



## Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 02:01 AM JST

PDB ID : 6K4M / pdb\_00006k4m  
EMDB ID : EMD-9915  
Title : Cryo-EM structure of Holo-bacterioferritin form-II from *Streptomyces coelicolor*  
Authors : Jobichen, C.; Sivaraman, J.  
Deposited on : 2019-05-24  
Resolution : 4.50 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

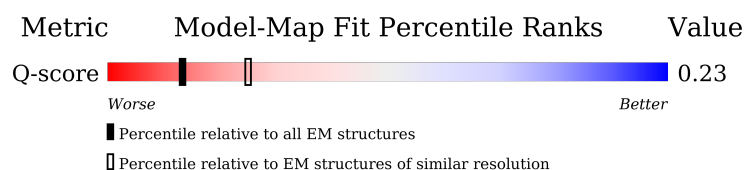
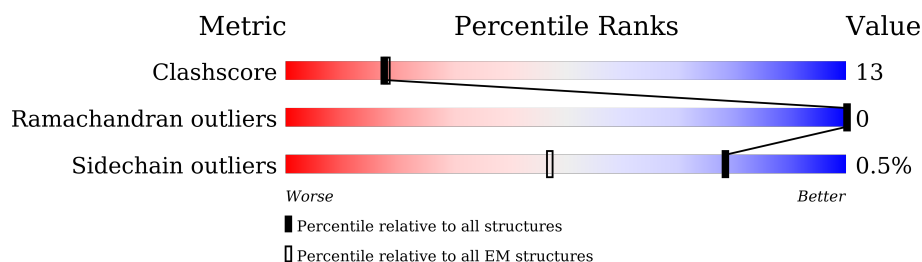
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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.



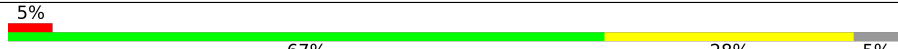
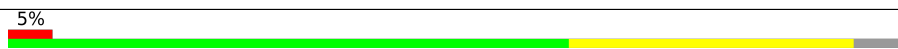
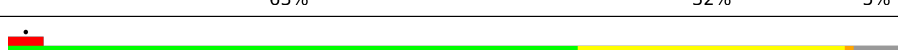
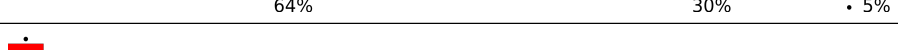
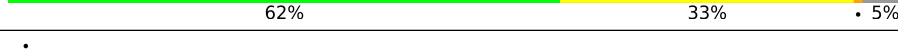
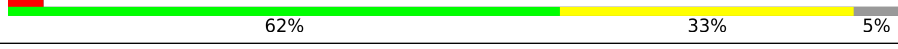
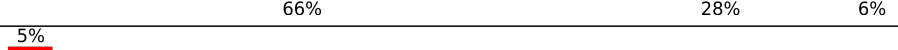
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 2937 ( 4.00 - 5.00 )                                     |

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    | <div> <div>5%</div> <div>62%</div> <div>32%</div> <div>5%</div> </div>  |
| 1   | B     | 167    | <div> <div>5%</div> <div>61%</div> <div>33%</div> <div>6%</div> </div>  |
| 1   | C     | 167    | <div> <div>•</div> <div>64%</div> <div>31%</div> <div>5%</div> </div>   |
| 1   | D     | 167    | <div> <div>•</div> <div>60%</div> <div>34%</div> <div>• 6%</div> </div> |

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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 31508 atoms, of which 0 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     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1290  | 814 | 222 | 250 | 4 |         |       |
| 1   | B     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | C     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1292  | 815 | 222 | 251 | 4 |         |       |
| 1   | D     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | F     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1295  | 817 | 223 | 251 | 4 |         |       |
| 1   | E     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1290  | 814 | 222 | 250 | 4 |         |       |
| 1   | G     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1295  | 817 | 223 | 251 | 4 |         |       |
| 1   | H     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1295  | 817 | 223 | 251 | 4 |         |       |
| 1   | I     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1290  | 814 | 222 | 250 | 4 |         |       |
| 1   | J     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1301  | 820 | 224 | 253 | 4 |         |       |
| 1   | K     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | L     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1292  | 815 | 222 | 251 | 4 |         |       |
| 1   | M     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | N     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1295  | 817 | 223 | 251 | 4 |         |       |
| 1   | O     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1292  | 815 | 222 | 251 | 4 |         |       |
| 1   | P     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | Q     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1292  | 815 | 222 | 251 | 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     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1295  | 817 | 223 | 251 | 4 |         |       |
| 1   | T     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1287  | 812 | 221 | 250 | 4 |         |       |
| 1   | U     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | V     | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1292  | 815 | 222 | 251 | 4 |         |       |
| 1   | W     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1285  | 811 | 221 | 249 | 4 |         |       |
| 1   | X     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1295  | 817 | 223 | 251 | 4 |         |       |

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

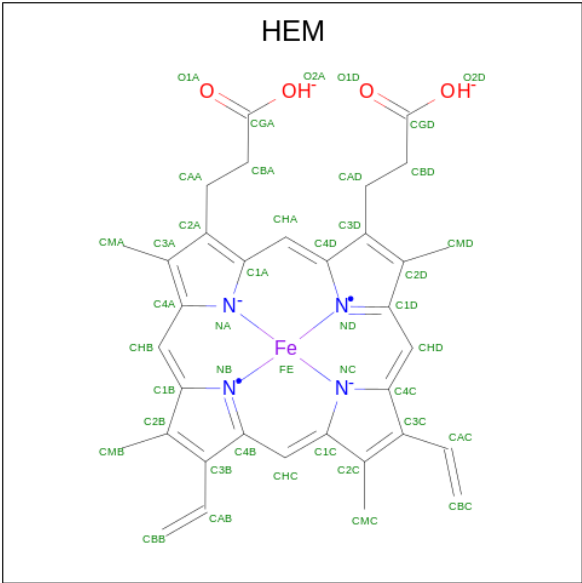
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 2   | A     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | B     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 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 | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | N     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | O     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | P     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | Q     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | R     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | S     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | T     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | U     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | V     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | W     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |
| 2   | X     | 1        | Total | Fe | 0       |
|     |       |          | 1     | 1  |         |

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

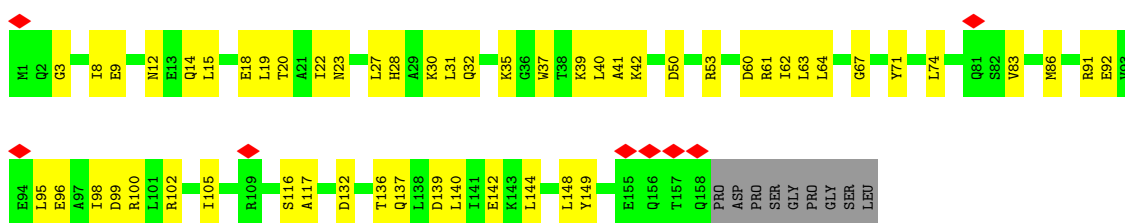


| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 3   | A     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | C     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | F     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | H     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | K     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | L     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | P     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | R     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | S     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | U     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | W     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |
| 3   | X     | 1        | Total<br>43 | C<br>34 | Fe<br>1 | N<br>4 | O<br>4 | 0       |

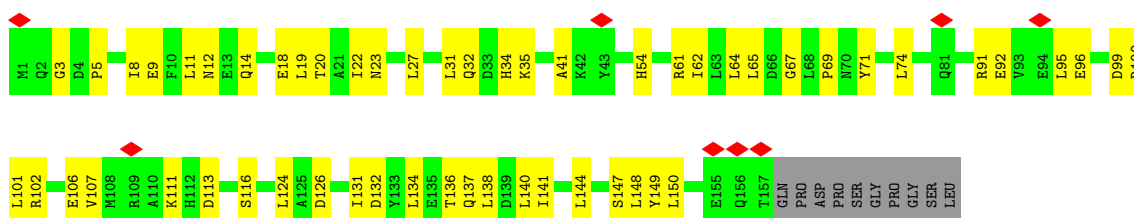
### 3 Residue-property plots [i](#)

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.

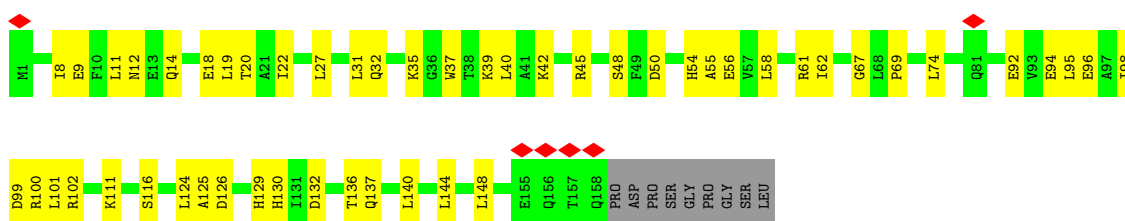
#### • Molecule 1: Bacterioferritin



#### • Molecule 1: Bacterioferritin



#### • Molecule 1: Bacterioferritin

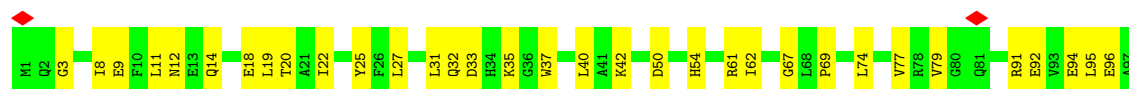


#### • Molecule 1: Bacterioferritin

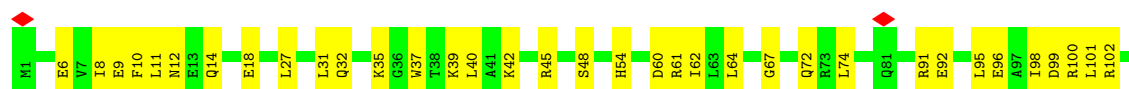




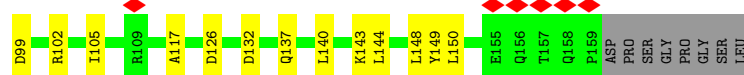
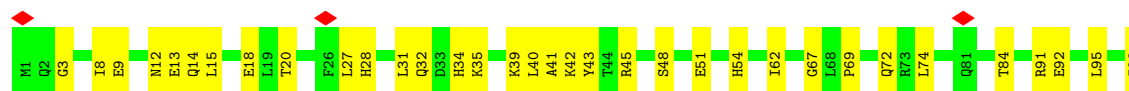
• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin





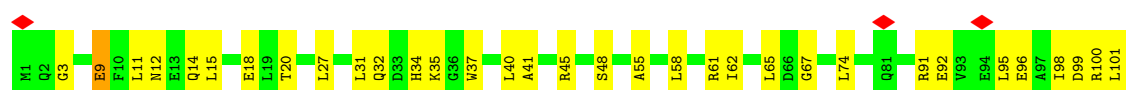
• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin



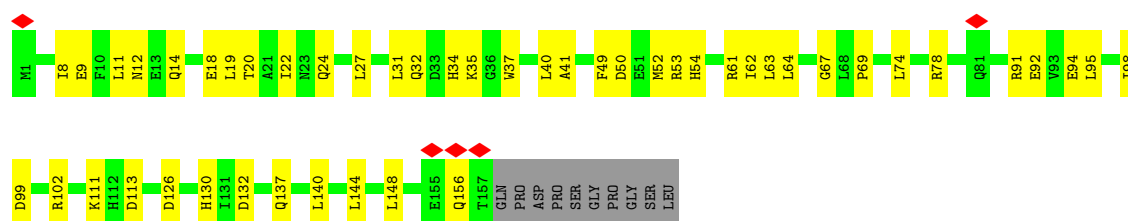
• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin

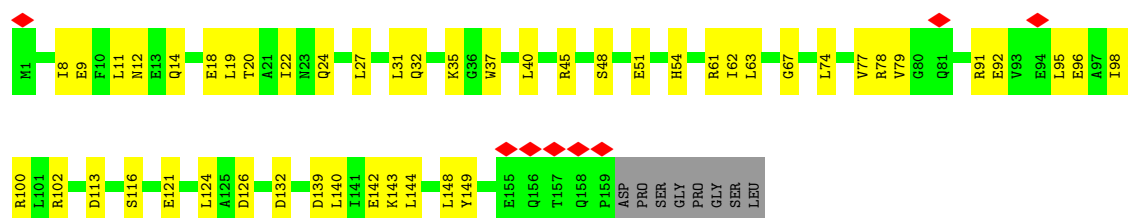


Chain M: 



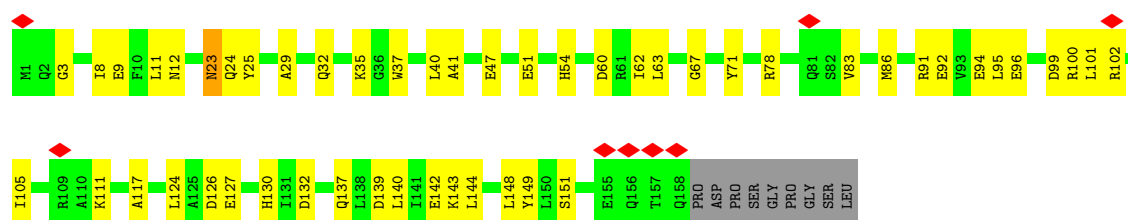
• Molecule 1: Bacterioferritin

Chain N: 



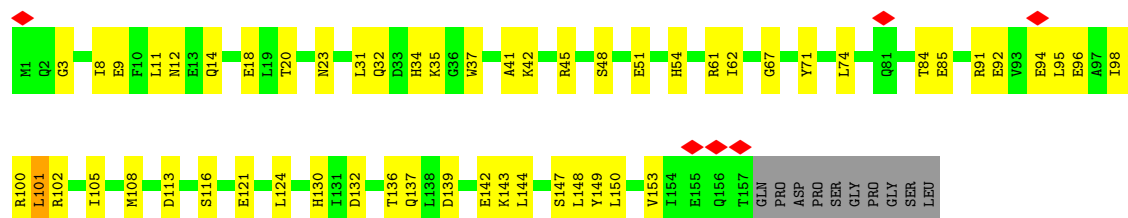
• Molecule 1: Bacterioferritin

Chain O: 



• Molecule 1: Bacterioferritin

Chain P: 



• Molecule 1: Bacterioferritin

Chain Q: 





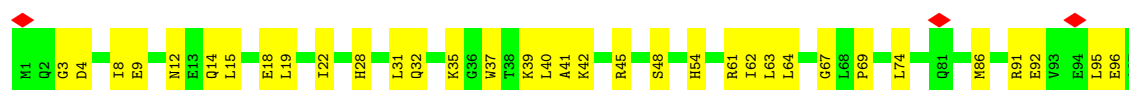
• Molecule 1: Bacterioferritin



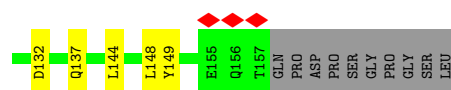
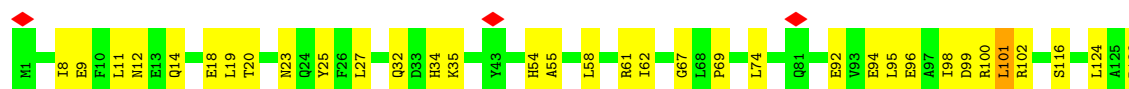
• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin

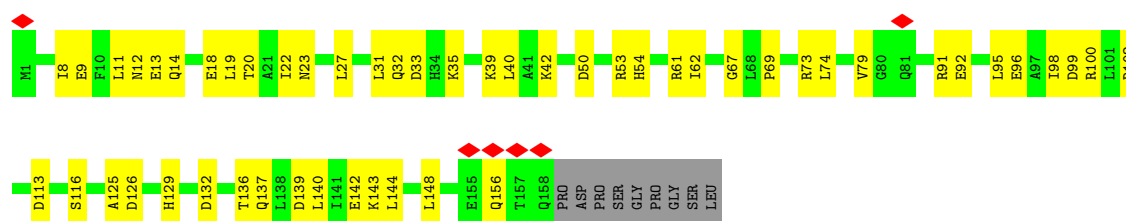


• Molecule 1: Bacterioferritin



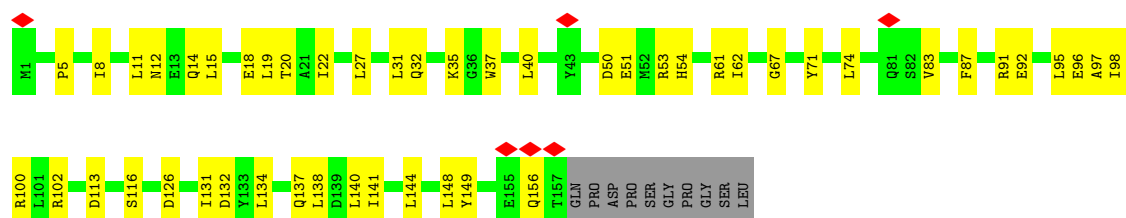
• Molecule 1: Bacterioferritin

Chain V:  63% 31% 5%



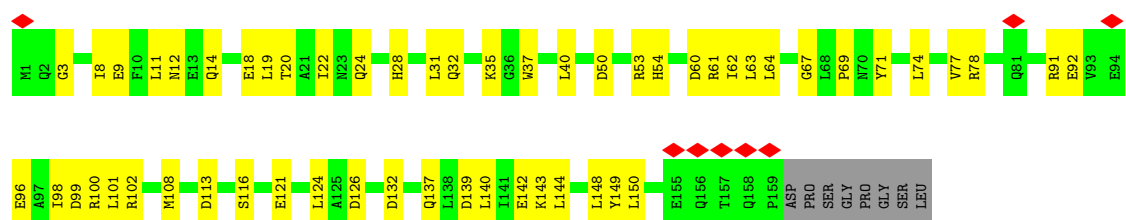
• Molecule 1: Bacterioferritin

Chain W:  64% 30% 6%



• Molecule 1: Bacterioferritin

Chain X:  5% 62% 34% 5%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, O                                | Depositor |
| Number of particles used             | 13793                                   | 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                    | 8.486                                   | Depositor |
| Minimum map value                    | -3.314                                  | Depositor |
| Average map value                    | 0.051                                   | Depositor |
| Map value standard deviation         | 0.650                                   | Depositor |
| Recommended contour level            | 2.22                                    | Depositor |
| Map size (Å)                         | 266.4, 266.4, 266.4                     | wwPDB     |
| Map dimensions                       | 240, 240, 240                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 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     | 0.29         | 0/1311  | 0.58        | 0/1771         |
| 1   | B     | 0.29         | 0/1306  | 0.54        | 0/1764         |
| 1   | C     | 0.28         | 0/1313  | 0.56        | 0/1774         |
| 1   | D     | 0.29         | 0/1306  | 0.57        | 0/1764         |
| 1   | E     | 0.28         | 0/1311  | 0.54        | 0/1771         |
| 1   | F     | 0.28         | 0/1316  | 0.56        | 0/1778         |
| 1   | G     | 0.28         | 0/1316  | 0.55        | 0/1778         |
| 1   | H     | 0.28         | 0/1316  | 0.54        | 0/1778         |
| 1   | I     | 0.29         | 0/1311  | 0.56        | 0/1771         |
| 1   | J     | 0.28         | 0/1322  | 0.56        | 0/1786         |
| 1   | K     | 0.27         | 0/1306  | 0.57        | 0/1764         |
| 1   | L     | 0.30         | 0/1313  | 0.56        | 0/1774         |
| 1   | M     | 0.29         | 0/1306  | 0.56        | 0/1764         |
| 1   | N     | 0.28         | 0/1316  | 0.55        | 0/1778         |
| 1   | O     | 0.29         | 0/1313  | 0.57        | 0/1774         |
| 1   | P     | 0.29         | 0/1306  | 0.57        | 1/1764 (0.1%)  |
| 1   | Q     | 0.28         | 0/1313  | 0.57        | 0/1774         |
| 1   | R     | 0.29         | 0/1306  | 0.56        | 0/1764         |
| 1   | S     | 0.29         | 0/1316  | 0.56        | 0/1778         |
| 1   | T     | 0.28         | 0/1308  | 0.56        | 0/1767         |
| 1   | U     | 0.30         | 0/1306  | 0.54        | 0/1764         |
| 1   | V     | 0.29         | 0/1313  | 0.53        | 0/1774         |
| 1   | W     | 0.29         | 0/1306  | 0.55        | 0/1764         |
| 1   | X     | 0.28         | 0/1316  | 0.57        | 0/1778         |
| All | All   | 0.29         | 0/31472 | 0.56        | 1/42516 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | D     | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| 1   | J     | 0                   | 2                   |
| 1   | M     | 0                   | 1                   |
| 1   | Q     | 0                   | 1                   |
| All | All   | 0                   | 6                   |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | P     | 153 | VAL  | N-CA-C | -5.58 | 107.69      | 113.10   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | D     | 111 | LYS  | Peptide |
| 1   | I     | 111 | LYS  | Peptide |
| 1   | J     | 111 | LYS  | Peptide |
| 1   | J     | 37  | TRP  | Peptide |
| 1   | M     | 111 | LYS  | Peptide |
| 1   | Q     | 111 | LYS  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1290  | 0        | 1264     | 38      | 0            |
| 1   | B     | 1285  | 0        | 1262     | 38      | 0            |
| 1   | C     | 1292  | 0        | 1269     | 32      | 0            |
| 1   | D     | 1285  | 0        | 1262     | 41      | 0            |
| 1   | E     | 1290  | 0        | 1264     | 35      | 0            |
| 1   | F     | 1295  | 0        | 1264     | 38      | 0            |
| 1   | G     | 1295  | 0        | 1265     | 34      | 0            |
| 1   | H     | 1295  | 0        | 1265     | 36      | 0            |
| 1   | I     | 1290  | 0        | 1264     | 36      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | J     | 1301  | 0        | 1276     | 38      | 0            |
| 1   | K     | 1285  | 0        | 1262     | 32      | 0            |
| 1   | L     | 1292  | 0        | 1269     | 36      | 0            |
| 1   | M     | 1285  | 0        | 1262     | 34      | 0            |
| 1   | N     | 1295  | 0        | 1265     | 32      | 0            |
| 1   | O     | 1292  | 0        | 1269     | 40      | 0            |
| 1   | P     | 1285  | 0        | 1262     | 41      | 0            |
| 1   | Q     | 1292  | 0        | 1269     | 42      | 0            |
| 1   | R     | 1285  | 0        | 1261     | 36      | 0            |
| 1   | S     | 1295  | 0        | 1264     | 41      | 0            |
| 1   | T     | 1287  | 0        | 1267     | 36      | 0            |
| 1   | U     | 1285  | 0        | 1261     | 25      | 0            |
| 1   | V     | 1292  | 0        | 1269     | 36      | 0            |
| 1   | W     | 1285  | 0        | 1262     | 36      | 0            |
| 1   | X     | 1295  | 0        | 1265     | 40      | 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            |
| 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    | 0        | 30       | 0       | 0            |
| 3   | C     | 43    | 0        | 30       | 1       | 0            |
| 3   | F     | 43    | 0        | 30       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | H     | 43    | 0        | 30       | 0       | 0            |
| 3   | K     | 43    | 0        | 30       | 0       | 0            |
| 3   | L     | 43    | 0        | 30       | 0       | 0            |
| 3   | P     | 43    | 0        | 30       | 0       | 0            |
| 3   | R     | 43    | 0        | 30       | 0       | 0            |
| 3   | S     | 43    | 0        | 30       | 1       | 0            |
| 3   | U     | 43    | 0        | 30       | 0       | 0            |
| 3   | W     | 43    | 0        | 30       | 1       | 0            |
| 3   | X     | 43    | 0        | 30       | 0       | 0            |
| All | All   | 31508 | 0        | 30722    | 838     | 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 13.

All (838) 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:P:32:GLN:HB2  | 1:P:37:TRP:HB2   | 1.71                     | 0.71              |
| 1:Q:14:GLN:HE21 | 1:Q:18:GLU:HG2   | 1.58                     | 0.67              |
| 1:F:77:VAL:H    | 1:E:72:GLN:HE22  | 1.41                     | 0.66              |
| 1:H:72:GLN:HE22 | 1:N:77:VAL:H     | 1.41                     | 0.66              |
| 1:A:32:GLN:HB2  | 1:A:37:TRP:HB2   | 1.77                     | 0.66              |
| 1:X:32:GLN:HB2  | 1:X:37:TRP:HB2   | 1.78                     | 0.65              |
| 1:I:72:GLN:HE22 | 1:S:77:VAL:H     | 1.43                     | 0.64              |
| 1:M:32:GLN:HB2  | 1:M:37:TRP:HB2   | 1.79                     | 0.64              |
| 1:K:32:GLN:HB2  | 1:K:37:TRP:HB2   | 1.78                     | 0.64              |
| 1:B:14:GLN:NE2  | 1:B:18:GLU:OE1   | 2.30                     | 0.64              |
| 1:B:144:LEU:HB3 | 1:B:148:LEU:HD11 | 1.80                     | 0.64              |
| 1:O:32:GLN:HA   | 1:O:35:LYS:HB2   | 1.80                     | 0.64              |
| 1:F:144:LEU:HB3 | 1:F:148:LEU:HD11 | 1.79                     | 0.63              |
| 1:I:12:ASN:HA   | 1:I:15:LEU:HD12  | 1.79                     | 0.63              |
| 1:L:14:GLN:NE2  | 1:L:18:GLU:OE2   | 2.29                     | 0.63              |
| 1:J:14:GLN:NE2  | 1:J:18:GLU:OE2   | 2.30                     | 0.63              |
| 1:F:137:GLN:HA  | 1:F:140:LEU:HD12 | 1.82                     | 0.62              |
| 1:D:14:GLN:NE2  | 1:D:18:GLU:OE2   | 2.33                     | 0.62              |
| 1:H:14:GLN:NE2  | 1:H:18:GLU:OE2   | 2.30                     | 0.62              |
| 1:E:14:GLN:NE2  | 1:E:18:GLU:OE2   | 2.33                     | 0.62              |
| 1:J:139:ASP:HA  | 1:J:142:GLU:HB3  | 1.82                     | 0.62              |
| 1:U:144:LEU:HB3 | 1:U:148:LEU:HD11 | 1.82                     | 0.62              |
| 1:P:144:LEU:HB3 | 1:P:148:LEU:HD11 | 1.82                     | 0.62              |
| 1:W:132:ASP:OD2 | 1:W:132:ASP:N    | 2.33                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:100:ARG:HD3  | 1:J:103:ARG:HH12 | 1.64                     | 0.61              |
| 1:J:139:ASP:N    | 1:J:139:ASP:OD1  | 2.33                     | 0.61              |
| 1:O:32:GLN:HB2   | 1:O:37:TRP:HB2   | 1.82                     | 0.61              |
| 1:M:9:GLU:HA     | 1:M:12:ASN:HB2   | 1.82                     | 0.61              |
| 1:A:14:GLN:NE2   | 1:A:18:GLU:OE2   | 2.33                     | 0.61              |
| 1:M:50:ASP:HB3   | 1:M:53:ARG:HH21  | 1.66                     | 0.61              |
| 1:O:83:VAL:HA    | 1:O:86:MET:HE2   | 1.81                     | 0.61              |
| 1:X:32:GLN:HA    | 1:X:35:LYS:HB2   | 1.82                     | 0.61              |
| 1:X:144:LEU:HB3  | 1:X:148:LEU:HD11 | 1.82                     | 0.61              |
| 1:E:32:GLN:HE22  | 1:E:40:LEU:HG    | 1.65                     | 0.61              |
| 1:N:32:GLN:HA    | 1:N:35:LYS:HB2   | 1.82                     | 0.61              |
| 1:R:9:GLU:HA     | 1:R:12:ASN:HB2   | 1.83                     | 0.61              |
| 1:D:156:GLN:HE22 | 1:J:40:LEU:HA    | 1.65                     | 0.61              |
| 1:Q:32:GLN:HA    | 1:Q:35:LYS:HB2   | 1.83                     | 0.61              |
| 1:E:32:GLN:HA    | 1:E:35:LYS:HB2   | 1.83                     | 0.60              |
| 1:K:9:GLU:HA     | 1:K:12:ASN:HB2   | 1.83                     | 0.60              |
| 1:I:144:LEU:HB3  | 1:I:148:LEU:HD11 | 1.81                     | 0.60              |
| 1:S:32:GLN:HA    | 1:S:35:LYS:HB2   | 1.83                     | 0.60              |
| 1:D:61:ARG:HA    | 1:D:64:LEU:HD12  | 1.83                     | 0.60              |
| 1:T:144:LEU:HD12 | 1:T:148:LEU:HD11 | 1.83                     | 0.60              |
| 1:L:50:ASP:HA    | 1:L:53:ARG:HE    | 1.66                     | 0.60              |
| 1:V:14:GLN:NE2   | 1:V:18:GLU:OE2   | 2.34                     | 0.60              |
| 1:H:32:GLN:HE22  | 1:H:40:LEU:HG    | 1.65                     | 0.60              |
| 1:A:32:GLN:HA    | 1:A:35:LYS:HB2   | 1.84                     | 0.60              |
| 1:O:71:TYR:HB3   | 1:P:23:ASN:HD22  | 1.67                     | 0.60              |
| 1:W:54:HIS:NE2   | 1:W:126:ASP:OD2  | 2.35                     | 0.60              |
| 1:D:132:ASP:OD1  | 1:D:132:ASP:N    | 2.31                     | 0.60              |
| 1:I:14:GLN:NE2   | 1:I:18:GLU:OE2   | 2.34                     | 0.60              |
| 1:I:32:GLN:HA    | 1:I:35:LYS:HB2   | 1.84                     | 0.60              |
| 1:Q:132:ASP:N    | 1:Q:132:ASP:OD1  | 2.33                     | 0.60              |
| 1:R:14:GLN:NE2   | 1:R:18:GLU:OE2   | 2.35                     | 0.60              |
| 1:B:8:ILE:HA     | 1:B:11:LEU:HD12  | 1.84                     | 0.59              |
| 1:O:105:ILE:HG23 | 1:O:117:ALA:HB1  | 1.84                     | 0.59              |
| 1:O:132:ASP:OD2  | 1:O:132:ASP:N    | 2.35                     | 0.59              |
| 1:D:96:GLU:HG3   | 1:D:100:ARG:HH22 | 1.67                     | 0.59              |
| 1:F:8:ILE:HA     | 1:F:11:LEU:HD12  | 1.85                     | 0.59              |
| 1:C:99:ASP:OD2   | 1:C:99:ASP:N     | 2.36                     | 0.59              |
| 1:R:8:ILE:HA     | 1:R:11:LEU:HD12  | 1.84                     | 0.59              |
| 1:T:14:GLN:NE2   | 1:T:18:GLU:OE2   | 2.33                     | 0.59              |
| 1:G:99:ASP:N     | 1:G:99:ASP:OD2   | 2.35                     | 0.59              |
| 1:A:99:ASP:OD2   | 1:A:99:ASP:N     | 2.36                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:14:GLN:NE2   | 1:F:18:GLU:OE2   | 2.36                     | 0.59              |
| 1:N:32:GLN:HB2   | 1:N:37:TRP:HB2   | 1.85                     | 0.59              |
| 1:Q:137:GLN:HA   | 1:Q:140:LEU:HD12 | 1.85                     | 0.59              |
| 1:O:144:LEU:HD12 | 1:O:148:LEU:HD11 | 1.84                     | 0.59              |
| 1:S:14:GLN:NE2   | 1:S:18:GLU:OE2   | 2.36                     | 0.59              |
| 1:J:50:ASP:HB3   | 1:J:53:ARG:HH21  | 1.68                     | 0.59              |
| 1:M:32:GLN:HA    | 1:M:35:LYS:HB2   | 1.85                     | 0.59              |
| 1:M:99:ASP:OD2   | 1:M:99:ASP:N     | 2.36                     | 0.59              |
| 1:A:20:THR:HG23  | 1:A:74:LEU:HD22  | 1.84                     | 0.59              |
| 1:I:32:GLN:HE22  | 1:I:40:LEU:HG    | 1.67                     | 0.59              |
| 1:T:32:GLN:HA    | 1:T:35:LYS:HB2   | 1.83                     | 0.59              |
| 1:A:23:ASN:HD22  | 1:B:71:TYR:HB3   | 1.68                     | 0.58              |
| 1:K:100:ARG:HD3  | 1:K:103:ARG:HH12 | 1.66                     | 0.58              |
| 1:S:61:ARG:HA    | 1:S:64:LEU:HD12  | 1.85                     | 0.58              |
| 1:X:14:GLN:NE2   | 1:X:18:GLU:OE2   | 2.33                     | 0.58              |
| 1:M:49:PHE:HA    | 1:M:52:MET:HE2   | 1.84                     | 0.58              |
| 1:R:32:GLN:HB2   | 1:R:37:TRP:HB2   | 1.85                     | 0.58              |
| 1:S:54:HIS:NE2   | 1:S:126:ASP:OD2  | 2.36                     | 0.58              |
| 1:B:61:ARG:HE    | 1:B:116:SER:HB3  | 1.69                     | 0.58              |
| 1:H:101:LEU:HB3  | 1:H:124:LEU:HD22 | 1.84                     | 0.58              |
| 1:L:32:GLN:HA    | 1:L:35:LYS:HB2   | 1.86                     | 0.58              |
| 1:R:61:ARG:HE    | 1:R:116:SER:HB3  | 1.69                     | 0.58              |
| 1:I:8:ILE:HA     | 1:I:11:LEU:HD12  | 1.85                     | 0.58              |
| 1:L:8:ILE:HA     | 1:L:11:LEU:HD12  | 1.85                     | 0.58              |
| 1:C:14:GLN:NE2   | 1:C:18:GLU:OE2   | 2.37                     | 0.58              |
| 1:K:14:GLN:NE2   | 1:K:18:GLU:OE1   | 2.36                     | 0.58              |
| 1:L:34:HIS:HB2   | 1:M:63:LEU:HD21  | 1.86                     | 0.58              |
| 1:N:14:GLN:NE2   | 1:N:18:GLU:OE2   | 2.36                     | 0.58              |
| 1:F:32:GLN:HE22  | 1:F:40:LEU:HG    | 1.68                     | 0.58              |
| 1:H:144:LEU:HB3  | 1:H:148:LEU:HD11 | 1.86                     | 0.58              |
| 1:X:54:HIS:NE2   | 1:X:126:ASP:OD2  | 2.36                     | 0.58              |
| 1:C:132:ASP:OD2  | 1:C:132:ASP:N    | 2.37                     | 0.58              |
| 1:N:144:LEU:HB3  | 1:N:148:LEU:HD11 | 1.86                     | 0.58              |
| 1:P:8:ILE:HA     | 1:P:11:LEU:HD12  | 1.86                     | 0.58              |
| 1:C:144:LEU:HB3  | 1:C:148:LEU:HD11 | 1.84                     | 0.57              |
| 1:D:99:ASP:OD1   | 1:D:99:ASP:N     | 2.37                     | 0.57              |
| 1:F:105:ILE:HA   | 1:F:108:MET:HE2  | 1.85                     | 0.57              |
| 1:G:12:ASN:HA    | 1:G:15:LEU:HD12  | 1.86                     | 0.57              |
| 1:G:143:LYS:HD3  | 1:G:144:LEU:HD22 | 1.86                     | 0.57              |
| 1:V:8:ILE:HA     | 1:V:11:LEU:HD12  | 1.86                     | 0.57              |
| 1:D:54:HIS:NE2   | 1:D:126:ASP:OD2  | 2.34                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:8:ILE:HA     | 1:S:11:LEU:HD12  | 1.86                     | 0.57              |
| 1:W:14:GLN:NE2   | 1:W:18:GLU:OE2   | 2.36                     | 0.57              |
| 1:A:96:GLU:HG3   | 1:A:100:ARG:HH22 | 1.69                     | 0.57              |
| 1:W:50:ASP:HB3   | 1:W:53:ARG:HH21  | 1.69                     | 0.57              |
| 1:A:105:ILE:HG23 | 1:A:117:ALA:HB1  | 1.86                     | 0.57              |
| 1:D:32:GLN:HA    | 1:D:35:LYS:HB2   | 1.87                     | 0.57              |
| 1:G:14:GLN:NE2   | 1:G:18:GLU:OE2   | 2.33                     | 0.57              |
| 1:L:144:LEU:HD12 | 1:L:148:LEU:HD11 | 1.85                     | 0.57              |
| 1:R:96:GLU:HG3   | 1:R:100:ARG:HH22 | 1.68                     | 0.57              |
| 1:S:20:THR:HG23  | 1:S:74:LEU:HD22  | 1.85                     | 0.57              |
| 1:W:99:ASP:OD1   | 1:W:99:ASP:N     | 2.38                     | 0.57              |
| 1:D:61:ARG:NH2   | 1:D:113:ASP:OD2  | 2.38                     | 0.57              |
| 1:P:99:ASP:OD2   | 1:P:99:ASP:N     | 2.37                     | 0.57              |
| 1:S:144:LEU:HB3  | 1:S:148:LEU:HD11 | 1.85                     | 0.57              |
| 1:E:61:ARG:HA    | 1:E:64:LEU:HD12  | 1.85                     | 0.57              |
| 1:N:32:GLN:HE22  | 1:N:40:LEU:HG    | 1.70                     | 0.57              |
| 1:P:132:ASP:OD2  | 1:P:132:ASP:N    | 2.37                     | 0.57              |
| 1:T:54:HIS:NE2   | 1:T:126:ASP:OD2  | 2.37                     | 0.57              |
| 1:G:132:ASP:OD1  | 1:G:132:ASP:N    | 2.37                     | 0.57              |
| 1:V:137:GLN:HA   | 1:V:140:LEU:HD12 | 1.85                     | 0.57              |
| 1:X:99:ASP:N     | 1:X:99:ASP:OD2   | 2.38                     | 0.57              |
| 1:C:20:THR:HG23  | 1:C:74:LEU:HD22  | 1.87                     | 0.57              |
| 1:D:20:THR:HG23  | 1:D:74:LEU:HD22  | 1.86                     | 0.57              |
| 1:E:99:ASP:OD2   | 1:E:99:ASP:N     | 2.38                     | 0.57              |
| 1:V:144:LEU:HB3  | 1:V:148:LEU:HD11 | 1.87                     | 0.57              |
| 1:J:63:LEU:HD21  | 1:K:34:HIS:HB2   | 1.86                     | 0.57              |
| 1:M:8:ILE:HA     | 1:M:11:LEU:HD12  | 1.87                     | 0.57              |
| 1:T:99:ASP:N     | 1:T:99:ASP:OD1   | 2.38                     | 0.57              |
| 1:E:96:GLU:HG3   | 1:E:100:ARG:HH22 | 1.69                     | 0.56              |
| 1:E:132:ASP:N    | 1:E:132:ASP:OD1  | 2.38                     | 0.56              |
| 1:H:100:ARG:HD2  | 1:H:103:ARG:HH22 | 1.70                     | 0.56              |
| 1:I:99:ASP:N     | 1:I:99:ASP:OD2   | 2.37                     | 0.56              |
| 1:S:132:ASP:OD1  | 1:S:132:ASP:N    | 2.38                     | 0.56              |
| 1:X:8:ILE:HA     | 1:X:11:LEU:HD12  | 1.87                     | 0.56              |
| 1:A:61:ARG:HA    | 1:A:64:LEU:HD12  | 1.85                     | 0.56              |
| 1:J:32:GLN:HA    | 1:J:35:LYS:HB2   | 1.86                     | 0.56              |
| 1:U:132:ASP:OD2  | 1:U:132:ASP:N    | 2.38                     | 0.56              |
| 1:X:19:LEU:HA    | 1:X:22:ILE:HD12  | 1.87                     | 0.56              |
| 1:B:106:GLU:HG3  | 1:B:107:VAL:HG23 | 1.88                     | 0.56              |
| 1:F:101:LEU:HB3  | 1:F:124:LEU:HD22 | 1.88                     | 0.56              |
| 1:N:19:LEU:HA    | 1:N:22:ILE:HD12  | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:132:ASP:OD1  | 1:N:132:ASP:N    | 2.38                     | 0.56              |
| 1:Q:50:ASP:HA    | 1:Q:53:ARG:HE    | 1.69                     | 0.56              |
| 1:B:132:ASP:OD1  | 1:B:132:ASP:N    | 2.39                     | 0.56              |
| 1:G:9:GLU:HA     | 1:G:12:ASN:HB2   | 1.86                     | 0.56              |
| 1:X:132:ASP:OD1  | 1:X:132:ASP:N    | 2.39                     | 0.56              |
| 1:N:54:HIS:NE2   | 1:N:126:ASP:OD2  | 2.38                     | 0.56              |
| 1:Q:49:PHE:HA    | 1:Q:52:MET:HG3   | 1.87                     | 0.56              |
| 1:F:132:ASP:OD2  | 1:F:132:ASP:N    | 2.33                     | 0.56              |
| 1:V:19:LEU:HA    | 1:V:22:ILE:HD12  | 1.88                     | 0.56              |
| 1:V:96:GLU:HG3   | 1:V:100:ARG:HH12 | 1.70                     | 0.56              |
| 1:C:19:LEU:HA    | 1:C:22:ILE:HD12  | 1.88                     | 0.56              |
| 1:C:32:GLN:HE22  | 1:C:40:LEU:HG    | 1.71                     | 0.56              |
| 1:D:9:GLU:HA     | 1:D:12:ASN:HB2   | 1.87                     | 0.56              |
| 1:S:156:GLN:HE22 | 1:W:40:LEU:HA    | 1.71                     | 0.56              |
| 1:V:61:ARG:HE    | 1:V:116:SER:HB3  | 1.71                     | 0.56              |
| 1:C:96:GLU:O     | 1:C:100:ARG:NH1  | 2.39                     | 0.55              |
| 1:J:132:ASP:N    | 1:J:132:ASP:OD1  | 2.38                     | 0.55              |
| 1:U:99:ASP:OD2   | 1:U:99:ASP:N     | 2.36                     | 0.55              |
| 1:L:96:GLU:O     | 1:L:100:ARG:NH1  | 2.39                     | 0.55              |
| 1:W:96:GLU:HG3   | 1:W:100:ARG:HH12 | 1.71                     | 0.55              |
| 1:L:94:GLU:OE2   | 1:L:130:HIS:ND1  | 2.39                     | 0.55              |
| 1:M:11:LEU:HD13  | 1:M:62:ILE:HG22  | 1.87                     | 0.55              |
| 1:D:19:LEU:HA    | 1:D:22:ILE:HD12  | 1.89                     | 0.55              |
| 1:T:61:ARG:HA    | 1:T:64:LEU:HD12  | 1.88                     | 0.55              |
| 1:U:55:ALA:HA    | 1:U:58:LEU:HD12  | 1.87                     | 0.55              |
| 1:J:61:ARG:HA    | 1:J:64:LEU:HD12  | 1.88                     | 0.55              |
| 1:T:98:ILE:O     | 1:T:102:ARG:N    | 2.37                     | 0.55              |
| 1:U:8:ILE:HA     | 1:U:11:LEU:HD12  | 1.89                     | 0.55              |
| 1:U:101:LEU:HB3  | 1:U:124:LEU:HD11 | 1.89                     | 0.55              |
| 1:A:83:VAL:HA    | 1:A:86:MET:HE2   | 1.89                     | 0.55              |
| 1:H:9:GLU:HA     | 1:H:12:ASN:HB2   | 1.89                     | 0.55              |
| 1:B:32:GLN:HA    | 1:B:35:LYS:HB2   | 1.88                     | 0.55              |
| 1:N:99:ASP:N     | 1:N:99:ASP:OD2   | 2.37                     | 0.55              |
| 1:T:63:LEU:HD21  | 1:U:34:HIS:HB2   | 1.88                     | 0.55              |
| 1:T:132:ASP:N    | 1:T:132:ASP:OD1  | 2.38                     | 0.55              |
| 1:B:11:LEU:HD13  | 1:B:62:ILE:HG22  | 1.89                     | 0.55              |
| 1:Q:96:GLU:O     | 1:Q:100:ARG:NH1  | 2.40                     | 0.55              |
| 1:S:99:ASP:N     | 1:S:99:ASP:OD2   | 2.38                     | 0.55              |
| 1:U:54:HIS:NE2   | 1:U:126:ASP:OD2  | 2.39                     | 0.55              |
| 1:J:101:LEU:HB3  | 1:J:124:LEU:HD22 | 1.88                     | 0.55              |
| 1:S:150:LEU:HB2  | 1:W:144:LEU:HD11 | 1.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:W:12:ASN:HA    | 1:W:15:LEU:HD12  | 1.88                     | 0.55              |
| 1:M:14:GLN:NE2   | 1:M:18:GLU:OE2   | 2.39                     | 0.55              |
| 1:P:32:GLN:HA    | 1:P:35:LYS:HB2   | 1.87                     | 0.55              |
| 1:D:32:GLN:HE22  | 1:D:40:LEU:HG    | 1.71                     | 0.54              |
| 1:J:32:GLN:HE22  | 1:J:40:LEU:HG    | 1.72                     | 0.54              |
| 1:R:54:HIS:NE2   | 1:R:126:ASP:OD2  | 2.35                     | 0.54              |
| 1:B:54:HIS:NE2   | 1:B:126:ASP:OD2  | 2.40                     | 0.54              |
| 1:L:99:ASP:N     | 1:L:99:ASP:OD2   | 2.37                     | 0.54              |
| 1:E:98:ILE:O     | 1:E:102:ARG:N    | 2.38                     | 0.54              |
| 1:S:32:GLN:HE22  | 1:S:40:LEU:HG    | 1.73                     | 0.54              |
| 1:F:54:HIS:NE2   | 1:F:126:ASP:OD2  | 2.32                     | 0.54              |
| 1:J:9:GLU:HA     | 1:J:12:ASN:HB2   | 1.90                     | 0.54              |
| 1:P:96:GLU:O     | 1:P:100:ARG:NH1  | 2.40                     | 0.54              |
| 1:P:98:ILE:O     | 1:P:102:ARG:N    | 2.37                     | 0.54              |
| 1:U:32:GLN:HA    | 1:U:35:LYS:HB2   | 1.89                     | 0.54              |
| 1:A:98:ILE:O     | 1:A:102:ARG:N    | 2.38                     | 0.54              |
| 1:L:132:ASP:N    | 1:L:132:ASP:OD2  | 2.38                     | 0.54              |
| 1:M:156:GLN:HE22 | 1:T:40:LEU:HA    | 1.72                     | 0.54              |
| 1:A:3:GLY:HA3    | 1:A:8:ILE:HD11   | 1.88                     | 0.54              |
| 1:D:39:LYS:NZ    | 1:D:154:ILE:O    | 2.41                     | 0.54              |
| 1:Q:99:ASP:OD2   | 1:Q:99:ASP:N     | 2.37                     | 0.54              |
| 1:A:19:LEU:HA    | 1:A:22:ILE:HD12  | 1.89                     | 0.54              |
| 1:O:3:GLY:HA3    | 1:O:8:ILE:HD11   | 1.89                     | 0.54              |
| 1:T:9:GLU:HA     | 1:T:12:ASN:HB2   | 1.89                     | 0.54              |
| 1:X:96:GLU:O     | 1:X:100:ARG:NH1  | 2.41                     | 0.54              |
| 1:P:121:GLU:HA   | 1:P:124:LEU:HB2  | 1.90                     | 0.54              |
| 1:M:144:LEU:HB3  | 1:M:148:LEU:HD11 | 1.90                     | 0.54              |
| 1:R:61:ARG:HA    | 1:R:64:LEU:HD12  | 1.90                     | 0.54              |
| 1:N:121:GLU:HA   | 1:N:124:LEU:HB2  | 1.91                     | 0.54              |
| 1:U:96:GLU:O     | 1:U:100:ARG:NH1  | 2.41                     | 0.54              |
| 1:X:140:LEU:HG   | 1:X:149:TYR:HE1  | 1.73                     | 0.54              |
| 1:G:3:GLY:HA3    | 1:G:8:ILE:HD11   | 1.89                     | 0.53              |
| 1:R:99:ASP:OD1   | 1:R:99:ASP:N     | 2.38                     | 0.53              |
| 1:R:113:ASP:OD2  | 1:R:116:SER:OG   | 2.26                     | 0.53              |
| 1:W:140:LEU:HG   | 1:W:149:TYR:HE1  | 1.73                     | 0.53              |
| 1:X:98:ILE:O     | 1:X:102:ARG:N    | 2.36                     | 0.53              |
| 1:A:63:LEU:HD21  | 1:B:34:HIS:HB2   | 1.89                     | 0.53              |
| 1:H:39:LYS:HA    | 1:H:42:LYS:HD3   | 1.90                     | 0.53              |
| 1:I:105:ILE:HG23 | 1:I:117:ALA:HB1  | 1.89                     | 0.53              |
| 1:H:32:GLN:HA    | 1:H:35:LYS:HB2   | 1.89                     | 0.53              |
| 1:T:139:ASP:HA   | 1:T:142:GLU:HB3  | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:9:GLU:HA     | 1:E:12:ASN:HB2   | 1.90                     | 0.53              |
| 1:N:96:GLU:O     | 1:N:100:ARG:NH1  | 2.42                     | 0.53              |
| 1:V:50:ASP:O     | 1:V:54:HIS:ND1   | 2.39                     | 0.53              |
| 1:V:156:GLN:HE22 | 1:X:40:LEU:HA    | 1.73                     | 0.53              |
| 1:A:50:ASP:HB3   | 1:A:53:ARG:HH21  | 1.73                     | 0.53              |
| 1:K:32:GLN:HG3   | 1:K:41:ALA:HB2   | 1.91                     | 0.53              |
| 1:M:20:THR:HG23  | 1:M:74:LEU:HD22  | 1.90                     | 0.53              |
| 1:O:51:GLU:HA    | 1:O:54:HIS:HB2   | 1.89                     | 0.53              |
| 1:U:14:GLN:NE2   | 1:U:18:GLU:OE1   | 2.41                     | 0.53              |
| 1:V:32:GLN:HE22  | 1:V:40:LEU:HG    | 1.73                     | 0.53              |
| 1:A:19:LEU:HB2   | 1:A:74:LEU:HD21  | 1.90                     | 0.53              |
| 1:I:132:ASP:OD1  | 1:I:132:ASP:N    | 2.38                     | 0.53              |
| 1:T:96:GLU:HG3   | 1:T:100:ARG:HH12 | 1.73                     | 0.53              |
| 1:W:113:ASP:OD2  | 1:W:116:SER:OG   | 2.27                     | 0.53              |
| 1:C:137:GLN:HA   | 1:C:140:LEU:HD12 | 1.91                     | 0.53              |
| 1:D:11:LEU:HD13  | 1:D:62:ILE:HG22  | 1.91                     | 0.53              |
| 1:L:19:LEU:HA    | 1:L:22:ILE:HD12  | 1.90                     | 0.53              |
| 1:Q:20:THR:HG23  | 1:Q:74:LEU:HD22  | 1.91                     | 0.53              |
| 1:V:99:ASP:OD2   | 1:V:99:ASP:N     | 2.40                     | 0.53              |
| 1:O:96:GLU:HG3   | 1:O:100:ARG:HH12 | 1.74                     | 0.53              |
| 1:P:139:ASP:HA   | 1:P:142:GLU:HB3  | 1.91                     | 0.53              |
| 1:B:147:SER:HA   | 1:B:150:LEU:HD12 | 1.91                     | 0.53              |
| 1:D:98:ILE:O     | 1:D:102:ARG:N    | 2.39                     | 0.53              |
| 1:E:39:LYS:HA    | 1:E:42:LYS:HD3   | 1.91                     | 0.53              |
| 1:X:137:GLN:OE1  | 1:X:149:TYR:OH   | 2.27                     | 0.53              |
| 1:X:20:THR:HG23  | 1:X:74:LEU:HD22  | 1.91                     | 0.52              |
| 1:G:39:LYS:HA    | 1:G:42:LYS:HD3   | 1.91                     | 0.52              |
| 1:O:63:LEU:HD21  | 1:P:34:HIS:HB2   | 1.91                     | 0.52              |
| 1:B:131:ILE:HA   | 1:B:134:LEU:HD13 | 1.91                     | 0.52              |
| 1:G:98:ILE:O     | 1:G:102:ARG:N    | 2.40                     | 0.52              |
| 1:O:29:ALA:HA    | 1:O:32:GLN:HE21  | 1.74                     | 0.52              |
| 1:O:99:ASP:OD2   | 1:O:99:ASP:N     | 2.41                     | 0.52              |
| 1:O:32:GLN:HG3   | 1:O:41:ALA:HB2   | 1.92                     | 0.52              |
| 1:X:50:ASP:O     | 1:X:54:HIS:ND1   | 2.43                     | 0.52              |
| 1:B:9:GLU:HA     | 1:B:12:ASN:HB2   | 1.92                     | 0.52              |
| 1:B:113:ASP:OD2  | 1:B:116:SER:OG   | 2.26                     | 0.52              |
| 1:L:137:GLN:HA   | 1:L:140:LEU:HD12 | 1.91                     | 0.52              |
| 1:P:147:SER:HA   | 1:P:150:LEU:HD12 | 1.91                     | 0.52              |
| 1:V:20:THR:HG23  | 1:V:74:LEU:HD22  | 1.91                     | 0.52              |
| 1:A:71:TYR:HB3   | 1:B:23:ASN:HD22  | 1.74                     | 0.52              |
| 1:F:20:THR:HG23  | 1:F:74:LEU:HD22  | 1.92                     | 0.52              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:P:14:GLN:NE2  | 1:P:18:GLU:OE1   | 2.43                     | 0.52              |
| 1:B:19:LEU:HA   | 1:B:22:ILE:HD12  | 1.92                     | 0.52              |
| 1:F:92:GLU:HA   | 1:F:95:LEU:HB2   | 1.90                     | 0.52              |
| 1:T:105:ILE:HA  | 1:T:108:MET:HB3  | 1.90                     | 0.52              |
| 1:D:50:ASP:HB3  | 1:D:53:ARG:HH21  | 1.75                     | 0.52              |
| 1:H:11:LEU:HD13 | 1:H:62:ILE:HG22  | 1.91                     | 0.52              |
| 1:I:54:HIS:NE2  | 1:I:126:ASP:OD2  | 2.43                     | 0.52              |
| 1:N:20:THR:HG23 | 1:N:74:LEU:HD22  | 1.92                     | 0.52              |
| 1:V:39:LYS:HA   | 1:V:42:LYS:HD3   | 1.92                     | 0.52              |
| 1:V:50:ASP:HA   | 1:V:53:ARG:HE    | 1.75                     | 0.52              |
| 1:X:108:MET:SD  | 1:X:116:SER:OG   | 2.66                     | 0.52              |
| 1:K:32:GLN:HA   | 1:K:35:LYS:HB2   | 1.92                     | 0.51              |
| 1:N:24:GLN:NE2  | 1:N:78:ARG:O     | 2.44                     | 0.51              |
| 1:O:23:ASN:OD1  | 1:O:23:ASN:N     | 2.36                     | 0.51              |
| 1:X:143:LYS:HD3 | 1:X:144:LEU:HD22 | 1.93                     | 0.51              |
| 1:A:132:ASP:OD1 | 1:A:132:ASP:N    | 2.40                     | 0.51              |
| 1:L:3:GLY:HA3   | 1:L:8:ILE:HD11   | 1.93                     | 0.51              |
| 1:P:105:ILE:HA  | 1:P:108:MET:HE2  | 1.92                     | 0.51              |
| 1:R:50:ASP:HB3  | 1:R:53:ARG:HH21  | 1.76                     | 0.51              |
| 1:R:92:GLU:HA   | 1:R:95:LEU:HB2   | 1.92                     | 0.51              |
| 1:B:92:GLU:HA   | 1:B:95:LEU:HB2   | 1.93                     | 0.51              |
| 1:H:50:ASP:O    | 1:H:54:HIS:ND1   | 2.43                     | 0.51              |
| 1:X:61:ARG:HE   | 1:X:116:SER:HB3  | 1.75                     | 0.51              |
| 1:G:144:LEU:HB3 | 1:G:148:LEU:HD11 | 1.93                     | 0.51              |
| 1:H:132:ASP:N   | 1:H:132:ASP:OD1  | 2.41                     | 0.51              |
| 1:N:140:LEU:HG  | 1:N:149:TYR:HE1  | 1.75                     | 0.51              |
| 1:Q:32:GLN:HE22 | 1:Q:40:LEU:HG    | 1.75                     | 0.51              |
| 1:S:105:ILE:HA  | 1:S:108:MET:HE2  | 1.91                     | 0.51              |
| 1:T:144:LEU:HB3 | 1:T:148:LEU:HD21 | 1.91                     | 0.51              |
| 1:E:137:GLN:OE1 | 1:E:149:TYR:OH   | 2.27                     | 0.51              |
| 1:I:9:GLU:HA    | 1:I:12:ASN:HB2   | 1.93                     | 0.51              |
| 1:J:61:ARG:HE   | 1:J:116:SER:HB3  | 1.76                     | 0.51              |
| 1:I:98:ILE:O    | 1:I:102:ARG:N    | 2.40                     | 0.51              |
| 1:J:32:GLN:HG3  | 1:J:41:ALA:HB2   | 1.93                     | 0.51              |
| 1:J:54:HIS:NE2  | 1:J:126:ASP:OD2  | 2.42                     | 0.51              |
| 1:W:61:ARG:HE   | 1:W:116:SER:HB3  | 1.76                     | 0.51              |
| 1:E:101:LEU:HG  | 1:E:124:LEU:HD22 | 1.92                     | 0.51              |
| 1:J:144:LEU:HB3 | 1:J:148:LEU:HD11 | 1.93                     | 0.51              |
| 1:R:144:LEU:HB3 | 1:R:148:LEU:HD11 | 1.92                     | 0.51              |
| 1:I:92:GLU:HA   | 1:I:95:LEU:HB2   | 1.93                     | 0.51              |
| 1:O:92:GLU:HA   | 1:O:95:LEU:HB2   | 1.93                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:92:GLU:HA    | 1:J:95:LEU:HB2   | 1.93                     | 0.51              |
| 1:W:92:GLU:HA    | 1:W:95:LEU:HB2   | 1.92                     | 0.51              |
| 1:T:61:ARG:HE    | 1:T:116:SER:HB3  | 1.76                     | 0.51              |
| 1:W:19:LEU:HA    | 1:W:22:ILE:HD12  | 1.92                     | 0.51              |
| 1:B:5:PRO:HA     | 1:B:8:ILE:HB     | 1.94                     | 0.50              |
| 1:F:19:LEU:HA    | 1:F:22:ILE:HD12  | 1.93                     | 0.50              |
| 1:I:34:HIS:HB2   | 1:S:63:LEU:HD21  | 1.93                     | 0.50              |
| 1:W:20:THR:HG23  | 1:W:74:LEU:HD22  | 1.92                     | 0.50              |
| 1:W:32:GLN:HA    | 1:W:35:LYS:HB2   | 1.94                     | 0.50              |
| 1:W:131:ILE:HA   | 1:W:134:LEU:HD13 | 1.94                     | 0.50              |
| 1:X:91:ARG:O     | 1:X:95:LEU:N     | 2.42                     | 0.50              |
| 1:A:40:LEU:HA    | 1:R:156:GLN:HE22 | 1.75                     | 0.50              |
| 1:L:61:ARG:HE    | 1:L:116:SER:HB3  | 1.76                     | 0.50              |
| 1:P:137:GLN:OE1  | 1:P:149:TYR:OH   | 2.29                     | 0.50              |
| 1:P:150:LEU:HB2  | 1:U:144:LEU:HD11 | 1.93                     | 0.50              |
| 1:S:9:GLU:HA     | 1:S:12:ASN:HB2   | 1.94                     | 0.50              |
| 1:X:92:GLU:HA    | 1:X:95:LEU:HB2   | 1.92                     | 0.50              |
| 1:D:140:LEU:HG   | 1:D:149:TYR:HE1  | 1.77                     | 0.50              |
| 1:J:19:LEU:HA    | 1:J:22:ILE:HD12  | 1.93                     | 0.50              |
| 1:K:143:LYS:HD3  | 1:K:144:LEU:HD22 | 1.93                     | 0.50              |
| 1:Q:144:LEU:HD12 | 1:Q:148:LEU:HD11 | 1.92                     | 0.50              |
| 1:R:98:ILE:O     | 1:R:102:ARG:N    | 2.38                     | 0.50              |
| 1:T:137:GLN:OE1  | 1:T:149:TYR:OH   | 2.30                     | 0.50              |
| 1:E:54:HIS:NE2   | 1:E:126:ASP:OD2  | 2.45                     | 0.50              |
| 1:U:19:LEU:O     | 1:U:23:ASN:ND2   | 2.40                     | 0.50              |
| 1:D:139:ASP:HA   | 1:D:142:GLU:HB3  | 1.93                     | 0.50              |
| 1:F:131:ILE:HA   | 1:F:134:LEU:HD13 | 1.93                     | 0.50              |
| 1:E:61:ARG:HE    | 1:E:116:SER:HB3  | 1.77                     | 0.50              |
| 1:F:32:GLN:HB2   | 1:F:37:TRP:HB2   | 1.94                     | 0.50              |
| 1:H:55:ALA:HA    | 1:H:58:LEU:HD12  | 1.94                     | 0.50              |
| 1:E:140:LEU:HD21 | 1:I:154:ILE:HG12 | 1.93                     | 0.50              |
| 1:O:96:GLU:O     | 1:O:100:ARG:NH1  | 2.45                     | 0.50              |
| 1:Q:92:GLU:HA    | 1:Q:95:LEU:HB2   | 1.94                     | 0.50              |
| 1:H:91:ARG:O     | 1:H:95:LEU:N     | 2.42                     | 0.50              |
| 1:H:140:LEU:HG   | 1:H:149:TYR:HE1  | 1.75                     | 0.50              |
| 1:J:140:LEU:HG   | 1:J:149:TYR:HE1  | 1.76                     | 0.50              |
| 1:K:101:LEU:HB3  | 1:K:124:LEU:HD22 | 1.93                     | 0.50              |
| 1:Q:19:LEU:HD22  | 1:Q:74:LEU:HD21  | 1.94                     | 0.50              |
| 1:T:32:GLN:HB2   | 1:T:37:TRP:HB2   | 1.92                     | 0.50              |
| 1:T:32:GLN:HG3   | 1:T:41:ALA:HB2   | 1.92                     | 0.50              |
| 1:V:113:ASP:OD1  | 1:V:116:SER:OG   | 2.28                     | 0.50              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:9:GLU:HA    | 1:A:12:ASN:HB2   | 1.94                     | 0.50              |
| 1:C:39:LYS:HA   | 1:C:42:LYS:HD3   | 1.94                     | 0.50              |
| 1:L:139:ASP:HA  | 1:L:142:GLU:HB2  | 1.94                     | 0.50              |
| 1:Q:139:ASP:HA  | 1:Q:142:GLU:HB3  | 1.94                     | 0.50              |
| 1:W:5:PRO:HA    | 1:W:8:ILE:HB     | 1.94                     | 0.50              |
| 1:E:62:ILE:O    | 1:E:67:GLY:N     | 2.44                     | 0.49              |
| 1:H:8:ILE:HA    | 1:H:11:LEU:HD12  | 1.93                     | 0.49              |
| 1:Q:117:ALA:HA  | 1:Q:120:PHE:HB2  | 1.93                     | 0.49              |
| 1:S:11:LEU:HD13 | 1:S:62:ILE:HG22  | 1.92                     | 0.49              |
| 1:C:94:GLU:OE2  | 1:C:130:HIS:ND1  | 2.45                     | 0.49              |
| 1:D:92:GLU:HA   | 1:D:95:LEU:HB2   | 1.94                     | 0.49              |
| 1:L:20:THR:HG23 | 1:L:74:LEU:HD22  | 1.93                     | 0.49              |
| 1:P:101:LEU:HB3 | 1:P:124:LEU:HD11 | 1.93                     | 0.49              |
| 1:E:91:ARG:O    | 1:E:95:LEU:N     | 2.43                     | 0.49              |
| 1:H:137:GLN:OE1 | 1:H:149:TYR:OH   | 2.30                     | 0.49              |
| 1:K:105:ILE:HA  | 1:K:108:MET:HB2  | 1.93                     | 0.49              |
| 1:D:62:ILE:O    | 1:D:67:GLY:N     | 2.45                     | 0.49              |
| 1:F:9:GLU:HA    | 1:F:12:ASN:HB2   | 1.95                     | 0.49              |
| 1:H:92:GLU:HA   | 1:H:95:LEU:HB2   | 1.94                     | 0.49              |
| 1:O:139:ASP:HA  | 1:O:142:GLU:HB3  | 1.95                     | 0.49              |
| 1:P:20:THR:HG23 | 1:P:74:LEU:HD22  | 1.94                     | 0.49              |
| 1:S:96:GLU:O    | 1:S:100:ARG:NH1  | 2.45                     | 0.49              |
| 1:G:92:GLU:HA   | 1:G:95:LEU:HB2   | 1.94                     | 0.49              |
| 1:Q:91:ARG:O    | 1:Q:95:LEU:N     | 2.43                     | 0.49              |
| 1:E:113:ASP:OD2 | 1:E:116:SER:OG   | 2.30                     | 0.49              |
| 1:U:98:ILE:O    | 1:U:102:ARG:N    | 2.39                     | 0.49              |
| 1:V:143:LYS:HD3 | 1:V:144:LEU:HD22 | 1.93                     | 0.49              |
| 1:W:91:ARG:O    | 1:W:95:LEU:N     | 2.43                     | 0.49              |
| 1:L:125:ALA:O   | 1:L:129:HIS:ND1  | 2.42                     | 0.49              |
| 1:M:19:LEU:HA   | 1:M:22:ILE:HD12  | 1.94                     | 0.49              |
| 1:M:54:HIS:NE2  | 1:M:126:ASP:OD2  | 2.36                     | 0.49              |
| 1:M:99:ASP:HA   | 1:M:102:ARG:HB2  | 1.95                     | 0.49              |
| 1:V:91:ARG:O    | 1:V:95:LEU:N     | 2.44                     | 0.49              |
| 1:V:92:GLU:HA   | 1:V:95:LEU:HB2   | 1.93                     | 0.49              |
| 1:A:137:GLN:OE1 | 1:A:149:TYR:OH   | 2.28                     | 0.49              |
| 1:C:55:ALA:HA   | 1:C:58:LEU:HD12  | 1.95                     | 0.49              |
| 1:F:96:GLU:HG3  | 1:F:100:ARG:HH12 | 1.78                     | 0.49              |
| 1:G:32:GLN:HA   | 1:G:35:LYS:HB2   | 1.95                     | 0.49              |
| 1:H:98:ILE:O    | 1:H:102:ARG:N    | 2.45                     | 0.49              |
| 1:O:99:ASP:HA   | 1:O:102:ARG:HB2  | 1.95                     | 0.49              |
| 1:G:54:HIS:NE2  | 1:G:126:ASP:OD2  | 2.39                     | 0.49              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:N:143:LYS:HD3 | 1:N:144:LEU:HD22 | 1.95                     | 0.49              |
| 1:Q:61:ARG:HA   | 1:Q:64:LEU:HD12  | 1.94                     | 0.49              |
| 1:S:32:GLN:HB2  | 1:S:37:TRP:HB2   | 1.94                     | 0.49              |
| 1:W:137:GLN:OE1 | 1:W:149:TYR:OH   | 2.29                     | 0.49              |
| 1:S:19:LEU:HA   | 1:S:22:ILE:HD12  | 1.94                     | 0.49              |
| 1:S:99:ASP:HA   | 1:S:102:ARG:HB2  | 1.94                     | 0.49              |
| 1:S:101:LEU:HB3 | 1:S:124:LEU:HD22 | 1.94                     | 0.49              |
| 1:M:32:GLN:HE22 | 1:M:40:LEU:HG    | 1.78                     | 0.48              |
| 1:P:92:GLU:HA   | 1:P:95:LEU:HB2   | 1.94                     | 0.48              |
| 1:Q:125:ALA:O   | 1:Q:129:HIS:ND1  | 2.42                     | 0.48              |
| 1:T:69:PRO:HB2  | 1:U:27:LEU:HD21  | 1.95                     | 0.48              |
| 1:B:96:GLU:O    | 1:B:100:ARG:NH1  | 2.47                     | 0.48              |
| 1:F:61:ARG:HE   | 1:F:116:SER:HB3  | 1.78                     | 0.48              |
| 1:E:92:GLU:HA   | 1:E:95:LEU:HB2   | 1.95                     | 0.48              |
| 1:K:98:ILE:O    | 1:K:102:ARG:N    | 2.44                     | 0.48              |
| 1:L:121:GLU:HA  | 1:L:124:LEU:HB2  | 1.95                     | 0.48              |
| 1:O:8:ILE:HA    | 1:O:11:LEU:HD12  | 1.95                     | 0.48              |
| 1:Q:96:GLU:HG3  | 1:Q:100:ARG:HH22 | 1.78                     | 0.48              |
| 1:S:1:MET:SD    | 1:S:1:MET:N      | 2.80                     | 0.48              |
| 1:S:62:ILE:O    | 1:S:67:GLY:N     | 2.45                     | 0.48              |
| 1:T:45:ARG:O    | 1:T:48:SER:OG    | 2.32                     | 0.48              |
| 1:X:9:GLU:HA    | 1:X:12:ASN:HB2   | 1.94                     | 0.48              |
| 1:C:54:HIS:NE2  | 1:C:126:ASP:OD2  | 2.46                     | 0.48              |
| 1:F:11:LEU:HD13 | 1:F:62:ILE:HG22  | 1.95                     | 0.48              |
| 1:G:150:LEU:HB2 | 1:I:144:LEU:HD11 | 1.94                     | 0.48              |
| 1:M:91:ARG:O    | 1:M:95:LEU:N     | 2.45                     | 0.48              |
| 1:V:54:HIS:NE2  | 1:V:126:ASP:OD2  | 2.46                     | 0.48              |
| 1:D:91:ARG:O    | 1:D:95:LEU:N     | 2.45                     | 0.48              |
| 1:I:137:GLN:OE1 | 1:I:149:TYR:OH   | 2.31                     | 0.48              |
| 1:W:62:ILE:O    | 1:W:67:GLY:N     | 2.46                     | 0.48              |
| 1:F:32:GLN:HA   | 1:F:35:LYS:HB2   | 1.95                     | 0.48              |
| 1:X:61:ARG:HA   | 1:X:64:LEU:HD12  | 1.95                     | 0.48              |
| 1:B:137:GLN:OE1 | 1:B:149:TYR:OH   | 2.31                     | 0.48              |
| 1:K:32:GLN:HE22 | 1:K:40:LEU:HG    | 1.78                     | 0.48              |
| 1:O:47:GLU:OE2  | 1:O:130:HIS:NE2  | 2.46                     | 0.48              |
| 1:T:62:ILE:O    | 1:T:67:GLY:N     | 2.42                     | 0.48              |
| 1:E:92:GLU:O    | 1:E:96:GLU:N     | 2.46                     | 0.48              |
| 1:P:32:GLN:HE21 | 1:P:41:ALA:HA    | 1.77                     | 0.48              |
| 1:W:144:LEU:HB3 | 1:W:148:LEU:HD11 | 1.95                     | 0.48              |
| 1:B:62:ILE:HD11 | 1:B:69:PRO:HG3   | 1.96                     | 0.48              |
| 1:G:137:GLN:OE1 | 1:G:149:TYR:OH   | 2.31                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:32:GLN:HB2  | 1:H:37:TRP:HB2   | 1.96                     | 0.48              |
| 1:L:27:LEU:O    | 1:L:31:LEU:N     | 2.46                     | 0.48              |
| 1:M:61:ARG:HA   | 1:M:64:LEU:HD12  | 1.95                     | 0.48              |
| 1:M:137:GLN:HA  | 1:M:140:LEU:HD12 | 1.95                     | 0.48              |
| 1:R:20:THR:HG23 | 1:R:74:LEU:HD22  | 1.96                     | 0.48              |
| 1:P:11:LEU:HD13 | 1:P:62:ILE:HG22  | 1.95                     | 0.48              |
| 1:U:9:GLU:HA    | 1:U:12:ASN:HB2   | 1.95                     | 0.48              |
| 1:I:140:LEU:HG  | 1:I:149:TYR:HE1  | 1.78                     | 0.48              |
| 1:J:157:THR:OG1 | 1:J:158:GLN:N    | 2.46                     | 0.48              |
| 1:O:91:ARG:O    | 1:O:95:LEU:N     | 2.43                     | 0.48              |
| 1:V:32:GLN:HA   | 1:V:35:LYS:HB2   | 1.96                     | 0.48              |
| 1:B:101:LEU:HB3 | 1:B:124:LEU:HD22 | 1.96                     | 0.47              |
| 1:C:98:ILE:O    | 1:C:102:ARG:N    | 2.42                     | 0.47              |
| 1:F:62:ILE:O    | 1:F:67:GLY:N     | 2.45                     | 0.47              |
| 1:N:92:GLU:HA   | 1:N:95:LEU:HB2   | 1.94                     | 0.47              |
| 1:V:27:LEU:O    | 1:V:31:LEU:N     | 2.47                     | 0.47              |
| 1:D:3:GLY:HA3   | 1:D:65:LEU:HB3   | 1.95                     | 0.47              |
| 1:K:55:ALA:HA   | 1:K:58:LEU:HD12  | 1.96                     | 0.47              |
| 1:K:92:GLU:HA   | 1:K:95:LEU:HB2   | 1.95                     | 0.47              |
| 1:U:62:ILE:O    | 1:U:67:GLY:N     | 2.47                     | 0.47              |
| 1:A:140:LEU:HG  | 1:A:149:TYR:HE1  | 1.79                     | 0.47              |
| 1:G:99:ASP:HA   | 1:G:102:ARG:HB2  | 1.96                     | 0.47              |
| 1:O:137:GLN:OE1 | 1:O:149:TYR:OH   | 2.31                     | 0.47              |
| 1:T:92:GLU:HA   | 1:T:95:LEU:HB2   | 1.96                     | 0.47              |
| 1:U:11:LEU:HD13 | 1:U:62:ILE:HG22  | 1.96                     | 0.47              |
| 1:X:50:ASP:OD2  | 1:X:53:ARG:NH2   | 2.46                     | 0.47              |
| 1:C:8:ILE:HA    | 1:C:11:LEU:HD12  | 1.96                     | 0.47              |
| 1:W:32:GLN:HB2  | 1:W:37:TRP:HB2   | 1.96                     | 0.47              |
| 1:B:140:LEU:HG  | 1:B:149:TYR:HE1  | 1.79                     | 0.47              |
| 1:C:45:ARG:O    | 1:C:48:SER:OG    | 2.32                     | 0.47              |
| 1:D:8:ILE:HA    | 1:D:11:LEU:HD12  | 1.96                     | 0.47              |
| 1:J:91:ARG:O    | 1:J:95:LEU:N     | 2.44                     | 0.47              |
| 1:N:98:ILE:O    | 1:N:102:ARG:N    | 2.40                     | 0.47              |
| 1:Q:5:PRO:HA    | 1:Q:8:ILE:HB     | 1.96                     | 0.47              |
| 1:R:91:ARG:O    | 1:R:95:LEU:N     | 2.40                     | 0.47              |
| 1:V:9:GLU:HA    | 1:V:12:ASN:HB2   | 1.95                     | 0.47              |
| 1:V:13:GLU:OE1  | 1:V:73:ARG:NH2   | 2.47                     | 0.47              |
| 1:X:121:GLU:HA  | 1:X:124:LEU:HB2  | 1.96                     | 0.47              |
| 1:F:61:ARG:NH2  | 1:F:113:ASP:OD1  | 2.47                     | 0.47              |
| 1:E:11:LEU:HD13 | 1:E:62:ILE:HG22  | 1.95                     | 0.47              |
| 1:E:61:ARG:NH2  | 1:E:113:ASP:OD1  | 2.47                     | 0.47              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:I:3:GLY:HA3   | 1:I:8:ILE:HD11   | 1.97                     | 0.47              |
| 1:N:27:LEU:O    | 1:N:31:LEU:N     | 2.48                     | 0.47              |
| 1:S:92:GLU:HA   | 1:S:95:LEU:HB2   | 1.95                     | 0.47              |
| 1:T:92:GLU:O    | 1:T:96:GLU:N     | 2.47                     | 0.47              |
| 1:X:139:ASP:HA  | 1:X:142:GLU:HB3  | 1.96                     | 0.47              |
| 1:C:9:GLU:HA    | 1:C:12:ASN:HB2   | 1.96                     | 0.47              |
| 1:C:62:ILE:O    | 1:C:67:GLY:N     | 2.46                     | 0.47              |
| 1:D:27:LEU:O    | 1:D:31:LEU:N     | 2.47                     | 0.47              |
| 1:G:28:HIS:HA   | 1:G:31:LEU:HB2   | 1.97                     | 0.47              |
| 1:H:54:HIS:HB3  | 1:H:123:ILE:HD12 | 1.97                     | 0.47              |
| 1:I:39:LYS:HA   | 1:I:42:LYS:HD3   | 1.97                     | 0.47              |
| 1:I:91:ARG:O    | 1:I:95:LEU:N     | 2.44                     | 0.47              |
| 1:J:137:GLN:OE1 | 1:J:149:TYR:OH   | 2.29                     | 0.47              |
| 1:M:62:ILE:HD11 | 1:M:69:PRO:HG3   | 1.95                     | 0.47              |
| 1:N:92:GLU:O    | 1:N:96:GLU:N     | 2.48                     | 0.47              |
| 1:P:14:GLN:HE21 | 1:P:18:GLU:HG2   | 1.80                     | 0.47              |
| 1:P:62:ILE:O    | 1:P:67:GLY:N     | 2.47                     | 0.47              |
| 1:R:121:GLU:HA  | 1:R:124:LEU:HB2  | 1.97                     | 0.47              |
| 1:V:62:ILE:O    | 1:V:67:GLY:N     | 2.44                     | 0.47              |
| 1:D:144:LEU:HB3 | 1:D:148:LEU:HD11 | 1.97                     | 0.47              |
| 1:E:32:GLN:HB2  | 1:E:37:TRP:HB2   | 1.95                     | 0.47              |
| 1:E:45:ARG:O    | 1:E:48:SER:OG    | 2.33                     | 0.47              |
| 1:J:28:HIS:HD2  | 1:J:31:LEU:HD12  | 1.80                     | 0.47              |
| 1:J:98:ILE:O    | 1:J:102:ARG:N    | 2.45                     | 0.47              |
| 1:S:139:ASP:HA  | 1:S:142:GLU:HB3  | 1.97                     | 0.47              |
| 1:A:92:GLU:O    | 1:A:96:GLU:N     | 2.48                     | 0.47              |
| 1:N:62:ILE:O    | 1:N:67:GLY:N     | 2.44                     | 0.47              |
| 1:P:9:GLU:HA    | 1:P:12:ASN:HB2   | 1.97                     | 0.47              |
| 1:Q:92:GLU:O    | 1:Q:96:GLU:N     | 2.48                     | 0.47              |
| 1:B:3:GLY:HA3   | 1:B:65:LEU:HB3   | 1.97                     | 0.47              |
| 1:G:140:LEU:HG  | 1:G:149:TYR:HE1  | 1.79                     | 0.47              |
| 1:O:9:GLU:HA    | 1:O:12:ASN:HB2   | 1.97                     | 0.47              |
| 1:P:51:GLU:HA   | 1:P:54:HIS:HB2   | 1.97                     | 0.47              |
| 1:R:61:ARG:NH2  | 1:R:113:ASP:OD1  | 2.49                     | 0.47              |
| 1:B:20:THR:HG23 | 1:B:74:LEU:HD22  | 1.96                     | 0.46              |
| 1:K:117:ALA:HA  | 1:K:120:PHE:HB2  | 1.96                     | 0.46              |
| 1:L:11:LEU:HD13 | 1:L:62:ILE:HG22  | 1.97                     | 0.46              |
| 1:S:98:ILE:HG13 | 1:S:124:LEU:HD11 | 1.97                     | 0.46              |
| 1:V:132:ASP:N   | 1:V:132:ASP:OD1  | 2.45                     | 0.46              |
| 1:X:62:ILE:O    | 1:X:67:GLY:N     | 2.46                     | 0.46              |
| 1:B:61:ARG:HA   | 1:B:64:LEU:HD12  | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:92:GLU:O     | 1:B:96:GLU:N     | 2.49                     | 0.46              |
| 1:F:91:ARG:O     | 1:F:95:LEU:N     | 2.40                     | 0.46              |
| 1:I:62:ILE:O     | 1:I:67:GLY:N     | 2.45                     | 0.46              |
| 1:J:62:ILE:O     | 1:J:67:GLY:N     | 2.46                     | 0.46              |
| 1:K:61:ARG:HE    | 1:K:116:SER:HB3  | 1.80                     | 0.46              |
| 1:O:62:ILE:O     | 1:O:67:GLY:N     | 2.47                     | 0.46              |
| 1:P:61:ARG:HE    | 1:P:116:SER:HB3  | 1.80                     | 0.46              |
| 1:S:92:GLU:O     | 1:S:96:GLU:N     | 2.49                     | 0.46              |
| 1:W:98:ILE:O     | 1:W:102:ARG:N    | 2.38                     | 0.46              |
| 1:G:32:GLN:HE22  | 1:G:40:LEU:HG    | 1.79                     | 0.46              |
| 1:M:144:LEU:HD11 | 1:X:150:LEU:HB2  | 1.96                     | 0.46              |
| 1:Q:98:ILE:O     | 1:Q:102:ARG:N    | 2.43                     | 0.46              |
| 1:T:98:ILE:HG23  | 1:T:124:LEU:HD11 | 1.96                     | 0.46              |
| 1:E:8:ILE:HA     | 1:E:11:LEU:HD12  | 1.98                     | 0.46              |
| 1:N:45:ARG:O     | 1:N:48:SER:OG    | 2.33                     | 0.46              |
| 1:N:139:ASP:HA   | 1:N:142:GLU:HB3  | 1.98                     | 0.46              |
| 1:A:92:GLU:HA    | 1:A:95:LEU:HB2   | 1.96                     | 0.46              |
| 1:G:62:ILE:O     | 1:G:67:GLY:N     | 2.46                     | 0.46              |
| 1:L:63:LEU:HD13  | 1:M:34:HIS:HB2   | 1.98                     | 0.46              |
| 1:Q:14:GLN:HG3   | 1:Q:58:LEU:HD11  | 1.96                     | 0.46              |
| 1:C:125:ALA:O    | 1:C:129:HIS:ND1  | 2.42                     | 0.46              |
| 1:C:132:ASP:O    | 1:C:136:THR:OG1  | 2.32                     | 0.46              |
| 1:M:92:GLU:HA    | 1:M:95:LEU:HB2   | 1.97                     | 0.46              |
| 1:A:91:ARG:O     | 1:A:95:LEU:N     | 2.45                     | 0.46              |
| 1:P:91:ARG:O     | 1:P:95:LEU:N     | 2.45                     | 0.46              |
| 1:E:6:GLU:O      | 1:E:10:PHE:N     | 2.47                     | 0.46              |
| 1:I:32:GLN:HG3   | 1:I:41:ALA:HB2   | 1.98                     | 0.46              |
| 1:V:139:ASP:HA   | 1:V:142:GLU:HB3  | 1.98                     | 0.46              |
| 1:X:28:HIS:HA    | 1:X:31:LEU:HB2   | 1.98                     | 0.46              |
| 1:O:92:GLU:O     | 1:O:96:GLU:N     | 2.49                     | 0.46              |
| 1:A:144:LEU:HB3  | 1:A:148:LEU:HD11 | 1.98                     | 0.46              |
| 1:G:45:ARG:O     | 1:G:48:SER:OG    | 2.34                     | 0.46              |
| 1:X:92:GLU:O     | 1:X:96:GLU:N     | 2.49                     | 0.46              |
| 1:X:24:GLN:NE2   | 1:X:78:ARG:O     | 2.49                     | 0.45              |
| 1:L:9:GLU:HA     | 1:L:12:ASN:HB2   | 1.97                     | 0.45              |
| 1:U:20:THR:HG23  | 1:U:74:LEU:HD22  | 1.98                     | 0.45              |
| 1:F:92:GLU:O     | 1:F:96:GLU:N     | 2.49                     | 0.45              |
| 1:S:45:ARG:O     | 1:S:48:SER:OG    | 2.34                     | 0.45              |
| 1:U:137:GLN:OE1  | 1:U:149:TYR:OH   | 2.32                     | 0.45              |
| 1:W:138:LEU:HA   | 1:W:141:ILE:HD12 | 1.97                     | 0.45              |
| 1:J:99:ASP:HA    | 1:J:102:ARG:HB2  | 1.98                     | 0.45              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:K:91:ARG:O    | 1:K:95:LEU:N     | 2.46                     | 0.45              |
| 1:K:144:LEU:HB3 | 1:K:148:LEU:HD11 | 1.98                     | 0.45              |
| 1:P:143:LYS:HG3 | 1:P:144:LEU:HD22 | 1.98                     | 0.45              |
| 1:R:27:LEU:HD12 | 1:R:27:LEU:HA    | 1.86                     | 0.45              |
| 1:I:32:GLN:HB2  | 1:I:37:TRP:HB2   | 1.99                     | 0.45              |
| 1:K:137:GLN:OE1 | 1:K:149:TYR:OH   | 2.34                     | 0.45              |
| 1:I:143:LYS:HG3 | 1:I:144:LEU:HD22 | 1.98                     | 0.45              |
| 1:R:62:ILE:O    | 1:R:67:GLY:N     | 2.47                     | 0.45              |
| 1:W:61:ARG:NH2  | 1:W:113:ASP:OD1  | 2.50                     | 0.45              |
| 1:K:132:ASP:OD1 | 1:K:132:ASP:N    | 2.49                     | 0.45              |
| 1:X:11:LEU:HD13 | 1:X:62:ILE:HG22  | 1.99                     | 0.45              |
| 1:T:91:ARG:O    | 1:T:95:LEU:N     | 2.45                     | 0.45              |
| 1:W:27:LEU:O    | 1:W:31:LEU:N     | 2.50                     | 0.45              |
| 1:W:51:GLU:HA   | 1:W:54:HIS:HB2   | 1.98                     | 0.45              |
| 1:C:32:GLN:HB2  | 1:C:37:TRP:HB2   | 1.99                     | 0.45              |
| 1:F:3:GLY:HA3   | 1:F:8:ILE:HD11   | 1.99                     | 0.45              |
| 1:G:20:THR:HG23 | 1:G:74:LEU:HD22  | 1.99                     | 0.45              |
| 1:U:61:ARG:HE   | 1:U:116:SER:HB3  | 1.81                     | 0.45              |
| 1:V:99:ASP:HA   | 1:V:102:ARG:HB2  | 1.98                     | 0.45              |
| 1:E:146:GLU:O   | 1:E:150:LEU:N    | 2.49                     | 0.45              |
| 1:G:32:GLN:HG3  | 1:G:41:ALA:HB2   | 1.98                     | 0.45              |
| 1:Q:32:GLN:HB2  | 1:Q:37:TRP:HB2   | 1.99                     | 0.45              |
| 1:Q:105:ILE:HA  | 1:Q:108:MET:HE3  | 1.99                     | 0.45              |
| 1:V:98:ILE:O    | 1:V:102:ARG:N    | 2.44                     | 0.45              |
| 1:W:8:ILE:HA    | 1:W:11:LEU:HD12  | 2.00                     | 0.45              |
| 1:X:62:ILE:HD11 | 1:X:69:PRO:HG3   | 1.98                     | 0.45              |
| 1:A:62:ILE:O    | 1:A:67:GLY:N     | 2.45                     | 0.44              |
| 1:K:3:GLY:HA3   | 1:K:65:LEU:HB3   | 1.99                     | 0.44              |
| 1:R:132:ASP:OD1 | 1:R:132:ASP:N    | 2.49                     | 0.44              |
| 1:V:62:ILE:HD11 | 1:V:69:PRO:HG3   | 1.98                     | 0.44              |
| 1:A:99:ASP:HA   | 1:A:102:ARG:HB2  | 1.98                     | 0.44              |
| 1:D:62:ILE:HD11 | 1:D:69:PRO:HG3   | 1.99                     | 0.44              |
| 1:G:74:LEU:HD23 | 1:G:74:LEU:HA    | 1.86                     | 0.44              |
| 1:K:12:ASN:HA   | 1:K:15:LEU:HG    | 1.99                     | 0.44              |
| 1:M:61:ARG:NH2  | 1:M:113:ASP:OD1  | 2.50                     | 0.44              |
| 1:P:113:ASP:OD1 | 1:P:116:SER:OG   | 2.30                     | 0.44              |
| 1:Q:39:LYS:HA   | 1:Q:42:LYS:HD3   | 1.99                     | 0.44              |
| 1:Q:108:MET:SD  | 1:Q:116:SER:OG   | 2.75                     | 0.44              |
| 1:S:98:ILE:O    | 1:S:102:ARG:N    | 2.42                     | 0.44              |
| 1:A:28:HIS:HA   | 1:A:31:LEU:HB2   | 1.98                     | 0.44              |
| 1:C:32:GLN:HA   | 1:C:35:LYS:HB2   | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:99:ASP:HA    | 1:D:102:ARG:HB2  | 1.99                     | 0.44              |
| 1:R:24:GLN:NE2   | 1:R:78:ARG:O     | 2.50                     | 0.44              |
| 1:T:12:ASN:HA    | 1:T:15:LEU:HD12  | 1.99                     | 0.44              |
| 1:C:101:LEU:HD22 | 1:C:124:LEU:HG   | 2.00                     | 0.44              |
| 1:G:72:GLN:HE22  | 1:X:77:VAL:H     | 1.65                     | 0.44              |
| 1:L:101:LEU:HB3  | 1:L:124:LEU:HD11 | 2.00                     | 0.44              |
| 1:B:132:ASP:O    | 1:B:136:THR:N    | 2.49                     | 0.44              |
| 1:L:62:ILE:O     | 1:L:67:GLY:N     | 2.50                     | 0.44              |
| 1:N:61:ARG:NH2   | 1:N:113:ASP:OD2  | 2.50                     | 0.44              |
| 1:A:139:ASP:HA   | 1:A:142:GLU:HB3  | 2.00                     | 0.44              |
| 3:C:202:HEM:C1C  | 1:D:52:MET:HE3   | 2.52                     | 0.44              |
| 1:D:137:GLN:OE1  | 1:D:149:TYR:OH   | 2.35                     | 0.44              |
| 1:J:39:LYS:HA    | 1:J:42:LYS:HD3   | 2.00                     | 0.44              |
| 1:J:113:ASP:OD2  | 1:J:116:SER:OG   | 2.34                     | 0.44              |
| 1:L:98:ILE:O     | 1:L:102:ARG:N    | 2.45                     | 0.44              |
| 1:O:11:LEU:HD13  | 1:O:62:ILE:HG22  | 1.99                     | 0.44              |
| 1:S:91:ARG:O     | 1:S:95:LEU:N     | 2.44                     | 0.44              |
| 1:A:12:ASN:HA    | 1:A:15:LEU:HG    | 2.00                     | 0.44              |
| 1:B:62:ILE:O     | 1:B:67:GLY:N     | 2.50                     | 0.44              |
| 1:E:99:ASP:HA    | 1:E:102:ARG:HB2  | 1.99                     | 0.44              |
| 1:K:20:THR:HG23  | 1:K:74:LEU:HD22  | 2.00                     | 0.44              |
| 1:N:61:ARG:HE    | 1:N:116:SER:HB3  | 1.82                     | 0.44              |
| 1:Q:9:GLU:HA     | 1:Q:12:ASN:HB2   | 1.98                     | 0.44              |
| 1:T:19:LEU:HA    | 1:T:22:ILE:HD12  | 1.99                     | 0.44              |
| 1:V:92:GLU:O     | 1:V:96:GLU:N     | 2.51                     | 0.44              |
| 1:V:125:ALA:O    | 1:V:129:HIS:ND1  | 2.40                     | 0.44              |
| 1:B:27:LEU:O     | 1:B:31:LEU:N     | 2.51                     | 0.44              |
| 1:D:92:GLU:O     | 1:D:96:GLU:N     | 2.50                     | 0.44              |
| 1:E:27:LEU:O     | 1:E:31:LEU:N     | 2.51                     | 0.44              |
| 1:H:99:ASP:HA    | 1:H:102:ARG:HB2  | 1.99                     | 0.44              |
| 1:L:132:ASP:O    | 1:L:136:THR:OG1  | 2.31                     | 0.44              |
| 1:Q:3:GLY:HA3    | 1:Q:8:ILE:HD11   | 2.00                     | 0.44              |
| 1:R:50:ASP:O     | 1:R:54:HIS:N     | 2.49                     | 0.44              |
| 1:C:62:ILE:HD11  | 1:C:69:PRO:HG3   | 1.99                     | 0.44              |
| 1:D:32:GLN:HB2   | 1:D:37:TRP:HB2   | 1.99                     | 0.44              |
| 1:F:99:ASP:HA    | 1:F:102:ARG:HB2  | 2.00                     | 0.44              |
| 1:D:134:LEU:HA   | 1:D:137:GLN:HB2  | 1.99                     | 0.43              |
| 1:G:105:ILE:HG23 | 1:G:117:ALA:HB1  | 1.99                     | 0.43              |
| 1:K:92:GLU:O     | 1:K:96:GLU:N     | 2.51                     | 0.43              |
| 1:M:132:ASP:OD1  | 1:M:132:ASP:N    | 2.50                     | 0.43              |
| 1:O:54:HIS:NE2   | 1:O:126:ASP:OD2  | 2.43                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:92:GLU:O     | 1:P:96:GLU:N     | 2.51                     | 0.43              |
| 1:Q:143:LYS:HG3  | 1:Q:144:LEU:HD22 | 2.00                     | 0.43              |
| 1:S:132:ASP:O    | 1:S:136:THR:N    | 2.46                     | 0.43              |
| 1:B:138:LEU:HA   | 1:B:141:ILE:HD12 | 1.98                     | 0.43              |
| 1:C:92:GLU:HA    | 1:C:95:LEU:HB2   | 1.99                     | 0.43              |
| 1:D:51:GLU:HA    | 1:D:54:HIS:HB2   | 2.00                     | 0.43              |
| 1:G:51:GLU:HA    | 1:G:54:HIS:HB2   | 1.99                     | 0.43              |
| 1:H:12:ASN:HA    | 1:H:15:LEU:HG    | 2.00                     | 0.43              |
| 1:J:28:HIS:HA    | 1:J:31:LEU:HB2   | 2.00                     | 0.43              |
| 1:K:45:ARG:O     | 1:K:48:SER:OG    | 2.35                     | 0.43              |
| 1:L:92:GLU:HA    | 1:L:95:LEU:HB2   | 2.00                     | 0.43              |
| 1:Q:108:MET:HE3  | 1:Q:108:MET:HB3  | 1.64                     | 0.43              |
| 1:T:143:LYS:HG3  | 1:T:144:LEU:HD22 | 2.00                     | 0.43              |
| 1:F:62:ILE:HD11  | 1:F:69:PRO:HG3   | 1.99                     | 0.43              |
| 1:H:54:HIS:NE2   | 1:H:126:ASP:OD2  | 2.33                     | 0.43              |
| 1:P:84:THR:OG1   | 1:P:85:GLU:OE1   | 2.36                     | 0.43              |
| 1:P:94:GLU:OE2   | 1:P:130:HIS:ND1  | 2.52                     | 0.43              |
| 1:C:56:GLU:HG3   | 1:D:26:PHE:HZ    | 1.82                     | 0.43              |
| 1:F:25:TYR:OH    | 1:F:94:GLU:OE2   | 2.35                     | 0.43              |
| 1:J:55:ALA:HA    | 1:J:58:LEU:HD12  | 2.00                     | 0.43              |
| 1:R:32:GLN:HA    | 1:R:35:LYS:HB2   | 1.99                     | 0.43              |
| 1:B:91:ARG:O     | 1:B:95:LEU:N     | 2.42                     | 0.43              |
| 1:F:33:ASP:N     | 1:F:33:ASP:OD1   | 2.49                     | 0.43              |
| 1:L:137:GLN:OE1  | 1:L:149:TYR:OH   | 2.30                     | 0.43              |
| 1:S:28:HIS:HA    | 1:S:31:LEU:HB2   | 2.00                     | 0.43              |
| 1:W:92:GLU:O     | 1:W:96:GLU:N     | 2.51                     | 0.43              |
| 1:C:61:ARG:HE    | 1:C:116:SER:HB3  | 1.83                     | 0.43              |
| 1:L:32:GLN:O     | 1:L:36:GLY:N     | 2.52                     | 0.43              |
| 1:Q:4:ASP:HB3    | 1:Q:7:VAL:HG23   | 2.00                     | 0.43              |
| 1:U:62:ILE:HD11  | 1:U:69:PRO:HG3   | 2.00                     | 0.43              |
| 1:F:132:ASP:O    | 1:F:136:THR:N    | 2.49                     | 0.43              |
| 1:H:138:LEU:HA   | 1:H:141:ILE:HD12 | 2.00                     | 0.43              |
| 1:Q:27:LEU:O     | 1:Q:31:LEU:N     | 2.50                     | 0.43              |
| 1:Q:99:ASP:HA    | 1:Q:102:ARG:HB2  | 2.01                     | 0.43              |
| 1:R:101:LEU:HD12 | 1:R:101:LEU:HA   | 1.81                     | 0.43              |
| 1:U:92:GLU:HA    | 1:U:95:LEU:HB2   | 2.01                     | 0.43              |
| 1:A:27:LEU:O     | 1:A:31:LEU:N     | 2.51                     | 0.43              |
| 1:J:51:GLU:HA    | 1:J:54:HIS:HB2   | 2.00                     | 0.43              |
| 1:N:99:ASP:HA    | 1:N:102:ARG:HB2  | 2.00                     | 0.43              |
| 1:R:124:LEU:HD23 | 1:R:124:LEU:HA   | 1.86                     | 0.43              |
| 1:F:150:LEU:HB2  | 1:R:144:LEU:HD11 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:143:LYS:HD3  | 1:H:144:LEU:HD22 | 2.00                     | 0.43              |
| 1:Q:23:ASN:HD22  | 1:R:71:TYR:HB3   | 1.84                     | 0.43              |
| 1:Q:137:GLN:OE1  | 1:Q:149:TYR:OH   | 2.32                     | 0.43              |
| 1:V:96:GLU:OE1   | 1:V:100:ARG:NH2  | 2.52                     | 0.43              |
| 1:B:61:ARG:NH2   | 1:B:113:ASP:OD1  | 2.52                     | 0.43              |
| 1:B:96:GLU:HG3   | 1:B:100:ARG:HH22 | 1.83                     | 0.43              |
| 1:F:50:ASP:O     | 1:F:54:HIS:N     | 2.50                     | 0.43              |
| 1:E:132:ASP:O    | 1:E:136:THR:OG1  | 2.31                     | 0.43              |
| 1:G:91:ARG:O     | 1:G:95:LEU:N     | 2.51                     | 0.43              |
| 1:I:96:GLU:O     | 1:I:100:ARG:NH1  | 2.52                     | 0.43              |
| 1:M:24:GLN:NE2   | 1:M:78:ARG:O     | 2.52                     | 0.43              |
| 1:N:9:GLU:HA     | 1:N:12:ASN:HB2   | 2.01                     | 0.43              |
| 1:P:42:LYS:HB3   | 1:P:42:LYS:HE2   | 1.85                     | 0.43              |
| 1:P:108:MET:HE2  | 1:P:108:MET:HB3  | 1.88                     | 0.43              |
| 1:S:27:LEU:O     | 1:S:31:LEU:N     | 2.52                     | 0.43              |
| 1:C:50:ASP:O     | 1:C:54:HIS:ND1   | 2.52                     | 0.42              |
| 1:D:28:HIS:HA    | 1:D:31:LEU:HB2   | 2.00                     | 0.42              |
| 1:D:37:TRP:HD1   | 1:D:154:ILE:HG22 | 1.83                     | 0.42              |
| 1:E:98:ILE:HG23  | 1:E:124:LEU:HD11 | 2.01                     | 0.42              |
| 1:I:1:MET:SD     | 1:I:1:MET:N      | 2.91                     | 0.42              |
| 1:K:27:LEU:O     | 1:K:31:LEU:N     | 2.50                     | 0.42              |
| 1:R:141:ILE:O    | 1:R:145:GLY:N    | 2.46                     | 0.42              |
| 1:T:117:ALA:HA   | 1:T:120:PHE:HB2  | 2.01                     | 0.42              |
| 1:A:132:ASP:O    | 1:A:136:THR:OG1  | 2.33                     | 0.42              |
| 1:B:32:GLN:HG3   | 1:B:41:ALA:HB2   | 2.02                     | 0.42              |
| 1:C:27:LEU:O     | 1:C:31:LEU:N     | 2.53                     | 0.42              |
| 1:F:98:ILE:O     | 1:F:102:ARG:N    | 2.48                     | 0.42              |
| 1:H:3:GLY:HA3    | 1:H:8:ILE:HD11   | 2.00                     | 0.42              |
| 1:H:108:MET:HB2  | 1:H:108:MET:HE3  | 1.76                     | 0.42              |
| 1:O:148:LEU:O    | 1:O:151:SER:OG   | 2.34                     | 0.42              |
| 1:G:40:LEU:HD12  | 1:G:43:TYR:HB3   | 2.01                     | 0.42              |
| 1:O:143:LYS:HD3  | 1:O:144:LEU:HD22 | 2.01                     | 0.42              |
| 1:Q:101:LEU:HD13 | 1:Q:124:LEU:HG   | 2.01                     | 0.42              |
| 1:S:84:THR:OG1   | 1:S:85:GLU:OE1   | 2.31                     | 0.42              |
| 1:H:92:GLU:O     | 1:H:96:GLU:N     | 2.52                     | 0.42              |
| 1:I:47:GLU:OE2   | 1:I:130:HIS:NE2  | 2.53                     | 0.42              |
| 1:P:132:ASP:O    | 1:P:136:THR:OG1  | 2.35                     | 0.42              |
| 1:Q:74:LEU:HD23  | 1:Q:74:LEU:HA    | 1.88                     | 0.42              |
| 1:X:101:LEU:HD12 | 1:X:101:LEU:HA   | 1.84                     | 0.42              |
| 1:M:98:ILE:O     | 1:M:102:ARG:N    | 2.44                     | 0.42              |
| 1:S:62:ILE:HD11  | 1:S:69:PRO:HG3   | 1.99                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:28:HIS:HA    | 1:T:31:LEU:HB2   | 2.00                     | 0.42              |
| 1:A:30:LYS:HA    | 1:A:30:LYS:HD2   | 1.86                     | 0.42              |
| 1:A:32:GLN:HG3   | 1:A:41:ALA:HB2   | 2.01                     | 0.42              |
| 1:C:111:LYS:HD2  | 1:C:111:LYS:HA   | 1.87                     | 0.42              |
| 1:F:137:GLN:OE1  | 1:F:149:TYR:OH   | 2.34                     | 0.42              |
| 1:K:99:ASP:HA    | 1:K:102:ARG:HB2  | 2.01                     | 0.42              |
| 1:R:92:GLU:O     | 1:R:96:GLU:N     | 2.52                     | 0.42              |
| 1:U:25:TYR:OH    | 1:U:94:GLU:OE2   | 2.36                     | 0.42              |
| 1:H:34:HIS:HB2   | 1:N:63:LEU:HD13  | 2.01                     | 0.42              |
| 1:M:50:ASP:O     | 1:M:54:HIS:N     | 2.51                     | 0.42              |
| 1:T:39:LYS:HA    | 1:T:42:LYS:HD3   | 2.00                     | 0.42              |
| 1:W:97:ALA:HA    | 1:W:100:ARG:NH2  | 2.34                     | 0.42              |
| 1:J:127:GLU:HA   | 1:J:130:HIS:HB3  | 2.02                     | 0.42              |
| 1:K:14:GLN:NE2   | 1:K:14:GLN:O     | 2.52                     | 0.42              |
| 1:L:39:LYS:HA    | 1:L:42:LYS:HD3   | 2.02                     | 0.42              |
| 1:R:19:LEU:HA    | 1:R:22:ILE:HD12  | 2.00                     | 0.42              |
| 1:J:27:LEU:O     | 1:J:31:LEU:N     | 2.50                     | 0.42              |
| 1:L:32:GLN:HE22  | 1:L:40:LEU:HG    | 1.85                     | 0.42              |
| 1:N:91:ARG:O     | 1:N:95:LEU:N     | 2.44                     | 0.42              |
| 1:W:83:VAL:O     | 1:W:87:PHE:N     | 2.50                     | 0.42              |
| 1:D:30:LYS:HA    | 1:D:30:LYS:HD2   | 1.89                     | 0.42              |
| 1:J:92:GLU:O     | 1:J:96:GLU:N     | 2.53                     | 0.42              |
| 1:O:144:LEU:HB3  | 1:O:148:LEU:HD21 | 2.01                     | 0.42              |
| 1:R:132:ASP:O    | 1:R:136:THR:N    | 2.50                     | 0.42              |
| 1:S:49:PHE:HZ    | 3:S:202:HEM:HBD2 | 1.85                     | 0.42              |
| 1:T:3:GLY:HA3    | 1:T:8:ILE:HD11   | 2.01                     | 0.42              |
| 1:V:27:LEU:HD11  | 1:W:71:TYR:CG    | 2.54                     | 0.42              |
| 1:C:101:LEU:HB3  | 1:C:124:LEU:HD11 | 2.02                     | 0.41              |
| 1:L:105:ILE:HA   | 1:L:108:MET:HB3  | 2.02                     | 0.41              |
| 1:O:25:TYR:OH    | 1:O:94:GLU:OE2   | 2.38                     | 0.41              |
| 1:T:74:LEU:HD23  | 1:T:74:LEU:HA    | 1.92                     | 0.41              |
| 1:A:14:GLN:NE2   | 1:A:14:GLN:O     | 2.52                     | 0.41              |
| 1:F:27:LEU:O     | 1:F:31:LEU:N     | 2.52                     | 0.41              |
| 1:I:92:GLU:O     | 1:I:96:GLU:N     | 2.53                     | 0.41              |
| 1:K:62:ILE:O     | 1:K:67:GLY:N     | 2.52                     | 0.41              |
| 1:M:94:GLU:OE2   | 1:M:130:HIS:ND1  | 2.53                     | 0.41              |
| 1:T:99:ASP:HA    | 1:T:102:ARG:HB2  | 2.00                     | 0.41              |
| 1:D:148:LEU:O    | 1:D:151:SER:OG   | 2.31                     | 0.41              |
| 1:I:111:LYS:HD2  | 1:I:111:LYS:HA   | 1.87                     | 0.41              |
| 1:K:11:LEU:HD13  | 1:K:62:ILE:HG22  | 2.01                     | 0.41              |
| 1:K:105:ILE:HG23 | 1:K:117:ALA:HB1  | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:140:LEU:HG   | 1:O:149:TYR:HE1  | 1.85                     | 0.41              |
| 1:F:139:ASP:HA   | 1:F:142:GLU:HB2  | 2.01                     | 0.41              |
| 1:G:62:ILE:HD11  | 1:G:69:PRO:HG3   | 2.03                     | 0.41              |
| 1:M:27:LEU:O     | 1:M:31:LEU:N     | 2.50                     | 0.41              |
| 1:M:32:GLN:HG3   | 1:M:41:ALA:HB2   | 2.02                     | 0.41              |
| 1:N:51:GLU:HA    | 1:N:54:HIS:HB2   | 2.02                     | 0.41              |
| 1:R:74:LEU:HD23  | 1:R:74:LEU:HA    | 1.88                     | 0.41              |
| 1:R:101:LEU:HD23 | 1:R:124:LEU:HG   | 2.01                     | 0.41              |
| 1:W:14:GLN:NE2   | 1:W:14:GLN:O     | 2.54                     | 0.41              |
| 1:B:99:ASP:HA    | 1:B:102:ARG:HB2  | 2.01                     | 0.41              |
| 1:C:99:ASP:HA    | 1:C:102:ARG:HB2  | 2.02                     | 0.41              |
| 1:H:117:ALA:HA   | 1:H:120:PHE:HB2  | 2.02                     | 0.41              |
| 1:N:74:LEU:HD23  | 1:N:74:LEU:HA    | 1.89                     | 0.41              |
| 1:Q:15:LEU:HD23  | 1:Q:58:LEU:HD13  | 2.03                     | 0.41              |
| 1:V:23:ASN:OD1   | 3:W:202:HEM:HBC1 | 2.20                     | 0.41              |
| 1:E:14:GLN:NE2   | 1:E:14:GLN:O     | 2.53                     | 0.41              |
| 1:I:24:GLN:NE2   | 1:I:78:ARG:O     | 2.54                     | 0.41              |
| 1:I:138:LEU:HA   | 1:I:141:ILE:HD12 | 2.01                     | 0.41              |
| 1:J:12:ASN:HA    | 1:J:15:LEU:HG    | 2.02                     | 0.41              |
| 1:P:31:LEU:HD23  | 1:P:31:LEU:HA    | 1.94                     | 0.41              |
| 1:Q:32:GLN:HG3   | 1:Q:41:ALA:HB2   | 2.02                     | 0.41              |
| 1:F:14:GLN:NE2   | 1:F:14:GLN:O     | 2.53                     | 0.41              |
| 1:H:62:ILE:O     | 1:H:67:GLY:N     | 2.49                     | 0.41              |
| 1:L:101:LEU:HD22 | 1:L:124:LEU:HG   | 2.03                     | 0.41              |
| 1:N:8:ILE:HA     | 1:N:11:LEU:HD12  | 2.02                     | 0.41              |
| 1:O:23:ASN:HD22  | 1:P:71:TYR:HB3   | 1.85                     | 0.41              |
| 1:O:24:GLN:NE2   | 1:O:78:ARG:O     | 2.53                     | 0.41              |
| 1:P:3:GLY:HA3    | 1:P:8:ILE:HD11   | 2.03                     | 0.41              |
| 1:S:3:GLY:HA3    | 1:S:65:LEU:HB3   | 2.02                     | 0.41              |
| 1:W:11:LEU:HD13  | 1:W:62:ILE:HG22  | 2.02                     | 0.41              |
| 1:A:61:ARG:HE    | 1:A:116:SER:HB3  | 1.85                     | 0.41              |
| 1:E:74:LEU:HD23  | 1:E:74:LEU:HA    | 1.89                     | 0.41              |
| 1:G:9:GLU:O      | 1:G:13:GLU:N     | 2.46                     | 0.41              |
| 1:G:34:HIS:HB2   | 1:X:63:LEU:HD21  | 2.01                     | 0.41              |
| 1:H:45:ARG:O     | 1:H:48:SER:OG    | 2.38                     | 0.41              |
| 1:H:106:GLU:HG3  | 1:H:107:VAL:HG23 | 2.03                     | 0.41              |
| 1:J:31:LEU:HD23  | 1:J:31:LEU:HA    | 1.96                     | 0.41              |
| 1:K:113:ASP:OD1  | 1:K:116:SER:OG   | 2.34                     | 0.41              |
| 1:O:127:GLU:HA   | 1:O:130:HIS:HB3  | 2.03                     | 0.41              |
| 1:O:144:LEU:HD13 | 1:O:144:LEU:HA   | 1.94                     | 0.41              |
| 1:S:14:GLN:NE2   | 1:S:14:GLN:O     | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:50:ASP:O     | 1:S:54:HIS:N     | 2.52                     | 0.41              |
| 1:S:96:GLU:HG3   | 1:S:100:ARG:HH12 | 1.85                     | 0.41              |
| 1:V:132:ASP:O    | 1:V:136:THR:N    | 2.51                     | 0.41              |
| 1:X:113:ASP:OD2  | 1:X:116:SER:OG   | 2.39                     | 0.41              |
| 1:G:27:LEU:HD11  | 1:X:71:TYR:CG    | 2.56                     | 0.41              |
| 1:J:11:LEU:HD13  | 1:J:62:ILE:HG22  | 2.03                     | 0.41              |
| 1:Q:28:HIS:HA    | 1:Q:31:LEU:HB2   | 2.03                     | 0.41              |
| 1:T:4:ASP:O      | 1:T:8:ILE:HG12   | 2.21                     | 0.41              |
| 1:V:33:ASP:OD1   | 1:V:33:ASP:N     | 2.53                     | 0.41              |
| 1:A:39:LYS:HA    | 1:A:42:LYS:HD3   | 2.02                     | 0.40              |
| 1:G:84:THR:H     | 1:G:84:THR:HG23  | 1.68                     | 0.40              |
| 1:O:101:LEU:HB3  | 1:O:124:LEU:HD22 | 2.02                     | 0.40              |
| 1:I:4:ASP:O      | 1:I:8:ILE:HG12   | 2.20                     | 0.40              |
| 1:M:62:ILE:O     | 1:M:67:GLY:N     | 2.52                     | 0.40              |
| 1:O:40:LEU:HA    | 1:W:156:GLN:HE22 | 1.87                     | 0.40              |
| 1:U:14:GLN:NE2   | 1:U:14:GLN:O     | 2.55                     | 0.40              |
| 1:X:101:LEU:HD23 | 1:X:124:LEU:HG   | 2.03                     | 0.40              |
| 1:D:74:LEU:HD23  | 1:D:74:LEU:HA    | 1.88                     | 0.40              |
| 1:D:133:TYR:O    | 1:D:136:THR:OG1  | 2.32                     | 0.40              |
| 1:E:105:ILE:HA   | 1:E:108:MET:HG2  | 2.02                     | 0.40              |
| 1:H:6:GLU:O      | 1:H:10:PHE:N     | 2.51                     | 0.40              |
| 1:I:28:HIS:HA    | 1:I:31:LEU:HB2   | 2.02                     | 0.40              |
| 1:P:45:ARG:O     | 1:P:48:SER:OG    | 2.39                     | 0.40              |
| 1:R:83:VAL:O     | 1:R:87:PHE:N     | 2.52                     | 0.40              |
| 1:X:3:GLY:HA3    | 1:X:8:ILE:HD11   | 2.04                     | 0.40              |
| 1:F:42:LYS:HE2   | 1:F:42:LYS:HB3   | 1.86                     | 0.40              |
| 1:L:71:TYR:CG    | 1:M:27:LEU:HD11  | 2.57                     | 0.40              |
| 1:Q:111:LYS:HD2  | 1:Q:111:LYS:HA   | 1.87                     | 0.40              |
| 1:B:111:LYS:HD2  | 1:B:111:LYS:HA   | 1.86                     | 0.40              |
| 1:H:111:LYS:HA   | 1:H:111:LYS:HD2  | 1.88                     | 0.40              |
| 1:I:124:LEU:HD23 | 1:I:124:LEU:HA   | 1.92                     | 0.40              |
| 1:L:62:ILE:HD11  | 1:L:69:PRO:HG3   | 2.04                     | 0.40              |
| 1:L:99:ASP:HA    | 1:L:102:ARG:HB2  | 2.04                     | 0.40              |
| 1:O:111:LYS:HD2  | 1:O:111:LYS:HA   | 1.86                     | 0.40              |
| 1:P:101:LEU:HD13 | 1:P:124:LEU:HG   | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 156/167 (93%)   | 154 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | B     | 155/167 (93%)   | 152 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | C     | 156/167 (93%)   | 153 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | D     | 155/167 (93%)   | 154 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | E     | 156/167 (93%)   | 153 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | F     | 157/167 (94%)   | 153 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | G     | 157/167 (94%)   | 155 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | H     | 157/167 (94%)   | 154 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | I     | 156/167 (93%)   | 153 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | J     | 157/167 (94%)   | 155 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | K     | 155/167 (93%)   | 152 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | L     | 156/167 (93%)   | 154 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | M     | 155/167 (93%)   | 153 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | N     | 157/167 (94%)   | 152 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | O     | 156/167 (93%)   | 153 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | P     | 155/167 (93%)   | 153 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | Q     | 156/167 (93%)   | 151 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | R     | 155/167 (93%)   | 152 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | S     | 157/167 (94%)   | 153 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | T     | 155/167 (93%)   | 153 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | U     | 155/167 (93%)   | 150 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | V     | 156/167 (93%)   | 154 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | W     | 155/167 (93%)   | 153 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | X     | 157/167 (94%)   | 154 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| All | All   | 3742/4008 (93%) | 3673 (98%) | 69 (2%) | 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     | 138/147 (94%) | 137 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | B     | 138/147 (94%) | 138 (100%) | 0        | 100         | 100 |
| 1   | C     | 139/147 (95%) | 139 (100%) | 0        | 100         | 100 |
| 1   | D     | 138/147 (94%) | 137 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | E     | 138/147 (94%) | 136 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | F     | 138/147 (94%) | 136 (99%)  | 2 (1%)   | 59          | 71  |
| 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%) | 139 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | K     | 138/147 (94%) | 137 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | L     | 139/147 (95%) | 138 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | M     | 138/147 (94%) | 138 (100%) | 0        | 100         | 100 |
| 1   | N     | 138/147 (94%) | 137 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | O     | 139/147 (95%) | 137 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | P     | 138/147 (94%) | 137 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | Q     | 139/147 (95%) | 139 (100%) | 0        | 100         | 100 |
| 1   | R     | 138/147 (94%) | 138 (100%) | 0        | 100         | 100 |
| 1   | S     | 138/147 (94%) | 137 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | T     | 139/147 (95%) | 138 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | U     | 138/147 (94%) | 137 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | V     | 139/147 (95%) | 138 (99%)  | 1 (1%)   | 76          | 79  |
| 1   | W     | 138/147 (94%) | 138 (100%) | 0        | 100         | 100 |
| 1   | X     | 138/147 (94%) | 137 (99%)  | 1 (1%)   | 76          | 79  |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |    |
|-----|-------|-----------------|-------------|----------|-------------|----|
| All | All   | 3320/3528 (94%) | 3302 (100%) | 18 (0%)  | 78          | 81 |

All (18) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 60  | ASP  |
| 1   | D     | 9   | GLU  |
| 1   | F     | 79  | VAL  |
| 1   | F     | 101 | LEU  |
| 1   | E     | 60  | ASP  |
| 1   | E     | 116 | SER  |
| 1   | J     | 50  | ASP  |
| 1   | K     | 9   | GLU  |
| 1   | L     | 126 | ASP  |
| 1   | N     | 79  | VAL  |
| 1   | O     | 23  | ASN  |
| 1   | O     | 60  | ASP  |
| 1   | P     | 101 | LEU  |
| 1   | S     | 19  | LEU  |
| 1   | T     | 86  | MET  |
| 1   | U     | 101 | LEU  |
| 1   | V     | 79  | VAL  |
| 1   | X     | 60  | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 14  | GLN  |
| 1   | A     | 118 | ASN  |
| 1   | B     | 23  | ASN  |
| 1   | B     | 118 | ASN  |
| 1   | C     | 14  | GLN  |
| 1   | C     | 118 | ASN  |
| 1   | C     | 156 | GLN  |
| 1   | D     | 14  | GLN  |
| 1   | D     | 118 | ASN  |
| 1   | D     | 156 | GLN  |
| 1   | F     | 14  | GLN  |
| 1   | E     | 14  | GLN  |
| 1   | E     | 32  | GLN  |
| 1   | E     | 72  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 118 | ASN  |
| 1   | G     | 12  | ASN  |
| 1   | G     | 72  | GLN  |
| 1   | G     | 118 | ASN  |
| 1   | G     | 129 | HIS  |
| 1   | G     | 156 | GLN  |
| 1   | H     | 72  | GLN  |
| 1   | I     | 14  | GLN  |
| 1   | I     | 72  | GLN  |
| 1   | I     | 118 | ASN  |
| 1   | J     | 32  | GLN  |
| 1   | K     | 32  | GLN  |
| 1   | K     | 81  | GLN  |
| 1   | K     | 118 | ASN  |
| 1   | K     | 156 | GLN  |
| 1   | L     | 118 | ASN  |
| 1   | M     | 14  | GLN  |
| 1   | M     | 156 | GLN  |
| 1   | N     | 14  | GLN  |
| 1   | O     | 32  | GLN  |
| 1   | O     | 118 | ASN  |
| 1   | P     | 14  | GLN  |
| 1   | P     | 23  | ASN  |
| 1   | P     | 81  | GLN  |
| 1   | P     | 118 | ASN  |
| 1   | Q     | 14  | GLN  |
| 1   | Q     | 118 | ASN  |
| 1   | Q     | 130 | HIS  |
| 1   | Q     | 156 | GLN  |
| 1   | R     | 14  | GLN  |
| 1   | R     | 118 | ASN  |
| 1   | S     | 14  | GLN  |
| 1   | S     | 156 | GLN  |
| 1   | T     | 130 | HIS  |
| 1   | U     | 14  | GLN  |
| 1   | U     | 118 | ASN  |
| 1   | V     | 118 | ASN  |
| 1   | V     | 156 | GLN  |
| 1   | W     | 14  | GLN  |
| 1   | W     | 118 | ASN  |
| 1   | X     | 14  | 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  | A     | 202 | 1    | 50,50,50     | 1.45 | 9 (18%)     | 66,82,82    | 1.33 | 7 (10%)     |
| 3   | HEM  | C     | 202 | 1    | 50,50,50     | 1.62 | 8 (16%)     | 66,82,82    | 1.29 | 9 (13%)     |
| 3   | HEM  | S     | 202 | 1    | 50,50,50     | 1.43 | 8 (16%)     | 66,82,82    | 1.09 | 4 (6%)      |
| 3   | HEM  | H     | 202 | 1    | 50,50,50     | 1.41 | 7 (14%)     | 66,82,82    | 1.21 | 7 (10%)     |
| 3   | HEM  | U     | 202 | 1    | 50,50,50     | 1.33 | 8 (16%)     | 66,82,82    | 1.13 | 5 (7%)      |
| 3   | HEM  | K     | 301 | -    | 50,50,50     | 1.35 | 9 (18%)     | 66,82,82    | 1.15 | 5 (7%)      |
| 3   | HEM  | P     | 202 | 1    | 50,50,50     | 1.57 | 8 (16%)     | 66,82,82    | 1.26 | 7 (10%)     |
| 3   | HEM  | F     | 202 | 1    | 50,50,50     | 1.40 | 8 (16%)     | 66,82,82    | 1.16 | 6 (9%)      |
| 3   | HEM  | X     | 301 | 1    | 50,50,50     | 1.44 | 8 (16%)     | 66,82,82    | 1.07 | 4 (6%)      |
| 3   | HEM  | R     | 301 | 1    | 50,50,50     | 1.38 | 9 (18%)     | 66,82,82    | 1.11 | 5 (7%)      |
| 3   | HEM  | W     | 202 | 1    | 50,50,50     | 1.47 | 8 (16%)     | 66,82,82    | 1.10 | 5 (7%)      |
| 3   | HEM  | L     | 202 | 1    | 50,50,50     | 1.37 | 7 (14%)     | 66,82,82    | 1.19 | 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  | A     | 202 | 1    | -       | 2/14/54/54 | -     |
| 3   | HEM  | C     | 202 | 1    | -       | 2/14/54/54 | -     |
| 3   | HEM  | S     | 202 | 1    | -       | 2/14/54/54 | -     |
| 3   | HEM  | H     | 202 | 1    | -       | 2/14/54/54 | -     |
| 3   | HEM  | U     | 202 | 1    | -       | 2/14/54/54 | -     |
| 3   | HEM  | K     | 301 | -    | -       | 2/14/54/54 | -     |
| 3   | HEM  | P     | 202 | 1    | -       | 1/14/54/54 | -     |
| 3   | HEM  | F     | 202 | 1    | -       | 2/14/54/54 | -     |
| 3   | HEM  | X     | 301 | 1    | -       | 0/14/54/54 | -     |
| 3   | HEM  | R     | 301 | 1    | -       | 1/14/54/54 | -     |
| 3   | HEM  | W     | 202 | 1    | -       | 2/14/54/54 | -     |
| 3   | HEM  | L     | 202 | 1    | -       | 3/14/54/54 | -     |

All (97) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | C     | 202 | HEM  | FE-ND   | 5.59 | 2.12        | 1.94     |
| 3   | C     | 202 | HEM  | FE-NB   | 4.63 | 2.09        | 1.94     |
| 3   | P     | 202 | HEM  | FE-ND   | 3.99 | 2.07        | 1.94     |
| 3   | W     | 202 | HEM  | FE-ND   | 3.86 | 2.06        | 1.94     |
| 3   | X     | 301 | HEM  | FE-NC   | 3.76 | 2.07        | 1.95     |
| 3   | W     | 202 | HEM  | FE-NB   | 3.75 | 2.06        | 1.94     |
| 3   | P     | 202 | HEM  | FE-NC   | 3.72 | 2.07        | 1.95     |
| 3   | P     | 202 | HEM  | FE-NB   | 3.65 | 2.06        | 1.94     |
| 3   | X     | 301 | HEM  | FE-NA   | 3.59 | 2.07        | 1.95     |
| 3   | A     | 202 | HEM  | FE-NC   | 3.54 | 2.07        | 1.95     |
| 3   | S     | 202 | HEM  | FE-NC   | 3.42 | 2.06        | 1.95     |
| 3   | P     | 202 | HEM  | FE-NA   | 3.39 | 2.06        | 1.95     |
| 3   | L     | 202 | HEM  | CAC-C3C | 3.27 | 1.56        | 1.47     |
| 3   | K     | 301 | HEM  | CAC-C3C | 3.27 | 1.56        | 1.47     |
| 3   | A     | 202 | HEM  | FE-NA   | 3.27 | 2.06        | 1.95     |
| 3   | C     | 202 | HEM  | CAC-C3C | 3.25 | 1.56        | 1.47     |
| 3   | A     | 202 | HEM  | CAB-C3B | 3.24 | 1.56        | 1.47     |
| 3   | U     | 202 | HEM  | CAB-C3B | 3.24 | 1.56        | 1.47     |
| 3   | A     | 202 | HEM  | CAC-C3C | 3.24 | 1.56        | 1.47     |
| 3   | L     | 202 | HEM  | FE-ND   | 3.22 | 2.04        | 1.94     |
| 3   | F     | 202 | HEM  | CAB-C3B | 3.21 | 1.56        | 1.47     |
| 3   | P     | 202 | HEM  | CAB-C3B | 3.21 | 1.56        | 1.47     |
| 3   | S     | 202 | HEM  | CAC-C3C | 3.19 | 1.56        | 1.47     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3   | L     | 202 | HEM  | FE-NB   | 3.19 | 2.04        | 1.94     |
| 3   | S     | 202 | HEM  | CAB-C3B | 3.18 | 1.56        | 1.47     |
| 3   | X     | 301 | HEM  | CAC-C3C | 3.17 | 1.56        | 1.47     |
| 3   | R     | 301 | HEM  | CAC-C3C | 3.17 | 1.56        | 1.47     |
| 3   | K     | 301 | HEM  | CAB-C3B | 3.16 | 1.56        | 1.47     |
| 3   | H     | 202 | HEM  | CAB-C3B | 3.16 | 1.56        | 1.47     |
| 3   | P     | 202 | HEM  | CAC-C3C | 3.16 | 1.56        | 1.47     |
| 3   | R     | 301 | HEM  | CAB-C3B | 3.14 | 1.56        | 1.47     |
| 3   | F     | 202 | HEM  | CAC-C3C | 3.14 | 1.56        | 1.47     |
| 3   | W     | 202 | HEM  | CAC-C3C | 3.12 | 1.55        | 1.47     |
| 3   | W     | 202 | HEM  | CAB-C3B | 3.12 | 1.55        | 1.47     |
| 3   | U     | 202 | HEM  | CAC-C3C | 3.12 | 1.55        | 1.47     |
| 3   | L     | 202 | HEM  | CAB-C3B | 3.11 | 1.55        | 1.47     |
| 3   | C     | 202 | HEM  | FE-NC   | 3.11 | 2.05        | 1.95     |
| 3   | F     | 202 | HEM  | FE-NB   | 3.10 | 2.04        | 1.94     |
| 3   | C     | 202 | HEM  | CAB-C3B | 3.07 | 1.55        | 1.47     |
| 3   | H     | 202 | HEM  | CAC-C3C | 3.06 | 1.55        | 1.47     |
| 3   | S     | 202 | HEM  | FE-NB   | 3.00 | 2.04        | 1.94     |
| 3   | R     | 301 | HEM  | FE-NC   | 2.99 | 2.05        | 1.95     |
| 3   | H     | 202 | HEM  | FE-NA   | 2.98 | 2.05        | 1.95     |
| 3   | X     | 301 | HEM  | CAB-C3B | 2.98 | 1.55        | 1.47     |
| 3   | K     | 301 | HEM  | FE-NC   | 2.96 | 2.05        | 1.95     |
| 3   | R     | 301 | HEM  | FE-NA   | 2.95 | 2.05        | 1.95     |
| 3   | A     | 202 | HEM  | FE-NB   | 2.92 | 2.03        | 1.94     |
| 3   | H     | 202 | HEM  | FE-NC   | 2.90 | 2.04        | 1.95     |
| 3   | H     | 202 | HEM  | FE-NB   | 2.88 | 2.03        | 1.94     |
| 3   | F     | 202 | HEM  | FE-NC   | 2.80 | 2.04        | 1.95     |
| 3   | F     | 202 | HEM  | FE-ND   | 2.78 | 2.03        | 1.94     |
| 3   | X     | 301 | HEM  | FE-NB   | 2.73 | 2.03        | 1.94     |
| 3   | S     | 202 | HEM  | FE-ND   | 2.72 | 2.03        | 1.94     |
| 3   | S     | 202 | HEM  | FE-NA   | 2.69 | 2.04        | 1.95     |
| 3   | W     | 202 | HEM  | FE-NC   | 2.65 | 2.04        | 1.95     |
| 3   | A     | 202 | HEM  | FE-ND   | 2.63 | 2.03        | 1.94     |
| 3   | H     | 202 | HEM  | FE-ND   | 2.63 | 2.03        | 1.94     |
| 3   | L     | 202 | HEM  | FE-NC   | 2.44 | 2.03        | 1.95     |
| 3   | F     | 202 | HEM  | FE-NA   | 2.43 | 2.03        | 1.95     |
| 3   | K     | 301 | HEM  | FE-NB   | 2.41 | 2.02        | 1.94     |
| 3   | U     | 202 | HEM  | FE-NC   | 2.37 | 2.03        | 1.95     |
| 3   | A     | 202 | HEM  | CMC-C2C | 2.37 | 1.55        | 1.50     |
| 3   | W     | 202 | HEM  | FE-NA   | 2.32 | 2.03        | 1.95     |
| 3   | R     | 301 | HEM  | FE-NB   | 2.31 | 2.02        | 1.94     |
| 3   | C     | 202 | HEM  | FE-NA   | 2.24 | 2.02        | 1.95     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3   | X     | 301 | HEM  | FE-ND   | 2.23  | 2.01        | 1.94     |
| 3   | U     | 202 | HEM  | FE-NA   | 2.22  | 2.02        | 1.95     |
| 3   | K     | 301 | HEM  | FE-NA   | 2.22  | 2.02        | 1.95     |
| 3   | R     | 301 | HEM  | FE-ND   | 2.20  | 2.01        | 1.94     |
| 3   | K     | 301 | HEM  | CMC-C2C | 2.18  | 1.55        | 1.50     |
| 3   | K     | 301 | HEM  | C2A-C3A | -2.16 | 1.33        | 1.38     |
| 3   | U     | 202 | HEM  | FE-NB   | 2.14  | 2.01        | 1.94     |
| 3   | A     | 202 | HEM  | C2A-C3A | -2.12 | 1.33        | 1.38     |
| 3   | W     | 202 | HEM  | CMB-C2B | 2.12  | 1.55        | 1.50     |
| 3   | K     | 301 | HEM  | CMB-C2B | 2.11  | 1.55        | 1.50     |
| 3   | W     | 202 | HEM  | CMC-C2C | 2.11  | 1.55        | 1.50     |
| 3   | R     | 301 | HEM  | CMB-C2B | 2.10  | 1.55        | 1.50     |
| 3   | X     | 301 | HEM  | CMB-C2B | 2.09  | 1.55        | 1.50     |
| 3   | P     | 202 | HEM  | CMC-C2C | 2.09  | 1.55        | 1.50     |
| 3   | F     | 202 | HEM  | CMB-C2B | 2.08  | 1.55        | 1.50     |
| 3   | C     | 202 | HEM  | CMC-C2C | 2.07  | 1.55        | 1.50     |
| 3   | R     | 301 | HEM  | CMC-C2C | 2.07  | 1.55        | 1.50     |
| 3   | F     | 202 | HEM  | CMC-C2C | 2.07  | 1.55        | 1.50     |
| 3   | X     | 301 | HEM  | CMC-C2C | 2.07  | 1.55        | 1.50     |
| 3   | S     | 202 | HEM  | CMB-C2B | 2.05  | 1.55        | 1.50     |
| 3   | U     | 202 | HEM  | CMB-C2B | 2.05  | 1.55        | 1.50     |
| 3   | L     | 202 | HEM  | CMC-C2C | 2.05  | 1.55        | 1.50     |
| 3   | P     | 202 | HEM  | CMB-C2B | 2.04  | 1.55        | 1.50     |
| 3   | U     | 202 | HEM  | CMC-C2C | 2.04  | 1.55        | 1.50     |
| 3   | H     | 202 | HEM  | CMB-C2B | 2.03  | 1.55        | 1.50     |
| 3   | L     | 202 | HEM  | CMB-C2B | 2.03  | 1.55        | 1.50     |
| 3   | U     | 202 | HEM  | FE-ND   | 2.03  | 2.01        | 1.94     |
| 3   | S     | 202 | HEM  | CMC-C2C | 2.02  | 1.55        | 1.50     |
| 3   | R     | 301 | HEM  | CMA-C3A | 2.02  | 1.55        | 1.50     |
| 3   | A     | 202 | HEM  | CMB-C2B | 2.01  | 1.55        | 1.50     |
| 3   | C     | 202 | HEM  | CMB-C2B | 2.01  | 1.55        | 1.50     |
| 3   | K     | 301 | HEM  | FE-ND   | 2.00  | 2.01        | 1.94     |

All (69) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | C     | 202 | HEM  | C4A-NA-C1A  | 3.61  | 108.89      | 105.35   |
| 3   | A     | 202 | HEM  | CAA-CBA-CGA | -3.44 | 106.20      | 113.60   |
| 3   | A     | 202 | HEM  | C4D-ND-C1D  | 3.24  | 108.42      | 105.07   |
| 3   | A     | 202 | HEM  | CMB-C2B-C1B | -3.06 | 120.37      | 125.04   |
| 3   | L     | 202 | HEM  | CAA-CBA-CGA | -3.05 | 107.04      | 113.60   |
| 3   | P     | 202 | HEM  | C1C-CHC-C4B | -2.84 | 119.92      | 126.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | L     | 202 | HEM  | C4A-NA-C1A  | 2.75  | 108.04      | 105.35   |
| 3   | C     | 202 | HEM  | C2A-C1A-NA  | -2.55 | 107.30      | 110.15   |
| 3   | H     | 202 | HEM  | CAC-C3C-C4C | 2.54  | 131.03      | 124.90   |
| 3   | X     | 301 | HEM  | C4D-ND-C1D  | 2.52  | 107.67      | 105.07   |
| 3   | R     | 301 | HEM  | C4D-ND-C1D  | 2.51  | 107.67      | 105.07   |
| 3   | L     | 202 | HEM  | CMB-C2B-C1B | -2.46 | 121.29      | 125.04   |
| 3   | C     | 202 | HEM  | CHA-C4D-ND  | -2.46 | 121.34      | 124.37   |
| 3   | U     | 202 | HEM  | C4C-CHD-C1D | -2.45 | 120.78      | 126.06   |
| 3   | A     | 202 | HEM  | C3D-C4D-ND  | -2.41 | 107.49      | 110.17   |
| 3   | C     | 202 | HEM  | CMB-C2B-C1B | -2.39 | 121.39      | 125.04   |
| 3   | U     | 202 | HEM  | CMB-C2B-C1B | -2.37 | 121.42      | 125.04   |
| 3   | K     | 301 | HEM  | CAD-CBD-CGD | -2.37 | 108.51      | 113.60   |
| 3   | H     | 202 | HEM  | C4C-NC-C1C  | 2.36  | 107.66      | 105.35   |
| 3   | F     | 202 | HEM  | CMB-C2B-C1B | -2.36 | 121.45      | 125.04   |
| 3   | P     | 202 | HEM  | CAA-CBA-CGA | -2.35 | 108.54      | 113.60   |
| 3   | U     | 202 | HEM  | C4D-ND-C1D  | 2.35  | 107.50      | 105.07   |
| 3   | C     | 202 | HEM  | CHA-C4D-C3D | 2.33  | 129.70      | 125.33   |
| 3   | K     | 301 | HEM  | C4D-ND-C1D  | 2.33  | 107.48      | 105.07   |
| 3   | P     | 202 | HEM  | C4D-ND-C1D  | 2.32  | 107.47      | 105.07   |
| 3   | R     | 301 | HEM  | CMB-C2B-C1B | -2.32 | 121.51      | 125.04   |
| 3   | H     | 202 | HEM  | CMB-C2B-C1B | -2.32 | 121.51      | 125.04   |
| 3   | C     | 202 | HEM  | C4C-CHD-C1D | -2.29 | 121.11      | 126.06   |
| 3   | H     | 202 | HEM  | C4D-ND-C1D  | 2.29  | 107.44      | 105.07   |
| 3   | P     | 202 | HEM  | C4A-CHB-C1B | -2.27 | 120.96      | 126.34   |
| 3   | W     | 202 | HEM  | C4D-ND-C1D  | 2.26  | 107.41      | 105.07   |
| 3   | F     | 202 | HEM  | C4A-NA-C1A  | 2.26  | 107.56      | 105.35   |
| 3   | W     | 202 | HEM  | C4A-NA-C1A  | 2.26  | 107.56      | 105.35   |
| 3   | X     | 301 | HEM  | CHD-C1D-ND  | 2.23  | 126.84      | 124.42   |
| 3   | W     | 202 | HEM  | CMB-C2B-C1B | -2.22 | 121.66      | 125.04   |
| 3   | P     | 202 | HEM  | CAD-CBD-CGD | -2.22 | 108.83      | 113.60   |
| 3   | S     | 202 | HEM  | C4D-ND-C1D  | 2.22  | 107.37      | 105.07   |
| 3   | H     | 202 | HEM  | CHD-C4C-C3C | 2.21  | 129.05      | 125.26   |
| 3   | K     | 301 | HEM  | CMB-C2B-C1B | -2.21 | 121.67      | 125.04   |
| 3   | P     | 202 | HEM  | C4C-NC-C1C  | 2.19  | 107.49      | 105.35   |
| 3   | P     | 202 | HEM  | CMB-C2B-C1B | -2.18 | 121.72      | 125.04   |
| 3   | X     | 301 | HEM  | CAD-CBD-CGD | -2.18 | 108.92      | 113.60   |
| 3   | S     | 202 | HEM  | CMB-C2B-C1B | -2.17 | 121.73      | 125.04   |
| 3   | R     | 301 | HEM  | CAD-CBD-CGD | -2.17 | 108.92      | 113.60   |
| 3   | L     | 202 | HEM  | C4D-ND-C1D  | 2.17  | 107.31      | 105.07   |
| 3   | F     | 202 | HEM  | C1B-NB-C4B  | 2.16  | 107.31      | 105.07   |
| 3   | W     | 202 | HEM  | CMC-C2C-C1C | -2.14 | 120.94      | 124.71   |
| 3   | K     | 301 | HEM  | CAA-CBA-CGA | -2.13 | 109.01      | 113.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3   | H     | 202 | HEM  | C4A-NA-C1A  | 2.13  | 107.43      | 105.35   |
| 3   | R     | 301 | HEM  | C4A-NA-C1A  | 2.12  | 107.42      | 105.35   |
| 3   | F     | 202 | HEM  | C1C-CHC-C4B | -2.10 | 121.53      | 126.06   |
| 3   | X     | 301 | HEM  | CMB-C2B-C1B | -2.09 | 121.85      | 125.04   |
| 3   | W     | 202 | HEM  | C4A-CHB-C1B | -2.09 | 121.39      | 126.34   |
| 3   | C     | 202 | HEM  | CAC-C3C-C4C | -2.09 | 119.86      | 124.90   |
| 3   | A     | 202 | HEM  | C3B-C2B-C1B | 2.08  | 108.03      | 106.49   |
| 3   | F     | 202 | HEM  | CMC-C2C-C1C | -2.07 | 121.07      | 124.71   |
| 3   | L     | 202 | HEM  | C2A-C1A-NA  | -2.06 | 107.84      | 110.15   |
| 3   | F     | 202 | HEM  | C4D-ND-C1D  | 2.05  | 107.19      | 105.07   |
| 3   | A     | 202 | HEM  | C2D-C1D-ND  | -2.05 | 107.43      | 109.88   |
| 3   | U     | 202 | HEM  | CAA-CBA-CGA | -2.05 | 109.19      | 113.60   |
| 3   | K     | 301 | HEM  | CBA-CAA-C2A | -2.05 | 106.94      | 112.63   |
| 3   | U     | 202 | HEM  | CAC-C3C-C4C | -2.04 | 119.97      | 124.90   |
| 3   | R     | 301 | HEM  | C3D-C4D-ND  | -2.03 | 107.91      | 110.17   |
| 3   | S     | 202 | HEM  | C4A-NA-C1A  | 2.02  | 107.33      | 105.35   |
| 3   | H     | 202 | HEM  | CAC-C3C-C2C | -2.02 | 121.94      | 128.60   |
| 3   | S     | 202 | HEM  | CMC-C2C-C1C | -2.02 | 121.15      | 124.71   |
| 3   | C     | 202 | HEM  | C4D-ND-C1D  | 2.02  | 107.16      | 105.07   |
| 3   | A     | 202 | HEM  | CMC-C2C-C1C | -2.02 | 121.16      | 124.71   |
| 3   | C     | 202 | HEM  | C4A-C3A-C2A | 2.00  | 109.18      | 106.83   |

There are no chirality outliers.

All (21) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | H     | 202 | HEM  | C3D-CAD-CBD-CGD |
| 3   | K     | 301 | HEM  | C2A-CAA-CBA-CGA |
| 3   | F     | 202 | HEM  | C3D-CAD-CBD-CGD |
| 3   | H     | 202 | HEM  | C4C-C3C-CAC-CBC |
| 3   | S     | 202 | HEM  | C2A-CAA-CBA-CGA |
| 3   | S     | 202 | HEM  | C3D-CAD-CBD-CGD |
| 3   | F     | 202 | HEM  | C2A-CAA-CBA-CGA |
| 3   | K     | 301 | HEM  | C3D-CAD-CBD-CGD |
| 3   | L     | 202 | HEM  | C3D-CAD-CBD-CGD |
| 3   | A     | 202 | HEM  | C2A-CAA-CBA-CGA |
| 3   | P     | 202 | HEM  | C2A-CAA-CBA-CGA |
| 3   | W     | 202 | HEM  | CAD-CBD-CGD-O2D |
| 3   | C     | 202 | HEM  | C2A-CAA-CBA-CGA |
| 3   | W     | 202 | HEM  | CAD-CBD-CGD-O1D |
| 3   | A     | 202 | HEM  | C3D-CAD-CBD-CGD |
| 3   | L     | 202 | HEM  | CAA-CBA-CGA-O1A |

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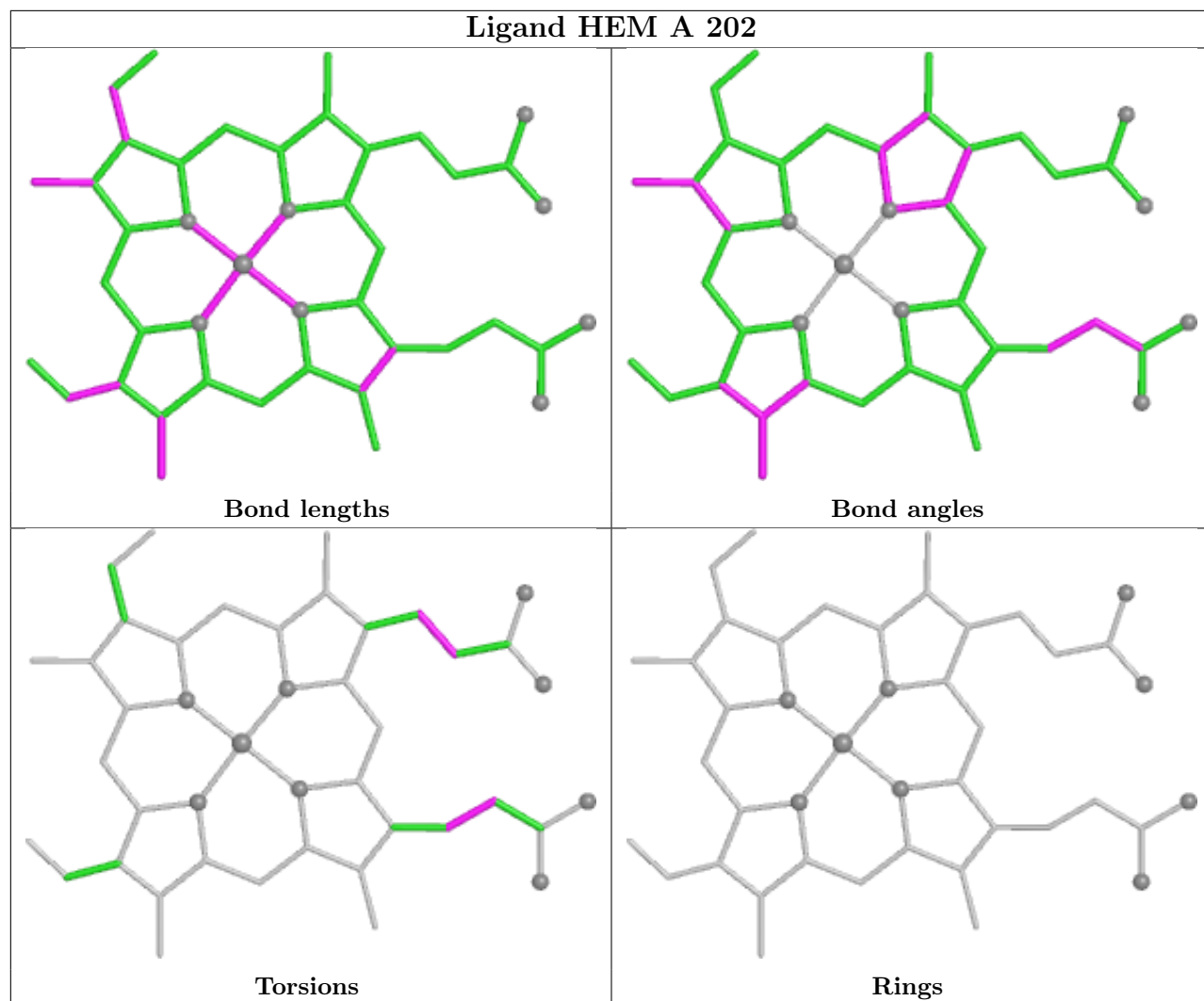
| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 3   | L     | 202 | HEM  | CAA-CBA-CGA-O2A |
| 3   | U     | 202 | HEM  | CAD-CBD-CGD-O2D |
| 3   | U     | 202 | HEM  | CAD-CBD-CGD-O1D |
| 3   | R     | 301 | HEM  | CAA-CBA-CGA-O1A |
| 3   | C     | 202 | HEM  | C1A-C2A-CAA-CBA |

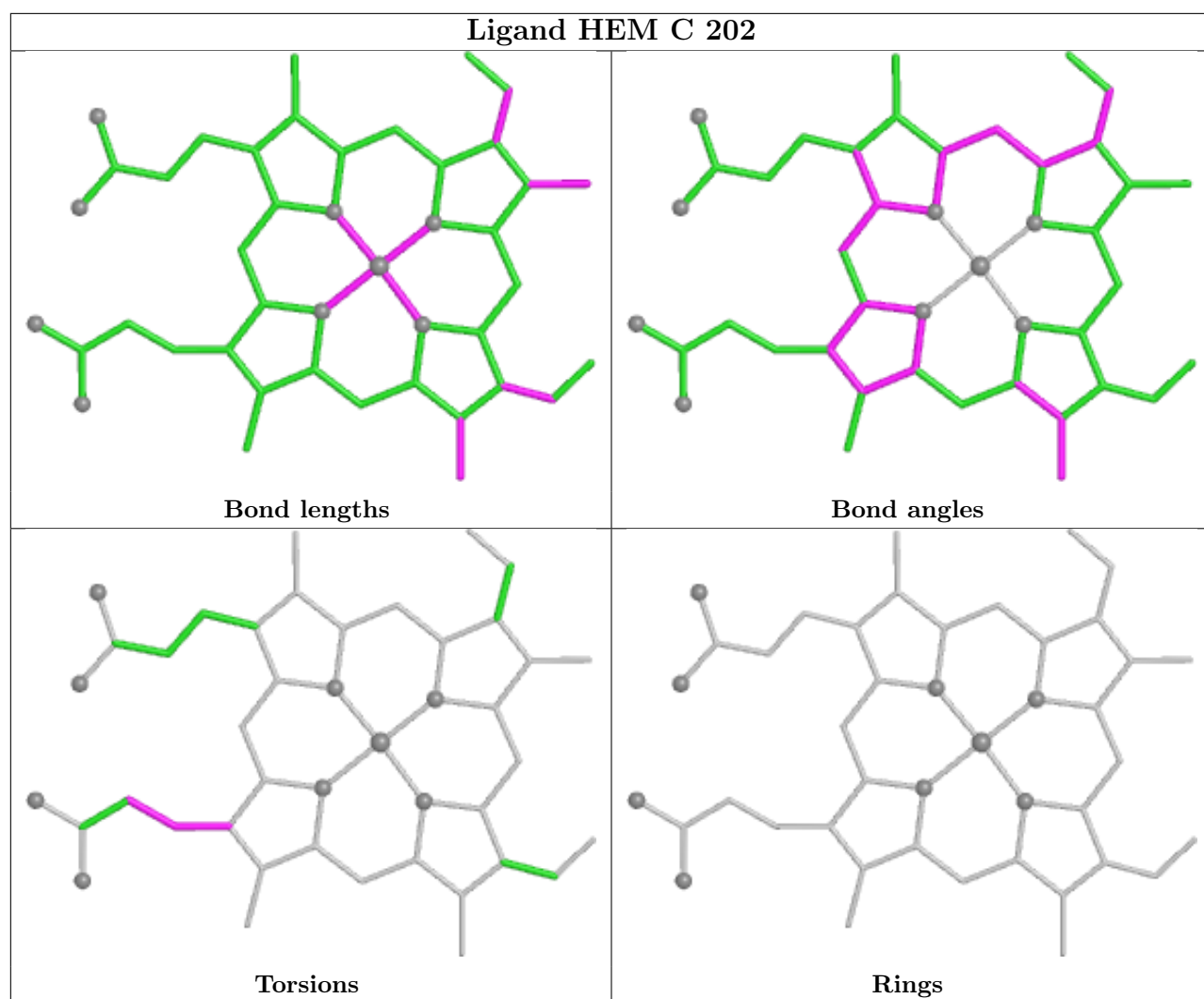
There are no ring outliers.

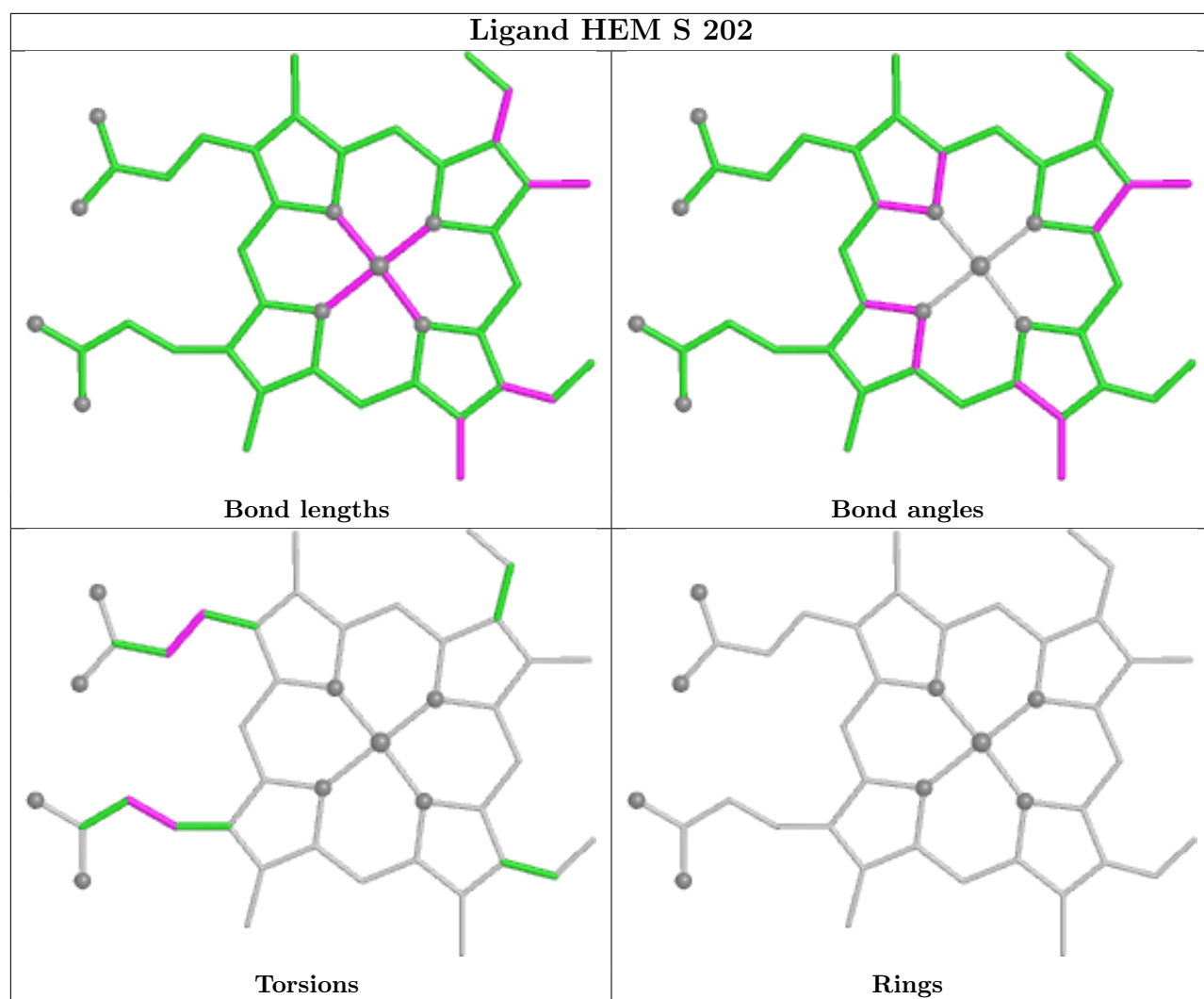
3 monomers are involved in 3 short contacts:

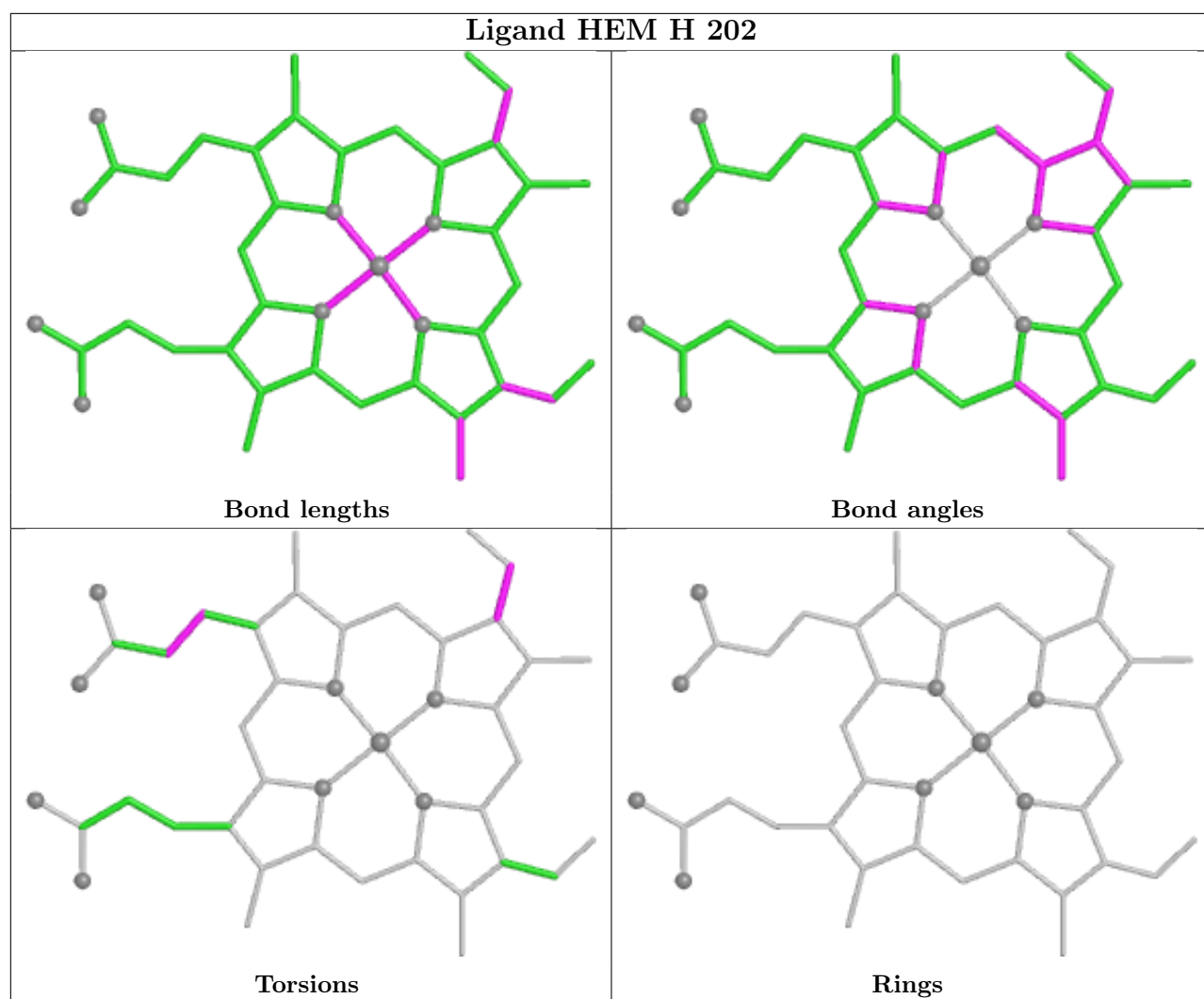
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | C     | 202 | HEM  | 1       | 0            |
| 3   | S     | 202 | HEM  | 1       | 0            |
| 3   | W     | 202 | HEM  | 1       | 0            |

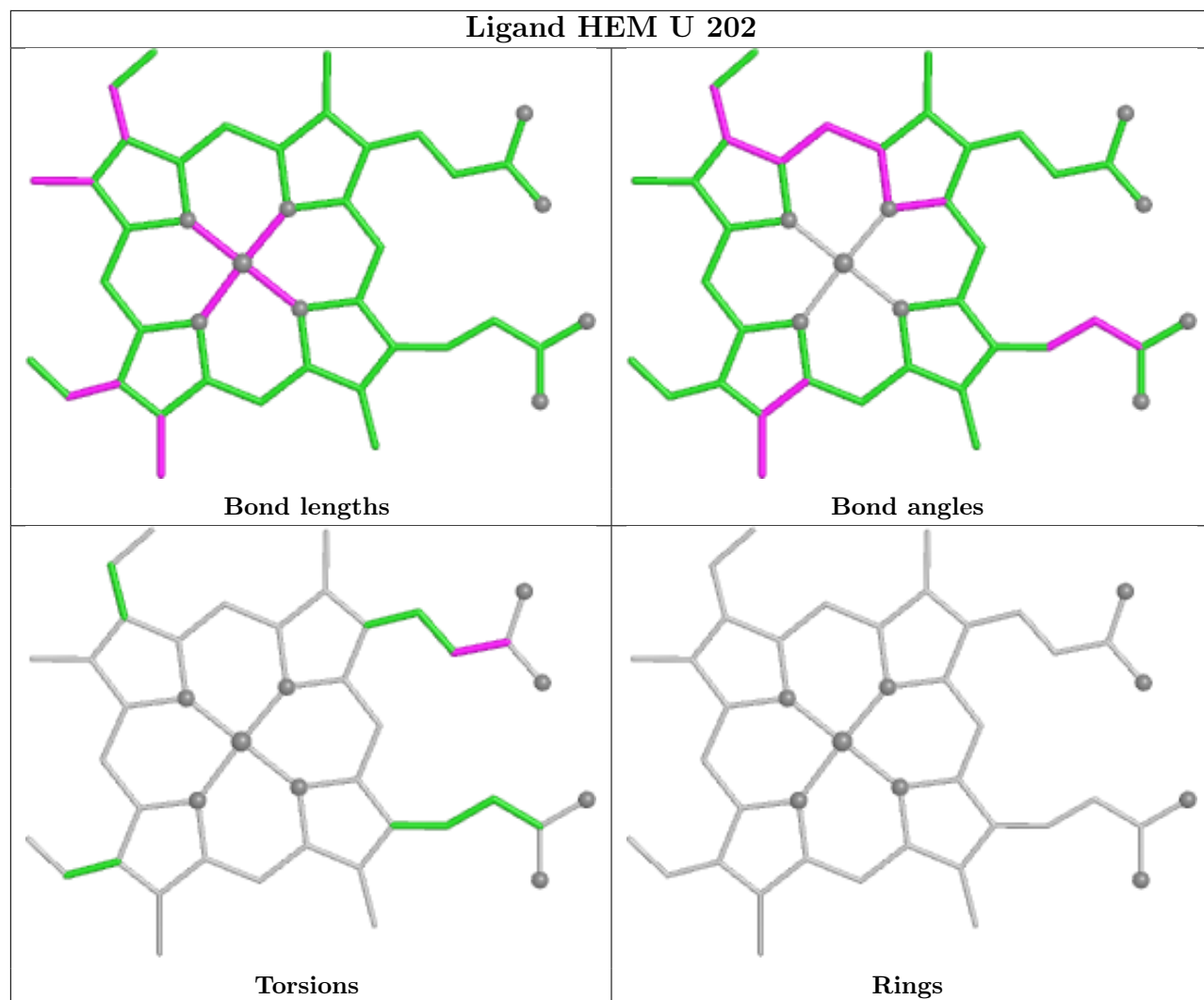
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

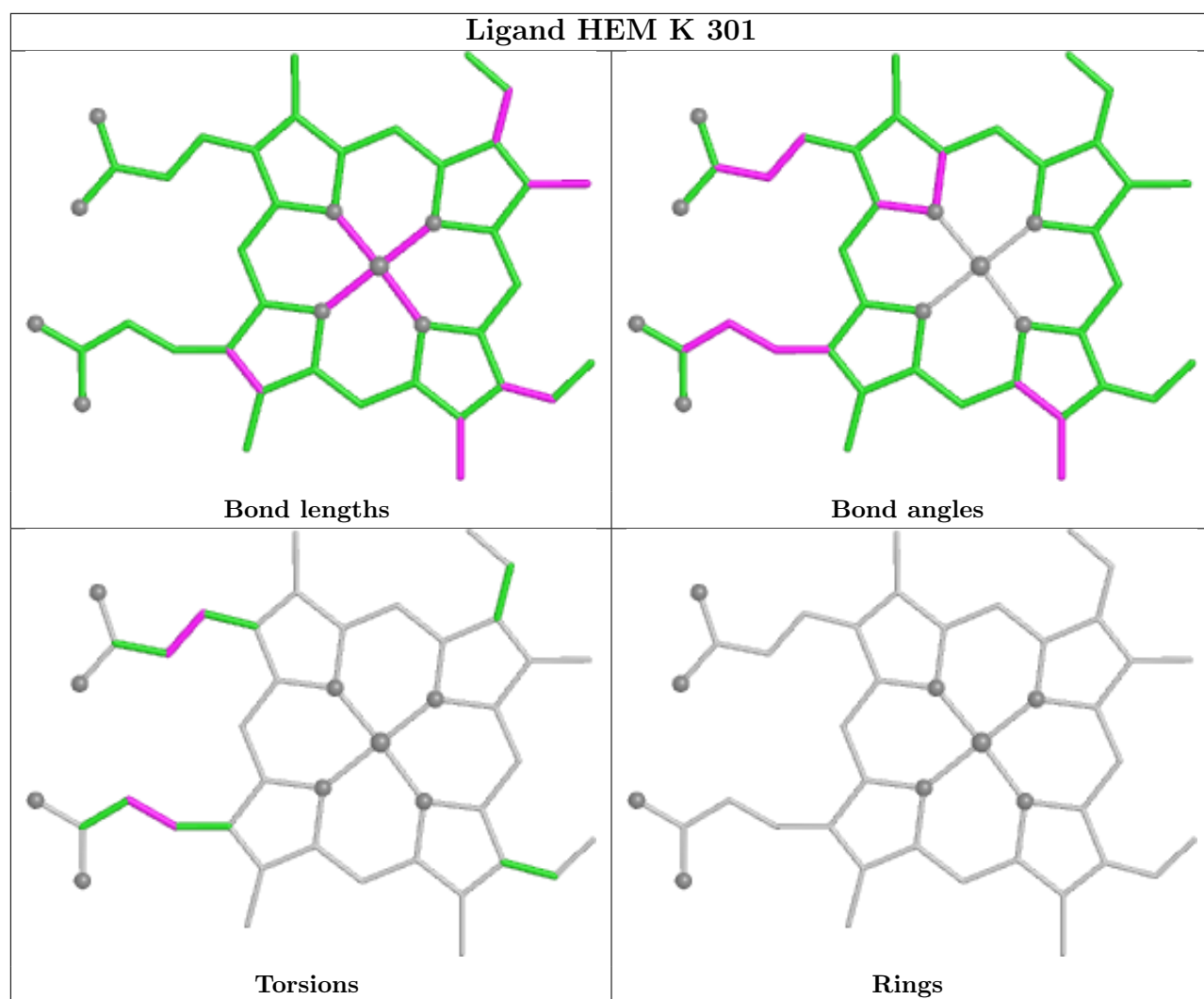


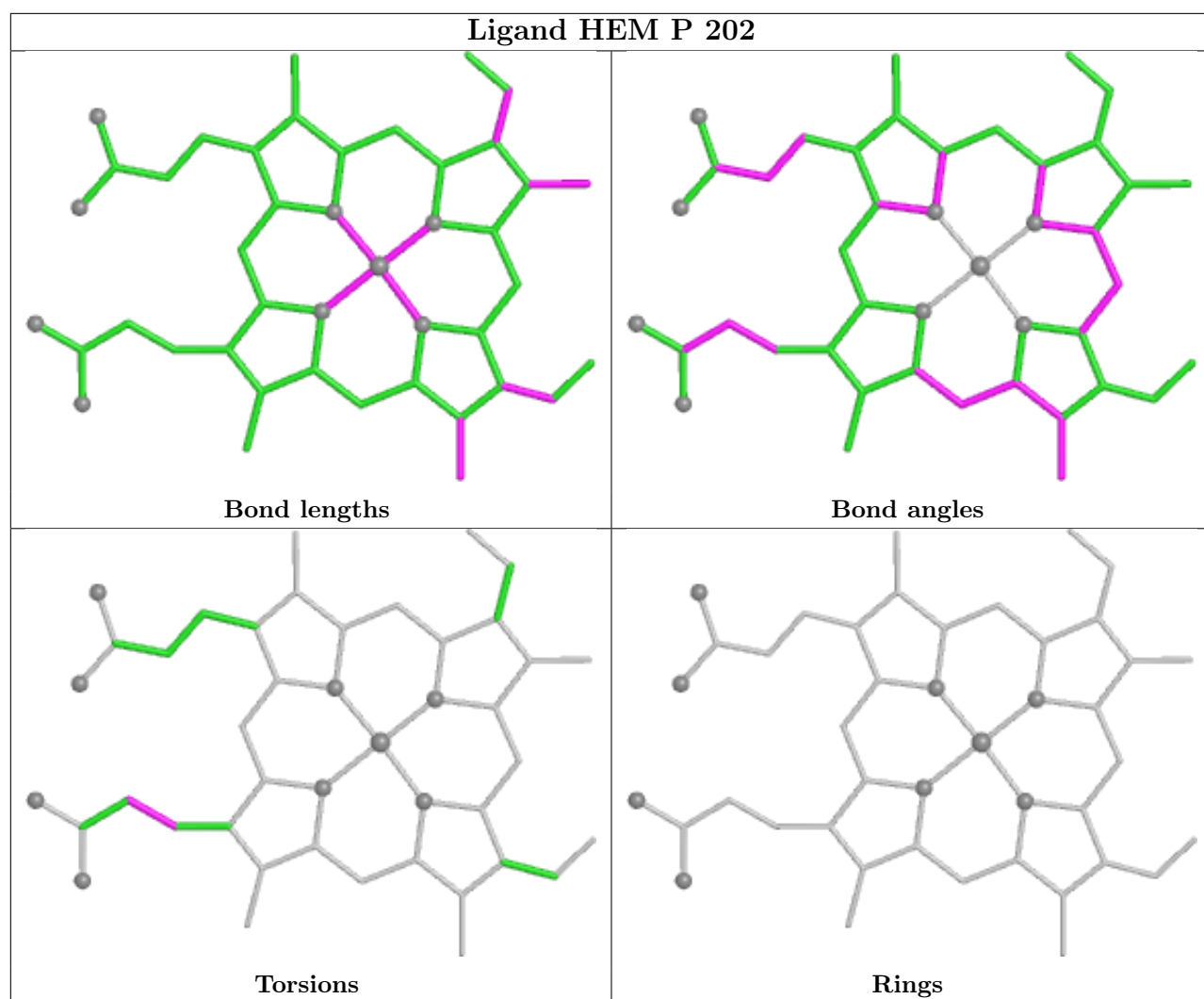


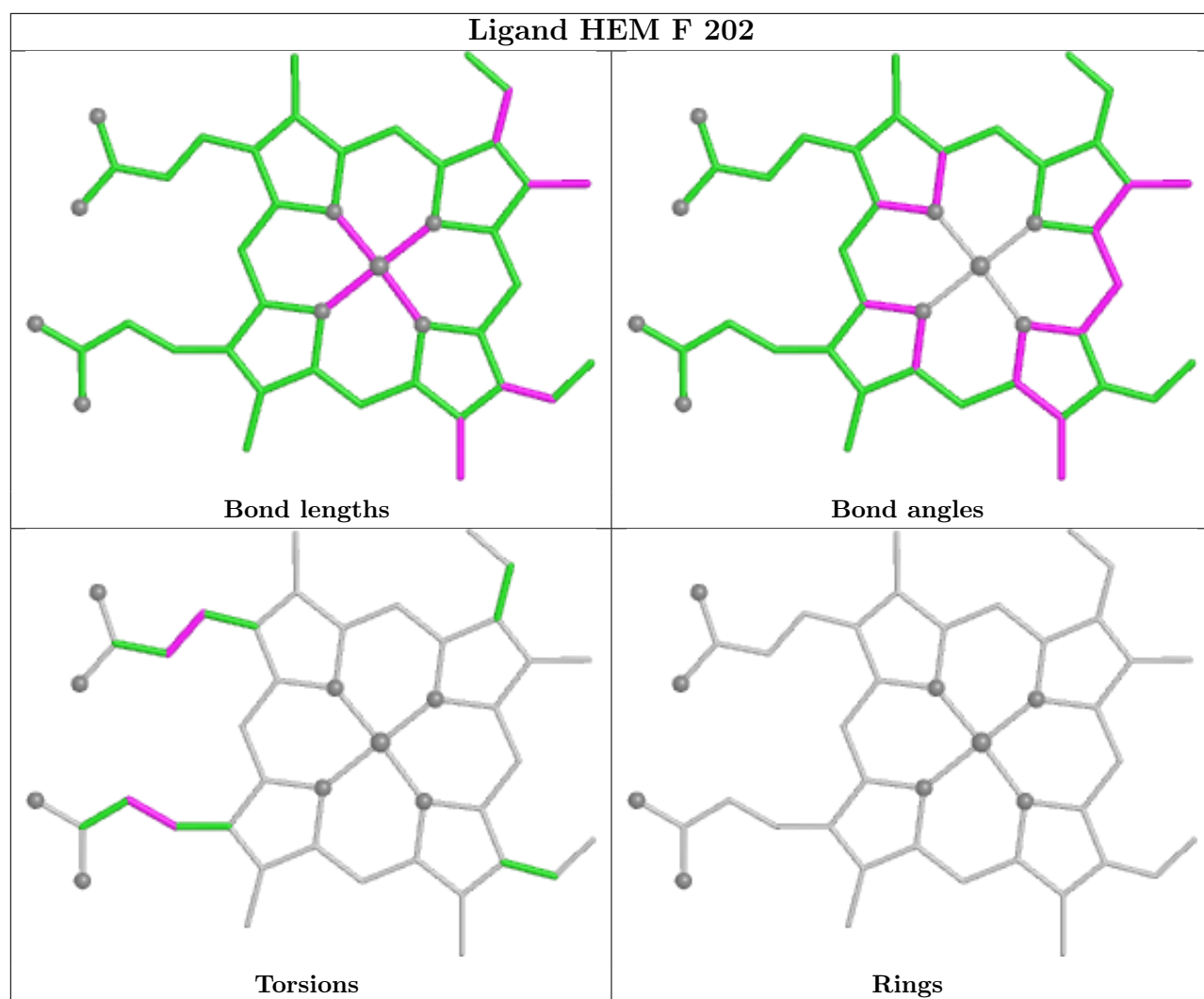


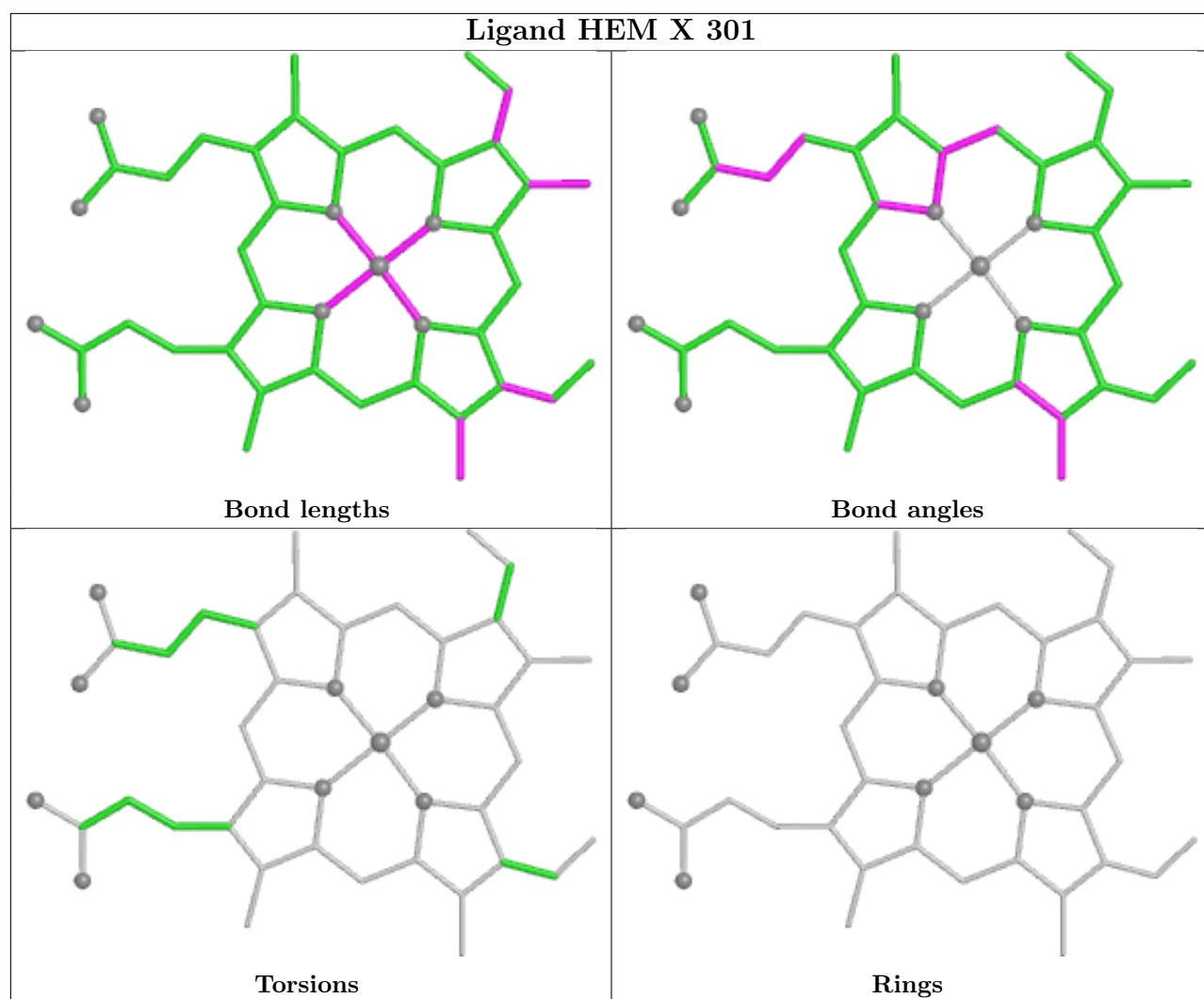


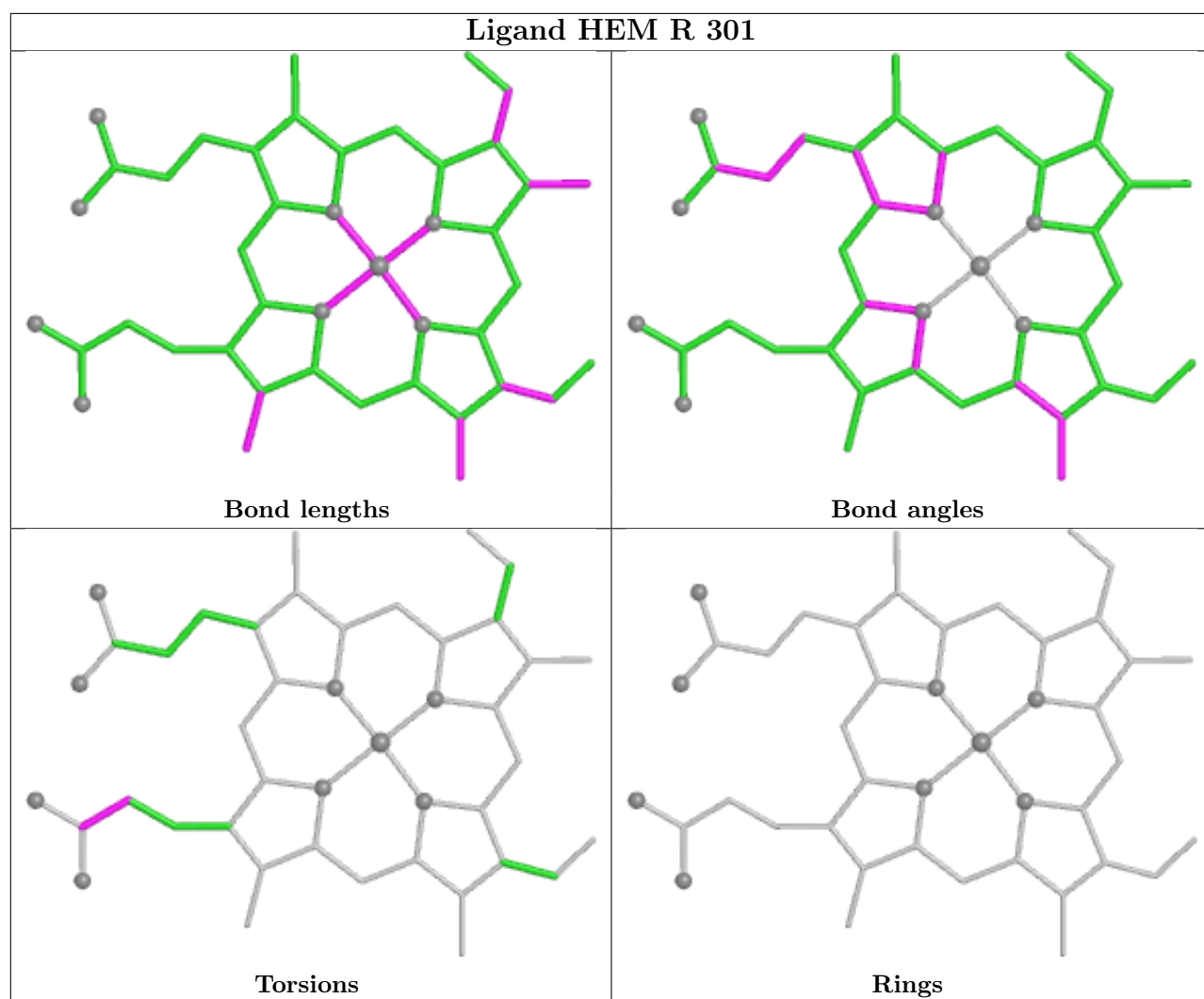


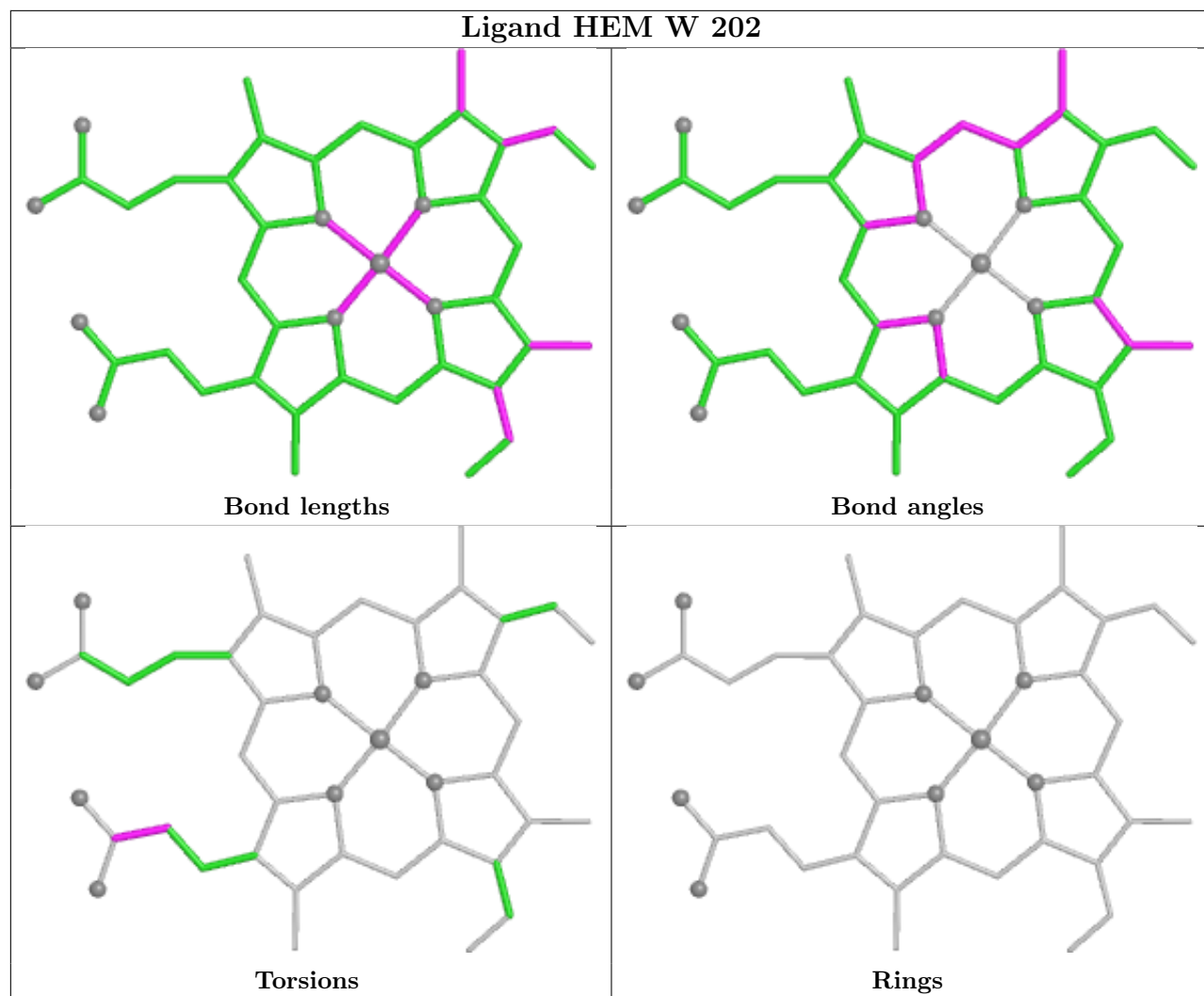


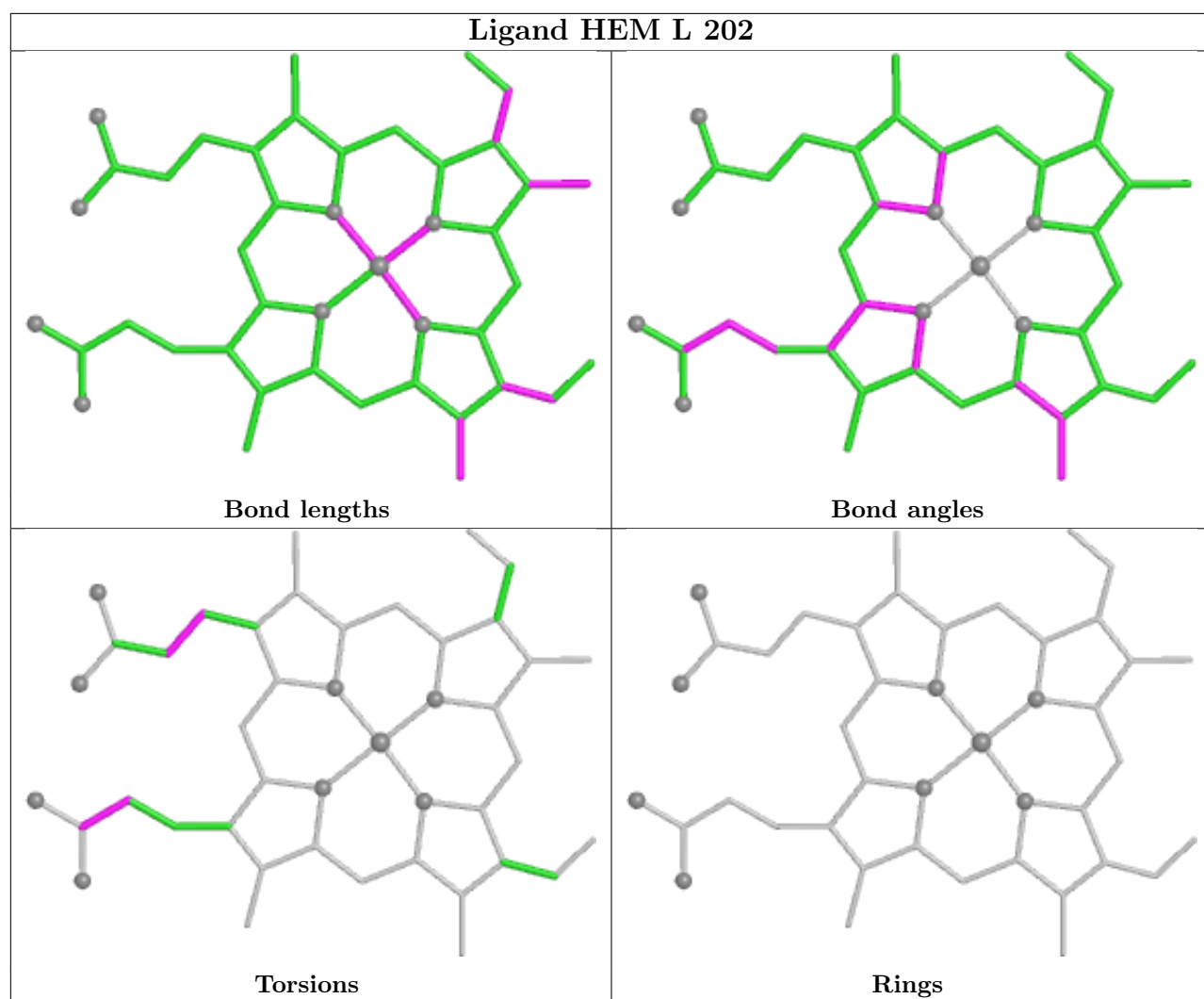












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

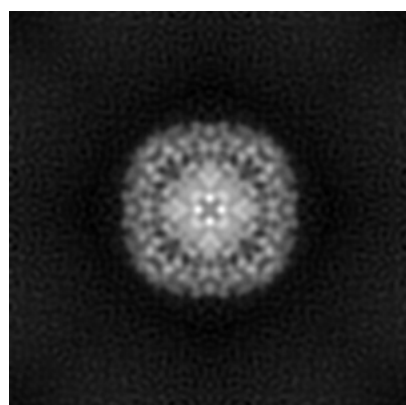
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9915. These allow visual inspection of the internal detail of the map and identification of artifacts.

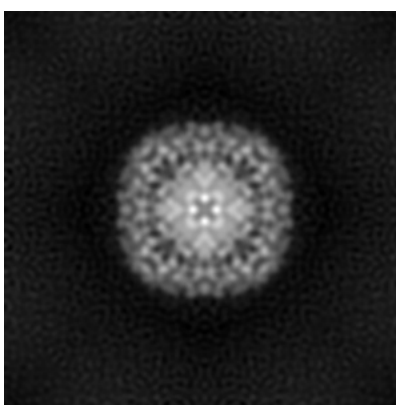
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

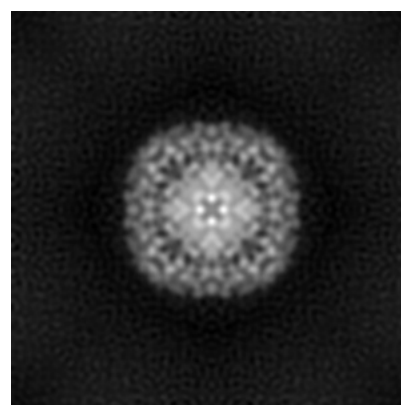
#### 6.1.1 Primary map



X



Y

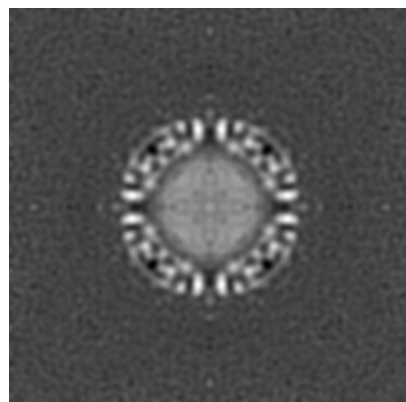


Z

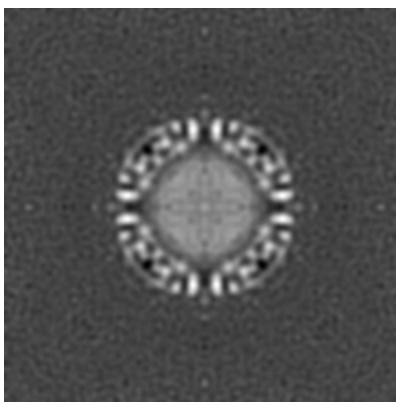
The images above show the map projected in three orthogonal directions.

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

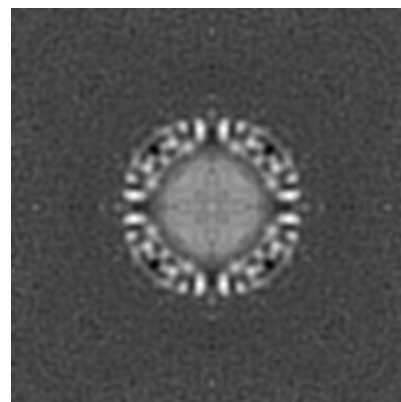
#### 6.2.1 Primary map



X Index: 120



Y Index: 120

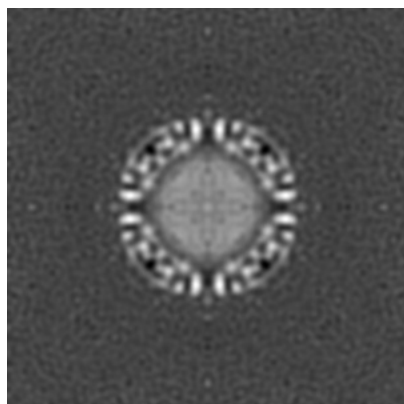


Z Index: 120

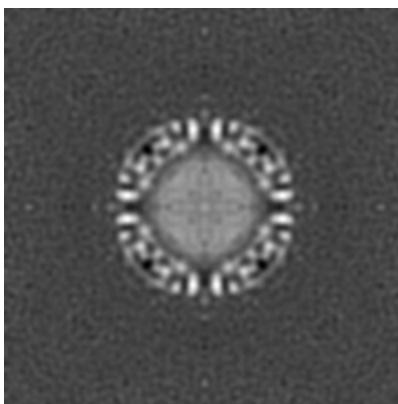
The images above show central slices of the map in three orthogonal directions.

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

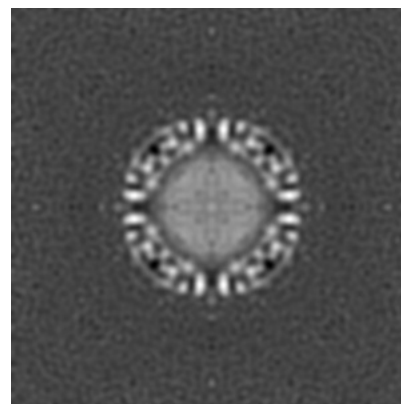
### 6.3.1 Primary map



X Index: 120



Y Index: 120

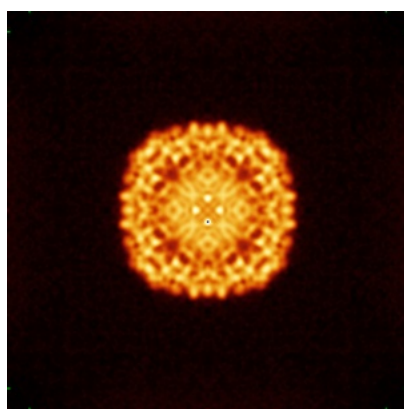


Z Index: 120

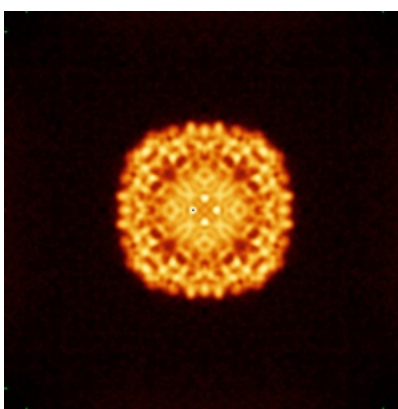
The images above show the largest variance slices of the map in three orthogonal directions.

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

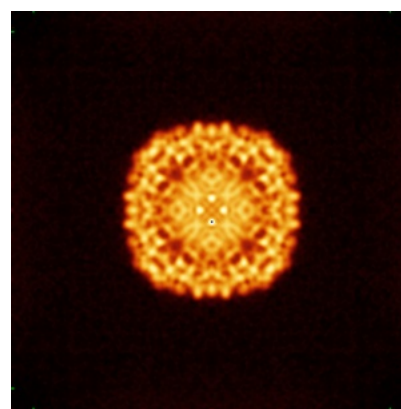
### 6.4.1 Primary map



X



Y

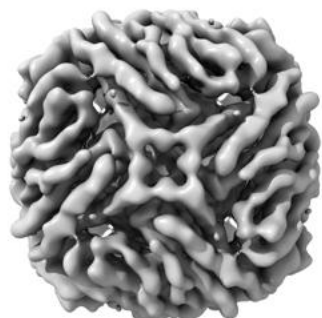


Z

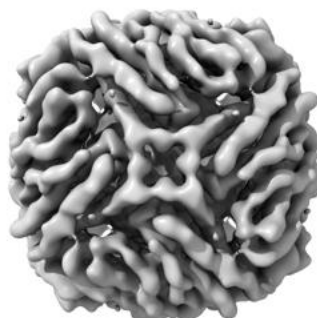
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

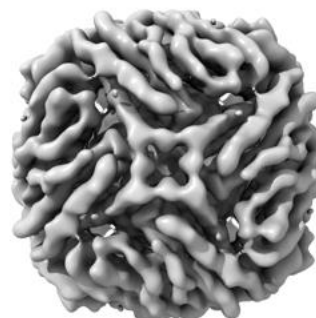
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

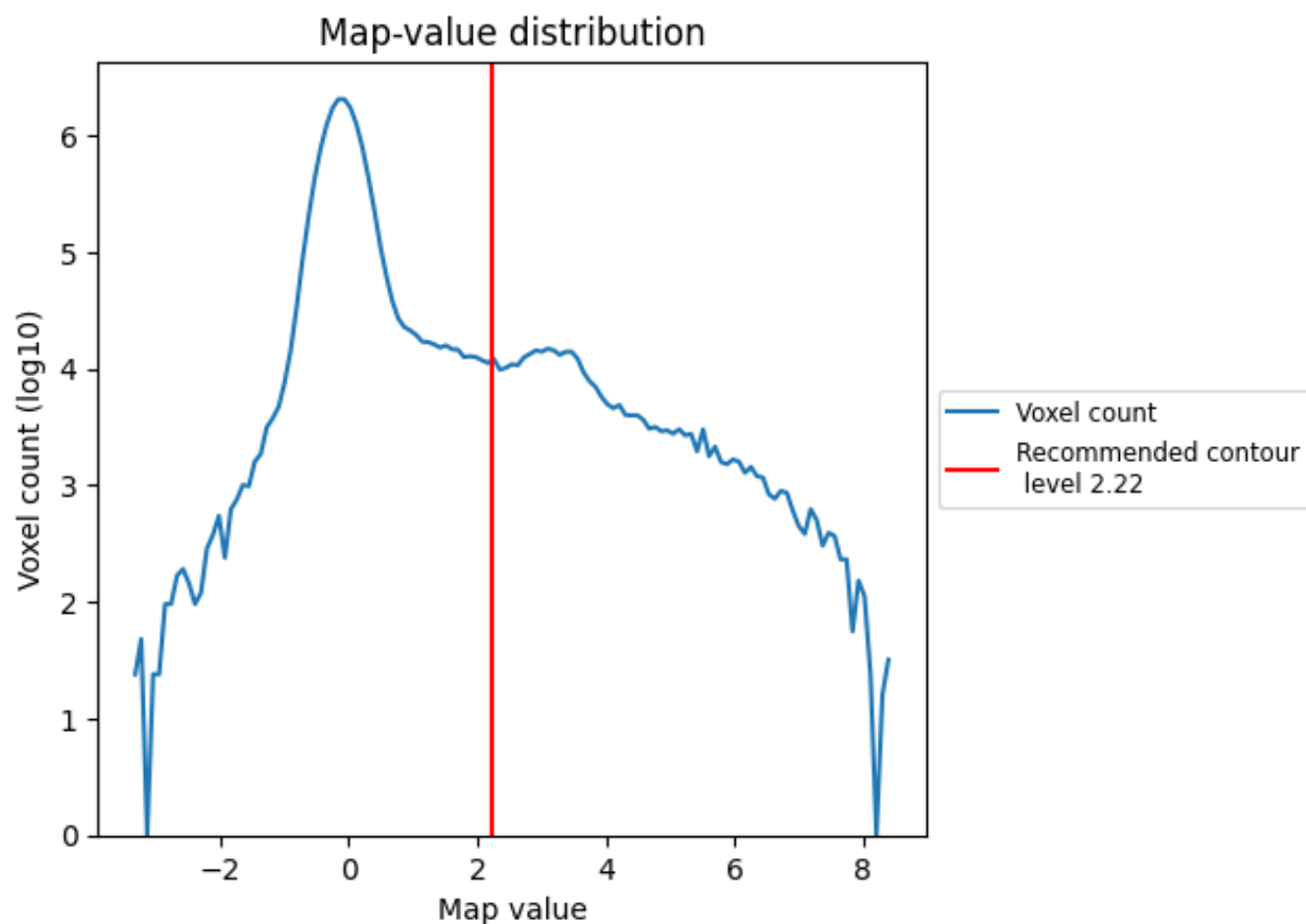
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

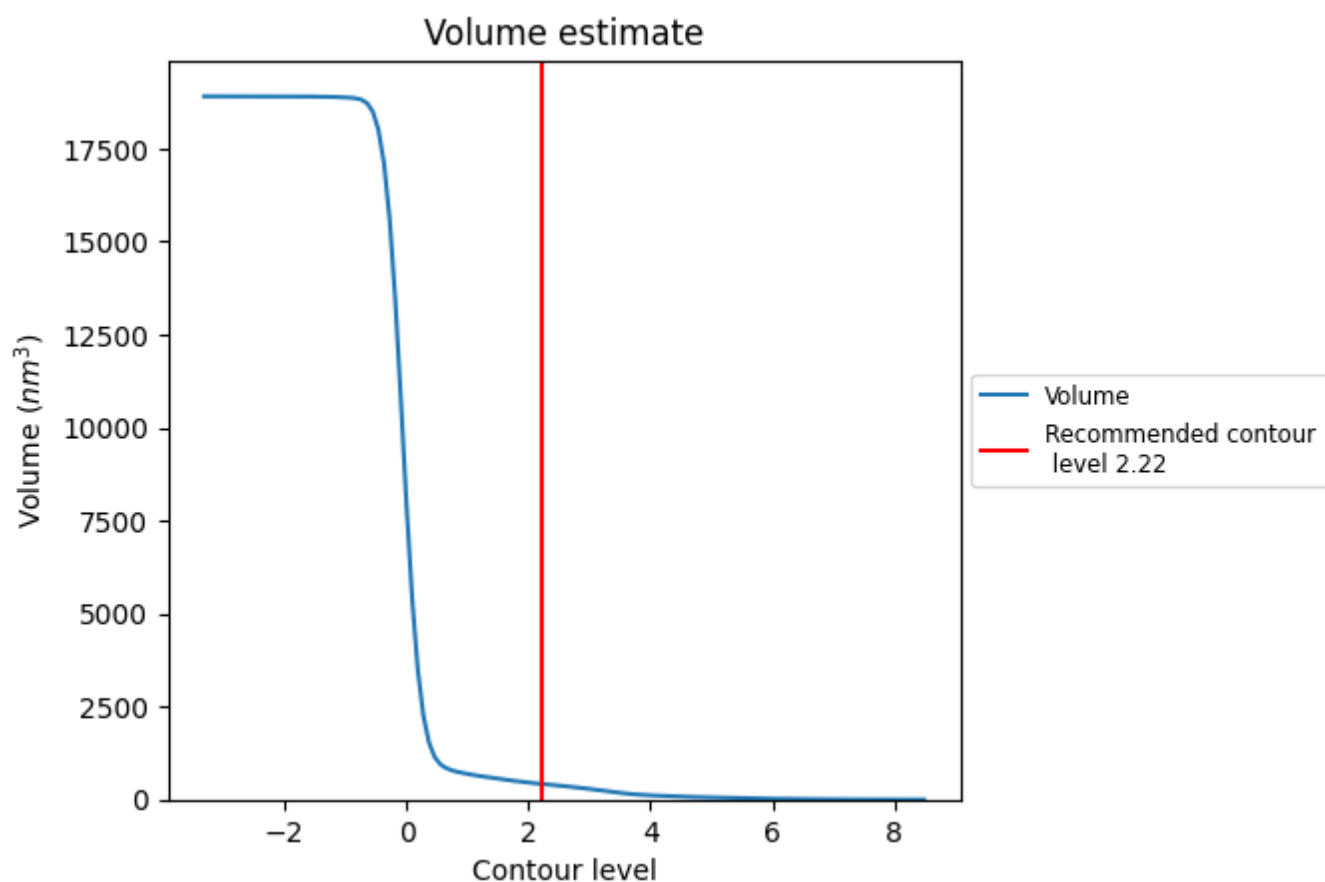
This section contains the results of statistical analysis of the map.

### 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.

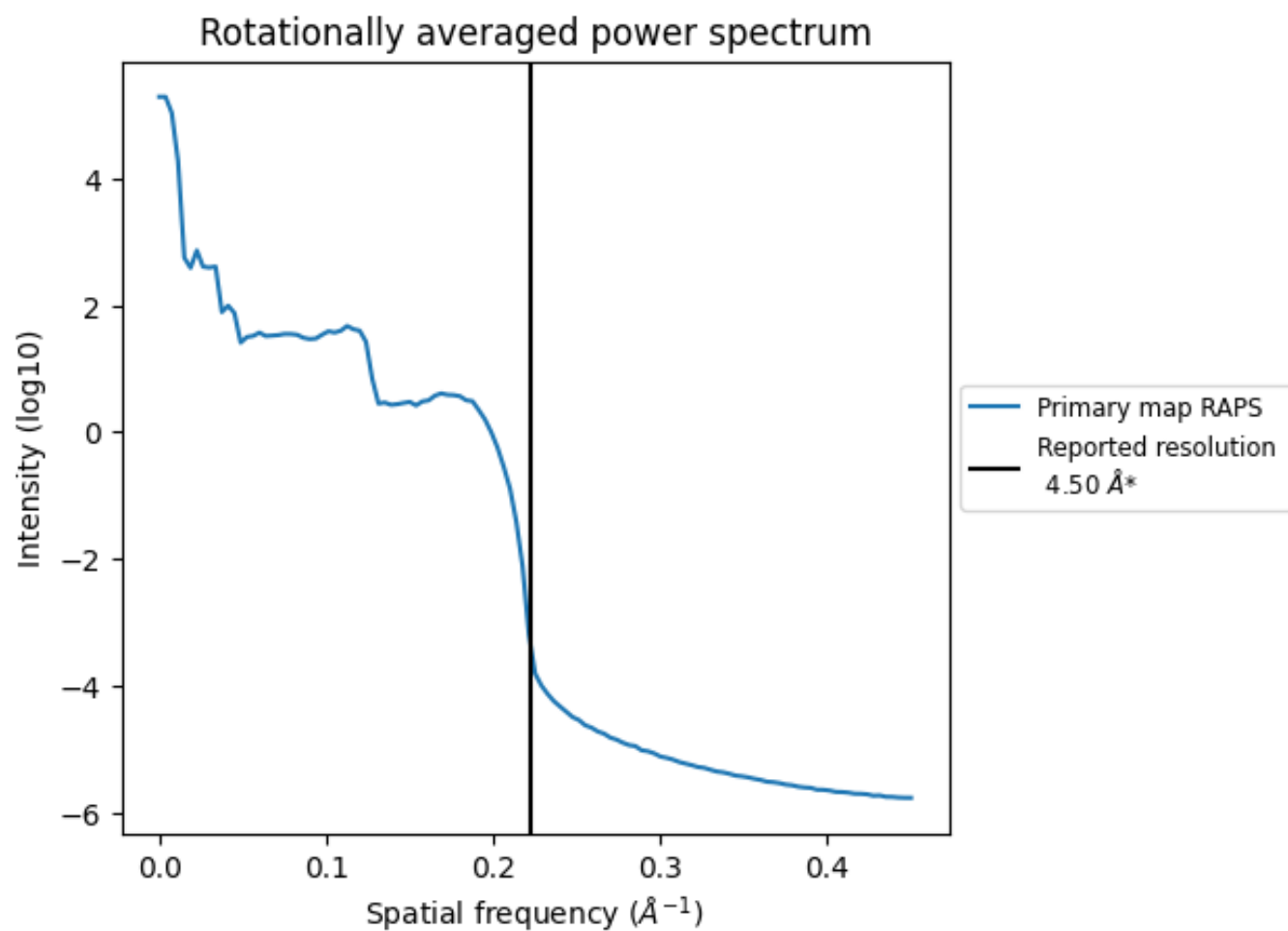
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 419 nm<sup>3</sup>; this corresponds to an approximate mass of 379 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 0.222 Å<sup>-1</sup>

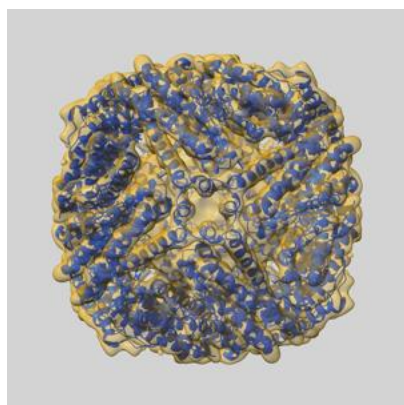
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

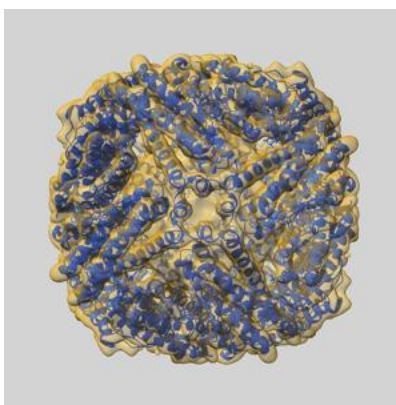
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9915 and PDB model 6K4M. Per-residue inclusion information can be found in section [3](#) on page [8](#).

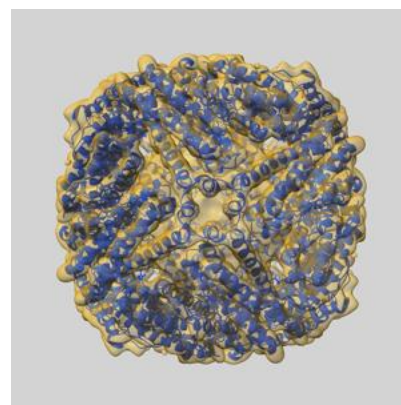
### 9.1 Map-model overlay [i](#)



X



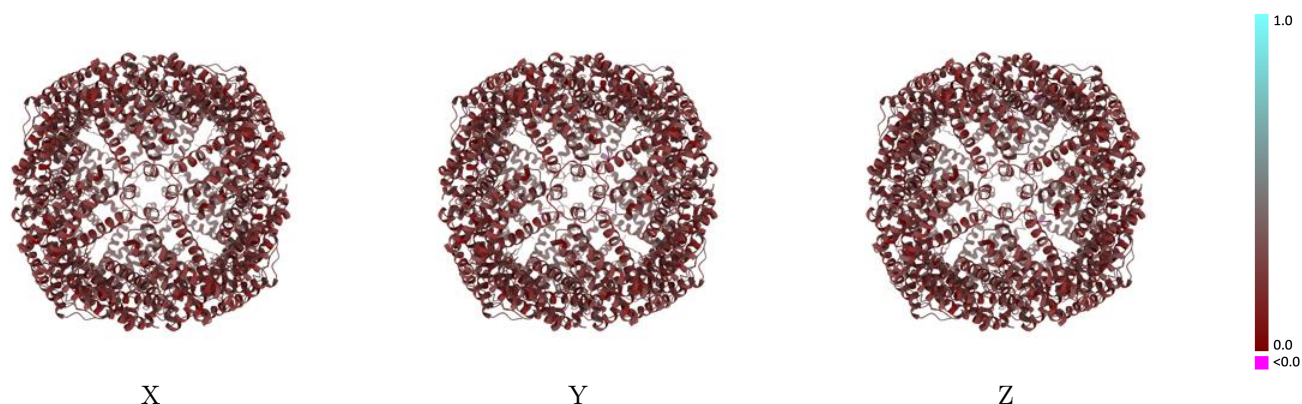
Y



Z

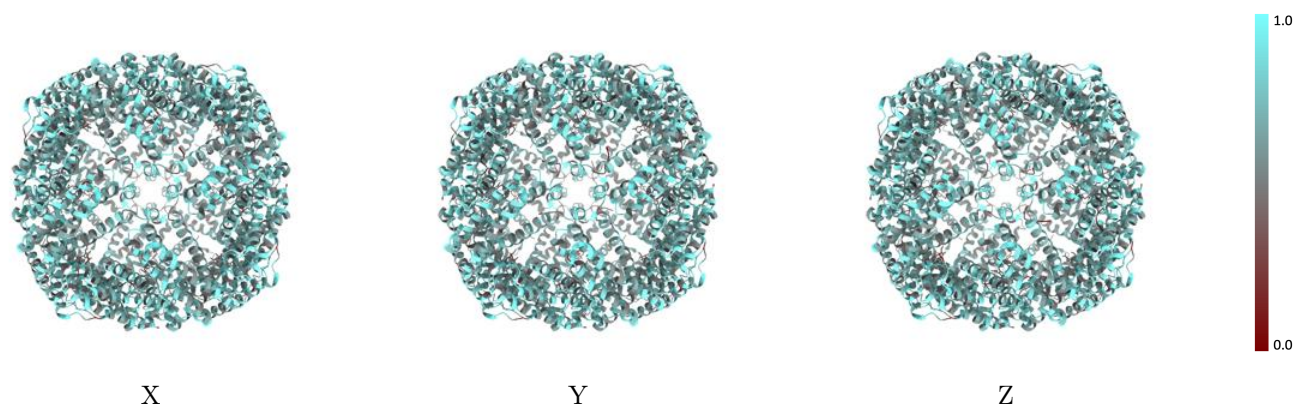
The images above show the 3D surface view of the map at the recommended contour level 2.22 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



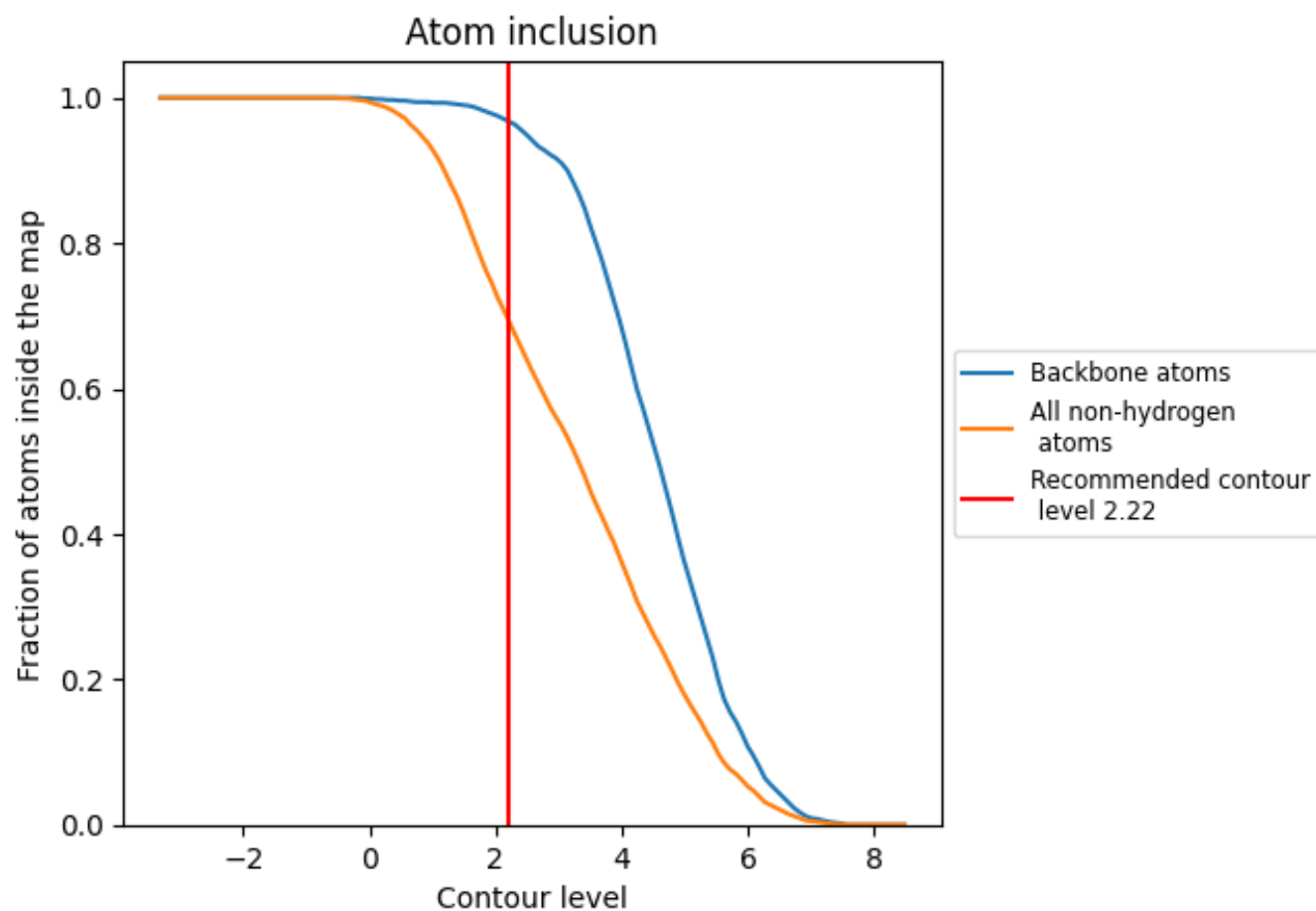
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.22).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 69% 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 (2.22) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6910   |  0.2300   |
| A     |  0.6860   |  0.2290   |
| B     |  0.6980   |  0.2320   |
| C     |  0.6840   |  0.2280   |
| D     |  0.7020   |  0.2320   |
| E     |  0.6960   |  0.2300   |
| F     |  0.6780   |  0.2290   |
| G     |  0.6900   |  0.2290   |
| H     |  0.6840   |  0.2290   |
| I     |  0.6990   |  0.2290   |
| J     |  0.6860   |  0.2300   |
| K     |  0.6840   |  0.2300   |
| L     |  0.6880   |  0.2260   |
| M     |  0.7070   |  0.2310   |
| N     |  0.6910  |  0.2300  |
| O     |  0.6950 |  0.2330 |
| P     |  0.6940 |  0.2330 |
| Q     |  0.6970 |  0.2290 |
| R     |  0.6910 |  0.2310 |
| S     |  0.6790 |  0.2320 |
| T     |  0.6940 |  0.2350 |
| U     |  0.6910 |  0.2300 |
| V     |  0.6940 |  0.2300 |
| W     |  0.6910 |  0.2310 |
| X     |  0.6810 |  0.2310 |

