



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 01:24 AM JST

PDB ID : 6K43 / pdb\_00006k43  
EMDB ID : EMD-9913  
Title : Cryo-EM structure of Holo-bacterioferritin-form-I from *Streptomyces coelicolor*  
Authors : Jobichen, C.; Sivaraman, J.  
Deposited on : 2019-05-23  
Resolution : 3.70 Å(reported)  
Based on initial model : 5XX9

This is a Full wwPDB EM 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

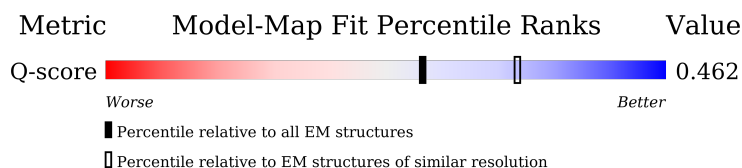
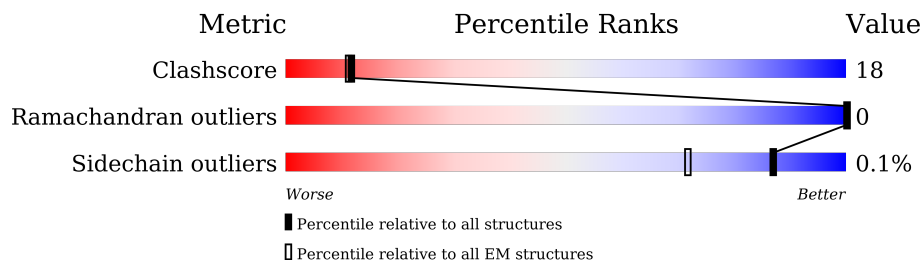
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 11569 ( 3.20 - 4.20 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 167    |                  |
| 1   | B     | 167    |                  |
| 1   | C     | 167    |                  |
| 1   | D     | 167    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 167    |                  |
| 1   | F     | 167    |                  |
| 1   | G     | 167    |                  |
| 1   | H     | 167    |                  |
| 1   | I     | 167    |                  |
| 1   | J     | 167    |                  |
| 1   | K     | 167    |                  |
| 1   | L     | 167    |                  |
| 1   | M     | 167    |                  |
| 1   | N     | 167    |                  |
| 1   | O     | 167    |                  |
| 1   | P     | 167    |                  |
| 1   | Q     | 167    |                  |
| 1   | R     | 167    |                  |
| 1   | S     | 167    |                  |
| 1   | T     | 167    |                  |
| 1   | U     | 167    |                  |
| 1   | V     | 167    |                  |
| 1   | W     | 167    |                  |
| 1   | X     | 167    |                  |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32168 atoms, of which 360 are hydrogens and 0 are deuteriums.

In the tables below, 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 Bacterioferritin.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1315  | 828 | 227 | 256 | 4 |         |       |
| 1   | B     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | C     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1318  | 832 | 226 | 256 | 4 |         |       |
| 1   | D     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | F     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1310  | 826 | 225 | 255 | 4 |         |       |
| 1   | E     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1304  | 823 | 225 | 252 | 4 |         |       |
| 1   | G     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1304  | 823 | 225 | 252 | 4 |         |       |
| 1   | H     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1304  | 823 | 225 | 252 | 4 |         |       |
| 1   | I     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1304  | 823 | 225 | 252 | 4 |         |       |
| 1   | J     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1315  | 828 | 227 | 256 | 4 |         |       |
| 1   | K     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | L     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1318  | 832 | 226 | 256 | 4 |         |       |
| 1   | M     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | N     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1310  | 826 | 225 | 255 | 4 |         |       |
| 1   | O     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1315  | 828 | 227 | 256 | 4 |         |       |
| 1   | P     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | Q     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1318  | 832 | 226 | 256 | 4 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | R     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | S     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1310  | 826 | 225 | 255 | 4 |         |       |
| 1   | T     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1315  | 828 | 227 | 256 | 4 |         |       |
| 1   | U     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | V     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1318  | 832 | 226 | 256 | 4 |         |       |
| 1   | W     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | X     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1310  | 826 | 225 | 255 | 4 |         |       |

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

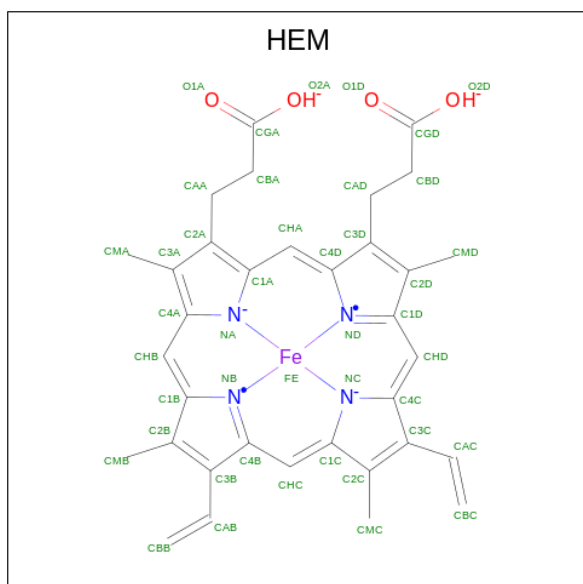
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 2   | A     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | B     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | C     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | D     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | F     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | E     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | G     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | H     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | I     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | J     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | K     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | L     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 2   | M     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | N     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | O     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | P     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | Q     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | R     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | S     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | T     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | U     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | V     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | W     | 1        | Total<br>1 | Fe<br>1 | 0       |
| 2   | X     | 1        | Total<br>1 | Fe<br>1 | 0       |

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).

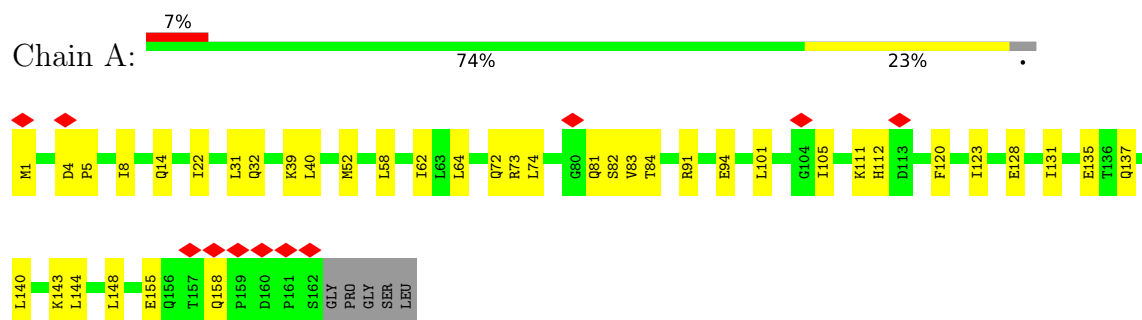


| Mol | Chain | Residues | Atoms       |         |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|--------|--------|---------|
| 3   | A     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | C     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | F     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | K     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | L     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | N     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | O     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | Q     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | S     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | U     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | V     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |
| 3   | X     | 1        | Total<br>73 | C<br>34 | Fe<br>1 | H<br>30 | N<br>4 | O<br>4 | 0       |

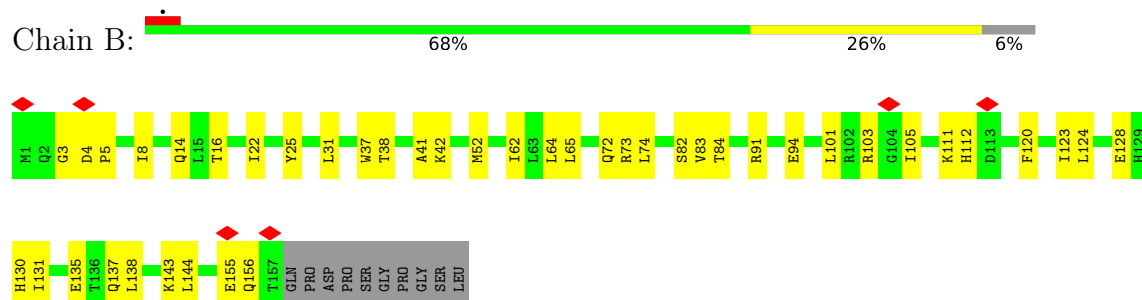
### 3 Residue-property plots [i](#)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

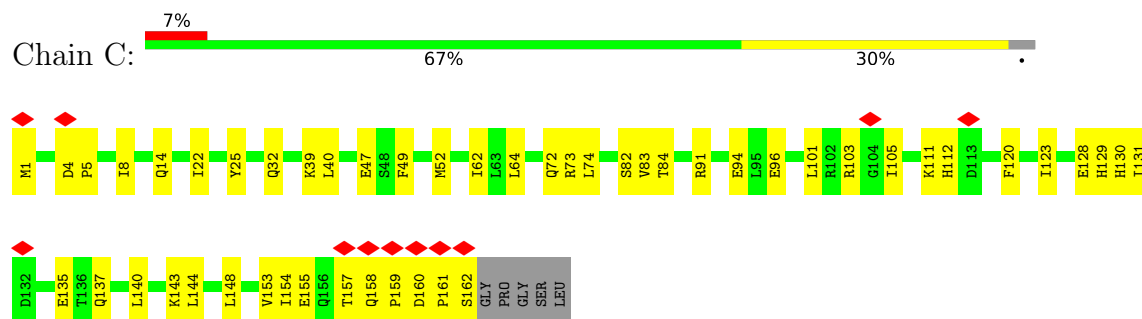
#### • Molecule 1: Bacterioferritin



#### • Molecule 1: Bacterioferritin

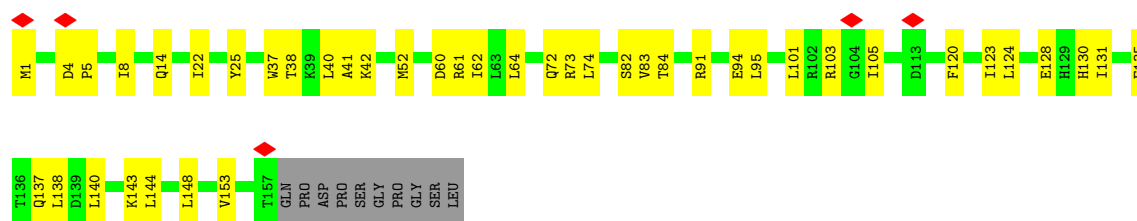


#### • Molecule 1: Bacterioferritin

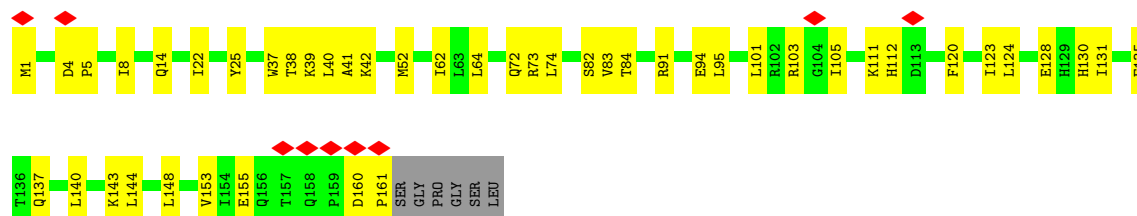


#### • Molecule 1: Bacterioferritin





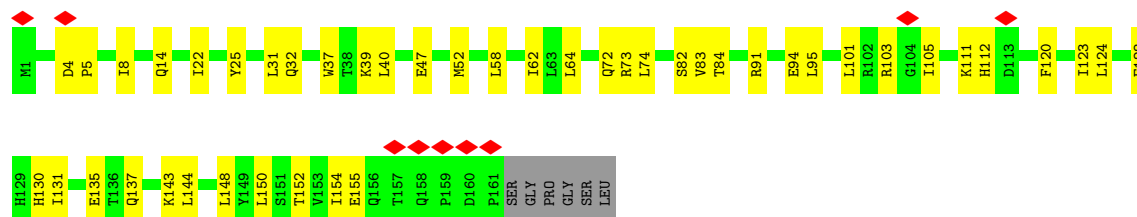
• Molecule 1: Bacterioferritin



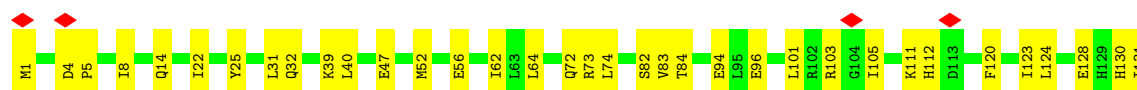
• Molecule 1: Bacterioferritin

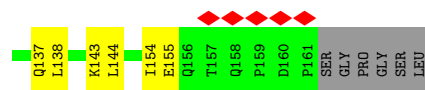


• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin

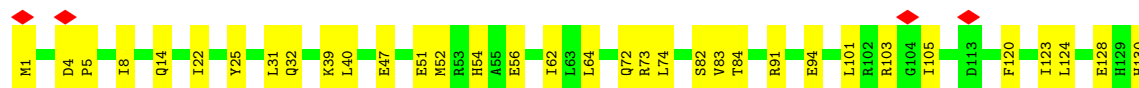




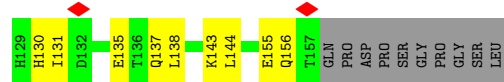
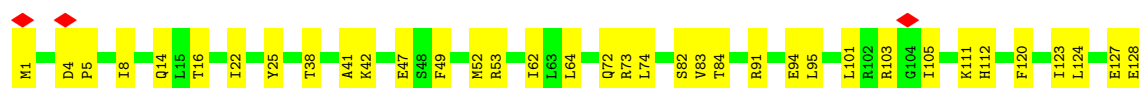
• Molecule 1: Bacterioferritin



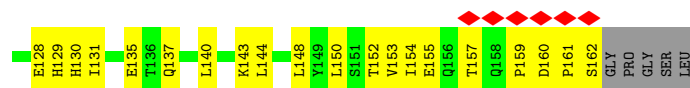
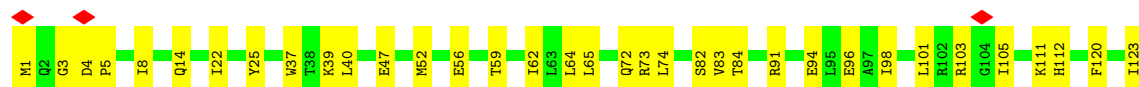
• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin

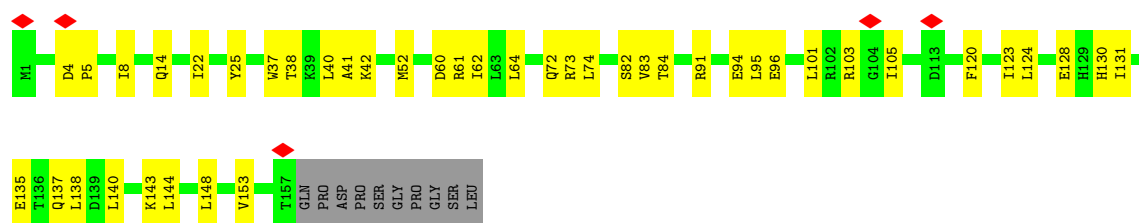


• Molecule 1: Bacterioferritin



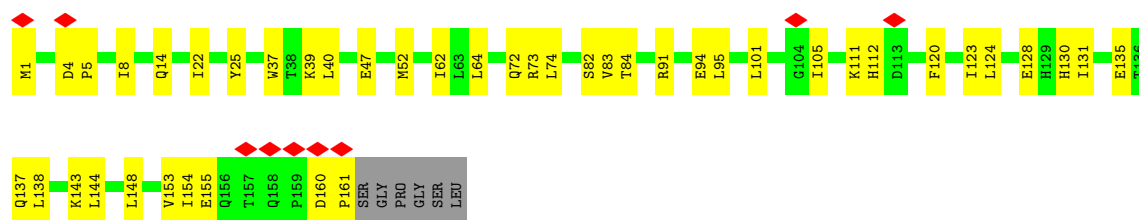
• Molecule 1: Bacterioferritin

Chain M: 



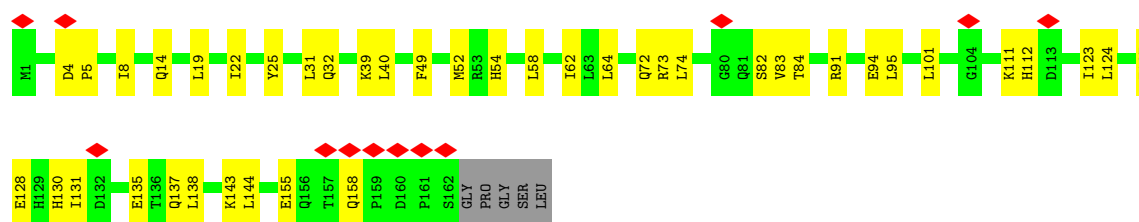
• Molecule 1: Bacterioferritin

Chain N: 



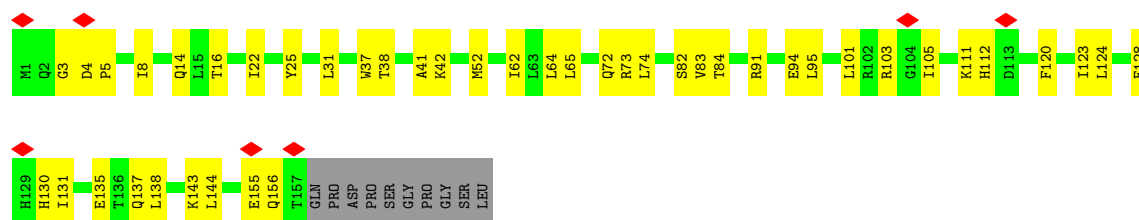
• Molecule 1: Bacterioferritin

Chain O: 



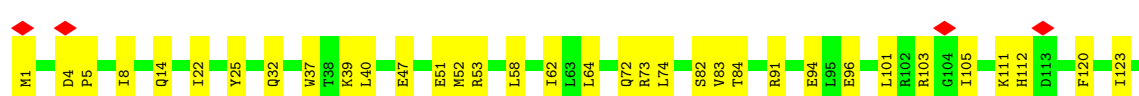
• Molecule 1: Bacterioferritin

Chain P: 



• Molecule 1: Bacterioferritin

Chain Q: 

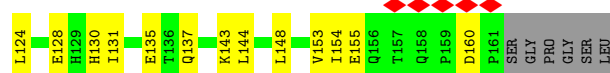




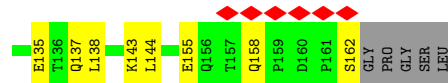
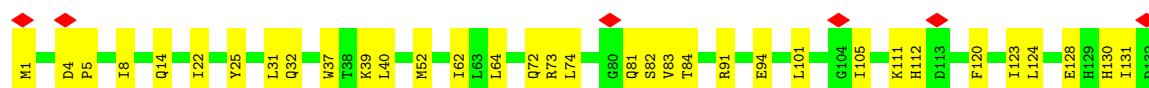
• Molecule 1: Bacterioferritin



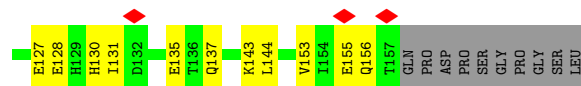
• Molecule 1: Bacterioferritin



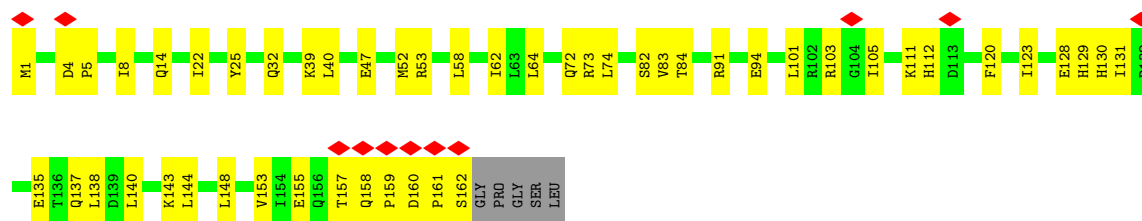
• Molecule 1: Bacterioferritin



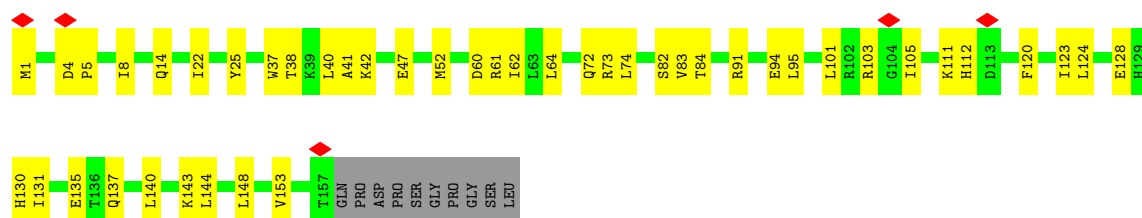
• Molecule 1: Bacterioferritin



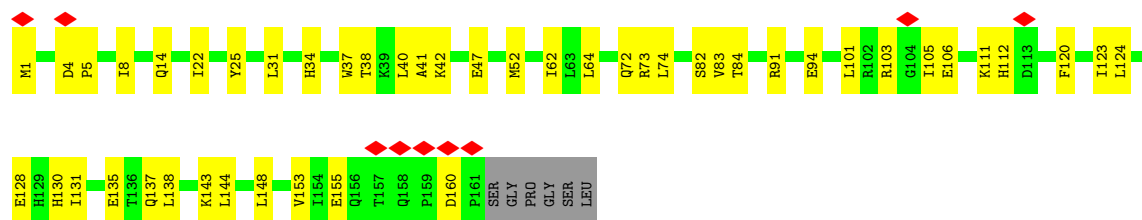
• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, O                                | Depositor |
| Number of particles used             | 19485                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 1.6                                     | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON II (4k x 4k)                 | Depositor |
| Maximum map value                    | 18.853                                  | Depositor |
| Minimum map value                    | -10.043                                 | Depositor |
| Average map value                    | 0.030                                   | Depositor |
| Map value standard deviation         | 1.242                                   | Depositor |
| Recommended contour level            | 5.1                                     | Depositor |
| Map size ( $\text{\AA}$ )            | 266.4, 266.4, 266.4                     | wwPDB     |
| Map dimensions                       | 240, 240, 240                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.11, 1.11, 1.11                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, HEM

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.31         | 0/1336      | 0.43        | 0/1805      |
| 1   | B     | 0.31         | 0/1306      | 0.43        | 0/1764      |
| 1   | C     | 0.31         | 0/1341      | 0.44        | 0/1814      |
| 1   | D     | 0.31         | 0/1306      | 0.43        | 0/1764      |
| 1   | E     | 0.31         | 0/1325      | 0.44        | 0/1790      |
| 1   | F     | 0.31         | 0/1332      | 0.43        | 0/1801      |
| 1   | G     | 0.31         | 0/1325      | 0.43        | 0/1790      |
| 1   | H     | 0.31         | 0/1325      | 0.43        | 0/1790      |
| 1   | I     | 0.31         | 0/1325      | 0.44        | 0/1790      |
| 1   | J     | 0.31         | 0/1336      | 0.44        | 0/1805      |
| 1   | K     | 0.32         | 0/1306      | 0.44        | 0/1764      |
| 1   | L     | 0.31         | 0/1341      | 0.44        | 0/1814      |
| 1   | M     | 0.31         | 0/1306      | 0.43        | 0/1764      |
| 1   | N     | 0.31         | 0/1332      | 0.43        | 0/1801      |
| 1   | O     | 0.32         | 0/1336      | 0.45        | 0/1805      |
| 1   | P     | 0.31         | 0/1306      | 0.42        | 0/1764      |
| 1   | Q     | 0.31         | 0/1341      | 0.44        | 0/1814      |
| 1   | R     | 0.31         | 0/1306      | 0.43        | 0/1764      |
| 1   | S     | 0.31         | 0/1332      | 0.43        | 0/1801      |
| 1   | T     | 0.31         | 0/1336      | 0.43        | 0/1805      |
| 1   | U     | 0.32         | 0/1306      | 0.45        | 0/1764      |
| 1   | V     | 0.31         | 0/1341      | 0.44        | 0/1814      |
| 1   | W     | 0.32         | 0/1306      | 0.43        | 0/1764      |
| 1   | X     | 0.31         | 0/1332      | 0.44        | 0/1801      |
| All | All   | 0.31         | 0/31784     | 0.44        | 0/42952     |

There are no bond length outliers.

There are no bond angle outliers.

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     | 1315  | 0        | 1280     | 42      | 0            |
| 1   | B     | 1285  | 0        | 1262     | 37      | 0            |
| 1   | C     | 1318  | 0        | 1289     | 55      | 0            |
| 1   | D     | 1285  | 0        | 1262     | 41      | 0            |
| 1   | E     | 1304  | 0        | 1268     | 44      | 0            |
| 1   | F     | 1310  | 0        | 1274     | 47      | 0            |
| 1   | G     | 1304  | 0        | 1268     | 42      | 0            |
| 1   | H     | 1304  | 0        | 1268     | 41      | 0            |
| 1   | I     | 1304  | 0        | 1268     | 42      | 0            |
| 1   | J     | 1315  | 0        | 1280     | 40      | 0            |
| 1   | K     | 1285  | 0        | 1262     | 44      | 0            |
| 1   | L     | 1318  | 0        | 1289     | 56      | 0            |
| 1   | M     | 1285  | 0        | 1262     | 44      | 0            |
| 1   | N     | 1310  | 0        | 1276     | 41      | 0            |
| 1   | O     | 1315  | 0        | 1280     | 38      | 0            |
| 1   | P     | 1285  | 0        | 1262     | 39      | 0            |
| 1   | Q     | 1318  | 0        | 1289     | 56      | 0            |
| 1   | R     | 1285  | 0        | 1261     | 42      | 0            |
| 1   | S     | 1310  | 0        | 1275     | 49      | 0            |
| 1   | T     | 1315  | 0        | 1280     | 43      | 0            |
| 1   | U     | 1285  | 0        | 1261     | 42      | 0            |
| 1   | V     | 1318  | 0        | 1289     | 52      | 0            |
| 1   | W     | 1285  | 0        | 1261     | 43      | 0            |
| 1   | X     | 1310  | 0        | 1276     | 45      | 0            |
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 1     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 1     | 0        | 0        | 0       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 2   | I     | 1     | 0        | 0        | 0       | 0            |
| 2   | J     | 1     | 0        | 0        | 0       | 0            |
| 2   | K     | 1     | 0        | 0        | 0       | 0            |
| 2   | L     | 1     | 0        | 0        | 0       | 0            |
| 2   | M     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | N     | 1     | 0        | 0        | 0       | 0            |
| 2   | O     | 1     | 0        | 0        | 0       | 0            |
| 2   | P     | 1     | 0        | 0        | 0       | 0            |
| 2   | Q     | 1     | 0        | 0        | 0       | 0            |
| 2   | R     | 1     | 0        | 0        | 0       | 0            |
| 2   | S     | 1     | 0        | 0        | 0       | 0            |
| 2   | T     | 1     | 0        | 0        | 0       | 0            |
| 2   | U     | 1     | 0        | 0        | 0       | 0            |
| 2   | V     | 1     | 0        | 0        | 0       | 0            |
| 2   | W     | 1     | 0        | 0        | 0       | 0            |
| 2   | X     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 43    | 30       | 30       | 11      | 0            |
| 3   | C     | 43    | 30       | 30       | 8       | 0            |
| 3   | F     | 43    | 30       | 30       | 6       | 0            |
| 3   | K     | 43    | 30       | 30       | 12      | 0            |
| 3   | L     | 43    | 30       | 30       | 8       | 0            |
| 3   | N     | 43    | 30       | 30       | 7       | 0            |
| 3   | O     | 43    | 30       | 30       | 10      | 0            |
| 3   | Q     | 43    | 30       | 30       | 5       | 0            |
| 3   | S     | 43    | 30       | 30       | 6       | 0            |
| 3   | U     | 43    | 30       | 30       | 11      | 0            |
| 3   | V     | 43    | 30       | 30       | 9       | 0            |
| 3   | X     | 43    | 30       | 30       | 4       | 0            |
| All | All   | 31808 | 360      | 30902    | 1104    | 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 18.

All (1104) 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:F:8:ILE:HG23 | 1:F:62:ILE:HD11 | 1.32                     | 1.12              |
| 1:U:8:ILE:HG23 | 1:U:62:ILE:HD11 | 1.32                     | 1.12              |
| 1:N:8:ILE:HG23 | 1:N:62:ILE:HD11 | 1.32                     | 1.09              |
| 1:P:8:ILE:HG23 | 1:P:62:ILE:HD11 | 1.32                     | 1.09              |
| 1:E:8:ILE:HG23 | 1:E:62:ILE:HD11 | 1.31                     | 1.09              |
| 1:H:8:ILE:HG23 | 1:H:62:ILE:HD11 | 1.30                     | 1.09              |
| 1:M:8:ILE:HG23 | 1:M:62:ILE:HD11 | 1.29                     | 1.08              |
| 1:B:8:ILE:HG23 | 1:B:62:ILE:HD11 | 1.32                     | 1.07              |
| 1:X:8:ILE:HG23 | 1:X:62:ILE:HD11 | 1.32                     | 1.07              |
| 1:D:8:ILE:HG23 | 1:D:62:ILE:HD11 | 1.30                     | 1.07              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:8:ILE:HG23   | 1:L:62:ILE:HD11  | 1.36                     | 1.07              |
| 1:C:8:ILE:HG23   | 1:C:62:ILE:HD11  | 1.33                     | 1.07              |
| 1:R:8:ILE:HG23   | 1:R:62:ILE:HD11  | 1.30                     | 1.07              |
| 1:W:8:ILE:HG23   | 1:W:62:ILE:HD11  | 1.30                     | 1.05              |
| 1:J:8:ILE:HG23   | 1:J:62:ILE:HD11  | 1.35                     | 1.04              |
| 1:S:8:ILE:HG23   | 1:S:62:ILE:HD11  | 1.31                     | 1.04              |
| 1:K:8:ILE:HG23   | 1:K:62:ILE:HD11  | 1.32                     | 1.04              |
| 1:T:8:ILE:HG23   | 1:T:62:ILE:HD11  | 1.34                     | 1.03              |
| 1:O:8:ILE:HG23   | 1:O:62:ILE:HD11  | 1.47                     | 0.96              |
| 1:A:8:ILE:HG23   | 1:A:62:ILE:HD11  | 1.48                     | 0.95              |
| 1:G:8:ILE:HG23   | 1:G:62:ILE:HD11  | 1.48                     | 0.95              |
| 1:Q:8:ILE:HG23   | 1:Q:62:ILE:HD11  | 1.47                     | 0.94              |
| 1:U:22:ILE:HD11  | 1:U:52:MET:HA    | 1.45                     | 0.94              |
| 1:Q:47:GLU:OE2   | 1:Q:130:HIS:CE1  | 2.20                     | 0.93              |
| 1:I:8:ILE:HG23   | 1:I:62:ILE:HD11  | 1.48                     | 0.93              |
| 1:V:8:ILE:HG23   | 1:V:62:ILE:HD11  | 1.48                     | 0.92              |
| 1:C:22:ILE:HD11  | 1:C:52:MET:HA    | 1.50                     | 0.92              |
| 1:B:22:ILE:HD11  | 1:B:52:MET:HA    | 1.50                     | 0.91              |
| 1:Q:1:MET:HE2    | 1:Q:1:MET:HA     | 1.53                     | 0.91              |
| 1:K:22:ILE:HD11  | 1:K:52:MET:HA    | 1.50                     | 0.91              |
| 1:Q:162:SER:N    | 1:R:60:ASP:OD2   | 2.06                     | 0.88              |
| 1:X:22:ILE:HD11  | 1:X:52:MET:HA    | 1.53                     | 0.88              |
| 1:A:101:LEU:HD11 | 1:A:123:ILE:HG22 | 1.55                     | 0.88              |
| 1:V:162:SER:N    | 1:W:60:ASP:OD2   | 2.06                     | 0.88              |
| 1:D:22:ILE:HD11  | 1:D:52:MET:HA    | 1.55                     | 0.88              |
| 1:E:101:LEU:HD11 | 1:E:123:ILE:HG22 | 1.56                     | 0.88              |
| 1:E:22:ILE:HD11  | 1:E:52:MET:HA    | 1.56                     | 0.88              |
| 1:T:22:ILE:HD11  | 1:T:52:MET:HA    | 1.53                     | 0.88              |
| 1:G:22:ILE:HD11  | 1:G:52:MET:HA    | 1.53                     | 0.87              |
| 1:C:162:SER:N    | 1:D:60:ASP:OD2   | 2.06                     | 0.87              |
| 1:J:101:LEU:HD11 | 1:J:123:ILE:HG22 | 1.56                     | 0.87              |
| 1:S:101:LEU:HD11 | 1:S:123:ILE:HG22 | 1.56                     | 0.87              |
| 1:I:101:LEU:HD11 | 1:I:123:ILE:HG22 | 1.57                     | 0.87              |
| 1:N:101:LEU:HD11 | 1:N:123:ILE:HG22 | 1.57                     | 0.87              |
| 1:F:101:LEU:HD11 | 1:F:123:ILE:HG22 | 1.57                     | 0.87              |
| 1:L:162:SER:N    | 1:M:60:ASP:OD2   | 2.06                     | 0.87              |
| 1:Q:22:ILE:HD11  | 1:Q:52:MET:HA    | 1.56                     | 0.87              |
| 1:Q:47:GLU:OE2   | 1:Q:130:HIS:ND1  | 2.07                     | 0.87              |
| 1:T:101:LEU:HD11 | 1:T:123:ILE:HG22 | 1.57                     | 0.87              |
| 1:B:101:LEU:HD11 | 1:B:123:ILE:HG22 | 1.57                     | 0.86              |
| 1:J:22:ILE:HD11  | 1:J:52:MET:HA    | 1.54                     | 0.86              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:101:LEU:HD11 | 1:H:123:ILE:HG22 | 1.56                     | 0.86              |
| 1:H:22:ILE:HD11  | 1:H:52:MET:HA    | 1.56                     | 0.86              |
| 1:I:22:ILE:HD11  | 1:I:52:MET:HA    | 1.56                     | 0.86              |
| 1:M:101:LEU:HD11 | 1:M:123:ILE:HG22 | 1.56                     | 0.86              |
| 1:G:101:LEU:HD11 | 1:G:123:ILE:HG22 | 1.57                     | 0.86              |
| 1:P:22:ILE:HD11  | 1:P:52:MET:HA    | 1.56                     | 0.86              |
| 1:K:101:LEU:HD11 | 1:K:123:ILE:HG22 | 1.58                     | 0.85              |
| 1:V:101:LEU:HD11 | 1:V:123:ILE:HG22 | 1.57                     | 0.85              |
| 1:R:101:LEU:HD11 | 1:R:123:ILE:HG22 | 1.56                     | 0.85              |
| 1:X:101:LEU:HD11 | 1:X:123:ILE:HG22 | 1.58                     | 0.85              |
| 1:D:101:LEU:HD11 | 1:D:123:ILE:HG22 | 1.56                     | 0.85              |
| 1:W:101:LEU:HD11 | 1:W:123:ILE:HG22 | 1.56                     | 0.85              |
| 1:F:22:ILE:HD11  | 1:F:52:MET:HA    | 1.56                     | 0.85              |
| 1:W:22:ILE:HD11  | 1:W:52:MET:HA    | 1.58                     | 0.85              |
| 1:M:22:ILE:HD11  | 1:M:52:MET:HA    | 1.59                     | 0.85              |
| 1:R:22:ILE:HD11  | 1:R:52:MET:HA    | 1.59                     | 0.85              |
| 1:S:22:ILE:HD11  | 1:S:52:MET:HA    | 1.56                     | 0.85              |
| 1:Q:101:LEU:HD11 | 1:Q:123:ILE:HG22 | 1.57                     | 0.84              |
| 1:A:22:ILE:HD11  | 1:A:52:MET:HA    | 1.57                     | 0.84              |
| 1:L:101:LEU:HD11 | 1:L:123:ILE:HG22 | 1.57                     | 0.84              |
| 1:N:22:ILE:HD11  | 1:N:52:MET:HA    | 1.59                     | 0.84              |
| 1:L:22:ILE:HD11  | 1:L:52:MET:HA    | 1.59                     | 0.84              |
| 1:P:101:LEU:HD11 | 1:P:123:ILE:HG22 | 1.58                     | 0.84              |
| 1:U:101:LEU:HD11 | 1:U:123:ILE:HG22 | 1.59                     | 0.83              |
| 1:O:101:LEU:HD11 | 1:O:123:ILE:HG22 | 1.60                     | 0.83              |
| 1:C:101:LEU:HD11 | 1:C:123:ILE:HG22 | 1.59                     | 0.83              |
| 1:L:91:ARG:NE    | 1:L:135:GLU:OE2  | 2.13                     | 0.82              |
| 1:A:91:ARG:NE    | 1:A:135:GLU:OE2  | 2.14                     | 0.81              |
| 1:F:91:ARG:NE    | 1:F:135:GLU:OE2  | 2.14                     | 0.81              |
| 1:M:91:ARG:NE    | 1:M:135:GLU:OE2  | 2.13                     | 0.81              |
| 1:W:91:ARG:NE    | 1:W:135:GLU:OE2  | 2.13                     | 0.81              |
| 1:I:91:ARG:NE    | 1:I:135:GLU:OE2  | 2.13                     | 0.81              |
| 1:C:91:ARG:NE    | 1:C:135:GLU:OE2  | 2.14                     | 0.81              |
| 1:G:91:ARG:NE    | 1:G:135:GLU:OE2  | 2.14                     | 0.81              |
| 1:J:91:ARG:NE    | 1:J:135:GLU:OE2  | 2.14                     | 0.81              |
| 1:B:91:ARG:NE    | 1:B:135:GLU:OE2  | 2.14                     | 0.81              |
| 1:P:91:ARG:NE    | 1:P:135:GLU:OE2  | 2.13                     | 0.81              |
| 1:R:91:ARG:NE    | 1:R:135:GLU:OE2  | 2.14                     | 0.81              |
| 1:S:91:ARG:NE    | 1:S:135:GLU:OE2  | 2.14                     | 0.81              |
| 1:K:91:ARG:NE    | 1:K:135:GLU:OE2  | 2.14                     | 0.80              |
| 1:V:91:ARG:NE    | 1:V:135:GLU:OE2  | 2.13                     | 0.80              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:91:ARG:NE    | 1:N:135:GLU:OE2  | 2.13                     | 0.80              |
| 1:Q:91:ARG:NE    | 1:Q:135:GLU:OE2  | 2.13                     | 0.80              |
| 1:U:91:ARG:NE    | 1:U:135:GLU:OE2  | 2.15                     | 0.80              |
| 3:Q:202:HEM:HBC2 | 3:Q:202:HEM:HMC2 | 1.63                     | 0.80              |
| 3:N:201:HEM:HHH  | 3:N:201:HEM:HBC2 | 1.63                     | 0.80              |
| 1:X:91:ARG:NE    | 1:X:135:GLU:OE2  | 2.14                     | 0.80              |
| 1:T:91:ARG:NE    | 1:T:135:GLU:OE2  | 2.15                     | 0.80              |
| 1:D:91:ARG:NE    | 1:D:135:GLU:OE2  | 2.14                     | 0.79              |
| 1:O:54:HIS:CE1   | 1:O:127:GLU:OE2  | 2.35                     | 0.79              |
| 1:V:39:LYS:NZ    | 1:V:155:GLU:OE2  | 2.15                     | 0.79              |
| 1:V:1:MET:HE2    | 1:V:1:MET:HA     | 1.64                     | 0.79              |
| 1:L:1:MET:HE2    | 1:L:1:MET:HA     | 1.64                     | 0.78              |
| 1:C:1:MET:HE2    | 1:C:1:MET:HA     | 1.64                     | 0.78              |
| 1:N:73:ARG:O     | 1:N:74:LEU:HD23  | 1.83                     | 0.78              |
| 3:O:202:HEM:HBC2 | 3:O:202:HEM:HMC2 | 1.66                     | 0.77              |
| 1:I:39:LYS:NZ    | 1:I:155:GLU:OE2  | 2.16                     | 0.77              |
| 1:N:39:LYS:NZ    | 1:N:155:GLU:OE1  | 2.14                     | 0.77              |
| 1:C:39:LYS:NZ    | 1:C:155:GLU:OE1  | 2.14                     | 0.77              |
| 1:L:39:LYS:NZ    | 1:L:155:GLU:OE1  | 2.14                     | 0.76              |
| 3:V:202:HEM:HMC2 | 3:V:202:HEM:HBC2 | 1.67                     | 0.76              |
| 1:K:73:ARG:O     | 1:K:74:LEU:HD23  | 1.85                     | 0.76              |
| 1:Q:39:LYS:NZ    | 1:Q:155:GLU:OE1  | 2.14                     | 0.76              |
| 3:F:202:HEM:HBC2 | 3:F:202:HEM:HMC2 | 1.68                     | 0.76              |
| 1:X:73:ARG:O     | 1:X:74:LEU:HD23  | 1.86                     | 0.76              |
| 1:R:73:ARG:O     | 1:R:74:LEU:HD23  | 1.86                     | 0.75              |
| 1:C:73:ARG:O     | 1:C:74:LEU:HD23  | 1.86                     | 0.75              |
| 1:F:73:ARG:O     | 1:F:74:LEU:HD23  | 1.86                     | 0.75              |
| 1:P:73:ARG:O     | 1:P:74:LEU:HD23  | 1.85                     | 0.75              |
| 1:D:73:ARG:O     | 1:D:74:LEU:HD23  | 1.86                     | 0.75              |
| 1:U:73:ARG:O     | 1:U:74:LEU:HD23  | 1.85                     | 0.75              |
| 1:B:73:ARG:O     | 1:B:74:LEU:HD23  | 1.86                     | 0.75              |
| 1:Q:73:ARG:O     | 1:Q:74:LEU:HD23  | 1.86                     | 0.75              |
| 1:A:39:LYS:NZ    | 1:A:155:GLU:OE1  | 2.17                     | 0.75              |
| 1:M:73:ARG:O     | 1:M:74:LEU:HD23  | 1.86                     | 0.74              |
| 1:V:73:ARG:O     | 1:V:74:LEU:HD23  | 1.86                     | 0.74              |
| 1:W:73:ARG:O     | 1:W:74:LEU:HD23  | 1.86                     | 0.74              |
| 1:S:73:ARG:O     | 1:S:74:LEU:HD23  | 1.86                     | 0.74              |
| 1:L:73:ARG:O     | 1:L:74:LEU:HD23  | 1.86                     | 0.74              |
| 1:G:39:LYS:NZ    | 1:G:155:GLU:OE2  | 2.16                     | 0.73              |
| 1:V:22:ILE:HD11  | 1:V:52:MET:HA    | 1.69                     | 0.73              |
| 1:H:8:ILE:HG23   | 1:H:62:ILE:CD1   | 2.16                     | 0.73              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:39:LYS:NZ    | 1:H:155:GLU:OE2  | 2.15                     | 0.72              |
| 1:P:64:LEU:O     | 1:P:64:LEU:HD23  | 1.90                     | 0.72              |
| 1:T:52:MET:HE1   | 3:U:201:HEM:C4C  | 2.24                     | 0.72              |
| 1:G:64:LEU:HD23  | 1:G:64:LEU:O     | 1.89                     | 0.72              |
| 1:L:64:LEU:HD23  | 1:L:64:LEU:O     | 1.89                     | 0.72              |
| 1:D:8:ILE:HG23   | 1:D:62:ILE:CD1   | 2.17                     | 0.72              |
| 1:B:64:LEU:HD23  | 1:B:64:LEU:O     | 1.90                     | 0.72              |
| 1:C:8:ILE:HG23   | 1:C:62:ILE:CD1   | 2.18                     | 0.72              |
| 1:O:39:LYS:NZ    | 1:O:155:GLU:OE1  | 2.17                     | 0.72              |
| 1:B:3:GLY:HA3    | 1:B:65:LEU:HD22  | 1.72                     | 0.71              |
| 1:O:64:LEU:HD23  | 1:O:64:LEU:O     | 1.90                     | 0.71              |
| 1:P:8:ILE:HG23   | 1:P:62:ILE:CD1   | 2.18                     | 0.71              |
| 1:Q:64:LEU:HD23  | 1:Q:64:LEU:O     | 1.91                     | 0.71              |
| 3:K:301:HEM:HBC2 | 3:K:301:HEM:HMC2 | 1.72                     | 0.71              |
| 1:V:157:THR:HG22 | 1:V:159:PRO:HG3  | 1.71                     | 0.71              |
| 1:Q:157:THR:HG22 | 1:Q:159:PRO:HG3  | 1.71                     | 0.71              |
| 1:O:91:ARG:NE    | 1:O:135:GLU:OE2  | 2.21                     | 0.71              |
| 1:I:64:LEU:HD23  | 1:I:64:LEU:O     | 1.90                     | 0.71              |
| 1:J:64:LEU:HD23  | 1:J:64:LEU:O     | 1.90                     | 0.71              |
| 1:A:64:LEU:O     | 1:A:64:LEU:HD23  | 1.91                     | 0.71              |
| 1:K:64:LEU:O     | 1:K:64:LEU:HD23  | 1.91                     | 0.71              |
| 1:P:3:GLY:HA3    | 1:P:65:LEU:HD22  | 1.73                     | 0.71              |
| 1:V:64:LEU:HD23  | 1:V:64:LEU:O     | 1.90                     | 0.70              |
| 1:E:8:ILE:HG23   | 1:E:62:ILE:CD1   | 2.17                     | 0.70              |
| 1:O:54:HIS:HE1   | 1:O:127:GLU:OE2  | 1.73                     | 0.70              |
| 1:Q:8:ILE:HG23   | 1:Q:62:ILE:CD1   | 2.21                     | 0.70              |
| 1:C:157:THR:HG22 | 1:C:159:PRO:HD3  | 1.73                     | 0.70              |
| 1:J:8:ILE:HG23   | 1:J:62:ILE:CD1   | 2.19                     | 0.70              |
| 1:C:64:LEU:HD23  | 1:C:64:LEU:O     | 1.91                     | 0.70              |
| 1:D:64:LEU:O     | 1:D:64:LEU:HD23  | 1.92                     | 0.70              |
| 1:M:8:ILE:HG23   | 1:M:62:ILE:CD1   | 2.16                     | 0.70              |
| 1:N:64:LEU:HD23  | 1:N:64:LEU:O     | 1.91                     | 0.70              |
| 1:E:64:LEU:HD23  | 1:E:64:LEU:O     | 1.92                     | 0.70              |
| 1:U:64:LEU:O     | 1:U:64:LEU:HD23  | 1.91                     | 0.70              |
| 1:H:64:LEU:O     | 1:H:64:LEU:HD23  | 1.92                     | 0.70              |
| 1:T:64:LEU:HD23  | 1:T:64:LEU:O     | 1.91                     | 0.70              |
| 1:X:64:LEU:HD23  | 1:X:64:LEU:O     | 1.91                     | 0.70              |
| 1:F:64:LEU:O     | 1:F:64:LEU:HD23  | 1.92                     | 0.70              |
| 1:V:8:ILE:HG23   | 1:V:62:ILE:CD1   | 2.22                     | 0.70              |
| 1:B:8:ILE:HG23   | 1:B:62:ILE:CD1   | 2.18                     | 0.70              |
| 1:O:8:ILE:HG23   | 1:O:62:ILE:CD1   | 2.21                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:8:ILE:HG23   | 1:K:62:ILE:CD1   | 2.18                     | 0.70              |
| 1:W:64:LEU:O     | 1:W:64:LEU:HD23  | 1.92                     | 0.69              |
| 1:N:8:ILE:HG23   | 1:N:62:ILE:CD1   | 2.18                     | 0.69              |
| 1:W:8:ILE:HG23   | 1:W:62:ILE:CD1   | 2.17                     | 0.69              |
| 3:N:201:HEM:HBB2 | 3:N:201:HEM:HMB2 | 1.75                     | 0.69              |
| 1:R:64:LEU:O     | 1:R:64:LEU:HD23  | 1.92                     | 0.69              |
| 1:S:64:LEU:HD23  | 1:S:64:LEU:O     | 1.92                     | 0.69              |
| 1:L:8:ILE:HG23   | 1:L:62:ILE:CD1   | 2.20                     | 0.69              |
| 3:V:202:HEM:HBB2 | 3:V:202:HEM:HMB2 | 1.74                     | 0.69              |
| 1:C:52:MET:HB3   | 3:C:202:HEM:HBA1 | 1.75                     | 0.69              |
| 1:T:39:LYS:NZ    | 1:T:155:GLU:OE2  | 2.18                     | 0.69              |
| 1:G:8:ILE:HG23   | 1:G:62:ILE:CD1   | 2.22                     | 0.68              |
| 1:A:8:ILE:HG23   | 1:A:62:ILE:CD1   | 2.22                     | 0.68              |
| 1:M:64:LEU:O     | 1:M:64:LEU:HD23  | 1.92                     | 0.68              |
| 1:I:8:ILE:HG23   | 1:I:62:ILE:CD1   | 2.22                     | 0.68              |
| 1:J:39:LYS:NZ    | 1:J:155:GLU:OE2  | 2.18                     | 0.68              |
| 1:L:157:THR:HG22 | 1:L:159:PRO:HG3  | 1.74                     | 0.68              |
| 1:R:8:ILE:HG23   | 1:R:62:ILE:CD1   | 2.17                     | 0.67              |
| 1:F:8:ILE:HG23   | 1:F:62:ILE:CD1   | 2.18                     | 0.67              |
| 1:U:8:ILE:HG23   | 1:U:62:ILE:CD1   | 2.18                     | 0.67              |
| 1:I:52:MET:HE1   | 3:S:202:HEM:NB   | 2.09                     | 0.67              |
| 3:S:202:HEM:HMB2 | 3:S:202:HEM:HBB2 | 1.74                     | 0.67              |
| 3:K:301:HEM:HHA  | 3:K:301:HEM:CBD  | 2.25                     | 0.66              |
| 3:O:202:HEM:HMA1 | 3:O:202:HEM:HBA1 | 1.76                     | 0.66              |
| 1:X:8:ILE:HG23   | 1:X:62:ILE:CD1   | 2.18                     | 0.66              |
| 1:K:53:ARG:HA    | 3:K:301:HEM:CBB  | 2.26                     | 0.66              |
| 3:K:301:HEM:HHA  | 3:K:301:HEM:CBA  | 2.26                     | 0.66              |
| 1:E:39:LYS:NZ    | 1:E:155:GLU:OE2  | 2.17                     | 0.66              |
| 3:C:202:HEM:HBB2 | 3:C:202:HEM:HMB1 | 1.77                     | 0.66              |
| 1:T:8:ILE:HG23   | 1:T:62:ILE:CD1   | 2.19                     | 0.65              |
| 1:L:3:GLY:HA3    | 1:L:65:LEU:HD22  | 1.77                     | 0.64              |
| 1:S:8:ILE:HG23   | 1:S:62:ILE:CD1   | 2.17                     | 0.64              |
| 3:L:202:HEM:HBA1 | 3:L:202:HEM:HMA1 | 1.79                     | 0.64              |
| 1:Q:4:ASP:HB3    | 1:Q:5:PRO:HD2    | 1.80                     | 0.64              |
| 3:Q:202:HEM:HBB2 | 3:Q:202:HEM:HMB2 | 1.79                     | 0.64              |
| 1:B:3:GLY:CA     | 1:B:65:LEU:HD22  | 2.28                     | 0.64              |
| 1:L:56:GLU:O     | 1:L:59:THR:HG22  | 1.98                     | 0.63              |
| 1:T:82:SER:OG    | 1:T:83:VAL:N     | 2.31                     | 0.63              |
| 3:U:201:HEM:HMC2 | 3:U:201:HEM:HBC2 | 1.79                     | 0.63              |
| 1:A:82:SER:OG    | 1:A:83:VAL:N     | 2.32                     | 0.63              |
| 3:C:202:HEM:HBC2 | 3:C:202:HEM:HMC1 | 1.81                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:72:GLN:O     | 1:J:72:GLN:HG3   | 2.00                     | 0.62              |
| 1:P:3:GLY:CA     | 1:P:65:LEU:HD22  | 2.28                     | 0.62              |
| 3:S:202:HEM:HMC2 | 3:S:202:HEM:HBC2 | 1.80                     | 0.62              |
| 1:U:51:GLU:OE1   | 1:U:54:HIS:HD2   | 1.82                     | 0.62              |
| 3:A:202:HEM:HBC2 | 3:A:202:HEM:HMC2 | 1.82                     | 0.62              |
| 1:C:128:GLU:O    | 1:C:131:ILE:HG22 | 1.98                     | 0.62              |
| 3:N:201:HEM:HBB2 | 3:N:201:HEM:CMB  | 2.30                     | 0.61              |
| 3:O:202:HEM:HBC2 | 3:O:202:HEM:CMC  | 2.30                     | 0.61              |
| 1:A:72:GLN:HG3   | 1:A:72:GLN:O     | 2.00                     | 0.61              |
| 3:F:202:HEM:HBC2 | 3:F:202:HEM:CMC  | 2.31                     | 0.61              |
| 1:O:128:GLU:O    | 1:O:131:ILE:HG22 | 2.01                     | 0.61              |
| 1:L:3:GLY:CA     | 1:L:65:LEU:HD22  | 2.31                     | 0.61              |
| 1:C:22:ILE:CD1   | 1:C:52:MET:HA    | 2.27                     | 0.60              |
| 1:F:101:LEU:CD1  | 1:F:123:ILE:HG22 | 2.31                     | 0.60              |
| 1:X:128:GLU:O    | 1:X:131:ILE:HG22 | 2.01                     | 0.60              |
| 1:Q:101:LEU:HD11 | 1:Q:123:ILE:CG2  | 2.32                     | 0.60              |
| 1:L:96:GLU:OE2   | 1:L:96:GLU:HA    | 2.02                     | 0.60              |
| 1:N:101:LEU:CD1  | 1:N:123:ILE:HG22 | 2.32                     | 0.60              |
| 1:O:22:ILE:HD11  | 1:O:52:MET:HA    | 1.82                     | 0.60              |
| 1:Q:4:ASP:O      | 1:Q:8:ILE:HG13   | 2.02                     | 0.60              |
| 1:N:52:MET:HE3   | 3:N:201:HEM:C4B  | 2.15                     | 0.59              |
| 1:E:101:LEU:HD11 | 1:E:123:ILE:CG2  | 2.32                     | 0.59              |
| 1:Q:96:GLU:OE2   | 1:Q:96:GLU:HA    | 2.03                     | 0.59              |
| 1:Q:101:LEU:CD1  | 1:Q:123:ILE:HG22 | 2.31                     | 0.59              |
| 1:D:101:LEU:CD1  | 1:D:123:ILE:HG22 | 2.32                     | 0.59              |
| 3:A:202:HEM:HBD2 | 3:A:202:HEM:HMD2 | 1.85                     | 0.59              |
| 1:U:156:GLN:O    | 1:U:156:GLN:HG3  | 2.02                     | 0.59              |
| 1:E:101:LEU:CD1  | 1:E:123:ILE:HG22 | 2.32                     | 0.59              |
| 1:O:82:SER:OG    | 1:O:83:VAL:N     | 2.32                     | 0.59              |
| 1:F:25:TYR:HE2   | 1:F:130:HIS:HE1  | 1.49                     | 0.58              |
| 1:J:101:LEU:HD11 | 1:J:123:ILE:CG2  | 2.32                     | 0.58              |
| 1:S:101:LEU:HD11 | 1:S:123:ILE:CG2  | 2.31                     | 0.58              |
| 1:R:101:LEU:HD11 | 1:R:123:ILE:CG2  | 2.31                     | 0.58              |
| 3:F:202:HEM:HHA  | 3:F:202:HEM:O1A  | 2.03                     | 0.58              |
| 1:A:101:LEU:HD11 | 1:A:123:ILE:CG2  | 2.32                     | 0.58              |
| 3:A:202:HEM:HMA2 | 3:A:202:HEM:HBA2 | 1.86                     | 0.58              |
| 1:C:96:GLU:OE2   | 1:C:96:GLU:HA    | 2.03                     | 0.58              |
| 1:I:101:LEU:HD11 | 1:I:123:ILE:CG2  | 2.33                     | 0.58              |
| 1:I:101:LEU:CD1  | 1:I:123:ILE:HG22 | 2.32                     | 0.58              |
| 3:K:301:HEM:HHA  | 3:K:301:HEM:HBD2 | 1.84                     | 0.58              |
| 1:B:101:LEU:CD1  | 1:B:123:ILE:HG22 | 2.32                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:101:LEU:HD11 | 1:T:123:ILE:CG2  | 2.32                     | 0.58              |
| 1:B:101:LEU:HD11 | 1:B:123:ILE:CG2  | 2.33                     | 0.58              |
| 1:K:128:GLU:O    | 1:K:131:ILE:HG22 | 2.03                     | 0.58              |
| 1:M:96:GLU:HA    | 1:M:96:GLU:OE2   | 2.04                     | 0.58              |
| 1:H:101:LEU:HD11 | 1:H:123:ILE:CG2  | 2.32                     | 0.58              |
| 1:S:155:GLU:OE2  | 1:S:155:GLU:HA   | 2.03                     | 0.58              |
| 1:T:72:GLN:O     | 1:T:72:GLN:HG3   | 2.02                     | 0.58              |
| 1:V:101:LEU:CD1  | 1:V:123:ILE:HG22 | 2.32                     | 0.58              |
| 3:V:202:HEM:HBB2 | 3:V:202:HEM:CMB  | 2.33                     | 0.58              |
| 1:F:155:GLU:OE2  | 1:F:155:GLU:HA   | 2.04                     | 0.57              |
| 1:L:82:SER:OG    | 1:L:83:VAL:N     | 2.37                     | 0.57              |
| 1:K:52:MET:HE1   | 3:K:301:HEM:C4D  | 2.39                     | 0.57              |
| 1:X:155:GLU:OE1  | 1:X:155:GLU:HA   | 2.04                     | 0.57              |
| 1:F:101:LEU:HD11 | 1:F:123:ILE:CG2  | 2.32                     | 0.57              |
| 3:L:202:HEM:HMB2 | 3:L:202:HEM:HBB2 | 1.85                     | 0.57              |
| 1:O:72:GLN:O     | 1:O:72:GLN:HG3   | 2.04                     | 0.57              |
| 1:M:101:LEU:CD1  | 1:M:123:ILE:HG22 | 2.33                     | 0.57              |
| 1:U:82:SER:OG    | 1:U:83:VAL:N     | 2.37                     | 0.57              |
| 3:U:201:HEM:HMB2 | 3:U:201:HEM:HBB2 | 1.85                     | 0.57              |
| 1:D:4:ASP:HB3    | 1:D:5:PRO:HD2    | 1.87                     | 0.57              |
| 1:S:4:ASP:HB3    | 1:S:5:PRO:HD2    | 1.87                     | 0.57              |
| 1:A:52:MET:HE1   | 3:A:202:HEM:C4A  | 2.40                     | 0.57              |
| 1:N:101:LEU:HD11 | 1:N:123:ILE:CG2  | 2.32                     | 0.57              |
| 1:R:101:LEU:CD1  | 1:R:123:ILE:HG22 | 2.32                     | 0.57              |
| 1:T:25:TYR:HE2   | 1:T:130:HIS:HE1  | 1.51                     | 0.57              |
| 1:U:128:GLU:O    | 1:U:131:ILE:HG22 | 2.05                     | 0.57              |
| 1:K:53:ARG:HA    | 3:K:301:HEM:HBB1 | 1.85                     | 0.56              |
| 3:X:201:HEM:HHB  | 3:X:201:HEM:CBA  | 2.35                     | 0.56              |
| 1:L:101:LEU:CD1  | 1:L:123:ILE:HG22 | 2.32                     | 0.56              |
| 1:B:156:GLN:O    | 1:B:156:GLN:HG3  | 2.05                     | 0.56              |
| 1:C:4:ASP:HB3    | 1:C:5:PRO:HD2    | 1.87                     | 0.56              |
| 1:H:96:GLU:HA    | 1:H:96:GLU:OE2   | 2.05                     | 0.56              |
| 1:U:22:ILE:CD1   | 1:U:52:MET:HA    | 2.28                     | 0.56              |
| 1:W:4:ASP:HB3    | 1:W:5:PRO:HD2    | 1.87                     | 0.56              |
| 1:K:101:LEU:HD11 | 1:K:123:ILE:CG2  | 2.34                     | 0.56              |
| 1:P:101:LEU:CD1  | 1:P:123:ILE:HG22 | 2.33                     | 0.56              |
| 1:L:4:ASP:HB3    | 1:L:5:PRO:HD2    | 1.88                     | 0.56              |
| 1:W:101:LEU:CD1  | 1:W:123:ILE:HG22 | 2.32                     | 0.56              |
| 1:S:4:ASP:O      | 1:S:8:ILE:HG13   | 2.06                     | 0.56              |
| 1:U:155:GLU:OE1  | 1:U:155:GLU:HA   | 2.06                     | 0.56              |
| 3:V:202:HEM:HBC2 | 3:V:202:HEM:CMC  | 2.36                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:101:LEU:HD11 | 1:W:123:ILE:CG2  | 2.32                     | 0.56              |
| 1:A:52:MET:HE1   | 3:A:202:HEM:NA   | 2.20                     | 0.56              |
| 1:C:4:ASP:O      | 1:C:8:ILE:HG13   | 2.06                     | 0.56              |
| 3:K:301:HEM:HBC2 | 3:K:301:HEM:CMC  | 2.36                     | 0.56              |
| 1:O:32:GLN:OE1   | 1:O:40:LEU:HB3   | 2.05                     | 0.56              |
| 1:P:101:LEU:HD11 | 1:P:123:ILE:CG2  | 2.33                     | 0.56              |
| 1:V:128:GLU:O    | 1:V:131:ILE:HG22 | 2.06                     | 0.56              |
| 1:E:96:GLU:OE2   | 1:E:96:GLU:HA    | 2.05                     | 0.55              |
| 1:G:101:LEU:CD1  | 1:G:123:ILE:HG22 | 2.33                     | 0.55              |
| 1:H:73:ARG:HG2   | 1:H:74:LEU:N     | 2.21                     | 0.55              |
| 1:K:156:GLN:O    | 1:K:156:GLN:HG3  | 2.06                     | 0.55              |
| 1:L:101:LEU:HD11 | 1:L:123:ILE:CG2  | 2.32                     | 0.55              |
| 1:C:101:LEU:HD11 | 1:C:123:ILE:CG2  | 2.34                     | 0.55              |
| 3:Q:202:HEM:HBC2 | 3:Q:202:HEM:CMC  | 2.36                     | 0.55              |
| 1:P:156:GLN:O    | 1:P:156:GLN:HG3  | 2.04                     | 0.55              |
| 1:T:52:MET:HE1   | 3:U:201:HEM:NC   | 2.22                     | 0.55              |
| 1:Q:1:MET:HA     | 1:Q:1:MET:CE     | 2.32                     | 0.55              |
| 1:L:128:GLU:O    | 1:L:131:ILE:HG22 | 2.06                     | 0.55              |
| 1:M:101:LEU:HD11 | 1:M:123:ILE:CG2  | 2.31                     | 0.55              |
| 1:E:73:ARG:HG2   | 1:E:74:LEU:N     | 2.21                     | 0.55              |
| 1:H:101:LEU:CD1  | 1:H:123:ILE:HG22 | 2.32                     | 0.55              |
| 1:R:4:ASP:HB3    | 1:R:5:PRO:HD2    | 1.89                     | 0.55              |
| 1:S:82:SER:OG    | 1:S:83:VAL:N     | 2.40                     | 0.55              |
| 3:U:201:HEM:HBC2 | 3:U:201:HEM:CMC  | 2.36                     | 0.55              |
| 1:I:4:ASP:HB3    | 1:I:5:PRO:HD2    | 1.89                     | 0.55              |
| 1:O:123:ILE:O    | 1:O:127:GLU:HG2  | 2.05                     | 0.55              |
| 1:E:128:GLU:CD   | 1:S:1:MET:HE1    | 2.32                     | 0.55              |
| 1:V:101:LEU:HD11 | 1:V:123:ILE:CG2  | 2.32                     | 0.55              |
| 1:D:101:LEU:HD11 | 1:D:123:ILE:CG2  | 2.31                     | 0.54              |
| 1:J:82:SER:OG    | 1:J:83:VAL:N     | 2.40                     | 0.54              |
| 1:K:82:SER:OG    | 1:K:83:VAL:N     | 2.39                     | 0.54              |
| 1:Q:25:TYR:HE2   | 1:Q:130:HIS:HE1  | 1.54                     | 0.54              |
| 3:K:301:HEM:HHA  | 3:K:301:HEM:HBA1 | 1.89                     | 0.54              |
| 1:C:157:THR:HG22 | 1:C:159:PRO:CD   | 2.37                     | 0.54              |
| 1:U:4:ASP:HB3    | 1:U:5:PRO:HD2    | 1.89                     | 0.54              |
| 3:U:201:HEM:CBD  | 3:U:201:HEM:HHA  | 2.36                     | 0.54              |
| 1:V:82:SER:OG    | 1:V:83:VAL:N     | 2.40                     | 0.54              |
| 1:X:101:LEU:HD11 | 1:X:123:ILE:CG2  | 2.34                     | 0.54              |
| 1:A:128:GLU:O    | 1:A:131:ILE:HG22 | 2.08                     | 0.54              |
| 1:F:4:ASP:HB3    | 1:F:5:PRO:HD2    | 1.89                     | 0.54              |
| 1:M:82:SER:OG    | 1:M:83:VAL:N     | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:16:THR:OG1   | 1:B:73:ARG:HD3   | 2.08                     | 0.54              |
| 1:C:82:SER:OG    | 1:C:83:VAL:N     | 2.40                     | 0.54              |
| 1:S:101:LEU:CD1  | 1:S:123:ILE:HG22 | 2.31                     | 0.54              |
| 1:W:82:SER:OG    | 1:W:83:VAL:N     | 2.40                     | 0.54              |
| 1:C:101:LEU:CD1  | 1:C:123:ILE:HG22 | 2.34                     | 0.54              |
| 1:F:148:LEU:HD12 | 1:F:148:LEU:O    | 2.08                     | 0.54              |
| 1:S:39:LYS:NZ    | 1:S:155:GLU:OE1  | 2.37                     | 0.54              |
| 1:V:4:ASP:HB3    | 1:V:5:PRO:HD2    | 1.90                     | 0.54              |
| 1:J:101:LEU:CD1  | 1:J:123:ILE:HG22 | 2.32                     | 0.54              |
| 1:L:4:ASP:O      | 1:L:8:ILE:HG13   | 2.07                     | 0.54              |
| 1:R:25:TYR:CE2   | 1:R:130:HIS:HE1  | 2.25                     | 0.54              |
| 1:V:72:GLN:O     | 1:V:72:GLN:HG3   | 2.08                     | 0.54              |
| 1:V:157:THR:CG2  | 1:V:159:PRO:HG3  | 2.37                     | 0.54              |
| 1:G:101:LEU:HD11 | 1:G:123:ILE:CG2  | 2.33                     | 0.54              |
| 1:M:72:GLN:HG3   | 1:M:72:GLN:O     | 2.08                     | 0.54              |
| 1:N:128:GLU:O    | 1:N:131:ILE:HG22 | 2.08                     | 0.54              |
| 1:V:4:ASP:O      | 1:V:8:ILE:HG13   | 2.07                     | 0.54              |
| 1:W:25:TYR:HE2   | 1:W:130:HIS:HE1  | 1.56                     | 0.54              |
| 1:X:148:LEU:HD12 | 1:X:148:LEU:O    | 2.08                     | 0.54              |
| 1:J:51:GLU:O     | 1:J:54:HIS:HB2   | 2.08                     | 0.53              |
| 1:N:72:GLN:O     | 1:N:72:GLN:HG3   | 2.08                     | 0.53              |
| 1:P:128:GLU:O    | 1:P:131:ILE:HG22 | 2.08                     | 0.53              |
| 1:E:128:GLU:O    | 1:E:131:ILE:HG22 | 2.08                     | 0.53              |
| 1:Q:128:GLU:O    | 1:Q:131:ILE:HG22 | 2.07                     | 0.53              |
| 1:R:148:LEU:HD12 | 1:R:148:LEU:O    | 2.08                     | 0.53              |
| 1:T:101:LEU:CD1  | 1:T:123:ILE:HG22 | 2.32                     | 0.53              |
| 1:W:72:GLN:HG3   | 1:W:72:GLN:O     | 2.08                     | 0.53              |
| 1:W:148:LEU:HD12 | 1:W:148:LEU:O    | 2.08                     | 0.53              |
| 1:M:148:LEU:HD12 | 1:M:148:LEU:O    | 2.08                     | 0.53              |
| 1:P:82:SER:OG    | 1:P:83:VAL:N     | 2.39                     | 0.53              |
| 1:P:155:GLU:OE2  | 1:P:155:GLU:HA   | 2.07                     | 0.53              |
| 1:Q:47:GLU:OE2   | 1:Q:130:HIS:CG   | 2.61                     | 0.53              |
| 1:W:4:ASP:O      | 1:W:8:ILE:HG13   | 2.08                     | 0.53              |
| 1:M:25:TYR:CE2   | 1:M:130:HIS:HE1  | 2.27                     | 0.53              |
| 1:N:4:ASP:HB3    | 1:N:5:PRO:HD2    | 1.89                     | 0.53              |
| 1:N:148:LEU:HD12 | 1:N:148:LEU:O    | 2.09                     | 0.53              |
| 1:P:16:THR:OG1   | 1:P:73:ARG:HD3   | 2.08                     | 0.53              |
| 1:Q:82:SER:OG    | 1:Q:83:VAL:N     | 2.40                     | 0.53              |
| 1:U:16:THR:OG1   | 1:U:73:ARG:HD3   | 2.08                     | 0.53              |
| 1:U:101:LEU:CD1  | 1:U:123:ILE:HG22 | 2.34                     | 0.53              |
| 1:A:101:LEU:CD1  | 1:A:123:ILE:HG22 | 2.32                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:148:LEU:HD12 | 1:E:148:LEU:O    | 2.09                     | 0.53              |
| 1:G:148:LEU:HD12 | 1:G:148:LEU:O    | 2.09                     | 0.53              |
| 1:W:25:TYR:CE2   | 1:W:130:HIS:HE1  | 2.26                     | 0.53              |
| 1:A:148:LEU:HD12 | 1:A:148:LEU:O    | 2.09                     | 0.53              |
| 3:U:201:HEM:CBA  | 3:U:201:HEM:HMA2 | 2.39                     | 0.53              |
| 1:V:148:LEU:HD12 | 1:V:148:LEU:O    | 2.09                     | 0.53              |
| 1:H:128:GLU:O    | 1:H:131:ILE:HG22 | 2.08                     | 0.53              |
| 1:I:25:TYR:CE2   | 1:I:130:HIS:HE1  | 2.27                     | 0.53              |
| 1:I:25:TYR:HE2   | 1:I:130:HIS:HE1  | 1.57                     | 0.53              |
| 1:R:25:TYR:HE2   | 1:R:130:HIS:HE1  | 1.57                     | 0.53              |
| 3:C:202:HEM:HBB2 | 3:C:202:HEM:CMB  | 2.38                     | 0.53              |
| 1:G:128:GLU:O    | 1:G:131:ILE:HG22 | 2.09                     | 0.53              |
| 1:J:148:LEU:O    | 1:J:148:LEU:HD12 | 2.09                     | 0.53              |
| 1:O:101:LEU:HD11 | 1:O:123:ILE:CG2  | 2.37                     | 0.53              |
| 1:Q:157:THR:HG22 | 1:Q:159:PRO:CG   | 2.39                     | 0.53              |
| 1:X:72:GLN:O     | 1:X:72:GLN:HG3   | 2.08                     | 0.53              |
| 1:D:4:ASP:O      | 1:D:8:ILE:HG13   | 2.08                     | 0.53              |
| 1:E:25:TYR:HE2   | 1:E:130:HIS:HE1  | 1.57                     | 0.53              |
| 1:N:25:TYR:CE2   | 1:N:130:HIS:HE1  | 2.27                     | 0.53              |
| 1:S:148:LEU:HD12 | 1:S:148:LEU:O    | 2.09                     | 0.53              |
| 1:D:128:GLU:O    | 1:D:131:ILE:HG22 | 2.09                     | 0.52              |
| 1:D:148:LEU:HD12 | 1:D:148:LEU:O    | 2.08                     | 0.52              |
| 1:F:72:GLN:O     | 1:F:72:GLN:HG3   | 2.08                     | 0.52              |
| 1:F:128:GLU:O    | 1:F:131:ILE:HG22 | 2.09                     | 0.52              |
| 1:E:73:ARG:HG2   | 1:E:74:LEU:H     | 1.74                     | 0.52              |
| 1:H:25:TYR:HE2   | 1:H:130:HIS:HE1  | 1.57                     | 0.52              |
| 1:H:82:SER:OG    | 1:H:83:VAL:N     | 2.41                     | 0.52              |
| 1:K:52:MET:HE1   | 3:K:301:HEM:CHA  | 2.39                     | 0.52              |
| 3:L:202:HEM:HMA1 | 3:L:202:HEM:CBA  | 2.40                     | 0.52              |
| 1:Q:157:THR:CG2  | 1:Q:159:PRO:HG3  | 2.37                     | 0.52              |
| 1:C:148:LEU:O    | 1:C:148:LEU:HD12 | 2.09                     | 0.52              |
| 1:D:82:SER:OG    | 1:D:83:VAL:N     | 2.40                     | 0.52              |
| 1:V:157:THR:HG22 | 1:V:159:PRO:CG   | 2.39                     | 0.52              |
| 1:B:82:SER:OG    | 1:B:83:VAL:N     | 2.40                     | 0.52              |
| 1:C:72:GLN:O     | 1:C:72:GLN:HG3   | 2.08                     | 0.52              |
| 1:F:82:SER:OG    | 1:F:83:VAL:N     | 2.41                     | 0.52              |
| 1:L:148:LEU:HD12 | 1:L:148:LEU:O    | 2.09                     | 0.52              |
| 1:R:72:GLN:HG3   | 1:R:72:GLN:O     | 2.08                     | 0.52              |
| 1:X:4:ASP:HB3    | 1:X:5:PRO:HD2    | 1.89                     | 0.52              |
| 1:H:25:TYR:CE2   | 1:H:130:HIS:HE1  | 2.27                     | 0.52              |
| 1:I:82:SER:OG    | 1:I:83:VAL:N     | 2.41                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:16:THR:OG1   | 1:K:73:ARG:HD3   | 2.09                     | 0.52              |
| 1:S:25:TYR:CE2   | 1:S:130:HIS:HE1  | 2.27                     | 0.52              |
| 1:W:128:GLU:O    | 1:W:131:ILE:HG22 | 2.09                     | 0.52              |
| 1:C:1:MET:HA     | 1:C:1:MET:CE     | 2.37                     | 0.52              |
| 1:D:72:GLN:O     | 1:D:72:GLN:HG3   | 2.08                     | 0.52              |
| 1:J:128:GLU:O    | 1:J:131:ILE:HG22 | 2.09                     | 0.52              |
| 1:L:72:GLN:O     | 1:L:72:GLN:HG3   | 2.09                     | 0.52              |
| 1:L:157:THR:CG2  | 1:L:159:PRO:HG3  | 2.40                     | 0.52              |
| 1:M:128:GLU:O    | 1:M:131:ILE:HG22 | 2.09                     | 0.52              |
| 1:X:25:TYR:CE2   | 1:X:130:HIS:HE1  | 2.27                     | 0.52              |
| 1:B:128:GLU:O    | 1:B:131:ILE:HG22 | 2.09                     | 0.52              |
| 1:B:155:GLU:OE1  | 1:B:155:GLU:HA   | 2.07                     | 0.52              |
| 1:E:25:TYR:CE2   | 1:E:130:HIS:HE1  | 2.26                     | 0.52              |
| 1:I:128:GLU:O    | 1:I:131:ILE:HG22 | 2.09                     | 0.52              |
| 1:M:4:ASP:HB3    | 1:M:5:PRO:HD2    | 1.92                     | 0.52              |
| 1:N:82:SER:OG    | 1:N:83:VAL:N     | 2.40                     | 0.52              |
| 1:R:82:SER:OG    | 1:R:83:VAL:N     | 2.41                     | 0.52              |
| 1:N:4:ASP:O      | 1:N:8:ILE:HG13   | 2.10                     | 0.52              |
| 1:Q:72:GLN:O     | 1:Q:72:GLN:HG3   | 2.08                     | 0.52              |
| 1:S:72:GLN:O     | 1:S:72:GLN:HG3   | 2.08                     | 0.52              |
| 1:U:25:TYR:CE2   | 1:U:130:HIS:HE1  | 2.28                     | 0.52              |
| 1:H:73:ARG:HG2   | 1:H:74:LEU:H     | 1.74                     | 0.52              |
| 1:X:4:ASP:O      | 1:X:8:ILE:HG13   | 2.10                     | 0.52              |
| 1:X:101:LEU:CD1  | 1:X:123:ILE:HG22 | 2.34                     | 0.52              |
| 3:A:202:HEM:HBC2 | 3:A:202:HEM:CMC  | 2.40                     | 0.52              |
| 1:D:25:TYR:CE2   | 1:D:130:HIS:HE1  | 2.28                     | 0.52              |
| 1:I:4:ASP:O      | 1:I:8:ILE:HG13   | 2.09                     | 0.52              |
| 1:M:4:ASP:O      | 1:M:8:ILE:HG13   | 2.09                     | 0.52              |
| 1:U:101:LEU:HD11 | 1:U:123:ILE:CG2  | 2.34                     | 0.52              |
| 1:O:25:TYR:CE2   | 1:O:130:HIS:HE1  | 2.27                     | 0.51              |
| 3:U:201:HEM:HBB2 | 3:U:201:HEM:CMB  | 2.40                     | 0.51              |
| 1:C:40:LEU:HD13  | 1:C:153:VAL:HG21 | 1.92                     | 0.51              |
| 1:F:25:TYR:CE2   | 1:F:130:HIS:HE1  | 2.28                     | 0.51              |
| 1:K:101:LEU:CD1  | 1:K:123:ILE:HG22 | 2.34                     | 0.51              |
| 3:K:301:HEM:HHA  | 3:K:301:HEM:HBA2 | 1.93                     | 0.51              |
| 1:R:4:ASP:O      | 1:R:8:ILE:HG13   | 2.10                     | 0.51              |
| 1:R:128:GLU:O    | 1:R:131:ILE:HG22 | 2.09                     | 0.51              |
| 1:Q:148:LEU:HD12 | 1:Q:148:LEU:O    | 2.09                     | 0.51              |
| 1:V:25:TYR:CE2   | 1:V:130:HIS:HE1  | 2.28                     | 0.51              |
| 1:B:25:TYR:CE2   | 1:B:130:HIS:HE1  | 2.28                     | 0.51              |
| 1:G:4:ASP:O      | 1:G:8:ILE:HG13   | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:73:ARG:HG2   | 1:J:74:LEU:N     | 2.25                     | 0.51              |
| 1:A:73:ARG:HG2   | 1:A:74:LEU:N     | 2.25                     | 0.51              |
| 1:C:25:TYR:CE2   | 1:C:130:HIS:HE1  | 2.27                     | 0.51              |
| 1:F:4:ASP:O      | 1:F:8:ILE:HG13   | 2.10                     | 0.51              |
| 1:M:25:TYR:HE2   | 1:M:130:HIS:HE1  | 1.59                     | 0.51              |
| 1:V:25:TYR:HE2   | 1:V:130:HIS:HE1  | 1.58                     | 0.51              |
| 1:J:25:TYR:CE2   | 1:J:130:HIS:HE1  | 2.28                     | 0.51              |
| 3:Q:202:HEM:HBB2 | 3:Q:202:HEM:CMB  | 2.39                     | 0.51              |
| 1:C:73:ARG:C     | 1:C:74:LEU:HD23  | 2.36                     | 0.51              |
| 1:F:39:LYS:NZ    | 1:F:155:GLU:OE1  | 2.33                     | 0.51              |
| 1:K:72:GLN:HG3   | 1:K:72:GLN:O     | 2.11                     | 0.51              |
| 1:G:25:TYR:CE2   | 1:G:130:HIS:HE1  | 2.29                     | 0.50              |
| 1:S:128:GLU:O    | 1:S:131:ILE:HG22 | 2.11                     | 0.50              |
| 1:Q:40:LEU:HD13  | 1:Q:153:VAL:HG21 | 1.92                     | 0.50              |
| 1:R:73:ARG:C     | 1:R:74:LEU:HD23  | 2.37                     | 0.50              |
| 1:F:40:LEU:HD13  | 1:F:153:VAL:HG21 | 1.92                     | 0.50              |
| 1:N:22:ILE:CD1   | 1:N:52:MET:HA    | 2.37                     | 0.50              |
| 1:N:25:TYR:HE2   | 1:N:130:HIS:HE1  | 1.59                     | 0.50              |
| 1:S:25:TYR:HE2   | 1:S:130:HIS:HE1  | 1.60                     | 0.50              |
| 1:B:25:TYR:HE2   | 1:B:130:HIS:HE1  | 1.60                     | 0.50              |
| 1:X:82:SER:OG    | 1:X:83:VAL:N     | 2.40                     | 0.50              |
| 1:L:73:ARG:C     | 1:L:74:LEU:HD23  | 2.37                     | 0.50              |
| 1:O:52:MET:SD    | 3:O:202:HEM:C4A  | 3.04                     | 0.50              |
| 1:T:25:TYR:CE2   | 1:T:130:HIS:HE1  | 2.30                     | 0.50              |
| 1:U:25:TYR:HE2   | 1:U:130:HIS:HE1  | 1.60                     | 0.50              |
| 1:W:73:ARG:C     | 1:W:74:LEU:HD23  | 2.37                     | 0.50              |
| 1:C:8:ILE:CG2    | 1:C:62:ILE:HD11  | 2.25                     | 0.50              |
| 1:K:4:ASP:O      | 1:K:8:ILE:HG13   | 2.11                     | 0.50              |
| 1:O:73:ARG:O     | 1:O:74:LEU:HG    | 2.12                     | 0.50              |
| 1:D:73:ARG:C     | 1:D:74:LEU:HD23  | 2.37                     | 0.50              |
| 1:Q:73:ARG:C     | 1:Q:74:LEU:HD23  | 2.37                     | 0.50              |
| 1:B:22:ILE:CD1   | 1:B:52:MET:HA    | 2.33                     | 0.50              |
| 1:E:83:VAL:HG23  | 1:E:84:THR:H     | 1.77                     | 0.50              |
| 1:J:25:TYR:HE2   | 1:J:130:HIS:HE1  | 1.60                     | 0.50              |
| 1:N:40:LEU:HD13  | 1:N:153:VAL:HG21 | 1.93                     | 0.49              |
| 1:V:73:ARG:C     | 1:V:74:LEU:HD23  | 2.37                     | 0.49              |
| 1:F:73:ARG:C     | 1:F:74:LEU:HD23  | 2.36                     | 0.49              |
| 1:O:49:PHE:O     | 1:O:52:MET:HB2   | 2.12                     | 0.49              |
| 1:O:101:LEU:CD1  | 1:O:123:ILE:HG22 | 2.36                     | 0.49              |
| 1:T:73:ARG:O     | 1:T:74:LEU:HG    | 2.12                     | 0.49              |
| 1:U:4:ASP:O      | 1:U:8:ILE:HG13   | 2.11                     | 0.49              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:U:22:ILE:HD11  | 1:U:52:MET:CA   | 2.31                     | 0.49              |
| 1:A:4:ASP:O      | 1:A:8:ILE:HG13  | 2.11                     | 0.49              |
| 1:K:25:TYR:CE2   | 1:K:130:HIS:HE1 | 2.31                     | 0.49              |
| 1:G:72:GLN:O     | 1:G:72:GLN:HG3  | 2.11                     | 0.49              |
| 1:S:73:ARG:C     | 1:S:74:LEU:HD23 | 2.36                     | 0.49              |
| 1:X:25:TYR:HE2   | 1:X:130:HIS:HE1 | 1.61                     | 0.49              |
| 1:X:47:GLU:HG3   | 1:X:130:HIS:NE2 | 2.27                     | 0.49              |
| 1:B:4:ASP:O      | 1:B:8:ILE:HG13  | 2.12                     | 0.49              |
| 1:E:72:GLN:O     | 1:E:72:GLN:HG3  | 2.12                     | 0.49              |
| 1:K:38:THR:O     | 1:K:41:ALA:N    | 2.46                     | 0.49              |
| 1:M:73:ARG:C     | 1:M:74:LEU:HD23 | 2.37                     | 0.49              |
| 1:U:38:THR:O     | 1:U:41:ALA:N    | 2.45                     | 0.49              |
| 1:X:38:THR:O     | 1:X:41:ALA:N    | 2.46                     | 0.49              |
| 1:K:25:TYR:HE2   | 1:K:130:HIS:HE1 | 1.61                     | 0.49              |
| 1:L:25:TYR:CE2   | 1:L:130:HIS:HE1 | 2.29                     | 0.49              |
| 1:X:22:ILE:CD1   | 1:X:52:MET:HA   | 2.34                     | 0.49              |
| 1:X:73:ARG:C     | 1:X:74:LEU:HD23 | 2.37                     | 0.49              |
| 1:D:25:TYR:HE2   | 1:D:130:HIS:HE1 | 1.60                     | 0.49              |
| 1:J:4:ASP:O      | 1:J:8:ILE:HG13  | 2.12                     | 0.49              |
| 1:L:25:TYR:HE2   | 1:L:130:HIS:HE1 | 1.60                     | 0.49              |
| 3:L:202:HEM:HBB2 | 3:L:202:HEM:CMB | 2.43                     | 0.49              |
| 1:I:83:VAL:HG23  | 1:I:84:THR:H    | 1.78                     | 0.49              |
| 1:C:25:TYR:HE2   | 1:C:130:HIS:HE1 | 1.61                     | 0.49              |
| 1:W:112:HIS:NE2  | 1:X:106:GLU:OE1 | 2.40                     | 0.49              |
| 3:C:202:HEM:HBC2 | 3:C:202:HEM:CMC | 2.44                     | 0.48              |
| 1:L:157:THR:HG22 | 1:L:159:PRO:CG  | 2.42                     | 0.48              |
| 1:P:4:ASP:O      | 1:P:8:ILE:HG13  | 2.13                     | 0.48              |
| 1:U:72:GLN:O     | 1:U:72:GLN:HG3  | 2.12                     | 0.48              |
| 1:A:4:ASP:HB3    | 1:A:5:PRO:HD2   | 1.96                     | 0.48              |
| 1:G:83:VAL:HG23  | 1:G:84:THR:H    | 1.79                     | 0.48              |
| 1:M:38:THR:O     | 1:M:41:ALA:N    | 2.47                     | 0.48              |
| 1:Q:94:GLU:OE1   | 1:Q:94:GLU:HA   | 2.13                     | 0.48              |
| 1:E:4:ASP:O      | 1:E:8:ILE:HG13  | 2.13                     | 0.48              |
| 1:K:42:LYS:HE2   | 1:K:42:LYS:HB3  | 1.60                     | 0.48              |
| 1:T:4:ASP:O      | 1:T:8:ILE:HG13  | 2.13                     | 0.48              |
| 1:W:38:THR:O     | 1:W:41:ALA:N    | 2.46                     | 0.48              |
| 1:A:32:GLN:OE1   | 1:A:40:LEU:HB3  | 2.14                     | 0.48              |
| 1:G:22:ILE:CD1   | 1:G:52:MET:HA   | 2.36                     | 0.48              |
| 1:O:4:ASP:O      | 1:O:8:ILE:HG13  | 2.13                     | 0.48              |
| 1:U:143:LYS:HG3  | 1:U:144:LEU:N   | 2.29                     | 0.48              |
| 1:B:72:GLN:O     | 1:B:72:GLN:HG3  | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:47:GLU:HG3   | 1:C:130:HIS:NE2  | 2.29                     | 0.48              |
| 3:S:202:HEM:HBC2 | 3:S:202:HEM:CMC  | 2.43                     | 0.48              |
| 1:J:158:GLN:HB3  | 1:J:162:SER:O    | 2.14                     | 0.48              |
| 1:P:38:THR:O     | 1:P:41:ALA:N     | 2.47                     | 0.48              |
| 1:V:40:LEU:HD13  | 1:V:153:VAL:HG21 | 1.95                     | 0.48              |
| 3:C:202:HEM:CHB  | 1:D:52:MET:HE2   | 2.44                     | 0.48              |
| 1:H:47:GLU:HG3   | 1:H:130:HIS:NE2  | 2.29                     | 0.48              |
| 1:P:25:TYR:CE2   | 1:P:130:HIS:HE1  | 2.31                     | 0.48              |
| 1:R:47:GLU:HG3   | 1:R:130:HIS:NE2  | 2.28                     | 0.48              |
| 1:T:32:GLN:OE1   | 1:T:40:LEU:HB3   | 2.14                     | 0.48              |
| 1:J:4:ASP:HB3    | 1:J:5:PRO:HD2    | 1.96                     | 0.47              |
| 1:G:52:MET:HE1   | 3:X:201:HEM:ND   | 2.29                     | 0.47              |
| 1:K:83:VAL:HG23  | 1:K:84:THR:N     | 2.29                     | 0.47              |
| 1:P:25:TYR:HE2   | 1:P:130:HIS:HE1  | 1.63                     | 0.47              |
| 1:P:72:GLN:O     | 1:P:72:GLN:HG3   | 2.13                     | 0.47              |
| 1:X:40:LEU:HD13  | 1:X:153:VAL:HG21 | 1.95                     | 0.47              |
| 1:A:83:VAL:HG13  | 1:A:84:THR:H     | 1.80                     | 0.47              |
| 1:D:38:THR:O     | 1:D:41:ALA:N     | 2.48                     | 0.47              |
| 1:G:25:TYR:HE2   | 1:G:130:HIS:HE1  | 1.62                     | 0.47              |
| 1:G:32:GLN:OE1   | 1:G:40:LEU:HB3   | 2.15                     | 0.47              |
| 1:L:59:THR:HA    | 1:L:62:ILE:HG22  | 1.95                     | 0.47              |
| 1:O:4:ASP:HB3    | 1:O:5:PRO:HD2    | 1.96                     | 0.47              |
| 1:O:83:VAL:HG13  | 1:O:84:THR:N     | 2.29                     | 0.47              |
| 1:Q:25:TYR:CE2   | 1:Q:130:HIS:HE1  | 2.31                     | 0.47              |
| 1:R:38:THR:O     | 1:R:41:ALA:N     | 2.48                     | 0.47              |
| 1:B:83:VAL:HG23  | 1:B:84:THR:N     | 2.29                     | 0.47              |
| 1:E:4:ASP:HB3    | 1:E:5:PRO:HD2    | 1.95                     | 0.47              |
| 1:Q:22:ILE:CD1   | 1:Q:52:MET:HA    | 2.38                     | 0.47              |
| 1:T:83:VAL:HG13  | 1:T:84:THR:H     | 1.80                     | 0.47              |
| 3:X:201:HEM:HHA  | 3:X:201:HEM:HBA2 | 1.95                     | 0.47              |
| 1:B:38:THR:O     | 1:B:41:ALA:N     | 2.47                     | 0.47              |
| 1:H:4:ASP:HB3    | 1:H:5:PRO:HD2    | 1.95                     | 0.47              |
| 1:K:22:ILE:CD1   | 1:K:52:MET:HA    | 2.34                     | 0.47              |
| 1:L:8:ILE:CG2    | 1:L:62:ILE:HD11  | 2.26                     | 0.47              |
| 1:O:83:VAL:HG13  | 1:O:84:THR:H     | 1.80                     | 0.47              |
| 1:P:42:LYS:HB3   | 1:P:42:LYS:HE2   | 1.60                     | 0.47              |
| 1:T:4:ASP:HB3    | 1:T:5:PRO:HD2    | 1.96                     | 0.47              |
| 1:T:83:VAL:HG13  | 1:T:84:THR:N     | 2.29                     | 0.47              |
| 1:X:22:ILE:HD11  | 1:X:52:MET:CA    | 2.37                     | 0.47              |
| 1:C:40:LEU:CD1   | 1:C:153:VAL:HG21 | 2.45                     | 0.47              |
| 1:H:72:GLN:O     | 1:H:72:GLN:HG3   | 2.13                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:4:ASP:HB3    | 1:P:5:PRO:HD2    | 1.96                     | 0.47              |
| 1:V:94:GLU:OE1   | 1:V:94:GLU:HA    | 2.15                     | 0.47              |
| 1:E:32:GLN:OE1   | 1:E:40:LEU:HB3   | 2.15                     | 0.47              |
| 1:N:47:GLU:HG3   | 1:N:130:HIS:NE2  | 2.30                     | 0.47              |
| 1:P:83:VAL:HG23  | 1:P:84:THR:N     | 2.30                     | 0.47              |
| 1:H:4:ASP:O      | 1:H:8:ILE:HG13   | 2.15                     | 0.46              |
| 1:K:143:LYS:HG3  | 1:K:144:LEU:N    | 2.30                     | 0.46              |
| 1:P:94:GLU:HA    | 1:P:94:GLU:OE1   | 2.15                     | 0.46              |
| 1:T:124:LEU:HD12 | 1:T:124:LEU:O    | 2.15                     | 0.46              |
| 1:A:73:ARG:HG2   | 1:A:74:LEU:H     | 1.80                     | 0.46              |
| 1:A:83:VAL:HG13  | 1:A:84:THR:N     | 2.29                     | 0.46              |
| 1:L:3:GLY:N      | 1:L:65:LEU:HD22  | 2.30                     | 0.46              |
| 1:O:143:LYS:HG3  | 1:O:144:LEU:N    | 2.31                     | 0.46              |
| 1:H:14:GLN:OE1   | 1:H:14:GLN:HA    | 2.16                     | 0.46              |
| 1:H:83:VAL:HG23  | 1:H:84:THR:H     | 1.81                     | 0.46              |
| 1:I:32:GLN:OE1   | 1:I:40:LEU:HB3   | 2.15                     | 0.46              |
| 1:J:32:GLN:OE1   | 1:J:40:LEU:HB3   | 2.14                     | 0.46              |
| 1:K:4:ASP:HB3    | 1:K:5:PRO:HD2    | 1.96                     | 0.46              |
| 1:U:40:LEU:HD13  | 1:U:153:VAL:HG21 | 1.98                     | 0.46              |
| 1:B:4:ASP:HB3    | 1:B:5:PRO:HD2    | 1.96                     | 0.46              |
| 1:L:14:GLN:HA    | 1:L:14:GLN:OE1   | 2.16                     | 0.46              |
| 1:O:25:TYR:HE2   | 1:O:130:HIS:HE1  | 1.64                     | 0.46              |
| 1:S:14:GLN:HA    | 1:S:14:GLN:OE1   | 2.16                     | 0.46              |
| 1:S:47:GLU:HG3   | 1:S:130:HIS:NE2  | 2.30                     | 0.46              |
| 1:U:83:VAL:HG23  | 1:U:84:THR:N     | 2.30                     | 0.46              |
| 1:V:8:ILE:CG2    | 1:V:62:ILE:HD11  | 2.34                     | 0.46              |
| 1:B:42:LYS:HB3   | 1:B:42:LYS:HE2   | 1.60                     | 0.46              |
| 1:G:14:GLN:OE1   | 1:G:14:GLN:HA    | 2.16                     | 0.46              |
| 1:J:14:GLN:HA    | 1:J:14:GLN:OE1   | 2.16                     | 0.46              |
| 1:J:73:ARG:HG2   | 1:J:74:LEU:H     | 1.80                     | 0.46              |
| 1:S:52:MET:HE3   | 3:S:202:HEM:C1C  | 2.43                     | 0.46              |
| 1:T:52:MET:HE1   | 3:U:201:HEM:CHD  | 2.45                     | 0.46              |
| 1:U:14:GLN:OE1   | 1:U:14:GLN:HA    | 2.16                     | 0.46              |
| 1:U:155:GLU:O    | 1:U:156:GLN:HB3  | 2.16                     | 0.46              |
| 1:W:14:GLN:OE1   | 1:W:14:GLN:HA    | 2.16                     | 0.46              |
| 1:F:111:LYS:O    | 1:F:112:HIS:HB2  | 2.16                     | 0.46              |
| 1:O:14:GLN:OE1   | 1:O:14:GLN:HA    | 2.16                     | 0.46              |
| 1:Q:40:LEU:CD1   | 1:Q:153:VAL:HG21 | 2.45                     | 0.46              |
| 1:S:111:LYS:O    | 1:S:112:HIS:HB2  | 2.16                     | 0.46              |
| 1:U:26:PHE:CZ    | 3:U:201:HEM:HMA1 | 2.51                     | 0.46              |
| 1:G:4:ASP:HB3    | 1:G:5:PRO:HD2    | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:47:GLU:HG3   | 1:I:130:HIS:NE2  | 2.31                     | 0.46              |
| 1:M:14:GLN:OE1   | 1:M:14:GLN:HA    | 2.15                     | 0.46              |
| 1:N:14:GLN:OE1   | 1:N:14:GLN:HA    | 2.16                     | 0.46              |
| 1:N:94:GLU:HA    | 1:N:94:GLU:OE1   | 2.15                     | 0.46              |
| 1:A:94:GLU:OE1   | 1:A:94:GLU:HA    | 2.16                     | 0.46              |
| 1:B:94:GLU:OE1   | 1:B:94:GLU:HA    | 2.15                     | 0.46              |
| 1:E:14:GLN:OE1   | 1:E:14:GLN:HA    | 2.16                     | 0.46              |
| 1:I:72:GLN:O     | 1:I:72:GLN:HG3   | 2.16                     | 0.46              |
| 1:Q:58:LEU:O     | 1:Q:62:ILE:HG22  | 2.16                     | 0.46              |
| 1:S:40:LEU:HD13  | 1:S:153:VAL:HG21 | 1.97                     | 0.46              |
| 1:W:40:LEU:HD13  | 1:W:153:VAL:HG21 | 1.98                     | 0.46              |
| 1:W:137:GLN:HA   | 1:W:137:GLN:OE1  | 2.16                     | 0.46              |
| 1:I:143:LYS:HG3  | 1:I:144:LEU:N    | 2.31                     | 0.46              |
| 1:L:94:GLU:OE1   | 1:L:94:GLU:HA    | 2.16                     | 0.46              |
| 1:M:137:GLN:OE1  | 1:M:137:GLN:HA   | 2.16                     | 0.46              |
| 1:P:14:GLN:OE1   | 1:P:14:GLN:HA    | 2.16                     | 0.46              |
| 1:P:143:LYS:HG3  | 1:P:144:LEU:N    | 2.31                     | 0.46              |
| 1:R:124:LEU:HD12 | 1:R:124:LEU:O    | 2.16                     | 0.46              |
| 1:T:14:GLN:OE1   | 1:T:14:GLN:HA    | 2.16                     | 0.46              |
| 1:F:14:GLN:OE1   | 1:F:14:GLN:HA    | 2.16                     | 0.46              |
| 1:N:111:LYS:O    | 1:N:112:HIS:HB2  | 2.16                     | 0.46              |
| 1:Q:14:GLN:HA    | 1:Q:14:GLN:OE1   | 2.16                     | 0.46              |
| 1:T:22:ILE:HD11  | 1:T:52:MET:CA    | 2.37                     | 0.46              |
| 1:T:128:GLU:O    | 1:T:131:ILE:HG22 | 2.16                     | 0.46              |
| 1:W:94:GLU:HA    | 1:W:94:GLU:OE1   | 2.16                     | 0.46              |
| 1:A:14:GLN:OE1   | 1:A:14:GLN:HA    | 2.16                     | 0.45              |
| 1:E:1:MET:HE1    | 1:E:64:LEU:HD21  | 1.98                     | 0.45              |
| 1:G:47:GLU:HG3   | 1:G:130:HIS:NE2  | 2.30                     | 0.45              |
| 1:N:143:LYS:HG3  | 1:N:144:LEU:N    | 2.31                     | 0.45              |
| 1:P:111:LYS:O    | 1:P:112:HIS:HB2  | 2.16                     | 0.45              |
| 3:Q:202:HEM:ND   | 1:R:52:MET:HE1   | 2.30                     | 0.45              |
| 1:R:42:LYS:HB3   | 1:R:42:LYS:HE2   | 1.60                     | 0.45              |
| 1:T:143:LYS:HG3  | 1:T:144:LEU:N    | 2.31                     | 0.45              |
| 1:V:137:GLN:HA   | 1:V:137:GLN:OE1  | 2.16                     | 0.45              |
| 3:V:202:HEM:C4D  | 1:W:52:MET:HE1   | 2.52                     | 0.45              |
| 1:X:42:LYS:HB3   | 1:X:42:LYS:HE2   | 1.61                     | 0.45              |
| 1:B:111:LYS:O    | 1:B:112:HIS:HB2  | 2.17                     | 0.45              |
| 1:B:124:LEU:HD12 | 1:B:124:LEU:O    | 2.16                     | 0.45              |
| 1:H:124:LEU:HD12 | 1:H:124:LEU:O    | 2.16                     | 0.45              |
| 1:H:143:LYS:HG3  | 1:H:144:LEU:N    | 2.31                     | 0.45              |
| 1:I:124:LEU:HD12 | 1:I:124:LEU:O    | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:40:LEU:HD13  | 1:L:153:VAL:HG21 | 1.97                     | 0.45              |
| 1:O:137:GLN:HA   | 1:O:137:GLN:OE1  | 2.16                     | 0.45              |
| 1:W:111:LYS:O    | 1:W:112:HIS:HB2  | 2.17                     | 0.45              |
| 1:A:137:GLN:HA   | 1:A:137:GLN:OE1  | 2.16                     | 0.45              |
| 1:D:143:LYS:HG3  | 1:D:144:LEU:N    | 2.30                     | 0.45              |
| 1:E:111:LYS:O    | 1:E:112:HIS:HB2  | 2.17                     | 0.45              |
| 1:G:111:LYS:O    | 1:G:112:HIS:HB2  | 2.17                     | 0.45              |
| 1:J:124:LEU:HD12 | 1:J:124:LEU:O    | 2.16                     | 0.45              |
| 1:V:14:GLN:OE1   | 1:V:14:GLN:HA    | 2.16                     | 0.45              |
| 1:V:155:GLU:OE1  | 1:V:155:GLU:HA   | 2.16                     | 0.45              |
| 1:B:143:LYS:HG3  | 1:B:144:LEU:N    | 2.31                     | 0.45              |
| 1:F:137:GLN:HA   | 1:F:137:GLN:OE1  | 2.16                     | 0.45              |
| 1:E:124:LEU:HD12 | 1:E:124:LEU:O    | 2.16                     | 0.45              |
| 1:H:111:LYS:O    | 1:H:112:HIS:HB2  | 2.17                     | 0.45              |
| 1:I:111:LYS:O    | 1:I:112:HIS:HB2  | 2.17                     | 0.45              |
| 1:I:137:GLN:OE1  | 1:I:137:GLN:HA   | 2.17                     | 0.45              |
| 1:R:137:GLN:HA   | 1:R:137:GLN:OE1  | 2.16                     | 0.45              |
| 1:U:47:GLU:HG3   | 1:U:130:HIS:NE2  | 2.31                     | 0.45              |
| 1:W:124:LEU:O    | 1:W:124:LEU:HD12 | 2.16                     | 0.45              |
| 1:A:111:LYS:O    | 1:A:112:HIS:HB2  | 2.17                     | 0.45              |
| 1:A:143:LYS:HG3  | 1:A:144:LEU:N    | 2.31                     | 0.45              |
| 1:B:14:GLN:HA    | 1:B:14:GLN:OE1   | 2.16                     | 0.45              |
| 1:D:14:GLN:OE1   | 1:D:14:GLN:HA    | 2.16                     | 0.45              |
| 1:F:42:LYS:HE2   | 1:F:42:LYS:HB3   | 1.61                     | 0.45              |
| 1:F:160:ASP:N    | 1:F:161:PRO:HD3  | 2.31                     | 0.45              |
| 1:H:1:MET:HE1    | 1:H:64:LEU:HD21  | 1.98                     | 0.45              |
| 1:J:47:GLU:HG3   | 1:J:130:HIS:NE2  | 2.31                     | 0.45              |
| 1:K:124:LEU:O    | 1:K:124:LEU:HD12 | 2.17                     | 0.45              |
| 1:K:155:GLU:OE2  | 1:K:155:GLU:HA   | 2.15                     | 0.45              |
| 1:L:111:LYS:O    | 1:L:112:HIS:HB2  | 2.17                     | 0.45              |
| 1:N:73:ARG:C     | 1:N:74:LEU:HD23  | 2.40                     | 0.45              |
| 1:N:160:ASP:N    | 1:N:161:PRO:HD3  | 2.30                     | 0.45              |
| 1:S:143:LYS:HG3  | 1:S:144:LEU:HD12 | 1.99                     | 0.45              |
| 3:V:202:HEM:ND   | 1:W:52:MET:HE1   | 2.31                     | 0.45              |
| 1:C:14:GLN:OE1   | 1:C:14:GLN:HA    | 2.16                     | 0.45              |
| 1:F:1:MET:HE1    | 1:F:64:LEU:HD21  | 1.99                     | 0.45              |
| 1:R:14:GLN:OE1   | 1:R:14:GLN:HA    | 2.16                     | 0.45              |
| 1:R:95:LEU:HD23  | 1:R:95:LEU:HA    | 1.85                     | 0.45              |
| 1:V:1:MET:HA     | 1:V:1:MET:CE     | 2.37                     | 0.45              |
| 1:X:14:GLN:OE1   | 1:X:14:GLN:HA    | 2.16                     | 0.45              |
| 1:F:22:ILE:CD1   | 1:F:52:MET:HA    | 2.36                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:143:LYS:HG3  | 1:E:144:LEU:HD12 | 1.98                     | 0.45              |
| 1:G:82:SER:OG    | 1:G:83:VAL:N     | 2.50                     | 0.45              |
| 1:I:14:GLN:OE1   | 1:I:14:GLN:HA    | 2.16                     | 0.45              |
| 1:I:58:LEU:O     | 1:I:62:ILE:HG22  | 2.17                     | 0.45              |
| 1:O:94:GLU:OE1   | 1:O:94:GLU:HA    | 2.16                     | 0.45              |
| 1:R:143:LYS:HG3  | 1:R:144:LEU:N    | 2.32                     | 0.45              |
| 1:S:94:GLU:HA    | 1:S:94:GLU:OE1   | 2.16                     | 0.45              |
| 1:S:137:GLN:OE1  | 1:S:137:GLN:HA   | 2.16                     | 0.45              |
| 1:T:137:GLN:HA   | 1:T:137:GLN:OE1  | 2.16                     | 0.45              |
| 1:W:47:GLU:HG3   | 1:W:130:HIS:NE2  | 2.31                     | 0.45              |
| 1:B:137:GLN:OE1  | 1:B:137:GLN:HA   | 2.16                     | 0.45              |
| 1:C:111:LYS:O    | 1:C:112:HIS:HB2  | 2.17                     | 0.45              |
| 1:H:94:GLU:OE1   | 1:H:94:GLU:HA    | 2.17                     | 0.45              |
| 1:J:56:GLU:HB2   | 3:K:301:HEM:O1D  | 2.16                     | 0.45              |
| 1:L:137:GLN:OE1  | 1:L:137:GLN:HA   | 2.17                     | 0.45              |
| 1:Q:161:PRO:HB2  | 1:R:60:ASP:OD2   | 2.17                     | 0.45              |
| 3:U:201:HEM:HHA  | 3:U:201:HEM:HBD2 | 1.99                     | 0.45              |
| 1:F:22:ILE:HD11  | 1:F:52:MET:CA    | 2.38                     | 0.45              |
| 1:F:94:GLU:HA    | 1:F:94:GLU:OE1   | 2.17                     | 0.45              |
| 1:F:143:LYS:HG3  | 1:F:144:LEU:N    | 2.32                     | 0.45              |
| 1:E:47:GLU:HG3   | 1:E:130:HIS:NE2  | 2.31                     | 0.45              |
| 1:G:137:GLN:OE1  | 1:G:137:GLN:HA   | 2.16                     | 0.45              |
| 1:K:14:GLN:OE1   | 1:K:14:GLN:HA    | 2.16                     | 0.45              |
| 1:T:111:LYS:O    | 1:T:112:HIS:HB2  | 2.16                     | 0.45              |
| 1:T:158:GLN:HG2  | 1:T:162:SER:O    | 2.17                     | 0.45              |
| 1:V:161:PRO:HB2  | 1:W:60:ASP:OD2   | 2.16                     | 0.45              |
| 1:W:42:LYS:HE2   | 1:W:42:LYS:HB3   | 1.60                     | 0.45              |
| 1:C:137:GLN:OE1  | 1:C:137:GLN:HA   | 2.16                     | 0.45              |
| 1:D:1:MET:HE1    | 1:F:128:GLU:CD   | 2.41                     | 0.45              |
| 1:G:124:LEU:HD12 | 1:G:124:LEU:O    | 2.16                     | 0.45              |
| 1:M:143:LYS:HG3  | 1:M:144:LEU:N    | 2.32                     | 0.45              |
| 1:Q:143:LYS:HG3  | 1:Q:144:LEU:HD12 | 1.99                     | 0.45              |
| 1:W:72:GLN:O     | 1:W:72:GLN:CG    | 2.65                     | 0.45              |
| 1:A:81:GLN:H     | 1:A:81:GLN:HG2   | 1.66                     | 0.44              |
| 1:D:124:LEU:HD12 | 1:D:124:LEU:O    | 2.16                     | 0.44              |
| 1:F:72:GLN:O     | 1:F:72:GLN:CG    | 2.65                     | 0.44              |
| 1:R:111:LYS:O    | 1:R:112:HIS:HB2  | 2.17                     | 0.44              |
| 1:V:58:LEU:O     | 1:V:62:ILE:HG22  | 2.17                     | 0.44              |
| 1:X:111:LYS:O    | 1:X:112:HIS:HB2  | 2.17                     | 0.44              |
| 1:D:94:GLU:HA    | 1:D:94:GLU:OE1   | 2.17                     | 0.44              |
| 1:F:40:LEU:CD1   | 1:F:153:VAL:HG21 | 2.47                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:58:LEU:O     | 1:G:62:ILE:HG22  | 2.17                     | 0.44              |
| 1:J:83:VAL:HG13  | 1:J:84:THR:N     | 2.32                     | 0.44              |
| 1:J:94:GLU:OE1   | 1:J:94:GLU:HA    | 2.17                     | 0.44              |
| 1:J:143:LYS:HG3  | 1:J:144:LEU:N    | 2.31                     | 0.44              |
| 1:V:111:LYS:O    | 1:V:112:HIS:HB2  | 2.17                     | 0.44              |
| 1:D:95:LEU:HD23  | 1:D:95:LEU:HA    | 1.86                     | 0.44              |
| 1:E:94:GLU:OE1   | 1:E:94:GLU:HA    | 2.17                     | 0.44              |
| 1:E:138:LEU:HD12 | 1:E:138:LEU:HA   | 1.80                     | 0.44              |
| 1:J:8:ILE:CG2    | 1:J:62:ILE:HD11  | 2.26                     | 0.44              |
| 1:L:47:GLU:HG3   | 1:L:130:HIS:NE2  | 2.31                     | 0.44              |
| 1:L:83:VAL:HG23  | 1:L:84:THR:N     | 2.33                     | 0.44              |
| 1:M:124:LEU:HD12 | 1:M:124:LEU:O    | 2.16                     | 0.44              |
| 1:X:137:GLN:OE1  | 1:X:137:GLN:HA   | 2.16                     | 0.44              |
| 1:C:96:GLU:OE2   | 1:C:96:GLU:CA    | 2.64                     | 0.44              |
| 1:F:124:LEU:O    | 1:F:124:LEU:HD12 | 2.17                     | 0.44              |
| 1:E:22:ILE:CD1   | 1:E:52:MET:HA    | 2.39                     | 0.44              |
| 1:N:72:GLN:O     | 1:N:72:GLN:CG    | 2.65                     | 0.44              |
| 1:N:124:LEU:HD12 | 1:N:124:LEU:O    | 2.17                     | 0.44              |
| 1:P:124:LEU:O    | 1:P:124:LEU:HD12 | 2.18                     | 0.44              |
| 1:Q:96:GLU:OE2   | 1:Q:96:GLU:CA    | 2.64                     | 0.44              |
| 1:Q:111:LYS:O    | 1:Q:112:HIS:HB2  | 2.17                     | 0.44              |
| 1:Q:137:GLN:OE1  | 1:Q:137:GLN:HA   | 2.17                     | 0.44              |
| 1:R:94:GLU:OE1   | 1:R:94:GLU:HA    | 2.17                     | 0.44              |
| 1:S:124:LEU:HD12 | 1:S:124:LEU:O    | 2.18                     | 0.44              |
| 1:T:94:GLU:OE1   | 1:T:94:GLU:HA    | 2.16                     | 0.44              |
| 1:U:49:PHE:O     | 1:U:52:MET:HB2   | 2.18                     | 0.44              |
| 1:X:143:LYS:HG3  | 1:X:144:LEU:N    | 2.32                     | 0.44              |
| 1:L:143:LYS:HG3  | 1:L:144:LEU:HD12 | 1.99                     | 0.44              |
| 1:M:72:GLN:O     | 1:M:72:GLN:CG    | 2.65                     | 0.44              |
| 1:U:95:LEU:HD23  | 1:U:95:LEU:HA    | 1.82                     | 0.44              |
| 1:V:40:LEU:CD1   | 1:V:153:VAL:HG21 | 2.47                     | 0.44              |
| 1:V:72:GLN:O     | 1:V:72:GLN:CG    | 2.65                     | 0.44              |
| 1:X:124:LEU:HD12 | 1:X:124:LEU:O    | 2.18                     | 0.44              |
| 1:C:94:GLU:OE1   | 1:C:94:GLU:HA    | 2.17                     | 0.44              |
| 1:E:73:ARG:O     | 1:E:74:LEU:HD23  | 2.18                     | 0.44              |
| 1:E:137:GLN:HA   | 1:E:137:GLN:OE1  | 2.17                     | 0.44              |
| 1:G:94:GLU:OE1   | 1:G:94:GLU:HA    | 2.16                     | 0.44              |
| 1:J:22:ILE:CD1   | 1:J:52:MET:HA    | 2.38                     | 0.44              |
| 1:M:83:VAL:HG13  | 1:M:84:THR:N     | 2.32                     | 0.44              |
| 1:P:95:LEU:HD23  | 1:P:95:LEU:HA    | 1.82                     | 0.44              |
| 1:S:83:VAL:HG13  | 1:S:84:THR:N     | 2.33                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:22:ILE:HD11  | 1:A:52:MET:CA    | 2.39                     | 0.44              |
| 1:C:49:PHE:O     | 1:C:52:MET:HB2   | 2.18                     | 0.44              |
| 1:C:161:PRO:HB2  | 1:D:60:ASP:OD2   | 2.18                     | 0.44              |
| 1:E:82:SER:OG    | 1:E:83:VAL:N     | 2.50                     | 0.44              |
| 1:I:94:GLU:HA    | 1:I:94:GLU:OE1   | 2.17                     | 0.44              |
| 1:L:72:GLN:O     | 1:L:72:GLN:CG    | 2.66                     | 0.44              |
| 3:L:202:HEM:C1A  | 1:M:52:MET:HE1   | 2.53                     | 0.44              |
| 1:M:96:GLU:OE2   | 1:M:96:GLU:CA    | 2.64                     | 0.44              |
| 1:N:1:MET:HE1    | 1:N:64:LEU:HD21  | 2.00                     | 0.44              |
| 1:P:137:GLN:OE1  | 1:P:137:GLN:HA   | 2.16                     | 0.44              |
| 1:Q:138:LEU:HD12 | 1:Q:138:LEU:HA   | 1.79                     | 0.44              |
| 1:D:137:GLN:OE1  | 1:D:137:GLN:HA   | 2.17                     | 0.44              |
| 1:G:95:LEU:HD23  | 1:G:95:LEU:HA    | 1.82                     | 0.44              |
| 1:N:105:ILE:HG13 | 1:N:120:PHE:HB3  | 2.00                     | 0.44              |
| 1:S:22:ILE:CD1   | 1:S:52:MET:HA    | 2.38                     | 0.44              |
| 1:S:105:ILE:HG13 | 1:S:120:PHE:HB3  | 2.00                     | 0.44              |
| 1:X:1:MET:HE1    | 1:X:64:LEU:HD21  | 2.00                     | 0.44              |
| 1:X:94:GLU:HA    | 1:X:94:GLU:OE1   | 2.17                     | 0.44              |
| 1:C:143:LYS:HG3  | 1:C:144:LEU:HD12 | 1.99                     | 0.44              |
| 1:D:72:GLN:O     | 1:D:72:GLN:CG    | 2.65                     | 0.44              |
| 1:J:73:ARG:O     | 1:J:74:LEU:HD23  | 2.18                     | 0.44              |
| 1:T:22:ILE:CD1   | 1:T:52:MET:HA    | 2.37                     | 0.44              |
| 1:V:83:VAL:HG23  | 1:V:84:THR:N     | 2.33                     | 0.44              |
| 1:W:83:VAL:HG13  | 1:W:84:THR:N     | 2.33                     | 0.44              |
| 1:X:72:GLN:O     | 1:X:72:GLN:CG    | 2.65                     | 0.44              |
| 1:X:83:VAL:HG13  | 1:X:84:THR:N     | 2.33                     | 0.44              |
| 1:F:83:VAL:HG13  | 1:F:84:THR:N     | 2.33                     | 0.43              |
| 1:L:161:PRO:HB2  | 1:M:60:ASP:OD2   | 2.17                     | 0.43              |
| 1:N:40:LEU:CD1   | 1:N:153:VAL:HG21 | 2.47                     | 0.43              |
| 3:O:202:HEM:HBB2 | 3:O:202:HEM:HMB2 | 1.99                     | 0.43              |
| 1:Q:155:GLU:OE2  | 1:Q:155:GLU:HA   | 2.18                     | 0.43              |
| 1:S:72:GLN:O     | 1:S:72:GLN:CG    | 2.65                     | 0.43              |
| 1:T:1:MET:HE1    | 1:T:64:LEU:HD21  | 2.00                     | 0.43              |
| 1:B:138:LEU:HD12 | 1:B:138:LEU:HA   | 1.78                     | 0.43              |
| 1:E:154:ILE:O    | 1:E:154:ILE:HG13 | 2.18                     | 0.43              |
| 1:H:73:ARG:O     | 1:H:74:LEU:HD23  | 2.18                     | 0.43              |
| 1:J:1:MET:HE1    | 1:J:64:LEU:HD21  | 2.00                     | 0.43              |
| 1:K:94:GLU:HA    | 1:K:94:GLU:OE1   | 2.17                     | 0.43              |
| 3:O:202:HEM:HBB2 | 3:O:202:HEM:CMB  | 2.48                     | 0.43              |
| 1:Q:72:GLN:O     | 1:Q:72:GLN:CG    | 2.66                     | 0.43              |
| 1:S:42:LYS:HE2   | 1:S:42:LYS:HB3   | 1.60                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:V:138:LEU:HD12 | 1:V:138:LEU:HA   | 1.78                     | 0.43              |
| 1:W:143:LYS:HG3  | 1:W:144:LEU:N    | 2.32                     | 0.43              |
| 1:A:1:MET:HE1    | 1:A:64:LEU:HD21  | 2.00                     | 0.43              |
| 1:F:105:ILE:HG13 | 1:F:120:PHE:HB3  | 2.00                     | 0.43              |
| 1:L:155:GLU:OE2  | 1:L:155:GLU:HA   | 2.18                     | 0.43              |
| 1:U:123:ILE:O    | 1:U:127:GLU:HG2  | 2.18                     | 0.43              |
| 1:X:105:ILE:HG13 | 1:X:120:PHE:HB3  | 2.00                     | 0.43              |
| 1:B:31:LEU:HD23  | 1:B:31:LEU:HA    | 1.87                     | 0.43              |
| 1:D:83:VAL:HG13  | 1:D:84:THR:N     | 2.33                     | 0.43              |
| 1:I:8:ILE:CG2    | 1:I:62:ILE:HD11  | 2.35                     | 0.43              |
| 1:O:58:LEU:O     | 1:O:62:ILE:HG22  | 2.18                     | 0.43              |
| 1:X:143:LYS:HG3  | 1:X:144:LEU:HD12 | 2.00                     | 0.43              |
| 3:X:201:HEM:HMB1 | 3:X:201:HEM:HBB2 | 2.00                     | 0.43              |
| 1:D:22:ILE:HD11  | 1:D:52:MET:CA    | 2.38                     | 0.43              |
| 1:F:8:ILE:CG2    | 1:F:62:ILE:HD11  | 2.24                     | 0.43              |
| 1:I:73:ARG:O     | 1:I:74:LEU:HD23  | 2.19                     | 0.43              |
| 1:M:101:LEU:HD23 | 1:M:101:LEU:HA   | 1.88                     | 0.43              |
| 1:M:138:LEU:HD12 | 1:M:138:LEU:HA   | 1.78                     | 0.43              |
| 1:R:83:VAL:HG13  | 1:R:84:THR:N     | 2.33                     | 0.43              |
| 3:A:202:HEM:CMB  | 3:A:202:HEM:HBB2 | 2.49                     | 0.43              |
| 1:C:72:GLN:O     | 1:C:72:GLN:CG    | 2.65                     | 0.43              |
| 1:C:143:LYS:HG3  | 1:C:144:LEU:N    | 2.33                     | 0.43              |
| 1:R:72:GLN:O     | 1:R:72:GLN:CG    | 2.65                     | 0.43              |
| 1:V:53:ARG:NH1   | 1:V:53:ARG:HB3   | 2.34                     | 0.43              |
| 1:V:143:LYS:HG3  | 1:V:144:LEU:HD12 | 1.99                     | 0.43              |
| 1:V:143:LYS:HG3  | 1:V:144:LEU:N    | 2.33                     | 0.43              |
| 1:A:58:LEU:O     | 1:A:62:ILE:HG22  | 2.19                     | 0.43              |
| 1:D:105:ILE:HG13 | 1:D:120:PHE:HB3  | 2.01                     | 0.43              |
| 1:H:56:GLU:HB2   | 3:N:201:HEM:O1A  | 1.96                     | 0.43              |
| 1:H:137:GLN:OE1  | 1:H:137:GLN:HA   | 2.17                     | 0.43              |
| 1:J:105:ILE:HG13 | 1:J:120:PHE:HB3  | 2.01                     | 0.43              |
| 1:L:96:GLU:OE2   | 1:L:96:GLU:CA    | 2.64                     | 0.43              |
| 1:M:105:ILE:HG13 | 1:M:120:PHE:HB3  | 2.00                     | 0.43              |
| 1:N:37:TRP:CD1   | 1:N:37:TRP:N     | 2.86                     | 0.43              |
| 1:U:94:GLU:HA    | 1:U:94:GLU:OE1   | 2.17                     | 0.43              |
| 1:X:40:LEU:CD1   | 1:X:153:VAL:HG21 | 2.49                     | 0.43              |
| 1:E:143:LYS:HG3  | 1:E:144:LEU:N    | 2.33                     | 0.43              |
| 1:H:96:GLU:OE2   | 1:H:96:GLU:CA    | 2.64                     | 0.43              |
| 1:K:47:GLU:HG3   | 1:K:130:HIS:NE2  | 2.34                     | 0.43              |
| 1:O:158:GLN:NE2  | 1:Q:129:HIS:HD2  | 2.17                     | 0.43              |
| 3:C:202:HEM:HBA2 | 3:C:202:HEM:CHA  | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:83:VAL:HG23  | 1:E:84:THR:N     | 2.33                     | 0.43              |
| 1:E:128:GLU:OE2  | 1:S:1:MET:HE1    | 2.19                     | 0.43              |
| 1:Q:83:VAL:HG23  | 1:Q:84:THR:N     | 2.34                     | 0.43              |
| 1:U:8:ILE:CG2    | 1:U:62:ILE:HD11  | 2.24                     | 0.43              |
| 1:B:22:ILE:HD11  | 1:B:52:MET:CA    | 2.37                     | 0.43              |
| 1:D:138:LEU:HD12 | 1:D:138:LEU:HA   | 1.81                     | 0.43              |
| 1:E:95:LEU:HD23  | 1:E:95:LEU:HA    | 1.86                     | 0.43              |
| 1:G:143:LYS:HG3  | 1:G:144:LEU:N    | 2.34                     | 0.43              |
| 1:L:37:TRP:CD1   | 1:L:37:TRP:N     | 2.87                     | 0.43              |
| 1:P:138:LEU:HA   | 1:P:138:LEU:HD12 | 1.78                     | 0.43              |
| 1:U:42:LYS:HE2   | 1:U:42:LYS:HB3   | 1.59                     | 0.43              |
| 1:V:103:ARG:HH11 | 1:V:103:ARG:HB2  | 1.84                     | 0.43              |
| 1:C:155:GLU:HA   | 1:C:155:GLU:OE2  | 2.18                     | 0.42              |
| 1:C:158:GLN:N    | 1:C:159:PRO:HD3  | 2.35                     | 0.42              |
| 1:E:96:GLU:OE2   | 1:E:96:GLU:CA    | 2.64                     | 0.42              |
| 1:H:31:LEU:HD23  | 1:H:31:LEU:HA    | 1.86                     | 0.42              |
| 1:K:137:GLN:OE1  | 1:K:137:GLN:HA   | 2.19                     | 0.42              |
| 1:N:83:VAL:HG13  | 1:N:84:THR:N     | 2.33                     | 0.42              |
| 1:O:111:LYS:O    | 1:O:112:HIS:HB2  | 2.17                     | 0.42              |
| 1:Q:47:GLU:O     | 1:Q:51:GLU:HG2   | 2.19                     | 0.42              |
| 1:U:137:GLN:OE1  | 1:U:137:GLN:HA   | 2.18                     | 0.42              |
| 1:A:22:ILE:CD1   | 1:A:52:MET:HA    | 2.37                     | 0.42              |
| 1:A:73:ARG:O     | 1:A:74:LEU:HD23  | 2.18                     | 0.42              |
| 1:D:140:LEU:HD23 | 1:D:140:LEU:HA   | 1.91                     | 0.42              |
| 1:G:143:LYS:HG3  | 1:G:144:LEU:HD12 | 1.99                     | 0.42              |
| 1:I:154:ILE:O    | 1:I:154:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:158:GLN:HE22 | 1:C:129:HIS:CD2  | 2.37                     | 0.42              |
| 3:A:202:HEM:HBB2 | 3:A:202:HEM:HMB1 | 2.01                     | 0.42              |
| 1:C:140:LEU:HD23 | 1:C:140:LEU:HA   | 1.91                     | 0.42              |
| 1:D:37:TRP:CD1   | 1:D:37:TRP:N     | 2.87                     | 0.42              |
| 1:D:42:LYS:HE2   | 1:D:42:LYS:HB3   | 1.60                     | 0.42              |
| 1:I:95:LEU:HD23  | 1:I:95:LEU:HA    | 1.82                     | 0.42              |
| 1:J:137:GLN:OE1  | 1:J:137:GLN:HA   | 2.19                     | 0.42              |
| 1:Q:143:LYS:HG3  | 1:Q:144:LEU:N    | 2.33                     | 0.42              |
| 1:R:112:HIS:NE2  | 1:S:106:GLU:OE1  | 2.39                     | 0.42              |
| 1:V:101:LEU:HD23 | 1:V:101:LEU:HA   | 1.89                     | 0.42              |
| 1:C:83:VAL:HG23  | 1:C:84:THR:N     | 2.34                     | 0.42              |
| 1:F:52:MET:HE3   | 3:F:202:HEM:NB   | 2.01                     | 0.42              |
| 1:K:138:LEU:HD12 | 1:K:138:LEU:HA   | 1.82                     | 0.42              |
| 1:N:95:LEU:HD23  | 1:N:95:LEU:HA    | 1.81                     | 0.42              |
| 1:V:140:LEU:HD23 | 1:V:140:LEU:HA   | 1.91                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:8:ILE:CG2    | 1:A:62:ILE:HD11  | 2.35                     | 0.42              |
| 1:K:95:LEU:HD23  | 1:K:95:LEU:HA    | 1.82                     | 0.42              |
| 1:K:103:ARG:HH11 | 1:K:103:ARG:HB2  | 1.85                     | 0.42              |
| 1:N:101:LEU:HD23 | 1:N:101:LEU:HA   | 1.88                     | 0.42              |
| 1:N:137:GLN:OE1  | 1:N:137:GLN:HA   | 2.19                     | 0.42              |
| 1:R:37:TRP:CD1   | 1:R:37:TRP:N     | 2.87                     | 0.42              |
| 1:W:95:LEU:HA    | 1:W:95:LEU:HD23  | 1.81                     | 0.42              |
| 1:F:37:TRP:CD1   | 1:F:37:TRP:N     | 2.86                     | 0.42              |
| 1:G:8:ILE:CG2    | 1:G:62:ILE:HD11  | 2.35                     | 0.42              |
| 1:G:83:VAL:HG23  | 1:G:84:THR:N     | 2.34                     | 0.42              |
| 1:I:103:ARG:HB2  | 1:I:103:ARG:HH11 | 1.85                     | 0.42              |
| 3:L:202:HEM:NA   | 1:M:52:MET:HE1   | 2.35                     | 0.42              |
| 3:N:201:HEM:HMB2 | 3:N:201:HEM:CBB  | 2.47                     | 0.42              |
| 1:O:19:LEU:HD22  | 3:O:202:HEM:CGA  | 2.49                     | 0.42              |
| 1:O:124:LEU:HD12 | 1:O:124:LEU:O    | 2.19                     | 0.42              |
| 1:Q:52:MET:HE2   | 1:Q:52:MET:HB3   | 1.93                     | 0.42              |
| 1:S:8:ILE:CG2    | 1:S:62:ILE:HD11  | 2.24                     | 0.42              |
| 1:S:103:ARG:HH11 | 1:S:103:ARG:HB2  | 1.85                     | 0.42              |
| 1:X:37:TRP:CD1   | 1:X:37:TRP:N     | 2.87                     | 0.42              |
| 3:A:202:HEM:HMD2 | 3:A:202:HEM:CBD  | 2.50                     | 0.42              |
| 1:F:101:LEU:HD23 | 1:F:101:LEU:HA   | 1.88                     | 0.42              |
| 1:H:32:GLN:OE1   | 1:H:40:LEU:HB3   | 2.19                     | 0.42              |
| 1:I:22:ILE:CD1   | 1:I:52:MET:HA    | 2.38                     | 0.42              |
| 1:I:52:MET:HE1   | 3:S:202:HEM:C1B  | 2.55                     | 0.42              |
| 1:J:22:ILE:HD11  | 1:J:52:MET:CA    | 2.38                     | 0.42              |
| 1:M:140:LEU:HD23 | 1:M:140:LEU:HA   | 1.91                     | 0.42              |
| 1:N:154:ILE:O    | 1:N:154:ILE:HG13 | 2.19                     | 0.42              |
| 1:P:31:LEU:HD23  | 1:P:31:LEU:HA    | 1.86                     | 0.42              |
| 1:R:140:LEU:HD23 | 1:R:140:LEU:HA   | 1.91                     | 0.42              |
| 1:B:103:ARG:HH11 | 1:B:103:ARG:HB2  | 1.85                     | 0.42              |
| 1:C:103:ARG:HH11 | 1:C:103:ARG:HB2  | 1.85                     | 0.42              |
| 1:C:154:ILE:O    | 1:C:154:ILE:HG13 | 2.20                     | 0.42              |
| 1:H:154:ILE:O    | 1:H:154:ILE:HG13 | 2.18                     | 0.42              |
| 1:J:143:LYS:HG3  | 1:J:144:LEU:HD12 | 2.02                     | 0.42              |
| 1:P:22:ILE:CD1   | 1:P:52:MET:HA    | 2.38                     | 0.42              |
| 1:Q:105:ILE:HG13 | 1:Q:120:PHE:HB3  | 2.02                     | 0.42              |
| 1:Q:158:GLN:N    | 1:Q:159:PRO:HD3  | 2.35                     | 0.42              |
| 1:C:157:THR:HG22 | 1:C:159:PRO:CG   | 2.50                     | 0.42              |
| 1:F:103:ARG:HH11 | 1:F:103:ARG:HB2  | 1.85                     | 0.42              |
| 1:F:140:LEU:HD23 | 1:F:140:LEU:HA   | 1.91                     | 0.42              |
| 1:K:105:ILE:HG13 | 1:K:120:PHE:HB3  | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:83:VAL:HG23  | 1:P:84:THR:H     | 1.85                     | 0.42              |
| 1:S:143:LYS:HG3  | 1:S:144:LEU:N    | 2.34                     | 0.42              |
| 1:S:154:ILE:O    | 1:S:154:ILE:HG13 | 2.20                     | 0.42              |
| 1:T:81:GLN:H     | 1:T:81:GLN:HG2   | 1.65                     | 0.42              |
| 1:C:162:SER:O    | 1:D:61:ARG:HB2   | 2.20                     | 0.42              |
| 1:K:1:MET:HE1    | 1:K:64:LEU:HD21  | 2.01                     | 0.42              |
| 1:L:143:LYS:HG3  | 1:L:144:LEU:N    | 2.34                     | 0.42              |
| 1:P:103:ARG:HB2  | 1:P:103:ARG:HH11 | 1.85                     | 0.42              |
| 1:U:124:LEU:O    | 1:U:124:LEU:HD12 | 2.19                     | 0.42              |
| 1:A:31:LEU:HA    | 1:A:31:LEU:HD23  | 1.87                     | 0.41              |
| 1:B:37:TRP:CD1   | 1:B:37:TRP:N     | 2.87                     | 0.41              |
| 1:E:72:GLN:O     | 1:E:72:GLN:CG    | 2.68                     | 0.41              |
| 1:M:37:TRP:CD1   | 1:M:37:TRP:N     | 2.87                     | 0.41              |
| 1:Q:154:ILE:O    | 1:Q:154:ILE:HG13 | 2.20                     | 0.41              |
| 1:R:40:LEU:HD13  | 1:R:153:VAL:HG21 | 2.01                     | 0.41              |
| 1:R:143:LYS:HG3  | 1:R:144:LEU:HD12 | 2.01                     | 0.41              |
| 1:S:37:TRP:CD1   | 1:S:37:TRP:N     | 2.87                     | 0.41              |
| 1:T:8:ILE:CG2    | 1:T:62:ILE:HD11  | 2.25                     | 0.41              |
| 3:V:202:HEM:HBA1 | 3:V:202:HEM:HMA1 | 2.02                     | 0.41              |
| 1:X:31:LEU:HD23  | 1:X:31:LEU:HA    | 1.86                     | 0.41              |
| 1:I:83:VAL:HG23  | 1:I:84:THR:N     | 2.34                     | 0.41              |
| 1:J:31:LEU:HD23  | 1:J:31:LEU:HA    | 1.86                     | 0.41              |
| 1:M:42:LYS:HB3   | 1:M:42:LYS:HE2   | 1.60                     | 0.41              |
| 1:P:37:TRP:CD1   | 1:P:37:TRP:N     | 2.86                     | 0.41              |
| 1:Q:32:GLN:OE1   | 1:Q:40:LEU:HB3   | 2.20                     | 0.41              |
| 1:Q:53:ARG:NH1   | 1:Q:53:ARG:HB3   | 2.35                     | 0.41              |
| 1:F:95:LEU:HA    | 1:F:95:LEU:HD23  | 1.81                     | 0.41              |
| 1:G:37:TRP:CD1   | 1:G:37:TRP:N     | 2.87                     | 0.41              |
| 1:L:1:MET:HA     | 1:L:1:MET:CE     | 2.37                     | 0.41              |
| 1:L:154:ILE:O    | 1:L:154:ILE:HG13 | 2.20                     | 0.41              |
| 3:O:202:HEM:HMA1 | 3:O:202:HEM:CBA  | 2.46                     | 0.41              |
| 1:Q:162:SER:O    | 1:R:61:ARG:HB2   | 2.20                     | 0.41              |
| 1:T:143:LYS:HG3  | 1:T:144:LEU:HD12 | 2.02                     | 0.41              |
| 1:T:158:GLN:NE2  | 1:V:129:HIS:HD2  | 2.18                     | 0.41              |
| 1:X:155:GLU:OE1  | 1:X:155:GLU:CA   | 2.68                     | 0.41              |
| 1:A:105:ILE:HG13 | 1:A:120:PHE:HB3  | 2.02                     | 0.41              |
| 1:K:83:VAL:HG23  | 1:K:84:THR:H     | 1.84                     | 0.41              |
| 1:K:111:LYS:O    | 1:K:112:HIS:HB2  | 2.20                     | 0.41              |
| 1:M:143:LYS:HG3  | 1:M:144:LEU:HD12 | 2.01                     | 0.41              |
| 1:N:138:LEU:HD12 | 1:N:138:LEU:HA   | 1.81                     | 0.41              |
| 1:R:105:ILE:HG13 | 1:R:120:PHE:HB3  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:103:ARG:HH11 | 1:U:103:ARG:HB2  | 1.85                     | 0.41              |
| 1:U:111:LYS:O    | 1:U:112:HIS:HB2  | 2.21                     | 0.41              |
| 1:W:143:LYS:HG3  | 1:W:144:LEU:HD12 | 2.02                     | 0.41              |
| 1:C:52:MET:O     | 3:C:202:HEM:CGA  | 2.68                     | 0.41              |
| 1:E:105:ILE:HG13 | 1:E:120:PHE:HB3  | 2.02                     | 0.41              |
| 1:L:140:LEU:HD23 | 1:L:140:LEU:HA   | 1.91                     | 0.41              |
| 1:M:40:LEU:HD13  | 1:M:153:VAL:HG21 | 2.02                     | 0.41              |
| 1:Q:103:ARG:HB2  | 1:Q:103:ARG:HH11 | 1.85                     | 0.41              |
| 1:R:101:LEU:HD23 | 1:R:101:LEU:HA   | 1.88                     | 0.41              |
| 1:T:105:ILE:HG13 | 1:T:120:PHE:HB3  | 2.03                     | 0.41              |
| 1:U:1:MET:HE1    | 1:U:64:LEU:HD21  | 2.01                     | 0.41              |
| 1:A:140:LEU:HD23 | 1:A:140:LEU:HA   | 1.92                     | 0.41              |
| 1:F:143:LYS:HG3  | 1:F:144:LEU:HD12 | 2.02                     | 0.41              |
| 1:H:103:ARG:HB2  | 1:H:103:ARG:HH11 | 1.86                     | 0.41              |
| 1:L:162:SER:O    | 1:M:61:ARG:HB2   | 2.21                     | 0.41              |
| 1:R:103:ARG:HB2  | 1:R:103:ARG:HH11 | 1.86                     | 0.41              |
| 1:V:47:GLU:HG3   | 1:V:130:HIS:NE2  | 2.35                     | 0.41              |
| 1:G:22:ILE:HD11  | 1:G:52:MET:CA    | 2.37                     | 0.41              |
| 1:I:22:ILE:HD11  | 1:I:52:MET:CA    | 2.39                     | 0.41              |
| 1:N:143:LYS:HG3  | 1:N:144:LEU:HD12 | 2.02                     | 0.41              |
| 3:O:202:HEM:C4A  | 1:P:52:MET:HE1   | 2.55                     | 0.41              |
| 3:V:202:HEM:CMA  | 3:V:202:HEM:CBA  | 2.98                     | 0.41              |
| 1:H:52:MET:HE1   | 3:N:201:HEM:C1C  | 2.56                     | 0.41              |
| 1:M:103:ARG:HB2  | 1:M:103:ARG:HH11 | 1.86                     | 0.41              |
| 1:B:105:ILE:HG13 | 1:B:120:PHE:HB3  | 2.03                     | 0.41              |
| 1:D:40:LEU:HD13  | 1:D:153:VAL:HG21 | 2.02                     | 0.41              |
| 1:D:103:ARG:HH11 | 1:D:103:ARG:HB2  | 1.85                     | 0.41              |
| 3:F:202:HEM:HBB2 | 3:F:202:HEM:HMB2 | 2.03                     | 0.41              |
| 1:G:31:LEU:HD23  | 1:G:31:LEU:HA    | 1.86                     | 0.41              |
| 1:G:103:ARG:HH11 | 1:G:103:ARG:HB2  | 1.85                     | 0.41              |
| 1:G:154:ILE:O    | 1:G:154:ILE:HG13 | 2.20                     | 0.41              |
| 1:H:83:VAL:HG23  | 1:H:84:THR:N     | 2.35                     | 0.41              |
| 1:H:105:ILE:HG13 | 1:H:120:PHE:HB3  | 2.02                     | 0.41              |
| 1:I:37:TRP:N     | 1:I:37:TRP:CD1   | 2.87                     | 0.41              |
| 1:I:60:ASP:OD2   | 1:S:30:LYS:NZ    | 2.50                     | 0.41              |
| 1:I:143:LYS:HG3  | 1:I:144:LEU:HD12 | 2.03                     | 0.41              |
| 1:L:52:MET:HE2   | 1:L:52:MET:HB3   | 1.77                     | 0.41              |
| 1:L:103:ARG:HH11 | 1:L:103:ARG:HB2  | 1.85                     | 0.41              |
| 1:M:94:GLU:HA    | 1:M:94:GLU:OE1   | 2.21                     | 0.41              |
| 1:O:95:LEU:HD23  | 1:O:95:LEU:HA    | 1.82                     | 0.41              |
| 1:P:105:ILE:HG13 | 1:P:120:PHE:HB3  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:31:LEU:HA    | 1:S:31:LEU:HD23  | 1.87                     | 0.41              |
| 1:T:37:TRP:CD1   | 1:T:37:TRP:N     | 2.88                     | 0.41              |
| 1:T:40:LEU:HD23  | 1:T:40:LEU:HA    | 1.86                     | 0.41              |
| 1:V:105:ILE:HG13 | 1:V:120:PHE:HB3  | 2.03                     | 0.41              |
| 1:W:103:ARG:HH11 | 1:W:103:ARG:HB2  | 1.85                     | 0.41              |
| 1:E:103:ARG:HH11 | 1:E:103:ARG:HB2  | 1.86                     | 0.41              |
| 1:H:72:GLN:O     | 1:H:72:GLN:CG    | 2.69                     | 0.41              |
| 1:I:138:LEU:HD12 | 1:I:138:LEU:HA   | 1.78                     | 0.41              |
| 1:I:155:GLU:OE1  | 1:I:155:GLU:HA   | 2.21                     | 0.41              |
| 1:J:103:ARG:HH11 | 1:J:103:ARG:HB2  | 1.86                     | 0.41              |
| 1:K:49:PHE:O     | 1:K:52:MET:HB2   | 2.21                     | 0.41              |
| 1:K:123:ILE:O    | 1:K:127:GLU:HG2  | 2.21                     | 0.41              |
| 1:L:98:ILE:HD13  | 1:L:98:ILE:HA    | 1.96                     | 0.41              |
| 1:O:138:LEU:HD12 | 1:O:138:LEU:HA   | 1.80                     | 0.41              |
| 1:S:155:GLU:OE2  | 1:S:155:GLU:CA   | 2.68                     | 0.41              |
| 1:T:138:LEU:HA   | 1:T:138:LEU:HD12 | 1.78                     | 0.41              |
| 1:W:37:TRP:CD1   | 1:W:37:TRP:N     | 2.87                     | 0.41              |
| 1:X:34:HIS:ND1   | 1:X:160:ASP:OD1  | 2.54                     | 0.41              |
| 1:A:52:MET:SD    | 3:A:202:HEM:C4D  | 3.12                     | 0.40              |
| 1:A:143:LYS:HG3  | 1:A:144:LEU:HD12 | 2.02                     | 0.40              |
| 3:A:202:HEM:HMA2 | 3:A:202:HEM:CBA  | 2.50                     | 0.40              |
| 1:C:105:ILE:HG13 | 1:C:120:PHE:HB3  | 2.02                     | 0.40              |
| 1:G:72:GLN:O     | 1:G:72:GLN:CG    | 2.69                     | 0.40              |
| 1:I:105:ILE:HG13 | 1:I:120:PHE:HB3  | 2.03                     | 0.40              |
| 1:L:105:ILE:HG13 | 1:L:120:PHE:HB3  | 2.02                     | 0.40              |
| 1:M:22:ILE:HD11  | 1:M:52:MET:CA    | 2.41                     | 0.40              |
| 1:Q:37:TRP:CD1   | 1:Q:37:TRP:N     | 2.87                     | 0.40              |
| 1:S:22:ILE:HD11  | 1:S:52:MET:CA    | 2.40                     | 0.40              |
| 1:S:40:LEU:CD1   | 1:S:153:VAL:HG21 | 2.51                     | 0.40              |
| 1:V:162:SER:O    | 1:W:61:ARG:HB2   | 2.20                     | 0.40              |
| 1:W:1:MET:HE1    | 1:X:128:GLU:CD   | 2.47                     | 0.40              |
| 1:X:103:ARG:HH11 | 1:X:103:ARG:HB2  | 1.85                     | 0.40              |
| 1:F:62:ILE:O     | 1:F:62:ILE:HG13  | 2.22                     | 0.40              |
| 1:S:34:HIS:ND1   | 1:S:160:ASP:OD1  | 2.54                     | 0.40              |
| 1:T:31:LEU:HD23  | 1:T:31:LEU:HA    | 1.87                     | 0.40              |
| 1:T:158:GLN:HE22 | 1:V:129:HIS:CD2  | 2.39                     | 0.40              |
| 1:V:32:GLN:OE1   | 1:V:40:LEU:HB3   | 2.20                     | 0.40              |
| 1:V:52:MET:HE3   | 3:V:202:HEM:C4D  | 2.21                     | 0.40              |
| 1:V:158:GLN:N    | 1:V:159:PRO:HD3  | 2.35                     | 0.40              |
| 1:W:140:LEU:HD23 | 1:W:140:LEU:HA   | 1.91                     | 0.40              |
| 1:A:101:LEU:HD23 | 1:A:101:LEU:HA   | 1.91                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:158:GLN:NE2  | 1:C:129:HIS:HD2  | 2.19                     | 0.40              |
| 1:C:101:LEU:HD23 | 1:C:101:LEU:HA   | 1.88                     | 0.40              |
| 1:F:38:THR:O     | 1:F:41:ALA:N     | 2.55                     | 0.40              |
| 3:F:202:HEM:C1B  | 1:E:52:MET:HE1   | 2.56                     | 0.40              |
| 1:H:143:LYS:HG3  | 1:H:144:LEU:HD12 | 2.03                     | 0.40              |
| 1:H:155:GLU:HA   | 1:H:155:GLU:OE1  | 2.21                     | 0.40              |
| 1:K:143:LYS:HG3  | 1:K:144:LEU:HD12 | 2.04                     | 0.40              |
| 3:L:202:HEM:CBA  | 3:L:202:HEM:CMA  | 2.98                     | 0.40              |
| 3:L:202:HEM:HBC2 | 3:L:202:HEM:CMC  | 2.51                     | 0.40              |
| 1:O:143:LYS:HG3  | 1:O:144:LEU:HD12 | 2.02                     | 0.40              |
| 1:X:138:LEU:HA   | 1:X:138:LEU:HD12 | 1.79                     | 0.40              |
| 1:D:143:LYS:HG3  | 1:D:144:LEU:HD12 | 2.03                     | 0.40              |
| 1:E:155:GLU:HA   | 1:E:155:GLU:OE1  | 2.22                     | 0.40              |
| 1:H:138:LEU:HA   | 1:H:138:LEU:HD12 | 1.80                     | 0.40              |
| 1:J:158:GLN:NE2  | 1:L:129:HIS:HD2  | 2.19                     | 0.40              |
| 1:L:40:LEU:CD1   | 1:L:153:VAL:HG21 | 2.51                     | 0.40              |
| 1:M:95:LEU:HD23  | 1:M:95:LEU:HA    | 1.85                     | 0.40              |
| 1:O:31:LEU:HD23  | 1:O:31:LEU:HA    | 1.87                     | 0.40              |
| 1:U:31:LEU:HD23  | 1:U:31:LEU:HA    | 1.86                     | 0.40              |
| 1:W:105:ILE:HG13 | 1:W:120:PHE:HB3  | 2.02                     | 0.40              |
| 1:C:32:GLN:OE1   | 1:C:40:LEU:HB3   | 2.22                     | 0.40              |
| 1:G:73:ARG:O     | 1:G:74:LEU:HG    | 2.21                     | 0.40              |
| 1:G:105:ILE:HG13 | 1:G:120:PHE:HB3  | 2.03                     | 0.40              |
| 1:G:150:LEU:C    | 1:G:152:THR:H    | 2.30                     | 0.40              |
| 1:K:62:ILE:O     | 1:K:62:ILE:HG13  | 2.22                     | 0.40              |
| 1:L:150:LEU:C    | 1:L:152:THR:H    | 2.30                     | 0.40              |
| 3:O:202:HEM:CBA  | 3:O:202:HEM:CMA  | 3.00                     | 0.40              |
| 1:S:95:LEU:HD23  | 1:S:95:LEU:HA    | 1.81                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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     | 160/167 (96%)   | 148 (92%)  | 12 (8%)  | 0        | 100         | 100 |
| 1   | B     | 155/167 (93%)   | 147 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 1   | C     | 160/167 (96%)   | 148 (92%)  | 12 (8%)  | 0        | 100         | 100 |
| 1   | D     | 155/167 (93%)   | 147 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 1   | E     | 159/167 (95%)   | 148 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| 1   | F     | 159/167 (95%)   | 147 (92%)  | 12 (8%)  | 0        | 100         | 100 |
| 1   | G     | 159/167 (95%)   | 148 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| 1   | H     | 159/167 (95%)   | 149 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 1   | I     | 159/167 (95%)   | 146 (92%)  | 13 (8%)  | 0        | 100         | 100 |
| 1   | J     | 160/167 (96%)   | 147 (92%)  | 13 (8%)  | 0        | 100         | 100 |
| 1   | K     | 155/167 (93%)   | 147 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 1   | L     | 160/167 (96%)   | 147 (92%)  | 13 (8%)  | 0        | 100         | 100 |
| 1   | M     | 155/167 (93%)   | 147 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 1   | N     | 159/167 (95%)   | 146 (92%)  | 13 (8%)  | 0        | 100         | 100 |
| 1   | O     | 160/167 (96%)   | 146 (91%)  | 14 (9%)  | 0        | 100         | 100 |
| 1   | P     | 155/167 (93%)   | 148 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 1   | Q     | 160/167 (96%)   | 147 (92%)  | 13 (8%)  | 0        | 100         | 100 |
| 1   | R     | 155/167 (93%)   | 147 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 1   | S     | 159/167 (95%)   | 148 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| 1   | T     | 160/167 (96%)   | 146 (91%)  | 14 (9%)  | 0        | 100         | 100 |
| 1   | U     | 155/167 (93%)   | 145 (94%)  | 10 (6%)  | 0        | 100         | 100 |
| 1   | V     | 160/167 (96%)   | 148 (92%)  | 12 (8%)  | 0        | 100         | 100 |
| 1   | W     | 155/167 (93%)   | 147 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 1   | X     | 159/167 (95%)   | 148 (93%)  | 11 (7%)  | 0        | 100         | 100 |
| All | All   | 3792/4008 (95%) | 3532 (93%) | 260 (7%) | 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 PDB entries followed by that with respect to all EM entries.

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     | 140/147 (95%)   | 140 (100%)  | 0        | 100         | 100 |
| 1   | B     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | C     | 142/147 (97%)   | 141 (99%)   | 1 (1%)   | 76          | 77  |
| 1   | D     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | E     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | F     | 140/147 (95%)   | 140 (100%)  | 0        | 100         | 100 |
| 1   | G     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | H     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | I     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | J     | 140/147 (95%)   | 140 (100%)  | 0        | 100         | 100 |
| 1   | K     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | L     | 142/147 (97%)   | 141 (99%)   | 1 (1%)   | 76          | 77  |
| 1   | M     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | N     | 140/147 (95%)   | 140 (100%)  | 0        | 100         | 100 |
| 1   | O     | 140/147 (95%)   | 140 (100%)  | 0        | 100         | 100 |
| 1   | P     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | Q     | 142/147 (97%)   | 141 (99%)   | 1 (1%)   | 76          | 77  |
| 1   | R     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | S     | 140/147 (95%)   | 140 (100%)  | 0        | 100         | 100 |
| 1   | T     | 140/147 (95%)   | 140 (100%)  | 0        | 100         | 100 |
| 1   | U     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | V     | 142/147 (97%)   | 141 (99%)   | 1 (1%)   | 76          | 77  |
| 1   | W     | 138/147 (94%)   | 138 (100%)  | 0        | 100         | 100 |
| 1   | X     | 140/147 (95%)   | 140 (100%)  | 0        | 100         | 100 |
| All | All   | 3344/3528 (95%) | 3340 (100%) | 4 (0%)   | 87          | 88  |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 160 | ASP  |
| 1   | L     | 160 | ASP  |
| 1   | Q     | 160 | ASP  |
| 1   | V     | 160 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 28  | HIS  |
| 1   | A     | 130 | HIS  |
| 1   | A     | 137 | GLN  |
| 1   | B     | 24  | GLN  |
| 1   | B     | 28  | HIS  |
| 1   | B     | 130 | HIS  |
| 1   | C     | 28  | HIS  |
| 1   | C     | 129 | HIS  |
| 1   | C     | 130 | HIS  |
| 1   | D     | 24  | GLN  |
| 1   | D     | 28  | HIS  |
| 1   | D     | 130 | HIS  |
| 1   | F     | 24  | GLN  |
| 1   | F     | 28  | HIS  |
| 1   | F     | 118 | ASN  |
| 1   | F     | 130 | HIS  |
| 1   | F     | 156 | GLN  |
| 1   | E     | 24  | GLN  |
| 1   | E     | 28  | HIS  |
| 1   | E     | 130 | HIS  |
| 1   | G     | 24  | GLN  |
| 1   | G     | 28  | HIS  |
| 1   | G     | 130 | HIS  |
| 1   | H     | 24  | GLN  |
| 1   | H     | 28  | HIS  |
| 1   | H     | 130 | HIS  |
| 1   | I     | 24  | GLN  |
| 1   | I     | 28  | HIS  |
| 1   | I     | 130 | HIS  |
| 1   | J     | 24  | GLN  |
| 1   | J     | 28  | HIS  |
| 1   | J     | 130 | HIS  |
| 1   | K     | 24  | GLN  |
| 1   | K     | 28  | HIS  |
| 1   | K     | 54  | HIS  |
| 1   | K     | 130 | HIS  |
| 1   | K     | 156 | GLN  |
| 1   | L     | 24  | GLN  |
| 1   | L     | 28  | HIS  |
| 1   | L     | 76  | HIS  |
| 1   | L     | 129 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L     | 130 | HIS  |
| 1   | M     | 24  | GLN  |
| 1   | M     | 28  | HIS  |
| 1   | M     | 130 | HIS  |
| 1   | N     | 24  | GLN  |
| 1   | N     | 28  | HIS  |
| 1   | N     | 118 | ASN  |
| 1   | N     | 130 | HIS  |
| 1   | O     | 24  | GLN  |
| 1   | O     | 28  | HIS  |
| 1   | O     | 54  | HIS  |
| 1   | O     | 130 | HIS  |
| 1   | P     | 28  | HIS  |
| 1   | P     | 81  | GLN  |
| 1   | P     | 130 | HIS  |
| 1   | Q     | 28  | HIS  |
| 1   | Q     | 54  | HIS  |
| 1   | Q     | 129 | HIS  |
| 1   | Q     | 130 | HIS  |
| 1   | R     | 24  | GLN  |
| 1   | R     | 28  | HIS  |
| 1   | R     | 130 | HIS  |
| 1   | S     | 24  | GLN  |
| 1   | S     | 28  | HIS  |
| 1   | S     | 118 | ASN  |
| 1   | S     | 130 | HIS  |
| 1   | S     | 156 | GLN  |
| 1   | T     | 24  | GLN  |
| 1   | T     | 28  | HIS  |
| 1   | T     | 130 | HIS  |
| 1   | U     | 24  | GLN  |
| 1   | U     | 28  | HIS  |
| 1   | U     | 54  | HIS  |
| 1   | U     | 130 | HIS  |
| 1   | V     | 24  | GLN  |
| 1   | V     | 28  | HIS  |
| 1   | V     | 72  | GLN  |
| 1   | V     | 129 | HIS  |
| 1   | V     | 130 | HIS  |
| 1   | W     | 24  | GLN  |
| 1   | W     | 28  | HIS  |
| 1   | W     | 76  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | W     | 130 | HIS  |
| 1   | X     | 24  | GLN  |
| 1   | X     | 28  | HIS  |
| 1   | X     | 118 | ASN  |
| 1   | X     | 130 | HIS  |
| 1   | X     | 156 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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$ |
| 3   | HEM  | Q     | 202 | 1    | 50,50,50     | 1.29 | 6 (12%)     | 66,82,82    | 1.04 | 2 (3%)      |
| 3   | HEM  | O     | 202 | 1    | 50,50,50     | 1.33 | 5 (10%)     | 66,82,82    | 1.19 | 5 (7%)      |
| 3   | HEM  | V     | 202 | 1    | 50,50,50     | 1.33 | 6 (12%)     | 66,82,82    | 1.29 | 8 (12%)     |
| 3   | HEM  | U     | 201 | 1    | 50,50,50     | 1.34 | 6 (12%)     | 66,82,82    | 1.34 | 10 (15%)    |
| 3   | HEM  | N     | 201 | 1    | 50,50,50     | 1.33 | 7 (14%)     | 66,82,82    | 1.19 | 5 (7%)      |
| 3   | HEM  | K     | 301 | -    | 50,50,50     | 1.42 | 6 (12%)     | 66,82,82    | 1.26 | 8 (12%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | HEM  | A     | 202 | 1    | 50,50,50     | 1.27 | 6 (12%)  | 66,82,82    | 1.20 | 6 (9%)   |
| 3   | HEM  | S     | 202 | 1    | 50,50,50     | 1.31 | 6 (12%)  | 66,82,82    | 1.22 | 6 (9%)   |
| 3   | HEM  | L     | 202 | 1    | 50,50,50     | 1.29 | 5 (10%)  | 66,82,82    | 1.17 | 5 (7%)   |
| 3   | HEM  | X     | 201 | 1    | 50,50,50     | 1.36 | 7 (14%)  | 66,82,82    | 1.30 | 9 (13%)  |
| 3   | HEM  | C     | 202 | 1    | 50,50,50     | 1.40 | 6 (12%)  | 66,82,82    | 1.13 | 5 (7%)   |
| 3   | HEM  | F     | 202 | 1    | 50,50,50     | 1.29 | 7 (14%)  | 66,82,82    | 1.18 | 5 (7%)   |

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 |
|-----|------|-------|-----|------|---------|------------|-------|
| 3   | HEM  | Q     | 202 | 1    | -       | 5/14/54/54 | -     |
| 3   | HEM  | O     | 202 | 1    | -       | 4/14/54/54 | -     |
| 3   | HEM  | V     | 202 | 1    | -       | 5/14/54/54 | -     |
| 3   | HEM  | U     | 201 | 1    | -       | 4/14/54/54 | -     |
| 3   | HEM  | N     | 201 | 1    | -       | 4/14/54/54 | -     |
| 3   | HEM  | K     | 301 | -    | -       | 4/14/54/54 | -     |
| 3   | HEM  | A     | 202 | 1    | -       | 4/14/54/54 | -     |
| 3   | HEM  | S     | 202 | 1    | -       | 3/14/54/54 | -     |
| 3   | HEM  | L     | 202 | 1    | -       | 4/14/54/54 | -     |
| 3   | HEM  | X     | 201 | 1    | -       | 4/14/54/54 | -     |
| 3   | HEM  | C     | 202 | 1    | -       | 4/14/54/54 | -     |
| 3   | HEM  | F     | 202 | 1    | -       | 1/14/54/54 | -     |

All (73) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | K     | 301 | HEM  | FE-NC   | 3.60 | 2.07        | 1.95     |
| 3   | K     | 301 | HEM  | FE-NA   | 3.58 | 2.07        | 1.95     |
| 3   | V     | 202 | HEM  | FE-ND   | 3.38 | 2.05        | 1.94     |
| 3   | C     | 202 | HEM  | FE-ND   | 3.29 | 2.05        | 1.94     |
| 3   | U     | 201 | HEM  | FE-ND   | 3.22 | 2.04        | 1.94     |
| 3   | C     | 202 | HEM  | FE-NC   | 3.20 | 2.06        | 1.95     |
| 3   | L     | 202 | HEM  | FE-NB   | 3.13 | 2.04        | 1.94     |
| 3   | O     | 202 | HEM  | FE-NC   | 3.10 | 2.05        | 1.95     |
| 3   | X     | 201 | HEM  | CAB-C3B | 3.09 | 1.55        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | S     | 202 | HEM  | FE-NC   | 3.07 | 2.05        | 1.95     |
| 3   | C     | 202 | HEM  | CAC-C3C | 3.01 | 1.55        | 1.47     |
| 3   | N     | 201 | HEM  | FE-NA   | 3.00 | 2.05        | 1.95     |
| 3   | K     | 301 | HEM  | CAC-C3C | 2.96 | 1.55        | 1.47     |
| 3   | X     | 201 | HEM  | FE-NB   | 2.96 | 2.04        | 1.94     |
| 3   | O     | 202 | HEM  | FE-NA   | 2.94 | 2.05        | 1.95     |
| 3   | N     | 201 | HEM  | FE-NB   | 2.94 | 2.03        | 1.94     |
| 3   | X     | 201 | HEM  | CAC-C3C | 2.94 | 1.55        | 1.47     |
| 3   | V     | 202 | HEM  | FE-NB   | 2.93 | 2.03        | 1.94     |
| 3   | S     | 202 | HEM  | FE-NA   | 2.93 | 2.05        | 1.95     |
| 3   | A     | 202 | HEM  | CAB-C3B | 2.93 | 1.55        | 1.47     |
| 3   | C     | 202 | HEM  | FE-NA   | 2.90 | 2.04        | 1.95     |
| 3   | C     | 202 | HEM  | FE-NB   | 2.89 | 2.03        | 1.94     |
| 3   | O     | 202 | HEM  | CAB-C3B | 2.88 | 1.55        | 1.47     |
| 3   | F     | 202 | HEM  | FE-NA   | 2.86 | 2.04        | 1.95     |
| 3   | L     | 202 | HEM  | CAC-C3C | 2.83 | 1.55        | 1.47     |
| 3   | L     | 202 | HEM  | FE-ND   | 2.83 | 2.03        | 1.94     |
| 3   | U     | 201 | HEM  | CAB-C3B | 2.80 | 1.55        | 1.47     |
| 3   | O     | 202 | HEM  | FE-ND   | 2.75 | 2.03        | 1.94     |
| 3   | U     | 201 | HEM  | FE-NB   | 2.73 | 2.03        | 1.94     |
| 3   | S     | 202 | HEM  | CAB-C3B | 2.68 | 1.54        | 1.47     |
| 3   | N     | 201 | HEM  | CAC-C3C | 2.68 | 1.54        | 1.47     |
| 3   | L     | 202 | HEM  | CAB-C3B | 2.66 | 1.54        | 1.47     |
| 3   | K     | 301 | HEM  | FE-NB   | 2.65 | 2.03        | 1.94     |
| 3   | N     | 201 | HEM  | FE-NC   | 2.64 | 2.04        | 1.95     |
| 3   | Q     | 202 | HEM  | FE-ND   | 2.61 | 2.02        | 1.94     |
| 3   | A     | 202 | HEM  | FE-ND   | 2.60 | 2.02        | 1.94     |
| 3   | A     | 202 | HEM  | FE-NB   | 2.59 | 2.02        | 1.94     |
| 3   | X     | 201 | HEM  | FE-ND   | 2.57 | 2.02        | 1.94     |
| 3   | X     | 201 | HEM  | FE-NA   | 2.55 | 2.03        | 1.95     |
| 3   | Q     | 202 | HEM  | FE-NC   | 2.54 | 2.03        | 1.95     |
| 3   | C     | 202 | HEM  | CAB-C3B | 2.54 | 1.54        | 1.47     |
| 3   | U     | 201 | HEM  | CAC-C3C | 2.53 | 1.54        | 1.47     |
| 3   | Q     | 202 | HEM  | CAB-C3B | 2.52 | 1.54        | 1.47     |
| 3   | F     | 202 | HEM  | CAB-C3B | 2.49 | 1.54        | 1.47     |
| 3   | V     | 202 | HEM  | CAB-C3B | 2.48 | 1.54        | 1.47     |
| 3   | S     | 202 | HEM  | CAC-C3C | 2.48 | 1.54        | 1.47     |
| 3   | K     | 301 | HEM  | CAB-C3B | 2.47 | 1.54        | 1.47     |
| 3   | O     | 202 | HEM  | CAC-C3C | 2.46 | 1.54        | 1.47     |
| 3   | A     | 202 | HEM  | CAC-C3C | 2.46 | 1.54        | 1.47     |
| 3   | X     | 201 | HEM  | FE-NC   | 2.45 | 2.03        | 1.95     |
| 3   | U     | 201 | HEM  | FE-NC   | 2.44 | 2.03        | 1.95     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | V     | 202 | HEM  | CAC-C3C | 2.41  | 1.54        | 1.47     |
| 3   | L     | 202 | HEM  | FE-NA   | 2.40  | 2.03        | 1.95     |
| 3   | F     | 202 | HEM  | CAC-C3C | 2.37  | 1.53        | 1.47     |
| 3   | N     | 201 | HEM  | CAB-C3B | 2.32  | 1.53        | 1.47     |
| 3   | Q     | 202 | HEM  | CAC-C3C | 2.32  | 1.53        | 1.47     |
| 3   | N     | 201 | HEM  | C3C-C2C | -2.27 | 1.32        | 1.37     |
| 3   | F     | 202 | HEM  | FE-NC   | 2.25  | 2.02        | 1.95     |
| 3   | V     | 202 | HEM  | FE-NC   | 2.24  | 2.02        | 1.95     |
| 3   | N     | 201 | HEM  | FE-ND   | 2.23  | 2.01        | 1.94     |
| 3   | F     | 202 | HEM  | FE-NB   | 2.19  | 2.01        | 1.94     |
| 3   | S     | 202 | HEM  | FE-ND   | 2.19  | 2.01        | 1.94     |
| 3   | U     | 201 | HEM  | FE-NA   | 2.18  | 2.02        | 1.95     |
| 3   | F     | 202 | HEM  | FE-ND   | 2.16  | 2.01        | 1.94     |
| 3   | K     | 301 | HEM  | FE-ND   | 2.13  | 2.01        | 1.94     |
| 3   | Q     | 202 | HEM  | FE-NB   | 2.12  | 2.01        | 1.94     |
| 3   | F     | 202 | HEM  | C2A-C3A | -2.11 | 1.33        | 1.38     |
| 3   | S     | 202 | HEM  | FE-NB   | 2.11  | 2.01        | 1.94     |
| 3   | Q     | 202 | HEM  | C2A-C3A | -2.09 | 1.33        | 1.38     |
| 3   | A     | 202 | HEM  | FE-NA   | 2.09  | 2.02        | 1.95     |
| 3   | V     | 202 | HEM  | C2A-C3A | -2.08 | 1.33        | 1.38     |
| 3   | A     | 202 | HEM  | CMC-C2C | 2.03  | 1.55        | 1.50     |
| 3   | X     | 201 | HEM  | C2A-C3A | -2.00 | 1.33        | 1.38     |

All (74) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | U     | 201 | HEM  | CAD-C3D-C4D | 3.05  | 130.00      | 124.66   |
| 3   | K     | 301 | HEM  | C4A-CHB-C1B | -3.04 | 119.13      | 126.34   |
| 3   | U     | 201 | HEM  | CHD-C1D-ND  | 2.98  | 127.65      | 124.42   |
| 3   | V     | 202 | HEM  | CHD-C1D-ND  | 2.97  | 127.64      | 124.42   |
| 3   | O     | 202 | HEM  | C4C-NC-C1C  | 2.92  | 108.21      | 105.35   |
| 3   | V     | 202 | HEM  | CAD-C3D-C4D | 2.90  | 129.72      | 124.66   |
| 3   | X     | 201 | HEM  | C4A-NA-C1A  | 2.87  | 108.16      | 105.35   |
| 3   | K     | 301 | HEM  | C1C-CHC-C4B | -2.82 | 119.98      | 126.06   |
| 3   | V     | 202 | HEM  | CAD-C3D-C2D | -2.77 | 122.72      | 127.88   |
| 3   | S     | 202 | HEM  | CHD-C1D-ND  | 2.76  | 127.42      | 124.42   |
| 3   | S     | 202 | HEM  | C3B-C2B-C1B | 2.69  | 108.48      | 106.49   |
| 3   | S     | 202 | HEM  | C1B-NB-C4B  | 2.68  | 107.84      | 105.07   |
| 3   | X     | 201 | HEM  | CHC-C1C-NC  | 2.66  | 127.31      | 124.44   |
| 3   | K     | 301 | HEM  | CHB-C1B-NB  | 2.65  | 127.64      | 124.37   |
| 3   | F     | 202 | HEM  | CHD-C1D-ND  | 2.63  | 127.27      | 124.42   |
| 3   | V     | 202 | HEM  | C4D-ND-C1D  | 2.59  | 107.75      | 105.07   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | U     | 201 | HEM  | C1D-C2D-C3D | 2.56  | 109.65      | 106.96   |
| 3   | C     | 202 | HEM  | C1B-NB-C4B  | 2.54  | 107.70      | 105.07   |
| 3   | U     | 201 | HEM  | C4D-ND-C1D  | 2.53  | 107.69      | 105.07   |
| 3   | U     | 201 | HEM  | C3B-C2B-C1B | 2.53  | 108.36      | 106.49   |
| 3   | X     | 201 | HEM  | CAA-C2A-C1A | 2.50  | 129.81      | 124.89   |
| 3   | A     | 202 | HEM  | CAA-C2A-C1A | -2.49 | 119.99      | 124.89   |
| 3   | A     | 202 | HEM  | CAA-CBA-CGA | -2.47 | 108.28      | 113.60   |
| 3   | O     | 202 | HEM  | C4D-ND-C1D  | 2.47  | 107.62      | 105.07   |
| 3   | Q     | 202 | HEM  | CHD-C1D-ND  | 2.36  | 126.98      | 124.42   |
| 3   | C     | 202 | HEM  | C4C-CHD-C1D | -2.35 | 120.98      | 126.06   |
| 3   | A     | 202 | HEM  | C3B-C2B-C1B | 2.35  | 108.23      | 106.49   |
| 3   | U     | 201 | HEM  | CAD-C3D-C2D | -2.34 | 123.52      | 127.88   |
| 3   | X     | 201 | HEM  | C3B-C2B-C1B | 2.33  | 108.22      | 106.49   |
| 3   | O     | 202 | HEM  | C3B-C2B-C1B | 2.33  | 108.21      | 106.49   |
| 3   | X     | 201 | HEM  | C4D-ND-C1D  | 2.32  | 107.47      | 105.07   |
| 3   | X     | 201 | HEM  | C2A-C1A-NA  | -2.29 | 107.59      | 110.15   |
| 3   | F     | 202 | HEM  | C4A-NA-C1A  | 2.28  | 107.58      | 105.35   |
| 3   | K     | 301 | HEM  | CMB-C2B-C1B | -2.27 | 121.58      | 125.04   |
| 3   | X     | 201 | HEM  | CMB-C2B-C1B | -2.26 | 121.59      | 125.04   |
| 3   | F     | 202 | HEM  | C1B-NB-C4B  | 2.23  | 107.37      | 105.07   |
| 3   | N     | 201 | HEM  | C1B-NB-C4B  | 2.22  | 107.36      | 105.07   |
| 3   | L     | 202 | HEM  | CAA-CBA-CGA | -2.21 | 108.84      | 113.60   |
| 3   | S     | 202 | HEM  | C4D-ND-C1D  | 2.21  | 107.36      | 105.07   |
| 3   | N     | 201 | HEM  | C3B-C2B-C1B | 2.21  | 108.13      | 106.49   |
| 3   | V     | 202 | HEM  | CAD-CBD-CGD | -2.19 | 108.90      | 113.60   |
| 3   | L     | 202 | HEM  | C3B-C2B-C1B | 2.18  | 108.10      | 106.49   |
| 3   | S     | 202 | HEM  | CHD-C4C-NC  | 2.16  | 126.78      | 124.44   |
| 3   | O     | 202 | HEM  | CAA-CBA-CGA | -2.16 | 108.96      | 113.60   |
| 3   | N     | 201 | HEM  | C4D-ND-C1D  | 2.16  | 107.30      | 105.07   |
| 3   | V     | 202 | HEM  | C3D-C4D-ND  | -2.16 | 107.76      | 110.17   |
| 3   | K     | 301 | HEM  | C3B-C2B-C1B | 2.15  | 108.08      | 106.49   |
| 3   | N     | 201 | HEM  | C4C-NC-C1C  | 2.15  | 107.45      | 105.35   |
| 3   | U     | 201 | HEM  | C4C-NC-C1C  | 2.15  | 107.45      | 105.35   |
| 3   | N     | 201 | HEM  | C3C-C2C-C1C | 2.14  | 109.12      | 107.08   |
| 3   | X     | 201 | HEM  | CAA-CBA-CGA | -2.13 | 109.02      | 113.60   |
| 3   | A     | 202 | HEM  | CAA-C2A-C3A | 2.13  | 131.94      | 127.07   |
| 3   | C     | 202 | HEM  | CBA-CAA-C2A | -2.13 | 106.71      | 112.63   |
| 3   | F     | 202 | HEM  | C4D-ND-C1D  | 2.12  | 107.26      | 105.07   |
| 3   | O     | 202 | HEM  | CAA-C2A-C1A | -2.12 | 120.72      | 124.89   |
| 3   | L     | 202 | HEM  | C4D-ND-C1D  | 2.10  | 107.25      | 105.07   |
| 3   | A     | 202 | HEM  | CAD-CBD-CGD | -2.10 | 109.08      | 113.60   |
| 3   | U     | 201 | HEM  | C1B-NB-C4B  | 2.10  | 107.24      | 105.07   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | V     | 202 | HEM  | C2A-C1A-NA  | -2.09 | 107.82      | 110.15   |
| 3   | K     | 301 | HEM  | CAA-C2A-C1A | 2.07  | 128.96      | 124.89   |
| 3   | Q     | 202 | HEM  | C4D-ND-C1D  | 2.06  | 107.20      | 105.07   |
| 3   | V     | 202 | HEM  | C1D-C2D-C3D | 2.06  | 109.12      | 106.96   |
| 3   | K     | 301 | HEM  | CHD-C1D-ND  | 2.04  | 126.64      | 124.42   |
| 3   | A     | 202 | HEM  | CAD-C3D-C4D | -2.04 | 121.09      | 124.66   |
| 3   | X     | 201 | HEM  | CHD-C1D-ND  | 2.03  | 126.63      | 124.42   |
| 3   | L     | 202 | HEM  | C4A-NA-C1A  | 2.03  | 107.34      | 105.35   |
| 3   | F     | 202 | HEM  | CHC-C4B-NB  | 2.03  | 126.62      | 124.42   |
| 3   | S     | 202 | HEM  | O2D-CGD-CBD | 2.03  | 120.54      | 114.03   |
| 3   | K     | 301 | HEM  | CHC-C4B-NB  | 2.02  | 126.62      | 124.42   |
| 3   | U     | 201 | HEM  | CAA-C2A-C1A | -2.02 | 120.91      | 124.89   |
| 3   | U     | 201 | HEM  | CAA-C2A-C3A | 2.02  | 131.69      | 127.07   |
| 3   | L     | 202 | HEM  | C1B-NB-C4B  | 2.02  | 107.16      | 105.07   |
| 3   | C     | 202 | HEM  | C4A-NA-C1A  | 2.01  | 107.31      | 105.35   |
| 3   | C     | 202 | HEM  | C3B-C2B-C1B | 2.00  | 107.97      | 106.49   |

There are no chirality outliers.

All (46) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | A     | 202 | HEM  | C3A-C2A-CAA-CBA |
| 3   | K     | 301 | HEM  | C1A-C2A-CAA-CBA |
| 3   | K     | 301 | HEM  | C2D-C3D-CAD-CBD |
| 3   | K     | 301 | HEM  | C4D-C3D-CAD-CBD |
| 3   | O     | 202 | HEM  | C2D-C3D-CAD-CBD |
| 3   | O     | 202 | HEM  | C4D-C3D-CAD-CBD |
| 3   | U     | 201 | HEM  | C2D-C3D-CAD-CBD |
| 3   | U     | 201 | HEM  | C4D-C3D-CAD-CBD |
| 3   | V     | 202 | HEM  | C1A-C2A-CAA-CBA |
| 3   | V     | 202 | HEM  | C3A-C2A-CAA-CBA |
| 3   | V     | 202 | HEM  | C2D-C3D-CAD-CBD |
| 3   | V     | 202 | HEM  | C4D-C3D-CAD-CBD |
| 3   | A     | 202 | HEM  | C2D-C3D-CAD-CBD |
| 3   | Q     | 202 | HEM  | C2D-C3D-CAD-CBD |
| 3   | L     | 202 | HEM  | C3A-C2A-CAA-CBA |
| 3   | O     | 202 | HEM  | C3A-C2A-CAA-CBA |
| 3   | U     | 201 | HEM  | C3A-C2A-CAA-CBA |
| 3   | A     | 202 | HEM  | C4D-C3D-CAD-CBD |
| 3   | Q     | 202 | HEM  | C4D-C3D-CAD-CBD |
| 3   | A     | 202 | HEM  | C1A-C2A-CAA-CBA |
| 3   | L     | 202 | HEM  | C1A-C2A-CAA-CBA |

*Continued on next page...*

*Continued from previous page...*

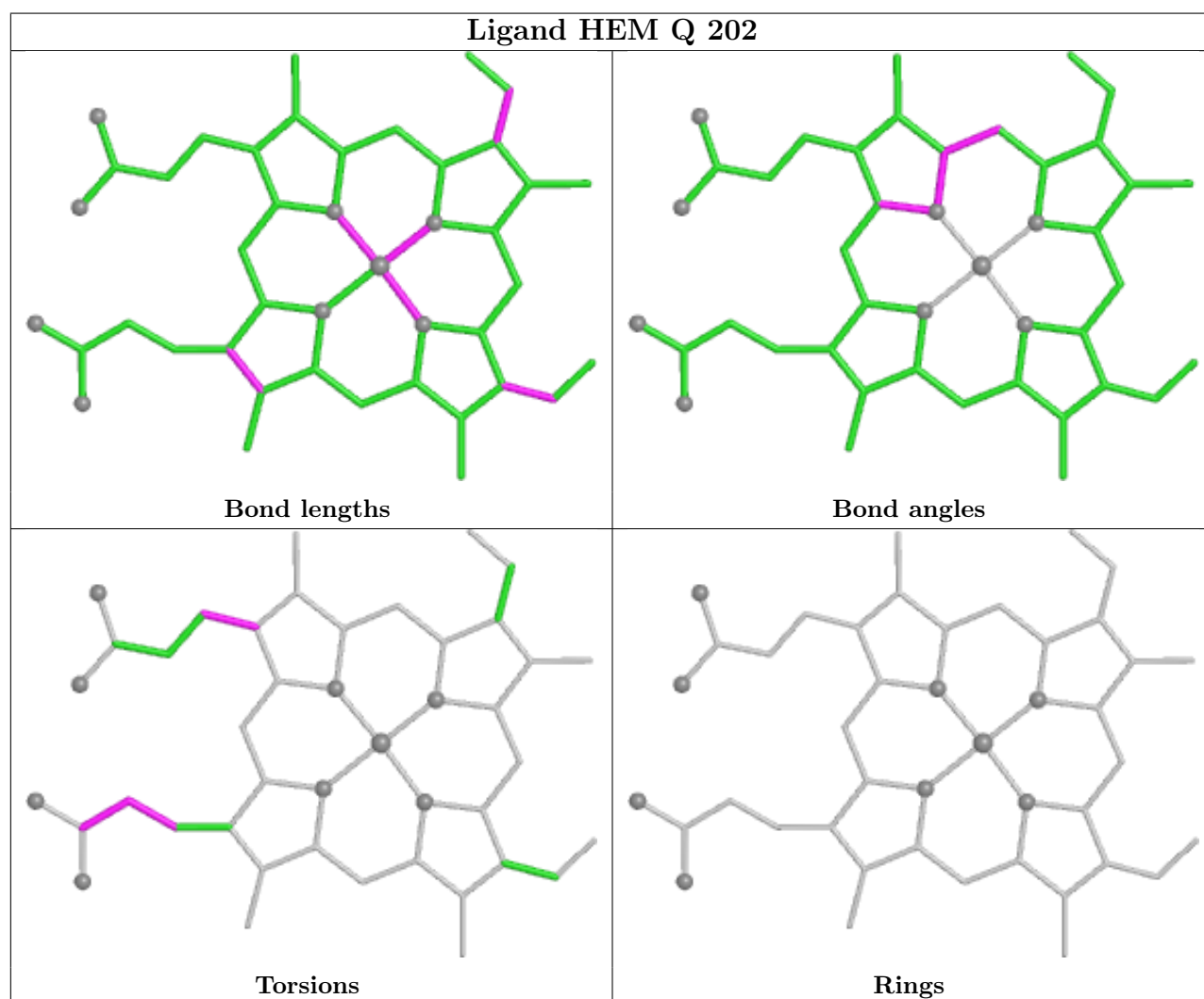
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | O     | 202 | HEM  | C1A-C2A-CAA-CBA |
| 3   | U     | 201 | HEM  | C1A-C2A-CAA-CBA |
| 3   | X     | 201 | HEM  | C1A-C2A-CAA-CBA |
| 3   | F     | 202 | HEM  | C3D-CAD-CBD-CGD |
| 3   | S     | 202 | HEM  | C2A-CAA-CBA-CGA |
| 3   | Q     | 202 | HEM  | C2A-CAA-CBA-CGA |
| 3   | S     | 202 | HEM  | C3D-CAD-CBD-CGD |
| 3   | K     | 301 | HEM  | C3A-C2A-CAA-CBA |
| 3   | X     | 201 | HEM  | C3A-C2A-CAA-CBA |
| 3   | C     | 202 | HEM  | C1A-C2A-CAA-CBA |
| 3   | C     | 202 | HEM  | C4D-C3D-CAD-CBD |
| 3   | C     | 202 | HEM  | C2D-C3D-CAD-CBD |
| 3   | N     | 201 | HEM  | C2A-CAA-CBA-CGA |
| 3   | N     | 201 | HEM  | C4C-C3C-CAC-CBC |
| 3   | X     | 201 | HEM  | C2D-C3D-CAD-CBD |
| 3   | X     | 201 | HEM  | C4D-C3D-CAD-CBD |
| 3   | V     | 202 | HEM  | C2A-CAA-CBA-CGA |
| 3   | N     | 201 | HEM  | C2D-C3D-CAD-CBD |
| 3   | C     | 202 | HEM  | C3A-C2A-CAA-CBA |
| 3   | S     | 202 | HEM  | C1A-C2A-CAA-CBA |
| 3   | N     | 201 | HEM  | C4D-C3D-CAD-CBD |
| 3   | Q     | 202 | HEM  | CAA-CBA-CGA-O2A |
| 3   | L     | 202 | HEM  | CAA-CBA-CGA-O1A |
| 3   | Q     | 202 | HEM  | CAA-CBA-CGA-O1A |
| 3   | L     | 202 | HEM  | CAA-CBA-CGA-O2A |

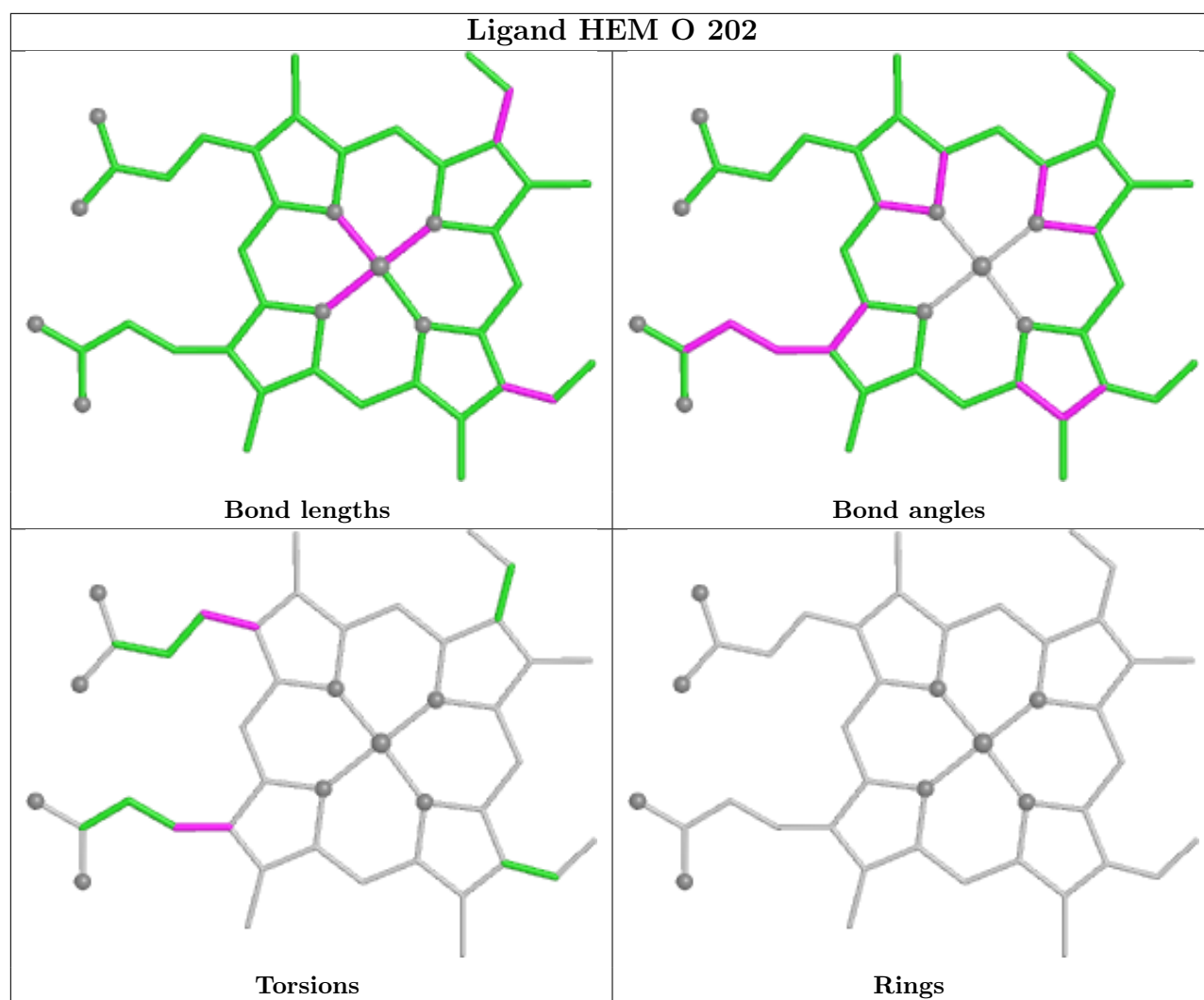
There are no ring outliers.

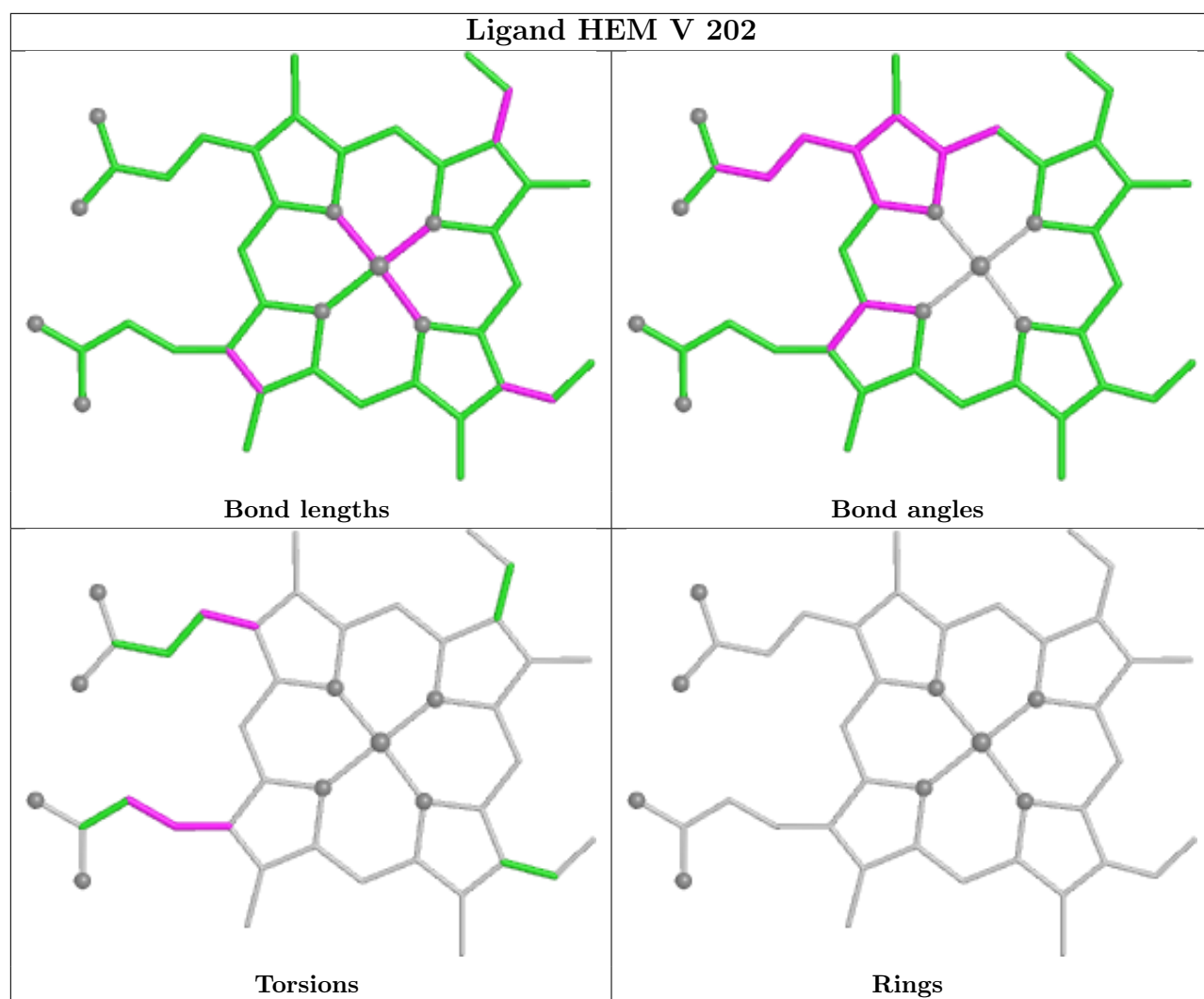
12 monomers are involved in 97 short contacts:

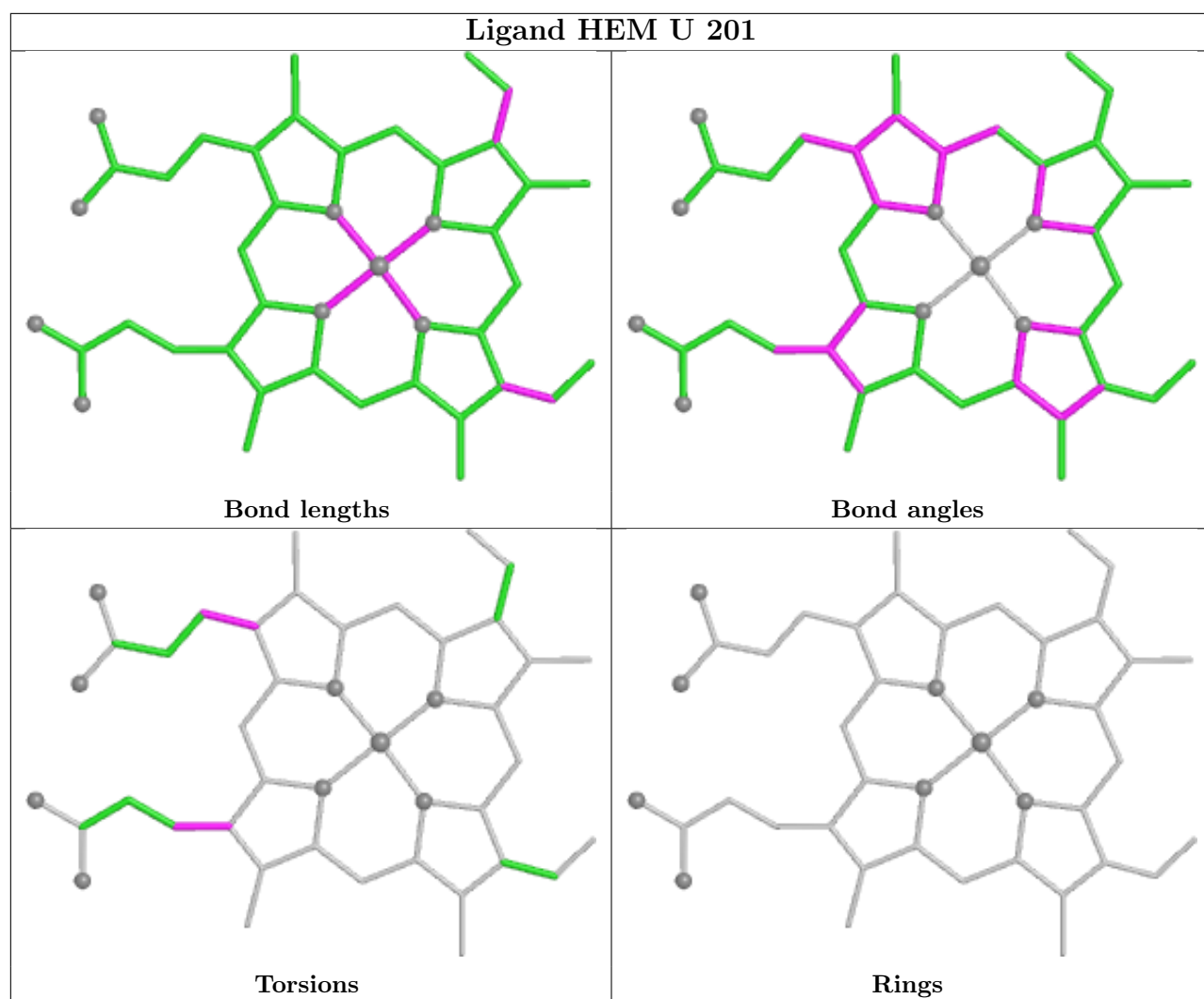
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | Q     | 202 | HEM  | 5       | 0            |
| 3   | O     | 202 | HEM  | 10      | 0            |
| 3   | V     | 202 | HEM  | 9       | 0            |
| 3   | U     | 201 | HEM  | 11      | 0            |
| 3   | N     | 201 | HEM  | 7       | 0            |
| 3   | K     | 301 | HEM  | 12      | 0            |
| 3   | A     | 202 | HEM  | 11      | 0            |
| 3   | S     | 202 | HEM  | 6       | 0            |
| 3   | L     | 202 | HEM  | 8       | 0            |
| 3   | X     | 201 | HEM  | 4       | 0            |
| 3   | C     | 202 | HEM  | 8       | 0            |
| 3   | F     | 202 | HEM  | 6       | 0            |

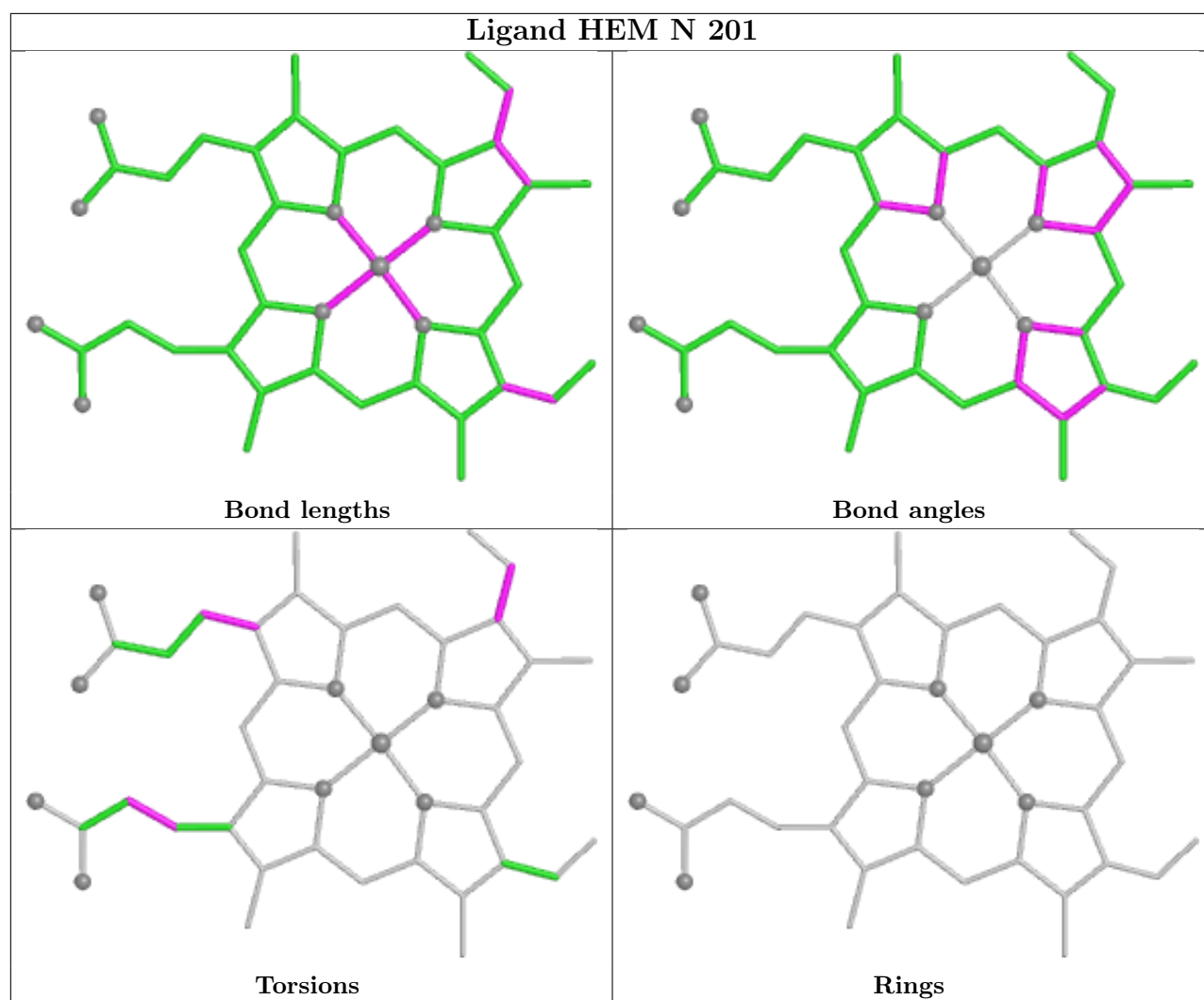
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

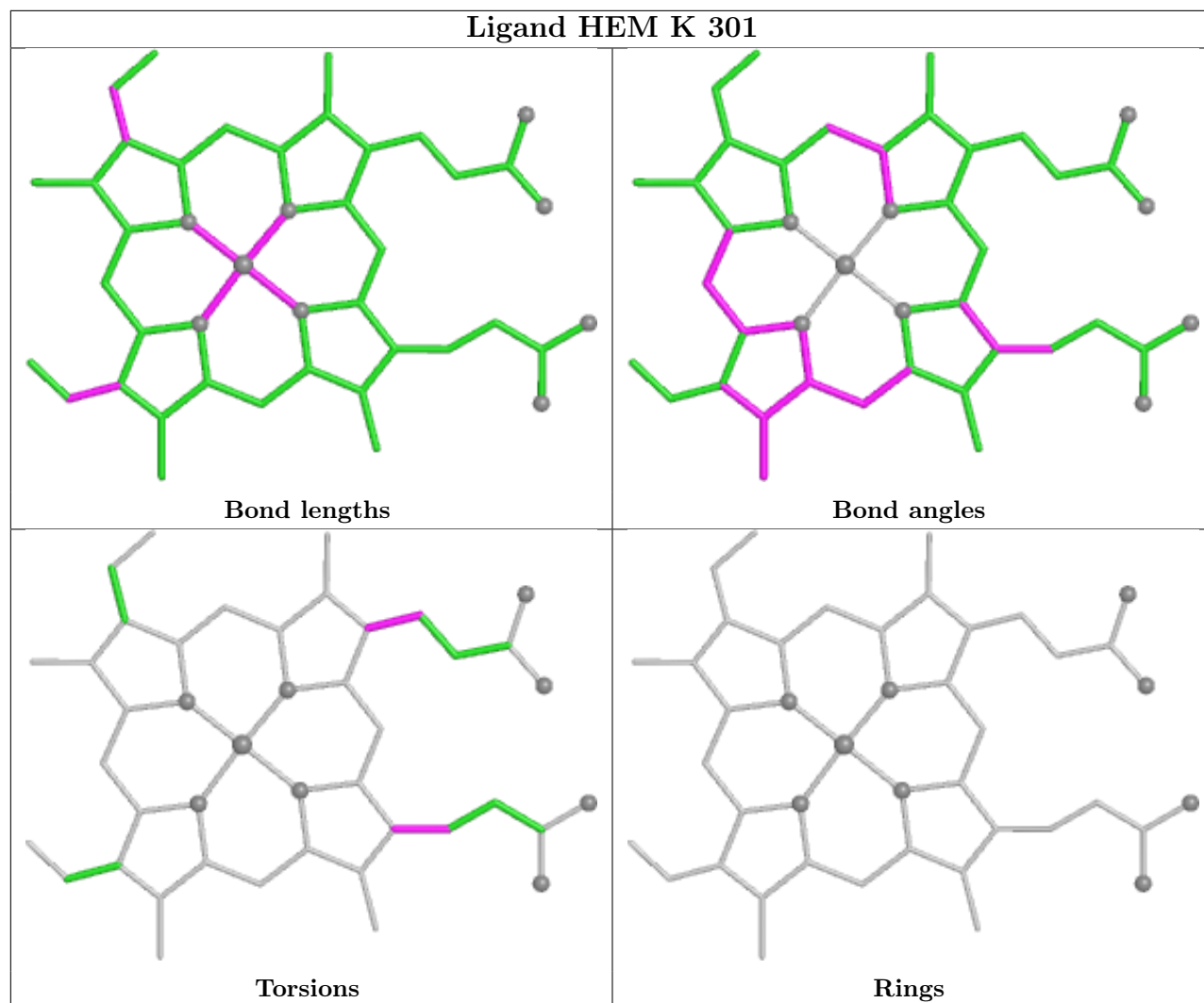


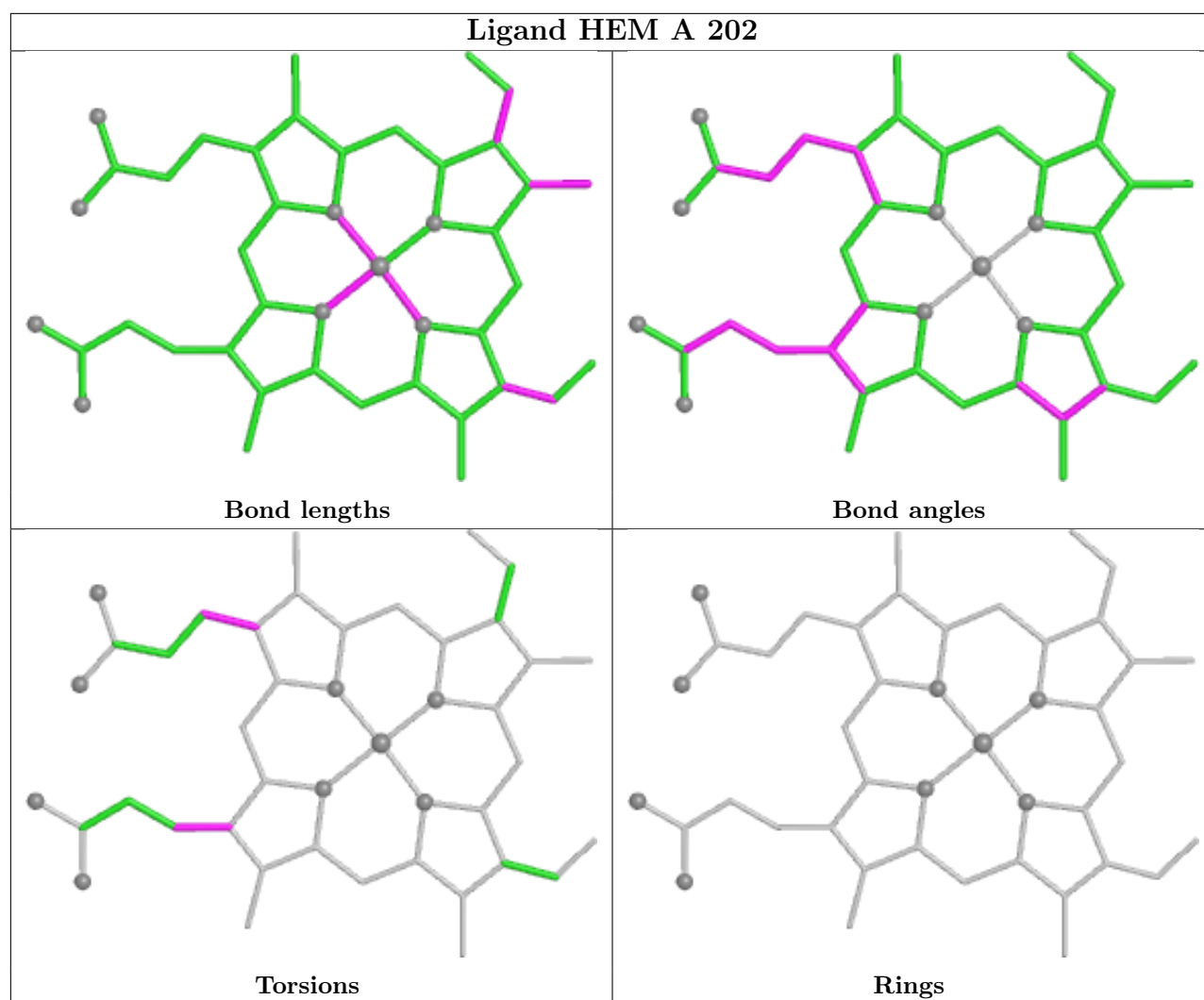


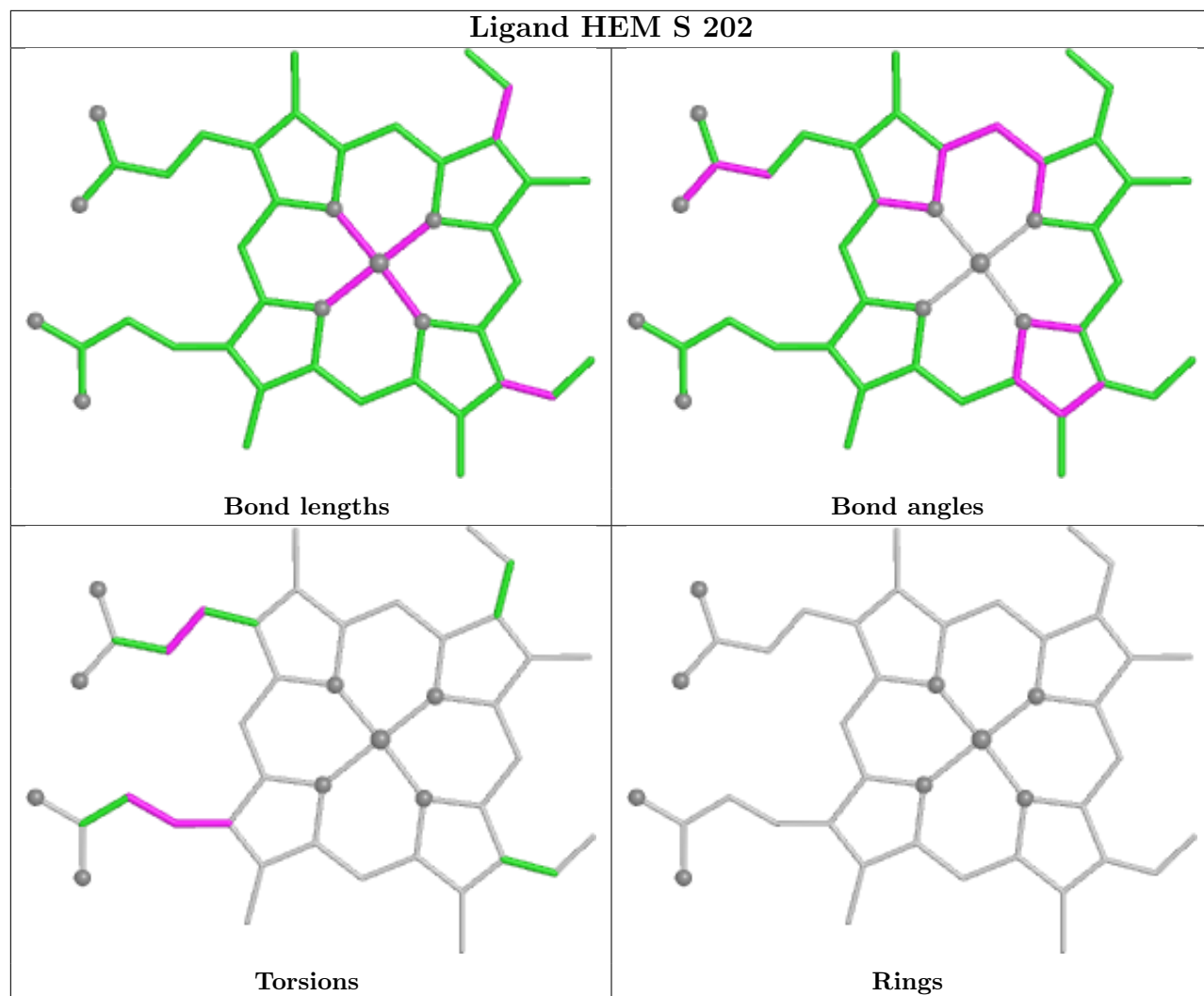


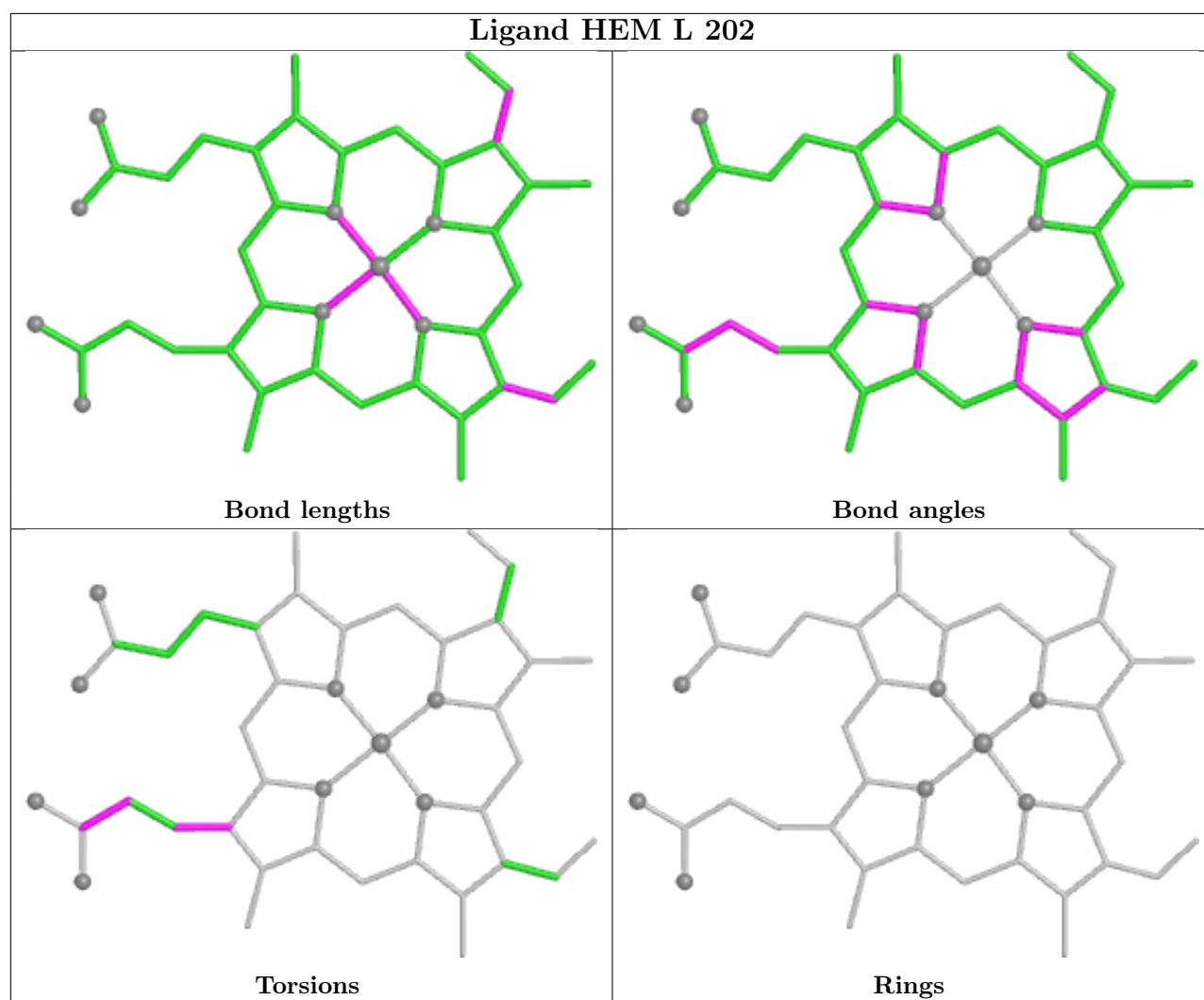


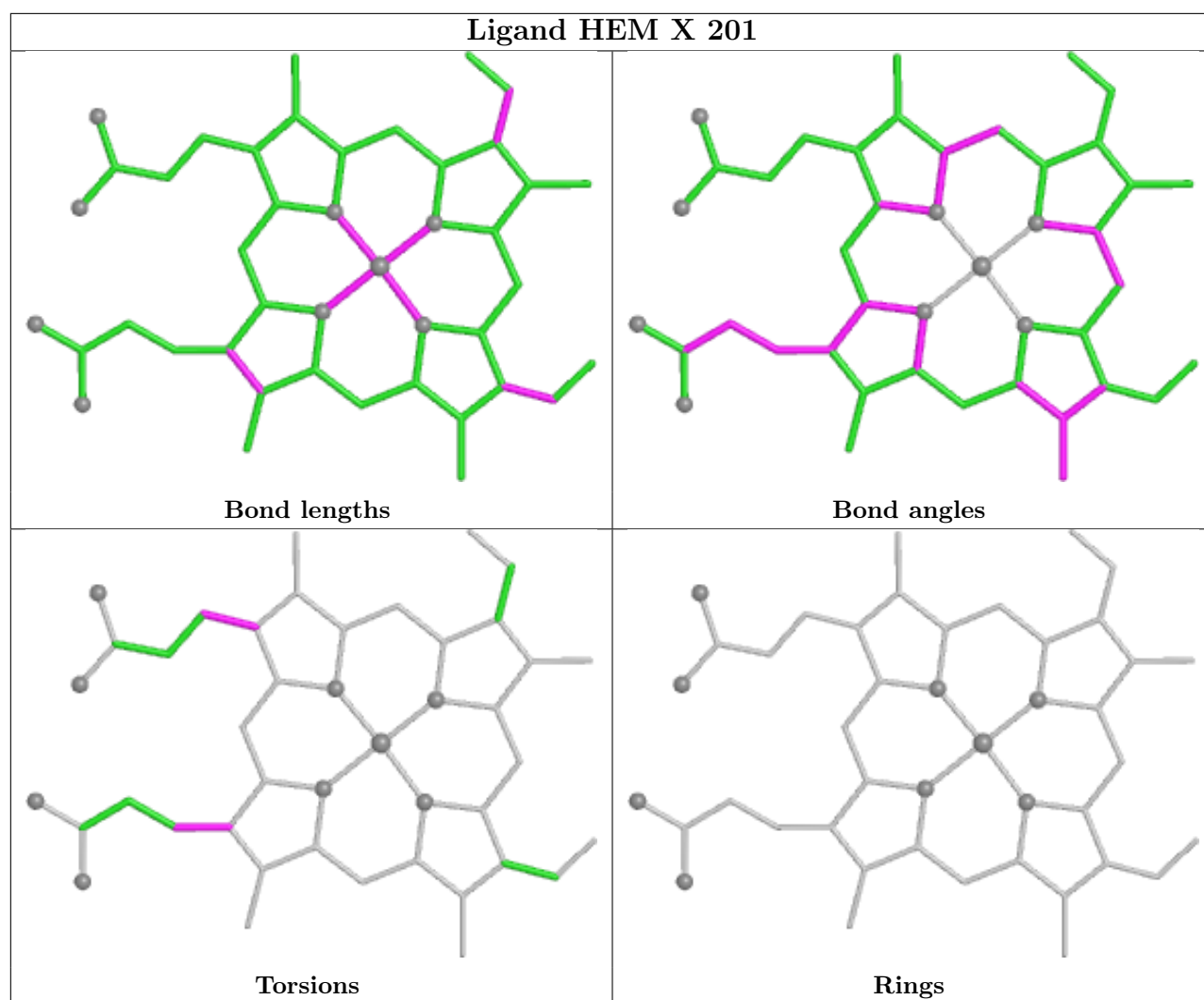


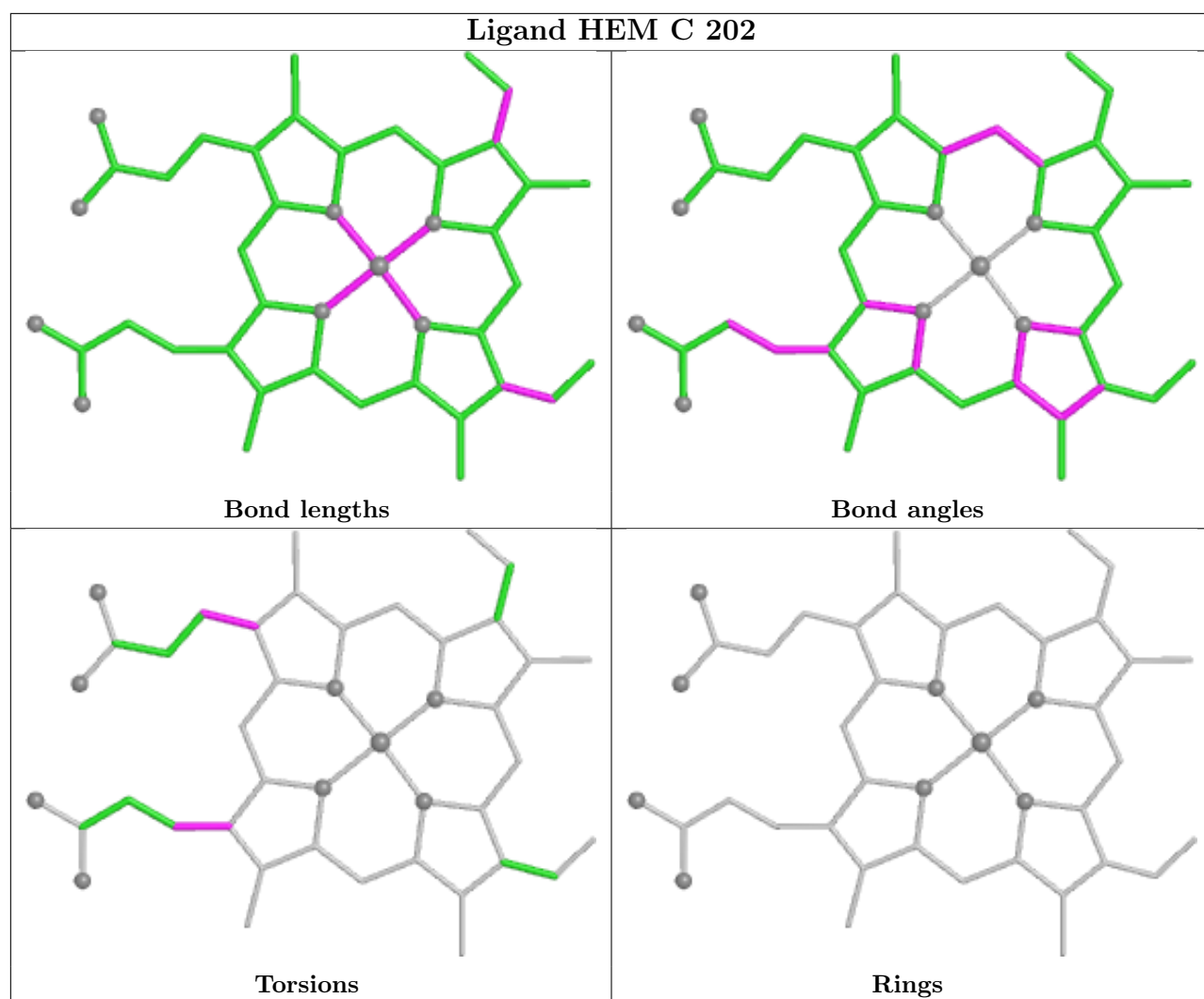


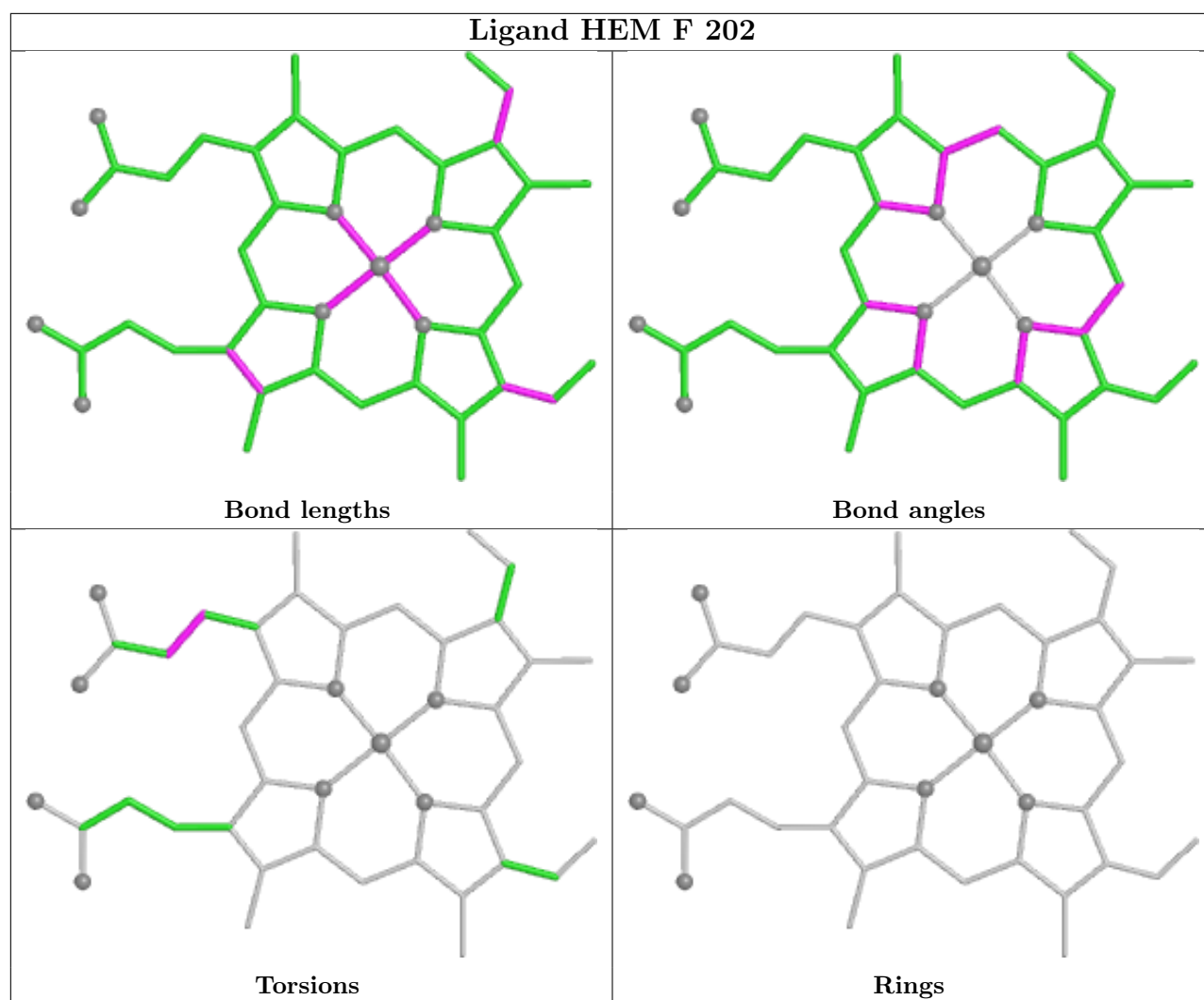












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

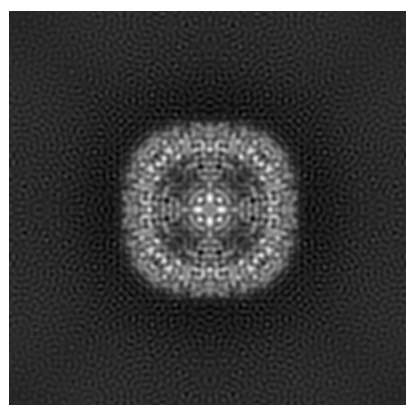
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9913. These allow visual inspection of the internal detail of the map and identification of artifacts.

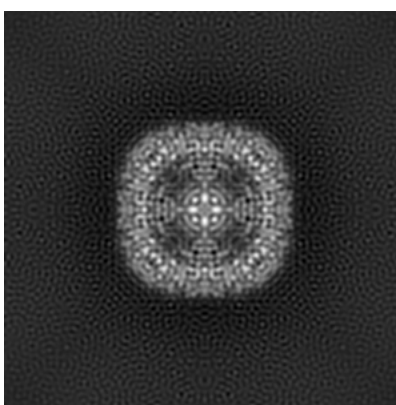
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

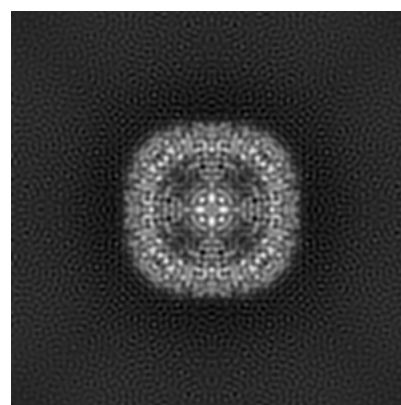
#### 6.1.1 Primary map



X



Y

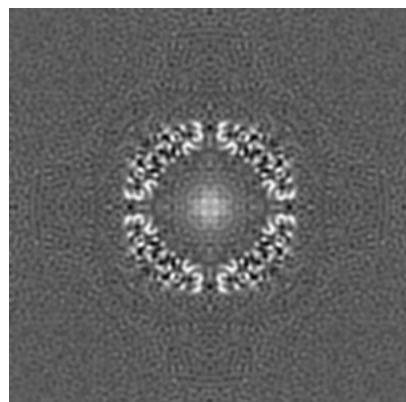


Z

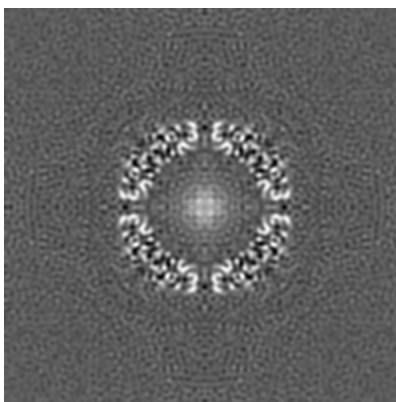
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

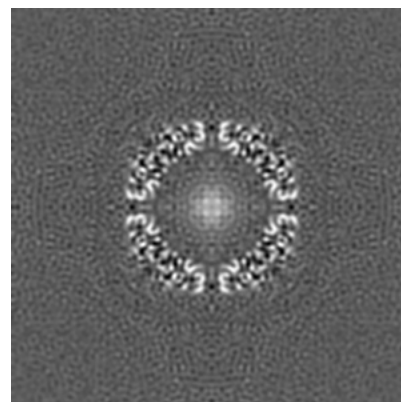
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

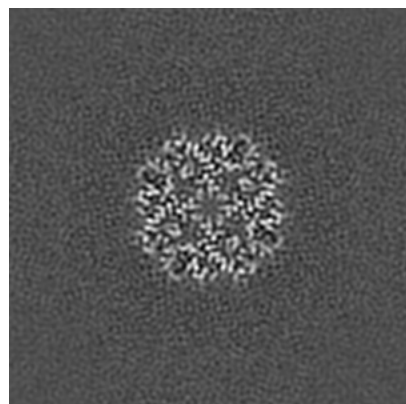


Z Index: 120

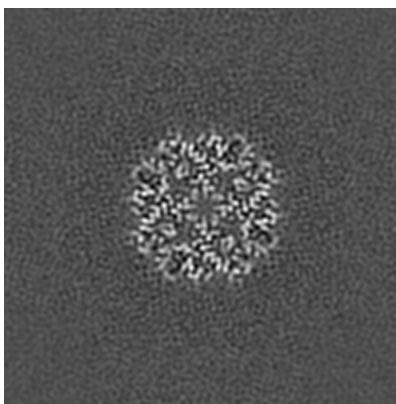
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

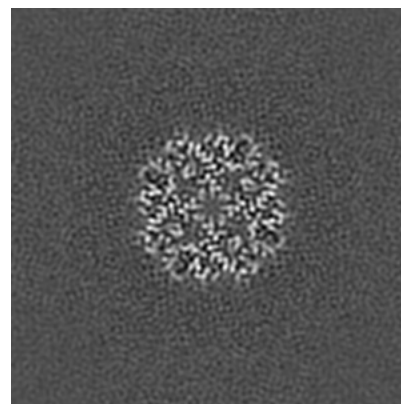
### 6.3.1 Primary map



X Index: 156



Y Index: 156

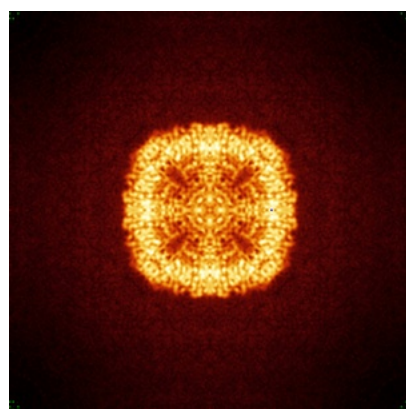


Z Index: 156

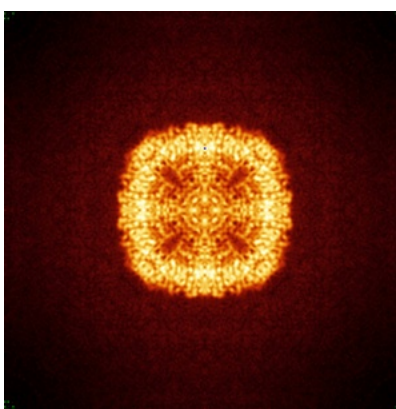
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

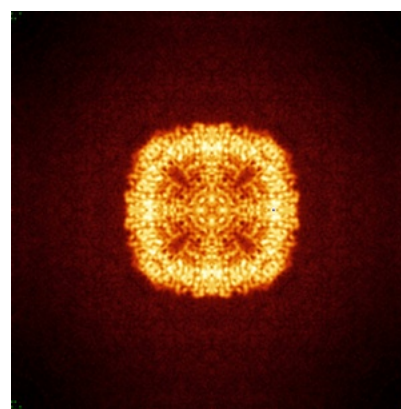
### 6.4.1 Primary map



X



Y



Z

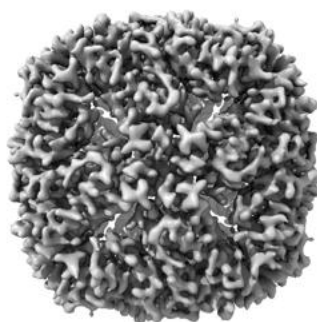
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

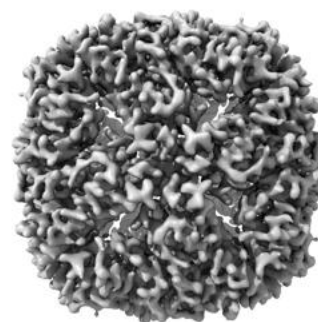
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

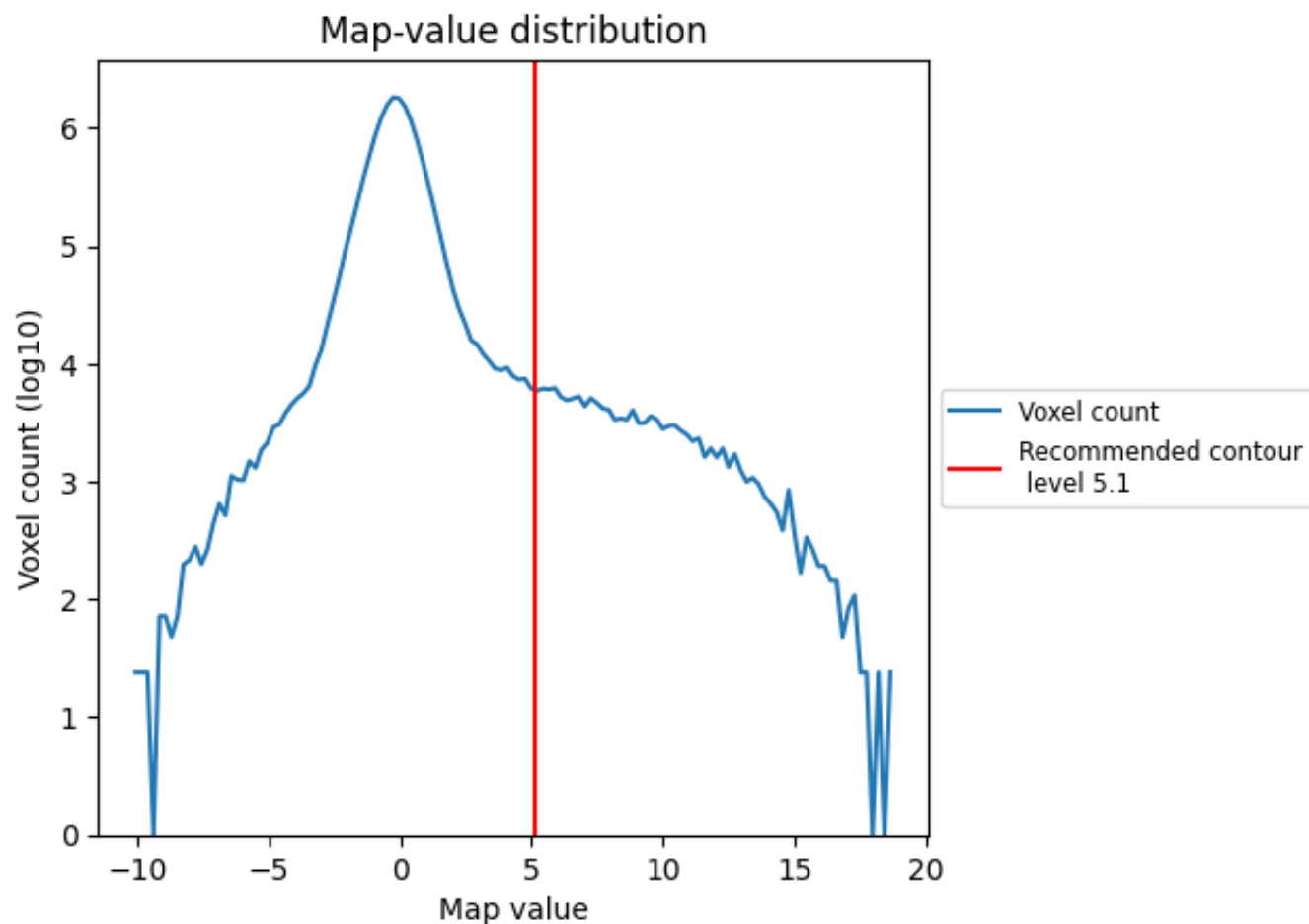
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

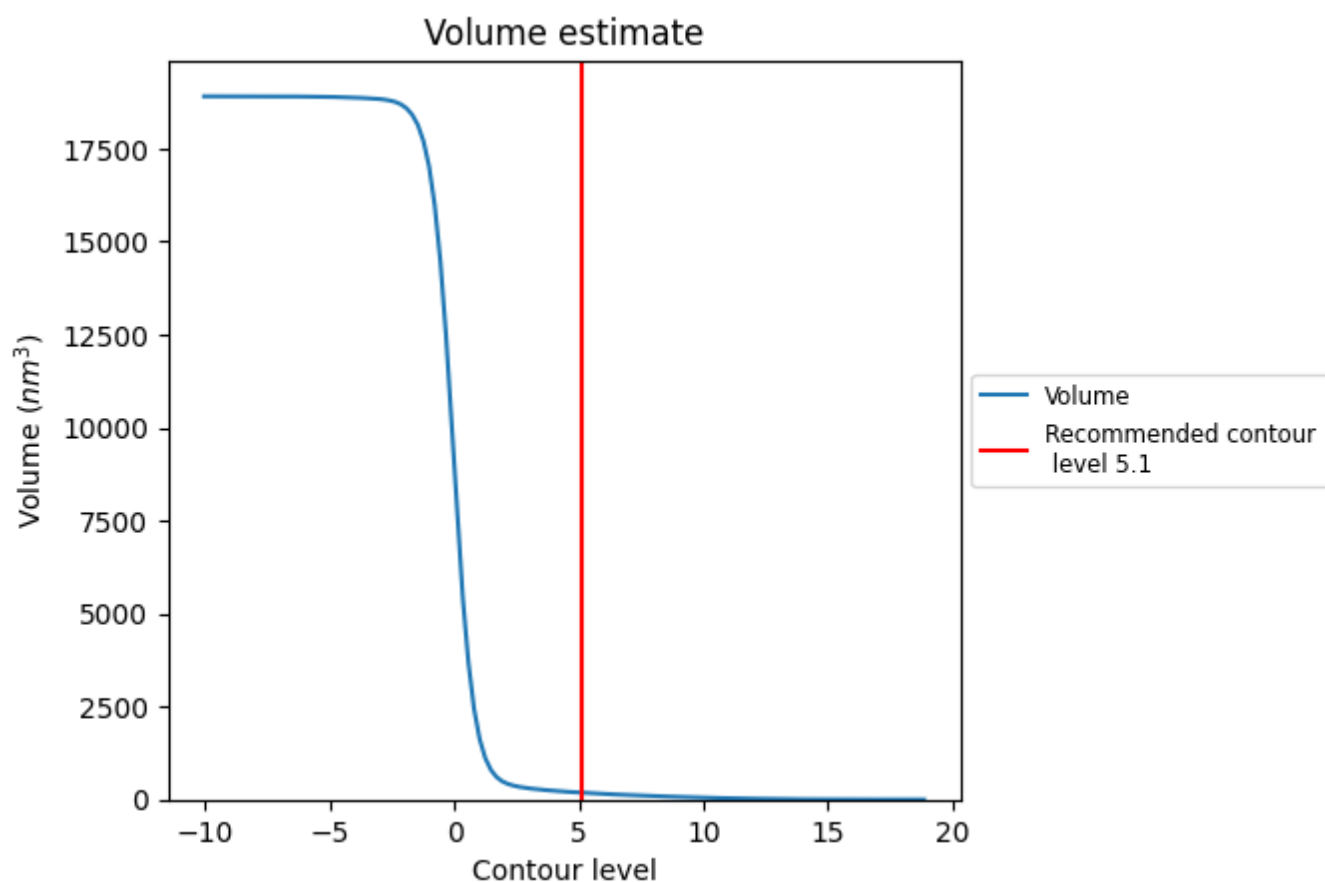
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

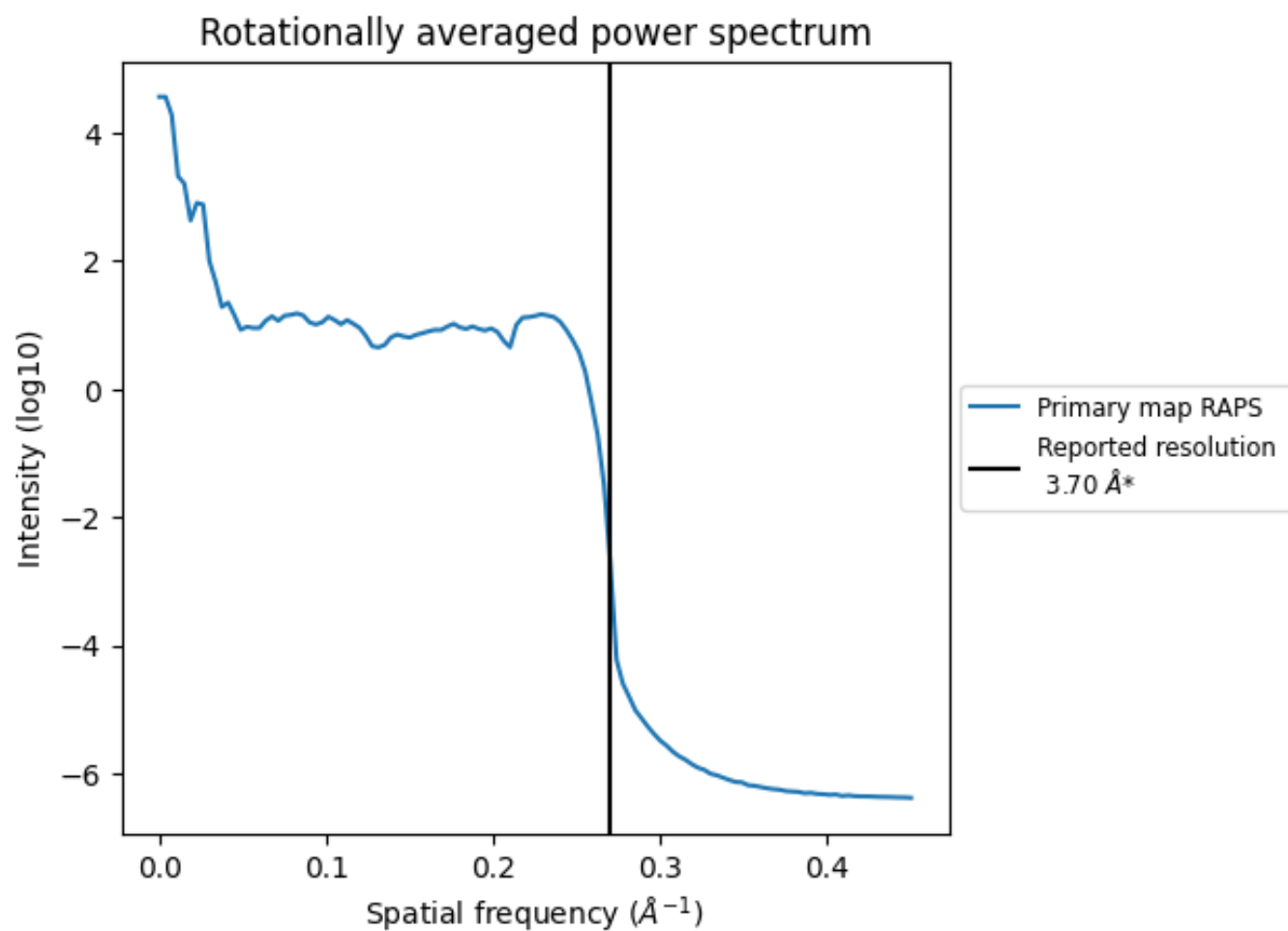
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 185 nm<sup>3</sup>; this corresponds to an approximate mass of 167 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

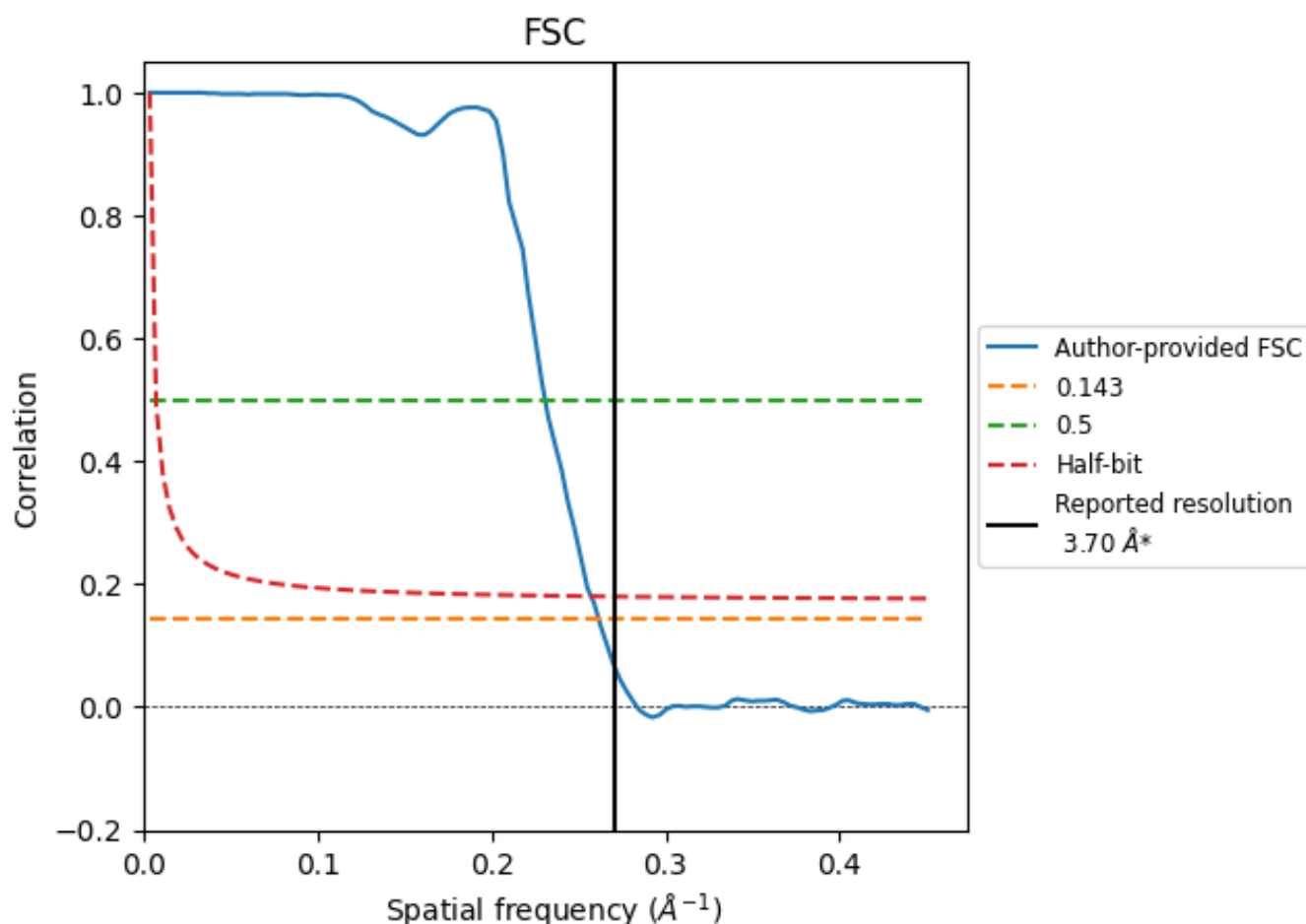


\*Reported resolution corresponds to spatial frequency of 0.270 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.270  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

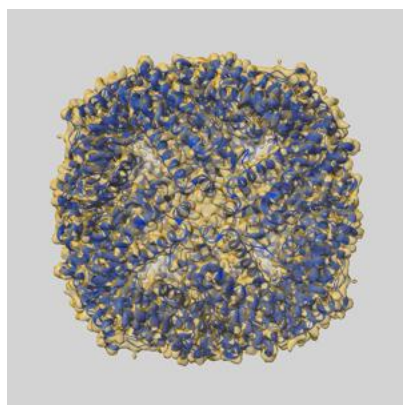
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.70                               | -    | -        |
| Author-provided FSC curve | 3.82                               | 4.33 | 3.89     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

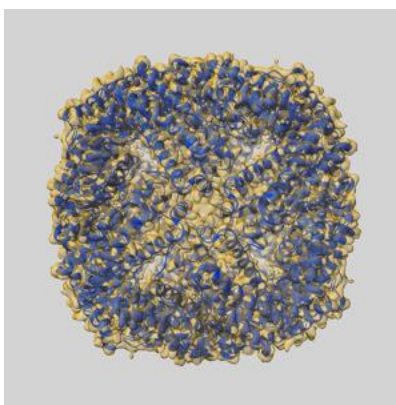
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9913 and PDB model 6K43. Per-residue inclusion information can be found in section [3](#) on page [8](#).

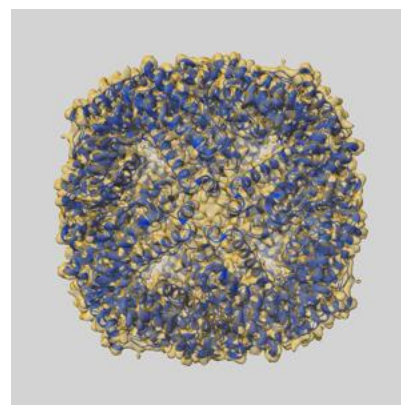
### 9.1 Map-model overlay [i](#)



X



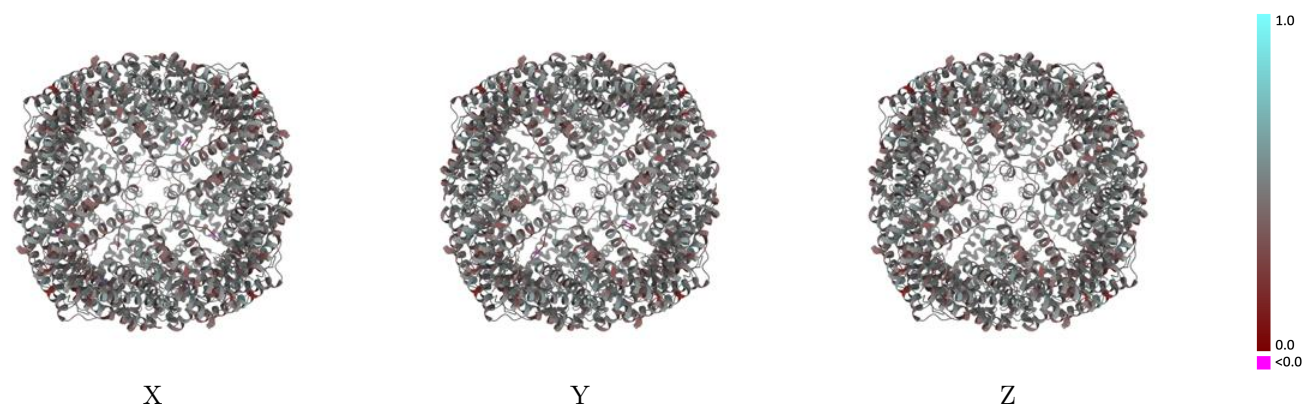
Y



Z

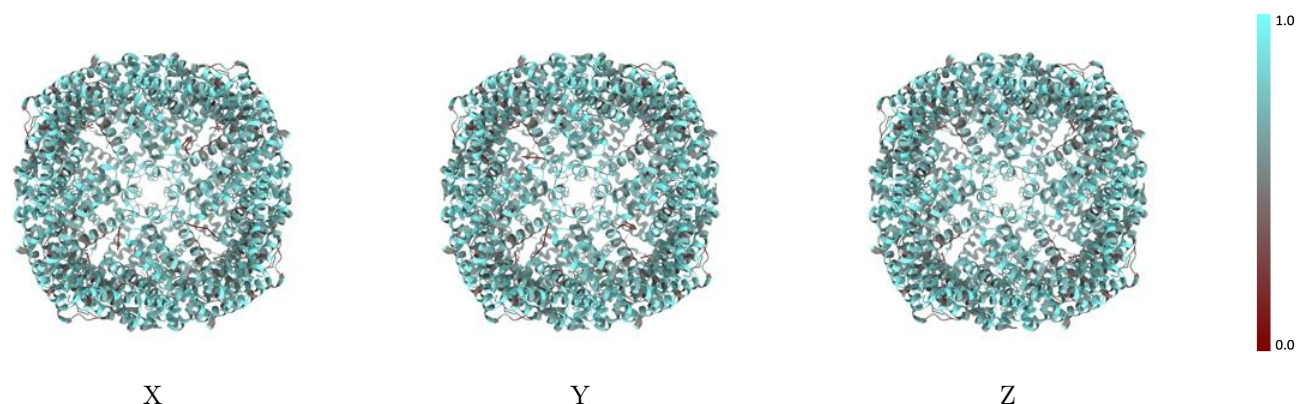
The images above show the 3D surface view of the map at the recommended contour level 5.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



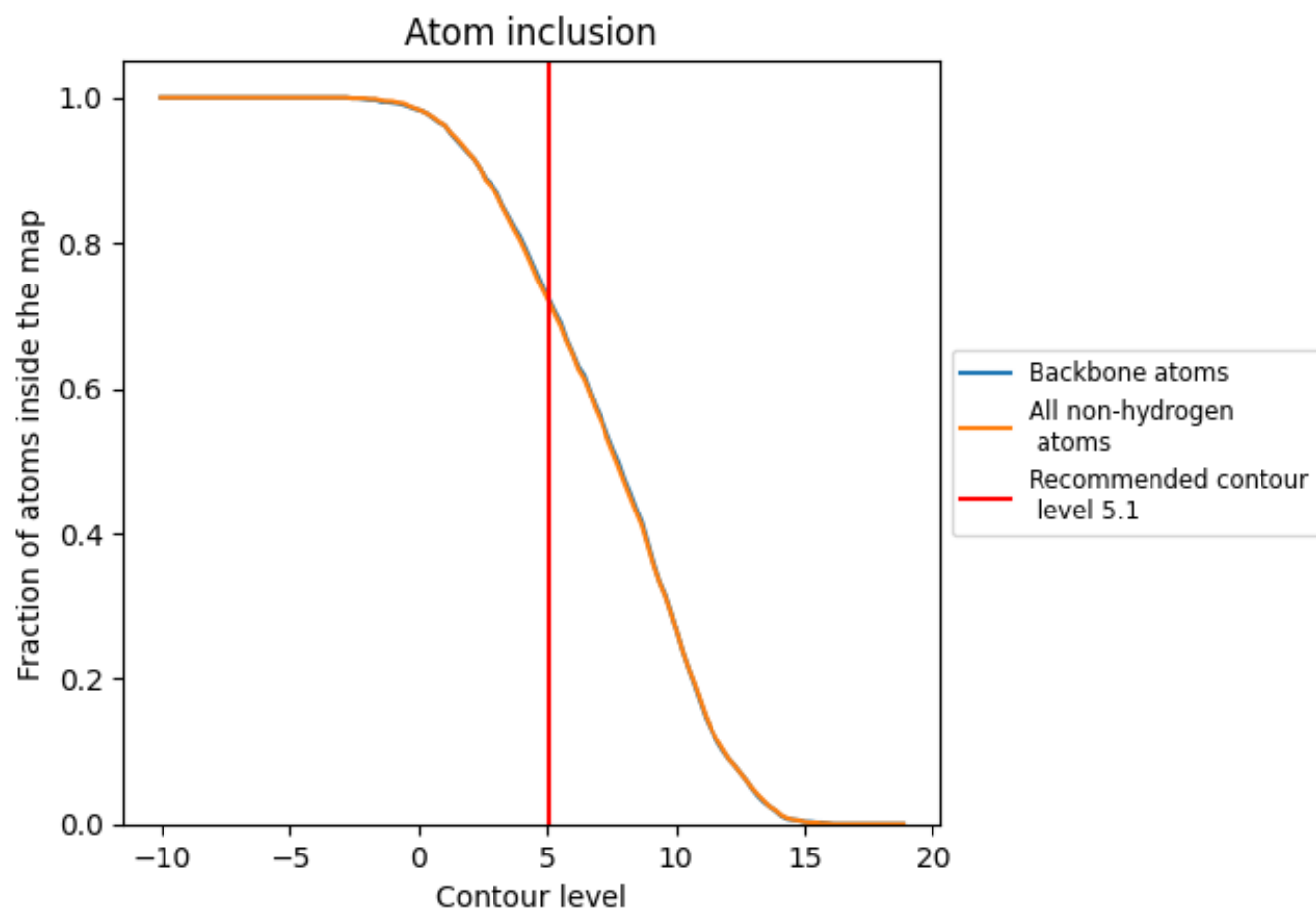
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7170   |  0.4620   |
| A     |  0.7140   |  0.4600   |
| B     |  0.7370   |  0.4660   |
| C     |  0.7120   |  0.4560   |
| D     |  0.7380   |  0.4660   |
| E     |  0.7260   |  0.4630   |
| F     |  0.7180   |  0.4600   |
| G     |  0.7240   |  0.4600   |
| H     |  0.7250   |  0.4620   |
| I     |  0.7210   |  0.4630   |
| J     |  0.7200   |  0.4610   |
| K     |  0.7280   |  0.4610   |
| L     |  0.7150   |  0.4580   |
| M     |  0.7370   |  0.4660   |
| N     |  0.7160  |  0.4640  |
| O     |  0.7110 |  0.4580 |
| P     |  0.7350 |  0.4620 |
| Q     |  0.7180 |  0.4570 |
| R     |  0.7370 |  0.4650 |
| S     |  0.7160 |  0.4580 |
| T     |  0.7140 |  0.4600 |
| U     |  0.7310 |  0.4610 |
| V     |  0.7170 |  0.4610 |
| W     |  0.7370 |  0.4680 |
| X     |  0.7190 |  0.4620 |

