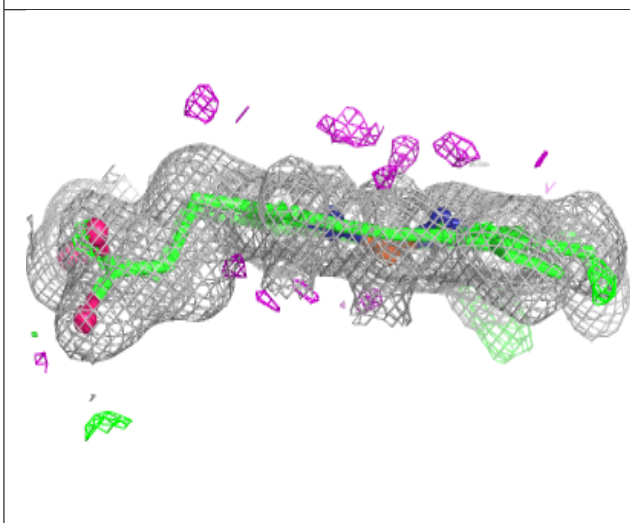
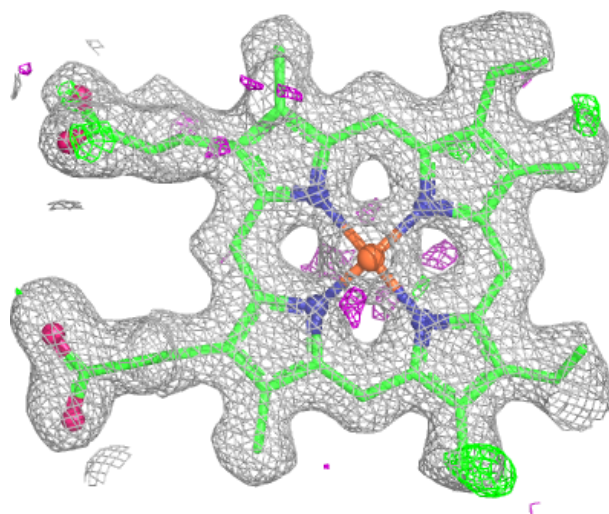
**Electron density around HDD D 801 (A):**

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



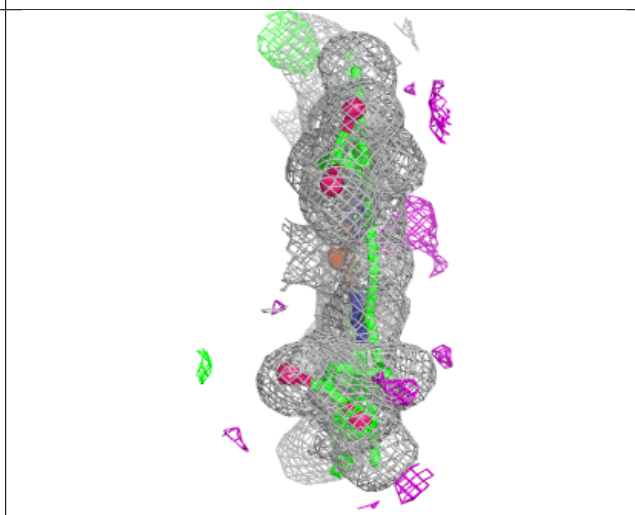
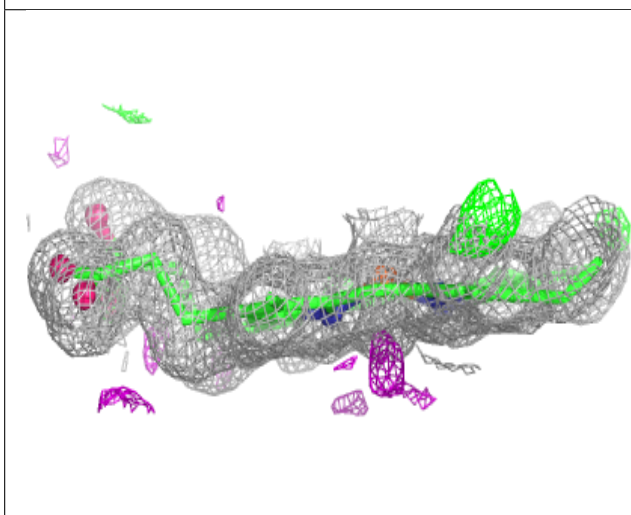
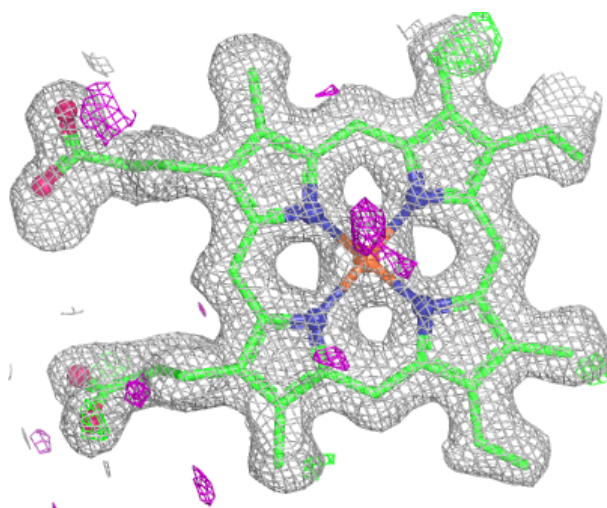
**Electron density around HEM A 802 (B):**

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



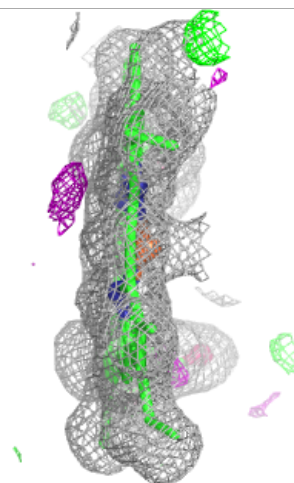
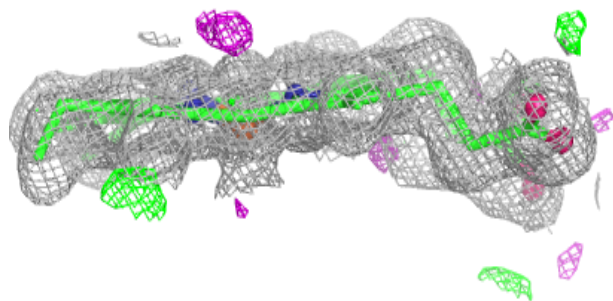
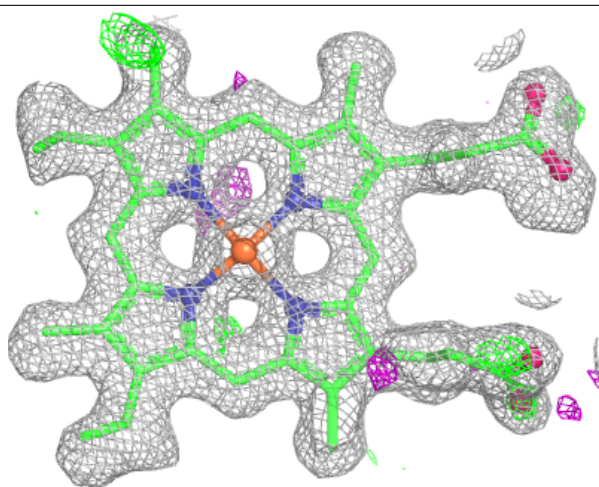
**Electron density around HEM B 802 (B):**

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



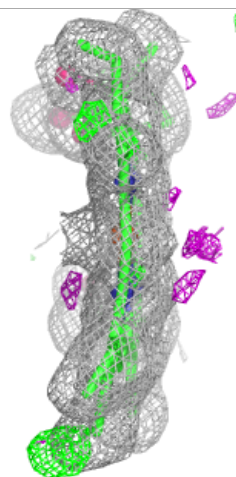
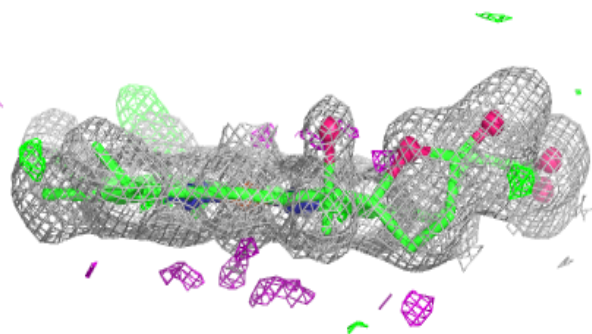
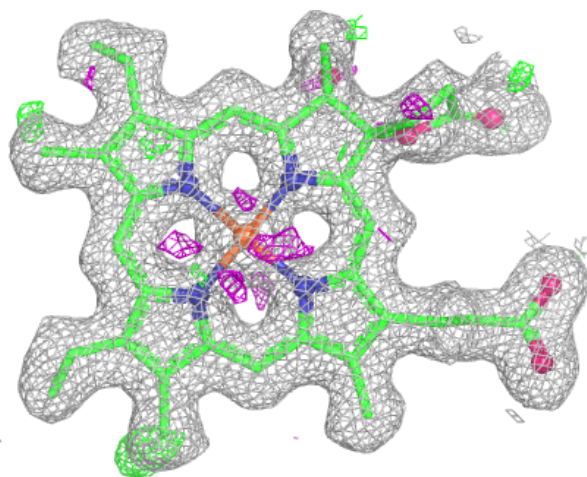
**Electron density around HEM C 802 (B):**

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



**Electron density around HDD A 801 (A):**

$2mF_o-DF_c$  (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.