



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:31 PM UTC

PDB ID : 8QYI / pdb\_00008qyi  
Title : OleP in complex with lithocholic acid in high salt crystallization conditions  
Authors : Fata, F.; Costanzo, A.; Freda, I.; Gugole, E.; Bulfaro, G.; Barbizzi, L.; Di Renzo, M.; Savino, C.; Vallone, B.; Montemiglio, L.C.  
Deposited on : 2023-10-26  
Resolution : 2.30 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>.

---

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

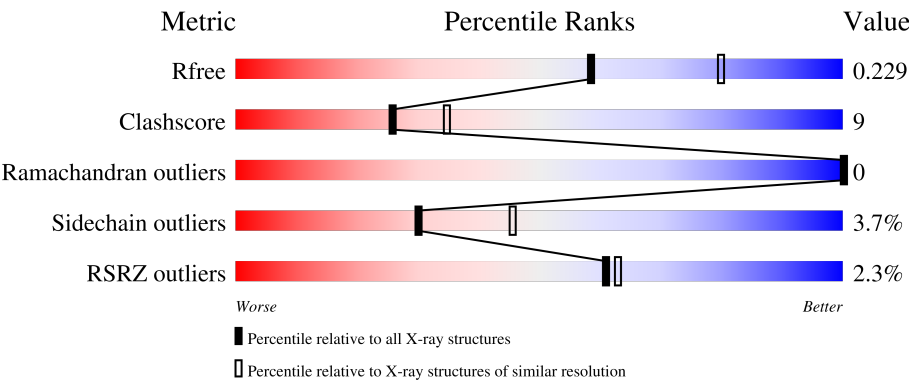
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                             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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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 <sub>free</sub>     | 180053                      | 6319 (2.30-2.30)                                      |
| Clashscore            | 190562                      | 6919 (2.30-2.30)                                      |
| Ramachandran outliers | 187476                      | 6854 (2.30-2.30)                                      |
| Sidechain outliers    | 187428                      | 6854 (2.30-2.30)                                      |
| RSRZ outliers         | 180081                      | 6325 (2.30-2.30)                                      |

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     | 398    | <div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%80%17%..</div>  |
| 1   | B     | 398    | <div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%81%18%..</div> |
| 1   | C     | 398    | <div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%84%15%. </div> |
| 1   | D     | 398    | <div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%77%21%. </div> |
| 1   | E     | 398    | <div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>3%74%23%..</div> |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 1   | F     | 398    |  |

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 |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | FMT  | A     | 505 | -         | -        | X       | -                |
| 4   | FMT  | B     | 513 | -         | -        | X       | -                |
| 4   | FMT  | D     | 505 | -         | -        | X       | -                |
| 4   | FMT  | D     | 514 | -         | -        | X       | -                |

## 2 Entry composition [i](#)

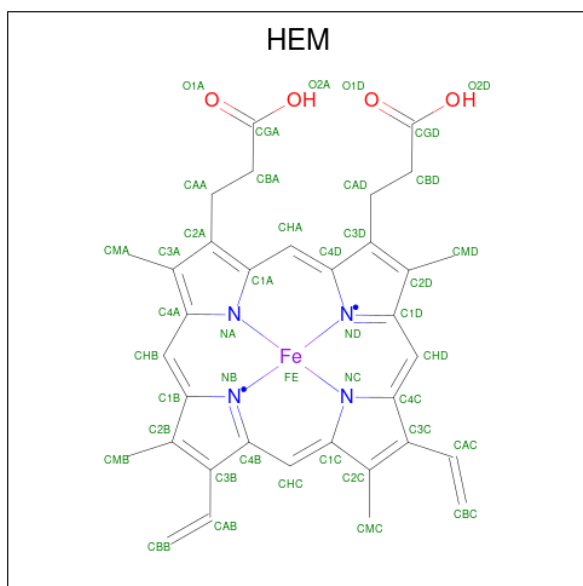
There are 6 unique types of molecules in this entry. The entry contains 20173 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P-450.

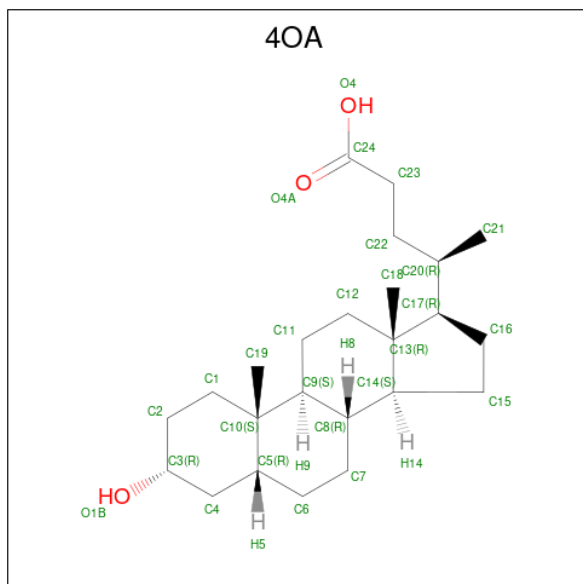
| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 396      | Total | C    | N   | O   | S  | 0       | 8       | 0     |
|     |       |          | 3133  | 1975 | 559 | 584 | 15 |         |         |       |
| 1   | B     | 396      | Total | C    | N   | O   | S  | 0       | 4       | 0     |
|     |       |          | 3108  | 1958 | 556 | 579 | 15 |         |         |       |
| 1   | C     | 398      | Total | C    | N   | O   | S  | 0       | 9       | 0     |
|     |       |          | 3156  | 1988 | 567 | 587 | 14 |         |         |       |
| 1   | D     | 397      | Total | C    | N   | O   | S  | 0       | 5       | 0     |
|     |       |          | 3122  | 1965 | 558 | 586 | 13 |         |         |       |
| 1   | E     | 394      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3081  | 1939 | 554 | 575 | 13 |         |         |       |
| 1   | F     | 396      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3094  | 1946 | 556 | 579 | 13 |         |         |       |

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



| Mol | Chain | Residues | Atoms |    |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|---------|---------|
| 2   | A     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |
| 2   | B     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |
| 2   | C     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |
| 2   | D     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |
| 2   | E     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |
| 2   | F     | 1        | Total | C  | Fe | N | O       |         |
|     |       |          | 43    | 34 | 1  | 4 | 4       |         |

- Molecule 3 is (3beta,5beta,14beta,17alpha)-3-hydroxycholan-24-oic acid (CCD ID: 40A) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



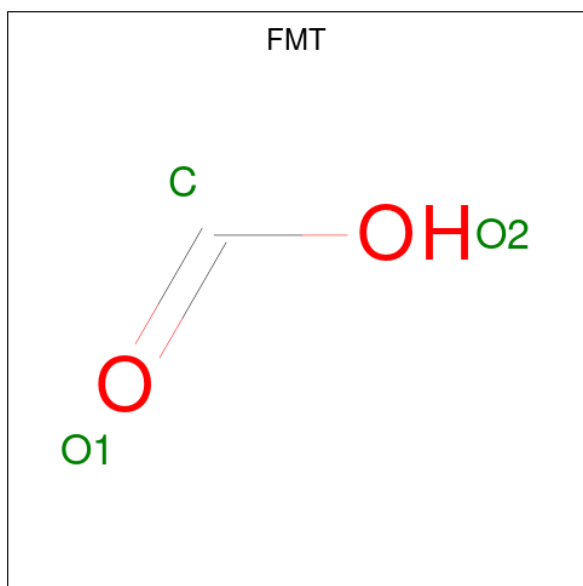
| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3   | A     | 1        | Total | C  | O |         |         |
|     |       |          | 27    | 24 | 3 |         |         |
| 3   | B     | 1        | Total | C  | O |         |         |
|     |       |          | 27    | 24 | 3 |         |         |
| 3   | C     | 1        | Total | C  | O |         |         |
|     |       |          | 27    | 24 | 3 |         |         |
| 3   | D     | 1        | Total | C  | O |         |         |
|     |       |          | 27    | 24 | 3 |         |         |
| 3   | E     | 1        | Total | C  | O |         |         |
|     |       |          | 27    | 24 | 3 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 3   | F     | 1        | Total | C  | O | 0       | 0       |
|     |       |          | 27    | 24 | 3 |         |         |

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | A     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | B     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | C     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|--------|---------|---------|
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | C     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | D     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | D     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | D     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | D     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |
| 4   | D     | 1        | Total<br>3 | C<br>1 | O<br>2 | 0       | 0       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | D     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | E     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |
| 4   | F     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 3     | 1 | 2 |         |         |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4   | F     | 1        | Total C O<br>3 1 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>3 1 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>3 1 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>3 1 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>3 1 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>3 1 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>3 1 2 | 0       | 0       |
| 4   | F     | 1        | Total C O<br>3 1 2 | 0       | 0       |

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5   | A     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | B     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | C     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | D     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | E     | 1        | Total Na<br>1 1 | 0       | 0       |
| 5   | F     | 1        | Total Na<br>1 1 | 0       | 0       |

- Molecule 6 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6   | A     | 139      | Total O<br>139 139 | 0       | 0       |
| 6   | B     | 147      | Total O<br>147 147 | 0       | 0       |
| 6   | C     | 199      | Total O<br>199 199 | 0       | 0       |

*Continued on next page...*

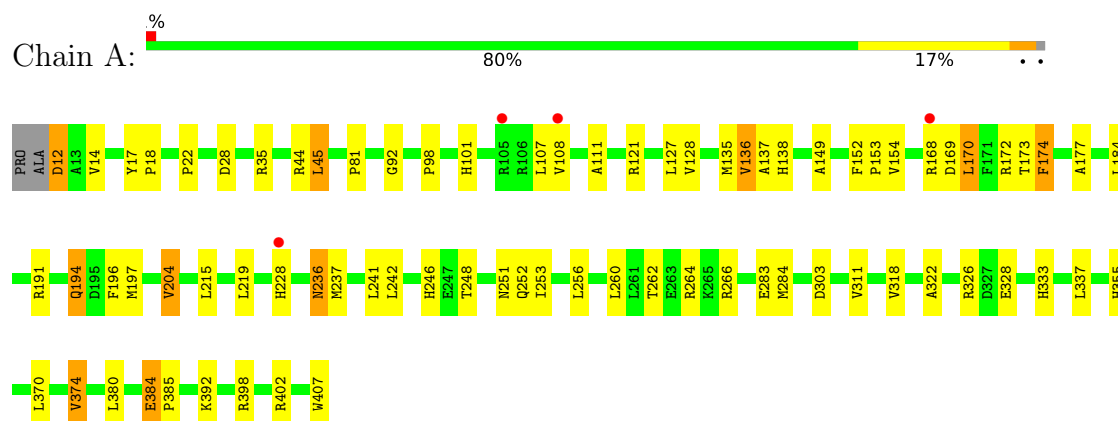
*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 6   | D     | 109      | Total<br>109 | O<br>109 | 0       | 0       |
| 6   | E     | 77       | Total<br>77  | O<br>77  | 0       | 0       |
| 6   | F     | 76       | Total<br>76  | O<br>76  | 0       | 0       |

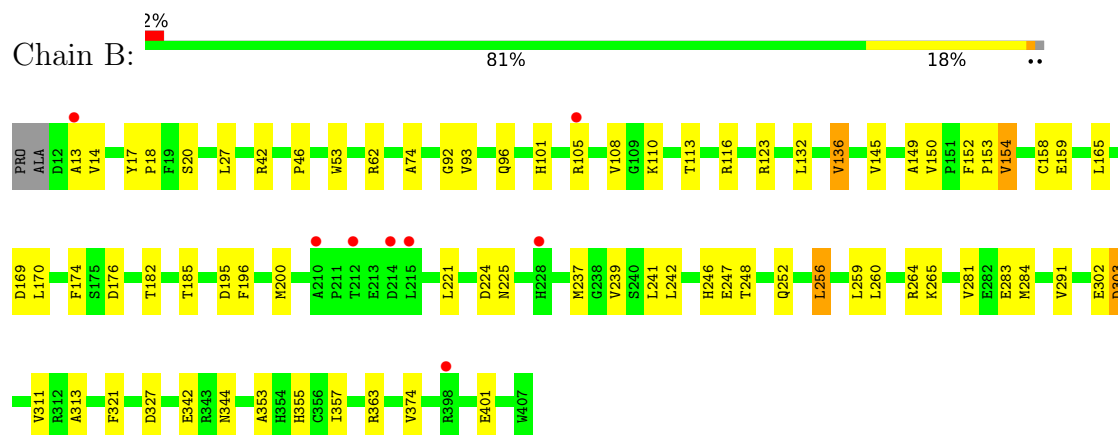
### 3 Residue-property plots [i](#)

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

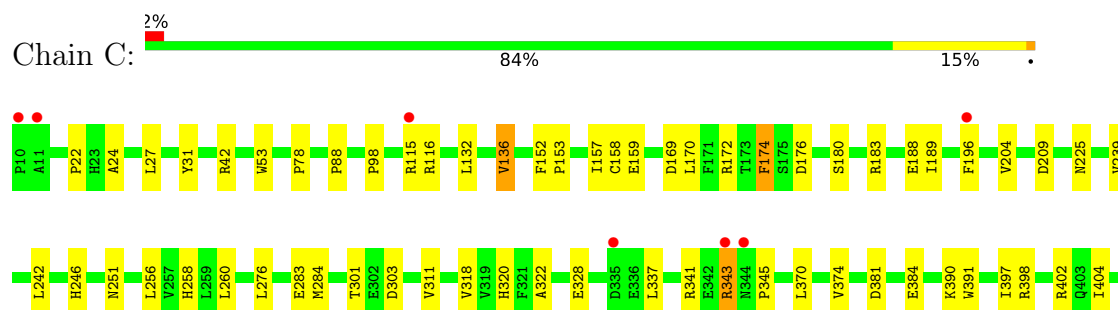
#### • Molecule 1: Cytochrome P-450



#### • Molecule 1: Cytochrome P-450

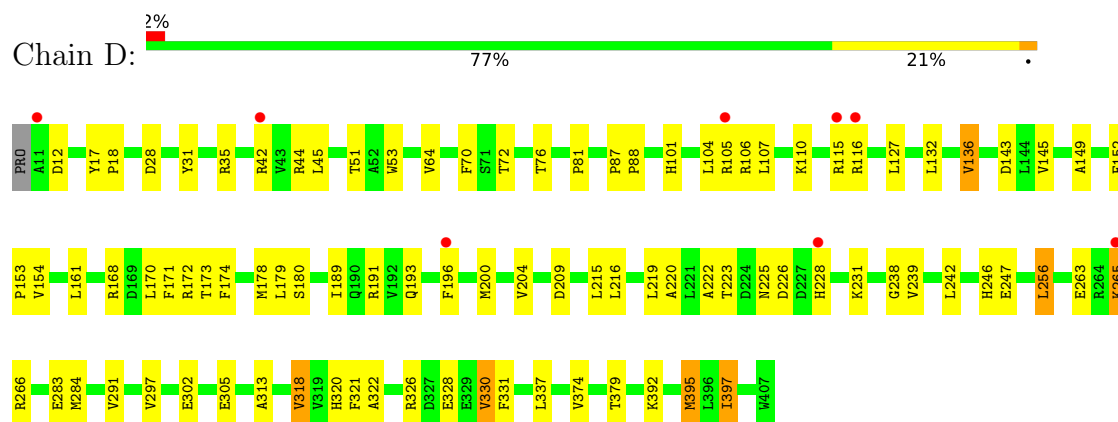


#### • Molecule 1: Cytochrome P-450

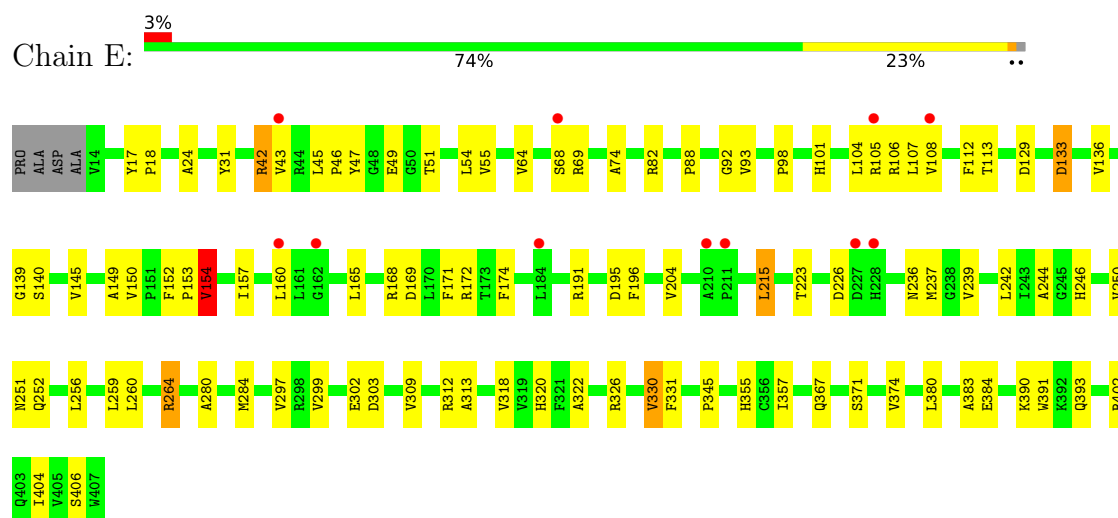


W407

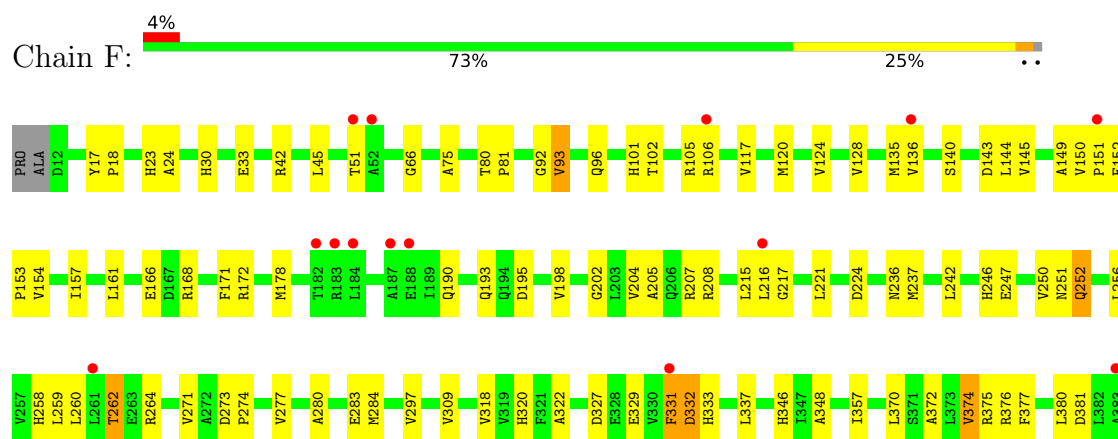
- Molecule 1: Cytochrome P-450

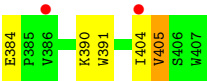


- Molecule 1: Cytochrome P-450



- Molecule 1: Cytochrome P-450





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 249.37Å 109.27Å 160.66Å<br>90.00° 129.60° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 80.01 – 2.30<br>80.01 – 2.30                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (80.01-2.30)<br>99.8 (80.01-2.30)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.10                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.94 (at 2.29Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.8.0267                                             | Depositor        |
| R, $R_{free}$                                                           | 0.173 , 0.222<br>0.188 , 0.229                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 7213 reflections (4.89%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 46.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.252                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 39.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.011 for -h-2*k,l                                          | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                        | EDS              |
| Total number of atoms                                                   | 20173                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 56.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6981e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FMT, 4OA, NA

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     | 1.19         | 5/3224 (0.2%)   | 1.48        | 16/4388 (0.4%)  |
| 1   | B     | 1.20         | 8/3187 (0.3%)   | 1.49        | 10/4339 (0.2%)  |
| 1   | C     | 1.20         | 5/3245 (0.2%)   | 1.49        | 13/4415 (0.3%)  |
| 1   | D     | 1.19         | 1/3204 (0.0%)   | 1.53        | 13/4362 (0.3%)  |
| 1   | E     | 1.16         | 1/3151 (0.0%)   | 1.57        | 21/4291 (0.5%)  |
| 1   | F     | 1.17         | 2/3164 (0.1%)   | 1.58        | 9/4309 (0.2%)   |
| All | All   | 1.18         | 22/19175 (0.1%) | 1.52        | 82/26104 (0.3%) |

All (22) bond length outliers are listed below:

| Mol | Chain | Res    | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|--------|------|---------|-------|-------------|----------|
| 1   | F     | 66     | GLY  | C-O     | -7.27 | 1.19        | 1.24     |
| 1   | C     | 88     | PRO  | C-O     | -7.12 | 1.16        | 1.23     |
| 1   | B     | 355    | HIS  | CE1-NE2 | 6.86  | 1.39        | 1.32     |
| 1   | B     | 46     | PRO  | C-O     | -6.35 | 1.16        | 1.24     |
| 1   | B     | 303    | ASP  | C-O     | -6.23 | 1.16        | 1.23     |
| 1   | A     | 253    | ILE  | C-O     | -6.08 | 1.17        | 1.24     |
| 1   | C     | 381    | ASP  | CG-OD1  | 5.82  | 1.36        | 1.25     |
| 1   | C     | 343[A] | ARG  | C-O     | 5.79  | 1.30        | 1.23     |
| 1   | C     | 343[B] | ARG  | C-O     | 5.79  | 1.30        | 1.23     |
| 1   | A     | 355    | HIS  | CE1-NE2 | 5.75  | 1.38        | 1.32     |
| 1   | B     | 281    | VAL  | C-O     | -5.69 | 1.17        | 1.24     |
| 1   | D     | 143    | ASP  | C-O     | 5.47  | 1.30        | 1.24     |
| 1   | B     | 353    | ALA  | C-O     | -5.46 | 1.17        | 1.24     |
| 1   | A     | 149    | ALA  | C-O     | -5.40 | 1.17        | 1.24     |
| 1   | B     | 101    | HIS  | CE1-NE2 | 5.40  | 1.38        | 1.32     |
| 1   | A     | 98     | PRO  | C-O     | -5.32 | 1.20        | 1.25     |
| 1   | E     | 355    | HIS  | CE1-NE2 | 5.30  | 1.37        | 1.32     |
| 1   | A     | 101    | HIS  | CE1-NE2 | 5.26  | 1.37        | 1.32     |
| 1   | B     | 363    | ARG  | C-O     | 5.22  | 1.30        | 1.24     |
| 1   | C     | 22     | PRO  | C-O     | -5.11 | 1.17        | 1.23     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 93  | VAL  | C-O   | 5.09  | 1.30        | 1.24     |
| 1   | B     | 74  | ALA  | C-O   | -5.04 | 1.17        | 1.24     |

All (82) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|-----------|-------|-------------|----------|
| 1   | F     | 273    | ASP  | CA-CB-CG  | 8.57  | 121.17      | 112.60   |
| 1   | B     | 169    | ASP  | CA-CB-CG  | 7.48  | 120.08      | 112.60   |
| 1   | E     | 129    | ASP  | CA-C-N    | 7.06  | 129.61      | 120.44   |
| 1   | E     | 129    | ASP  | C-N-CA    | 7.06  | 129.61      | 120.44   |
| 1   | A     | 174    | PHE  | CA-C-N    | 7.05  | 129.61      | 120.44   |
| 1   | A     | 174    | PHE  | C-N-CA    | 7.05  | 129.61      | 120.44   |
| 1   | E     | 226    | ASP  | CA-CB-CG  | 6.66  | 119.25      | 112.60   |
| 1   | C     | 276    | LEU  | CA-C-N    | 6.63  | 125.63      | 120.33   |
| 1   | C     | 276    | LEU  | C-N-CA    | 6.63  | 125.63      | 120.33   |
| 1   | F     | 274    | PRO  | CA-C-N    | 6.52  | 129.01      | 120.28   |
| 1   | F     | 274    | PRO  | C-N-CA    | 6.52  | 129.01      | 120.28   |
| 1   | E     | 345    | PRO  | CA-C-O    | -6.43 | 116.55      | 121.31   |
| 1   | E     | 244    | ALA  | CA-C-N    | 6.20  | 127.89      | 120.14   |
| 1   | E     | 244    | ALA  | C-N-CA    | 6.20  | 127.89      | 120.14   |
| 1   | A     | 173    | THR  | CA-CB-OG1 | -6.19 | 100.31      | 109.60   |
| 1   | C     | 98     | PRO  | CA-C-O    | -6.19 | 116.44      | 120.90   |
| 1   | E     | 226    | ASP  | N-CA-C    | -6.15 | 97.69       | 110.80   |
| 1   | E     | 154    | VAL  | N-CA-C    | -6.12 | 104.33      | 111.00   |
| 1   | E     | 239    | VAL  | CA-C-N    | 5.83  | 128.41      | 120.54   |
| 1   | E     | 239    | VAL  | C-N-CA    | 5.83  | 128.41      | 120.54   |
| 1   | A     | 333    | HIS  | CA-C-N    | 5.76  | 128.28      | 120.38   |
| 1   | A     | 333    | HIS  | C-N-CA    | 5.76  | 128.28      | 120.38   |
| 1   | C     | 301    | THR  | CA-CB-OG1 | -5.76 | 100.96      | 109.60   |
| 1   | F     | 329    | GLU  | CB-CG-CD  | 5.69  | 122.28      | 112.60   |
| 1   | A     | 228    | HIS  | CB-CA-C   | 5.68  | 119.10      | 109.55   |
| 1   | C     | 158    | CYS  | CA-C-O    | -5.66 | 114.56      | 120.55   |
| 1   | A     | 236    | ASN  | CA-CB-CG  | -5.65 | 106.95      | 112.60   |
| 1   | D     | 115[A] | ARG  | N-CA-C    | 5.65  | 117.89      | 111.11   |
| 1   | D     | 115[B] | ARG  | N-CA-C    | 5.65  | 117.89      | 111.11   |
| 1   | B     | 182    | THR  | CA-C-N    | 5.64  | 128.30      | 120.29   |
| 1   | B     | 182    | THR  | C-N-CA    | 5.64  | 128.30      | 120.29   |
| 1   | C     | 225    | ASN  | CA-CB-CG  | 5.59  | 118.19      | 112.60   |
| 1   | C     | 322    | ALA  | CA-C-O    | -5.55 | 113.83      | 120.10   |
| 1   | E     | 367    | GLN  | CA-C-O    | -5.53 | 115.00      | 120.70   |
| 1   | E     | 251    | ASN  | CA-CB-CG  | -5.53 | 107.07      | 112.60   |
| 1   | E     | 133    | ASP  | CA-C-N    | 5.51  | 127.98      | 120.54   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 133 | ASP  | C-N-CA    | 5.51  | 127.98      | 120.54   |
| 1   | F     | 190 | GLN  | CA-C-N    | 5.50  | 127.59      | 120.44   |
| 1   | F     | 190 | GLN  | C-N-CA    | 5.50  | 127.59      | 120.44   |
| 1   | E     | 113 | THR  | CA-C-O    | -5.47 | 115.85      | 121.87   |
| 1   | C     | 78  | PRO  | CB-CA-C   | -5.40 | 104.19      | 111.85   |
| 1   | A     | 262 | THR  | CA-CB-OG1 | -5.37 | 101.55      | 109.60   |
| 1   | D     | 173 | THR  | CA-CB-OG1 | -5.36 | 101.55      | 109.60   |
| 1   | B     | 158 | CYS  | CA-C-O    | -5.35 | 115.20      | 120.82   |
| 1   | D     | 231 | LYS  | CA-C-N    | 5.34  | 126.03      | 119.99   |
| 1   | D     | 231 | LYS  | C-N-CA    | 5.34  | 126.03      | 119.99   |
| 1   | F     | 195 | ASP  | CA-C-O    | -5.34 | 115.22      | 120.82   |
| 1   | A     | 136 | VAL  | CA-C-O    | -5.27 | 114.78      | 120.47   |
| 1   | B     | 195 | ASP  | CA-CB-CG  | 5.25  | 117.85      | 112.60   |
| 1   | D     | 51  | THR  | CA-CB-OG1 | -5.25 | 101.73      | 109.60   |
| 1   | D     | 87  | PRO  | O-C-N     | -5.24 | 118.90      | 121.31   |
| 1   | B     | 344 | ASN  | O-C-N     | -5.24 | 116.65      | 121.42   |
| 1   | A     | 384 | GLU  | CB-CA-C   | 5.23  | 117.04      | 109.45   |
| 1   | A     | 28  | ASP  | CB-CA-C   | 5.21  | 117.48      | 109.50   |
| 1   | D     | 72  | THR  | CA-CB-OG1 | -5.21 | 101.78      | 109.60   |
| 1   | A     | 204 | VAL  | CA-C-O    | -5.20 | 115.34      | 120.85   |
| 1   | D     | 395 | MET  | CA-C-N    | 5.19  | 128.99      | 120.63   |
| 1   | D     | 395 | MET  | C-N-CA    | 5.19  | 128.99      | 120.63   |
| 1   | A     | 385 | PRO  | CA-C-N    | 5.18  | 127.56      | 120.46   |
| 1   | A     | 385 | PRO  | C-N-CA    | 5.18  | 127.56      | 120.46   |
| 1   | B     | 20  | SER  | CA-C-N    | 5.18  | 127.85      | 120.49   |
| 1   | B     | 20  | SER  | C-N-CA    | 5.18  | 127.85      | 120.49   |
| 1   | D     | 28  | ASP  | CB-CA-C   | 5.18  | 118.36      | 109.82   |
| 1   | C     | 328 | GLU  | CB-CG-CD  | 5.17  | 121.39      | 112.60   |
| 1   | E     | 303 | ASP  | CA-CB-CG  | 5.16  | 117.76      | 112.60   |
| 1   | F     | 202 | GLY  | CA-C-O    | -5.16 | 115.44      | 120.75   |
| 1   | D     | 51  | THR  | CA-C-O    | -5.14 | 115.30      | 121.11   |
| 1   | C     | 169 | ASP  | N-CA-C    | -5.14 | 105.76      | 111.36   |
| 1   | B     | 113 | THR  | CA-CB-OG1 | -5.13 | 101.90      | 109.60   |
| 1   | C     | 174 | PHE  | CA-CB-CG  | 5.13  | 118.93      | 113.80   |
| 1   | C     | 341 | ARG  | CB-CA-C   | -5.13 | 102.15      | 109.84   |
| 1   | A     | 248 | THR  | CA-C-N    | 5.09  | 127.10      | 120.28   |
| 1   | A     | 248 | THR  | C-N-CA    | 5.09  | 127.10      | 120.28   |
| 1   | B     | 200 | MET  | CA-C-O    | -5.06 | 115.18      | 120.55   |
| 1   | C     | 98  | PRO  | N-CA-C    | -5.06 | 105.61      | 110.47   |
| 1   | F     | 171 | PHE  | CA-CB-CG  | 5.04  | 118.84      | 113.80   |
| 1   | E     | 139 | GLY  | CA-C-O    | -5.02 | 118.77      | 122.23   |
| 1   | E     | 223 | THR  | CA-C-N    | 5.02  | 127.00      | 120.28   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | E     | 223 | THR  | C-N-CA    | 5.02  | 127.00      | 120.28   |
| 1   | E     | 98  | PRO  | CA-C-O    | -5.01 | 117.29      | 120.90   |
| 1   | D     | 379 | THR  | CA-CB-OG1 | -5.01 | 102.08      | 109.60   |
| 1   | E     | 371 | SER  | CA-C-O    | -5.01 | 115.54      | 120.90   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3133  | 0        | 3132     | 60      | 0            |
| 1   | B     | 3108  | 0        | 3100     | 52      | 0            |
| 1   | C     | 3156  | 0        | 3159     | 41      | 0            |
| 1   | D     | 3122  | 0        | 3107     | 79      | 0            |
| 1   | E     | 3081  | 0        | 3064     | 57      | 0            |
| 1   | F     | 3094  | 0        | 3073     | 58      | 0            |
| 2   | A     | 43    | 0        | 30       | 3       | 0            |
| 2   | B     | 43    | 0        | 30       | 4       | 0            |
| 2   | C     | 43    | 0        | 30       | 3       | 0            |
| 2   | D     | 43    | 0        | 30       | 4       | 0            |
| 2   | E     | 43    | 0        | 30       | 5       | 0            |
| 2   | F     | 43    | 0        | 30       | 3       | 0            |
| 3   | A     | 27    | 0        | 39       | 2       | 0            |
| 3   | B     | 27    | 0        | 39       | 1       | 0            |
| 3   | C     | 27    | 0        | 39       | 1       | 0            |
| 3   | D     | 27    | 0        | 39       | 0       | 0            |
| 3   | E     | 27    | 0        | 39       | 3       | 0            |
| 3   | F     | 27    | 0        | 39       | 1       | 0            |
| 4   | A     | 66    | 0        | 22       | 2       | 0            |
| 4   | B     | 66    | 0        | 23       | 8       | 0            |
| 4   | C     | 72    | 0        | 24       | 2       | 0            |
| 4   | D     | 39    | 0        | 13       | 5       | 0            |
| 4   | E     | 30    | 0        | 10       | 1       | 0            |
| 4   | F     | 33    | 0        | 11       | 0       | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5   | B     | 1     | 0        | 0        | 0       | 0            |
| 5   | C     | 1     | 0        | 0        | 0       | 0            |
| 5   | D     | 1     | 0        | 0        | 0       | 0            |
| 5   | E     | 1     | 0        | 0        | 0       | 0            |
| 5   | F     | 1     | 0        | 0        | 0       | 0            |
| 6   | A     | 139   | 0        | 0        | 2       | 0            |
| 6   | B     | 147   | 0        | 0        | 0       | 0            |
| 6   | C     | 199   | 0        | 0        | 4       | 0            |
| 6   | D     | 109   | 0        | 0        | 4       | 0            |
| 6   | E     | 77    | 0        | 0        | 1       | 0            |
| 6   | F     | 76    | 0        | 0        | 3       | 0            |
| All | All   | 20173 | 0        | 19152    | 365     | 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 9.

All (365) 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:A:108:VAL:HG23 | 1:A:215[B]:LEU:CD1  | 1.60                     | 1.31              |
| 1:A:108:VAL:CG2  | 1:A:215[B]:LEU:HD11 | 1.67                     | 1.22              |
| 1:A:108:VAL:CG2  | 1:A:215[B]:LEU:HD21 | 1.94                     | 0.98              |
| 1:A:108:VAL:HG21 | 1:A:215[B]:LEU:HD21 | 1.43                     | 0.97              |
| 1:D:174:PHE:HB3  | 1:D:196:PHE:CD2     | 2.03                     | 0.94              |
| 1:D:174:PHE:HB3  | 1:D:196:PHE:HD2     | 1.29                     | 0.94              |
| 1:B:174:PHE:HB3  | 1:B:196:PHE:HD2     | 1.33                     | 0.89              |
| 1:B:105:ARG:HD2  | 1:B:357:ILE:HD12    | 1.56                     | 0.88              |
| 1:D:76:THR:HA    | 1:D:88:PRO:HG2      | 1.58                     | 0.84              |
| 1:E:42:ARG:HG3   | 1:E:51:THR:HG22     | 1.60                     | 0.84              |
| 1:C:174:PHE:HB3  | 1:C:196:PHE:HD2     | 1.44                     | 0.82              |
| 1:B:174:PHE:HB3  | 1:B:196:PHE:CD2     | 2.15                     | 0.81              |
| 1:F:145:VAL:HA   | 1:F:149:ALA:HB3     | 1.64                     | 0.80              |
| 1:A:260:LEU:HG   | 1:A:284[A]:MET:HE1  | 1.63                     | 0.79              |
| 1:C:402:ARG:HD3  | 1:C:404:ILE:HG13    | 1.63                     | 0.79              |
| 1:E:42:ARG:HG3   | 1:E:51:THR:CG2      | 2.12                     | 0.78              |
| 1:D:101:HIS:NE2  | 1:D:105:ARG:HD2     | 1.99                     | 0.77              |
| 1:D:174:PHE:CB   | 1:D:196:PHE:CD2     | 2.67                     | 0.77              |
| 1:D:152:PHE:HB3  | 1:D:153:PRO:HD3     | 1.67                     | 0.76              |
| 1:A:154:VAL:HG11 | 1:A:168:ARG:HD3     | 1.69                     | 0.75              |
| 1:B:260:LEU:HG   | 1:B:284[A]:MET:HE1  | 1.67                     | 0.75              |
| 1:D:228:HIS:HB2  | 6:D:682:HOH:O       | 1.87                     | 0.73              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:D:174:PHE:CB     | 1:D:196:PHE:HD2     | 2.00                     | 0.73              |
| 1:A:108:VAL:CG2    | 1:A:215[B]:LEU:CD2  | 2.67                     | 0.73              |
| 1:A:172:ARG:HD2    | 1:A:246:HIS:HE1     | 1.54                     | 0.72              |
| 1:D:242:LEU:O      | 1:D:246:HIS:HD2     | 1.72                     | 0.72              |
| 1:D:12:ASP:HB2     | 1:D:44:ARG:HH22     | 1.55                     | 0.72              |
| 1:B:174:PHE:CB     | 1:B:196:PHE:CD2     | 2.73                     | 0.72              |
| 1:C:174:PHE:CB     | 1:C:196:PHE:HD2     | 2.03                     | 0.71              |
| 1:D:222:ALA:O      | 1:D:226:ASP:HB2     | 1.90                     | 0.71              |
| 1:B:174:PHE:CB     | 1:B:196:PHE:HD2     | 2.04                     | 0.71              |
| 1:E:108:VAL:HG12   | 1:E:215:LEU:HD11    | 1.74                     | 0.69              |
| 1:A:108:VAL:HG23   | 1:A:215[B]:LEU:CG   | 2.22                     | 0.69              |
| 1:A:108:VAL:HG23   | 1:A:215[B]:LEU:HD11 | 0.76                     | 0.68              |
| 1:D:174:PHE:CD2    | 1:D:196:PHE:CD2     | 2.82                     | 0.67              |
| 1:F:242:LEU:O      | 1:F:246:HIS:HD2     | 1.78                     | 0.67              |
| 1:F:280:ALA:O      | 1:F:284:MET:HG3     | 1.94                     | 0.67              |
| 1:D:326:ARG:HD3    | 6:D:652:HOH:O       | 1.93                     | 0.67              |
| 1:E:256:LEU:HD22   | 1:E:284:MET:HB3     | 1.77                     | 0.67              |
| 1:F:161:LEU:HD23   | 1:F:215:LEU:HD12    | 1.77                     | 0.67              |
| 1:C:174:PHE:HB3    | 1:C:196:PHE:CD2     | 2.30                     | 0.67              |
| 1:C:174:PHE:CB     | 1:C:196:PHE:CD2     | 2.78                     | 0.66              |
| 1:D:12:ASP:HB2     | 1:D:44:ARG:NH2      | 2.10                     | 0.66              |
| 1:C:256:LEU:HD22   | 1:C:284:MET:HB3     | 1.75                     | 0.66              |
| 1:D:291:VAL:HB     | 4:D:514:FMT:H       | 1.76                     | 0.66              |
| 1:D:35:ARG:NH2     | 6:D:602:HOH:O       | 2.27                     | 0.66              |
| 1:E:384:GLU:OE1    | 1:E:402:ARG:NH1     | 2.27                     | 0.66              |
| 1:A:108:VAL:HG21   | 1:A:215[B]:LEU:CD2  | 2.21                     | 0.66              |
| 1:A:326:ARG:HD3    | 6:A:665:HOH:O       | 1.95                     | 0.65              |
| 1:D:291:VAL:HB     | 4:D:514:FMT:C       | 2.27                     | 0.65              |
| 2:D:501:HEM:HHC    | 2:D:501:HEM:HBB2    | 1.78                     | 0.65              |
| 1:C:283:GLU:HG3    | 1:C:337:LEU:HD12    | 1.79                     | 0.65              |
| 1:C:174:PHE:CD2    | 1:C:196:PHE:CD2     | 2.84                     | 0.65              |
| 1:A:108:VAL:CG2    | 1:A:215[B]:LEU:CD1  | 2.47                     | 0.64              |
| 1:A:108:VAL:CG2    | 1:A:215[B]:LEU:CG   | 2.76                     | 0.64              |
| 1:C:251:ASN:HD22   | 1:C:397:ILE:HD12    | 1.62                     | 0.64              |
| 1:B:152:PHE:HB3    | 1:B:153:PRO:HD3     | 1.78                     | 0.64              |
| 1:A:328:GLU:HB2    | 4:A:505:FMT:C       | 2.28                     | 0.63              |
| 1:D:256:LEU:HD22   | 1:D:284:MET:HB3     | 1.79                     | 0.63              |
| 2:F:501:HEM:HMB2   | 2:F:501:HEM:HBB2    | 1.81                     | 0.63              |
| 1:A:251:ASN:HD21   | 1:A:392:LYS:NZ      | 1.97                     | 0.63              |
| 1:E:191[A]:ARG:NH2 | 4:E:512:FMT:O1      | 2.32                     | 0.63              |
| 1:C:196:PHE:HD1    | 1:C:239:VAL:HG22    | 1.63                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E:157:ILE:HD12   | 1:E:160:LEU:HD23   | 1.80                     | 0.62              |
| 1:E:191[A]:ARG:CZ  | 1:E:195:ASP:OD1    | 2.47                     | 0.62              |
| 1:E:256:LEU:HD22   | 1:E:284:MET:CB     | 2.30                     | 0.62              |
| 2:B:501:HEM:HHC    | 2:B:501:HEM:HBB2   | 1.82                     | 0.62              |
| 1:D:101:HIS:HE1    | 2:D:501:HEM:O2D    | 1.83                     | 0.62              |
| 1:A:197:MET:HG3    | 6:A:700:HOH:O      | 2.00                     | 0.61              |
| 1:C:174:PHE:HD2    | 1:C:196:PHE:CD2    | 2.18                     | 0.61              |
| 1:A:260:LEU:CG     | 1:A:284[A]:MET:HE1 | 2.30                     | 0.61              |
| 1:B:291:VAL:HB     | 4:B:513:FMT:C      | 2.31                     | 0.61              |
| 1:D:392:LYS:HB3    | 1:D:395:MET:CE     | 2.31                     | 0.61              |
| 1:B:321:PHE:HD2    | 4:B:513:FMT:H      | 1.66                     | 0.60              |
| 1:D:174:PHE:HD2    | 1:D:196:PHE:CD2    | 2.18                     | 0.60              |
| 1:D:110:LYS:O      | 1:D:116:ARG:HG3    | 2.00                     | 0.60              |
| 1:D:392:LYS:HD3    | 1:D:395:MET:HE1    | 1.82                     | 0.60              |
| 1:F:150:VAL:HB     | 1:F:151:PRO:HD3    | 1.81                     | 0.60              |
| 1:A:121:ARG:HD2    | 1:D:42:ARG:HH21    | 1.67                     | 0.59              |
| 1:C:390:LYS:NZ     | 6:C:604:HOH:O      | 2.34                     | 0.59              |
| 1:D:196:PHE:HD1    | 1:D:239:VAL:HG22   | 1.67                     | 0.59              |
| 1:E:259:LEU:HB2    | 1:E:284:MET:CE     | 2.32                     | 0.59              |
| 1:C:343[B]:ARG:NH1 | 1:C:345:PRO:HG3    | 2.18                     | 0.59              |
| 1:F:247:GLU:O      | 1:F:251:ASN:ND2    | 2.35                     | 0.59              |
| 1:E:31:TYR:CZ      | 1:E:320:HIS:CD2    | 2.91                     | 0.58              |
| 1:B:174:PHE:HB2    | 1:B:196:PHE:CE2    | 2.38                     | 0.58              |
| 1:B:196:PHE:HD1    | 1:B:239:VAL:HG22   | 1.67                     | 0.58              |
| 1:F:166:GLU:O      | 1:F:166:GLU:HG2    | 2.02                     | 0.58              |
| 1:C:251:ASN:HD22   | 1:C:397:ILE:CD1    | 2.16                     | 0.58              |
| 1:C:116:ARG:NH1    | 6:C:606:HOH:O      | 2.37                     | 0.58              |
| 1:E:191[A]:ARG:NH2 | 1:E:195:ASP:OD1    | 2.37                     | 0.58              |
| 1:F:102:THR:O      | 1:F:106[A]:ARG:HG3 | 2.03                     | 0.58              |
| 1:F:320:HIS:CE1    | 1:F:322:ALA:HB3    | 2.39                     | 0.58              |
| 1:D:283:GLU:HG3    | 1:D:337:LEU:HD12   | 1.86                     | 0.57              |
| 1:B:242:LEU:O      | 1:B:246:HIS:HD2    | 1.86                     | 0.57              |
| 1:F:135:MET:HE1    | 1:F:144:LEU:HD13   | 1.85                     | 0.57              |
| 1:D:174:PHE:HB2    | 1:D:196:PHE:CE2    | 2.38                     | 0.57              |
| 1:C:170:LEU:HD23   | 1:C:170:LEU:C      | 2.30                     | 0.57              |
| 1:C:196:PHE:CD1    | 1:C:239:VAL:HG22   | 2.40                     | 0.57              |
| 1:D:174:PHE:CB     | 1:D:196:PHE:CE2    | 2.88                     | 0.57              |
| 1:F:101:HIS:HD2    | 6:F:606:HOH:O      | 1.86                     | 0.57              |
| 1:B:256:LEU:HD22   | 1:B:284[A]:MET:HB3 | 1.87                     | 0.56              |
| 1:F:236:ASN:OD1    | 3:F:502:4OA:O4A    | 2.23                     | 0.56              |
| 1:A:266:ARG:HD3    | 1:A:337:LEU:HD23   | 1.87                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:D:145:VAL:HA     | 1:D:149:ALA:HB3    | 1.86                     | 0.56              |
| 1:E:133:ASP:O      | 1:E:136:VAL:HG22   | 2.04                     | 0.56              |
| 1:A:251:ASN:HD21   | 1:A:392:LYS:HZ3    | 1.54                     | 0.56              |
| 1:D:132:LEU:O      | 1:D:136:VAL:HG13   | 2.05                     | 0.56              |
| 1:E:69:ARG:HD2     | 1:E:302:GLU:CD     | 2.31                     | 0.55              |
| 1:D:154:VAL:HG11   | 1:D:168:ARG:HD2    | 1.88                     | 0.55              |
| 1:C:42:ARG:HG2     | 1:C:53:TRP:CZ3     | 2.41                     | 0.55              |
| 1:B:93[A]:VAL:HG21 | 1:B:237:MET:SD     | 2.47                     | 0.55              |
| 1:D:196:PHE:CD1    | 1:D:239:VAL:HG13   | 2.42                     | 0.55              |
| 1:F:207:ARG:HG2    | 1:F:217:GLY:HA2    | 1.89                     | 0.55              |
| 1:F:246:HIS:O      | 1:F:250:VAL:HG23   | 2.07                     | 0.55              |
| 1:A:172:ARG:HD2    | 1:A:246:HIS:CE1    | 2.40                     | 0.55              |
| 1:A:170:LEU:C      | 1:A:170:LEU:HD23   | 2.32                     | 0.55              |
| 1:B:123:ARG:HD3    | 1:B:159:GLU:OE1    | 2.07                     | 0.55              |
| 1:A:12:ASP:HB2     | 1:A:44:ARG:HH12    | 1.72                     | 0.55              |
| 1:A:236:ASN:HD21   | 3:A:502:4OA:C24    | 2.20                     | 0.55              |
| 2:C:501:HEM:HBC2   | 2:C:501:HEM:HMC2   | 1.89                     | 0.54              |
| 2:B:501:HEM:HBC2   | 2:B:501:HEM:HMC2   | 1.90                     | 0.54              |
| 1:F:172:ARG:HD2    | 1:F:246:HIS:CE1    | 2.43                     | 0.54              |
| 1:D:191:ARG:HD3    | 6:E:620:HOH:O      | 2.06                     | 0.54              |
| 1:C:172:ARG:HD2    | 1:C:246:HIS:CE1    | 2.43                     | 0.54              |
| 1:A:45:LEU:HD22    | 1:A:81:PRO:CB      | 2.38                     | 0.54              |
| 1:B:260:LEU:CG     | 1:B:284[A]:MET:HE1 | 2.35                     | 0.54              |
| 1:B:260:LEU:CD2    | 1:B:284[A]:MET:HE1 | 2.38                     | 0.53              |
| 1:D:170:LEU:C      | 1:D:170:LEU:HD23   | 2.33                     | 0.53              |
| 1:D:263:GLU:HB3    | 1:D:265[A]:LYS:HZ3 | 1.73                     | 0.53              |
| 1:D:297:VAL:HG22   | 1:D:318:VAL:HG23   | 1.91                     | 0.53              |
| 1:C:283:GLU:HG3    | 1:C:337:LEU:CD1    | 2.38                     | 0.53              |
| 1:F:221:LEU:O      | 1:F:224:ASP:HB2    | 2.09                     | 0.53              |
| 1:F:258:HIS:O      | 1:F:262:THR:OG1    | 2.27                     | 0.52              |
| 1:E:101:HIS:HE1    | 2:E:501:HEM:O2D    | 1.91                     | 0.52              |
| 1:C:188:GLU:HB2    | 6:C:608:HOH:O      | 2.09                     | 0.52              |
| 1:D:179:LEU:HD11   | 1:D:247:GLU:HG3    | 1.92                     | 0.52              |
| 1:D:101:HIS:HD2    | 6:D:601:HOH:O      | 1.93                     | 0.52              |
| 1:E:145:VAL:HG21   | 1:E:402:ARG:HA     | 1.91                     | 0.52              |
| 1:F:105:ARG:HD3    | 1:F:357:ILE:HD12   | 1.91                     | 0.52              |
| 1:D:152:PHE:CB     | 1:D:153:PRO:HD3    | 2.36                     | 0.52              |
| 1:A:242:LEU:O      | 1:A:246:HIS:HD2    | 1.91                     | 0.51              |
| 1:D:178:MET:HE3    | 1:D:193:GLN:HG2    | 1.93                     | 0.51              |
| 1:F:17:TYR:CD1     | 1:F:18:PRO:HA      | 2.46                     | 0.51              |
| 1:F:178:MET:HE3    | 1:F:193:GLN:HG2    | 1.92                     | 0.51              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:45:LEU:HD22    | 1:A:81:PRO:HB3     | 1.92                     | 0.51              |
| 1:D:107:LEU:HD22   | 1:D:219:LEU:HD23   | 1.92                     | 0.51              |
| 2:D:501:HEM:HBC2   | 2:D:501:HEM:HMC2   | 1.93                     | 0.51              |
| 1:B:150:VAL:O      | 1:B:154:VAL:HG13   | 2.11                     | 0.51              |
| 1:C:159[A]:GLU:OE2 | 4:C:520:FMT:O2     | 2.29                     | 0.51              |
| 1:E:150:VAL:O      | 1:E:154:VAL:HG13   | 2.11                     | 0.51              |
| 1:D:31:TYR:CZ      | 1:D:320:HIS:CD2    | 2.99                     | 0.50              |
| 1:D:174:PHE:HB2    | 1:D:196:PHE:HE2    | 1.74                     | 0.50              |
| 1:B:17:TYR:CD1     | 1:B:18:PRO:HA      | 2.47                     | 0.50              |
| 1:A:191:ARG:NH2    | 1:A:194[A]:GLN:OE1 | 2.45                     | 0.50              |
| 1:E:42:ARG:HG3     | 1:E:51:THR:HG21    | 1.93                     | 0.50              |
| 1:F:161:LEU:O      | 1:F:216:LEU:HB2    | 2.12                     | 0.50              |
| 1:F:283:GLU:HG3    | 1:F:337:LEU:HD12   | 1.92                     | 0.50              |
| 1:B:291:VAL:HB     | 4:B:513:FMT:H      | 1.92                     | 0.50              |
| 1:F:332:ASP:O      | 1:F:333:HIS:C      | 2.55                     | 0.50              |
| 1:A:256:LEU:HD22   | 1:A:284[A]:MET:HB3 | 1.93                     | 0.49              |
| 2:A:501:HEM:HBB2   | 2:A:501:HEM:HMB2   | 1.93                     | 0.49              |
| 1:E:55:VAL:HG21    | 1:E:64:VAL:HG21    | 1.93                     | 0.49              |
| 1:A:35:ARG:HH11    | 4:A:505:FMT:C      | 2.26                     | 0.49              |
| 1:F:24:ALA:HA      | 1:F:391:TRP:CE2    | 2.47                     | 0.49              |
| 2:F:501:HEM:HBB2   | 2:F:501:HEM:CMB    | 2.42                     | 0.49              |
| 1:B:256:LEU:HD22   | 1:B:284[B]:MET:HB3 | 1.94                     | 0.49              |
| 1:D:168:ARG:HA     | 1:D:171:PHE:CE2    | 2.46                     | 0.49              |
| 1:E:152:PHE:HB3    | 1:E:153:PRO:HD3    | 1.93                     | 0.49              |
| 1:F:30:HIS:HD2     | 1:F:33:GLU:OE2     | 1.95                     | 0.49              |
| 1:F:42:ARG:HG2     | 1:F:51:THR:OG1     | 2.12                     | 0.49              |
| 1:C:27:LEU:HD13    | 6:C:695:HOH:O      | 2.13                     | 0.49              |
| 1:E:264:ARG:NH2    | 1:E:380:LEU:O      | 2.46                     | 0.48              |
| 1:B:92:GLY:O       | 1:B:96:GLN:HG2     | 2.13                     | 0.48              |
| 1:F:259:LEU:HB2    | 1:F:284:MET:CE     | 2.43                     | 0.48              |
| 1:D:172:ARG:HD2    | 1:D:246:HIS:HE1    | 1.77                     | 0.48              |
| 1:F:124:VAL:O      | 1:F:128:VAL:HG23   | 2.13                     | 0.48              |
| 1:F:154:VAL:HG11   | 1:F:168:ARG:HD2    | 1.95                     | 0.48              |
| 1:B:110:LYS:NZ     | 1:B:116:ARG:HE     | 2.10                     | 0.48              |
| 2:A:501:HEM:C1A    | 3:A:502:4OA:H6     | 2.48                     | 0.48              |
| 1:B:196:PHE:CD1    | 1:B:239:VAL:HG22   | 2.46                     | 0.48              |
| 1:A:22:PRO:HB2     | 1:A:398:ARG:HD3    | 1.96                     | 0.48              |
| 1:E:242:LEU:O      | 1:E:246:HIS:HD2    | 1.96                     | 0.48              |
| 1:B:176:ASP:OD1    | 1:B:247:GLU:OE2    | 2.32                     | 0.48              |
| 1:D:242:LEU:O      | 1:D:246:HIS:CD2    | 2.61                     | 0.48              |
| 1:A:92:GLY:HA2     | 1:A:236:ASN:HD22   | 1.79                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:B:196:PHE:CD1   | 1:B:239:VAL:HG13   | 2.49                     | 0.48              |
| 1:D:265[A]:LYS:NZ | 1:D:265[A]:LYS:HB2 | 2.28                     | 0.47              |
| 1:E:236:ASN:HD21  | 3:E:502:4OA:C24    | 2.27                     | 0.47              |
| 1:C:152:PHE:HB3   | 1:C:153:PRO:HD3    | 1.95                     | 0.47              |
| 1:D:107:LEU:HD21  | 1:D:222:ALA:CB     | 2.45                     | 0.47              |
| 1:F:260:LEU:HG    | 1:F:284:MET:HE1    | 1.96                     | 0.47              |
| 1:B:259:LEU:HB2   | 1:B:284[A]:MET:HE2 | 1.96                     | 0.47              |
| 1:D:263:GLU:HB3   | 1:D:265[A]:LYS:NZ  | 2.29                     | 0.47              |
| 1:E:43:VAL:HG21   | 1:E:54:LEU:HB2     | 1.97                     | 0.47              |
| 1:E:330:VAL:HG22  | 1:E:331:PHE:CD2    | 2.50                     | 0.47              |
| 1:F:172:ARG:HD2   | 1:F:246:HIS:HE1    | 1.78                     | 0.47              |
| 1:F:208:ARG:NH2   | 6:F:604:HOH:O      | 2.46                     | 0.47              |
| 1:A:17:TYR:HA     | 1:A:18:PRO:C       | 2.39                     | 0.47              |
| 1:A:152:PHE:HB3   | 1:A:153:PRO:HD3    | 1.96                     | 0.47              |
| 1:B:248:THR:O     | 1:B:252:GLN:HB2    | 2.15                     | 0.47              |
| 1:D:179:LEU:HD13  | 1:D:397:ILE:HD11   | 1.96                     | 0.47              |
| 1:D:200:MET:HE3   | 1:D:238:GLY:C      | 2.38                     | 0.47              |
| 1:A:172:ARG:CD    | 1:A:246:HIS:CE1    | 2.98                     | 0.47              |
| 1:A:322:ALA:O     | 1:A:326:ARG:HG2    | 2.15                     | 0.47              |
| 1:B:237:MET:HE3   | 1:B:241:LEU:HG     | 1.95                     | 0.47              |
| 1:C:132:LEU:O     | 1:C:136:VAL:HG13   | 2.15                     | 0.47              |
| 1:D:322:ALA:O     | 1:D:326:ARG:HG2    | 2.15                     | 0.47              |
| 1:E:24:ALA:HA     | 1:E:391:TRP:CE2    | 2.50                     | 0.47              |
| 1:A:303:ASP:HA    | 1:A:311:VAL:O      | 2.15                     | 0.47              |
| 1:B:42:ARG:HG2    | 1:B:53:TRP:CZ3     | 2.50                     | 0.46              |
| 1:C:174:PHE:HB2   | 1:C:196:PHE:CE2    | 2.50                     | 0.46              |
| 1:A:256:LEU:HD22  | 1:A:284[B]:MET:HB3 | 1.95                     | 0.46              |
| 1:D:17:TYR:HA     | 1:D:18:PRO:C       | 2.41                     | 0.46              |
| 1:F:101:HIS:HE1   | 2:F:501:HEM:O2D    | 1.98                     | 0.46              |
| 1:D:104:LEU:O     | 1:D:107:LEU:HB2    | 2.15                     | 0.46              |
| 1:F:75:ALA:HA     | 1:F:80:THR:HG21    | 1.97                     | 0.46              |
| 4:B:514:FMT:O1    | 4:B:517:FMT:C      | 2.63                     | 0.46              |
| 1:C:31:TYR:CZ     | 1:C:320:HIS:CD2    | 3.04                     | 0.46              |
| 1:D:45:LEU:HD12   | 1:D:81:PRO:CB      | 2.46                     | 0.46              |
| 1:E:252:GLN:HA    | 1:E:252:GLN:OE1    | 2.16                     | 0.46              |
| 1:B:321:PHE:CD2   | 4:B:513:FMT:H      | 2.50                     | 0.46              |
| 1:B:327:ASP:OD1   | 1:B:327:ASP:C      | 2.59                     | 0.46              |
| 1:E:322:ALA:O     | 1:E:326:ARG:HG2    | 2.15                     | 0.46              |
| 2:E:501:HEM:HBC2  | 2:E:501:HEM:HMC2   | 1.99                     | 0.45              |
| 1:A:172:ARG:CD    | 1:A:246:HIS:HE1    | 2.27                     | 0.45              |
| 1:B:174:PHE:HB2   | 1:B:196:PHE:HE2    | 1.80                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:B:145:VAL:HA     | 1:B:149:ALA:HB3     | 1.98                     | 0.45              |
| 1:D:265[A]:LYS:HB2 | 1:D:265[A]:LYS:HZ2  | 1.81                     | 0.45              |
| 1:C:242:LEU:O      | 1:C:246:HIS:HD2     | 1.99                     | 0.45              |
| 1:E:172:ARG:NH1    | 1:E:246:HIS:HE1     | 2.14                     | 0.45              |
| 1:E:260:LEU:HG     | 1:E:284:MET:HE1     | 1.99                     | 0.45              |
| 1:F:93:VAL:HG21    | 1:F:237:MET:HE1     | 1.97                     | 0.45              |
| 1:B:170:LEU:HD12   | 1:B:170:LEU:HA      | 1.64                     | 0.45              |
| 1:D:161:LEU:O      | 1:D:216:LEU:HG      | 2.17                     | 0.45              |
| 1:F:161:LEU:HB3    | 1:F:216:LEU:HD13    | 1.98                     | 0.45              |
| 1:B:174:PHE:CB     | 1:B:196:PHE:CE2     | 2.98                     | 0.45              |
| 2:E:501:HEM:HBB2   | 2:E:501:HEM:HMB2    | 1.99                     | 0.45              |
| 1:A:137:ALA:O      | 1:A:138:HIS:C       | 2.58                     | 0.45              |
| 1:E:312:ARG:O      | 1:E:313:ALA:C       | 2.58                     | 0.45              |
| 1:F:375:ARG:HG3    | 1:F:376:ARG:HG3     | 1.99                     | 0.45              |
| 1:A:111:ALA:HB2    | 1:A:215[A]:LEU:HD21 | 1.99                     | 0.45              |
| 1:C:176:ASP:OD1    | 1:C:183:ARG:NH2     | 2.50                     | 0.45              |
| 1:D:64:VAL:HA      | 1:D:70:PHE:CD2      | 2.52                     | 0.45              |
| 1:A:111:ALA:CB     | 1:A:215[A]:LEU:HD21 | 2.47                     | 0.44              |
| 2:D:501:HEM:HBC2   | 2:D:501:HEM:CMC     | 2.47                     | 0.44              |
| 1:E:168:ARG:O      | 1:E:169:ASP:C       | 2.60                     | 0.44              |
| 1:E:46:PRO:HB2     | 1:E:47:TYR:CD2      | 2.52                     | 0.44              |
| 3:C:502:4OA:H21A   | 3:C:502:4OA:H12     | 1.99                     | 0.44              |
| 1:E:68:SER:O       | 1:E:69:ARG:C        | 2.61                     | 0.44              |
| 1:B:13:ALA:O       | 1:C:115[B]:ARG:NE   | 2.51                     | 0.44              |
| 2:C:501:HEM:HBC2   | 2:C:501:HEM:CMC     | 2.47                     | 0.44              |
| 1:E:17:TYR:HA      | 1:E:18:PRO:C        | 2.42                     | 0.44              |
| 1:F:117:VAL:O      | 1:F:120:MET:HG2     | 2.16                     | 0.44              |
| 1:F:346:HIS:HD2    | 1:F:348:ALA:H       | 1.65                     | 0.44              |
| 1:D:330:VAL:HG22   | 1:D:331:PHE:CE2     | 2.53                     | 0.44              |
| 1:E:172:ARG:HH11   | 1:E:246:HIS:HE1     | 1.64                     | 0.44              |
| 1:F:372:ALA:O      | 1:F:376:ARG:HB2     | 2.18                     | 0.44              |
| 1:B:110:LYS:HZ3    | 1:B:116:ARG:HE      | 1.65                     | 0.44              |
| 1:B:185:THR:HB     | 4:B:511:FMT:O2      | 2.18                     | 0.44              |
| 1:B:256:LEU:HD13   | 1:B:284[B]:MET:HE3  | 2.00                     | 0.44              |
| 2:B:501:HEM:C1A    | 3:B:502:4OA:H6      | 2.53                     | 0.44              |
| 1:D:172:ARG:HD2    | 1:D:246:HIS:CE1     | 2.53                     | 0.44              |
| 1:D:392:LYS:HB3    | 1:D:395:MET:HE3     | 2.00                     | 0.44              |
| 2:A:501:HEM:HMC2   | 2:A:501:HEM:HBC2    | 1.99                     | 0.43              |
| 1:F:327:ASP:H      | 1:F:331:PHE:HE1     | 1.66                     | 0.43              |
| 1:A:174:PHE:HB3    | 1:A:196:PHE:CD2     | 2.53                     | 0.43              |
| 1:B:108:VAL:HG23   | 1:B:357:ILE:HD11    | 1.99                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:B:321:PHE:H       | 4:B:513:FMT:C       | 2.30                     | 0.43              |
| 1:C:258:HIS:HE1     | 4:C:510:FMT:O2      | 2.00                     | 0.43              |
| 1:E:104:LEU:O       | 1:E:107:LEU:HB3     | 2.18                     | 0.43              |
| 1:E:384:GLU:CD      | 1:E:402:ARG:NH1     | 2.76                     | 0.43              |
| 1:D:180:SER:OG      | 1:D:189:ILE:HD11    | 2.19                     | 0.43              |
| 1:F:152:PHE:HB3     | 1:F:153:PRO:HD3     | 2.00                     | 0.43              |
| 1:B:132:LEU:O       | 1:B:136:VAL:HG13    | 2.18                     | 0.43              |
| 1:D:321:PHE:HB2     | 4:D:514:FMT:H       | 2.00                     | 0.43              |
| 1:F:150:VAL:O       | 1:F:154:VAL:CG2     | 2.67                     | 0.43              |
| 1:B:62:ARG:HE       | 4:B:506:FMT:C       | 2.30                     | 0.43              |
| 1:A:108:VAL:CG2     | 1:A:215[A]:LEU:HD13 | 2.48                     | 0.43              |
| 1:B:27:LEU:HD23     | 1:B:27:LEU:HA       | 1.91                     | 0.43              |
| 1:E:145:VAL:HA      | 1:E:149:ALA:HB3     | 1.99                     | 0.43              |
| 3:E:502:4OA:H21A    | 3:E:502:4OA:H18B    | 2.00                     | 0.43              |
| 1:B:264:ARG:O       | 1:B:265:LYS:C       | 2.61                     | 0.43              |
| 1:A:215[B]:LEU:HD12 | 1:A:215[B]:LEU:HA   | 1.78                     | 0.43              |
| 1:A:135[A]:MET:HE2  | 1:A:407:TRP:CZ3     | 2.54                     | 0.43              |
| 1:D:42:ARG:NH2      | 1:D:53:TRP:CZ2      | 2.86                     | 0.43              |
| 1:F:161:LEU:CD2     | 1:F:215:LEU:HD12    | 2.48                     | 0.43              |
| 1:D:392:LYS:HB3     | 1:D:395:MET:HE2     | 2.01                     | 0.43              |
| 1:B:150:VAL:O       | 1:B:154:VAL:CG1     | 2.67                     | 0.42              |
| 1:D:220:ALA:O       | 1:D:223:THR:OG1     | 2.37                     | 0.42              |
| 1:F:92:GLY:O        | 1:F:96:GLN:HG2      | 2.18                     | 0.42              |
| 1:A:121:ARG:CD      | 1:D:42:ARG:HH21     | 2.32                     | 0.42              |
| 1:B:283:GLU:OE1     | 1:B:283:GLU:HA      | 2.19                     | 0.42              |
| 1:B:303:ASP:HA      | 1:B:311:VAL:O       | 2.19                     | 0.42              |
| 1:D:265[B]:LYS:HG3  | 1:D:266:ARG:N       | 2.34                     | 0.42              |
| 1:F:81:PRO:O        | 1:F:297:VAL:HG21    | 2.19                     | 0.42              |
| 1:A:370:LEU:O       | 1:A:374:VAL:HB      | 2.19                     | 0.42              |
| 1:B:302:GLU:HA      | 1:B:313:ALA:HB2     | 2.01                     | 0.42              |
| 1:C:260:LEU:CD1     | 1:C:370[B]:LEU:HD11 | 2.49                     | 0.42              |
| 1:A:283:GLU:HA      | 1:A:283:GLU:OE1     | 2.19                     | 0.42              |
| 1:F:205:ALA:O       | 1:F:208:ARG:HB2     | 2.20                     | 0.42              |
| 1:A:260:LEU:CD2     | 1:A:284[A]:MET:HE1  | 2.49                     | 0.42              |
| 2:C:501:HEM:HBB2    | 2:C:501:HEM:HMB2    | 2.02                     | 0.42              |
| 1:E:112:PHE:CZ      | 1:E:160:LEU:HD21    | 2.55                     | 0.42              |
| 1:C:384:GLU:OE2     | 1:C:402:ARG:HD2     | 2.20                     | 0.42              |
| 1:E:46:PRO:HB2      | 1:E:47:TYR:CE2      | 2.55                     | 0.42              |
| 1:E:92:GLY:HA2      | 1:E:236:ASN:HD22    | 1.84                     | 0.42              |
| 1:D:161:LEU:HD23    | 1:D:215:LEU:HD12    | 2.02                     | 0.42              |
| 1:D:283:GLU:OE1     | 1:D:283:GLU:HA      | 2.20                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E:383:ALA:HB3    | 1:E:404:ILE:HG22   | 2.02                     | 0.42              |
| 1:A:384:GLU:OE2    | 1:A:402:ARG:HD3    | 2.20                     | 0.42              |
| 2:E:501:HEM:C1A    | 3:E:502:4OA:H6     | 2.55                     | 0.42              |
| 1:D:196:PHE:CD1    | 1:D:239:VAL:HG22   | 2.52                     | 0.42              |
| 1:D:283:GLU:HG3    | 1:D:337:LEU:CD1    | 2.49                     | 0.41              |
| 1:E:93:VAL:HB      | 1:E:237:MET:HE1    | 2.01                     | 0.41              |
| 1:A:45:LEU:HD22    | 1:A:81:PRO:HB2     | 2.02                     | 0.41              |
| 1:F:271:VAL:HA     | 1:F:374:VAL:HG13   | 2.01                     | 0.41              |
| 1:A:264:ARG:NH1    | 1:A:380:LEU:O      | 2.53                     | 0.41              |
| 1:E:31:TYR:CE1     | 1:E:320:HIS:CD2    | 3.08                     | 0.41              |
| 1:E:168:ARG:HA     | 1:E:171:PHE:CE2    | 2.54                     | 0.41              |
| 1:F:377:PHE:O      | 1:F:380:LEU:HB2    | 2.20                     | 0.41              |
| 1:A:107:LEU:HD21   | 1:A:219:LEU:CD2    | 2.50                     | 0.41              |
| 1:D:35:ARG:HH11    | 4:D:505:FMT:C      | 2.33                     | 0.41              |
| 1:E:246:HIS:O      | 1:E:250:VAL:HG23   | 2.21                     | 0.41              |
| 1:E:259:LEU:HB2    | 1:E:284:MET:HE2    | 2.01                     | 0.41              |
| 1:F:327:ASP:C      | 1:F:327:ASP:OD1    | 2.64                     | 0.41              |
| 1:C:157:ILE:HD12   | 1:C:157:ILE:HA     | 1.96                     | 0.41              |
| 1:C:402:ARG:HD3    | 1:C:404:ILE:CG1    | 2.40                     | 0.41              |
| 1:A:128:VAL:HG23   | 1:A:152:PHE:CE1    | 2.55                     | 0.41              |
| 1:F:143:ASP:HA     | 1:F:404:ILE:HA     | 2.02                     | 0.41              |
| 1:A:168:ARG:O      | 1:A:169:ASP:C      | 2.64                     | 0.41              |
| 2:B:501:HEM:HBC2   | 2:B:501:HEM:CMC    | 2.51                     | 0.41              |
| 1:C:303:ASP:HA     | 1:C:311:VAL:O      | 2.20                     | 0.41              |
| 1:D:302:GLU:HA     | 1:D:313:ALA:HB2    | 2.02                     | 0.41              |
| 1:D:170:LEU:HA     | 1:E:106:ARG:HE     | 1.86                     | 0.41              |
| 1:E:191[A]:ARG:HA  | 1:E:191[A]:ARG:HD2 | 1.85                     | 0.41              |
| 1:E:280:ALA:O      | 1:E:284:MET:HG3    | 2.21                     | 0.41              |
| 1:A:196:PHE:CZ     | 1:A:242:LEU:HD23   | 2.56                     | 0.41              |
| 1:B:17:TYR:HA      | 1:B:18:PRO:C       | 2.46                     | 0.41              |
| 1:B:252:GLN:OE1    | 1:B:252:GLN:HA     | 2.20                     | 0.41              |
| 1:C:24:ALA:HA      | 1:C:391:TRP:CE2    | 2.56                     | 0.41              |
| 1:D:328[B]:GLU:HB2 | 4:D:505:FMT:O1     | 2.20                     | 0.41              |
| 1:E:140:SER:OG     | 1:E:406:SER:HA     | 2.20                     | 0.41              |
| 1:F:17:TYR:HA      | 1:F:18:PRO:C       | 2.44                     | 0.41              |
| 1:F:252:GLN:O      | 1:F:256:LEU:HD13   | 2.21                     | 0.41              |
| 1:F:381:ASP:O      | 1:F:405:VAL:HG22   | 2.21                     | 0.41              |
| 1:D:330:VAL:HG22   | 1:D:331:PHE:CD2    | 2.56                     | 0.41              |
| 1:E:82:ARG:HD3     | 1:E:88:PRO:HD3     | 2.02                     | 0.41              |
| 1:C:397:ILE:HG21   | 1:C:397:ILE:HD13   | 1.81                     | 0.40              |
| 1:D:101:HIS:O      | 1:D:105:ARG:HG3    | 2.21                     | 0.40              |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:165:LEU:HD12 | 1:E:165:LEU:HA   | 1.94                     | 0.40              |
| 1:E:174:PHE:HB3  | 1:E:196:PHE:CD2  | 2.56                     | 0.40              |
| 1:C:42:ARG:HG2   | 1:C:53:TRP:CE3   | 2.56                     | 0.40              |
| 1:E:74:ALA:HB3   | 1:E:299:VAL:HB   | 2.04                     | 0.40              |
| 2:E:501:HEM:HBC2 | 2:E:501:HEM:CMC  | 2.51                     | 0.40              |
| 1:F:30:HIS:HE1   | 6:F:662:HOH:O    | 2.05                     | 0.40              |
| 1:F:252:GLN:OE1  | 1:F:252:GLN:HA   | 2.20                     | 0.40              |
| 1:C:180:SER:OG   | 1:C:189:ILE:HD11 | 2.21                     | 0.40              |
| 1:E:105:ARG:CZ   | 1:E:357:ILE:HB   | 2.52                     | 0.40              |
| 1:F:157:ILE:HD12 | 1:F:157:ILE:HA   | 1.89                     | 0.40              |
| 1:A:177:ALA:HA   | 1:A:184:LEU:HD12 | 2.03                     | 0.40              |
| 1:A:237:MET:HE3  | 1:A:241:LEU:HG   | 2.04                     | 0.40              |
| 1:D:106:ARG:HA   | 1:D:106:ARG:HD2  | 1.95                     | 0.40              |
| 1:C:172:ARG:HD2  | 1:C:246:HIS:HE1  | 1.86                     | 0.40              |
| 1:F:327:ASP:N    | 1:F:331:PHE:HE1  | 2.19                     | 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     | 402/398 (101%)   | 385 (96%)  | 17 (4%) | 0        | 100         | 100 |
| 1   | B     | 398/398 (100%)   | 387 (97%)  | 11 (3%) | 0        | 100         | 100 |
| 1   | C     | 405/398 (102%)   | 395 (98%)  | 10 (2%) | 0        | 100         | 100 |
| 1   | D     | 400/398 (100%)   | 374 (94%)  | 26 (6%) | 0        | 100         | 100 |
| 1   | E     | 393/398 (99%)    | 378 (96%)  | 15 (4%) | 0        | 100         | 100 |
| 1   | F     | 395/398 (99%)    | 376 (95%)  | 19 (5%) | 0        | 100         | 100 |
| All | All   | 2393/2388 (100%) | 2295 (96%) | 98 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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     | 340/333 (102%)   | 328 (96%)  | 12 (4%)  | 32          | 48 |
| 1   | B     | 336/333 (101%)   | 325 (97%)  | 11 (3%)  | 33          | 50 |
| 1   | C     | 342/333 (103%)   | 336 (98%)  | 6 (2%)   | 51          | 70 |
| 1   | D     | 337/333 (101%)   | 324 (96%)  | 13 (4%)  | 28          | 43 |
| 1   | E     | 332/333 (100%)   | 318 (96%)  | 14 (4%)  | 26          | 40 |
| 1   | F     | 333/333 (100%)   | 314 (94%)  | 19 (6%)  | 18          | 27 |
| All | All   | 2020/1998 (101%) | 1945 (96%) | 75 (4%)  | 30          | 45 |

All (75) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 12     | ASP  |
| 1   | A     | 14     | VAL  |
| 1   | A     | 45     | LEU  |
| 1   | A     | 127    | LEU  |
| 1   | A     | 136    | VAL  |
| 1   | A     | 170    | LEU  |
| 1   | A     | 194[A] | GLN  |
| 1   | A     | 194[B] | GLN  |
| 1   | A     | 204    | VAL  |
| 1   | A     | 252    | GLN  |
| 1   | A     | 318    | VAL  |
| 1   | A     | 374    | VAL  |
| 1   | B     | 14     | VAL  |
| 1   | B     | 136    | VAL  |
| 1   | B     | 154    | VAL  |
| 1   | B     | 165    | LEU  |
| 1   | B     | 221    | LEU  |
| 1   | B     | 224    | ASP  |
| 1   | B     | 225    | ASN  |
| 1   | B     | 256    | LEU  |
| 1   | B     | 342    | GLU  |
| 1   | B     | 374    | VAL  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | B     | 401    | GLU  |
| 1   | C     | 136    | VAL  |
| 1   | C     | 204    | VAL  |
| 1   | C     | 209    | ASP  |
| 1   | C     | 318    | VAL  |
| 1   | C     | 374    | VAL  |
| 1   | C     | 398    | ARG  |
| 1   | D     | 127    | LEU  |
| 1   | D     | 136    | VAL  |
| 1   | D     | 204    | VAL  |
| 1   | D     | 209    | ASP  |
| 1   | D     | 225    | ASN  |
| 1   | D     | 256    | LEU  |
| 1   | D     | 265[A] | LYS  |
| 1   | D     | 265[B] | LYS  |
| 1   | D     | 305    | GLU  |
| 1   | D     | 318    | VAL  |
| 1   | D     | 330    | VAL  |
| 1   | D     | 374    | VAL  |
| 1   | D     | 397    | ILE  |
| 1   | E     | 42     | ARG  |
| 1   | E     | 45     | LEU  |
| 1   | E     | 49     | GLU  |
| 1   | E     | 154    | VAL  |
| 1   | E     | 204    | VAL  |
| 1   | E     | 215    | LEU  |
| 1   | E     | 264    | ARG  |
| 1   | E     | 297    | VAL  |
| 1   | E     | 309    | VAL  |
| 1   | E     | 318    | VAL  |
| 1   | E     | 330    | VAL  |
| 1   | E     | 374    | VAL  |
| 1   | E     | 390    | LYS  |
| 1   | E     | 393    | GLN  |
| 1   | F     | 23     | HIS  |
| 1   | F     | 45     | LEU  |
| 1   | F     | 136    | VAL  |
| 1   | F     | 140    | SER  |
| 1   | F     | 198    | VAL  |
| 1   | F     | 204    | VAL  |
| 1   | F     | 252    | GLN  |
| 1   | F     | 262    | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 264 | ARG  |
| 1   | F     | 277 | VAL  |
| 1   | F     | 309 | VAL  |
| 1   | F     | 318 | VAL  |
| 1   | F     | 331 | PHE  |
| 1   | F     | 332 | ASP  |
| 1   | F     | 370 | LEU  |
| 1   | F     | 374 | VAL  |
| 1   | F     | 384 | GLU  |
| 1   | F     | 390 | LYS  |
| 1   | F     | 405 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 236 | ASN  |
| 1   | A     | 246 | HIS  |
| 1   | A     | 251 | ASN  |
| 1   | A     | 258 | HIS  |
| 1   | A     | 320 | HIS  |
| 1   | A     | 340 | HIS  |
| 1   | A     | 351 | HIS  |
| 1   | B     | 96  | GLN  |
| 1   | B     | 193 | GLN  |
| 1   | B     | 246 | HIS  |
| 1   | B     | 320 | HIS  |
| 1   | B     | 351 | HIS  |
| 1   | B     | 393 | GLN  |
| 1   | C     | 30  | HIS  |
| 1   | C     | 193 | GLN  |
| 1   | C     | 246 | HIS  |
| 1   | C     | 258 | HIS  |
| 1   | C     | 320 | HIS  |
| 1   | C     | 351 | HIS  |
| 1   | D     | 193 | GLN  |
| 1   | D     | 246 | HIS  |
| 1   | D     | 351 | HIS  |
| 1   | E     | 101 | HIS  |
| 1   | E     | 194 | GLN  |
| 1   | E     | 236 | ASN  |
| 1   | E     | 246 | HIS  |
| 1   | E     | 320 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 351 | HIS  |
| 1   | F     | 30  | HIS  |
| 1   | F     | 101 | HIS  |
| 1   | F     | 193 | GLN  |
| 1   | F     | 225 | ASN  |
| 1   | F     | 236 | ASN  |
| 1   | F     | 246 | HIS  |
| 1   | F     | 340 | HIS  |
| 1   | F     | 344 | ASN  |
| 1   | F     | 346 | HIS  |
| 1   | F     | 351 | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 120 ligands modelled in this entry, 6 are monoatomic - leaving 114 for Mogul analysis.

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 | $\# Z  > 2$ |
| 4   | FMT  | E     | 507 | -    | 2,2,2        | 0.22 | 0           | 1,1,1       | 0.12 | 0           |
| 4   | FMT  | F     | 513 | -    | 2,2,2        | 0.37 | 0           | 1,1,1       | 0.12 | 0           |
| 4   | FMT  | B     | 521 | -    | 2,2,2        | 0.50 | 0           | 1,1,1       | 0.05 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | FMT  | B     | 503 | -    | 2,2,2        | 0.44 | 0        | 1,1,1       | 0.05 | 0        |
| 4   | FMT  | D     | 506 | -    | 2,2,2        | 0.41 | 0        | 1,1,1       | 0.04 | 0        |
| 4   | FMT  | C     | 518 | -    | 2,2,2        | 0.35 | 0        | 1,1,1       | 0.09 | 0        |
| 3   | 4OA  | B     | 502 | -    | 30,30,30     | 0.50 | 0        | 47,47,47    | 0.69 | 0        |
| 4   | FMT  | B     | 512 | -    | 2,2,2        | 0.66 | 0        | 1,1,1       | 0.11 | 0        |
| 4   | FMT  | C     | 513 | -    | 2,2,2        | 0.54 | 0        | 1,1,1       | 0.02 | 0        |
| 4   | FMT  | B     | 506 | -    | 2,2,2        | 0.62 | 0        | 1,1,1       | 0.08 | 0        |
| 4   | FMT  | A     | 520 | -    | 2,2,2        | 0.51 | 0        | 1,1,1       | 0.07 | 0        |
| 4   | FMT  | A     | 518 | -    | 2,2,2        | 0.69 | 0        | 1,1,1       | 0.03 | 0        |
| 4   | FMT  | A     | 504 | -    | 2,2,2        | 0.21 | 0        | 1,1,1       | 0.21 | 0        |
| 4   | FMT  | B     | 520 | -    | 2,2,2        | 0.52 | 0        | 1,1,1       | 0.01 | 0        |
| 4   | FMT  | A     | 512 | -    | 2,2,2        | 0.51 | 0        | 1,1,1       | 0.02 | 0        |
| 4   | FMT  | C     | 524 | -    | 2,2,2        | 0.61 | 0        | 1,1,1       | 0.06 | 0        |
| 2   | HEM  | F     | 501 | 1    | 50,50,50     | 1.47 | 4 (8%)   | 67,82,82    | 1.71 | 12 (17%) |
| 4   | FMT  | E     | 512 | -    | 2,2,2        | 0.30 | 0        | 1,1,1       | 0.12 | 0        |
| 4   | FMT  | F     | 505 | -    | 2,2,2        | 0.69 | 0        | 1,1,1       | 0.03 | 0        |
| 4   | FMT  | A     | 523 | -    | 2,2,2        | 0.44 | 0        | 1,1,1       | 0.03 | 0        |
| 4   | FMT  | D     | 507 | -    | 2,2,2        | 0.59 | 0        | 1,1,1       | 0.17 | 0        |
| 4   | FMT  | A     | 506 | -    | 2,2,2        | 0.31 | 0        | 1,1,1       | 0.10 | 0        |
| 4   | FMT  | B     | 508 | -    | 2,2,2        | 0.43 | 0        | 1,1,1       | 0.05 | 0        |
| 4   | FMT  | E     | 509 | -    | 2,2,2        | 0.43 | 0        | 1,1,1       | 0.11 | 0        |
| 2   | HEM  | A     | 501 | 1    | 50,50,50     | 1.61 | 9 (18%)  | 67,82,82    | 1.55 | 15 (22%) |
| 4   | FMT  | A     | 513 | -    | 2,2,2        | 0.57 | 0        | 1,1,1       | 0.06 | 0        |
| 4   | FMT  | A     | 505 | -    | 2,2,2        | 0.47 | 0        | 1,1,1       | 0.05 | 0        |
| 4   | FMT  | E     | 508 | -    | 2,2,2        | 0.40 | 0        | 1,1,1       | 0.08 | 0        |
| 4   | FMT  | B     | 505 | -    | 2,2,2        | 0.44 | 0        | 1,1,1       | 0.07 | 0        |
| 4   | FMT  | D     | 515 | -    | 2,2,2        | 0.45 | 0        | 1,1,1       | 0.07 | 0        |
| 4   | FMT  | B     | 523 | -    | 2,2,2        | 0.45 | 0        | 1,1,1       | 0.03 | 0        |
| 4   | FMT  | C     | 510 | -    | 2,2,2        | 0.25 | 0        | 1,1,1       | 0.20 | 0        |
| 4   | FMT  | B     | 518 | -    | 2,2,2        | 0.57 | 0        | 1,1,1       | 0.01 | 0        |
| 4   | FMT  | C     | 525 | -    | 2,2,2        | 0.48 | 0        | 1,1,1       | 0.04 | 0        |
| 4   | FMT  | A     | 514 | -    | 2,2,2        | 0.42 | 0        | 1,1,1       | 0.10 | 0        |
| 4   | FMT  | A     | 508 | -    | 2,2,2        | 0.49 | 0        | 1,1,1       | 0.01 | 0        |
| 4   | FMT  | B     | 513 | -    | 2,2,2        | 1.28 | 0        | 1,1,1       | 0.64 | 0        |
| 4   | FMT  | C     | 504 | -    | 2,2,2        | 0.35 | 0        | 1,1,1       | 0.15 | 0        |
| 4   | FMT  | B     | 514 | -    | 2,2,2        | 0.59 | 0        | 1,1,1       | 0.28 | 0        |
| 4   | FMT  | B     | 511 | -    | 2,2,2        | 0.40 | 0        | 1,1,1       | 0.07 | 0        |
| 4   | FMT  | B     | 519 | -    | 2,2,2        | 0.21 | 0        | 1,1,1       | 0.20 | 0        |
| 4   | FMT  | D     | 512 | -    | 2,2,2        | 0.70 | 0        | 1,1,1       | 0.06 | 0        |
| 4   | FMT  | F     | 508 | -    | 2,2,2        | 0.34 | 0        | 1,1,1       | 0.10 | 0        |
| 4   | FMT  | A     | 509 | -    | 2,2,2        | 0.39 | 0        | 1,1,1       | 0.11 | 0        |
| 4   | FMT  | A     | 503 | -    | 2,2,2        | 0.33 | 0        | 1,1,1       | 0.10 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | FMT  | F     | 507 | -    | 2,2,2        | 0.35 | 0        | 1,1,1       | 0.05 | 0        |
| 3   | 4OA  | E     | 502 | -    | 30,30,30     | 0.52 | 0        | 47,47,47    | 0.60 | 0        |
| 4   | FMT  | C     | 526 | -    | 2,2,2        | 0.32 | 0        | 1,1,1       | 0.14 | 0        |
| 4   | FMT  | A     | 517 | -    | 2,2,2        | 0.87 | 0        | 1,1,1       | 0.27 | 0        |
| 4   | FMT  | D     | 508 | -    | 2,2,2        | 0.54 | 0        | 1,1,1       | 0.04 | 0        |
| 4   | FMT  | E     | 510 | -    | 2,2,2        | 0.27 | 0        | 1,1,1       | 0.18 | 0        |
| 4   | FMT  | F     | 503 | -    | 2,2,2        | 0.35 | 0        | 1,1,1       | 0.09 | 0        |
| 3   | 4OA  | F     | 502 | -    | 30,30,30     | 0.52 | 0        | 47,47,47    | 0.77 | 0        |
| 4   | FMT  | D     | 505 | -    | 2,2,2        | 0.37 | 0        | 1,1,1       | 0.13 | 0        |
| 2   | HEM  | B     | 501 | 1    | 50,50,50     | 1.68 | 13 (26%) | 67,82,82    | 1.64 | 19 (28%) |
| 4   | FMT  | B     | 504 | -    | 2,2,2        | 0.28 | 0        | 1,1,1       | 0.18 | 0        |
| 3   | 4OA  | D     | 502 | -    | 30,30,30     | 0.61 | 0        | 47,47,47    | 0.76 | 0        |
| 4   | FMT  | A     | 507 | -    | 2,2,2        | 0.28 | 0        | 1,1,1       | 0.15 | 0        |
| 4   | FMT  | C     | 522 | -    | 2,2,2        | 0.37 | 0        | 1,1,1       | 0.12 | 0        |
| 4   | FMT  | C     | 523 | -    | 2,2,2        | 0.26 | 0        | 1,1,1       | 0.20 | 0        |
| 4   | FMT  | D     | 504 | -    | 2,2,2        | 0.27 | 0        | 1,1,1       | 0.17 | 0        |
| 4   | FMT  | D     | 514 | -    | 2,2,2        | 0.69 | 0        | 1,1,1       | 0.28 | 0        |
| 4   | FMT  | E     | 506 | -    | 2,2,2        | 0.60 | 0        | 1,1,1       | 0.02 | 0        |
| 4   | FMT  | E     | 505 | -    | 2,2,2        | 0.86 | 0        | 1,1,1       | 0.22 | 0        |
| 4   | FMT  | E     | 511 | -    | 2,2,2        | 0.63 | 0        | 1,1,1       | 0.11 | 0        |
| 4   | FMT  | C     | 519 | -    | 2,2,2        | 0.25 | 0        | 1,1,1       | 0.19 | 0        |
| 4   | FMT  | F     | 509 | -    | 2,2,2        | 0.27 | 0        | 1,1,1       | 0.14 | 0        |
| 4   | FMT  | D     | 513 | -    | 2,2,2        | 0.44 | 0        | 1,1,1       | 0.19 | 0        |
| 4   | FMT  | F     | 512 | -    | 2,2,2        | 0.37 | 0        | 1,1,1       | 0.12 | 0        |
| 4   | FMT  | F     | 504 | -    | 2,2,2        | 0.36 | 0        | 1,1,1       | 0.10 | 0        |
| 4   | FMT  | A     | 521 | -    | 2,2,2        | 0.30 | 0        | 1,1,1       | 0.09 | 0        |
| 4   | FMT  | B     | 524 | -    | 2,2,2        | 0.24 | 0        | 1,1,1       | 0.21 | 0        |
| 4   | FMT  | C     | 507 | -    | 2,2,2        | 0.07 | 0        | 1,1,1       | 0.24 | 0        |
| 4   | FMT  | A     | 519 | -    | 2,2,2        | 0.22 | 0        | 1,1,1       | 0.22 | 0        |
| 2   | HEM  | E     | 501 | 1    | 50,50,50     | 1.56 | 9 (18%)  | 67,82,82    | 1.43 | 10 (14%) |
| 4   | FMT  | C     | 505 | -    | 2,2,2        | 0.39 | 0        | 1,1,1       | 0.10 | 0        |
| 4   | FMT  | C     | 509 | -    | 2,2,2        | 0.45 | 0        | 1,1,1       | 0.02 | 0        |
| 3   | 4OA  | C     | 502 | -    | 30,30,30     | 0.58 | 0        | 47,47,47    | 0.86 | 0        |
| 4   | FMT  | B     | 509 | -    | 2,2,2        | 0.28 | 0        | 1,1,1       | 0.18 | 0        |
| 4   | FMT  | D     | 503 | -    | 2,2,2        | 0.80 | 0        | 1,1,1       | 0.29 | 0        |
| 4   | FMT  | F     | 506 | -    | 2,2,2        | 0.10 | 0        | 1,1,1       | 0.32 | 0        |
| 4   | FMT  | E     | 503 | -    | 2,2,2        | 0.28 | 0        | 1,1,1       | 0.14 | 0        |
| 4   | FMT  | C     | 516 | -    | 2,2,2        | 0.42 | 0        | 1,1,1       | 0.12 | 0        |
| 4   | FMT  | D     | 511 | -    | 2,2,2        | 0.28 | 0        | 1,1,1       | 0.20 | 0        |
| 4   | FMT  | A     | 515 | -    | 2,2,2        | 0.54 | 0        | 1,1,1       | 0.29 | 0        |
| 3   | 4OA  | A     | 502 | -    | 30,30,30     | 0.49 | 0        | 47,47,47    | 0.50 | 0        |
| 2   | HEM  | C     | 501 | 1    | 50,50,50     | 1.49 | 8 (16%)  | 67,82,82    | 1.69 | 12 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | FMT  | A     | 522 | -    | 2,2,2        | 0.29 | 0        | 1,1,1       | 0.09 | 0        |
| 4   | FMT  | F     | 510 | -    | 2,2,2        | 0.30 | 0        | 1,1,1       | 0.15 | 0        |
| 4   | FMT  | B     | 515 | -    | 2,2,2        | 0.45 | 0        | 1,1,1       | 0.05 | 0        |
| 4   | FMT  | B     | 517 | -    | 2,2,2        | 0.34 | 0        | 1,1,1       | 0.08 | 0        |
| 4   | FMT  | A     | 516 | -    | 2,2,2        | 0.37 | 0        | 1,1,1       | 0.12 | 0        |
| 4   | FMT  | A     | 524 | -    | 2,2,2        | 0.60 | 0        | 1,1,1       | 0.07 | 0        |
| 4   | FMT  | B     | 522 | -    | 2,2,2        | 0.57 | 0        | 1,1,1       | 0.02 | 0        |
| 4   | FMT  | D     | 510 | -    | 2,2,2        | 0.37 | 0        | 1,1,1       | 0.02 | 0        |
| 4   | FMT  | A     | 511 | -    | 2,2,2        | 0.29 | 0        | 1,1,1       | 0.18 | 0        |
| 4   | FMT  | C     | 521 | -    | 2,2,2        | 0.53 | 0        | 1,1,1       | 0.02 | 0        |
| 4   | FMT  | C     | 503 | -    | 2,2,2        | 0.39 | 0        | 1,1,1       | 0.07 | 0        |
| 4   | FMT  | E     | 504 | -    | 2,2,2        | 0.92 | 0        | 1,1,1       | 0.26 | 0        |
| 4   | FMT  | C     | 508 | -    | 2,2,2        | 0.23 | 0        | 1,1,1       | 0.15 | 0        |
| 4   | FMT  | C     | 512 | -    | 2,2,2        | 0.05 | 0        | 1,1,1       | 0.27 | 0        |
| 4   | FMT  | C     | 506 | -    | 2,2,2        | 0.53 | 0        | 1,1,1       | 0.05 | 0        |
| 4   | FMT  | C     | 520 | -    | 2,2,2        | 0.37 | 0        | 1,1,1       | 0.10 | 0        |
| 4   | FMT  | F     | 511 | -    | 2,2,2        | 0.39 | 0        | 1,1,1       | 0.08 | 0        |
| 4   | FMT  | C     | 511 | -    | 2,2,2        | 0.25 | 0        | 1,1,1       | 0.22 | 0        |
| 4   | FMT  | B     | 507 | -    | 2,2,2        | 0.34 | 0        | 1,1,1       | 0.11 | 0        |
| 4   | FMT  | A     | 510 | -    | 2,2,2        | 0.26 | 0        | 1,1,1       | 0.19 | 0        |
| 2   | HEM  | D     | 501 | 1    | 50,50,50     | 1.68 | 10 (20%) | 67,82,82    | 2.04 | 23 (34%) |
| 4   | FMT  | D     | 509 | -    | 2,2,2        | 0.37 | 0        | 1,1,1       | 0.07 | 0        |
| 4   | FMT  | B     | 516 | -    | 2,2,2        | 0.47 | 0        | 1,1,1       | 0.00 | 0        |
| 4   | FMT  | C     | 515 | -    | 2,2,2        | 0.36 | 0        | 1,1,1       | 0.15 | 0        |
| 4   | FMT  | B     | 510 | -    | 2,2,2        | 0.40 | 0        | 1,1,1       | 0.08 | 0        |
| 4   | FMT  | C     | 517 | -    | 2,2,2        | 0.35 | 0        | 1,1,1       | 0.10 | 0        |
| 4   | FMT  | C     | 514 | -    | 2,2,2        | 0.25 | 0        | 1,1,1       | 0.18 | 0        |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | HEM  | B     | 501 | 1    | -       | 1/14/54/54 | -       |
| 3   | 4OA  | B     | 502 | -    | -       | 3/9/67/67  | 0/4/4/4 |
| 2   | HEM  | D     | 501 | 1    | -       | 1/14/54/54 | -       |
| 2   | HEM  | E     | 501 | 1    | -       | 0/14/54/54 | -       |
| 2   | HEM  | A     | 501 | 1    | -       | 0/14/54/54 | -       |
| 2   | HEM  | F     | 501 | 1    | -       | 1/14/54/54 | -       |
| 3   | 4OA  | D     | 502 | -    | -       | 1/9/67/67  | 0/4/4/4 |
| 3   | 4OA  | A     | 502 | -    | -       | 3/9/67/67  | 0/4/4/4 |

Continued on next page...

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 2   | HEM  | C     | 501 | 1    | -       | 0/14/54/54 | -       |
| 3   | 4OA  | F     | 502 | -    | -       | 7/9/67/67  | 0/4/4/4 |
| 3   | 4OA  | E     | 502 | -    | -       | 4/9/67/67  | 0/4/4/4 |
| 3   | 4OA  | C     | 502 | -    | -       | 3/9/67/67  | 0/4/4/4 |

All (53) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | E     | 501 | HEM  | FE-NB   | 5.11  | 2.10        | 1.94     |
| 2   | F     | 501 | HEM  | FE-NC   | 4.84  | 2.11        | 1.95     |
| 2   | F     | 501 | HEM  | FE-NB   | 4.75  | 2.09        | 1.94     |
| 2   | C     | 501 | HEM  | FE-NB   | 4.29  | 2.08        | 1.94     |
| 2   | B     | 501 | HEM  | FE-NB   | 4.28  | 2.08        | 1.94     |
| 2   | A     | 501 | HEM  | C1B-NB  | -3.97 | 1.33        | 1.40     |
| 2   | D     | 501 | HEM  | FE-ND   | -3.92 | 1.82        | 1.94     |
| 2   | B     | 501 | HEM  | FE-NC   | 3.86  | 2.07        | 1.95     |
| 2   | A     | 501 | HEM  | FE-NB   | 3.79  | 2.06        | 1.94     |
| 2   | A     | 501 | HEM  | FE-NC   | 3.78  | 2.07        | 1.95     |
| 2   | E     | 501 | HEM  | FE-NC   | 3.75  | 2.07        | 1.95     |
| 2   | A     | 501 | HEM  | C4B-NB  | -3.54 | 1.31        | 1.38     |
| 2   | B     | 501 | HEM  | C1B-NB  | -3.47 | 1.34        | 1.40     |
| 2   | D     | 501 | HEM  | C4D-ND  | -3.45 | 1.34        | 1.40     |
| 2   | C     | 501 | HEM  | C1B-NB  | -3.43 | 1.34        | 1.40     |
| 2   | F     | 501 | HEM  | C1B-NB  | -3.38 | 1.34        | 1.40     |
| 2   | E     | 501 | HEM  | C4D-ND  | -3.26 | 1.34        | 1.40     |
| 2   | E     | 501 | HEM  | C1B-NB  | -3.25 | 1.34        | 1.40     |
| 2   | B     | 501 | HEM  | C4A-NA  | -3.24 | 1.33        | 1.39     |
| 2   | D     | 501 | HEM  | C1B-NB  | -3.23 | 1.34        | 1.40     |
| 2   | C     | 501 | HEM  | FE-NC   | 3.21  | 2.05        | 1.95     |
| 2   | D     | 501 | HEM  | FE-NC   | 3.10  | 2.05        | 1.95     |
| 2   | B     | 501 | HEM  | C1C-NC  | -3.09 | 1.33        | 1.39     |
| 2   | B     | 501 | HEM  | C4D-ND  | -3.08 | 1.34        | 1.40     |
| 2   | D     | 501 | HEM  | C3C-C4C | -3.00 | 1.40        | 1.46     |
| 2   | D     | 501 | HEM  | C1C-C2C | -2.97 | 1.39        | 1.45     |
| 2   | A     | 501 | HEM  | C1C-NC  | -2.94 | 1.34        | 1.39     |
| 2   | F     | 501 | HEM  | C1C-C2C | -2.94 | 1.39        | 1.45     |
| 2   | D     | 501 | HEM  | CHA-C1A | -2.93 | 1.32        | 1.39     |
| 2   | B     | 501 | HEM  | C4B-NB  | -2.76 | 1.33        | 1.38     |
| 2   | A     | 501 | HEM  | C3C-C4C | -2.72 | 1.41        | 1.46     |
| 2   | D     | 501 | HEM  | C1D-ND  | -2.66 | 1.33        | 1.38     |
| 2   | A     | 501 | HEM  | C1C-C2C | -2.43 | 1.40        | 1.45     |
| 2   | E     | 501 | HEM  | C4C-NC  | -2.43 | 1.35        | 1.39     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | D     | 501 | HEM  | FE-NB   | 2.40  | 2.02        | 1.94     |
| 2   | C     | 501 | HEM  | C4B-NB  | -2.39 | 1.34        | 1.38     |
| 2   | E     | 501 | HEM  | C1D-ND  | -2.36 | 1.34        | 1.38     |
| 2   | E     | 501 | HEM  | C1C-C2C | -2.36 | 1.40        | 1.45     |
| 2   | E     | 501 | HEM  | C4B-NB  | -2.35 | 1.34        | 1.38     |
| 2   | C     | 501 | HEM  | C4D-ND  | -2.25 | 1.36        | 1.40     |
| 2   | C     | 501 | HEM  | C1A-C2A | -2.24 | 1.40        | 1.44     |
| 2   | E     | 501 | HEM  | C1C-NC  | -2.21 | 1.35        | 1.39     |
| 2   | B     | 501 | HEM  | C3D-C2D | -2.18 | 1.32        | 1.36     |
| 2   | B     | 501 | HEM  | C1D-ND  | -2.18 | 1.34        | 1.38     |
| 2   | A     | 501 | HEM  | C4D-ND  | -2.16 | 1.36        | 1.40     |
| 2   | B     | 501 | HEM  | FE-ND   | -2.15 | 1.88        | 1.94     |
| 2   | D     | 501 | HEM  | C4C-NC  | -2.12 | 1.35        | 1.39     |
| 2   | C     | 501 | HEM  | C3C-C4C | -2.11 | 1.42        | 1.46     |
| 2   | B     | 501 | HEM  | C1C-C2C | -2.07 | 1.41        | 1.45     |
| 2   | B     | 501 | HEM  | C3C-C4C | -2.03 | 1.42        | 1.46     |
| 2   | C     | 501 | HEM  | C1C-NC  | -2.02 | 1.35        | 1.39     |
| 2   | A     | 501 | HEM  | C1D-ND  | -2.01 | 1.34        | 1.38     |
| 2   | B     | 501 | HEM  | O2D-CGD | -2.01 | 1.24        | 1.30     |

All (91) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | D     | 501 | HEM  | CHB-C1B-NB  | 5.46  | 131.12      | 124.37   |
| 2   | C     | 501 | HEM  | CHC-C4B-NB  | 5.37  | 130.21      | 124.42   |
| 2   | F     | 501 | HEM  | CHC-C4B-NB  | 5.26  | 130.08      | 124.42   |
| 2   | D     | 501 | HEM  | CHC-C4B-NB  | 5.05  | 129.85      | 124.42   |
| 2   | A     | 501 | HEM  | CHD-C1D-ND  | 5.02  | 129.83      | 124.42   |
| 2   | C     | 501 | HEM  | C1B-NB-C4B  | 4.68  | 110.75      | 105.21   |
| 2   | F     | 501 | HEM  | CAC-C3C-C4C | 4.46  | 135.47      | 124.82   |
| 2   | A     | 501 | HEM  | CHC-C4B-NB  | 4.38  | 129.14      | 124.42   |
| 2   | F     | 501 | HEM  | CHD-C1D-ND  | 4.37  | 129.12      | 124.42   |
| 2   | D     | 501 | HEM  | CHA-C4D-ND  | 4.23  | 129.60      | 124.37   |
| 2   | E     | 501 | HEM  | CHC-C4B-NB  | 4.17  | 128.91      | 124.42   |
| 2   | D     | 501 | HEM  | C1B-NB-C4B  | 4.03  | 109.98      | 105.21   |
| 2   | F     | 501 | HEM  | C1B-NB-C4B  | 3.87  | 109.79      | 105.21   |
| 2   | C     | 501 | HEM  | CHD-C1D-ND  | 3.75  | 128.45      | 124.42   |
| 2   | A     | 501 | HEM  | CHD-C1D-C2D | -3.72 | 119.16      | 125.03   |
| 2   | D     | 501 | HEM  | CMD-C2D-C1D | 3.66  | 130.75      | 125.03   |
| 2   | B     | 501 | HEM  | CHD-C1D-ND  | 3.62  | 128.31      | 124.42   |
| 2   | D     | 501 | HEM  | C3B-C4B-NB  | -3.56 | 106.91      | 109.47   |
| 2   | F     | 501 | HEM  | CAC-C3C-C2C | -3.54 | 116.93      | 128.43   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | E     | 501 | HEM  | CHD-C1D-ND  | 3.49  | 128.18      | 124.42   |
| 2   | D     | 501 | HEM  | CHD-C1D-C2D | -3.40 | 119.67      | 125.03   |
| 2   | B     | 501 | HEM  | CMD-C2D-C1D | 3.36  | 130.28      | 125.03   |
| 2   | D     | 501 | HEM  | CHD-C1D-ND  | 3.34  | 128.01      | 124.42   |
| 2   | D     | 501 | HEM  | CHA-C4D-C3D | -3.25 | 119.23      | 125.23   |
| 2   | E     | 501 | HEM  | CHD-C1D-C2D | -3.25 | 119.90      | 125.03   |
| 2   | D     | 501 | HEM  | CAD-C3D-C4D | 3.24  | 130.35      | 124.70   |
| 2   | C     | 501 | HEM  | CHD-C1D-C2D | -3.16 | 120.04      | 125.03   |
| 2   | E     | 501 | HEM  | C1B-NB-C4B  | 3.14  | 108.93      | 105.21   |
| 2   | B     | 501 | HEM  | CHA-C4D-ND  | 3.11  | 128.21      | 124.37   |
| 2   | C     | 501 | HEM  | CAD-C3D-C4D | 3.10  | 130.10      | 124.70   |
| 2   | A     | 501 | HEM  | C1B-NB-C4B  | 3.02  | 108.78      | 105.21   |
| 2   | F     | 501 | HEM  | CHA-C4D-ND  | 3.00  | 128.08      | 124.37   |
| 2   | B     | 501 | HEM  | C1B-NB-C4B  | 2.92  | 108.67      | 105.21   |
| 2   | B     | 501 | HEM  | CMB-C2B-C1B | 2.87  | 129.52      | 125.03   |
| 2   | B     | 501 | HEM  | CAD-C3D-C4D | 2.86  | 129.69      | 124.70   |
| 2   | B     | 501 | HEM  | CHA-C4D-C3D | -2.86 | 119.95      | 125.23   |
| 2   | B     | 501 | HEM  | CAB-C3B-C2B | -2.78 | 119.39      | 128.43   |
| 2   | C     | 501 | HEM  | C3B-C4B-NB  | -2.69 | 107.54      | 109.47   |
| 2   | A     | 501 | HEM  | O2A-CGA-CBA | 2.67  | 122.45      | 114.00   |
| 2   | D     | 501 | HEM  | C1A-CHA-C4D | -2.67 | 119.98      | 126.25   |
| 2   | B     | 501 | HEM  | C3B-C4B-NB  | -2.63 | 107.58      | 109.47   |
| 2   | A     | 501 | HEM  | C1A-CHA-C4D | -2.61 | 120.12      | 126.25   |
| 2   | D     | 501 | HEM  | CHB-C1B-C2B | -2.58 | 119.61      | 126.95   |
| 2   | F     | 501 | HEM  | C4B-C3B-C2B | -2.58 | 104.91      | 107.28   |
| 2   | B     | 501 | HEM  | CHB-C1B-NB  | 2.58  | 127.56      | 124.37   |
| 2   | D     | 501 | HEM  | CMB-C2B-C1B | 2.55  | 129.03      | 125.03   |
| 2   | D     | 501 | HEM  | O2D-CGD-O1D | -2.54 | 116.81      | 123.33   |
| 2   | C     | 501 | HEM  | CHA-C4D-ND  | 2.53  | 127.49      | 124.37   |
| 2   | F     | 501 | HEM  | CHD-C1D-C2D | -2.50 | 121.08      | 125.03   |
| 2   | D     | 501 | HEM  | CAB-C3B-C2B | -2.48 | 120.36      | 128.43   |
| 2   | C     | 501 | HEM  | CHB-C1B-NB  | 2.44  | 127.38      | 124.37   |
| 2   | E     | 501 | HEM  | CBD-CAD-C3D | -2.41 | 105.88      | 112.53   |
| 2   | B     | 501 | HEM  | O2A-CGA-CBA | 2.40  | 121.60      | 114.00   |
| 2   | E     | 501 | HEM  | C1A-CHA-C4D | -2.40 | 120.60      | 126.25   |
| 2   | D     | 501 | HEM  | CBD-CAD-C3D | -2.31 | 106.16      | 112.53   |
| 2   | B     | 501 | HEM  | O2D-CGD-CBD | 2.29  | 121.23      | 114.00   |
| 2   | D     | 501 | HEM  | CMB-C2B-C3B | -2.29 | 122.89      | 128.43   |
| 2   | D     | 501 | HEM  | CAD-C3D-C2D | -2.28 | 123.60      | 127.87   |
| 2   | C     | 501 | HEM  | CAD-C3D-C2D | -2.27 | 123.62      | 127.87   |
| 2   | B     | 501 | HEM  | O2D-CGD-O1D | -2.25 | 117.53      | 123.33   |
| 2   | C     | 501 | HEM  | C1A-CHA-C4D | -2.25 | 120.96      | 126.25   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2   | F     | 501 | HEM  | O2A-CGA-O1A | -2.24 | 117.58      | 123.33   |
| 2   | D     | 501 | HEM  | CHD-C4C-NC  | 2.23  | 126.88      | 124.45   |
| 2   | E     | 501 | HEM  | CHA-C4D-ND  | 2.22  | 127.12      | 124.37   |
| 2   | A     | 501 | HEM  | CAB-C3B-C2B | 2.21  | 135.63      | 128.43   |
| 2   | B     | 501 | HEM  | CAB-C3B-C4B | 2.21  | 134.16      | 124.39   |
| 2   | B     | 501 | HEM  | CHD-C1D-C2D | -2.21 | 121.55      | 125.03   |
| 2   | A     | 501 | HEM  | C4B-C3B-C2B | -2.20 | 105.26      | 107.28   |
| 2   | A     | 501 | HEM  | CBD-CAD-C3D | -2.20 | 106.46      | 112.53   |
| 2   | F     | 501 | HEM  | CHC-C4B-C3B | -2.18 | 120.71      | 125.07   |
| 2   | E     | 501 | HEM  | O2A-CGA-O1A | -2.18 | 117.72      | 123.33   |
| 2   | B     | 501 | HEM  | CHD-C4C-NC  | 2.17  | 126.82      | 124.45   |
| 2   | B     | 501 | HEM  | C1A-CHA-C4D | -2.17 | 121.15      | 126.25   |
| 2   | D     | 501 | HEM  | C3B-C2B-C1B | 2.14  | 108.02      | 106.41   |
| 2   | A     | 501 | HEM  | O2A-CGA-O1A | -2.12 | 117.87      | 123.33   |
| 2   | F     | 501 | HEM  | C1A-CHA-C4D | -2.11 | 121.29      | 126.25   |
| 2   | A     | 501 | HEM  | CHA-C1A-NA  | 2.10  | 127.68      | 123.86   |
| 2   | A     | 501 | HEM  | CAD-C3D-C4D | 2.10  | 128.35      | 124.70   |
| 2   | D     | 501 | HEM  | CAB-C3B-C4B | 2.10  | 133.66      | 124.39   |
| 2   | B     | 501 | HEM  | CMB-C2B-C3B | -2.08 | 123.39      | 128.43   |
| 2   | E     | 501 | HEM  | C1D-C2D-C3D | -2.08 | 104.80      | 106.98   |
| 2   | C     | 501 | HEM  | CHD-C4C-NC  | 2.07  | 126.71      | 124.45   |
| 2   | D     | 501 | HEM  | C2D-C1D-ND  | 2.07  | 112.30      | 109.90   |
| 2   | A     | 501 | HEM  | CHC-C4B-C3B | -2.07 | 120.94      | 125.07   |
| 2   | A     | 501 | HEM  | C4C-CHD-C1D | -2.05 | 121.66      | 126.02   |
| 2   | E     | 501 | HEM  | CHA-C1A-NA  | 2.04  | 127.56      | 123.86   |
| 2   | B     | 501 | HEM  | C4C-CHD-C1D | -2.03 | 121.71      | 126.02   |
| 2   | F     | 501 | HEM  | CHD-C4C-C3C | 2.02  | 128.62      | 125.21   |
| 2   | A     | 501 | HEM  | CHA-C4D-ND  | 2.02  | 126.86      | 124.37   |
| 2   | C     | 501 | HEM  | C4C-CHD-C1D | -2.01 | 121.75      | 126.02   |
| 2   | D     | 501 | HEM  | C1C-CHC-C4B | -2.00 | 121.77      | 126.02   |

There are no chirality outliers.

All (24) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | D     | 502 | 4OA  | C21-C20-C22-C23 |
| 3   | F     | 502 | 4OA  | C17-C20-C22-C23 |
| 3   | B     | 502 | 4OA  | C17-C20-C22-C23 |
| 3   | F     | 502 | 4OA  | C13-C17-C20-C22 |
| 3   | E     | 502 | 4OA  | C17-C20-C22-C23 |
| 2   | B     | 501 | HEM  | C4B-C3B-CAB-CBB |
| 2   | D     | 501 | HEM  | C4B-C3B-CAB-CBB |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 2   | F     | 501 | HEM  | C4C-C3C-CAC-CBC |
| 3   | F     | 502 | 4OA  | C16-C17-C20-C22 |
| 3   | F     | 502 | 4OA  | C13-C17-C20-C21 |
| 3   | F     | 502 | 4OA  | C21-C20-C22-C23 |
| 3   | E     | 502 | 4OA  | C21-C20-C22-C23 |
| 3   | C     | 502 | 4OA  | C22-C23-C24-O4  |
| 3   | B     | 502 | 4OA  | C22-C23-C24-O4A |
| 3   | C     | 502 | 4OA  | C17-C20-C22-C23 |
| 3   | B     | 502 | 4OA  | C22-C23-C24-O4  |
| 3   | E     | 502 | 4OA  | C22-C23-C24-O4A |
| 3   | A     | 502 | 4OA  | C22-C23-C24-O4  |
| 3   | C     | 502 | 4OA  | C22-C23-C24-O4A |
| 3   | F     | 502 | 4OA  | C22-C23-C24-O4  |
| 3   | A     | 502 | 4OA  | C22-C23-C24-O4A |
| 3   | F     | 502 | 4OA  | C22-C23-C24-O4A |
| 3   | E     | 502 | 4OA  | C22-C23-C24-O4  |
| 3   | A     | 502 | 4OA  | C17-C20-C22-C23 |

There are no ring outliers.

22 monomers are involved in 45 short contacts:

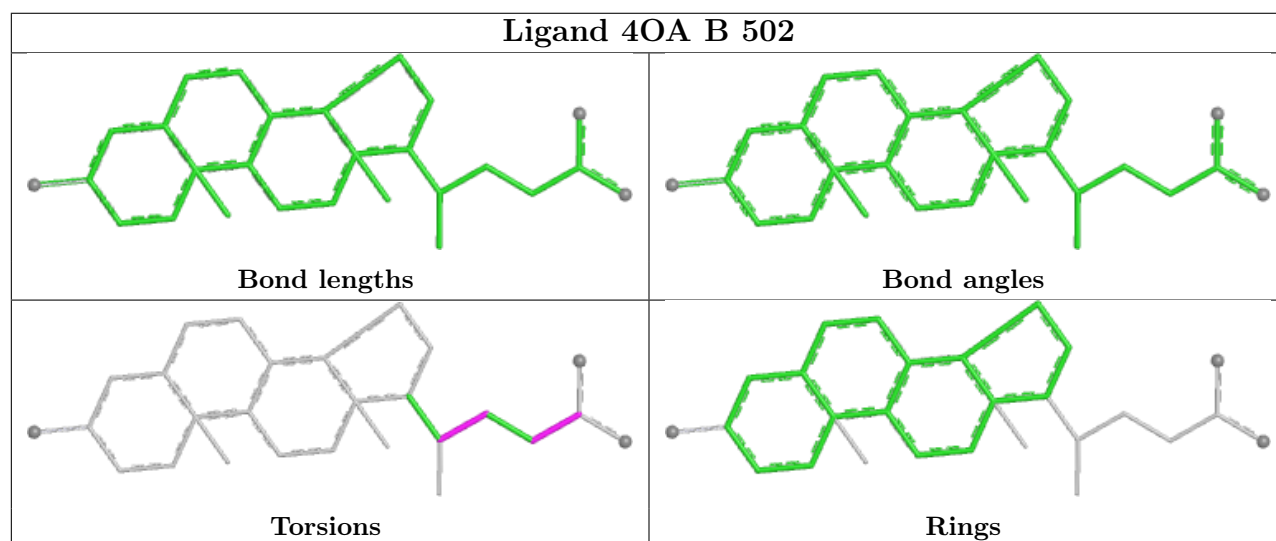
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | B     | 502 | 4OA  | 1       | 0            |
| 4   | B     | 506 | FMT  | 1       | 0            |
| 2   | F     | 501 | HEM  | 3       | 0            |
| 4   | E     | 512 | FMT  | 1       | 0            |
| 2   | A     | 501 | HEM  | 3       | 0            |
| 4   | A     | 505 | FMT  | 2       | 0            |
| 4   | C     | 510 | FMT  | 1       | 0            |
| 4   | B     | 513 | FMT  | 5       | 0            |
| 4   | B     | 514 | FMT  | 1       | 0            |
| 4   | B     | 511 | FMT  | 1       | 0            |
| 3   | E     | 502 | 4OA  | 3       | 0            |
| 3   | F     | 502 | 4OA  | 1       | 0            |
| 4   | D     | 505 | FMT  | 2       | 0            |
| 2   | B     | 501 | HEM  | 4       | 0            |
| 4   | D     | 514 | FMT  | 3       | 0            |
| 2   | E     | 501 | HEM  | 5       | 0            |
| 3   | C     | 502 | 4OA  | 1       | 0            |
| 3   | A     | 502 | 4OA  | 2       | 0            |
| 2   | C     | 501 | HEM  | 3       | 0            |
| 4   | B     | 517 | FMT  | 1       | 0            |

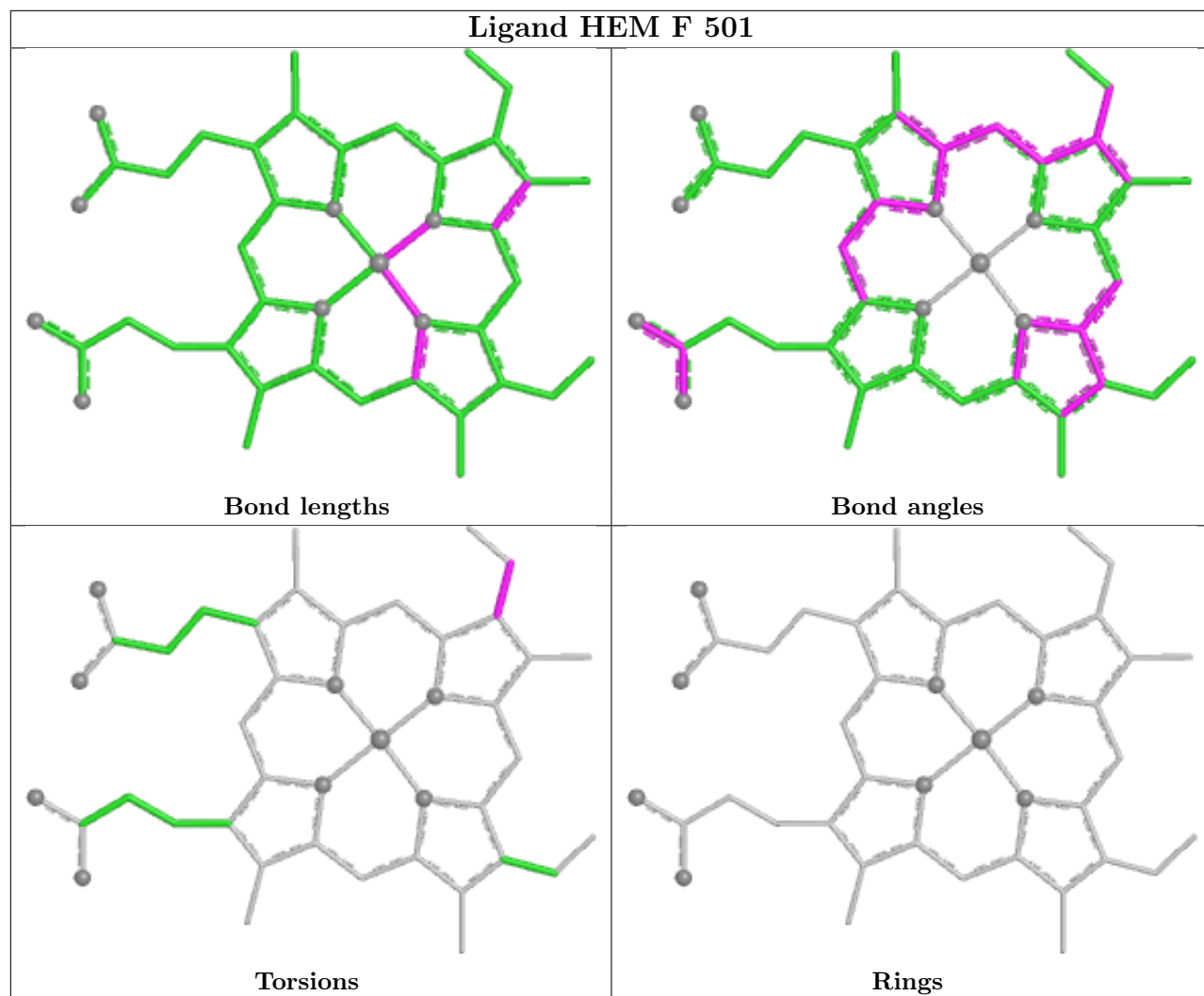
*Continued on next page...*

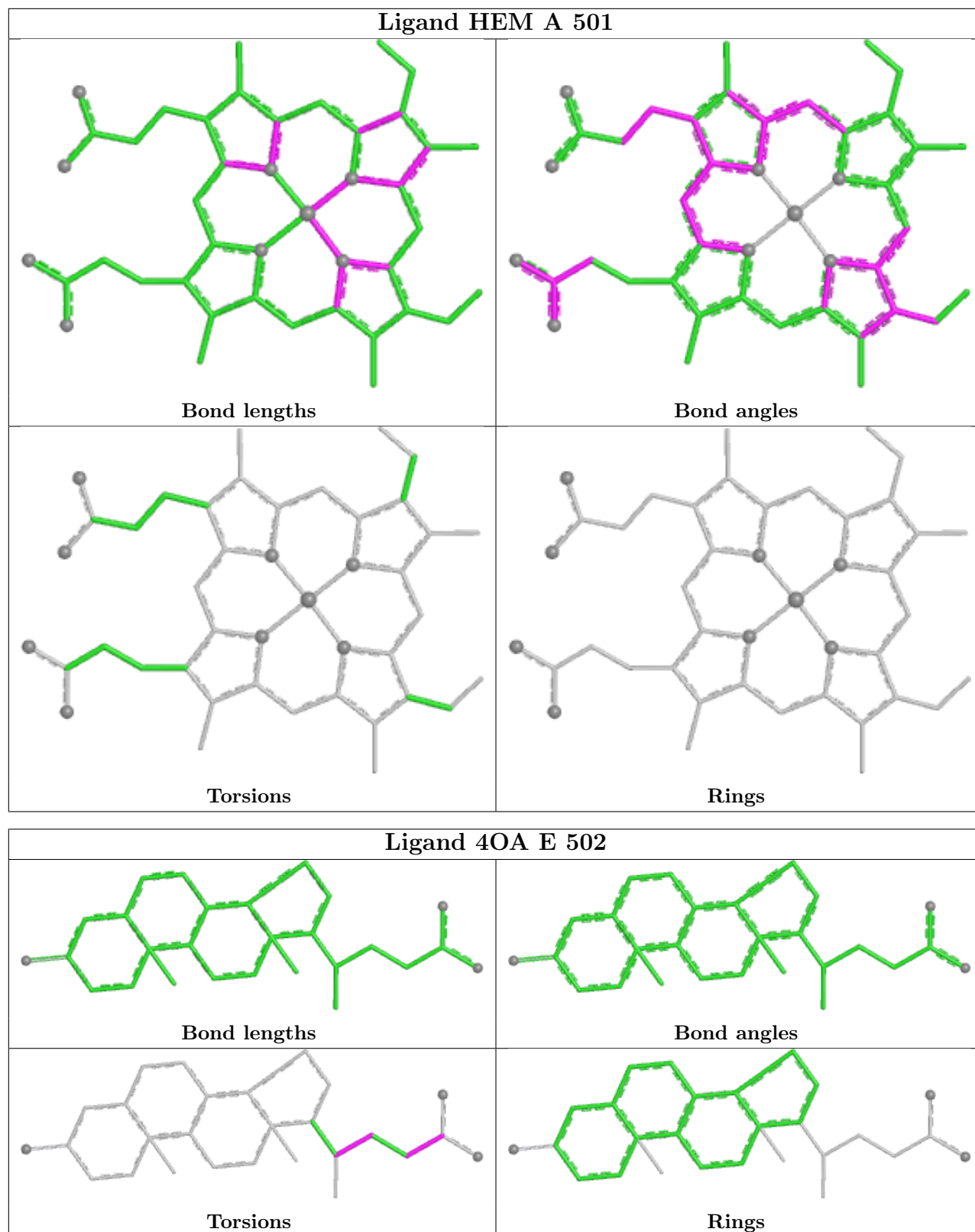
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | C     | 520 | FMT  | 1       | 0            |
| 2   | D     | 501 | HEM  | 4       | 0            |

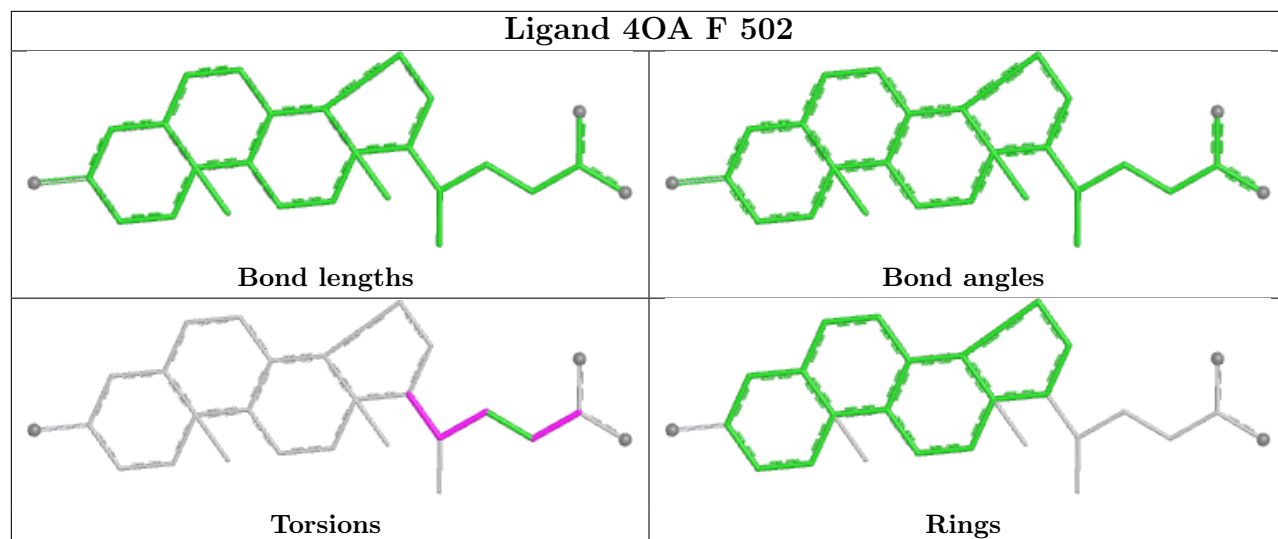
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



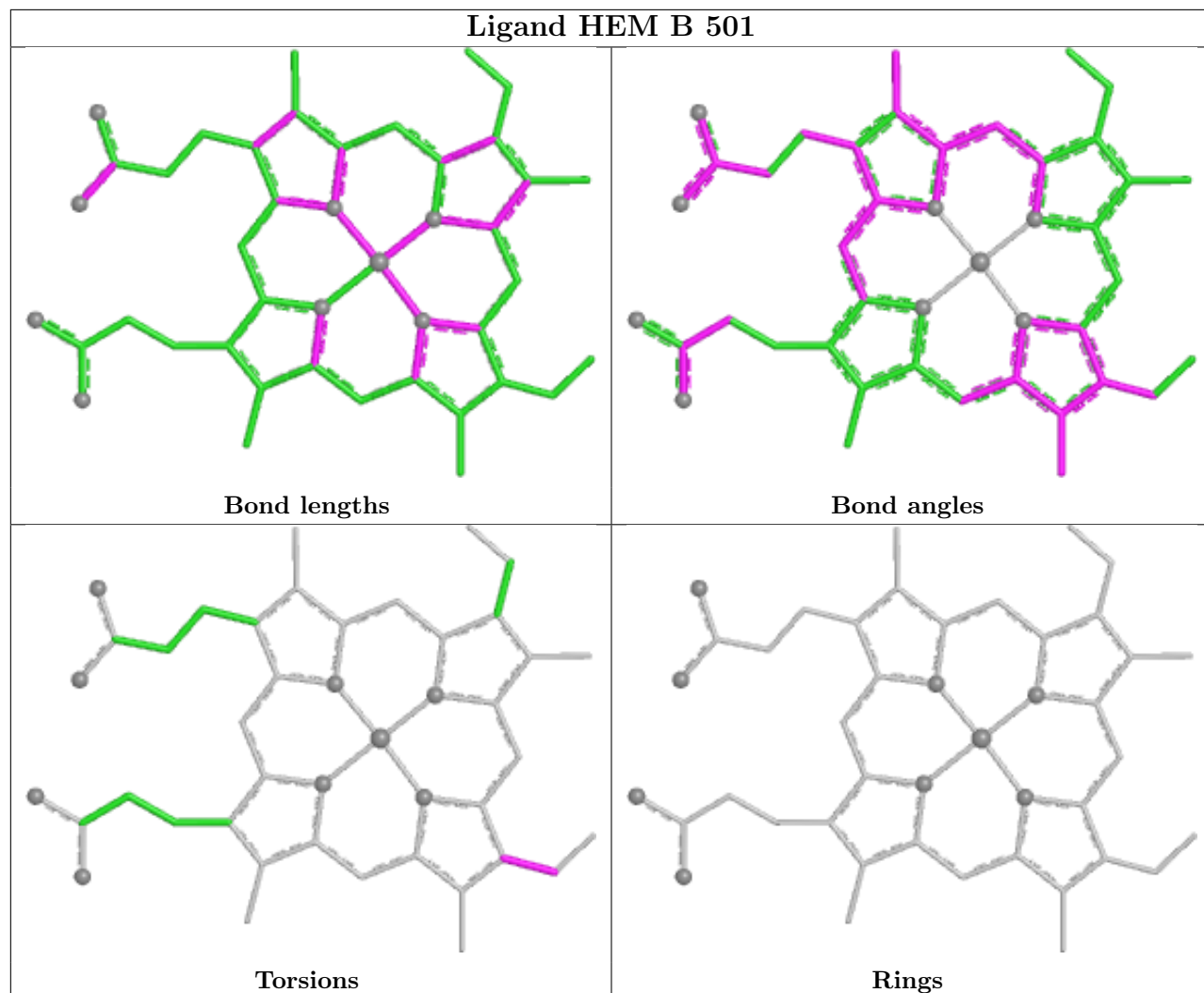




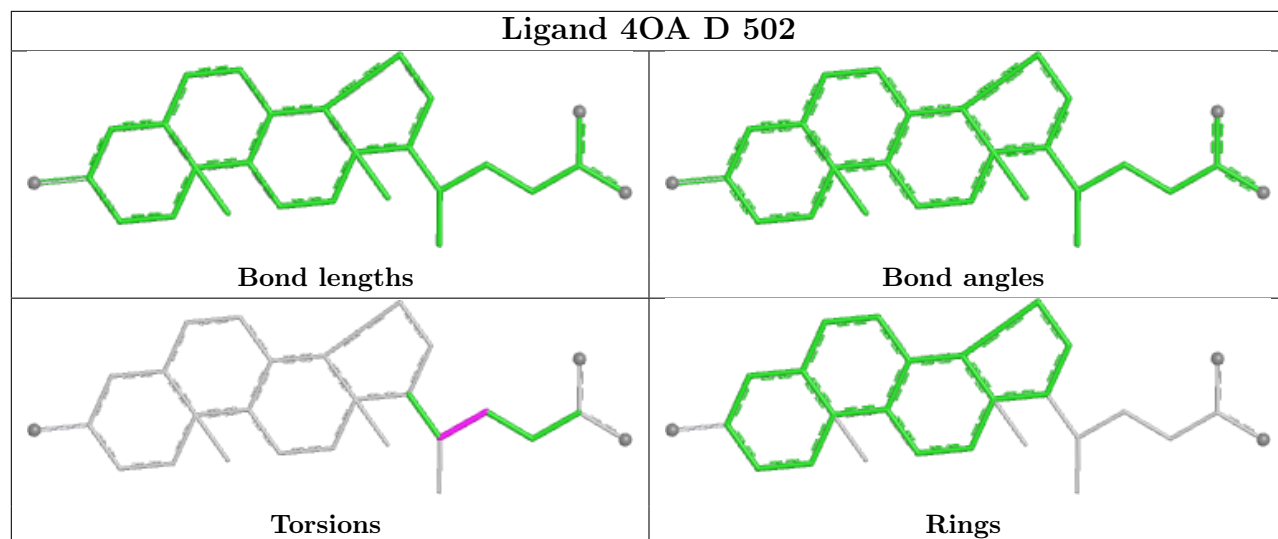
## Ligand 4OA F 502



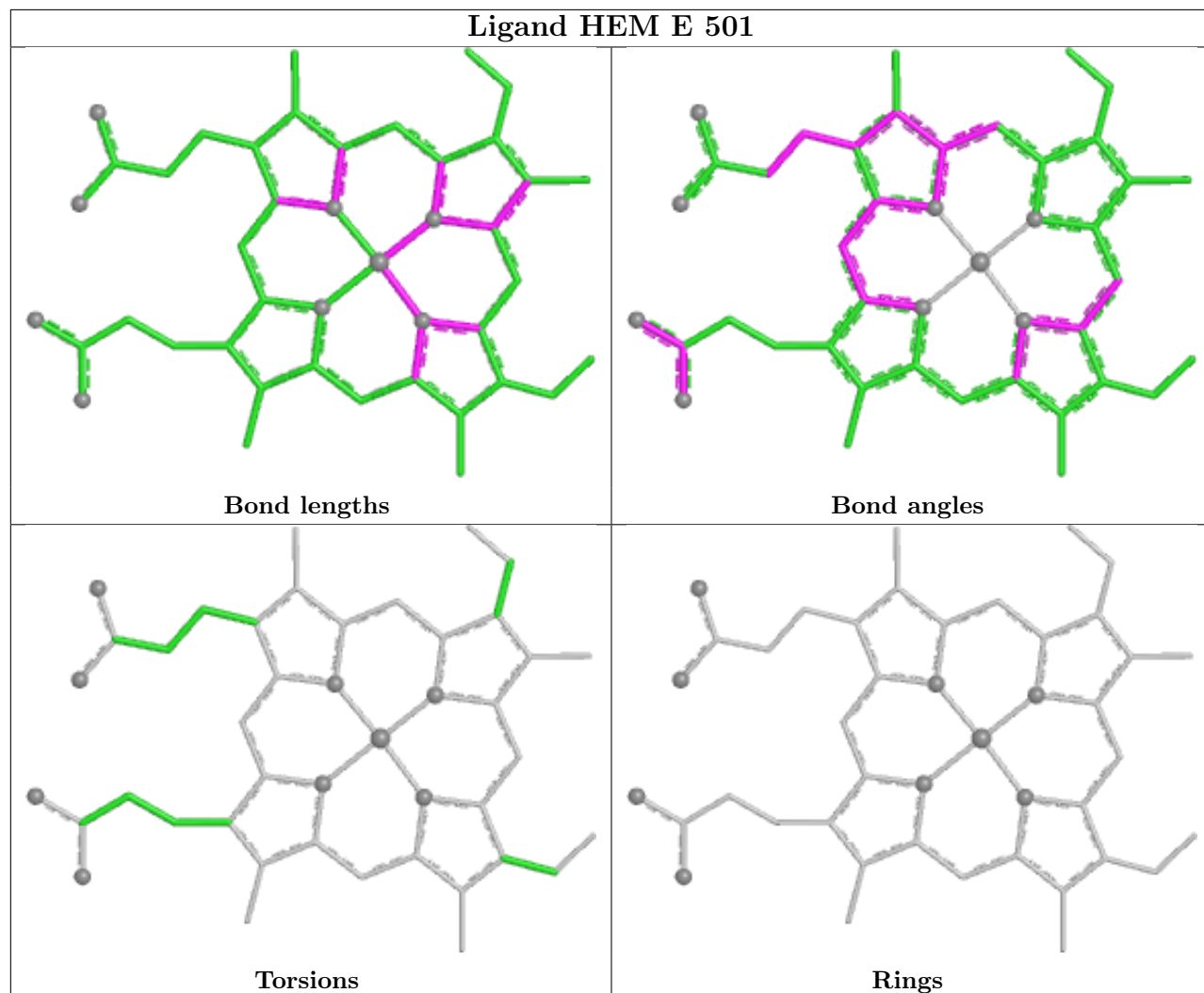
## Ligand HEM B 501



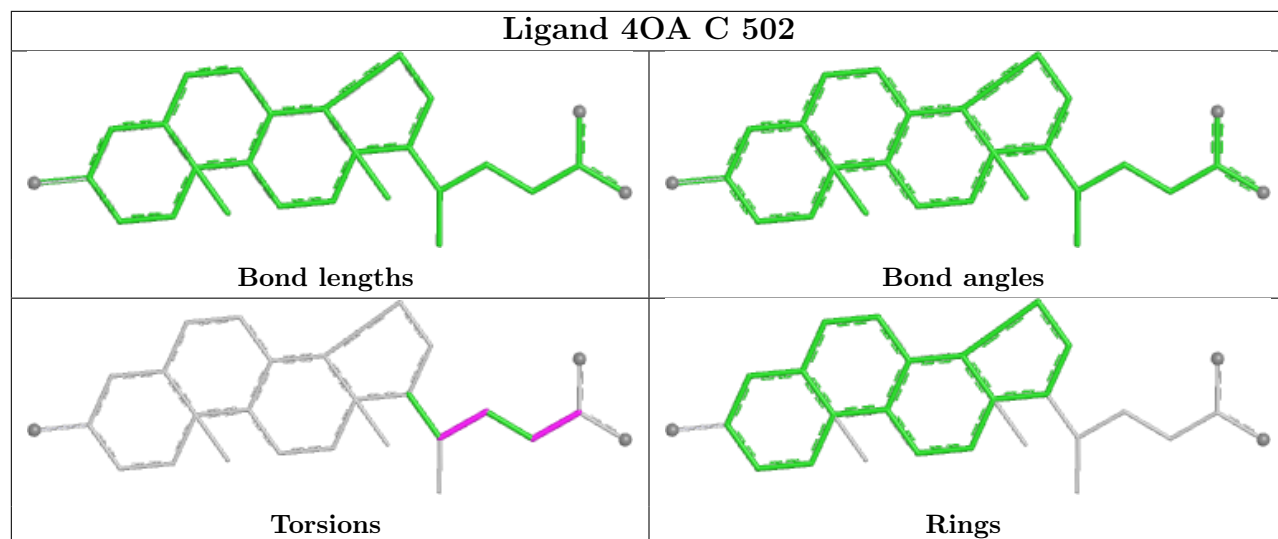
## Ligand 4OA D 502



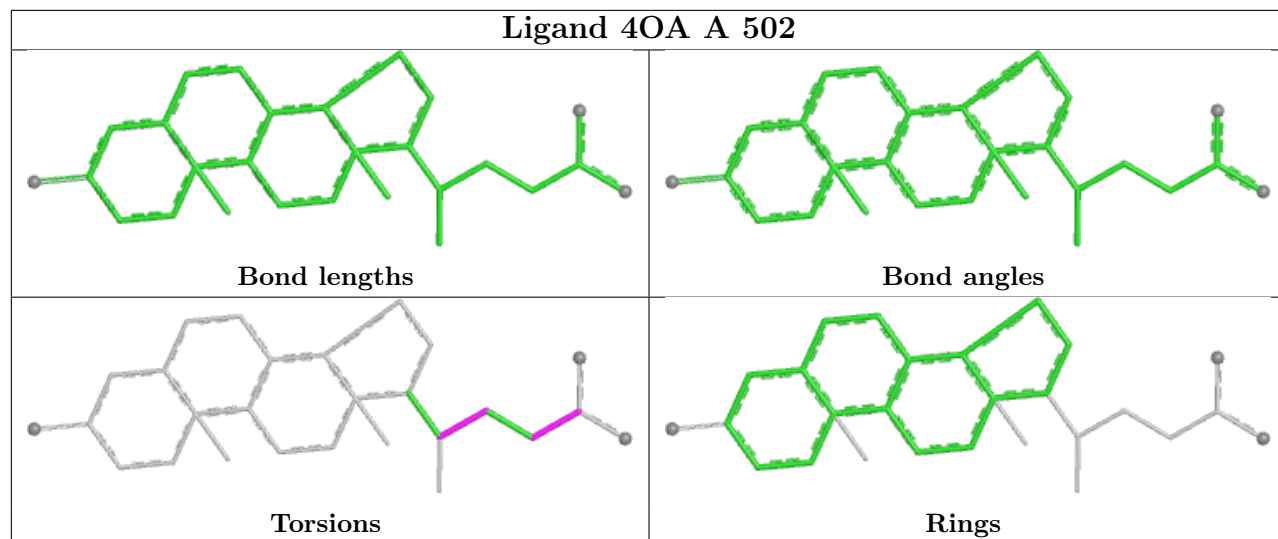
## Ligand HEM E 501

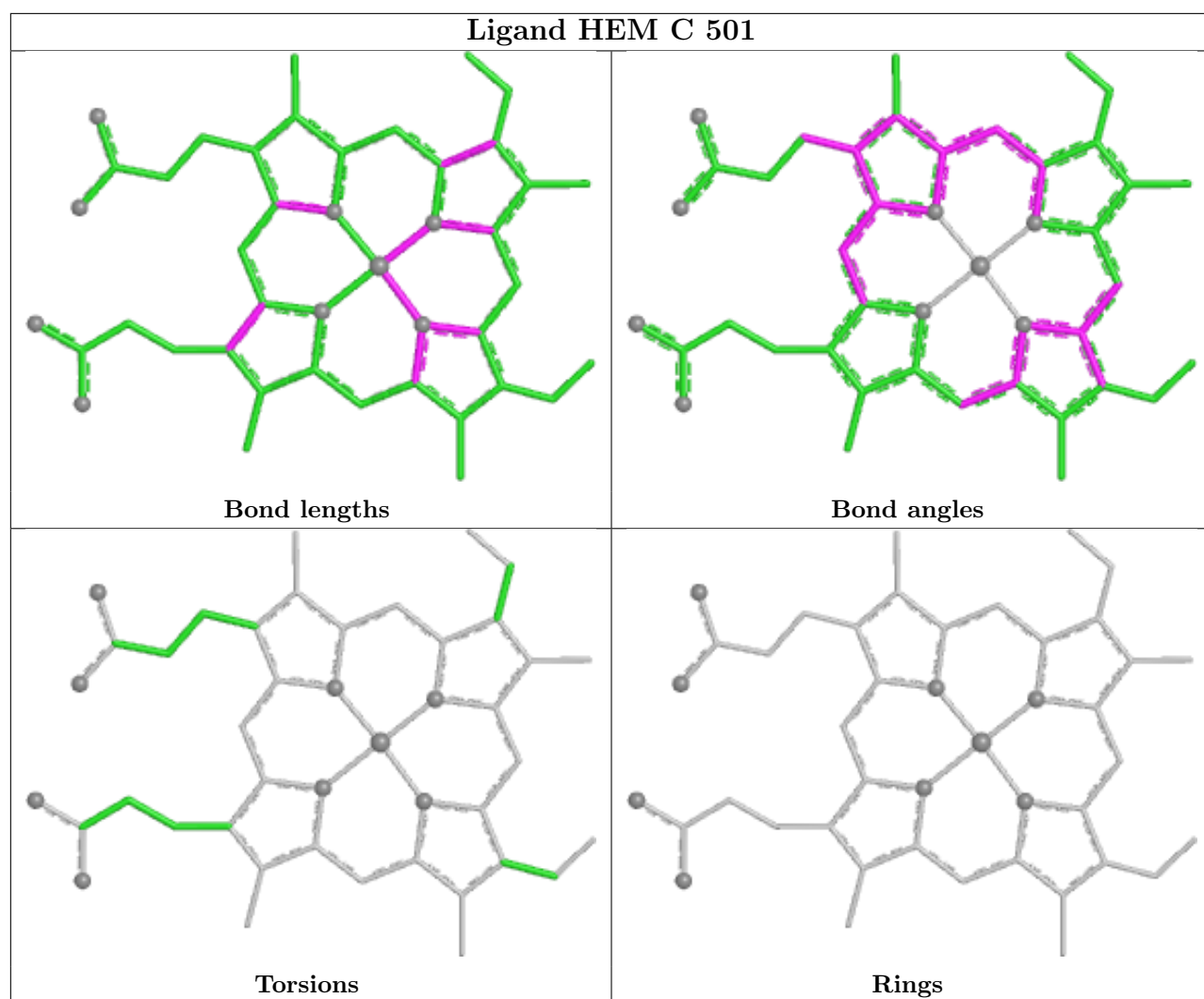


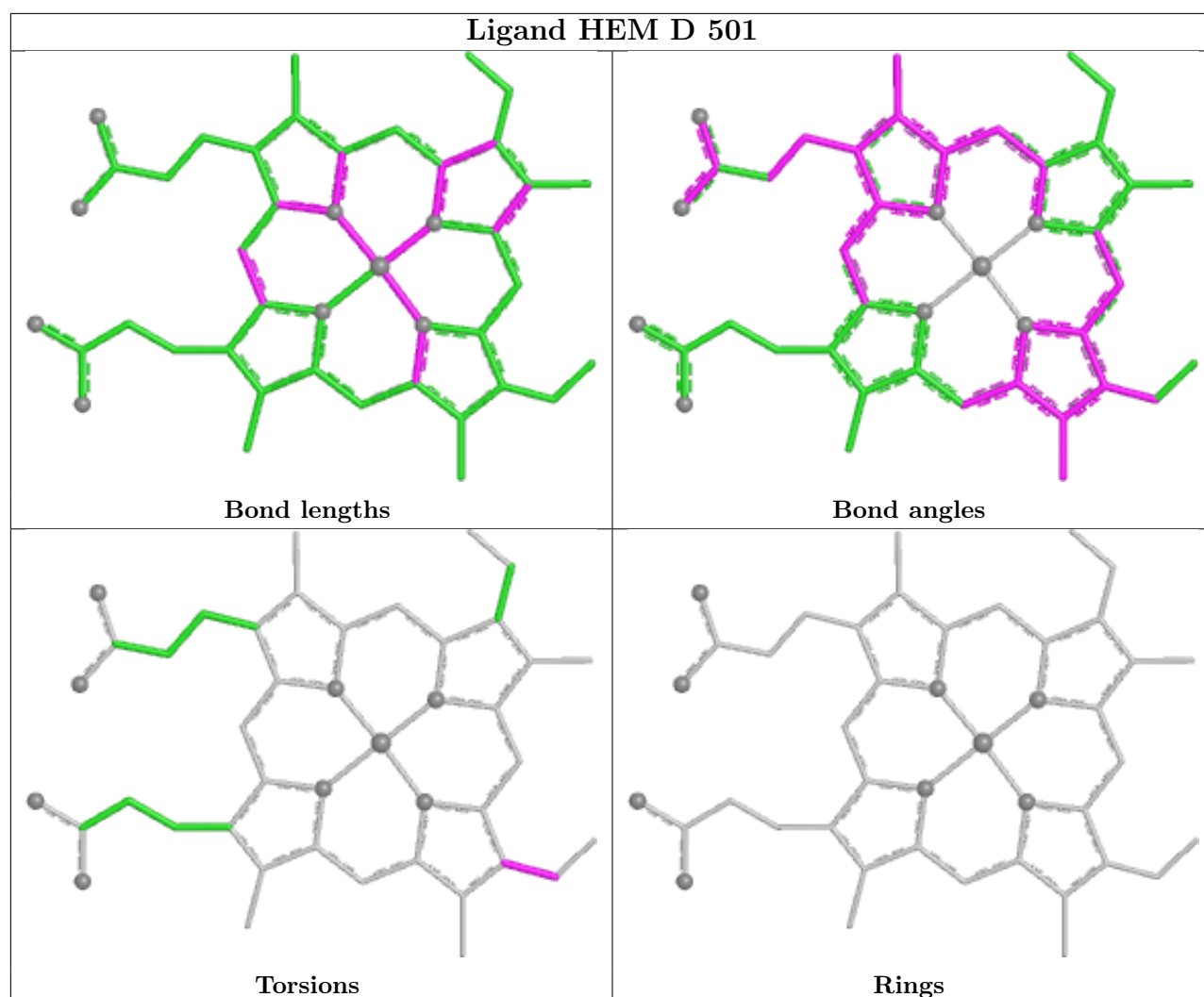
## Ligand 4OA C 502



## Ligand 4OA A 502







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |       | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-------|-----------------------|---------|
| 1   | A     | 396/398 (99%)   | -0.16  | 4 (1%)    | 79 80 | 27, 47, 74, 99        | 8 (2%)  |
| 1   | B     | 396/398 (99%)   | -0.16  | 8 (2%)    | 65 66 | 24, 47, 75, 131       | 4 (1%)  |
| 1   | C     | 398/398 (100%)  | -0.25  | 7 (1%)    | 67 69 | 17, 43, 63, 102       | 9 (2%)  |
| 1   | D     | 397/398 (99%)   | -0.01  | 8 (2%)    | 65 66 | 28, 54, 78, 117       | 5 (1%)  |
| 1   | E     | 394/398 (98%)   | 0.28   | 11 (2%)   | 55 57 | 37, 62, 92, 125       | 1 (0%)  |
| 1   | F     | 396/398 (99%)   | 0.32   | 16 (4%)   | 42 44 | 31, 63, 105, 116      | 1 (0%)  |
| All | All   | 2377/2388 (99%) | 0.00   | 54 (2%)   | 61 63 | 17, 53, 90, 131       | 28 (1%) |

All (54) RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | C     | 11     | ALA  | 7.0  |
| 1   | F     | 51     | THR  | 5.2  |
| 1   | E     | 108    | VAL  | 4.7  |
| 1   | F     | 52     | ALA  | 4.5  |
| 1   | E     | 43     | VAL  | 4.1  |
| 1   | E     | 228    | HIS  | 3.8  |
| 1   | F     | 331    | PHE  | 3.7  |
| 1   | C     | 10     | PRO  | 3.7  |
| 1   | D     | 228    | HIS  | 3.7  |
| 1   | B     | 215    | LEU  | 3.5  |
| 1   | E     | 210    | ALA  | 3.5  |
| 1   | B     | 214    | ASP  | 3.3  |
| 1   | C     | 343[A] | ARG  | 3.2  |
| 1   | A     | 168    | ARG  | 3.0  |
| 1   | F     | 106[A] | ARG  | 3.0  |
| 1   | D     | 116    | ARG  | 3.0  |
| 1   | B     | 13     | ALA  | 2.9  |
| 1   | C     | 344    | ASN  | 2.8  |
| 1   | E     | 160    | LEU  | 2.7  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | B     | 210    | ALA  | 2.7  |
| 1   | D     | 265[A] | LYS  | 2.6  |
| 1   | F     | 383    | ALA  | 2.6  |
| 1   | D     | 11     | ALA  | 2.6  |
| 1   | D     | 115[A] | ARG  | 2.6  |
| 1   | E     | 184    | LEU  | 2.5  |
| 1   | B     | 228    | HIS  | 2.5  |
| 1   | A     | 105    | ARG  | 2.5  |
| 1   | D     | 42     | ARG  | 2.4  |
| 1   | E     | 227    | ASP  | 2.4  |
| 1   | C     | 196    | PHE  | 2.4  |
| 1   | B     | 212    | THR  | 2.4  |
| 1   | F     | 184    | LEU  | 2.4  |
| 1   | F     | 187    | ALA  | 2.3  |
| 1   | A     | 108    | VAL  | 2.3  |
| 1   | E     | 68     | SER  | 2.3  |
| 1   | F     | 136    | VAL  | 2.3  |
| 1   | E     | 105    | ARG  | 2.2  |
| 1   | E     | 162    | GLY  | 2.2  |
| 1   | F     | 182    | THR  | 2.2  |
| 1   | F     | 151    | PRO  | 2.2  |
| 1   | E     | 211    | PRO  | 2.2  |
| 1   | F     | 188    | GLU  | 2.2  |
| 1   | F     | 261    | LEU  | 2.2  |
| 1   | F     | 386    | VAL  | 2.2  |
| 1   | B     | 398    | ARG  | 2.1  |
| 1   | F     | 216    | LEU  | 2.1  |
| 1   | C     | 335    | ASP  | 2.1  |
| 1   | A     | 228    | HIS  | 2.1  |
| 1   | C     | 115[A] | ARG  | 2.1  |
| 1   | F     | 404    | ILE  | 2.1  |
| 1   | D     | 196    | PHE  | 2.0  |
| 1   | B     | 105    | ARG  | 2.0  |
| 1   | D     | 105    | ARG  | 2.0  |
| 1   | F     | 183    | ARG  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | FMT  | A     | 511 | 3/3   | 0.61 | 0.15 | 83,83,83,89                | 0     |
| 4   | FMT  | F     | 510 | 3/3   | 0.65 | 0.12 | 88,88,91,97                | 0     |
| 4   | FMT  | E     | 510 | 3/3   | 0.66 | 0.14 | 86,86,95,95                | 0     |
| 4   | FMT  | F     | 512 | 3/3   | 0.67 | 0.22 | 74,74,88,91                | 0     |
| 4   | FMT  | C     | 511 | 3/3   | 0.68 | 0.13 | 77,77,81,85                | 0     |
| 4   | FMT  | A     | 510 | 3/3   | 0.68 | 0.15 | 85,85,91,94                | 0     |
| 4   | FMT  | C     | 514 | 3/3   | 0.69 | 0.12 | 84,84,86,88                | 0     |
| 4   | FMT  | C     | 523 | 3/3   | 0.71 | 0.14 | 89,89,90,93                | 0     |
| 4   | FMT  | A     | 504 | 3/3   | 0.71 | 0.12 | 81,81,83,84                | 0     |
| 4   | FMT  | A     | 519 | 3/3   | 0.72 | 0.17 | 78,78,86,87                | 0     |
| 4   | FMT  | F     | 513 | 3/3   | 0.72 | 0.36 | 96,96,96,102               | 0     |
| 4   | FMT  | F     | 511 | 3/3   | 0.73 | 0.21 | 72,72,78,86                | 0     |
| 4   | FMT  | B     | 504 | 3/3   | 0.74 | 0.15 | 89,89,91,92                | 0     |
| 4   | FMT  | D     | 505 | 3/3   | 0.75 | 0.24 | 73,73,84,86                | 0     |
| 4   | FMT  | C     | 526 | 3/3   | 0.75 | 0.15 | 76,76,82,83                | 0     |
| 4   | FMT  | E     | 509 | 3/3   | 0.77 | 0.18 | 80,80,84,90                | 0     |
| 4   | FMT  | C     | 525 | 3/3   | 0.79 | 0.21 | 67,67,71,74                | 0     |
| 4   | FMT  | B     | 515 | 3/3   | 0.80 | 0.14 | 65,65,76,77                | 0     |
| 4   | FMT  | C     | 519 | 3/3   | 0.80 | 0.19 | 91,91,96,99                | 0     |
| 4   | FMT  | D     | 513 | 3/3   | 0.80 | 0.15 | 46,46,46,47                | 3     |
| 4   | FMT  | F     | 508 | 3/3   | 0.81 | 0.14 | 67,67,76,81                | 0     |
| 4   | FMT  | D     | 512 | 3/3   | 0.81 | 0.27 | 56,56,63,72                | 0     |
| 4   | FMT  | A     | 512 | 3/3   | 0.81 | 0.22 | 62,62,78,82                | 0     |
| 4   | FMT  | B     | 522 | 3/3   | 0.81 | 0.21 | 74,74,76,90                | 0     |
| 4   | FMT  | A     | 518 | 3/3   | 0.81 | 0.20 | 54,54,70,73                | 0     |
| 4   | FMT  | B     | 519 | 3/3   | 0.83 | 0.17 | 79,79,83,84                | 0     |
| 4   | FMT  | A     | 515 | 3/3   | 0.83 | 0.14 | 48,48,56,56                | 0     |
| 4   | FMT  | C     | 524 | 3/3   | 0.83 | 0.22 | 48,48,54,57                | 3     |
| 4   | FMT  | D     | 509 | 3/3   | 0.83 | 0.17 | 78,78,82,84                | 0     |
| 4   | FMT  | F     | 503 | 3/3   | 0.83 | 0.23 | 80,80,83,90                | 0     |
| 4   | FMT  | B     | 506 | 3/3   | 0.84 | 0.20 | 59,59,67,73                | 0     |
| 4   | FMT  | B     | 510 | 3/3   | 0.84 | 0.18 | 81,81,86,86                | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | FMT  | A     | 514 | 3/3   | 0.84 | 0.13 | 71,71,74,83                 | 0     |
| 4   | FMT  | B     | 524 | 3/3   | 0.85 | 0.17 | 88,88,88,89                 | 0     |
| 4   | FMT  | B     | 514 | 3/3   | 0.85 | 0.18 | 47,47,50,55                 | 0     |
| 4   | FMT  | E     | 506 | 3/3   | 0.86 | 0.28 | 64,64,66,79                 | 0     |
| 4   | FMT  | B     | 518 | 3/3   | 0.86 | 0.15 | 58,58,70,79                 | 0     |
| 4   | FMT  | C     | 516 | 3/3   | 0.86 | 0.17 | 64,64,75,77                 | 0     |
| 4   | FMT  | B     | 503 | 3/3   | 0.86 | 0.20 | 69,69,80,89                 | 0     |
| 4   | FMT  | C     | 522 | 3/3   | 0.86 | 0.14 | 80,80,84,87                 | 0     |
| 4   | FMT  | C     | 510 | 3/3   | 0.86 | 0.14 | 69,69,73,76                 | 0     |
| 4   | FMT  | B     | 521 | 3/3   | 0.86 | 0.16 | 66,66,70,75                 | 0     |
| 4   | FMT  | D     | 515 | 3/3   | 0.86 | 0.13 | 71,71,79,85                 | 0     |
| 4   | FMT  | E     | 503 | 3/3   | 0.86 | 0.17 | 66,66,72,76                 | 0     |
| 4   | FMT  | D     | 504 | 3/3   | 0.87 | 0.11 | 73,73,79,80                 | 0     |
| 4   | FMT  | A     | 503 | 3/3   | 0.87 | 0.20 | 69,69,75,76                 | 0     |
| 4   | FMT  | E     | 505 | 3/3   | 0.87 | 0.25 | 60,60,60,79                 | 0     |
| 4   | FMT  | C     | 506 | 3/3   | 0.87 | 0.19 | 60,60,76,81                 | 0     |
| 4   | FMT  | A     | 523 | 3/3   | 0.87 | 0.24 | 66,66,80,86                 | 0     |
| 4   | FMT  | A     | 507 | 3/3   | 0.87 | 0.17 | 73,73,73,75                 | 0     |
| 4   | FMT  | C     | 513 | 3/3   | 0.88 | 0.21 | 59,59,70,80                 | 0     |
| 4   | FMT  | F     | 505 | 3/3   | 0.88 | 0.23 | 64,64,69,81                 | 0     |
| 4   | FMT  | C     | 509 | 3/3   | 0.88 | 0.14 | 65,65,72,78                 | 0     |
| 4   | FMT  | F     | 509 | 3/3   | 0.88 | 0.12 | 54,54,58,60                 | 0     |
| 4   | FMT  | E     | 508 | 3/3   | 0.88 | 0.15 | 73,73,80,81                 | 0     |
| 4   | FMT  | B     | 507 | 3/3   | 0.88 | 0.15 | 65,65,70,72                 | 0     |
| 4   | FMT  | A     | 516 | 3/3   | 0.88 | 0.19 | 69,69,79,83                 | 0     |
| 4   | FMT  | E     | 511 | 3/3   | 0.88 | 0.23 | 59,59,60,69                 | 0     |
| 4   | FMT  | D     | 507 | 3/3   | 0.89 | 0.15 | 56,56,63,65                 | 0     |
| 4   | FMT  | F     | 506 | 3/3   | 0.89 | 0.11 | 58,58,61,65                 | 0     |
| 4   | FMT  | D     | 508 | 3/3   | 0.89 | 0.16 | 57,57,62,70                 | 0     |
| 4   | FMT  | B     | 505 | 3/3   | 0.89 | 0.14 | 61,61,80,82                 | 0     |
| 4   | FMT  | A     | 508 | 3/3   | 0.89 | 0.19 | 61,61,70,75                 | 0     |
| 4   | FMT  | C     | 520 | 3/3   | 0.89 | 0.18 | 70,70,76,77                 | 0     |
| 4   | FMT  | B     | 520 | 3/3   | 0.89 | 0.15 | 57,57,70,75                 | 0     |
| 4   | FMT  | A     | 505 | 3/3   | 0.89 | 0.14 | 52,52,61,62                 | 0     |
| 4   | FMT  | C     | 508 | 3/3   | 0.90 | 0.17 | 62,62,67,70                 | 0     |
| 4   | FMT  | A     | 513 | 3/3   | 0.90 | 0.19 | 61,61,64,77                 | 0     |
| 4   | FMT  | B     | 511 | 3/3   | 0.90 | 0.28 | 71,71,72,82                 | 0     |
| 4   | FMT  | B     | 513 | 3/3   | 0.90 | 0.14 | 30,30,34,48                 | 0     |
| 4   | FMT  | C     | 512 | 3/3   | 0.90 | 0.17 | 51,51,53,53                 | 0     |
| 4   | FMT  | C     | 503 | 3/3   | 0.90 | 0.16 | 64,64,65,76                 | 0     |
| 4   | FMT  | B     | 508 | 3/3   | 0.90 | 0.12 | 52,52,59,67                 | 0     |
| 4   | FMT  | C     | 515 | 3/3   | 0.90 | 0.15 | 56,56,68,68                 | 0     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4   | FMT  | D     | 514 | 3/3   | 0.91 | 0.21 | 45,45,49,57                 | 0     |
| 4   | FMT  | B     | 509 | 3/3   | 0.91 | 0.12 | 66,66,70,71                 | 0     |
| 4   | FMT  | A     | 509 | 3/3   | 0.91 | 0.11 | 71,71,77,79                 | 0     |
| 4   | FMT  | A     | 506 | 3/3   | 0.91 | 0.14 | 59,59,61,63                 | 0     |
| 4   | FMT  | B     | 523 | 3/3   | 0.91 | 0.17 | 57,57,71,73                 | 0     |
| 4   | FMT  | A     | 517 | 3/3   | 0.91 | 0.20 | 32,32,38,47                 | 3     |
| 4   | FMT  | B     | 512 | 3/3   | 0.92 | 0.17 | 59,59,63,77                 | 0     |
| 4   | FMT  | C     | 507 | 3/3   | 0.92 | 0.15 | 56,56,56,60                 | 0     |
| 4   | FMT  | D     | 503 | 3/3   | 0.92 | 0.20 | 50,50,50,63                 | 0     |
| 4   | FMT  | E     | 504 | 3/3   | 0.92 | 0.20 | 48,48,50,66                 | 0     |
| 4   | FMT  | E     | 512 | 3/3   | 0.92 | 0.17 | 84,84,91,95                 | 0     |
| 4   | FMT  | A     | 524 | 3/3   | 0.92 | 0.25 | 61,61,67,80                 | 0     |
| 4   | FMT  | A     | 520 | 3/3   | 0.92 | 0.19 | 60,60,62,67                 | 0     |
| 5   | NA   | E     | 513 | 1/1   | 0.92 | 0.14 | 61,61,61,61                 | 0     |
| 4   | FMT  | C     | 504 | 3/3   | 0.93 | 0.11 | 59,59,61,64                 | 0     |
| 4   | FMT  | A     | 521 | 3/3   | 0.93 | 0.24 | 71,71,72,75                 | 0     |
| 4   | FMT  | C     | 518 | 3/3   | 0.93 | 0.20 | 65,65,71,74                 | 0     |
| 4   | FMT  | E     | 507 | 3/3   | 0.94 | 0.11 | 69,69,71,72                 | 0     |
| 4   | FMT  | D     | 506 | 3/3   | 0.94 | 0.15 | 63,63,66,72                 | 0     |
| 3   | 4OA  | A     | 502 | 27/27 | 0.94 | 0.10 | 35,38,54,59                 | 0     |
| 4   | FMT  | C     | 505 | 3/3   | 0.94 | 0.15 | 58,58,61,64                 | 0     |
| 4   | FMT  | F     | 507 | 3/3   | 0.94 | 0.14 | 67,67,73,81                 | 0     |
| 4   | FMT  | B     | 516 | 3/3   | 0.94 | 0.16 | 64,64,73,83                 | 0     |
| 3   | 4OA  | D     | 502 | 27/27 | 0.95 | 0.10 | 41,45,70,78                 | 0     |
| 3   | 4OA  | E     | 502 | 27/27 | 0.95 | 0.10 | 42,46,64,65                 | 0     |
| 4   | FMT  | C     | 517 | 3/3   | 0.95 | 0.26 | 67,67,67,69                 | 0     |
| 4   | FMT  | F     | 504 | 3/3   | 0.95 | 0.14 | 65,65,69,74                 | 0     |
| 4   | FMT  | C     | 521 | 3/3   | 0.95 | 0.13 | 55,55,61,66                 | 0     |
| 4   | FMT  | D     | 510 | 3/3   | 0.95 | 0.28 | 57,57,67,72                 | 0     |
| 5   | NA   | C     | 527 | 1/1   | 0.95 | 0.16 | 44,44,44,44                 | 0     |
| 5   | NA   | D     | 516 | 1/1   | 0.95 | 0.11 | 50,50,50,50                 | 0     |
| 4   | FMT  | D     | 511 | 3/3   | 0.95 | 0.17 | 70,70,72,75                 | 0     |
| 5   | NA   | F     | 514 | 1/1   | 0.95 | 0.09 | 55,55,55,55                 | 0     |
| 3   | 4OA  | B     | 502 | 27/27 | 0.96 | 0.08 | 33,36,54,58                 | 0     |
| 3   | 4OA  | C     | 502 | 27/27 | 0.96 | 0.10 | 35,40,69,77                 | 0     |
| 4   | FMT  | B     | 517 | 3/3   | 0.96 | 0.10 | 51,51,53,58                 | 0     |
| 3   | 4OA  | F     | 502 | 27/27 | 0.96 | 0.09 | 45,49,64,72                 | 0     |
| 2   | HEM  | F     | 501 | 43/43 | 0.97 | 0.09 | 44,50,58,77                 | 0     |
| 5   | NA   | B     | 525 | 1/1   | 0.98 | 0.10 | 43,43,43,43                 | 0     |
| 2   | HEM  | E     | 501 | 43/43 | 0.98 | 0.07 | 37,42,50,52                 | 0     |
| 4   | FMT  | A     | 522 | 3/3   | 0.98 | 0.07 | 45,45,46,50                 | 0     |
| 2   | HEM  | D     | 501 | 43/43 | 0.98 | 0.06 | 27,33,46,48                 | 0     |

*Continued on next page...*

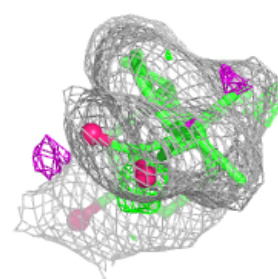
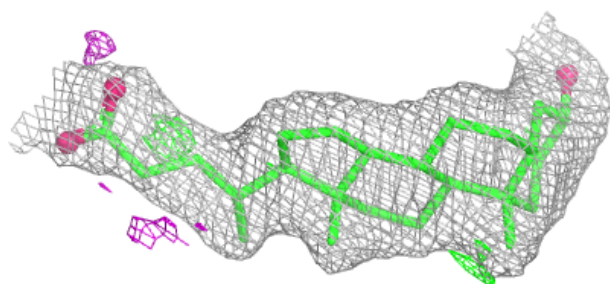
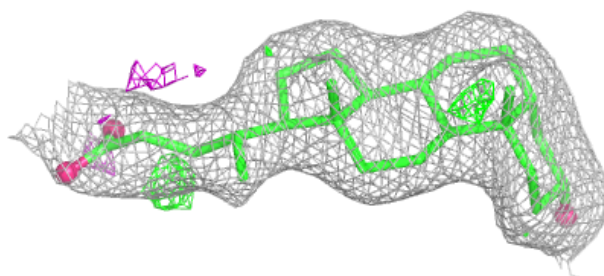
*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5   | NA   | A     | 525 | 1/1   | 0.98 | 0.12 | 50,50,50,50                 | 0     |
| 2   | HEM  | A     | 501 | 43/43 | 0.99 | 0.05 | 30,33,36,46                 | 0     |
| 2   | HEM  | B     | 501 | 43/43 | 0.99 | 0.06 | 28,32,38,50                 | 0     |
| 2   | HEM  | C     | 501 | 43/43 | 0.99 | 0.06 | 32,34,38,49                 | 0     |

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

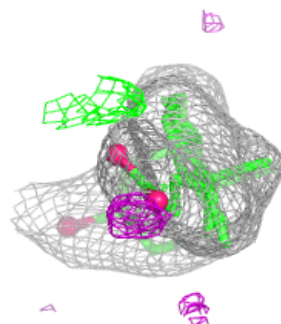
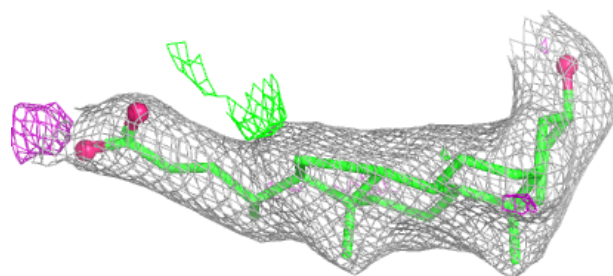
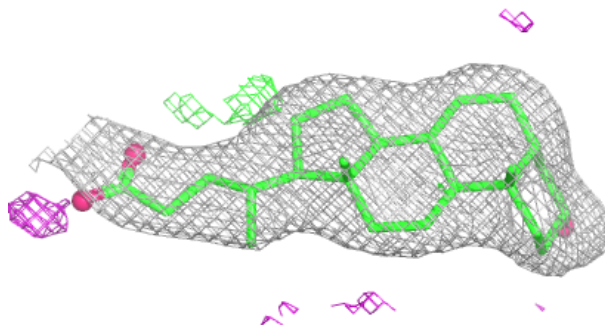
**Electron density around 4OA A 502:**

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

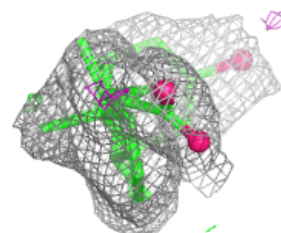
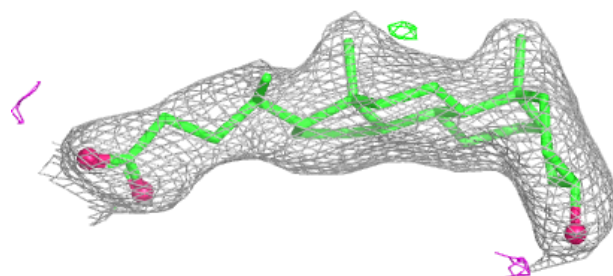
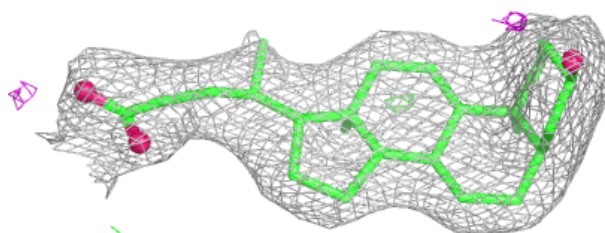


**Electron density around 4OA D 502:**

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

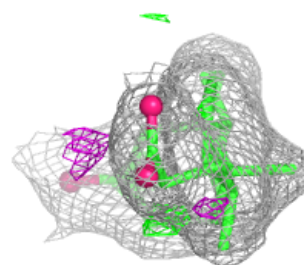
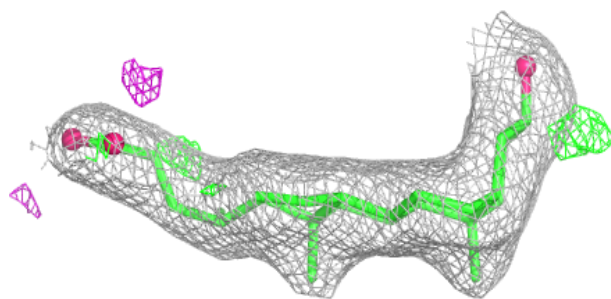
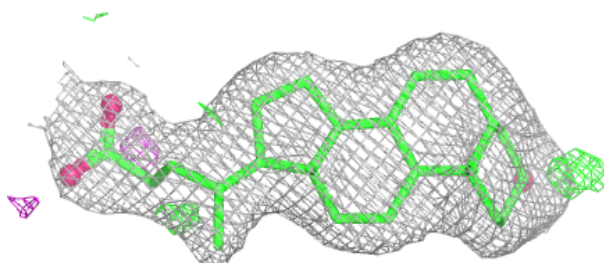
**Electron density around 4OA E 502:**

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

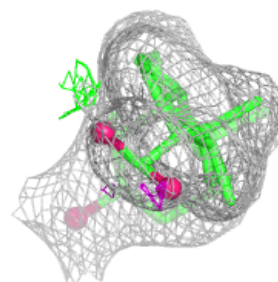
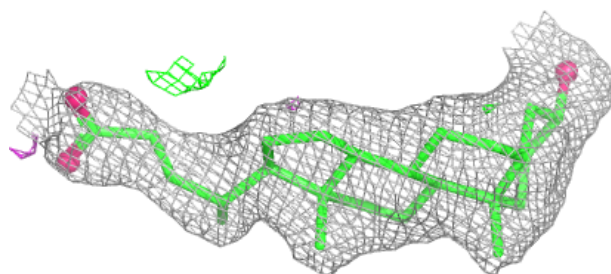
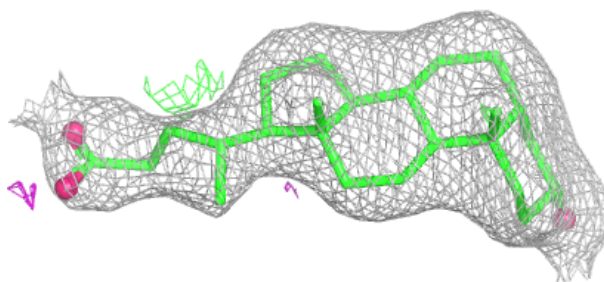


**Electron density around 4OA B 502:**

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

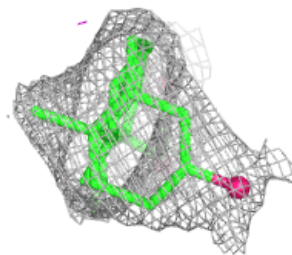
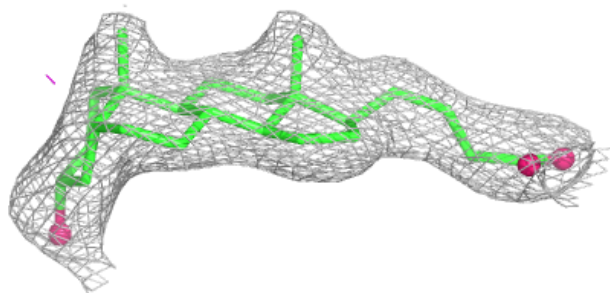
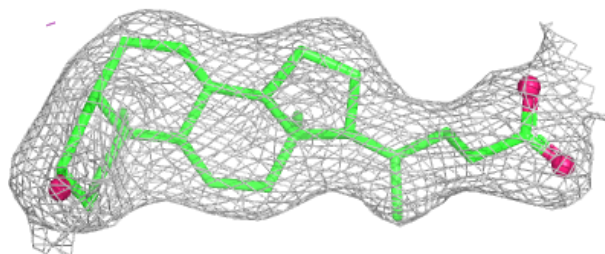
**Electron density around 4OA C 502:**

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



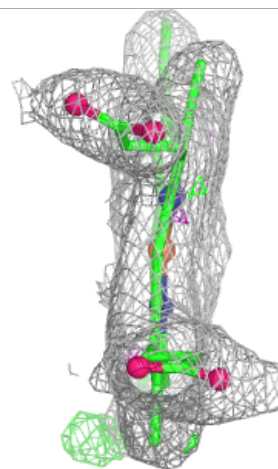
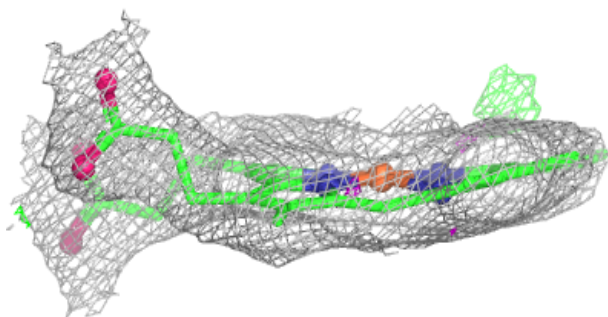
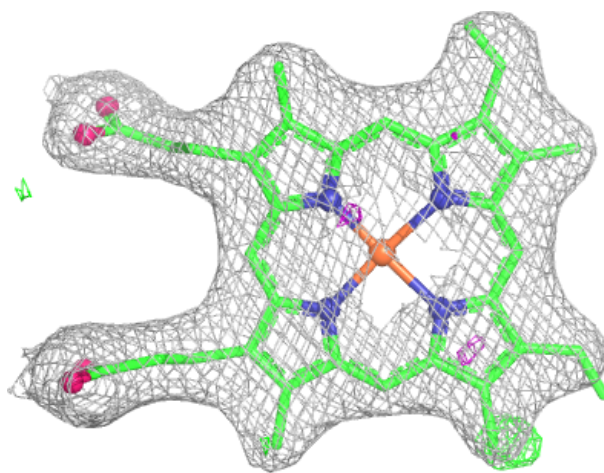
**Electron density around 4OA F 502:**

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



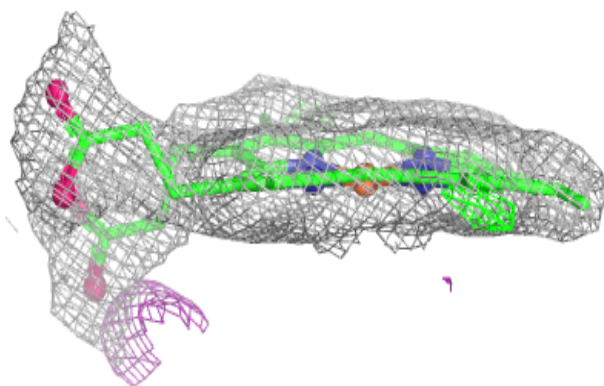
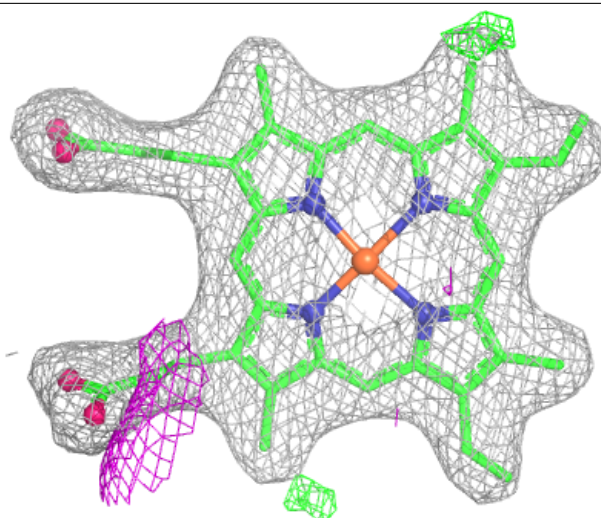
**Electron density around HEM F 501:**

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



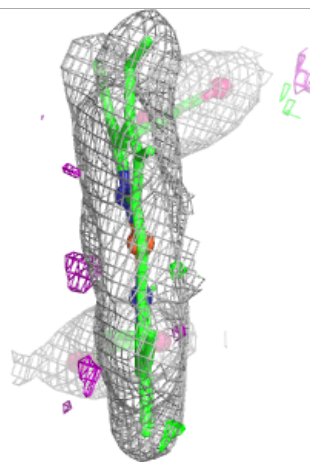
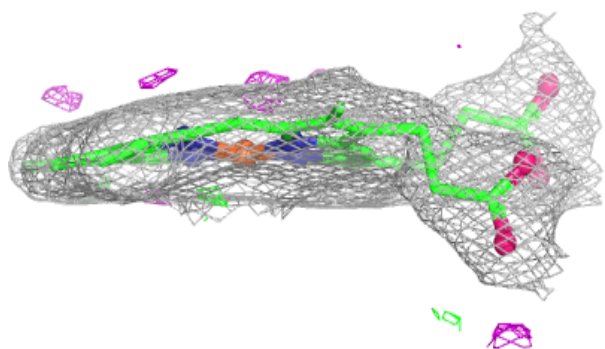
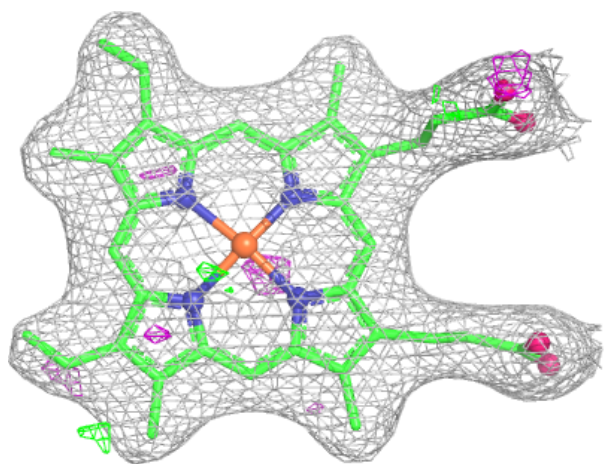
**Electron density around HEM E 501:**

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



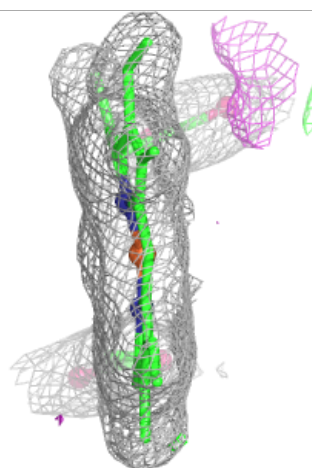
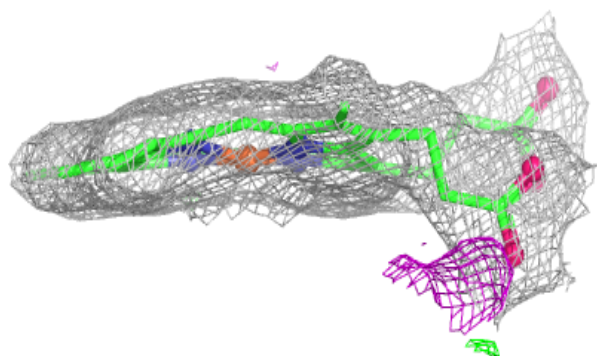
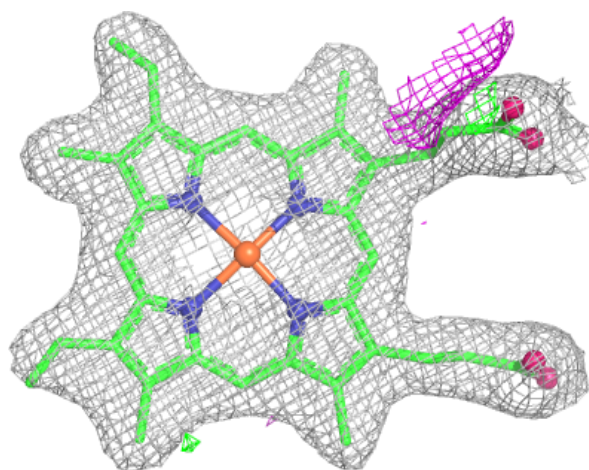
**Electron density around HEM D 501:**

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



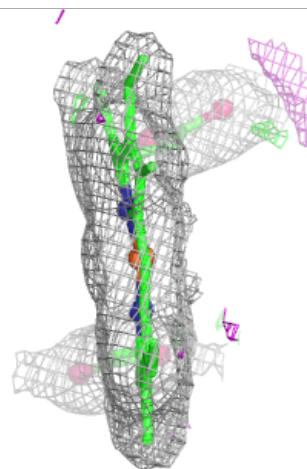
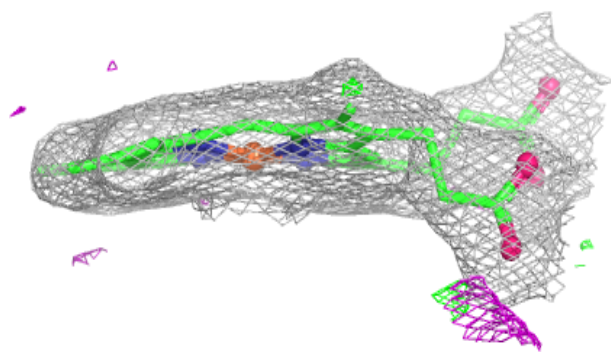
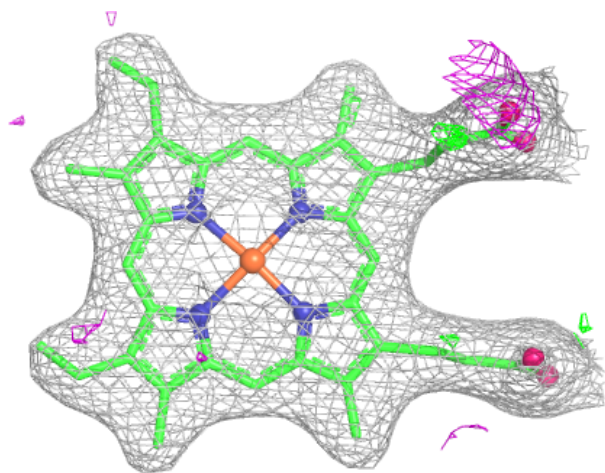
**Electron density around HEM A 501:**

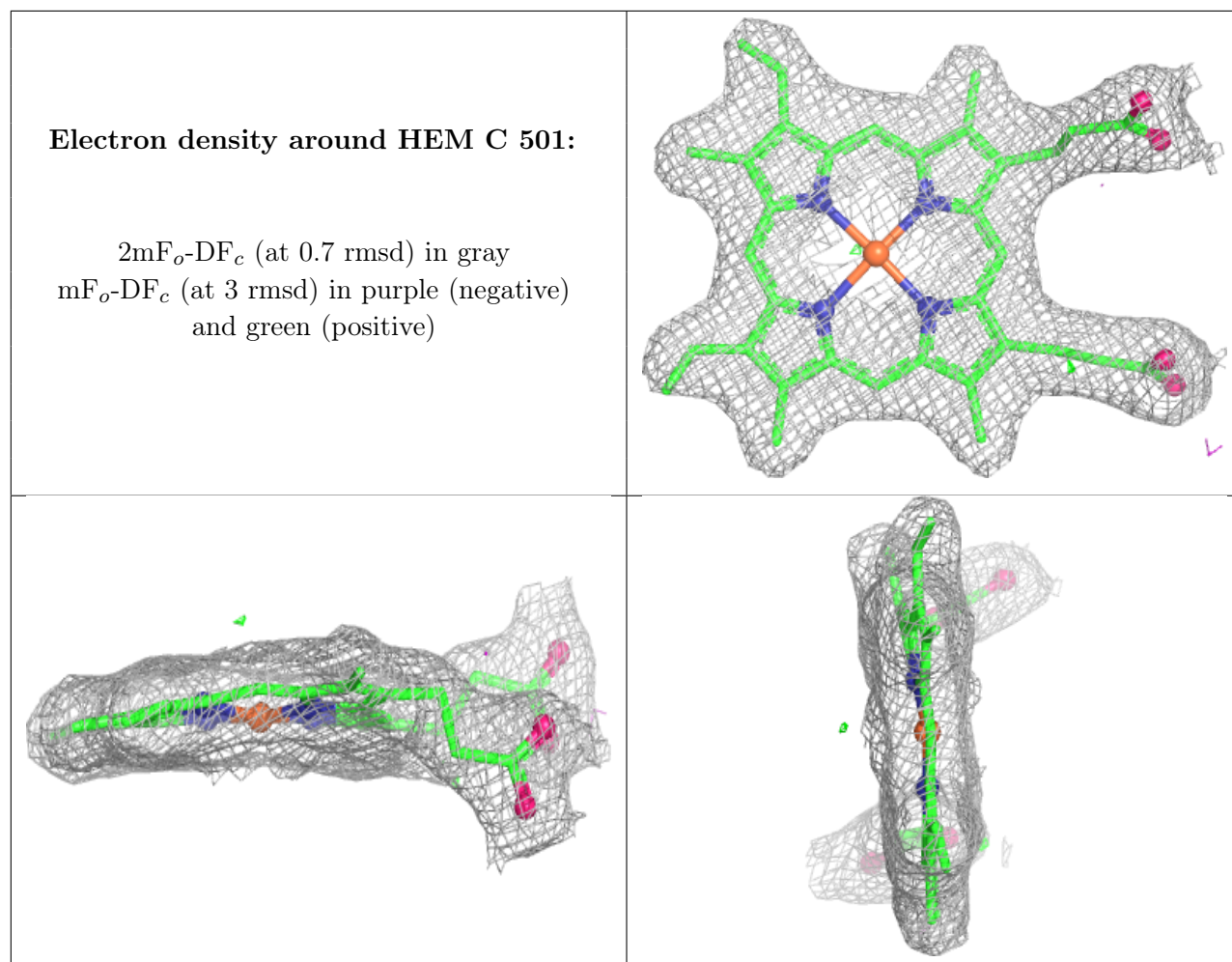
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM B 501:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.