



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:55 AM UTC

PDB ID : 2JD6 / pdb\_00002jd6  
Title : Crystal Structure of the as isolated Ferritin from the Hyperthermophilic Archaeal Anaerobe Pyrococcus furiosus  
Authors : Tatur, J.; Hagen, W.R.; Matias, P.M.  
Deposited on : 2007-01-05  
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | NOT EXECUTED                                                     |
| EDS                            | : | NOT EXECUTED                                                     |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

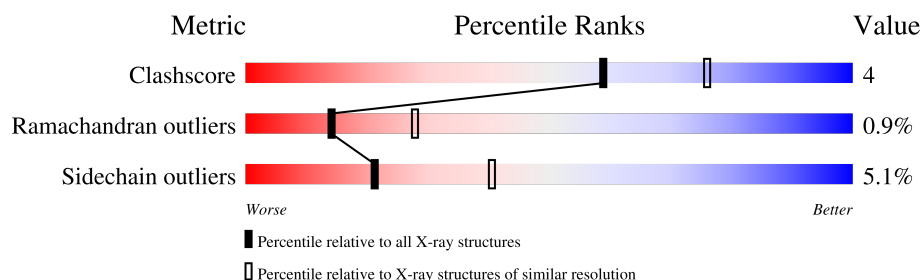
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| Clashscore            | 190562                      | 1044 (2.76-2.76)                                      |
| Ramachandran outliers | 187476                      | 1024 (2.76-2.76)                                      |
| Sidechain outliers    | 187428                      | 1024 (2.76-2.76)                                      |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 0     | 174    |                  |
| 1   | 1     | 174    |                  |
| 1   | 2     | 174    |                  |
| 1   | 3     | 174    |                  |
| 1   | 4     | 174    |                  |
| 1   | 5     | 174    |                  |
| 1   | 6     | 174    |                  |
| 1   | 7     | 174    |                  |

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| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 1   | 8     | 174    |  85% 9% . .     |
| 1   | 9     | 174    |  82% 11% . .    |
| 1   | A     | 174    |  78% 17% . .    |
| 1   | B     | 174    |  82% 11% . .    |
| 1   | C     | 174    |  84% 11% . .    |
| 1   | D     | 174    |  82% 13% . .    |
| 1   | E     | 174    |  86% 9% . .     |
| 1   | F     | 174    |  84% 11% . .    |
| 1   | G     | 174    |  87% 7% . .     |
| 1   | H     | 174    |  80% 14% . .    |
| 1   | I     | 174    |  80% 15% . .    |
| 1   | J     | 174    |  86% 9% . .     |
| 1   | K     | 174    |  83% 9% . . . |
| 1   | L     | 174    |  83% 10% . .  |
| 1   | M     | 174    |  76% 18% . .  |
| 1   | N     | 174    |  82% 12% . .  |
| 1   | O     | 174    |  80% 13% . .  |
| 1   | P     | 174    |  77% 18% . .  |
| 1   | Q     | 174    |  84% 11% .    |
| 1   | R     | 174    |  82% 12% . .  |
| 1   | S     | 174    |  83% 12% . .  |
| 1   | T     | 174    |  85% 8% . .   |
| 1   | U     | 174    |  84% 10% . .  |
| 1   | V     | 174    |  81% 14% . .  |
| 1   | W     | 174    |  80% 16% . .  |

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| Mol | Chain | Length | Quality of chain                                                                               |
|-----|-------|--------|------------------------------------------------------------------------------------------------|
| 1   | X     | 174    |  86% 9% . .  |
| 1   | Y     | 174    |  80% 13% . . |
| 1   | Z     | 174    |  80% 13% . . |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50819 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called FERRITIN HOMOLOG.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | 0     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | 1     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | 2     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | 3     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | 4     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | 5     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | 6     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | 7     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | 8     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | 9     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | A     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | B     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | C     | 167      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1388  | 900 | 221 | 262 | 5 |         |         |       |
| 1   | D     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | E     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | F     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | G     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | H     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | I     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | J     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | K     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | L     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | M     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | N     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | O     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | P     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | Q     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | R     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | S     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | T     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | U     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | V     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | W     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | X     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | Y     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |
| 1   | Z     | 167      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | 0     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | 1     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | 2     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | 3     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | 4     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | 5     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | 6     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | 7     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | 8     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | 9     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | A     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | B     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | C     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | D     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | E     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | F     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | G     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | H     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | I     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | J     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | K     | 1        | Total Fe<br>1 1 | 0       | 0       |
| 2   | L     | 1        | Total Fe<br>1 1 | 0       | 0       |

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | 1     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | 1     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | 2     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | 2     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | 3     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | 3     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | 4     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | 5     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | 6     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | 7     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | 8     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | E     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | F     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | G     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | H     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | I     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | J     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | K     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | M     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | O     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | Q     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | R     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | S     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | S     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | T     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | V     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | V     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | W     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | W     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | X     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | Z     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | 0     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 4   | 1     | 23       | Total | O  | 0       | 0       |
|     |       |          | 23    | 23 |         |         |
| 4   | 2     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 4   | 3     | 25       | Total | O  | 0       | 0       |
|     |       |          | 25    | 25 |         |         |
| 4   | 4     | 25       | Total | O  | 0       | 0       |
|     |       |          | 25    | 25 |         |         |
| 4   | 5     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 4   | 6     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 4   | 7     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 4   | 8     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 4   | 9     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 4   | A     | 40       | Total | O  | 0       | 0       |
|     |       |          | 40    | 40 |         |         |
| 4   | B     | 26       | Total | O  | 0       | 0       |
|     |       |          | 26    | 26 |         |         |
| 4   | C     | 19       | Total | O  | 0       | 0       |
|     |       |          | 19    | 19 |         |         |
| 4   | D     | 29       | Total | O  | 0       | 0       |
|     |       |          | 29    | 29 |         |         |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4   | E     | 37       | Total O<br>37 37 | 0       | 0       |
| 4   | F     | 24       | Total O<br>24 24 | 0       | 0       |
| 4   | G     | 31       | Total O<br>31 31 | 0       | 0       |
| 4   | H     | 10       | Total O<br>10 10 | 0       | 0       |
| 4   | I     | 30       | Total O<br>30 30 | 0       | 0       |
| 4   | J     | 31       | Total O<br>31 31 | 0       | 0       |
| 4   | K     | 12       | Total O<br>12 12 | 0       | 0       |
| 4   | L     | 20       | Total O<br>20 20 | 0       | 0       |
| 4   | M     | 20       | Total O<br>20 20 | 0       | 0       |
| 4   | N     | 24       | Total O<br>24 24 | 0       | 0       |
| 4   | O     | 14       | Total O<br>14 14 | 0       | 0       |
| 4   | P     | 13       | Total O<br>13 13 | 0       | 0       |
| 4   | Q     | 18       | Total O<br>18 18 | 0       | 0       |
| 4   | R     | 20       | Total O<br>20 20 | 0       | 0       |
| 4   | S     | 28       | Total O<br>28 28 | 0       | 0       |
| 4   | T     | 19       | Total O<br>19 19 | 0       | 0       |
| 4   | U     | 27       | Total O<br>27 27 | 0       | 0       |
| 4   | V     | 18       | Total O<br>18 18 | 0       | 0       |
| 4   | W     | 23       | Total O<br>23 23 | 0       | 0       |
| 4   | X     | 24       | Total O<br>24 24 | 0       | 0       |
| 4   | Y     | 31       | Total O<br>31 31 | 0       | 0       |

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| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4   | Z     | 7        | Total | O | 0       | 0       |
|     |       |          | 7     | 7 |         |         |

### 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. 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. 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.

Note EDS was not executed.

#### • Molecule 1: FERRITIN HOMOLOG

Chain 0:  86% 9% ..



#### • Molecule 1: FERRITIN HOMOLOG

Chain 1:  82% 13% ..



#### • Molecule 1: FERRITIN HOMOLOG

Chain 2:  88% 8% .



#### • Molecule 1: FERRITIN HOMOLOG

Chain 3:  80% 14% ..



#### • Molecule 1: FERRITIN HOMOLOG

Chain 4:  82% 11% ..



#### • Molecule 1: FERRITIN HOMOLOG

Chain 5:  83% 12% ..



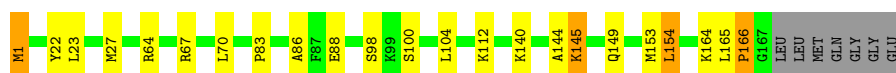
• Molecule 1: FERRITIN HOMOLOG

Chain 6: 79% 14% . .



• Molecule 1: FERRITIN HOMOLOG

Chain 7: 83% 11% . .



• Molecule 1: FERRITIN HOMOLOG

Chain 8: 85% 9% . .



• Molecule 1: FERRITIN HOMOLOG

Chain 9: 82% 11% . .



• Molecule 1: FERRITIN HOMOLOG

Chain A: 78% 17% . .



• Molecule 1: FERRITIN HOMOLOG

Chain B: 82% 11% . .

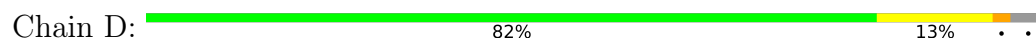


• Molecule 1: FERRITIN HOMOLOG

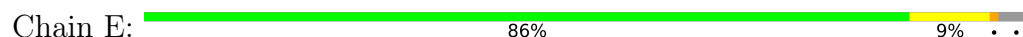
Chain C: 84% 11% . .



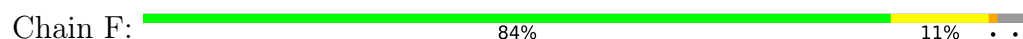
• Molecule 1: FERRITIN HOMOLOG



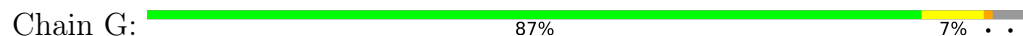
• Molecule 1: FERRITIN HOMOLOG



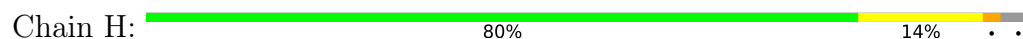
• Molecule 1: FERRITIN HOMOLOG



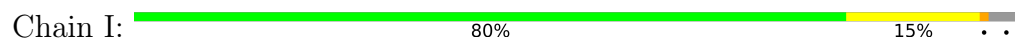
• Molecule 1: FERRITIN HOMOLOG



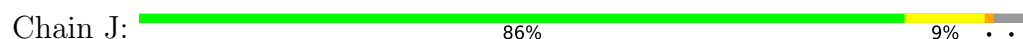
• Molecule 1: FERRITIN HOMOLOG



• Molecule 1: FERRITIN HOMOLOG



• Molecule 1: FERRITIN HOMOLOG





- Molecule 1: FERRITIN HOMOLOG

Chain K: 83% 9% . . .



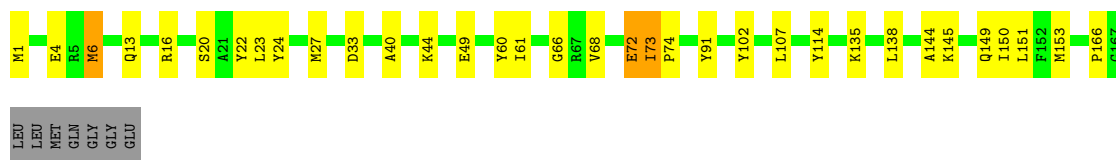
- Molecule 1: FERRITIN HOMOLOG

Chain L: 83% 10% . .



- Molecule 1: FERRITIN HOMOLOG

Chain M: 76% 18% . .



- Molecule 1: FERRITIN HOMOLOG

Chain N: 82% 12% . .



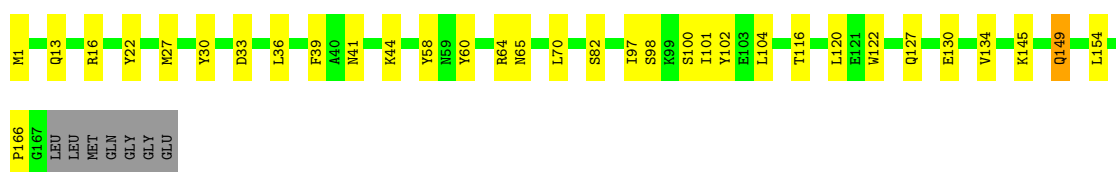
- Molecule 1: FERRITIN HOMOLOG

Chain O: 80% 13% . .



- Molecule 1: FERRITIN HOMOLOG

Chain P: 77% 18% . .



- Molecule 1: FERRITIN HOMOLOG

Chain Q:  84% 11% .



• Molecule 1: FERRITIN HOMOLOG

Chain R:  82% 12% . .



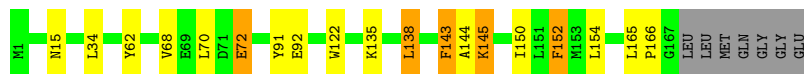
• Molecule 1: FERRITIN HOMOLOG

Chain S:  83% 12% . .



• Molecule 1: FERRITIN HOMOLOG

Chain T:  85% 8% . .



• Molecule 1: FERRITIN HOMOLOG

Chain U:  84% 10% . .



• Molecule 1: FERRITIN HOMOLOG

Chain V:  81% 14% . .



• Molecule 1: FERRITIN HOMOLOG

Chain W:  80% 16% . .

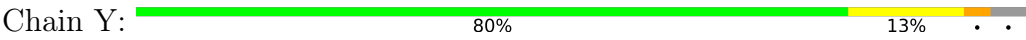


• Molecule 1: FERRITIN HOMOLOG

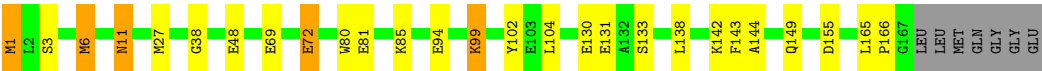
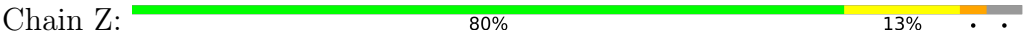
Chain X:  86% 9% . .



● Molecule 1: FERRITIN HOMOLOG



● Molecule 1: FERRITIN HOMOLOG



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property                                                 | Value                                           | Source    |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group                                              | C 2 2 21                                        | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 254.10Å 341.42Å 265.52Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)                                           | 204.12 – 2.75                                   | Depositor |
| % Data completeness<br>(in resolution range)             | 99.6 (204.12-2.75)                              | Depositor |
| $R_{merge}$                                              | 0.08                                            | Depositor |
| $R_{sym}$                                                | (Not available)                                 | Depositor |
| Refinement program                                       | REFMAC 5.3.0021                                 | Depositor |
| R, $R_{free}$                                            | 0.195 , 0.247                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 50819                                           | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 33.0                                            | wwPDB-VP  |

## 5 Model quality [i](#)

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

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

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   | 0     | 0.78         | 0/1417        | 0.97        | 0/1908        |
| 1   | 1     | 0.77         | 0/1417        | 0.93        | 0/1908        |
| 1   | 2     | 0.72         | 0/1417        | 0.92        | 0/1908        |
| 1   | 3     | 0.87         | 0/1417        | 1.02        | 4/1908 (0.2%) |
| 1   | 4     | 0.76         | 0/1417        | 0.96        | 0/1908        |
| 1   | 5     | 0.75         | 0/1417        | 0.94        | 2/1908 (0.1%) |
| 1   | 6     | 0.77         | 0/1417        | 0.96        | 0/1908        |
| 1   | 7     | 0.75         | 0/1417        | 0.96        | 0/1908        |
| 1   | 8     | 0.80         | 0/1417        | 0.96        | 0/1908        |
| 1   | 9     | 0.71         | 0/1417        | 0.90        | 0/1908        |
| 1   | A     | 0.88         | 0/1417        | 1.03        | 4/1908 (0.2%) |
| 1   | B     | 0.86         | 0/1417        | 1.01        | 1/1908 (0.1%) |
| 1   | C     | 0.89         | 0/1425        | 0.95        | 1/1919 (0.1%) |
| 1   | D     | 0.91         | 0/1417        | 1.03        | 1/1908 (0.1%) |
| 1   | E     | 0.82         | 0/1417        | 0.97        | 0/1908        |
| 1   | F     | 0.91         | 1/1417 (0.1%) | 0.96        | 1/1908 (0.1%) |
| 1   | G     | 0.82         | 0/1417        | 0.97        | 0/1908        |
| 1   | H     | 0.74         | 0/1417        | 0.95        | 0/1908        |
| 1   | I     | 0.85         | 0/1417        | 0.96        | 2/1908 (0.1%) |
| 1   | J     | 0.82         | 0/1417        | 0.97        | 4/1908 (0.2%) |
| 1   | K     | 0.74         | 0/1417        | 0.98        | 5/1908 (0.3%) |
| 1   | L     | 0.78         | 0/1417        | 0.99        | 0/1908        |
| 1   | M     | 0.76         | 0/1417        | 0.98        | 2/1908 (0.1%) |
| 1   | N     | 0.76         | 0/1417        | 0.92        | 0/1908        |
| 1   | O     | 0.81         | 0/1417        | 0.99        | 1/1908 (0.1%) |
| 1   | P     | 0.76         | 0/1417        | 0.92        | 1/1908 (0.1%) |
| 1   | Q     | 0.82         | 0/1417        | 0.95        | 2/1908 (0.1%) |
| 1   | R     | 0.71         | 0/1417        | 0.92        | 2/1908 (0.1%) |
| 1   | S     | 0.87         | 0/1417        | 1.00        | 2/1908 (0.1%) |
| 1   | T     | 0.85         | 0/1417        | 1.01        | 2/1908 (0.1%) |
| 1   | U     | 0.88         | 0/1417        | 1.00        | 3/1908 (0.2%) |
| 1   | V     | 0.89         | 0/1417        | 1.06        | 4/1908 (0.2%) |

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | W     | 0.94         | 0/1417         | 0.97        | 0/1908          |
| 1   | X     | 0.87         | 0/1417         | 0.97        | 1/1908 (0.1%)   |
| 1   | Y     | 0.79         | 0/1417         | 0.96        | 1/1908 (0.1%)   |
| 1   | Z     | 0.72         | 0/1417         | 0.93        | 0/1908          |
| All | All   | 0.81         | 1/51020 (0.0%) | 0.97        | 46/68699 (0.1%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 106 | ALA  | CA-CB | -5.32 | 1.45        | 1.53     |

All (46) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | M     | 73  | ILE  | CA-C-N | 6.75  | 126.51      | 119.76   |
| 1   | M     | 73  | ILE  | C-N-CA | 6.75  | 126.51      | 119.76   |
| 1   | Y     | 82  | SER  | N-CA-C | 6.66  | 114.12      | 108.13   |
| 1   | V     | 73  | ILE  | CA-C-N | -6.65 | 113.80      | 120.31   |
| 1   | V     | 73  | ILE  | C-N-CA | -6.65 | 113.80      | 120.31   |
| 1   | V     | 28  | ALA  | N-CA-C | -6.21 | 104.42      | 111.07   |
| 1   | A     | 75  | LYS  | CA-C-N | 6.15  | 126.71      | 120.38   |
| 1   | A     | 75  | LYS  | C-N-CA | 6.15  | 126.71      | 120.38   |
| 1   | S     | 73  | ILE  | CA-C-N | 5.99  | 125.93      | 119.76   |
| 1   | S     | 73  | ILE  | C-N-CA | 5.99  | 125.93      | 119.76   |
| 1   | K     | 73  | ILE  | CA-C-N | 5.98  | 125.94      | 119.78   |
| 1   | K     | 73  | ILE  | C-N-CA | 5.98  | 125.94      | 119.78   |
| 1   | U     | 124 | ILE  | N-CA-C | -5.87 | 105.02      | 110.53   |
| 1   | P     | 82  | SER  | N-CA-C | 5.83  | 113.38      | 108.13   |
| 1   | Q     | 73  | ILE  | CA-C-N | 5.78  | 126.11      | 119.92   |
| 1   | Q     | 73  | ILE  | C-N-CA | 5.78  | 126.11      | 119.92   |
| 1   | 3     | 15  | ASN  | N-CA-C | 5.71  | 117.50      | 111.28   |
| 1   | U     | 104 | LEU  | N-CA-C | -5.69 | 105.16      | 111.36   |
| 1   | C     | 82  | SER  | N-CA-C | 5.62  | 113.19      | 108.13   |
| 1   | I     | 42  | TRP  | N-CA-C | -5.59 | 105.09      | 111.07   |
| 1   | T     | 122 | TRP  | N-CA-C | -5.59 | 105.19      | 111.28   |
| 1   | J     | 92  | GLU  | N-CA-C | -5.55 | 105.22      | 111.28   |
| 1   | 5     | 162 | ALA  | CA-C-N | 5.53  | 125.45      | 119.76   |
| 1   | 5     | 162 | ALA  | C-N-CA | 5.53  | 125.45      | 119.76   |
| 1   | X     | 82  | SER  | N-CA-C | 5.51  | 113.09      | 108.13   |
| 1   | 3     | 82  | SER  | N-CA-C | 5.50  | 113.17      | 108.22   |
| 1   | O     | 64  | ARG  | N-CA-C | -5.49 | 106.17      | 112.92   |
| 1   | B     | 42  | TRP  | N-CA-C | -5.46 | 105.32      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | 3     | 140 | LYS  | N-CA-C | -5.46 | 105.41      | 111.36   |
| 1   | K     | 165 | LEU  | N-CA-C | 5.44  | 120.15      | 112.75   |
| 1   | T     | 92  | GLU  | N-CA-C | -5.44 | 105.35      | 111.28   |
| 1   | J     | 81  | GLU  | N-CA-C | 5.42  | 117.19      | 111.28   |
| 1   | R     | 73  | ILE  | CA-C-N | 5.32  | 125.32      | 119.89   |
| 1   | R     | 73  | ILE  | C-N-CA | 5.32  | 125.32      | 119.89   |
| 1   | I     | 94  | GLU  | N-CA-C | -5.32 | 105.56      | 111.36   |
| 1   | U     | 25  | PHE  | N-CA-C | -5.30 | 105.58      | 111.36   |
| 1   | 3     | 22  | TYR  | N-CA-C | -5.30 | 105.58      | 111.36   |
| 1   | A     | 147 | SER  | CA-C-N | 5.23  | 126.38      | 119.84   |
| 1   | A     | 147 | SER  | C-N-CA | 5.23  | 126.38      | 119.84   |
| 1   | K     | 42  | TRP  | N-CA-C | -5.21 | 105.60      | 111.28   |
| 1   | K     | 82  | SER  | N-CA-C | 5.21  | 112.82      | 108.13   |
| 1   | D     | 8   | LYS  | N-CA-C | -5.15 | 105.85      | 111.82   |
| 1   | J     | 64  | ARG  | N-CA-C | -5.12 | 107.20      | 112.93   |
| 1   | F     | 37  | GLU  | N-CA-C | 5.03  | 116.76      | 111.28   |
| 1   | V     | 82  | SER  | N-CA-C | 5.01  | 113.90      | 108.14   |
| 1   | J     | 122 | TRP  | N-CA-C | -5.00 | 105.93      | 112.23   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 1383  | 0        | 1352     | 10      | 0            |
| 1   | 1     | 1383  | 0        | 1352     | 14      | 0            |
| 1   | 2     | 1383  | 0        | 1352     | 8       | 0            |
| 1   | 3     | 1383  | 0        | 1352     | 16      | 0            |
| 1   | 4     | 1383  | 0        | 1352     | 15      | 0            |
| 1   | 5     | 1383  | 0        | 1352     | 11      | 0            |
| 1   | 6     | 1383  | 0        | 1352     | 15      | 0            |
| 1   | 7     | 1383  | 0        | 1352     | 15      | 0            |
| 1   | 8     | 1383  | 0        | 1352     | 11      | 0            |
| 1   | 9     | 1383  | 0        | 1352     | 17      | 0            |
| 1   | A     | 1383  | 0        | 1352     | 16      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | B     | 1383  | 0        | 1352     | 18      | 0            |
| 1   | C     | 1388  | 0        | 1358     | 13      | 0            |
| 1   | D     | 1383  | 0        | 1352     | 14      | 0            |
| 1   | E     | 1383  | 0        | 1352     | 10      | 0            |
| 1   | F     | 1383  | 0        | 1352     | 9       | 0            |
| 1   | G     | 1383  | 0        | 1352     | 8       | 0            |
| 1   | H     | 1383  | 0        | 1352     | 16      | 0            |
| 1   | I     | 1383  | 0        | 1352     | 16      | 0            |
| 1   | J     | 1383  | 0        | 1352     | 8       | 0            |
| 1   | K     | 1383  | 0        | 1352     | 18      | 0            |
| 1   | L     | 1383  | 0        | 1352     | 10      | 0            |
| 1   | M     | 1383  | 0        | 1352     | 17      | 0            |
| 1   | N     | 1383  | 0        | 1352     | 18      | 0            |
| 1   | O     | 1383  | 0        | 1352     | 21      | 0            |
| 1   | P     | 1383  | 0        | 1352     | 22      | 0            |
| 1   | Q     | 1383  | 0        | 1352     | 6       | 0            |
| 1   | R     | 1383  | 0        | 1352     | 16      | 0            |
| 1   | S     | 1383  | 0        | 1352     | 8       | 0            |
| 1   | T     | 1383  | 0        | 1352     | 10      | 0            |
| 1   | U     | 1383  | 0        | 1352     | 7       | 0            |
| 1   | V     | 1383  | 0        | 1352     | 15      | 0            |
| 1   | W     | 1383  | 0        | 1352     | 14      | 0            |
| 1   | X     | 1383  | 0        | 1352     | 7       | 0            |
| 1   | Y     | 1383  | 0        | 1352     | 21      | 0            |
| 1   | Z     | 1383  | 0        | 1352     | 17      | 0            |
| 2   | 0     | 1     | 0        | 0        | 0       | 0            |
| 2   | 1     | 1     | 0        | 0        | 0       | 0            |
| 2   | 2     | 1     | 0        | 0        | 0       | 0            |
| 2   | 3     | 1     | 0        | 0        | 0       | 0            |
| 2   | 4     | 1     | 0        | 0        | 0       | 0            |
| 2   | 5     | 1     | 0        | 0        | 0       | 0            |
| 2   | 6     | 1     | 0        | 0        | 0       | 0            |
| 2   | 7     | 1     | 0        | 0        | 0       | 0            |
| 2   | 8     | 1     | 0        | 0        | 0       | 0            |
| 2   | 9     | 1     | 0        | 0        | 0       | 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            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 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            |
| 2   | Y     | 1     | 0        | 0        | 0       | 0            |
| 2   | Z     | 1     | 0        | 0        | 0       | 0            |
| 3   | 1     | 10    | 0        | 0        | 0       | 0            |
| 3   | 2     | 10    | 0        | 0        | 0       | 0            |
| 3   | 3     | 10    | 0        | 0        | 0       | 0            |
| 3   | 4     | 5     | 0        | 0        | 0       | 0            |
| 3   | 5     | 5     | 0        | 0        | 0       | 0            |
| 3   | 6     | 5     | 0        | 0        | 0       | 0            |
| 3   | 7     | 5     | 0        | 0        | 0       | 0            |
| 3   | 8     | 5     | 0        | 0        | 0       | 0            |
| 3   | A     | 15    | 0        | 0        | 0       | 0            |
| 3   | B     | 5     | 0        | 0        | 0       | 0            |
| 3   | C     | 10    | 0        | 0        | 0       | 0            |
| 3   | E     | 5     | 0        | 0        | 0       | 0            |
| 3   | F     | 5     | 0        | 0        | 0       | 0            |
| 3   | G     | 10    | 0        | 0        | 0       | 0            |
| 3   | H     | 5     | 0        | 0        | 0       | 0            |
| 3   | I     | 5     | 0        | 0        | 0       | 0            |
| 3   | J     | 15    | 0        | 0        | 0       | 0            |
| 3   | K     | 5     | 0        | 0        | 0       | 0            |
| 3   | M     | 5     | 0        | 0        | 0       | 0            |
| 3   | O     | 5     | 0        | 0        | 0       | 0            |
| 3   | Q     | 5     | 0        | 0        | 0       | 0            |
| 3   | R     | 5     | 0        | 0        | 0       | 0            |
| 3   | S     | 10    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | T     | 5     | 0        | 0        | 0       | 0            |
| 3   | V     | 10    | 0        | 0        | 0       | 0            |
| 3   | W     | 10    | 0        | 0        | 0       | 0            |
| 3   | X     | 5     | 0        | 0        | 0       | 0            |
| 3   | Z     | 5     | 0        | 0        | 0       | 0            |
| 4   | 0     | 18    | 0        | 0        | 0       | 0            |
| 4   | 1     | 23    | 0        | 0        | 0       | 0            |
| 4   | 2     | 19    | 0        | 0        | 0       | 0            |
| 4   | 3     | 25    | 0        | 0        | 0       | 0            |
| 4   | 4     | 25    | 0        | 0        | 0       | 0            |
| 4   | 5     | 13    | 0        | 0        | 0       | 0            |
| 4   | 6     | 14    | 0        | 0        | 0       | 0            |
| 4   | 7     | 19    | 0        | 0        | 0       | 0            |
| 4   | 8     | 13    | 0        | 0        | 0       | 0            |
| 4   | 9     | 26    | 0        | 0        | 0       | 0            |
| 4   | A     | 40    | 0        | 0        | 2       | 0            |
| 4   | B     | 26    | 0        | 0        | 0       | 0            |
| 4   | C     | 19    | 0        | 0        | 0       | 0            |
| 4   | D     | 29    | 0        | 0        | 1       | 0            |
| 4   | E     | 37    | 0        | 0        | 1       | 0            |
| 4   | F     | 24    | 0        | 0        | 0       | 0            |
| 4   | G     | 31    | 0        | 0        | 0       | 0            |
| 4   | H     | 10    | 0        | 0        | 0       | 0            |
| 4   | I     | 30    | 0        | 0        | 0       | 0            |
| 4   | J     | 31    | 0        | 0        | 0       | 0            |
| 4   | K     | 12    | 0        | 0        | 0       | 0            |
| 4   | L     | 20    | 0        | 0        | 0       | 0            |
| 4   | M     | 20    | 0        | 0        | 0       | 0            |
| 4   | N     | 24    | 0        | 0        | 0       | 0            |
| 4   | O     | 14    | 0        | 0        | 0       | 0            |
| 4   | P     | 13    | 0        | 0        | 1       | 0            |
| 4   | Q     | 18    | 0        | 0        | 0       | 0            |
| 4   | R     | 20    | 0        | 0        | 0       | 0            |
| 4   | S     | 28    | 0        | 0        | 0       | 0            |
| 4   | T     | 19    | 0        | 0        | 1       | 0            |
| 4   | U     | 27    | 0        | 0        | 0       | 0            |
| 4   | V     | 18    | 0        | 0        | 0       | 0            |
| 4   | W     | 23    | 0        | 0        | 0       | 0            |
| 4   | X     | 24    | 0        | 0        | 0       | 0            |
| 4   | Y     | 31    | 0        | 0        | 0       | 0            |
| 4   | Z     | 7     | 0        | 0        | 0       | 0            |
| All | All   | 50819 | 0        | 48678    | 424     | 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 4.

All (424) 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:N:149:GLN:HE21 | 1:N:149:GLN:H    | 0.98                     | 0.95              |
| 1:B:144:ALA:HB2  | 1:B:150:ILE:HG21 | 1.48                     | 0.95              |
| 1:D:144:ALA:HB2  | 1:D:150:ILE:HG21 | 1.53                     | 0.90              |
| 1:B:144:ALA:HB2  | 1:B:150:ILE:CG2  | 2.05                     | 0.86              |
| 1:3:6:MET:HE2    | 1:3:116:THR:HG21 | 1.58                     | 0.84              |
| 1:N:149:GLN:H    | 1:N:149:GLN:NE2  | 1.76                     | 0.83              |
| 1:6:32:GLU:HG3   | 1:O:58:TYR:OH    | 1.78                     | 0.82              |
| 1:E:149:GLN:HE21 | 1:X:149:GLN:HG3  | 1.43                     | 0.82              |
| 1:9:149:GLN:H    | 1:9:149:GLN:HE21 | 1.25                     | 0.81              |
| 1:P:116:THR:O    | 1:P:120:LEU:HD12 | 1.82                     | 0.78              |
| 1:K:149:GLN:H    | 1:K:149:GLN:HE21 | 1.32                     | 0.78              |
| 1:8:81:GLU:HB2   | 1:8:85:LYS:HD3   | 1.65                     | 0.78              |
| 1:3:6:MET:CE     | 1:3:116:THR:HG21 | 2.13                     | 0.78              |
| 1:T:15:ASN:HB2   | 4:T:2008:HOH:O   | 1.85                     | 0.77              |
| 1:6:149:GLN:HE21 | 1:6:149:GLN:H    | 1.29                     | 0.77              |
| 1:L:6:MET:HE2    | 1:L:107:LEU:HG   | 1.69                     | 0.73              |
| 1:O:11:ASN:HD21  | 1:O:68:VAL:HA    | 1.51                     | 0.73              |
| 1:5:72:GLU:OE2   | 1:N:72:GLU:OE1   | 2.06                     | 0.73              |
| 1:Z:81:GLU:H     | 1:Z:85:LYS:HD2   | 1.54                     | 0.72              |
| 1:M:91:TYR:CZ    | 1:M:135:LYS:HD3  | 2.25                     | 0.71              |
| 1:D:144:ALA:HB2  | 1:D:150:ILE:CG2  | 2.20                     | 0.71              |
| 1:9:15:ASN:HD21  | 1:9:71:ASP:H     | 1.38                     | 0.70              |
| 1:N:138:LEU:HD23 | 1:N:138:LEU:C    | 2.18                     | 0.69              |
| 1:Y:6:MET:HE3    | 1:Y:108:ALA:HA   | 1.75                     | 0.69              |
| 1:N:140:LYS:HB3  | 1:N:154:LEU:HD11 | 1.75                     | 0.68              |
| 1:G:138:LEU:C    | 1:G:138:LEU:HD23 | 2.20                     | 0.67              |
| 1:H:81:GLU:HB2   | 1:H:85:LYS:HG3   | 1.77                     | 0.67              |
| 1:E:149:GLN:NE2  | 1:X:149:GLN:HG3  | 2.07                     | 0.66              |
| 1:A:138:LEU:C    | 1:A:138:LEU:HD23 | 2.20                     | 0.66              |
| 1:F:6:MET:HE2    | 1:F:107:LEU:HG   | 1.77                     | 0.66              |
| 1:F:144:ALA:HB2  | 1:F:150:ILE:HG21 | 1.79                     | 0.65              |
| 1:5:13:GLN:OE1   | 1:5:16:ARG:HD2   | 1.98                     | 0.64              |
| 1:A:138:LEU:HD23 | 1:A:138:LEU:O    | 1.98                     | 0.64              |
| 1:S:138:LEU:C    | 1:S:138:LEU:HD23 | 2.23                     | 0.64              |
| 1:K:15:ASN:HD21  | 1:K:71:ASP:H     | 1.46                     | 0.63              |
| 1:N:149:GLN:HE21 | 1:N:149:GLN:N    | 1.83                     | 0.63              |
| 1:U:94:GLU:OE1   | 1:U:130:GLU:HB3  | 2.00                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:147:SER:OG   | 1:X:149:GLN:HG2  | 1.99                     | 0.62              |
| 1:C:144:ALA:HB2  | 1:C:150:ILE:HG21 | 1.80                     | 0.62              |
| 1:K:131:GLU:OE1  | 1:R:1:MET:HE2    | 2.00                     | 0.62              |
| 1:6:140:LYS:HB3  | 1:6:154:LEU:HD11 | 1.82                     | 0.61              |
| 1:Y:5:ARG:HD2    | 1:Y:111:GLU:OE2  | 2.00                     | 0.61              |
| 1:W:9:ALA:HB1    | 1:W:104:LEU:CD2  | 2.30                     | 0.61              |
| 1:I:11:ASN:HD21  | 1:I:68:VAL:HA    | 1.65                     | 0.61              |
| 1:K:149:GLN:H    | 1:K:149:GLN:NE2  | 1.99                     | 0.61              |
| 1:O:81:GLU:HB2   | 1:O:85:LYS:HG2   | 1.83                     | 0.61              |
| 1:9:149:GLN:H    | 1:9:149:GLN:NE2  | 1.98                     | 0.61              |
| 1:1:58:TYR:OH    | 1:J:32:GLU:HG3   | 2.01                     | 0.60              |
| 1:C:72:GLU:OE1   | 1:U:72:GLU:OE1   | 2.20                     | 0.60              |
| 1:G:140:LYS:HD3  | 1:G:154:LEU:HD21 | 1.83                     | 0.60              |
| 1:I:5:ARG:H      | 1:I:5:ARG:HD3    | 1.66                     | 0.60              |
| 1:S:91:TYR:CZ    | 1:S:135:LYS:HD3  | 2.37                     | 0.60              |
| 1:3:144:ALA:HB2  | 1:3:150:ILE:HG21 | 1.84                     | 0.59              |
| 1:1:1:MET:HE3    | 1:1:65:ASN:HB2   | 1.84                     | 0.59              |
| 1:V:91:TYR:CZ    | 1:V:135:LYS:HD3  | 2.38                     | 0.59              |
| 1:I:6:MET:HE3    | 1:I:108:ALA:HA   | 1.84                     | 0.59              |
| 1:7:140:LYS:HB3  | 1:7:154:LEU:HD11 | 1.85                     | 0.58              |
| 1:I:6:MET:CE     | 1:I:108:ALA:HA   | 2.33                     | 0.58              |
| 1:B:64:ARG:O     | 1:B:65:ASN:HB3   | 2.03                     | 0.58              |
| 1:B:72:GLU:OE1   | 1:T:72:GLU:OE1   | 2.21                     | 0.58              |
| 1:3:15:ASN:HD21  | 1:3:71:ASP:H     | 1.51                     | 0.58              |
| 1:D:91:TYR:CZ    | 1:D:135:LYS:HD3  | 2.38                     | 0.58              |
| 1:1:144:ALA:HB2  | 1:1:150:ILE:CG2  | 2.34                     | 0.58              |
| 1:C:6:MET:HE2    | 1:C:107:LEU:HG   | 1.86                     | 0.58              |
| 1:Y:91:TYR:CZ    | 1:Y:135:LYS:HD3  | 2.38                     | 0.58              |
| 1:Y:95:LYS:O     | 1:Y:99:LYS:HG3   | 2.03                     | 0.58              |
| 1:D:62:TYR:CE2   | 1:D:68:VAL:HG23  | 2.38                     | 0.58              |
| 1:M:13:GLN:NE2   | 1:M:16:ARG:HH11  | 2.01                     | 0.58              |
| 1:O:145:LYS:C    | 1:O:147:SER:H    | 2.10                     | 0.58              |
| 1:4:72:GLU:OE1   | 1:M:72:GLU:OE1   | 2.22                     | 0.57              |
| 1:M:40:ALA:O     | 1:M:44:LYS:HG3   | 2.04                     | 0.57              |
| 1:O:6:MET:HE3    | 1:O:6:MET:HA     | 1.85                     | 0.57              |
| 1:3:144:ALA:HB2  | 1:3:150:ILE:CG2  | 2.33                     | 0.57              |
| 1:8:140:LYS:HB3  | 1:8:154:LEU:HD11 | 1.87                     | 0.57              |
| 1:N:138:LEU:HD23 | 1:N:138:LEU:O    | 2.05                     | 0.57              |
| 1:1:144:ALA:HB2  | 1:1:150:ILE:HG21 | 1.87                     | 0.57              |
| 1:8:1:MET:HE2    | 1:9:131:GLU:OE1  | 2.05                     | 0.57              |
| 1:8:143:PHE:HZ   | 1:M:151:LEU:HD23 | 1.68                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:91:TYR:CZ    | 1:T:135:LYS:HD3  | 2.40                     | 0.57              |
| 1:7:67:ARG:HD3   | 1:P:33:ASP:OD2   | 2.05                     | 0.57              |
| 1:V:14:LEU:C     | 1:V:14:LEU:HD23  | 2.30                     | 0.56              |
| 1:T:138:LEU:C    | 1:T:138:LEU:HD23 | 2.31                     | 0.56              |
| 1:V:138:LEU:C    | 1:V:138:LEU:HD23 | 2.31                     | 0.56              |
| 1:Y:48:GLU:OE2   | 1:Y:165:LEU:HB2  | 2.05                     | 0.56              |
| 1:D:14:LEU:C     | 1:D:14:LEU:HD23  | 2.30                     | 0.56              |
| 1:B:144:ALA:CB   | 1:B:150:ILE:CG2  | 2.81                     | 0.56              |
| 1:F:72:GLU:OE1   | 1:X:72:GLU:OE1   | 2.24                     | 0.56              |
| 1:2:135:LYS:NZ   | 1:2:139:ASP:OD1  | 2.37                     | 0.56              |
| 1:C:8:LYS:HD2    | 1:Y:74:PRO:HG3   | 1.86                     | 0.56              |
| 1:H:144:ALA:HB2  | 1:H:150:ILE:CG2  | 2.36                     | 0.56              |
| 1:Y:149:GLN:H    | 1:Y:149:GLN:HE21 | 1.54                     | 0.55              |
| 1:4:91:TYR:CZ    | 1:4:135:LYS:HD3  | 2.41                     | 0.55              |
| 1:6:13:GLN:HB2   | 1:6:104:LEU:HD11 | 1.88                     | 0.55              |
| 1:Y:144:ALA:O    | 1:Y:145:LYS:C    | 2.50                     | 0.55              |
| 1:4:15:ASN:ND2   | 1:4:71:ASP:HB2   | 2.22                     | 0.55              |
| 1:P:36:LEU:HB3   | 1:P:39:PHE:HD1   | 1.70                     | 0.55              |
| 1:R:11:ASN:ND2   | 1:R:69:GLU:H     | 2.05                     | 0.55              |
| 1:3:1:MET:HE2    | 1:Y:91:TYR:OH    | 2.07                     | 0.54              |
| 1:7:23:LEU:HD11  | 1:7:27:MET:HE3   | 1.89                     | 0.54              |
| 1:0:91:TYR:CE2   | 1:0:95:LYS:HE2   | 2.43                     | 0.54              |
| 1:R:138:LEU:C    | 1:R:138:LEU:HD23 | 2.33                     | 0.54              |
| 1:0:144:ALA:HB2  | 1:0:150:ILE:HG21 | 1.90                     | 0.54              |
| 1:9:149:GLN:HE21 | 1:9:149:GLN:N    | 2.00                     | 0.54              |
| 1:6:69:GLU:HB2   | 1:O:78:LYS:HE3   | 1.90                     | 0.53              |
| 1:I:44:LYS:HB2   | 1:I:163:PRO:HG3  | 1.90                     | 0.53              |
| 1:M:138:LEU:C    | 1:M:138:LEU:HD23 | 2.33                     | 0.53              |
| 1:W:13:GLN:HB2   | 1:W:104:LEU:HD11 | 1.90                     | 0.53              |
| 1:Z:99:LYS:HA    | 1:Z:102:TYR:HD2  | 1.73                     | 0.53              |
| 1:8:67:ARG:NH2   | 1:Q:78:LYS:O     | 2.42                     | 0.53              |
| 1:Z:94:GLU:OE1   | 1:Z:130:GLU:HB3  | 2.08                     | 0.53              |
| 1:X:17:GLU:O     | 1:X:20:SER:HB2   | 2.08                     | 0.53              |
| 1:4:153:MET:HE1  | 1:R:149:GLN:HG3  | 1.91                     | 0.53              |
| 1:P:130:GLU:O    | 1:P:134:VAL:HG23 | 2.08                     | 0.53              |
| 1:H:144:ALA:O    | 1:H:145:LYS:C    | 2.52                     | 0.53              |
| 1:Y:138:LEU:O    | 1:Y:138:LEU:HD23 | 2.09                     | 0.52              |
| 1:W:6:MET:HE3    | 1:W:108:ALA:HA   | 1.90                     | 0.52              |
| 1:N:144:ALA:HB2  | 1:N:150:ILE:HG21 | 1.91                     | 0.52              |
| 1:H:65:ASN:OD1   | 1:R:135:LYS:HE3  | 2.09                     | 0.52              |
| 1:K:6:MET:HE2    | 1:K:107:LEU:HG   | 1.91                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:138:LEU:HD23 | 1:G:138:LEU:O    | 2.09                     | 0.52              |
| 1:H:144:ALA:HB2  | 1:H:150:ILE:HG21 | 1.91                     | 0.52              |
| 1:2:138:LEU:C    | 1:2:138:LEU:HD23 | 2.34                     | 0.52              |
| 1:4:165:LEU:O    | 1:4:166:PRO:C    | 2.53                     | 0.52              |
| 1:A:15:ASN:HB2   | 4:A:2021:HOH:O   | 2.08                     | 0.52              |
| 1:U:107:LEU:O    | 1:U:111:GLU:HG3  | 2.10                     | 0.52              |
| 1:4:135:LYS:HE3  | 1:9:65:ASN:HD21  | 1.75                     | 0.52              |
| 1:Y:138:LEU:HD23 | 1:Y:138:LEU:C    | 2.35                     | 0.52              |
| 1:9:15:ASN:ND2   | 1:9:71:ASP:H     | 2.06                     | 0.52              |
| 1:A:144:ALA:HB2  | 1:A:150:ILE:CG2  | 2.40                     | 0.52              |
| 1:T:144:ALA:O    | 1:T:145:LYS:C    | 2.54                     | 0.51              |
| 1:Y:165:LEU:HB3  | 1:Y:166:PRO:HD3  | 1.92                     | 0.51              |
| 1:3:91:TYR:CZ    | 1:3:135:LYS:HD3  | 2.45                     | 0.51              |
| 1:Y:6:MET:HE3    | 1:Y:108:ALA:CA   | 2.39                     | 0.51              |
| 1:5:116:THR:O    | 1:5:120:LEU:HD12 | 2.09                     | 0.51              |
| 1:I:88:GLU:HG2   | 1:I:138:LEU:HD11 | 1.92                     | 0.51              |
| 1:V:165:LEU:O    | 1:V:166:PRO:C    | 2.52                     | 0.51              |
| 1:D:144:ALA:CB   | 1:D:150:ILE:CG2  | 2.88                     | 0.51              |
| 1:4:6:MET:HE3    | 1:4:108:ALA:HA   | 1.92                     | 0.51              |
| 1:A:91:TYR:CZ    | 1:A:135:LYS:HD3  | 2.45                     | 0.51              |
| 1:A:138:LEU:C    | 1:A:138:LEU:CD2  | 2.84                     | 0.51              |
| 1:I:40:ALA:O     | 1:I:44:LYS:HG3   | 2.11                     | 0.51              |
| 1:N:91:TYR:CZ    | 1:N:135:LYS:HD3  | 2.45                     | 0.50              |
| 1:7:144:ALA:O    | 1:7:145:LYS:C    | 2.54                     | 0.50              |
| 1:0:144:ALA:HB2  | 1:0:150:ILE:CG2  | 2.41                     | 0.50              |
| 1:H:140:LYS:HD3  | 1:H:154:LEU:HD21 | 1.94                     | 0.50              |
| 1:E:138:LEU:C    | 1:E:138:LEU:HD23 | 2.36                     | 0.50              |
| 1:5:69:GLU:OE2   | 1:N:75:LYS:NZ    | 2.37                     | 0.50              |
| 1:H:102:TYR:CE1  | 1:K:114:TYR:HB2  | 2.47                     | 0.50              |
| 1:7:22:TYR:OH    | 1:P:70:LEU:HB3   | 2.11                     | 0.50              |
| 1:I:6:MET:HE2    | 1:I:107:LEU:HG   | 1.92                     | 0.50              |
| 1:0:67:ARG:NH2   | 1:I:30:TYR:HA    | 2.26                     | 0.50              |
| 1:B:138:LEU:C    | 1:B:138:LEU:HD23 | 2.37                     | 0.50              |
| 1:5:135:LYS:NZ   | 1:5:139:ASP:OD1  | 2.45                     | 0.50              |
| 1:B:144:ALA:HB2  | 1:B:150:ILE:HG22 | 1.93                     | 0.50              |
| 1:L:91:TYR:CZ    | 1:L:135:LYS:HD3  | 2.46                     | 0.50              |
| 1:D:6:MET:HE2    | 1:D:107:LEU:HG   | 1.94                     | 0.49              |
| 1:P:13:GLN:OE1   | 1:P:16:ARG:HD2   | 2.12                     | 0.49              |
| 1:I:22:TYR:CD2   | 1:I:76:PRO:HD3   | 2.47                     | 0.49              |
| 1:A:135:LYS:NZ   | 1:A:139:ASP:OD2  | 2.45                     | 0.49              |
| 1:O:6:MET:HE2    | 1:O:10:LEU:HG    | 1.93                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:94:GLU:OE1   | 1:E:94:GLU:HA    | 2.11                     | 0.49              |
| 1:H:72:GLU:OE1   | 1:Z:72:GLU:OE1   | 2.31                     | 0.49              |
| 1:0:131:GLU:OE1  | 1:Z:1:MET:CE     | 2.61                     | 0.49              |
| 1:4:25:PHE:O     | 1:4:28:ALA:HB3   | 2.12                     | 0.49              |
| 1:8:81:GLU:HB2   | 1:8:85:LYS:CD    | 2.42                     | 0.49              |
| 1:1:58:TYR:OH    | 1:J:32:GLU:CG    | 2.60                     | 0.49              |
| 1:V:62:TYR:CE2   | 1:V:68:VAL:HG23  | 2.48                     | 0.49              |
| 1:Y:60:TYR:HB2   | 1:Y:119:PHE:CE1  | 2.48                     | 0.49              |
| 1:Y:149:GLN:H    | 1:Y:149:GLN:NE2  | 2.10                     | 0.49              |
| 1:7:22:TYR:CZ    | 1:P:70:LEU:HB3   | 2.48                     | 0.48              |
| 1:2:165:LEU:HD13 | 1:K:165:LEU:HD12 | 1.95                     | 0.48              |
| 1:Z:99:LYS:HA    | 1:Z:102:TYR:CD2  | 2.47                     | 0.48              |
| 1:1:78:LYS:HE3   | 1:J:69:GLU:OE1   | 2.14                     | 0.48              |
| 1:V:91:TYR:CE2   | 1:V:95:LYS:HE3   | 2.49                     | 0.48              |
| 1:W:5:ARG:HD2    | 1:W:111:GLU:OE2  | 2.13                     | 0.48              |
| 1:Y:81:GLU:HB2   | 1:Y:85:LYS:HG3   | 1.95                     | 0.48              |
| 1:Z:27:MET:HG2   | 1:Z:80:TRP:CH2   | 2.48                     | 0.48              |
| 1:9:72:GLU:OE1   | 1:R:72:GLU:OE1   | 2.31                     | 0.48              |
| 1:1:46:GLN:NE2   | 1:1:130:GLU:OE1  | 2.45                     | 0.48              |
| 1:3:51:ILE:O     | 1:3:54:ALA:HB3   | 2.13                     | 0.48              |
| 1:F:48:GLU:OE2   | 1:F:165:LEU:HB2  | 2.14                     | 0.48              |
| 1:G:138:LEU:C    | 1:G:138:LEU:CD2  | 2.86                     | 0.48              |
| 1:X:91:TYR:CZ    | 1:X:135:LYS:HD3  | 2.49                     | 0.48              |
| 1:3:15:ASN:OD1   | 1:3:71:ASP:HB2   | 2.12                     | 0.48              |
| 1:F:91:TYR:CZ    | 1:F:135:LYS:HD3  | 2.48                     | 0.48              |
| 1:A:94:GLU:OE1   | 1:A:130:GLU:HB3  | 2.13                     | 0.48              |
| 1:K:144:ALA:O    | 1:K:145:LYS:C    | 2.56                     | 0.48              |
| 1:R:60:TYR:CZ    | 1:R:64:ARG:HG3   | 2.48                     | 0.48              |
| 1:2:72:GLU:OE1   | 1:K:72:GLU:OE1   | 2.31                     | 0.48              |
| 1:9:41:ASN:HA    | 1:9:44:LYS:HD2   | 1.94                     | 0.48              |
| 1:B:1:MET:HE3    | 1:B:65:ASN:HB2   | 1.96                     | 0.48              |
| 1:E:67:ARG:NH2   | 4:E:2019:HOH:O   | 2.46                     | 0.48              |
| 1:I:60:TYR:HB2   | 1:I:119:PHE:CE1  | 2.48                     | 0.48              |
| 1:T:62:TYR:CE2   | 1:T:68:VAL:HG23  | 2.48                     | 0.48              |
| 1:4:144:ALA:O    | 1:4:145:LYS:C    | 2.56                     | 0.48              |
| 1:O:6:MET:HE3    | 1:O:9:ALA:HB3    | 1.96                     | 0.48              |
| 1:P:97:ILE:O     | 1:P:101:ILE:HG12 | 2.13                     | 0.48              |
| 1:0:67:ARG:HH22  | 1:I:30:TYR:HA    | 1.79                     | 0.48              |
| 1:7:22:TYR:CE1   | 1:P:70:LEU:HD13  | 2.49                     | 0.47              |
| 1:M:114:TYR:HB2  | 1:P:102:TYR:CD1  | 2.49                     | 0.47              |
| 1:K:149:GLN:HE21 | 1:K:149:GLN:N    | 2.06                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:138:LEU:HD23 | 1:Z:138:LEU:O    | 2.15                     | 0.47              |
| 1:3:165:LEU:C    | 1:3:167:GLY:H    | 2.22                     | 0.47              |
| 1:R:62:TYR:CE2   | 1:R:68:VAL:HG23  | 2.49                     | 0.47              |
| 1:W:143:PHE:CG   | 1:W:143:PHE:O    | 2.67                     | 0.47              |
| 1:J:81:GLU:HB2   | 1:J:85:LYS:HG3   | 1.97                     | 0.47              |
| 1:7:70:LEU:HB3   | 1:P:22:TYR:CZ    | 2.50                     | 0.47              |
| 1:8:25:PHE:O     | 1:8:28:ALA:HB3   | 2.14                     | 0.47              |
| 1:B:3:SER:CB     | 1:B:6:MET:H      | 2.28                     | 0.47              |
| 1:V:46:GLN:NE2   | 1:V:49:GLU:OE1   | 2.48                     | 0.47              |
| 1:1:43:MET:HE2   | 1:1:87:PHE:CZ    | 2.50                     | 0.47              |
| 1:3:147:SER:O    | 1:3:148:PRO:C    | 2.58                     | 0.47              |
| 1:D:60:TYR:HB2   | 1:D:119:PHE:CE1  | 2.50                     | 0.47              |
| 1:P:149:GLN:H    | 1:P:149:GLN:HG2  | 1.44                     | 0.47              |
| 1:T:144:ALA:HB2  | 1:T:150:ILE:HG21 | 1.97                     | 0.47              |
| 1:Y:150:ILE:O    | 1:Y:154:LEU:HB2  | 2.15                     | 0.47              |
| 1:6:165:LEU:O    | 1:6:167:GLY:N    | 2.48                     | 0.46              |
| 1:7:70:LEU:HD13  | 1:P:22:TYR:CE1   | 2.49                     | 0.46              |
| 1:9:64:ARG:HD2   | 1:9:64:ARG:HA    | 1.66                     | 0.46              |
| 1:E:13:GLN:OE1   | 1:E:100:SER:HB3  | 2.15                     | 0.46              |
| 1:E:135:LYS:NZ   | 1:E:139:ASP:OD1  | 2.47                     | 0.46              |
| 1:B:165:LEU:O    | 1:B:166:PRO:C    | 2.59                     | 0.46              |
| 1:W:138:LEU:HD23 | 1:W:138:LEU:O    | 2.13                     | 0.46              |
| 1:1:77:PRO:HB2   | 1:1:80:TRP:CZ2   | 2.51                     | 0.46              |
| 1:D:5:ARG:NH2    | 4:D:2002:HOH:O   | 2.41                     | 0.46              |
| 1:N:27:MET:HG2   | 1:N:80:TRP:CH2   | 2.50                     | 0.46              |
| 1:W:64:ARG:O     | 1:W:65:ASN:HB3   | 2.15                     | 0.46              |
| 1:6:64:ARG:HD2   | 1:6:64:ARG:HA    | 1.64                     | 0.46              |
| 1:Z:11:ASN:HD21  | 1:Z:69:GLU:H     | 1.63                     | 0.46              |
| 1:P:122:TRP:HB2  | 4:P:2012:HOH:O   | 2.16                     | 0.46              |
| 1:4:48:GLU:OE2   | 1:4:165:LEU:HB2  | 2.16                     | 0.46              |
| 1:5:91:TYR:CZ    | 1:5:135:LYS:HD3  | 2.51                     | 0.46              |
| 1:D:72:GLU:OE1   | 1:V:72:GLU:OE1   | 2.34                     | 0.46              |
| 1:G:111:GLU:O    | 1:G:112:LYS:HB2  | 2.15                     | 0.46              |
| 1:1:138:LEU:C    | 1:1:138:LEU:HD23 | 2.41                     | 0.46              |
| 1:2:156:LYS:O    | 1:2:159:SER:OG   | 2.27                     | 0.46              |
| 1:7:64:ARG:HA    | 1:7:64:ARG:HD2   | 1.80                     | 0.46              |
| 1:B:145:LYS:O    | 1:B:146:ASP:C    | 2.59                     | 0.46              |
| 1:D:144:ALA:O    | 1:D:145:LYS:C    | 2.58                     | 0.46              |
| 1:H:138:LEU:C    | 1:H:138:LEU:HD23 | 2.41                     | 0.46              |
| 1:O:64:ARG:HD2   | 1:O:64:ARG:HA    | 1.64                     | 0.46              |
| 1:5:17:GLU:O     | 1:5:20:SER:HB2   | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:8:64:ARG:HD2   | 1:8:64:ARG:HA    | 1.67                     | 0.46              |
| 1:A:107:LEU:O    | 1:A:108:ALA:C    | 2.58                     | 0.46              |
| 1:Y:82:SER:HB2   | 1:Y:83:PRO:HD2   | 1.98                     | 0.46              |
| 1:9:69:GLU:OE2   | 1:R:75:LYS:NZ    | 2.48                     | 0.45              |
| 1:9:153:MET:HE1  | 1:Q:153:MET:SD   | 2.55                     | 0.45              |
| 1:9:165:LEU:HB3  | 1:9:166:PRO:HD3  | 1.99                     | 0.45              |
| 1:M:23:LEU:O     | 1:M:27:MET:HG3   | 2.16                     | 0.45              |
| 1:T:165:LEU:O    | 1:T:166:PRO:C    | 2.58                     | 0.45              |
| 1:V:6:MET:HE2    | 1:V:107:LEU:HG   | 1.97                     | 0.45              |
| 1:W:144:ALA:O    | 1:W:145:LYS:C    | 2.59                     | 0.45              |
| 1:1:94:GLU:OE2   | 1:1:94:GLU:HA    | 2.16                     | 0.45              |
| 1:R:11:ASN:HD21  | 1:R:68:VAL:HA    | 1.82                     | 0.45              |
| 1:A:120:LEU:O    | 1:A:121:GLU:C    | 2.59                     | 0.45              |
| 1:3:150:ILE:HA   | 1:3:153:MET:HE3  | 1.99                     | 0.45              |
| 1:1:144:ALA:O    | 1:1:145:LYS:C    | 2.60                     | 0.45              |
| 1:I:88:GLU:CG    | 1:I:138:LEU:HD11 | 2.47                     | 0.45              |
| 1:N:138:LEU:C    | 1:N:138:LEU:CD2  | 2.90                     | 0.45              |
| 1:6:70:LEU:HD12  | 1:O:26:ALA:HB2   | 1.99                     | 0.45              |
| 1:J:149:GLN:H    | 1:J:149:GLN:HE21 | 1.64                     | 0.45              |
| 1:Z:11:ASN:ND2   | 1:Z:69:GLU:H     | 2.14                     | 0.45              |
| 1:6:42:TRP:CD1   | 1:6:158:LEU:HD22 | 2.51                     | 0.44              |
| 1:1:143:PHE:HE2  | 1:O:152:PHE:HB2  | 1.82                     | 0.44              |
| 1:C:64:ARG:O     | 1:C:65:ASN:HB3   | 2.16                     | 0.44              |
| 1:C:102:TYR:HB3  | 1:D:114:TYR:CE1  | 2.51                     | 0.44              |
| 1:M:73:ILE:HA    | 1:M:74:PRO:HD3   | 1.81                     | 0.44              |
| 1:5:70:LEU:HD13  | 1:N:22:TYR:CE1   | 2.52                     | 0.44              |
| 1:Z:81:GLU:H     | 1:Z:85:LYS:CD    | 2.26                     | 0.44              |
| 1:6:32:GLU:HG2   | 1:6:40:ALA:HB1   | 1.99                     | 0.44              |
| 1:Z:38:GLY:HA3   | 1:Z:155:ASP:O    | 2.17                     | 0.44              |
| 1:4:22:TYR:CE1   | 1:M:73:ILE:HD11  | 2.53                     | 0.44              |
| 1:L:145:LYS:O    | 1:L:146:ASP:C    | 2.61                     | 0.44              |
| 1:A:85:LYS:HG3   | 4:A:2029:HOH:O   | 2.17                     | 0.44              |
| 1:E:165:LEU:HD12 | 1:E:165:LEU:HA   | 1.79                     | 0.44              |
| 1:6:23:LEU:O     | 1:6:26:ALA:HB3   | 2.18                     | 0.44              |
| 1:B:97:ILE:O     | 1:B:100:SER:HB2  | 2.18                     | 0.44              |
| 1:E:138:LEU:HD23 | 1:E:138:LEU:O    | 2.18                     | 0.44              |
| 1:G:165:LEU:O    | 1:G:166:PRO:C    | 2.59                     | 0.44              |
| 1:P:58:TYR:CD1   | 1:P:58:TYR:C     | 2.95                     | 0.44              |
| 1:P:116:THR:HG22 | 1:P:120:LEU:HD11 | 2.00                     | 0.44              |
| 1:7:165:LEU:HD12 | 1:7:165:LEU:HA   | 1.77                     | 0.43              |
| 1:B:58:TYR:CD1   | 1:B:58:TYR:C     | 2.95                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:103:GLU:HG2  | 1:Y:16:ARG:NH2   | 2.33                     | 0.43              |
| 1:L:15:ASN:ND2   | 1:L:71:ASP:HB2   | 2.33                     | 0.43              |
| 1:M:6:MET:HE2    | 1:M:107:LEU:HG   | 2.00                     | 0.43              |
| 1:M:102:TYR:CE1  | 1:O:114:TYR:HB2  | 2.53                     | 0.43              |
| 1:O:6:MET:HE3    | 1:O:108:ALA:HB2  | 2.00                     | 0.43              |
| 1:C:144:ALA:HB2  | 1:C:150:ILE:CG2  | 2.47                     | 0.43              |
| 1:F:56:ARG:HB2   | 1:F:123:PHE:HZ   | 1.83                     | 0.43              |
| 1:H:156:LYS:O    | 1:H:157:GLU:C    | 2.61                     | 0.43              |
| 1:T:152:PHE:C    | 1:T:152:PHE:CD2  | 2.96                     | 0.43              |
| 1:W:138:LEU:HD23 | 1:W:138:LEU:C    | 2.42                     | 0.43              |
| 1:Q:60:TYR:HB2   | 1:Q:119:PHE:CE1  | 2.53                     | 0.43              |
| 1:Y:6:MET:HE2    | 1:Y:107:LEU:HG   | 2.00                     | 0.43              |
| 1:O:13:GLN:O     | 1:O:17:GLU:HG2   | 2.19                     | 0.43              |
| 1:D:69:GLU:HG3   | 1:V:78:LYS:HD2   | 2.01                     | 0.43              |
| 1:E:34:LEU:HD23  | 1:E:34:LEU:HA    | 1.78                     | 0.43              |
| 1:L:140:LYS:HD2  | 1:L:154:LEU:HD21 | 1.99                     | 0.43              |
| 1:W:97:ILE:O     | 1:W:101:ILE:HG12 | 2.19                     | 0.43              |
| 1:7:83:PRO:O     | 1:7:86:ALA:HB3   | 2.18                     | 0.43              |
| 1:F:144:ALA:HB2  | 1:F:150:ILE:CG2  | 2.47                     | 0.43              |
| 1:P:1:MET:HE1    | 1:P:65:ASN:HB2   | 1.99                     | 0.43              |
| 1:P:127:GLN:HA   | 1:P:130:GLU:HB2  | 1.99                     | 0.43              |
| 1:Q:64:ARG:HA    | 1:Q:64:ARG:HD2   | 1.80                     | 0.43              |
| 1:3:48:GLU:OE2   | 1:3:165:LEU:HB3  | 2.18                     | 0.43              |
| 1:A:144:ALA:HB2  | 1:A:150:ILE:HG21 | 2.01                     | 0.43              |
| 1:L:18:LEU:O     | 1:L:21:ALA:HB3   | 2.19                     | 0.43              |
| 1:R:94:GLU:OE1   | 1:R:94:GLU:HA    | 2.18                     | 0.43              |
| 1:N:165:LEU:O    | 1:N:166:PRO:C    | 2.62                     | 0.43              |
| 1:R:64:ARG:HA    | 1:R:64:ARG:HD2   | 1.83                     | 0.43              |
| 1:5:78:LYS:HE3   | 1:N:69:GLU:HB2   | 2.01                     | 0.43              |
| 1:B:3:SER:HB2    | 1:B:6:MET:H      | 1.83                     | 0.43              |
| 1:O:6:MET:HE1    | 1:O:104:LEU:CD2  | 2.49                     | 0.43              |
| 1:P:41:ASN:HA    | 1:P:44:LYS:HD2   | 2.00                     | 0.43              |
| 1:V:13:GLN:HG2   | 1:V:57:PHE:CZ    | 2.54                     | 0.43              |
| 1:3:165:LEU:O    | 1:3:167:GLY:N    | 2.52                     | 0.43              |
| 1:A:145:LYS:O    | 1:A:146:ASP:C    | 2.62                     | 0.43              |
| 1:B:64:ARG:HA    | 1:B:64:ARG:HD2   | 1.68                     | 0.43              |
| 1:O:64:ARG:O     | 1:O:65:ASN:HB3   | 2.19                     | 0.43              |
| 1:B:144:ALA:O    | 1:B:145:LYS:C    | 2.61                     | 0.43              |
| 1:U:64:ARG:HA    | 1:U:64:ARG:HD2   | 1.91                     | 0.43              |
| 1:U:144:ALA:O    | 1:U:145:LYS:C    | 2.62                     | 0.43              |
| 1:7:149:GLN:O    | 1:7:153:MET:HG3  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:60:TYR:CZ    | 1:P:64:ARG:HG3   | 2.55                     | 0.42              |
| 1:9:38:GLY:HA3   | 1:9:155:ASP:O    | 2.19                     | 0.42              |
| 1:G:24:TYR:CD2   | 1:G:46:GLN:HG3   | 2.54                     | 0.42              |
| 1:H:102:TYR:CD1  | 1:K:114:TYR:HB2  | 2.55                     | 0.42              |
| 1:M:61:ILE:HG23  | 1:M:66:GLY:HA3   | 2.00                     | 0.42              |
| 1:U:91:TYR:CZ    | 1:U:135:LYS:HD3  | 2.54                     | 0.42              |
| 1:W:91:TYR:CE2   | 1:W:95:LYS:HE3   | 2.54                     | 0.42              |
| 1:Y:165:LEU:HB3  | 1:Y:166:PRO:CD   | 2.50                     | 0.42              |
| 1:2:48:GLU:OE2   | 1:2:163:PRO:HB2  | 2.19                     | 0.42              |
| 1:4:67:ARG:HD3   | 1:M:33:ASP:CG    | 2.43                     | 0.42              |
| 1:4:135:LYS:CE   | 1:9:65:ASN:HD21  | 2.32                     | 0.42              |
| 1:C:165:LEU:HD12 | 1:C:165:LEU:HA   | 1.80                     | 0.42              |
| 1:C:165:LEU:HB3  | 1:C:166:PRO:HD3  | 2.01                     | 0.42              |
| 1:I:14:LEU:HD23  | 1:I:14:LEU:C     | 2.45                     | 0.42              |
| 1:K:64:ARG:HA    | 1:K:64:ARG:HD2   | 1.73                     | 0.42              |
| 1:N:142:LYS:C    | 1:N:144:ALA:H    | 2.28                     | 0.42              |
| 1:2:138:LEU:HD23 | 1:2:138:LEU:O    | 2.20                     | 0.42              |
| 1:I:150:ILE:HA   | 1:I:153:MET:HE3  | 2.01                     | 0.42              |
| 1:N:117:ARG:NH1  | 1:N:121:GLU:OE1  | 2.51                     | 0.42              |
| 1:P:27:MET:O     | 1:P:30:TYR:HB3   | 2.19                     | 0.42              |
| 1:S:97:ILE:O     | 1:S:100:SER:HB2  | 2.20                     | 0.42              |
| 1:4:6:MET:HE2    | 1:4:107:LEU:HD23 | 2.02                     | 0.42              |
| 1:K:48:GLU:OE2   | 1:K:165:LEU:HB2  | 2.19                     | 0.42              |
| 1:A:69:GLU:OE2   | 1:S:75:LYS:NZ    | 2.48                     | 0.42              |
| 1:S:145:LYS:HB3  | 1:S:146:ASP:H    | 1.76                     | 0.42              |
| 1:W:91:TYR:CZ    | 1:W:95:LYS:HE3   | 2.55                     | 0.42              |
| 1:2:62:TYR:HE1   | 1:K:33:ASP:HB2   | 1.85                     | 0.42              |
| 1:7:165:LEU:O    | 1:7:166:PRO:C    | 2.63                     | 0.42              |
| 1:6:165:LEU:HB3  | 1:6:166:PRO:HD3  | 2.01                     | 0.41              |
| 1:H:3:SER:O      | 1:H:4:GLU:C      | 2.63                     | 0.41              |
| 1:5:114:TYR:HB3  | 1:6:124:ILE:HD13 | 2.03                     | 0.41              |
| 1:6:3:SER:OG     | 1:6:6:MET:HB2    | 2.20                     | 0.41              |
| 1:M:60:TYR:O     | 1:M:61:ILE:C     | 2.60                     | 0.41              |
| 1:M:144:ALA:HB1  | 1:M:150:ILE:HB   | 2.00                     | 0.41              |
| 1:X:64:ARG:HA    | 1:X:64:ARG:HD2   | 1.76                     | 0.41              |
| 1:B:22:TYR:CZ    | 1:T:70:LEU:HB3   | 2.55                     | 0.41              |
| 1:O:6:MET:HE3    | 1:O:6:MET:CA     | 2.51                     | 0.41              |
| 1:R:19:TYR:CD1   | 1:R:74:PRO:HG2   | 2.55                     | 0.41              |
| 1:3:165:LEU:C    | 1:3:167:GLY:N    | 2.79                     | 0.41              |
| 1:5:143:PHE:HE2  | 1:J:152:PHE:HB2  | 1.84                     | 0.41              |
| 1:8:165:LEU:HD13 | 1:Q:165:LEU:HD13 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:104:LEU:HB3  | 1:J:120:LEU:HD11 | 2.01                     | 0.41              |
| 1:A:60:TYR:O     | 1:A:61:ILE:C     | 2.64                     | 0.41              |
| 1:F:2:LEU:HD22   | 1:F:6:MET:HB3    | 2.02                     | 0.41              |
| 1:H:13:GLN:HG2   | 1:H:57:PHE:CZ    | 2.55                     | 0.41              |
| 1:O:55:LEU:HD23  | 1:O:55:LEU:HA    | 1.91                     | 0.41              |
| 1:Q:140:LYS:HD3  | 1:Q:154:LEU:HD21 | 2.02                     | 0.41              |
| 1:V:138:LEU:HD23 | 1:V:138:LEU:O    | 2.20                     | 0.41              |
| 1:W:4:GLU:O      | 1:W:8:LYS:HG3    | 2.21                     | 0.41              |
| 1:9:20:SER:O     | 1:9:21:ALA:C     | 2.64                     | 0.41              |
| 1:K:138:LEU:HD23 | 1:K:138:LEU:C    | 2.46                     | 0.41              |
| 1:L:144:ALA:HB2  | 1:L:150:ILE:HG21 | 2.02                     | 0.41              |
| 1:R:138:LEU:C    | 1:R:138:LEU:CD2  | 2.93                     | 0.41              |
| 1:W:6:MET:HE2    | 1:W:107:LEU:HG   | 2.02                     | 0.41              |
| 1:0:131:GLU:OE1  | 1:Z:1:MET:HE2    | 2.20                     | 0.41              |
| 1:7:1:MET:HE2    | 1:Z:131:GLU:OE1  | 2.21                     | 0.41              |
| 1:L:144:ALA:HB2  | 1:L:150:ILE:CG2  | 2.51                     | 0.41              |
| 1:S:165:LEU:HA   | 1:S:165:LEU:HD12 | 1.81                     | 0.41              |
| 1:V:64:ARG:HA    | 1:V:64:ARG:HD2   | 1.73                     | 0.41              |
| 1:1:131:GLU:OE1  | 1:6:1:MET:HE2    | 2.21                     | 0.41              |
| 1:4:106:ALA:O    | 1:4:110:GLU:HG3  | 2.21                     | 0.41              |
| 1:8:165:LEU:O    | 1:8:166:PRO:C    | 2.64                     | 0.41              |
| 1:K:73:ILE:HA    | 1:K:74:PRO:HD3   | 1.90                     | 0.41              |
| 1:O:11:ASN:HD22  | 1:O:11:ASN:HA    | 1.73                     | 0.41              |
| 1:O:58:TYR:CD1   | 1:O:58:TYR:C     | 2.99                     | 0.41              |
| 1:R:165:LEU:O    | 1:R:166:PRO:C    | 2.64                     | 0.41              |
| 1:U:20:SER:O     | 1:U:21:ALA:C     | 2.64                     | 0.41              |
| 1:V:165:LEU:HA   | 1:V:165:LEU:HD12 | 1.79                     | 0.41              |
| 1:0:149:GLN:HG3  | 1:H:149:GLN:HG2  | 2.03                     | 0.41              |
| 1:9:135:LYS:HE3  | 1:9:139:ASP:OD2  | 2.21                     | 0.41              |
| 1:C:5:ARG:HD3    | 1:C:5:ARG:N      | 2.35                     | 0.41              |
| 1:J:104:LEU:HB3  | 1:J:120:LEU:CD1  | 2.51                     | 0.41              |
| 1:L:64:ARG:HA    | 1:L:64:ARG:HD2   | 1.89                     | 0.41              |
| 1:R:13:GLN:OE1   | 1:R:100:SER:HB3  | 2.20                     | 0.41              |
| 1:8:2:LEU:HD22   | 1:8:6:MET:HB3    | 2.03                     | 0.41              |
| 1:A:147:SER:HA   | 1:A:148:PRO:HD2  | 1.84                     | 0.41              |
| 1:D:144:ALA:CB   | 1:D:150:ILE:HG21 | 2.37                     | 0.41              |
| 1:G:22:TYR:CD1   | 1:G:76:PRO:HD3   | 2.56                     | 0.41              |
| 1:O:145:LYS:O    | 1:O:147:SER:N    | 2.44                     | 0.41              |
| 1:C:64:ARG:O     | 1:C:65:ASN:CB    | 2.70                     | 0.40              |
| 1:V:56:ARG:HH11  | 1:V:56:ARG:HG2   | 1.86                     | 0.40              |
| 1:Z:3:SER:OG     | 1:Z:6:MET:HB2    | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Z:142:LYS:C    | 1:Z:144:ALA:N    | 2.79                     | 0.40              |
| 1:B:22:TYR:CD2   | 1:B:76:PRO:HD3   | 2.56                     | 0.40              |
| 1:F:165:LEU:O    | 1:F:167:GLY:N    | 2.55                     | 0.40              |
| 1:H:58:TYR:CD1   | 1:H:58:TYR:C     | 2.99                     | 0.40              |
| 1:N:3:SER:OG     | 1:N:6:MET:HB2    | 2.21                     | 0.40              |
| 1:3:72:GLU:OE1   | 1:L:72:GLU:OE1   | 2.40                     | 0.40              |
| 1:C:165:LEU:HB3  | 1:C:166:PRO:CD   | 2.51                     | 0.40              |
| 1:I:5:ARG:HD3    | 1:I:5:ARG:N      | 2.35                     | 0.40              |
| 1:K:15:ASN:ND2   | 1:K:71:ASP:H     | 2.13                     | 0.40              |
| 1:P:116:THR:HG22 | 1:P:120:LEU:CD1  | 2.51                     | 0.40              |
| 1:Z:48:GLU:OE2   | 1:Z:165:LEU:HB2  | 2.21                     | 0.40              |
| 1:O:6:MET:HE1    | 1:O:104:LEU:HD23 | 2.02                     | 0.40              |
| 1:S:138:LEU:C    | 1:S:138:LEU:CD2  | 2.93                     | 0.40              |
| 1:H:60:TYR:CZ    | 1:H:64:ARG:HG3   | 2.57                     | 0.40              |
| 1:K:154:LEU:HD23 | 1:K:154:LEU:HA   | 1.74                     | 0.40              |
| 1:M:20:SER:O     | 1:M:24:TYR:CD2   | 2.75                     | 0.40              |
| 1:O:13:GLN:HG2   | 1:O:57:PHE:CZ    | 2.56                     | 0.40              |
| 1:S:120:LEU:O    | 1:S:121:GLU:C    | 2.65                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | 0     | 165/174 (95%) | 160 (97%) | 4 (2%)  | 1 (1%)   | 21          | 38 |
| 1   | 1     | 165/174 (95%) | 161 (98%) | 3 (2%)  | 1 (1%)   | 21          | 38 |
| 1   | 2     | 165/174 (95%) | 160 (97%) | 3 (2%)  | 2 (1%)   | 10          | 20 |
| 1   | 3     | 165/174 (95%) | 159 (96%) | 5 (3%)  | 1 (1%)   | 21          | 38 |
| 1   | 4     | 165/174 (95%) | 159 (96%) | 4 (2%)  | 2 (1%)   | 10          | 20 |
| 1   | 5     | 165/174 (95%) | 158 (96%) | 5 (3%)  | 2 (1%)   | 10          | 20 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | 6     | 165/174 (95%)   | 156 (94%)  | 7 (4%)   | 2 (1%)   | 10          | 20  |
| 1   | 7     | 165/174 (95%)   | 162 (98%)  | 1 (1%)   | 2 (1%)   | 10          | 20  |
| 1   | 8     | 165/174 (95%)   | 160 (97%)  | 3 (2%)   | 2 (1%)   | 10          | 20  |
| 1   | 9     | 165/174 (95%)   | 161 (98%)  | 2 (1%)   | 2 (1%)   | 10          | 20  |
| 1   | A     | 165/174 (95%)   | 163 (99%)  | 1 (1%)   | 1 (1%)   | 21          | 38  |
| 1   | B     | 165/174 (95%)   | 159 (96%)  | 3 (2%)   | 3 (2%)   | 6           | 13  |
| 1   | C     | 166/174 (95%)   | 159 (96%)  | 5 (3%)   | 2 (1%)   | 10          | 20  |
| 1   | D     | 165/174 (95%)   | 160 (97%)  | 2 (1%)   | 3 (2%)   | 6           | 13  |
| 1   | E     | 165/174 (95%)   | 163 (99%)  | 1 (1%)   | 1 (1%)   | 21          | 38  |
| 1   | F     | 165/174 (95%)   | 161 (98%)  | 3 (2%)   | 1 (1%)   | 21          | 38  |
| 1   | G     | 165/174 (95%)   | 162 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 1   | H     | 165/174 (95%)   | 160 (97%)  | 4 (2%)   | 1 (1%)   | 21          | 38  |
| 1   | I     | 165/174 (95%)   | 159 (96%)  | 4 (2%)   | 2 (1%)   | 10          | 20  |
| 1   | J     | 165/174 (95%)   | 161 (98%)  | 3 (2%)   | 1 (1%)   | 21          | 38  |
| 1   | K     | 165/174 (95%)   | 162 (98%)  | 2 (1%)   | 1 (1%)   | 21          | 38  |
| 1   | L     | 165/174 (95%)   | 161 (98%)  | 2 (1%)   | 2 (1%)   | 10          | 20  |
| 1   | M     | 165/174 (95%)   | 155 (94%)  | 8 (5%)   | 2 (1%)   | 10          | 20  |
| 1   | N     | 165/174 (95%)   | 160 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 1   | O     | 165/174 (95%)   | 159 (96%)  | 4 (2%)   | 2 (1%)   | 10          | 20  |
| 1   | P     | 165/174 (95%)   | 158 (96%)  | 5 (3%)   | 2 (1%)   | 10          | 20  |
| 1   | Q     | 165/174 (95%)   | 159 (96%)  | 4 (2%)   | 2 (1%)   | 10          | 20  |
| 1   | R     | 165/174 (95%)   | 160 (97%)  | 3 (2%)   | 2 (1%)   | 10          | 20  |
| 1   | S     | 165/174 (95%)   | 161 (98%)  | 3 (2%)   | 1 (1%)   | 21          | 38  |
| 1   | T     | 165/174 (95%)   | 161 (98%)  | 2 (1%)   | 2 (1%)   | 10          | 20  |
| 1   | U     | 165/174 (95%)   | 162 (98%)  | 1 (1%)   | 2 (1%)   | 10          | 20  |
| 1   | V     | 165/174 (95%)   | 158 (96%)  | 6 (4%)   | 1 (1%)   | 21          | 38  |
| 1   | W     | 165/174 (95%)   | 161 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 1   | X     | 165/174 (95%)   | 161 (98%)  | 3 (2%)   | 1 (1%)   | 21          | 38  |
| 1   | Y     | 165/174 (95%)   | 160 (97%)  | 3 (2%)   | 2 (1%)   | 10          | 20  |
| 1   | Z     | 165/174 (95%)   | 158 (96%)  | 5 (3%)   | 2 (1%)   | 10          | 20  |
| All | All   | 5941/6264 (95%) | 5759 (97%) | 126 (2%) | 56 (1%)  | 14          | 28  |

All (56) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 145 | LYS  |
| 1   | 3     | 166 | PRO  |
| 1   | 4     | 145 | LYS  |
| 1   | 7     | 145 | LYS  |
| 1   | 8     | 145 | LYS  |
| 1   | H     | 145 | LYS  |
| 1   | K     | 145 | LYS  |
| 1   | O     | 146 | ASP  |
| 1   | P     | 145 | LYS  |
| 1   | R     | 145 | LYS  |
| 1   | S     | 145 | LYS  |
| 1   | T     | 145 | LYS  |
| 1   | U     | 145 | LYS  |
| 1   | X     | 145 | LYS  |
| 1   | Y     | 145 | LYS  |
| 1   | Z     | 143 | PHE  |
| 1   | 9     | 145 | LYS  |
| 1   | 9     | 166 | PRO  |
| 1   | B     | 146 | ASP  |
| 1   | D     | 145 | LYS  |
| 1   | O     | 145 | LYS  |
| 1   | Q     | 145 | LYS  |
| 1   | V     | 166 | PRO  |
| 1   | 0     | 145 | LYS  |
| 1   | 5     | 145 | LYS  |
| 1   | E     | 145 | LYS  |
| 1   | F     | 166 | PRO  |
| 1   | I     | 36  | LEU  |
| 1   | U     | 166 | PRO  |
| 1   | Y     | 143 | PHE  |
| 1   | 1     | 145 | LYS  |
| 1   | 6     | 145 | LYS  |
| 1   | 6     | 166 | PRO  |
| 1   | B     | 145 | LYS  |
| 1   | L     | 146 | ASP  |
| 1   | M     | 145 | LYS  |
| 1   | M     | 166 | PRO  |
| 1   | T     | 143 | PHE  |
| 1   | 7     | 166 | PRO  |
| 1   | I     | 166 | PRO  |
| 1   | Q     | 166 | PRO  |
| 1   | A     | 166 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 145 | LYS  |
| 1   | J     | 166 | PRO  |
| 1   | L     | 145 | LYS  |
| 1   | 5     | 166 | PRO  |
| 1   | D     | 165 | LEU  |
| 1   | D     | 166 | PRO  |
| 1   | R     | 166 | PRO  |
| 1   | 2     | 166 | PRO  |
| 1   | 8     | 166 | PRO  |
| 1   | B     | 166 | PRO  |
| 1   | C     | 166 | PRO  |
| 1   | P     | 166 | PRO  |
| 1   | Z     | 166 | PRO  |
| 1   | 4     | 166 | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | 0     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 19          | 36 |
| 1   | 1     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 19          | 36 |
| 1   | 2     | 142/147 (97%) | 140 (99%) | 2 (1%)   | 59          | 75 |
| 1   | 3     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 19          | 36 |
| 1   | 4     | 142/147 (97%) | 135 (95%) | 7 (5%)   | 22          | 43 |
| 1   | 5     | 142/147 (97%) | 137 (96%) | 5 (4%)   | 32          | 56 |
| 1   | 6     | 142/147 (97%) | 131 (92%) | 11 (8%)  | 12          | 22 |
| 1   | 7     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 19          | 36 |
| 1   | 8     | 142/147 (97%) | 135 (95%) | 7 (5%)   | 22          | 43 |
| 1   | 9     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 19          | 36 |
| 1   | A     | 142/147 (97%) | 132 (93%) | 10 (7%)  | 14          | 26 |
| 1   | B     | 142/147 (97%) | 136 (96%) | 6 (4%)   | 26          | 49 |
| 1   | C     | 143/147 (97%) | 138 (96%) | 5 (4%)   | 32          | 56 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | D     | 142/147 (97%)   | 134 (94%)  | 8 (6%)   | 19          | 36 |
| 1   | E     | 142/147 (97%)   | 134 (94%)  | 8 (6%)   | 19          | 36 |
| 1   | F     | 142/147 (97%)   | 135 (95%)  | 7 (5%)   | 22          | 43 |
| 1   | G     | 142/147 (97%)   | 136 (96%)  | 6 (4%)   | 26          | 49 |
| 1   | H     | 142/147 (97%)   | 132 (93%)  | 10 (7%)  | 14          | 26 |
| 1   | I     | 142/147 (97%)   | 137 (96%)  | 5 (4%)   | 32          | 56 |
| 1   | J     | 142/147 (97%)   | 136 (96%)  | 6 (4%)   | 26          | 49 |
| 1   | K     | 142/147 (97%)   | 133 (94%)  | 9 (6%)   | 16          | 30 |
| 1   | L     | 142/147 (97%)   | 134 (94%)  | 8 (6%)   | 19          | 36 |
| 1   | M     | 142/147 (97%)   | 133 (94%)  | 9 (6%)   | 16          | 30 |
| 1   | N     | 142/147 (97%)   | 134 (94%)  | 8 (6%)   | 19          | 36 |
| 1   | O     | 142/147 (97%)   | 134 (94%)  | 8 (6%)   | 19          | 36 |
| 1   | P     | 142/147 (97%)   | 137 (96%)  | 5 (4%)   | 32          | 56 |
| 1   | Q     | 142/147 (97%)   | 133 (94%)  | 9 (6%)   | 16          | 30 |
| 1   | R     | 142/147 (97%)   | 135 (95%)  | 7 (5%)   | 22          | 43 |
| 1   | S     | 142/147 (97%)   | 132 (93%)  | 10 (7%)  | 14          | 26 |
| 1   | T     | 142/147 (97%)   | 136 (96%)  | 6 (4%)   | 26          | 49 |
| 1   | U     | 142/147 (97%)   | 136 (96%)  | 6 (4%)   | 26          | 49 |
| 1   | V     | 142/147 (97%)   | 137 (96%)  | 5 (4%)   | 32          | 56 |
| 1   | W     | 142/147 (97%)   | 133 (94%)  | 9 (6%)   | 16          | 30 |
| 1   | X     | 142/147 (97%)   | 133 (94%)  | 9 (6%)   | 16          | 30 |
| 1   | Y     | 142/147 (97%)   | 138 (97%)  | 4 (3%)   | 38          | 61 |
| 1   | Z     | 142/147 (97%)   | 134 (94%)  | 8 (6%)   | 19          | 36 |
| All | All   | 5113/5292 (97%) | 4850 (95%) | 263 (5%) | 21          | 40 |

All (263) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 5   | ARG  |
| 1   | 0     | 6   | MET  |
| 1   | 0     | 22  | TYR  |
| 1   | 0     | 79  | GLU  |
| 1   | 0     | 85  | LYS  |
| 1   | 0     | 104 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 110 | GLU  |
| 1   | 0     | 149 | GLN  |
| 1   | 1     | 1   | MET  |
| 1   | 1     | 5   | ARG  |
| 1   | 1     | 6   | MET  |
| 1   | 1     | 15  | ASN  |
| 1   | 1     | 72  | GLU  |
| 1   | 1     | 104 | LEU  |
| 1   | 1     | 133 | SER  |
| 1   | 1     | 149 | GLN  |
| 1   | 2     | 6   | MET  |
| 1   | 2     | 140 | LYS  |
| 1   | 3     | 1   | MET  |
| 1   | 3     | 5   | ARG  |
| 1   | 3     | 49  | GLU  |
| 1   | 3     | 68  | VAL  |
| 1   | 3     | 72  | GLU  |
| 1   | 3     | 79  | GLU  |
| 1   | 3     | 104 | LEU  |
| 1   | 3     | 130 | GLU  |
| 1   | 4     | 1   | MET  |
| 1   | 4     | 6   | MET  |
| 1   | 4     | 15  | ASN  |
| 1   | 4     | 72  | GLU  |
| 1   | 4     | 75  | LYS  |
| 1   | 4     | 104 | LEU  |
| 1   | 4     | 149 | GLN  |
| 1   | 5     | 72  | GLU  |
| 1   | 5     | 79  | GLU  |
| 1   | 5     | 100 | SER  |
| 1   | 5     | 104 | LEU  |
| 1   | 5     | 133 | SER  |
| 1   | 6     | 1   | MET  |
| 1   | 6     | 6   | MET  |
| 1   | 6     | 15  | ASN  |
| 1   | 6     | 22  | TYR  |
| 1   | 6     | 68  | VAL  |
| 1   | 6     | 72  | GLU  |
| 1   | 6     | 83  | PRO  |
| 1   | 6     | 100 | SER  |
| 1   | 6     | 133 | SER  |
| 1   | 6     | 149 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 6     | 154 | LEU  |
| 1   | 7     | 1   | MET  |
| 1   | 7     | 88  | GLU  |
| 1   | 7     | 98  | SER  |
| 1   | 7     | 100 | SER  |
| 1   | 7     | 104 | LEU  |
| 1   | 7     | 112 | LYS  |
| 1   | 7     | 154 | LEU  |
| 1   | 7     | 164 | LYS  |
| 1   | 8     | 1   | MET  |
| 1   | 8     | 6   | MET  |
| 1   | 8     | 20  | SER  |
| 1   | 8     | 104 | LEU  |
| 1   | 8     | 133 | SER  |
| 1   | 8     | 136 | LYS  |
| 1   | 8     | 154 | LEU  |
| 1   | 9     | 1   | MET  |
| 1   | 9     | 5   | ARG  |
| 1   | 9     | 15  | ASN  |
| 1   | 9     | 72  | GLU  |
| 1   | 9     | 78  | LYS  |
| 1   | 9     | 136 | LYS  |
| 1   | 9     | 149 | GLN  |
| 1   | 9     | 165 | LEU  |
| 1   | A     | 1   | MET  |
| 1   | A     | 6   | MET  |
| 1   | A     | 22  | TYR  |
| 1   | A     | 34  | LEU  |
| 1   | A     | 58  | TYR  |
| 1   | A     | 72  | GLU  |
| 1   | A     | 100 | SER  |
| 1   | A     | 110 | GLU  |
| 1   | A     | 138 | LEU  |
| 1   | A     | 149 | GLN  |
| 1   | B     | 5   | ARG  |
| 1   | B     | 34  | LEU  |
| 1   | B     | 72  | GLU  |
| 1   | B     | 104 | LEU  |
| 1   | B     | 149 | GLN  |
| 1   | B     | 154 | LEU  |
| 1   | C     | 1   | MET  |
| 1   | C     | 34  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 49  | GLU  |
| 1   | C     | 149 | GLN  |
| 1   | C     | 154 | LEU  |
| 1   | D     | 6   | MET  |
| 1   | D     | 34  | LEU  |
| 1   | D     | 72  | GLU  |
| 1   | D     | 85  | LYS  |
| 1   | D     | 100 | SER  |
| 1   | D     | 110 | GLU  |
| 1   | D     | 133 | SER  |
| 1   | D     | 149 | GLN  |
| 1   | E     | 1   | MET  |
| 1   | E     | 4   | GLU  |
| 1   | E     | 6   | MET  |
| 1   | E     | 67  | ARG  |
| 1   | E     | 104 | LEU  |
| 1   | E     | 110 | GLU  |
| 1   | E     | 149 | GLN  |
| 1   | E     | 154 | LEU  |
| 1   | F     | 1   | MET  |
| 1   | F     | 6   | MET  |
| 1   | F     | 72  | GLU  |
| 1   | F     | 99  | LYS  |
| 1   | F     | 146 | ASP  |
| 1   | F     | 149 | GLN  |
| 1   | F     | 156 | LYS  |
| 1   | G     | 1   | MET  |
| 1   | G     | 22  | TYR  |
| 1   | G     | 72  | GLU  |
| 1   | G     | 104 | LEU  |
| 1   | G     | 110 | GLU  |
| 1   | G     | 138 | LEU  |
| 1   | H     | 1   | MET  |
| 1   | H     | 4   | GLU  |
| 1   | H     | 6   | MET  |
| 1   | H     | 22  | TYR  |
| 1   | H     | 67  | ARG  |
| 1   | H     | 72  | GLU  |
| 1   | H     | 79  | GLU  |
| 1   | H     | 110 | GLU  |
| 1   | H     | 154 | LEU  |
| 1   | H     | 165 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | I     | 22  | TYR  |
| 1   | I     | 72  | GLU  |
| 1   | I     | 79  | GLU  |
| 1   | I     | 104 | LEU  |
| 1   | I     | 149 | GLN  |
| 1   | J     | 22  | TYR  |
| 1   | J     | 49  | GLU  |
| 1   | J     | 72  | GLU  |
| 1   | J     | 112 | LYS  |
| 1   | J     | 149 | GLN  |
| 1   | J     | 165 | LEU  |
| 1   | K     | 1   | MET  |
| 1   | K     | 6   | MET  |
| 1   | K     | 15  | ASN  |
| 1   | K     | 33  | ASP  |
| 1   | K     | 72  | GLU  |
| 1   | K     | 100 | SER  |
| 1   | K     | 104 | LEU  |
| 1   | K     | 149 | GLN  |
| 1   | K     | 165 | LEU  |
| 1   | L     | 1   | MET  |
| 1   | L     | 6   | MET  |
| 1   | L     | 37  | GLU  |
| 1   | L     | 72  | GLU  |
| 1   | L     | 75  | LYS  |
| 1   | L     | 104 | LEU  |
| 1   | L     | 112 | LYS  |
| 1   | L     | 149 | GLN  |
| 1   | M     | 1   | MET  |
| 1   | M     | 4   | GLU  |
| 1   | M     | 6   | MET  |
| 1   | M     | 22  | TYR  |
| 1   | M     | 49  | GLU  |
| 1   | M     | 68  | VAL  |
| 1   | M     | 72  | GLU  |
| 1   | M     | 149 | GLN  |
| 1   | M     | 153 | MET  |
| 1   | N     | 6   | MET  |
| 1   | N     | 22  | TYR  |
| 1   | N     | 65  | ASN  |
| 1   | N     | 72  | GLU  |
| 1   | N     | 130 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 133 | SER  |
| 1   | N     | 146 | ASP  |
| 1   | N     | 149 | GLN  |
| 1   | O     | 1   | MET  |
| 1   | O     | 11  | ASN  |
| 1   | O     | 49  | GLU  |
| 1   | O     | 99  | LYS  |
| 1   | O     | 100 | SER  |
| 1   | O     | 147 | SER  |
| 1   | O     | 164 | LYS  |
| 1   | O     | 165 | LEU  |
| 1   | P     | 98  | SER  |
| 1   | P     | 100 | SER  |
| 1   | P     | 104 | LEU  |
| 1   | P     | 149 | GLN  |
| 1   | P     | 154 | LEU  |
| 1   | Q     | 1   | MET  |
| 1   | Q     | 5   | ARG  |
| 1   | Q     | 75  | LYS  |
| 1   | Q     | 100 | SER  |
| 1   | Q     | 104 | LEU  |
| 1   | Q     | 110 | GLU  |
| 1   | Q     | 133 | SER  |
| 1   | Q     | 149 | GLN  |
| 1   | Q     | 156 | LYS  |
| 1   | R     | 1   | MET  |
| 1   | R     | 6   | MET  |
| 1   | R     | 20  | SER  |
| 1   | R     | 72  | GLU  |
| 1   | R     | 111 | GLU  |
| 1   | R     | 133 | SER  |
| 1   | R     | 138 | LEU  |
| 1   | S     | 1   | MET  |
| 1   | S     | 5   | ARG  |
| 1   | S     | 34  | LEU  |
| 1   | S     | 49  | GLU  |
| 1   | S     | 83  | PRO  |
| 1   | S     | 99  | LYS  |
| 1   | S     | 111 | GLU  |
| 1   | S     | 147 | SER  |
| 1   | S     | 149 | GLN  |
| 1   | S     | 152 | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 34  | LEU  |
| 1   | T     | 72  | GLU  |
| 1   | T     | 138 | LEU  |
| 1   | T     | 143 | PHE  |
| 1   | T     | 152 | PHE  |
| 1   | T     | 154 | LEU  |
| 1   | U     | 1   | MET  |
| 1   | U     | 34  | LEU  |
| 1   | U     | 72  | GLU  |
| 1   | U     | 104 | LEU  |
| 1   | U     | 133 | SER  |
| 1   | U     | 149 | GLN  |
| 1   | V     | 1   | MET  |
| 1   | V     | 6   | MET  |
| 1   | V     | 136 | LYS  |
| 1   | V     | 149 | GLN  |
| 1   | V     | 154 | LEU  |
| 1   | W     | 1   | MET  |
| 1   | W     | 34  | LEU  |
| 1   | W     | 72  | GLU  |
| 1   | W     | 79  | GLU  |
| 1   | W     | 110 | GLU  |
| 1   | W     | 143 | PHE  |
| 1   | W     | 149 | GLN  |
| 1   | W     | 152 | PHE  |
| 1   | W     | 154 | LEU  |
| 1   | X     | 1   | MET  |
| 1   | X     | 6   | MET  |
| 1   | X     | 49  | GLU  |
| 1   | X     | 72  | GLU  |
| 1   | X     | 99  | LYS  |
| 1   | X     | 104 | LEU  |
| 1   | X     | 110 | GLU  |
| 1   | X     | 130 | GLU  |
| 1   | X     | 149 | GLN  |
| 1   | Y     | 1   | MET  |
| 1   | Y     | 5   | ARG  |
| 1   | Y     | 149 | GLN  |
| 1   | Y     | 154 | LEU  |
| 1   | Z     | 1   | MET  |
| 1   | Z     | 6   | MET  |
| 1   | Z     | 11  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Z     | 72  | GLU  |
| 1   | Z     | 99  | LYS  |
| 1   | Z     | 104 | LEU  |
| 1   | Z     | 133 | SER  |
| 1   | Z     | 149 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 125 | ASN  |
| 1   | 0     | 127 | GLN  |
| 1   | 0     | 149 | GLN  |
| 1   | 1     | 149 | GLN  |
| 1   | 2     | 59  | ASN  |
| 1   | 2     | 127 | GLN  |
| 1   | 3     | 15  | ASN  |
| 1   | 4     | 125 | ASN  |
| 1   | 4     | 127 | GLN  |
| 1   | 4     | 149 | GLN  |
| 1   | 5     | 127 | GLN  |
| 1   | 6     | 125 | ASN  |
| 1   | 6     | 149 | GLN  |
| 1   | 8     | 149 | GLN  |
| 1   | 9     | 15  | ASN  |
| 1   | 9     | 65  | ASN  |
| 1   | 9     | 127 | GLN  |
| 1   | 9     | 149 | GLN  |
| 1   | A     | 127 | GLN  |
| 1   | C     | 65  | ASN  |
| 1   | C     | 125 | ASN  |
| 1   | C     | 149 | GLN  |
| 1   | D     | 149 | GLN  |
| 1   | E     | 149 | GLN  |
| 1   | H     | 149 | GLN  |
| 1   | I     | 11  | ASN  |
| 1   | I     | 149 | GLN  |
| 1   | J     | 127 | GLN  |
| 1   | J     | 149 | GLN  |
| 1   | K     | 15  | ASN  |
| 1   | K     | 149 | GLN  |
| 1   | L     | 127 | GLN  |
| 1   | M     | 13  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 41  | ASN  |
| 1   | M     | 127 | GLN  |
| 1   | M     | 149 | GLN  |
| 1   | N     | 65  | ASN  |
| 1   | N     | 127 | GLN  |
| 1   | N     | 149 | GLN  |
| 1   | O     | 11  | ASN  |
| 1   | O     | 149 | GLN  |
| 1   | P     | 59  | ASN  |
| 1   | P     | 149 | GLN  |
| 1   | Q     | 149 | GLN  |
| 1   | R     | 11  | ASN  |
| 1   | R     | 149 | GLN  |
| 1   | S     | 127 | GLN  |
| 1   | T     | 127 | GLN  |
| 1   | V     | 127 | GLN  |
| 1   | V     | 149 | GLN  |
| 1   | W     | 59  | ASN  |
| 1   | W     | 125 | ASN  |
| 1   | W     | 127 | GLN  |
| 1   | W     | 149 | GLN  |
| 1   | Y     | 125 | ASN  |
| 1   | Y     | 127 | GLN  |
| 1   | Y     | 149 | GLN  |
| 1   | Z     | 11  | ASN  |
| 1   | Z     | 15  | ASN  |

### 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 76 ligands modelled in this entry, 36 are monoatomic - leaving 40 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   | SO4  | V     | 1668 | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.38 | 0        |
| 3   | SO4  | A     | 1169 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.30 | 0        |
| 3   | SO4  | V     | 1669 | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.36 | 0        |
| 3   | SO4  | B     | 1168 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.29 | 0        |
| 3   | SO4  | X     | 1668 | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.48 | 0        |
| 3   | SO4  | C     | 1169 | -    | 4,4,4        | 0.21 | 0        | 6,6,6       | 0.37 | 0        |
| 3   | SO4  | H     | 1168 | -    | 4,4,4        | 0.36 | 0        | 6,6,6       | 0.44 | 0        |
| 3   | SO4  | 3     | 1669 | -    | 4,4,4        | 0.41 | 0        | 6,6,6       | 0.44 | 0        |
| 3   | SO4  | 3     | 1668 | -    | 4,4,4        | 0.31 | 0        | 6,6,6       | 0.20 | 0        |
| 3   | SO4  | A     | 1168 | -    | 4,4,4        | 0.38 | 0        | 6,6,6       | 0.33 | 0        |
| 3   | SO4  | F     | 1168 | -    | 4,4,4        | 0.19 | 0        | 6,6,6       | 0.35 | 0        |
| 3   | SO4  | G     | 1169 | -    | 4,4,4        | 0.32 | 0        | 6,6,6       | 0.20 | 0        |
| 3   | SO4  | Q     | 1168 | -    | 4,4,4        | 0.28 | 0        | 6,6,6       | 0.39 | 0        |
| 3   | SO4  | T     | 1668 | -    | 4,4,4        | 0.50 | 0        | 6,6,6       | 0.65 | 0        |
| 3   | SO4  | O     | 1168 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.21 | 0        |
| 3   | SO4  | W     | 1668 | -    | 4,4,4        | 0.39 | 0        | 6,6,6       | 0.54 | 0        |
| 3   | SO4  | G     | 1168 | -    | 4,4,4        | 0.40 | 0        | 6,6,6       | 0.34 | 0        |
| 3   | SO4  | 4     | 1668 | -    | 4,4,4        | 0.38 | 0        | 6,6,6       | 0.29 | 0        |
| 3   | SO4  | 8     | 1668 | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.25 | 0        |
| 3   | SO4  | I     | 1168 | -    | 4,4,4        | 0.21 | 0        | 6,6,6       | 0.58 | 0        |
| 3   | SO4  | A     | 1170 | -    | 4,4,4        | 0.42 | 0        | 6,6,6       | 0.35 | 0        |
| 3   | SO4  | M     | 1168 | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.23 | 0        |
| 3   | SO4  | S     | 1668 | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.32 | 0        |
| 3   | SO4  | 2     | 1668 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.37 | 0        |
| 3   | SO4  | S     | 1669 | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.40 | 0        |
| 3   | SO4  | J     | 1168 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.50 | 0        |
| 3   | SO4  | 2     | 1669 | -    | 4,4,4        | 0.29 | 0        | 6,6,6       | 0.27 | 0        |
| 3   | SO4  | 1     | 1668 | -    | 4,4,4        | 0.28 | 0        | 6,6,6       | 0.28 | 0        |
| 3   | SO4  | 6     | 1668 | -    | 4,4,4        | 0.38 | 0        | 6,6,6       | 0.46 | 0        |
| 3   | SO4  | 1     | 1669 | -    | 4,4,4        | 0.27 | 0        | 6,6,6       | 0.64 | 0        |
| 3   | SO4  | Z     | 1668 | -    | 4,4,4        | 0.31 | 0        | 6,6,6       | 0.27 | 0        |
| 3   | SO4  | 5     | 1668 | -    | 4,4,4        | 0.26 | 0        | 6,6,6       | 0.42 | 0        |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | SO4  | C     | 1168 | -    | 4,4,4        | 0.25 | 0        | 6,6,6       | 0.21 | 0        |
| 3   | SO4  | R     | 1168 | -    | 4,4,4        | 0.28 | 0        | 6,6,6       | 0.28 | 0        |
| 3   | SO4  | W     | 1669 | -    | 4,4,4        | 0.33 | 0        | 6,6,6       | 0.21 | 0        |
| 3   | SO4  | J     | 1170 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.75 | 0        |
| 3   | SO4  | 7     | 1668 | -    | 4,4,4        | 0.30 | 0        | 6,6,6       | 0.27 | 0        |
| 3   | SO4  | E     | 1168 | -    | 4,4,4        | 0.35 | 0        | 6,6,6       | 0.60 | 0        |
| 3   | SO4  | K     | 1168 | -    | 4,4,4        | 0.31 | 0        | 6,6,6       | 0.31 | 0        |
| 3   | SO4  | J     | 1169 | -    | 4,4,4        | 0.23 | 0        | 6,6,6       | 0.39 | 0        |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.