



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:16 am BST

PDB ID : 2JD7  
Title : Crystal Structure of the Fe-soaked Ferritin from the Hyperthermophilic Archaeal Anaerobe *Pyrococcus furiosus*  
Authors : Tatur, J.; Hagen, W.R.; Matias, P.M.  
Deposited on : 2007-01-05  
Resolution : 2.80 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

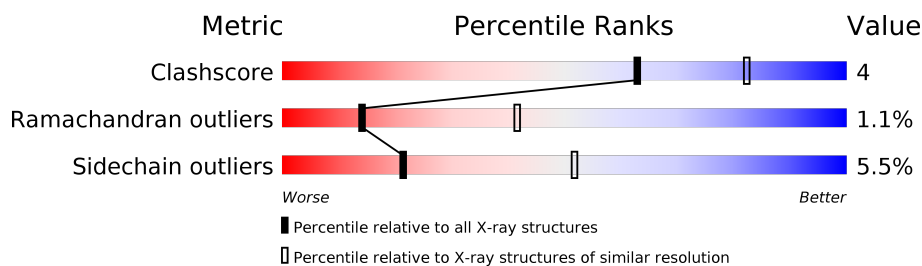
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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            | 141614                      | 3569 (2.80-2.80)                                      |
| Ramachandran outliers | 138981                      | 3498 (2.80-2.80)                                      |
| Sidechain outliers    | 138945                      | 3500 (2.80-2.80)                                      |


























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 on 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    | 79% 16% . .      |
| 1   | 1     | 174    | 79% 17% .        |
| 1   | 2     | 174    | 81% 12% . .      |
| 1   | 3     | 174    | 82% 12% . .      |
| 1   | 4     | 174    | 83% 12% . .      |
| 1   | 5     | 174    | 90% 6% . .       |
| 1   | 6     | 174    | 85% 10% . .      |
| 1   | 7     | 174    | 79% 13% . .      |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | 8     | 174    |  83% 11% . .   |
| 1   | 9     | 174    |  80% 14% . .   |
| 1   | A     | 174    |  84% 10% . .   |
| 1   | B     | 174    |  82% 12% . .   |
| 1   | C     | 174    |  84% 11% . .   |
| 1   | D     | 174    |  84% 10% . .   |
| 1   | E     | 174    |  82% 12% . .   |
| 1   | F     | 174    |  81% 13% . .   |
| 1   | G     | 174    |  88% 7% . .    |
| 1   | H     | 174    |  76% 17% . .   |
| 1   | I     | 174    |  78% 15% . .   |
| 1   | J     | 174    |  90% 5% . .    |
| 1   | K     | 174    |  85% 10% . . |
| 1   | L     | 174    |  87% 9% . .  |
| 1   | M     | 174    |  75% 21% . . |
| 1   | N     | 174    |  83% 10% . . |
| 1   | O     | 174    |  74% 20% . . |
| 1   | P     | 174    |  76% 18% . . |
| 1   | Q     | 174    |  82% 13% . . |
| 1   | R     | 174    |  84% 10% . . |
| 1   | S     | 174    |  84% 11% . . |
| 1   | T     | 174    |  85% 10% . . |
| 1   | U     | 174    |  88% 7% . .  |
| 1   | V     | 174    |  82% 11% . . |
| 1   | W     | 174    |  84% 10% . . |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | X     | 174    | <div><div></div><div>87%</div><div>9%</div><div></div><div></div></div>  |
| 1   | Y     | 174    | <div><div></div><div>81%</div><div>14%</div><div></div><div></div></div> |
| 1   | Z     | 174    | <div><div></div><div>80%</div><div>16%</div><div></div><div></div></div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50409 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       | 0       | 0     |
|     |       |          | 1383  | 897 | 220 | 261 | 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       | 1       | 0     |
|     |       |          | 1388  | 900 | 221 | 262 | 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       | 1       | 0     |
|     |       |          | 1388  | 900 | 221 | 262 | 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       | 1       | 0     |
|     |       |          | 1388  | 900 | 221 | 262 | 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 (three-letter code: FE) (formula: Fe).

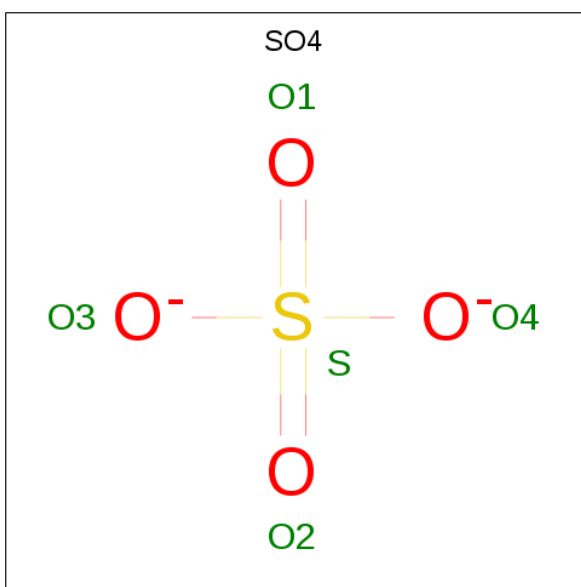
| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | P     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | K     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | B     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | 6     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | W     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | N     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | X     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | 2     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | S     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | J     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | E     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | V     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | A     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | 5     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | R     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | M     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | 1     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | D     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | I     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | Z     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | 4     | 3        | Total Fe<br>3 3 | 0       | 0       |
| 2   | U     | 3        | Total Fe<br>3 3 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | 9     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | L     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | 0     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | G     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | Q     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | H     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | C     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | 7     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | T     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | 8     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | O     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | Y     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | 3     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |
| 2   | F     | 3        | Total<br>3 | Fe<br>3 | 0       | 0       |

- Molecule 3 is SULFATE ION (three-letter code: 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   | 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   | 8     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 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   | C     | 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 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | I     | 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   | O     | 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   | T     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | V     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | V     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | W     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | Y     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | Y     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | 0     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 4   | 1     | 10       | Total | O  | 0       | 0       |
|     |       |          | 10    | 10 |         |         |
| 4   | 2     | 7        | Total | O  | 0       | 0       |
|     |       |          | 7     | 7  |         |         |
| 4   | 3     | 15       | Total | O  | 0       | 0       |
|     |       |          | 15    | 15 |         |         |
| 4   | 4     | 8        | Total | O  | 0       | 0       |
|     |       |          | 8     | 8  |         |         |
| 4   | 5     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |
| 4   | 6     | 8        | Total | O  | 0       | 0       |
|     |       |          | 8     | 8  |         |         |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4   | 7     | 11       | Total O<br>11 11 | 0       | 0       |
| 4   | 8     | 9        | Total O<br>9 9   | 0       | 0       |
| 4   | 9     | 7        | Total O<br>7 7   | 0       | 0       |
| 4   | A     | 13       | Total O<br>13 13 | 0       | 0       |
| 4   | B     | 17       | Total O<br>17 17 | 0       | 0       |
| 4   | C     | 8        | Total O<br>8 8   | 0       | 0       |
| 4   | D     | 16       | Total O<br>16 16 | 0       | 0       |
| 4   | E     | 18       | Total O<br>18 18 | 0       | 0       |
| 4   | F     | 21       | Total O<br>21 21 | 0       | 0       |
| 4   | G     | 14       | Total O<br>14 14 | 0       | 0       |
| 4   | H     | 2        | Total O<br>2 2   | 0       | 0       |
| 4   | I     | 5        | Total O<br>5 5   | 0       | 0       |
| 4   | J     | 16       | Total O<br>16 16 | 0       | 0       |
| 4   | K     | 4        | Total O<br>4 4   | 0       | 0       |
| 4   | L     | 9        | Total O<br>9 9   | 0       | 0       |
| 4   | M     | 11       | Total O<br>11 11 | 0       | 0       |
| 4   | N     | 3        | Total O<br>3 3   | 0       | 0       |
| 4   | O     | 5        | Total O<br>5 5   | 0       | 0       |
| 4   | P     | 5        | Total O<br>5 5   | 0       | 0       |
| 4   | Q     | 9        | Total O<br>9 9   | 0       | 0       |
| 4   | R     | 5        | Total O<br>5 5   | 0       | 0       |

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| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | S     | 17       | Total | O  | 0       | 0       |
|     |       |          | 17    | 17 |         |         |
| 4   | T     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 4   | U     | 18       | Total | O  | 0       | 0       |
|     |       |          | 18    | 18 |         |         |
| 4   | V     | 13       | Total | O  | 0       | 0       |
|     |       |          | 13    | 13 |         |         |
| 4   | W     | 9        | Total | O  | 0       | 0       |
|     |       |          | 9     | 9  |         |         |
| 4   | X     | 14       | Total | O  | 0       | 0       |
|     |       |          | 14    | 14 |         |         |
| 4   | Y     | 11       | Total | O  | 0       | 0       |
|     |       |          | 11    | 11 |         |         |
| 4   | Z     | 5        | Total | O  | 0       | 0       |
|     |       |          | 5     | 5  |         |         |

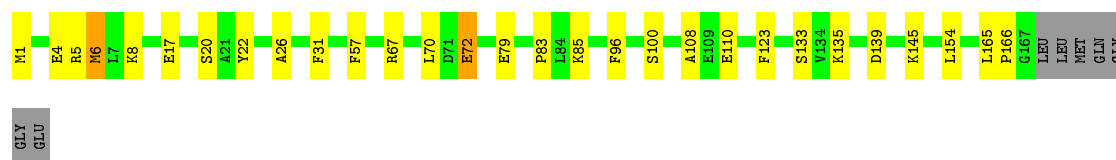
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

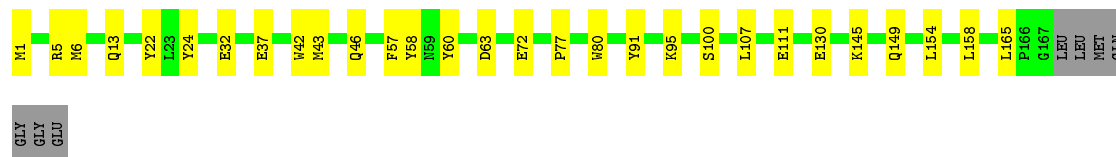
#### • Molecule 1: FERRITIN HOMOLOG

Chain 0: 




#### • Molecule 1: FERRITIN HOMOLOG

Chain 1: 




#### • Molecule 1: FERRITIN HOMOLOG

Chain 2: 




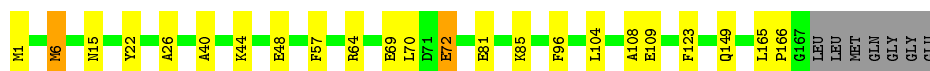
#### • Molecule 1: FERRITIN HOMOLOG

Chain 3: 



#### • Molecule 1: FERRITIN HOMOLOG

Chain 4: 



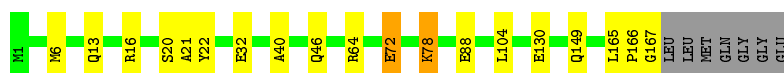
- Molecule 1: FERRITIN HOMOLOG

Chain 5: 90% 6% . .



- Molecule 1: FERRITIN HOMOLOG

Chain 6: 85% 10% . .



- Molecule 1: FERRITIN HOMOLOG

Chain 7: 79% 13% . .



- Molecule 1: FERRITIN HOMOLOG

Chain 8: 83% 11% . .



- Molecule 1: FERRITIN HOMOLOG

Chain 9: 80% 14% . .



- Molecule 1: FERRITIN HOMOLOG

Chain A: 84% 10% . .



- Molecule 1: FERRITIN HOMOLOG

Chain B: 82% 12% . .



• Molecule 1: FERRITIN HOMOLOG

Chain C: 84% 11% . .



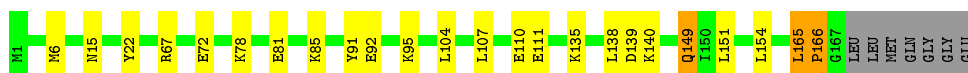
• Molecule 1: FERRITIN HOMOLOG

Chain D: 84% 10% . .



• Molecule 1: FERRITIN HOMOLOG

Chain E: 82% 12% . .



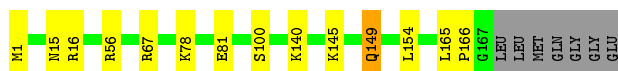
• Molecule 1: FERRITIN HOMOLOG

Chain F: 81% 13% . .



• Molecule 1: FERRITIN HOMOLOG

Chain G: 88% 7% . .



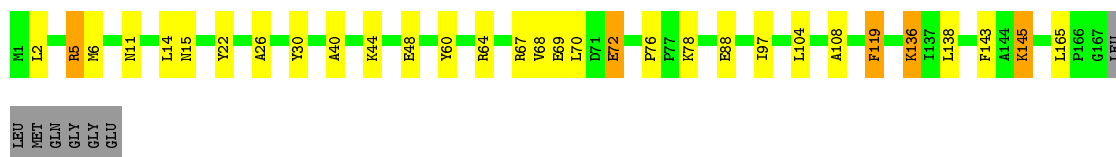
• Molecule 1: FERRITIN HOMOLOG

Chain H: 76% 17% . .



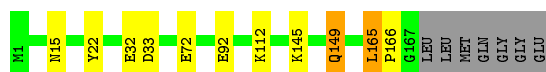
• Molecule 1: FERRITIN HOMOLOG

Chain I: 78% 15% . .



• Molecule 1: FERRITIN HOMOLOG

Chain J: 90% 5% . .



• Molecule 1: FERRITIN HOMOLOG

Chain K: 85% 10% . .



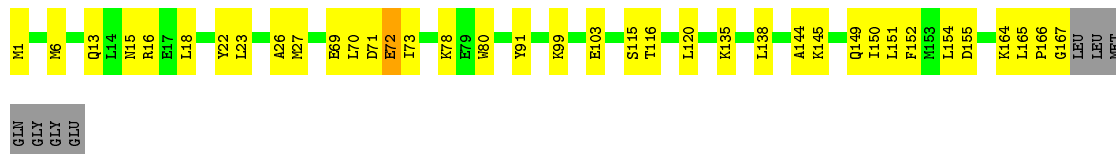
• Molecule 1: FERRITIN HOMOLOG

Chain L: 87% 9% . .



• Molecule 1: FERRITIN HOMOLOG

Chain M: 75% 21% . .



• Molecule 1: FERRITIN HOMOLOG

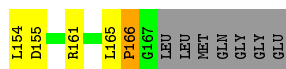
Chain N: 83% 10% . .



• Molecule 1: FERRITIN HOMOLOG

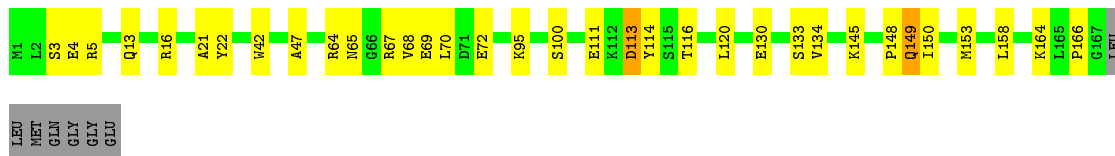
Chain O: 74% 20% . .





## ● Molecule 1: FERRITIN HOMOLOG

Chain P: 76% 18% . .



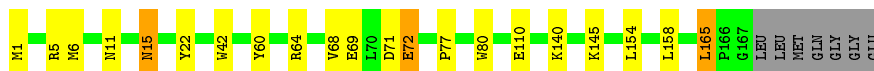
## ● Molecule 1: FERRITIN HOMOLOG

Chain Q: 82% 13% . .



## ● Molecule 1: FERRITIN HOMOLOG

Chain R: 84% 10% . .



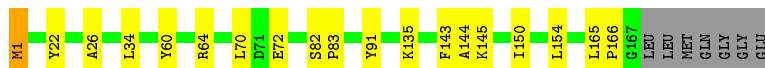
## ● Molecule 1: FERRITIN HOMOLOG

Chain S: 84% 11% . .



## ● Molecule 1: FERRITIN HOMOLOG

Chain T: 85% 10% . .



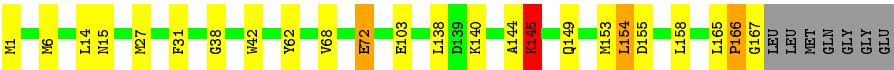
## ● Molecule 1: FERRITIN HOMOLOG

Chain U: 88% 7% . .

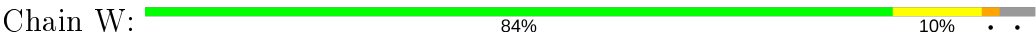


## ● Molecule 1: FERRITIN HOMOLOG

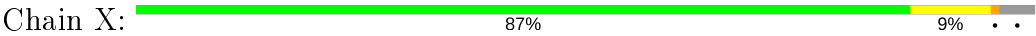
Chain V: 82% 11% . . .



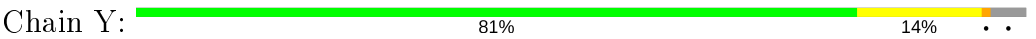
• Molecule 1: FERRITIN HOMOLOG



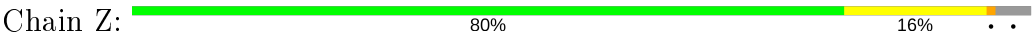
• Molecule 1: FERRITIN HOMOLOG



• 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, $\alpha$ , $\beta$ , $\gamma$ | 254.30 Å   342.88 Å   266.22 Å<br>90.00°   90.00°   90.00° | Depositor |
| Resolution (Å)   | 204.12 – 2.80  | Depositor |
| % Data completeness<br>(in resolution range)             | 99.1 (204.12-2.80)   | Depositor |
| $R_{merge}$  | 0.08   | Depositor |
| $R_{sym}$  | (Not available)  | Depositor |
| Refinement program                                       | REFMAC 5.3.0021  | Depositor |
| R, $R_{free}$  | 0.199 , 0.250  | Depositor |
| Estimated twinning fraction                              | No twinning to report.                                     | Xtriage   |
| Total number of atoms                                    | 50409  | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 39.0   | 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: FE, SO4

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     | 0.69         | 0/1417        | 0.72        | 0/1908        |
| 1   | 1     | 0.70         | 0/1417        | 0.70        | 0/1908        |
| 1   | 2     | 0.68         | 0/1417        | 0.69        | 0/1908        |
| 1   | 3     | 0.74         | 0/1417        | 0.76        | 0/1908        |
| 1   | 4     | 0.73         | 0/1417        | 0.72        | 0/1908        |
| 1   | 5     | 0.68         | 0/1417        | 0.67        | 0/1908        |
| 1   | 6     | 0.67         | 0/1417        | 0.68        | 0/1908        |
| 1   | 7     | 0.71         | 0/1417        | 0.69        | 0/1908        |
| 1   | 8     | 0.74         | 0/1417        | 0.72        | 0/1908        |
| 1   | 9     | 0.68         | 0/1417        | 0.68        | 0/1908        |
| 1   | A     | 0.77         | 0/1417        | 0.75        | 0/1908        |
| 1   | B     | 0.82         | 1/1417 (0.1%) | 0.80        | 2/1908 (0.1%) |
| 1   | C     | 0.78         | 0/1417        | 0.76        | 0/1908        |
| 1   | D     | 0.76         | 0/1417        | 0.80        | 1/1908 (0.1%) |
| 1   | E     | 0.74         | 0/1417        | 0.74        | 0/1908        |
| 1   | F     | 0.78         | 0/1417        | 0.73        | 0/1908        |
| 1   | G     | 0.77         | 0/1425        | 0.76        | 1/1919 (0.1%) |
| 1   | H     | 0.68         | 0/1417        | 0.69        | 0/1908        |
| 1   | I     | 0.75         | 1/1417 (0.1%) | 0.75        | 0/1908        |
| 1   | J     | 0.74         | 1/1417 (0.1%) | 0.71        | 0/1908        |
| 1   | K     | 0.67         | 0/1417        | 0.71        | 0/1908        |
| 1   | L     | 0.71         | 0/1417        | 0.71        | 0/1908        |
| 1   | M     | 0.71         | 0/1417        | 0.73        | 0/1908        |
| 1   | N     | 0.69         | 0/1417        | 0.69        | 0/1908        |
| 1   | O     | 0.72         | 0/1417        | 0.72        | 0/1908        |
| 1   | P     | 0.72         | 0/1417        | 0.73        | 2/1908 (0.1%) |
| 1   | Q     | 0.75         | 1/1417 (0.1%) | 0.71        | 0/1908        |
| 1   | R     | 0.65         | 0/1417        | 0.65        | 0/1908        |
| 1   | S     | 0.76         | 1/1417 (0.1%) | 0.75        | 0/1908        |
| 1   | T     | 0.79         | 0/1425        | 0.75        | 0/1919        |
| 1   | U     | 0.80         | 0/1417        | 0.74        | 0/1908        |
| 1   | V     | 0.78         | 0/1417        | 0.78        | 0/1908        |

| Mol | Chain | Bond lengths |                | Bond angles |                |
|-----|-------|--------------|----------------|-------------|----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5        |
| 1   | W     | 0.84         | 0/1425         | 0.80        | 0/1919         |
| 1   | X     | 0.73         | 0/1417         | 0.73        | 0/1908         |
| 1   | Y     | 0.77         | 0/1417         | 0.78        | 1/1908 (0.1%)  |
| 1   | Z     | 0.65         | 0/1417         | 0.69        | 0/1908         |
| All | All   | 0.73         | 5/51036 (0.0%) | 0.73        | 7/68721 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 1                   |
| 1   | E     | 0                   | 1                   |
| 1   | U     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | Q     | 92  | GLU  | CG-CD | 6.07 | 1.61        | 1.51     |
| 1   | J     | 92  | GLU  | CG-CD | 5.89 | 1.60        | 1.51     |
| 1   | S     | 4   | GLU  | CG-CD | 5.54 | 1.60        | 1.51     |
| 1   | B     | 81  | GLU  | CG-CD | 5.49 | 1.60        | 1.51     |
| 1   | I     | 15  | ASN  | CB-CG | 5.38 | 1.63        | 1.51     |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 64  | ARG  | NE-CZ-NH2 | -7.66 | 116.47      | 120.30   |
| 1   | B     | 64  | ARG  | NE-CZ-NH1 | 6.32  | 123.46      | 120.30   |
| 1   | D     | 5   | ARG  | NE-CZ-NH2 | -5.96 | 117.32      | 120.30   |
| 1   | P     | 113 | ASP  | CB-CG-OD1 | 5.51  | 123.26      | 118.30   |
| 1   | P     | 67  | ARG  | NE-CZ-NH1 | 5.27  | 122.93      | 120.30   |
| 1   | Y     | 56  | ARG  | NE-CZ-NH2 | -5.07 | 117.77      | 120.30   |
| 1   | G     | 16  | ARG  | NE-CZ-NH2 | -5.02 | 117.79      | 120.30   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 78  | LYS  | Peptide |
| 1   | E     | 78  | LYS  | Peptide |
| 1   | U     | 1   | MET  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 1383  | 0        | 1352     | 14      | 0            |
| 1   | 1     | 1383  | 0        | 1352     | 12      | 0            |
| 1   | 2     | 1383  | 0        | 1352     | 15      | 0            |
| 1   | 3     | 1383  | 0        | 1352     | 14      | 0            |
| 1   | 4     | 1383  | 0        | 1352     | 14      | 0            |
| 1   | 5     | 1383  | 0        | 1352     | 7       | 0            |
| 1   | 6     | 1383  | 0        | 1352     | 13      | 0            |
| 1   | 7     | 1383  | 0        | 1352     | 18      | 0            |
| 1   | 8     | 1383  | 0        | 1352     | 8       | 0            |
| 1   | 9     | 1383  | 0        | 1352     | 14      | 0            |
| 1   | A     | 1383  | 0        | 1352     | 8       | 0            |
| 1   | B     | 1383  | 0        | 1352     | 16      | 0            |
| 1   | C     | 1383  | 0        | 1352     | 12      | 0            |
| 1   | D     | 1383  | 0        | 1352     | 9       | 0            |
| 1   | E     | 1383  | 0        | 1352     | 13      | 0            |
| 1   | F     | 1383  | 0        | 1352     | 13      | 0            |
| 1   | G     | 1388  | 0        | 1358     | 9       | 0            |
| 1   | H     | 1383  | 0        | 1352     | 24      | 0            |
| 1   | I     | 1383  | 0        | 1352     | 22      | 0            |
| 1   | J     | 1383  | 0        | 1352     | 5       | 0            |
| 1   | K     | 1383  | 0        | 1352     | 8       | 0            |
| 1   | L     | 1383  | 0        | 1352     | 8       | 0            |
| 1   | M     | 1383  | 0        | 1352     | 20      | 0            |
| 1   | N     | 1383  | 0        | 1352     | 19      | 0            |
| 1   | O     | 1383  | 0        | 1352     | 29      | 0            |
| 1   | P     | 1383  | 0        | 1352     | 22      | 0            |
| 1   | Q     | 1383  | 0        | 1352     | 10      | 0            |
| 1   | R     | 1383  | 0        | 1352     | 10      | 0            |
| 1   | S     | 1383  | 0        | 1352     | 8       | 0            |
| 1   | T     | 1388  | 0        | 1358     | 10      | 0            |
| 1   | U     | 1383  | 0        | 1352     | 6       | 0            |

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

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | 2     | 5     | 0        | 0        | 0       | 0            |
| 3   | 3     | 10    | 0        | 0        | 0       | 0            |
| 3   | 8     | 5     | 0        | 0        | 0       | 0            |
| 3   | A     | 5     | 0        | 0        | 0       | 0            |
| 3   | B     | 10    | 0        | 0        | 0       | 0            |
| 3   | C     | 15    | 0        | 0        | 0       | 0            |
| 3   | G     | 10    | 0        | 0        | 0       | 0            |
| 3   | H     | 5     | 0        | 0        | 0       | 0            |
| 3   | I     | 10    | 0        | 0        | 0       | 0            |
| 3   | J     | 5     | 0        | 0        | 0       | 0            |
| 3   | O     | 5     | 0        | 0        | 0       | 0            |
| 3   | R     | 5     | 0        | 0        | 0       | 0            |
| 3   | S     | 5     | 0        | 0        | 0       | 0            |
| 3   | T     | 5     | 0        | 0        | 0       | 0            |
| 3   | V     | 10    | 0        | 0        | 0       | 0            |
| 3   | W     | 5     | 0        | 0        | 0       | 0            |
| 3   | Y     | 10    | 0        | 0        | 1       | 0            |
| 4   | 0     | 7     | 0        | 0        | 0       | 0            |
| 4   | 1     | 10    | 0        | 0        | 0       | 0            |
| 4   | 2     | 7     | 0        | 0        | 1       | 0            |
| 4   | 3     | 15    | 0        | 0        | 2       | 0            |
| 4   | 4     | 8     | 0        | 0        | 0       | 0            |
| 4   | 5     | 5     | 0        | 0        | 0       | 0            |
| 4   | 6     | 8     | 0        | 0        | 0       | 0            |
| 4   | 7     | 11    | 0        | 0        | 0       | 0            |
| 4   | 8     | 9     | 0        | 0        | 0       | 0            |
| 4   | 9     | 7     | 0        | 0        | 0       | 0            |
| 4   | A     | 13    | 0        | 0        | 1       | 0            |
| 4   | B     | 17    | 0        | 0        | 2       | 0            |
| 4   | C     | 8     | 0        | 0        | 1       | 0            |
| 4   | D     | 16    | 0        | 0        | 1       | 0            |
| 4   | E     | 18    | 0        | 0        | 2       | 0            |
| 4   | F     | 21    | 0        | 0        | 1       | 0            |
| 4   | G     | 14    | 0        | 0        | 1       | 0            |
| 4   | H     | 2     | 0        | 0        | 2       | 0            |
| 4   | I     | 5     | 0        | 0        | 0       | 0            |
| 4   | J     | 16    | 0        | 0        | 1       | 0            |
| 4   | K     | 4     | 0        | 0        | 1       | 0            |
| 4   | L     | 9     | 0        | 0        | 1       | 0            |
| 4   | M     | 11    | 0        | 0        | 0       | 0            |
| 4   | N     | 3     | 0        | 0        | 0       | 0            |
| 4   | O     | 5     | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | P     | 5     | 0        | 0        | 0       | 0            |
| 4   | Q     | 9     | 0        | 0        | 0       | 0            |
| 4   | R     | 5     | 0        | 0        | 0       | 0            |
| 4   | S     | 17    | 0        | 0        | 1       | 0            |
| 4   | T     | 13    | 0        | 0        | 0       | 0            |
| 4   | U     | 18    | 0        | 0        | 1       | 0            |
| 4   | V     | 13    | 0        | 0        | 2       | 0            |
| 4   | W     | 9     | 0        | 0        | 0       | 0            |
| 4   | X     | 14    | 0        | 0        | 1       | 0            |
| 4   | Y     | 11    | 0        | 0        | 0       | 0            |
| 4   | Z     | 5     | 0        | 0        | 0       | 0            |
| All | All   | 50409 | 0        | 48690    | 417     | 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 (417) 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:S:15:ASN:HB3   | 4:S:2004:HOH:O   | 1.48                     | 1.11              |
| 1:A:2:LEU:O      | 1:A:3:SER:HB3    | 1.50                     | 1.07              |
| 1:V:15:ASN:HB3   | 4:V:2002:HOH:O   | 1.51                     | 1.06              |
| 1:5:69:GLU:HG3   | 1:N:78:LYS:HD2   | 1.36                     | 1.05              |
| 1:B:15:ASN:HB3   | 4:B:2001:HOH:O   | 1.55                     | 1.05              |
| 1:H:15:ASN:HB3   | 4:H:2001:HOH:O   | 1.66                     | 0.95              |
| 1:G:166:PRO:HB2  | 4:G:2014:HOH:O   | 1.63                     | 0.95              |
| 1:4:69:GLU:HG3   | 1:M:78:LYS:HD2   | 1.49                     | 0.95              |
| 1:N:149:GLN:HE21 | 1:N:149:GLN:H    | 1.16                     | 0.92              |
| 1:N:56:ARG:HG2   | 1:N:56:ARG:HH11  | 1.34                     | 0.92              |
| 1:Z:81:GLU:H     | 1:Z:85:LYS:HD2   | 1.34                     | 0.92              |
| 1:V:167:GLY:HA3  | 4:V:2012:HOH:O   | 1.70                     | 0.92              |
| 1:P:116:THR:O    | 1:P:120:LEU:HD12 | 1.68                     | 0.91              |
| 1:X:15:ASN:HB3   | 4:X:2003:HOH:O   | 1.71                     | 0.90              |
| 1:H:145:LYS:HB2  | 4:H:2002:HOH:O   | 1.73                     | 0.86              |
| 1:U:15:ASN:HB2   | 4:U:2008:HOH:O   | 1.75                     | 0.85              |
| 1:2:5:ARG:HD2    | 4:2:2003:HOH:O   | 1.77                     | 0.82              |
| 1:O:15:ASN:HB2   | 4:O:2001:HOH:O   | 1.82                     | 0.80              |
| 1:O:67:ARG:NH2   | 1:I:30:TYR:HA    | 1.97                     | 0.80              |
| 1:P:13:GLN:OE1   | 1:P:16:ARG:HD2   | 1.83                     | 0.78              |
| 1:J:15:ASN:HB2   | 4:J:2002:HOH:O   | 1.82                     | 0.77              |
| 1:K:149:GLN:HE21 | 1:K:149:GLN:H    | 1.35                     | 0.74              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:3:165:LEU:O    | 1:3:167:GLY:N    | 2.21                     | 0.74              |
| 1:P:116:THR:HG22 | 1:P:120:LEU:HD11 | 1.68                     | 0.73              |
| 1:8:104:LEU:HD22 | 1:8:120:LEU:HD11 | 1.72                     | 0.72              |
| 1:4:40:ALA:O     | 1:4:44:LYS:HG3   | 1.90                     | 0.72              |
| 1:X:91:TYR:CZ    | 1:X:135:LYS:HD3  | 2.25                     | 0.71              |
| 1:N:138:LEU:HD23 | 1:N:138:LEU:C    | 2.10                     | 0.71              |
| 1:1:58:TYR:OH    | 1:J:32:GLU:HG3   | 1.91                     | 0.71              |
| 1:O:11:ASN:OD1   | 1:O:69:GLU:N     | 2.22                     | 0.70              |
| 1:H:81:GLU:HB2   | 1:H:85:LYS:HG3   | 1.73                     | 0.70              |
| 1:F:144:ALA:HB2  | 1:F:150:ILE:HG21 | 1.73                     | 0.70              |
| 1:N:56:ARG:HG2   | 1:N:56:ARG:NH1   | 2.07                     | 0.70              |
| 1:H:144:ALA:HB2  | 1:H:150:ILE:CG2  | 2.21                     | 0.70              |
| 1:O:11:ASN:ND2   | 1:O:61:ILE:HD13  | 2.08                     | 0.69              |
| 1:D:62:TYR:CE2   | 1:D:68:VAL:HG23  | 2.28                     | 0.68              |
| 1:D:72:GLU:OE1   | 1:V:72:GLU:OE1   | 2.11                     | 0.68              |
| 1:I:6:MET:HE3    | 1:I:108:ALA:HA   | 1.76                     | 0.67              |
| 1:9:15:ASN:HD21  | 1:9:71:ASP:H     | 1.42                     | 0.67              |
| 1:P:113:ASP:OD2  | 1:P:116:THR:OG1  | 2.11                     | 0.66              |
| 1:7:165:LEU:O    | 1:7:167:GLY:N    | 2.28                     | 0.66              |
| 1:Q:144:ALA:HB2  | 1:Q:150:ILE:HG21 | 1.78                     | 0.65              |
| 1:F:48:GLU:OE2   | 1:F:165:LEU:HB2  | 1.96                     | 0.65              |
| 1:Z:3:SER:OG     | 1:Z:6:MET:HB2    | 1.97                     | 0.65              |
| 1:M:91:TYR:CZ    | 1:M:135:LYS:HD3  | 2.32                     | 0.65              |
| 1:F:88:GLU:HG3   | 1:F:138:LEU:HD11 | 1.79                     | 0.65              |
| 1:O:11:ASN:HD21  | 1:O:68:VAL:HA    | 1.62                     | 0.64              |
| 1:6:78:LYS:HD3   | 1:O:69:GLU:HG3   | 1.79                     | 0.64              |
| 1:R:11:ASN:HD21  | 1:R:68:VAL:HA    | 1.63                     | 0.64              |
| 1:D:112:LYS:HE3  | 1:Y:99:LYS:HE2   | 1.77                     | 0.64              |
| 1:3:136:LYS:HE3  | 1:K:37:GLU:OE2   | 1.97                     | 0.64              |
| 1:6:32:GLU:HG2   | 1:6:40:ALA:HB1   | 1.80                     | 0.64              |
| 1:I:11:ASN:HD21  | 1:I:68:VAL:HA    | 1.62                     | 0.64              |
| 1:C:72:GLU:OE1   | 1:U:72:GLU:OE1   | 2.16                     | 0.63              |
| 1:3:149:GLN:NE2  | 1:3:149:GLN:H    | 1.96                     | 0.63              |
| 1:I:88:GLU:HG3   | 1:I:138:LEU:HD11 | 1.81                     | 0.63              |
| 1:O:46:GLN:HB2   | 1:O:161:ARG:HH12 | 1.64                     | 0.62              |
| 1:5:72:GLU:OE2   | 1:N:72:GLU:OE1   | 2.18                     | 0.62              |
| 1:1:46:GLN:NE2   | 1:1:130:GLU:OE1  | 2.32                     | 0.62              |
| 1:4:22:TYR:CE1   | 1:M:73:ILE:HD11  | 2.34                     | 0.62              |
| 1:Y:5:ARG:HD2    | 1:Y:111:GLU:OE2  | 2.00                     | 0.62              |
| 1:0:135:LYS:HE3  | 1:0:139:ASP:OD2  | 2.00                     | 0.61              |
| 1:Q:99:LYS:O     | 1:Q:103:GLU:HG2  | 1.99                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:13:GLN:OE1   | 1:P:13:GLN:HA    | 2.00                     | 0.61              |
| 1:C:78:LYS:O     | 1:U:67:ARG:NH2   | 2.34                     | 0.61              |
| 1:O:72:GLU:OE1   | 1:I:72:GLU:OE1   | 2.19                     | 0.60              |
| 1:B:149:GLN:HE21 | 1:B:149:GLN:H    | 1.48                     | 0.60              |
| 1:O:11:ASN:HD22  | 1:O:61:ILE:HD13  | 1.66                     | 0.60              |
| 1:Z:81:GLU:N     | 1:Z:85:LYS:HD2   | 2.13                     | 0.60              |
| 1:9:149:GLN:H    | 1:9:149:GLN:HE21 | 1.49                     | 0.60              |
| 1:X:138:LEU:HD23 | 1:X:138:LEU:O    | 2.02                     | 0.60              |
| 1:P:42:TRP:CD1   | 1:P:158:LEU:HD22 | 2.37                     | 0.59              |
| 1:Y:64:ARG:O     | 1:Y:65:ASN:HB3   | 2.01                     | 0.59              |
| 1:B:37:GLU:HG3   | 4:B:2002:HOH:O   | 2.00                     | 0.59              |
| 1:B:14:LEU:C     | 1:B:14:LEU:HD23  | 2.23                     | 0.59              |
| 1:7:91:TYR:CZ    | 1:7:135:LYS:HD3  | 2.37                     | 0.59              |
| 1:E:140:LYS:HD3  | 1:E:154:LEU:HD21 | 1.85                     | 0.59              |
| 1:Y:6:MET:HE3    | 1:Y:108:ALA:HB2  | 1.85                     | 0.59              |
| 1:M:13:GLN:NE2   | 1:M:16:ARG:HH11  | 2.01                     | 0.59              |
| 1:5:165:LEU:HB3  | 1:5:166:PRO:HD3  | 1.86                     | 0.58              |
| 1:4:72:GLU:OE1   | 1:M:72:GLU:OE1   | 2.21                     | 0.58              |
| 1:I:37:GLU:OE2   | 1:I:136:LYS:HD3  | 2.03                     | 0.58              |
| 1:T:91:TYR:CZ    | 1:T:135:LYS:HD3  | 2.39                     | 0.58              |
| 1:J:149:GLN:H    | 1:J:149:GLN:HE21 | 1.51                     | 0.58              |
| 1:A:2:LEU:O      | 1:A:3:SER:CB     | 2.35                     | 0.57              |
| 1:I:6:MET:CE     | 1:I:108:ALA:HA   | 2.33                     | 0.57              |
| 1:F:144:ALA:HB2  | 1:F:150:ILE:CG2  | 2.34                     | 0.57              |
| 1:W:4:GLU:O      | 1:W:8:LYS:HG2    | 2.04                     | 0.57              |
| 1:2:144:ALA:HB2  | 1:2:150:ILE:CG2  | 2.35                     | 0.57              |
| 1:7:117:ARG:HG3  | 1:7:117:ARG:HH11 | 1.69                     | 0.57              |
| 1:E:149:GLN:HE21 | 1:X:149:GLN:HG3  | 1.70                     | 0.57              |
| 1:3:149:GLN:HE21 | 1:3:149:GLN:H    | 1.52                     | 0.56              |
| 1:4:48:GLU:OE2   | 1:4:165:LEU:HB2  | 2.06                     | 0.56              |
| 1:3:78:LYS:HE3   | 1:L:69:GLU:HB2   | 1.87                     | 0.56              |
| 1:O:67:ARG:HG2   | 1:O:67:ARG:HH11  | 1.70                     | 0.56              |
| 1:Y:138:LEU:HD23 | 1:Y:138:LEU:O    | 2.05                     | 0.56              |
| 1:Z:138:LEU:O    | 1:Z:138:LEU:HD23 | 2.06                     | 0.56              |
| 1:5:17:GLU:O     | 1:5:20:SER:HB2   | 2.06                     | 0.56              |
| 1:R:77:PRO:HB2   | 1:R:80:TRP:CZ2   | 2.41                     | 0.56              |
| 1:V:144:ALA:O    | 1:V:145:LYS:C    | 2.44                     | 0.55              |
| 1:K:15:ASN:HB2   | 4:K:2002:HOH:O   | 2.06                     | 0.55              |
| 1:3:6:MET:CE     | 1:3:116:THR:HG21 | 2.37                     | 0.55              |
| 1:E:81:GLU:HB2   | 1:E:85:LYS:HG3   | 1.89                     | 0.55              |
| 1:W:13:GLN:HB2   | 1:W:104:LEU:HD11 | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:144:ALA:HB2  | 1:L:150:ILE:CG2  | 2.37                     | 0.55              |
| 1:T:144:ALA:HB2  | 1:T:150:ILE:HG21 | 1.87                     | 0.55              |
| 1:1:107:LEU:O    | 1:1:111:GLU:HG3  | 2.07                     | 0.54              |
| 1:I:11:ASN:ND2   | 1:I:69:GLU:H     | 2.03                     | 0.54              |
| 1:Y:48:GLU:OE2   | 1:Y:165:LEU:HB2  | 2.08                     | 0.54              |
| 1:Z:13:GLN:OE1   | 1:Z:13:GLN:HA    | 2.08                     | 0.54              |
| 1:6:165:LEU:O    | 1:6:167:GLY:N    | 2.41                     | 0.54              |
| 1:O:99:LYS:HA    | 1:O:102:TYR:HD2  | 1.71                     | 0.54              |
| 1:I:48:GLU:OE2   | 1:I:165:LEU:HB3  | 2.08                     | 0.54              |
| 1:F:69:GLU:HB2   | 1:X:78:LYS:HD2   | 1.89                     | 0.54              |
| 1:W:5:ARG:HD2    | 1:W:111:GLU:OE2  | 2.08                     | 0.54              |
| 1:A:91:TYR:CZ    | 1:A:135:LYS:HG2  | 2.43                     | 0.53              |
| 1:0:67:ARG:HH22  | 1:I:30:TYR:HA    | 1.71                     | 0.53              |
| 1:1:165:LEU:HD13 | 1:J:165:LEU:HD12 | 1.91                     | 0.53              |
| 1:O:81:GLU:HB2   | 1:O:85:LYS:HG2   | 1.90                     | 0.53              |
| 1:F:15:ASN:HD21  | 1:F:71:ASP:H     | 1.55                     | 0.53              |
| 1:E:91:TYR:CZ    | 1:E:135:LYS:HD3  | 2.43                     | 0.53              |
| 1:F:92:GLU:HG2   | 4:F:2012:HOH:O   | 2.09                     | 0.53              |
| 1:O:38:GLY:HA3   | 1:O:155:ASP:O    | 2.09                     | 0.53              |
| 1:L:144:ALA:HB2  | 1:L:150:ILE:HG21 | 1.90                     | 0.53              |
| 1:1:42:TRP:CD1   | 1:1:158:LEU:HD22 | 2.44                     | 0.53              |
| 1:6:72:GLU:OE1   | 1:O:72:GLU:OE1   | 2.28                     | 0.52              |
| 1:7:65:ASN:HD21  | 1:Z:135:LYS:HE3  | 1.74                     | 0.52              |
| 1:O:6:MET:HE2    | 1:O:10:LEU:HG    | 1.91                     | 0.52              |
| 1:G:165:LEU:HD13 | 1:Y:165:LEU:HD13 | 1.90                     | 0.52              |
| 1:3:15:ASN:HD21  | 1:3:71:ASP:H     | 1.58                     | 0.52              |
| 1:V:14:LEU:C     | 1:V:14:LEU:HD23  | 2.30                     | 0.52              |
| 1:B:70:LEU:HD12  | 1:T:26:ALA:HB2   | 1.92                     | 0.52              |
| 1:H:165:LEU:O    | 1:H:166:PRO:C    | 2.48                     | 0.52              |
| 1:Q:165:LEU:O    | 1:Q:167:GLY:N    | 2.43                     | 0.52              |
| 1:9:165:LEU:O    | 1:9:167:GLY:N    | 2.43                     | 0.51              |
| 1:H:144:ALA:HB2  | 1:H:150:ILE:HG21 | 1.92                     | 0.51              |
| 1:U:107:LEU:O    | 1:U:111:GLU:HG3  | 2.10                     | 0.51              |
| 1:R:15:ASN:HD21  | 1:R:71:ASP:H     | 1.59                     | 0.51              |
| 1:9:40:ALA:O     | 1:9:44:LYS:HG3   | 2.11                     | 0.51              |
| 1:S:91:TYR:CZ    | 1:S:135:LYS:HD3  | 2.46                     | 0.51              |
| 1:N:60:TYR:CZ    | 1:N:64:ARG:HG3   | 2.46                     | 0.51              |
| 1:V:14:LEU:HD23  | 1:V:14:LEU:O     | 2.11                     | 0.51              |
| 1:0:57:PHE:CE2   | 1:0:123:PHE:CZ   | 2.98                     | 0.51              |
| 1:3:78:LYS:HD3   | 4:3:2010:HOH:O   | 2.10                     | 0.51              |
| 1:B:138:LEU:HD23 | 1:B:138:LEU:C    | 2.31                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:X:135:LYS:NZ   | 1:X:139:ASP:OD1  | 2.42                     | 0.50              |
| 1:H:18:LEU:O     | 1:H:21:ALA:HB3   | 2.11                     | 0.50              |
| 1:H:144:ALA:HB2  | 1:H:150:ILE:HG22 | 1.94                     | 0.50              |
| 1:Y:91:TYR:CZ    | 1:Y:135:LYS:HD3  | 2.47                     | 0.50              |
| 1:Y:5:ARG:HG3    | 3:Y:1669:SO4:O4  | 2.12                     | 0.50              |
| 1:2:149:GLN:O    | 1:2:153:MET:HG3  | 2.12                     | 0.50              |
| 1:M:15:ASN:ND2   | 1:M:71:ASP:HB2   | 2.26                     | 0.50              |
| 1:3:97:ILE:HD11  | 4:3:2004:HOH:O   | 2.10                     | 0.50              |
| 1:R:140:LYS:HB3  | 1:R:154:LEU:HD11 | 1.94                     | 0.50              |
| 1:H:13:GLN:OE1   | 1:H:16:ARG:NH1   | 2.43                     | 0.49              |
| 1:7:22:TYR:CE1   | 1:P:70:LEU:HD13  | 2.47                     | 0.49              |
| 1:4:149:GLN:HA   | 1:P:150:ILE:HD11 | 1.94                     | 0.49              |
| 1:8:6:MET:CE     | 1:8:108:ALA:HA   | 2.42                     | 0.49              |
| 1:H:17:GLU:O     | 1:H:20:SER:HB2   | 2.12                     | 0.49              |
| 1:M:27:MET:HG2   | 1:M:80:TRP:CH2   | 2.47                     | 0.49              |
| 1:O:149:GLN:O    | 1:O:152:PHE:HB3  | 2.13                     | 0.49              |
| 1:W:6:MET:HE3    | 1:W:108:ALA:HA   | 1.95                     | 0.49              |
| 1:7:22:TYR:OH    | 1:P:70:LEU:HB3   | 2.13                     | 0.49              |
| 1:B:149:GLN:NE2  | 1:B:149:GLN:H    | 2.10                     | 0.49              |
| 1:E:135:LYS:NZ   | 1:E:139:ASP:OD1  | 2.46                     | 0.48              |
| 1:L:91:TYR:CZ    | 1:L:135:LYS:HD3  | 2.48                     | 0.48              |
| 1:P:5:ARG:NH1    | 1:P:111:GLU:OE2  | 2.45                     | 0.48              |
| 1:Q:144:ALA:HB2  | 1:Q:150:ILE:CG2  | 2.43                     | 0.48              |
| 1:7:117:ARG:HG3  | 1:7:117:ARG:NH1  | 2.28                     | 0.48              |
| 1:9:149:GLN:H    | 1:9:149:GLN:NE2  | 2.10                     | 0.48              |
| 1:6:13:GLN:HB2   | 1:6:104:LEU:HD11 | 1.95                     | 0.48              |
| 1:8:25:PHE:O     | 1:8:28:ALA:HB3   | 2.13                     | 0.48              |
| 1:9:38:GLY:N     | 1:9:155:ASP:OD1  | 2.47                     | 0.48              |
| 1:9:15:ASN:ND2   | 1:9:71:ASP:H     | 2.10                     | 0.48              |
| 1:C:64:ARG:O     | 1:C:65:ASN:HB3   | 2.13                     | 0.48              |
| 1:R:60:TYR:CZ    | 1:R:64:ARG:HG3   | 2.48                     | 0.48              |
| 1:0:6:MET:HE3    | 1:0:108:ALA:HB2  | 1.95                     | 0.48              |
| 1:7:104:LEU:HD22 | 1:7:120:LEU:HD11 | 1.94                     | 0.48              |
| 1:M:152:PHE:O    | 1:M:155:ASP:HB3  | 2.14                     | 0.48              |
| 1:7:84:LEU:HA    | 1:7:141:LEU:HD13 | 1.96                     | 0.48              |
| 1:A:15:ASN:HB2   | 4:A:2004:HOH:O   | 2.14                     | 0.48              |
| 1:7:72:GLU:OE1   | 1:P:72:GLU:OE1   | 2.32                     | 0.48              |
| 1:T:165:LEU:O    | 1:T:166:PRO:C    | 2.52                     | 0.47              |
| 1:2:144:ALA:HB2  | 1:2:150:ILE:HG22 | 1.96                     | 0.47              |
| 1:P:130:GLU:O    | 1:P:134:VAL:HG23 | 2.13                     | 0.47              |
| 1:Q:42:TRP:CD1   | 1:Q:158:LEU:HD22 | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:75:LYS:HD2   | 1:Z:71:ASP:HA    | 1.97                     | 0.47              |
| 1:V:165:LEU:O    | 1:V:166:PRO:C    | 2.53                     | 0.47              |
| 1:9:13:GLN:OE1   | 1:9:16:ARG:HD2   | 2.14                     | 0.47              |
| 1:P:116:THR:C    | 1:P:120:LEU:HD12 | 2.31                     | 0.47              |
| 1:8:140:LYS:HB3  | 1:8:154:LEU:HD11 | 1.95                     | 0.47              |
| 1:N:138:LEU:O    | 1:N:138:LEU:HD23 | 2.14                     | 0.47              |
| 1:N:56:ARG:NH1   | 1:N:56:ARG:CG    | 2.76                     | 0.47              |
| 1:6:72:GLU:HB3   | 1:O:75:LYS:H     | 1.79                     | 0.47              |
| 1:V:165:LEU:O    | 1:V:167:GLY:N    | 2.48                     | 0.47              |
| 1:E:138:LEU:HD23 | 1:E:138:LEU:C    | 2.34                     | 0.47              |
| 1:Z:91:TYR:CZ    | 1:Z:135:LYS:HD3  | 2.49                     | 0.47              |
| 1:Y:165:LEU:O    | 1:Y:166:PRO:C    | 2.53                     | 0.47              |
| 1:F:91:TYR:CZ    | 1:F:135:LYS:HD3  | 2.49                     | 0.47              |
| 1:O:11:ASN:HD22  | 1:O:61:ILE:CD1   | 2.27                     | 0.47              |
| 1:V:38:GLY:HA3   | 1:V:155:ASP:O    | 2.14                     | 0.47              |
| 1:9:72:GLU:OE1   | 1:R:72:GLU:OE1   | 2.33                     | 0.46              |
| 1:Z:38:GLY:HA3   | 1:Z:155:ASP:O    | 2.15                     | 0.46              |
| 1:6:78:LYS:O     | 1:O:67:ARG:NH2   | 2.47                     | 0.46              |
| 1:G:165:LEU:O    | 1:G:166:PRO:C    | 2.53                     | 0.46              |
| 1:P:116:THR:HG22 | 1:P:120:LEU:CD1  | 2.43                     | 0.46              |
| 1:X:138:LEU:HD23 | 1:X:138:LEU:C    | 2.36                     | 0.46              |
| 1:C:165:LEU:HB3  | 1:C:166:PRO:HD3  | 1.96                     | 0.46              |
| 1:E:138:LEU:O    | 1:E:138:LEU:HD23 | 2.16                     | 0.46              |
| 1:4:70:LEU:HD12  | 1:M:26:ALA:HB2   | 1.96                     | 0.46              |
| 1:T:144:ALA:O    | 1:T:145:LYS:C    | 2.53                     | 0.46              |
| 1:2:156:LYS:O    | 1:2:159:SER:OG   | 2.28                     | 0.46              |
| 1:B:14:LEU:O     | 1:B:14:LEU:HD23  | 2.15                     | 0.46              |
| 1:C:135:LYS:HE3  | 1:C:139:ASP:OD2  | 2.16                     | 0.46              |
| 1:P:64:ARG:HD2   | 1:P:64:ARG:HA    | 1.62                     | 0.46              |
| 1:R:42:TRP:CD1   | 1:R:158:LEU:HD22 | 2.50                     | 0.46              |
| 1:9:46:GLN:NE2   | 1:9:130:GLU:OE1  | 2.48                     | 0.46              |
| 1:7:22:TYR:CZ    | 1:P:70:LEU:HB3   | 2.50                     | 0.46              |
| 1:F:88:GLU:HG3   | 1:F:138:LEU:CD1  | 2.46                     | 0.46              |
| 1:N:138:LEU:CD2  | 1:N:138:LEU:C    | 2.83                     | 0.46              |
| 1:B:26:ALA:HB2   | 1:T:70:LEU:HD12  | 1.98                     | 0.46              |
| 1:D:62:TYR:CE2   | 1:D:68:VAL:CG2   | 2.98                     | 0.46              |
| 1:I:22:TYR:CD2   | 1:I:76:PRO:HD3   | 2.51                     | 0.46              |
| 1:N:3:SER:OG     | 1:N:6:MET:HB2    | 2.16                     | 0.46              |
| 1:S:17:GLU:O     | 1:S:20:SER:HB2   | 2.15                     | 0.46              |
| 1:T:82:SER:HB2   | 1:T:83:PRO:HD2   | 1.98                     | 0.46              |
| 1:W:91:TYR:CZ    | 1:W:135:LYS:HD3  | 2.50                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:9:107:LEU:O    | 1:9:111:GLU:HG3  | 2.16                     | 0.46              |
| 1:B:3:SER:CB     | 1:B:6:MET:H      | 2.29                     | 0.46              |
| 1:C:144:ALA:HB1  | 1:C:150:ILE:HB   | 1.97                     | 0.46              |
| 1:E:15:ASN:HB2   | 4:E:2006:HOH:O   | 2.16                     | 0.46              |
| 1:6:72:GLU:HB3   | 1:O:75:LYS:N     | 2.30                     | 0.46              |
| 1:V:27:MET:O     | 1:V:31:PHE:HD2   | 1.98                     | 0.46              |
| 1:4:26:ALA:HB2   | 1:M:70:LEU:HD12  | 1.98                     | 0.45              |
| 1:E:151:LEU:HD12 | 1:E:151:LEU:HA   | 1.81                     | 0.45              |
| 1:I:2:LEU:HG     | 1:I:64:ARG:HB3   | 1.98                     | 0.45              |
| 1:4:22:TYR:HE1   | 1:M:18:LEU:HD13  | 1.80                     | 0.45              |
| 1:Y:165:LEU:HA   | 1:Y:165:LEU:HD12 | 1.81                     | 0.45              |
| 1:7:48:GLU:OE1   | 1:7:164:LYS:HB2  | 2.17                     | 0.45              |
| 1:9:20:SER:O     | 1:9:21:ALA:C     | 2.55                     | 0.45              |
| 1:F:17:GLU:O     | 1:F:20:SER:HB2   | 2.16                     | 0.45              |
| 1:M:116:THR:HG22 | 1:M:120:LEU:HD12 | 1.98                     | 0.45              |
| 1:5:70:LEU:HD13  | 1:N:22:TYR:CE1   | 2.52                     | 0.45              |
| 1:P:3:SER:O      | 1:P:4:GLU:C      | 2.54                     | 0.45              |
| 1:D:140:LYS:HB3  | 1:D:154:LEU:HD11 | 1.99                     | 0.45              |
| 1:I:64:ARG:HD2   | 1:I:64:ARG:HA    | 1.65                     | 0.45              |
| 1:M:13:GLN:NE2   | 1:M:16:ARG:NH1   | 2.63                     | 0.45              |
| 1:N:27:MET:HG2   | 1:N:80:TRP:CH2   | 2.52                     | 0.45              |
| 1:O:102:TYR:CD1  | 1:P:114:TYR:HD1  | 2.34                     | 0.45              |
| 1:H:71:ASP:OD1   | 1:Z:75:LYS:NZ    | 2.49                     | 0.45              |
| 1:I:14:LEU:C     | 1:I:14:LEU:HD23  | 2.37                     | 0.45              |
| 1:2:46:GLN:NE2   | 1:2:130:GLU:OE1  | 2.46                     | 0.45              |
| 1:4:81:GLU:HB2   | 1:4:85:LYS:HG3   | 1.98                     | 0.45              |
| 1:8:95:LYS:O     | 1:8:99:LYS:HG3   | 2.16                     | 0.45              |
| 1:1:91:TYR:CZ    | 1:1:95:LYS:HE2   | 2.52                     | 0.45              |
| 1:C:56:ARG:HD3   | 4:C:2003:HOH:O   | 2.16                     | 0.45              |
| 1:G:56:ARG:HG2   | 1:G:56:ARG:HH11  | 1.82                     | 0.45              |
| 1:O:6:MET:HE3    | 1:O:9:ALA:HB3    | 1.98                     | 0.45              |
| 1:3:26:ALA:HA    | 1:L:70:LEU:HD12  | 1.98                     | 0.45              |
| 1:E:165:LEU:O    | 1:E:166:PRO:C    | 2.55                     | 0.45              |
| 1:O:154:LEU:O    | 1:O:155:ASP:C    | 2.55                     | 0.45              |
| 1:R:11:ASN:ND2   | 1:R:69:GLU:H     | 2.14                     | 0.45              |
| 1:F:149:GLN:HG2  | 1:S:149:GLN:HG3  | 1.98                     | 0.45              |
| 1:V:140:LYS:HB3  | 1:V:154:LEU:HD11 | 1.98                     | 0.45              |
| 1:D:2:LEU:HB2    | 4:D:2007:HOH:O   | 2.15                     | 0.44              |
| 1:G:140:LYS:HD3  | 1:G:154:LEU:HD21 | 1.99                     | 0.44              |
| 1:O:165:LEU:O    | 1:O:166:PRO:C    | 2.56                     | 0.44              |
| 1:6:64:ARG:HD2   | 1:6:64:ARG:HA    | 1.79                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:144:ALA:HB1  | 1:B:150:ILE:HB   | 1.98                     | 0.44              |
| 1:H:144:ALA:O    | 1:H:146:ASP:N    | 2.49                     | 0.44              |
| 1:M:138:LEU:C    | 1:M:138:LEU:HD23 | 2.38                     | 0.44              |
| 1:H:6:MET:HE3    | 1:H:108:ALA:HB2  | 2.00                     | 0.44              |
| 1:2:149:GLN:HG3  | 1:H:150:ILE:HD11 | 2.00                     | 0.44              |
| 1:4:6:MET:HE3    | 1:4:108:ALA:HB2  | 1.99                     | 0.44              |
| 1:9:38:GLY:HA3   | 1:9:155:ASP:O    | 2.18                     | 0.44              |
| 1:2:149:GLN:HE21 | 1:G:149:GLN:HG2  | 1.83                     | 0.44              |
| 1:M:13:GLN:HE21  | 1:M:16:ARG:NH1   | 2.14                     | 0.44              |
| 1:7:144:ALA:O    | 1:7:145:LYS:C    | 2.56                     | 0.44              |
| 1:8:143:PHE:HZ   | 1:M:151:LEU:HD23 | 1.82                     | 0.44              |
| 1:F:72:GLU:OE1   | 1:X:72:GLU:OE1   | 2.36                     | 0.44              |
| 1:H:147:SER:HA   | 1:H:148:PRO:HD2  | 1.71                     | 0.44              |
| 1:R:140:LYS:HD3  | 1:R:154:LEU:HD21 | 2.00                     | 0.44              |
| 1:Z:64:ARG:HD2   | 1:Z:64:ARG:HA    | 1.81                     | 0.44              |
| 1:1:13:GLN:HG2   | 1:1:57:PHE:CZ    | 2.53                     | 0.44              |
| 1:4:64:ARG:HD2   | 1:4:64:ARG:HA    | 1.87                     | 0.44              |
| 1:8:67:ARG:NH2   | 1:Q:78:LYS:O     | 2.51                     | 0.44              |
| 1:D:11:ASN:O     | 1:D:12:ASP:C     | 2.54                     | 0.44              |
| 1:N:144:ALA:O    | 1:N:145:LYS:C    | 2.57                     | 0.44              |
| 1:5:69:GLU:OE2   | 1:N:75:LYS:NZ    | 2.35                     | 0.43              |
| 1:H:102:TYR:CE1  | 1:K:114:TYR:HB2  | 2.53                     | 0.43              |
| 1:M:165:LEU:C    | 1:M:167:GLY:H    | 2.20                     | 0.43              |
| 1:O:55:LEU:HA    | 1:O:55:LEU:HD23  | 1.82                     | 0.43              |
| 1:1:58:TYR:HH    | 1:J:32:GLU:HG3   | 1.83                     | 0.43              |
| 1:W:150:ILE:O    | 1:W:154:LEU:HB2  | 2.17                     | 0.43              |
| 1:N:149:GLN:NE2  | 1:N:149:GLN:H    | 1.98                     | 0.43              |
| 1:W:34:LEU:HD12  | 1:W:34:LEU:HA    | 1.82                     | 0.43              |
| 1:A:144:ALA:HB2  | 1:A:150:ILE:CG2  | 2.48                     | 0.43              |
| 1:Y:116:THR:O    | 1:Y:120:LEU:HG   | 2.18                     | 0.43              |
| 1:I:5:ARG:H      | 1:I:5:ARG:HD3    | 1.83                     | 0.43              |
| 1:0:67:ARG:NH1   | 1:0:67:ARG:HG2   | 2.33                     | 0.43              |
| 1:6:46:GLN:NE2   | 1:6:130:GLU:OE1  | 2.52                     | 0.43              |
| 1:I:40:ALA:O     | 1:I:44:LYS:HG3   | 2.19                     | 0.43              |
| 1:B:64:ARG:HD2   | 1:B:64:ARG:HA    | 1.72                     | 0.43              |
| 1:G:149:GLN:NE2  | 1:G:149:GLN:H    | 2.17                     | 0.43              |
| 1:O:64:ARG:HA    | 1:O:64:ARG:HD2   | 1.71                     | 0.43              |
| 1:V:62:TYR:CE2   | 1:V:68:VAL:HG23  | 2.53                     | 0.43              |
| 1:Y:6:MET:HE3    | 1:Y:108:ALA:CB   | 2.49                     | 0.43              |
| 1:4:57:PHE:CE2   | 1:4:123:PHE:CZ   | 3.06                     | 0.43              |
| 1:Z:34:LEU:HD12  | 1:Z:36:LEU:HD12  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:0:135:LYS:HE3   | 1:0:139:ASP:CG   | 2.39                     | 0.43              |
| 1:2:144:ALA:HB2   | 1:2:150:ILE:HG21 | 2.00                     | 0.43              |
| 1:3:6:MET:HE1     | 1:3:116:THR:HG21 | 2.01                     | 0.43              |
| 1:I:67:ARG:NH1    | 1:I:68:VAL:O     | 2.52                     | 0.43              |
| 1:Q:107:LEU:HA    | 1:Q:107:LEU:HD12 | 1.83                     | 0.43              |
| 1:0:17:GLU:O      | 1:0:20:SER:HB2   | 2.19                     | 0.43              |
| 1:0:31:PHE:HE1    | 1:0:83:PRO:HB3   | 1.83                     | 0.43              |
| 1:I:97:ILE:HD13   | 1:I:97:ILE:HA    | 1.92                     | 0.43              |
| 1:2:15:ASN:HD21   | 1:2:71:ASP:H     | 1.66                     | 0.42              |
| 1:7:58:TYR:CD1    | 1:7:58:TYR:C     | 2.93                     | 0.42              |
| 1:C:93:HIS:O      | 1:C:96:PHE:HB3   | 2.19                     | 0.42              |
| 1:2:138:LEU:HD23  | 1:2:138:LEU:C    | 2.40                     | 0.42              |
| 1:G:15[B]:ASN:ND2 | 1:Y:22:TYR:OH    | 2.51                     | 0.42              |
| 1:O:85:LYS:HD2    | 1:O:85:LYS:HA    | 1.44                     | 0.42              |
| 1:A:3:SER:O       | 1:A:4:GLU:C      | 2.57                     | 0.42              |
| 1:0:70:LEU:HD12   | 1:I:26:ALA:HA    | 2.02                     | 0.42              |
| 1:U:57:PHE:CE1    | 1:U:119:PHE:HE2  | 2.38                     | 0.42              |
| 1:F:165:LEU:O     | 1:F:167:GLY:N    | 2.52                     | 0.42              |
| 1:M:13:GLN:HE21   | 1:M:16:ARG:HH11  | 1.65                     | 0.42              |
| 1:S:81:GLU:HB2    | 1:S:85:LYS:HG3   | 2.01                     | 0.42              |
| 1:B:165:LEU:O     | 1:B:166:PRO:C    | 2.55                     | 0.42              |
| 1:C:144:ALA:HB2   | 1:C:150:ILE:HG21 | 2.02                     | 0.42              |
| 1:H:14:LEU:HD23   | 1:H:14:LEU:O     | 2.20                     | 0.42              |
| 1:Z:55:LEU:HA     | 1:Z:55:LEU:HD23  | 1.64                     | 0.42              |
| 1:G:149:GLN:H     | 1:G:149:GLN:HE21 | 1.66                     | 0.42              |
| 1:H:38:GLY:HA3    | 1:H:155:ASP:O    | 2.20                     | 0.42              |
| 1:2:165:LEU:HB3   | 1:2:166:PRO:HD3  | 2.02                     | 0.42              |
| 1:8:27:MET:O      | 1:8:30:TYR:HB3   | 2.20                     | 0.42              |
| 1:H:60:TYR:CZ     | 1:H:64:ARG:HG3   | 2.55                     | 0.42              |
| 1:Y:138:LEU:C     | 1:Y:138:LEU:HD23 | 2.39                     | 0.42              |
| 1:A:147:SER:HA    | 1:A:148:PRO:HD2  | 1.91                     | 0.42              |
| 1:M:23:LEU:O      | 1:M:27:MET:HG3   | 2.20                     | 0.42              |
| 1:O:55:LEU:O      | 1:O:58:TYR:HB3   | 2.20                     | 0.42              |
| 1:C:23:LEU:O      | 1:C:26:ALA:HB3   | 2.20                     | 0.42              |
| 1:H:58:TYR:CD1    | 1:H:58:TYR:C     | 2.93                     | 0.42              |
| 1:N:135:LYS:HZ3   | 1:N:139:ASP:CG   | 2.23                     | 0.42              |
| 1:2:91:TYR:CZ     | 1:2:135:LYS:HD3  | 2.55                     | 0.41              |
| 1:E:107:LEU:O     | 1:E:111:GLU:HG3  | 2.20                     | 0.41              |
| 1:H:143:PHE:C     | 1:H:145:LYS:H    | 2.23                     | 0.41              |
| 1:H:144:ALA:O     | 1:H:145:LYS:C    | 2.58                     | 0.41              |
| 1:K:138:LEU:C     | 1:K:138:LEU:HD23 | 2.41                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:97:ILE:HA    | 1:N:97:ILE:HD13  | 1.91                     | 0.41              |
| 1:O:99:LYS:HA    | 1:O:102:TYR:CD2  | 2.54                     | 0.41              |
| 1:P:148:PRO:HD2  | 1:P:149:GLN:OE1  | 2.20                     | 0.41              |
| 1:Q:87:PHE:CE1   | 1:Q:137:ILE:HG21 | 2.55                     | 0.41              |
| 1:6:20:SER:O     | 1:6:21:ALA:C     | 2.57                     | 0.41              |
| 1:7:64:ARG:O     | 1:7:65:ASN:CB    | 2.68                     | 0.41              |
| 1:7:83:PRO:O     | 1:7:86:ALA:HB3   | 2.20                     | 0.41              |
| 1:D:22:TYR:CD2   | 1:D:76:PRO:HD3   | 2.55                     | 0.41              |
| 1:Z:99:LYS:HA    | 1:Z:102:TYR:HD2  | 1.85                     | 0.41              |
| 1:Z:20:SER:O     | 1:Z:24:TYR:CD2   | 2.73                     | 0.41              |
| 1:0:26:ALA:HA    | 1:I:70:LEU:HD12  | 2.01                     | 0.41              |
| 1:3:82:SER:O     | 1:3:83:PRO:C     | 2.58                     | 0.41              |
| 1:B:55:LEU:HA    | 1:B:55:LEU:HD23  | 1.93                     | 0.41              |
| 1:C:154:LEU:HD23 | 1:C:154:LEU:HA   | 1.82                     | 0.41              |
| 1:O:6:MET:HE2    | 1:O:6:MET:O      | 2.20                     | 0.41              |
| 1:V:138:LEU:C    | 1:V:138:LEU:HD23 | 2.41                     | 0.41              |
| 1:E:72:GLU:CD    | 1:W:72:GLU:OE1   | 2.59                     | 0.41              |
| 1:0:67:ARG:HD3   | 1:I:78:LYS:HE2   | 2.02                     | 0.41              |
| 1:O:99:LYS:HB3   | 1:O:99:LYS:HE2   | 1.84                     | 0.41              |
| 1:A:117:ARG:HG3  | 1:A:117:ARG:O    | 2.19                     | 0.41              |
| 1:K:144:ALA:O    | 1:K:145:LYS:C    | 2.59                     | 0.41              |
| 1:P:68:VAL:HG12  | 1:P:69:GLU:N     | 2.36                     | 0.41              |
| 1:S:13:GLN:HG2   | 1:S:57:PHE:CZ    | 2.55                     | 0.41              |
| 1:X:64:ARG:HD2   | 1:X:64:ARG:HA    | 1.93                     | 0.41              |
| 1:R:15:ASN:ND2   | 1:R:71:ASP:H     | 2.19                     | 0.41              |
| 1:Y:6:MET:HE3    | 1:Y:108:ALA:CA   | 2.51                     | 0.41              |
| 1:O:18:LEU:HA    | 1:O:18:LEU:HD23  | 1.95                     | 0.41              |
| 1:T:1:MET:CE     | 1:U:131:GLU:OE1  | 2.68                     | 0.41              |
| 1:3:38:GLY:HA3   | 1:3:155:ASP:O    | 2.21                     | 0.41              |
| 1:6:32:GLU:HG2   | 1:6:40:ALA:CB    | 2.48                     | 0.41              |
| 1:K:154:LEU:HA   | 1:K:154:LEU:HD23 | 1.86                     | 0.41              |
| 1:M:144:ALA:HB1  | 1:M:150:ILE:HB   | 2.03                     | 0.41              |
| 1:P:21:ALA:HA    | 1:P:47:ALA:HA    | 2.02                     | 0.41              |
| 1:S:64:ARG:HA    | 1:S:64:ARG:HD2   | 1.74                     | 0.41              |
| 1:3:6:MET:O      | 1:3:7:LEU:C      | 2.59                     | 0.41              |
| 1:B:135:LYS:HE3  | 1:B:139:ASP:OD2  | 2.21                     | 0.41              |
| 1:D:14:LEU:HD23  | 1:D:14:LEU:C     | 2.41                     | 0.41              |
| 1:K:147:SER:HA   | 1:K:148:PRO:HD2  | 1.85                     | 0.41              |
| 1:T:60:TYR:CZ    | 1:T:64:ARG:HG3   | 2.55                     | 0.41              |
| 1:1:24:TYR:HD1   | 1:1:43:MET:SD    | 2.43                     | 0.41              |
| 1:1:60:TYR:O     | 1:1:63:ASP:HB2   | 2.21                     | 0.41              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:2:48:GLU:OE2  | 1:2:163:PRO:HB2  | 2.21                     | 0.41              |
| 1:1:60:TYR:HB2  | 1:1:119:PHE:CE1  | 2.56                     | 0.41              |
| 1:Q:46:GLN:O    | 1:Q:50:GLU:HG2   | 2.21                     | 0.41              |
| 1:1:77:PRO:HB2  | 1:1:80:TRP:CZ2   | 2.55                     | 0.40              |
| 1:4:165:LEU:O   | 1:4:166:PRO:C    | 2.58                     | 0.40              |
| 1:5:64:ARG:HA   | 1:5:64:ARG:HD2   | 1.63                     | 0.40              |
| 1:9:154:LEU:HA  | 1:9:154:LEU:HD23 | 1.94                     | 0.40              |
| 1:E:95:LYS:HD3  | 4:E:2016:HOH:O   | 2.21                     | 0.40              |
| 1:L:10:LEU:HB3  | 1:L:61:ILE:HD11  | 2.03                     | 0.40              |
| 1:B:22:TYR:CZ   | 1:T:70:LEU:HB3   | 2.56                     | 0.40              |
| 1:Z:82:SER:O    | 1:Z:83:PRO:C     | 2.59                     | 0.40              |
| 1:7:135:LYS:NZ  | 1:7:139:ASP:OD1  | 2.54                     | 0.40              |
| 1:L:114:TYR:HB3 | 1:Q:124:ILE:HD13 | 2.03                     | 0.40              |
| 1:L:15:ASN:HB2  | 4:L:2002:HOH:O   | 2.20                     | 0.40              |
| 1:S:57:PHE:O    | 1:S:61:ILE:HG13  | 2.21                     | 0.40              |
| 1:W:31:PHE:O    | 1:W:32:GLU:C     | 2.59                     | 0.40              |
| 1:Y:81:GLU:HB2  | 1:Y:85:LYS:HG3   | 2.03                     | 0.40              |
| 1:7:117:ARG:HD2 | 1:7:117:ARG:HA   | 1.65                     | 0.40              |
| 1:H:64:ARG:HA   | 1:H:64:ARG:HD2   | 1.86                     | 0.40              |
| 1:6:13:GLN:OE1  | 1:6:16:ARG:HD2   | 2.22                     | 0.40              |
| 1:N:46:GLN:NE2  | 1:N:130:GLU:OE1  | 2.54                     | 0.40              |
| 1:2:60:TYR:CZ   | 1:2:64:ARG:HG3   | 2.56                     | 0.40              |
| 1:C:64:ARG:HA   | 1:C:64:ARG:HD2   | 1.86                     | 0.40              |
| 1:P:13:GLN:HA   | 1:P:16:ARG:HB2   | 2.03                     | 0.40              |
| 1:V:42:TRP:CD1  | 1:V:158:LEU:HD22 | 2.57                     | 0.40              |
| 1:Y:144:ALA:O   | 1:Y:146:ASP:N    | 2.55                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | 0     | 165/174 (95%) | 161 (98%) | 1 (1%)  | 3 (2%)   | 8           | 28  |
| 1   | 1     | 165/174 (95%) | 159 (96%) | 5 (3%)  | 1 (1%)   | 25          | 56  |
| 1   | 2     | 165/174 (95%) | 160 (97%) | 2 (1%)  | 3 (2%)   | 8           | 28  |
| 1   | 3     | 165/174 (95%) | 160 (97%) | 2 (1%)  | 3 (2%)   | 8           | 28  |
| 1   | 4     | 165/174 (95%) | 157 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 1   | 5     | 165/174 (95%) | 161 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | 6     | 165/174 (95%) | 157 (95%) | 7 (4%)  | 1 (1%)   | 25          | 56  |
| 1   | 7     | 165/174 (95%) | 160 (97%) | 3 (2%)  | 2 (1%)   | 13          | 39  |
| 1   | 8     | 165/174 (95%) | 158 (96%) | 5 (3%)  | 2 (1%)   | 13          | 39  |
| 1   | 9     | 165/174 (95%) | 160 (97%) | 3 (2%)  | 2 (1%)   | 13          | 39  |
| 1   | A     | 165/174 (95%) | 158 (96%) | 2 (1%)  | 5 (3%)   | 4           | 15  |
| 1   | B     | 165/174 (95%) | 160 (97%) | 4 (2%)  | 1 (1%)   | 25          | 56  |
| 1   | C     | 165/174 (95%) | 157 (95%) | 7 (4%)  | 1 (1%)   | 25          | 56  |
| 1   | D     | 165/174 (95%) | 159 (96%) | 3 (2%)  | 3 (2%)   | 8           | 28  |
| 1   | E     | 165/174 (95%) | 161 (98%) | 2 (1%)  | 2 (1%)   | 13          | 39  |
| 1   | F     | 165/174 (95%) | 158 (96%) | 5 (3%)  | 2 (1%)   | 13          | 39  |
| 1   | G     | 166/174 (95%) | 158 (95%) | 7 (4%)  | 1 (1%)   | 25          | 56  |
| 1   | H     | 165/174 (95%) | 157 (95%) | 6 (4%)  | 2 (1%)   | 13          | 39  |
| 1   | I     | 165/174 (95%) | 159 (96%) | 5 (3%)  | 1 (1%)   | 25          | 56  |
| 1   | J     | 165/174 (95%) | 161 (98%) | 2 (1%)  | 2 (1%)   | 13          | 39  |
| 1   | K     | 165/174 (95%) | 160 (97%) | 4 (2%)  | 1 (1%)   | 25          | 56  |
| 1   | L     | 165/174 (95%) | 156 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | M     | 165/174 (95%) | 153 (93%) | 9 (6%)  | 3 (2%)   | 8           | 28  |
| 1   | N     | 165/174 (95%) | 163 (99%) | 1 (1%)  | 1 (1%)   | 25          | 56  |
| 1   | O     | 165/174 (95%) | 155 (94%) | 6 (4%)  | 4 (2%)   | 6           | 20  |
| 1   | P     | 165/174 (95%) | 158 (96%) | 4 (2%)  | 3 (2%)   | 8           | 28  |
| 1   | Q     | 165/174 (95%) | 160 (97%) | 3 (2%)  | 2 (1%)   | 13          | 39  |
| 1   | R     | 165/174 (95%) | 158 (96%) | 5 (3%)  | 2 (1%)   | 13          | 39  |
| 1   | S     | 165/174 (95%) | 160 (97%) | 3 (2%)  | 2 (1%)   | 13          | 39  |
| 1   | T     | 166/174 (95%) | 160 (96%) | 5 (3%)  | 1 (1%)   | 25          | 56  |
| 1   | U     | 165/174 (95%) | 159 (96%) | 4 (2%)  | 2 (1%)   | 13          | 39  |
| 1   | V     | 165/174 (95%) | 159 (96%) | 4 (2%)  | 2 (1%)   | 13          | 39  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | W     | 166/174 (95%)   | 163 (98%)  | 2 (1%)   | 1 (1%)   | 25          | 56 |
| 1   | X     | 165/174 (95%)   | 159 (96%)  | 4 (2%)   | 2 (1%)   | 13          | 39 |
| 1   | Y     | 165/174 (95%)   | 158 (96%)  | 6 (4%)   | 1 (1%)   | 25          | 56 |
| 1   | Z     | 165/174 (95%)   | 158 (96%)  | 6 (4%)   | 1 (1%)   | 25          | 56 |
| All | All   | 5943/6264 (95%) | 5720 (96%) | 158 (3%) | 65 (1%)  | 14          | 41 |

All (65) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 145 | LYS  |
| 1   | 3     | 166 | PRO  |
| 1   | 7     | 166 | PRO  |
| 1   | 9     | 145 | LYS  |
| 1   | A     | 3   | SER  |
| 1   | D     | 145 | LYS  |
| 1   | P     | 145 | LYS  |
| 1   | Q     | 145 | LYS  |
| 1   | S     | 145 | LYS  |
| 1   | V     | 145 | LYS  |
| 1   | V     | 166 | PRO  |
| 1   | 0     | 166 | PRO  |
| 1   | 7     | 145 | LYS  |
| 1   | 8     | 145 | LYS  |
| 1   | F     | 166 | PRO  |
| 1   | G     | 145 | LYS  |
| 1   | H     | 145 | LYS  |
| 1   | I     | 145 | LYS  |
| 1   | M     | 115 | SER  |
| 1   | M     | 145 | LYS  |
| 1   | P     | 65  | ASN  |
| 1   | U     | 145 | LYS  |
| 1   | W     | 145 | LYS  |
| 1   | X     | 145 | LYS  |
| 1   | Y     | 145 | LYS  |
| 1   | Z     | 145 | LYS  |
| 1   | 6     | 166 | PRO  |
| 1   | A     | 165 | LEU  |
| 1   | A     | 166 | PRO  |
| 1   | D     | 166 | PRO  |
| 1   | F     | 145 | LYS  |
| 1   | J     | 145 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 145 | LYS  |
| 1   | O     | 145 | LYS  |
| 1   | O     | 146 | ASP  |
| 1   | R     | 165 | LEU  |
| 1   | 0     | 145 | LYS  |
| 1   | 9     | 166 | PRO  |
| 1   | A     | 146 | ASP  |
| 1   | A     | 147 | SER  |
| 1   | C     | 166 | PRO  |
| 1   | D     | 165 | LEU  |
| 1   | O     | 147 | SER  |
| 1   | P     | 166 | PRO  |
| 1   | R     | 145 | LYS  |
| 1   | 2     | 144 | ALA  |
| 1   | 2     | 145 | LYS  |
| 1   | 2     | 166 | PRO  |
| 1   | 3     | 145 | LYS  |
| 1   | H     | 146 | ASP  |
| 1   | O     | 166 | PRO  |
| 1   | T     | 143 | PHE  |
| 1   | U     | 166 | PRO  |
| 1   | 3     | 148 | PRO  |
| 1   | J     | 166 | PRO  |
| 1   | X     | 166 | PRO  |
| 1   | 0     | 165 | LEU  |
| 1   | E     | 165 | LEU  |
| 1   | M     | 166 | PRO  |
| 1   | S     | 165 | LEU  |
| 1   | B     | 166 | PRO  |
| 1   | E     | 166 | PRO  |
| 1   | Q     | 166 | PRO  |
| 1   | 8     | 166 | PRO  |
| 1   | N     | 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%) | 128 (90%) | 14 (10%) | 8           | 23 |
| 1   | 1     | 142/147 (97%) | 133 (94%) | 9 (6%)   | 18          | 46 |
| 1   | 2     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 21          | 51 |
| 1   | 3     | 142/147 (97%) | 132 (93%) | 10 (7%)  | 15          | 40 |
| 1   | 4     | 142/147 (97%) | 135 (95%) | 7 (5%)   | 25          | 57 |
| 1   | 5     | 142/147 (97%) | 138 (97%) | 4 (3%)   | 43          | 77 |
| 1   | 6     | 142/147 (97%) | 136 (96%) | 6 (4%)   | 30          | 63 |
| 1   | 7     | 142/147 (97%) | 128 (90%) | 14 (10%) | 8           | 23 |
| 1   | 8     | 142/147 (97%) | 132 (93%) | 10 (7%)  | 15          | 40 |
| 1   | 9     | 142/147 (97%) | 133 (94%) | 9 (6%)   | 18          | 46 |
| 1   | A     | 142/147 (97%) | 135 (95%) | 7 (5%)   | 25          | 57 |
| 1   | B     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 21          | 51 |
| 1   | C     | 142/147 (97%) | 136 (96%) | 6 (4%)   | 30          | 63 |
| 1   | D     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 21          | 51 |
| 1   | E     | 142/147 (97%) | 135 (95%) | 7 (5%)   | 25          | 57 |
| 1   | F     | 142/147 (97%) | 132 (93%) | 10 (7%)  | 15          | 40 |
| 1   | G     | 143/147 (97%) | 137 (96%) | 6 (4%)   | 30          | 63 |
| 1   | H     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 21          | 51 |
| 1   | I     | 142/147 (97%) | 135 (95%) | 7 (5%)   | 25          | 57 |
| 1   | J     | 142/147 (97%) | 136 (96%) | 6 (4%)   | 30          | 63 |
| 1   | K     | 142/147 (97%) | 132 (93%) | 10 (7%)  | 15          | 40 |
| 1   | L     | 142/147 (97%) | 135 (95%) | 7 (5%)   | 25          | 57 |
| 1   | M     | 142/147 (97%) | 132 (93%) | 10 (7%)  | 15          | 40 |
| 1   | N     | 142/147 (97%) | 137 (96%) | 5 (4%)   | 36          | 70 |
| 1   | O     | 142/147 (97%) | 130 (92%) | 12 (8%)  | 10          | 31 |
| 1   | P     | 142/147 (97%) | 135 (95%) | 7 (5%)   | 25          | 57 |
| 1   | Q     | 142/147 (97%) | 133 (94%) | 9 (6%)   | 18          | 46 |
| 1   | R     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 21          | 51 |
| 1   | S     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 21          | 51 |
| 1   | T     | 143/147 (97%) | 138 (96%) | 5 (4%)   | 36          | 70 |
| 1   | U     | 142/147 (97%) | 137 (96%) | 5 (4%)   | 36          | 70 |
| 1   | V     | 142/147 (97%) | 134 (94%) | 8 (6%)   | 21          | 51 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | W     | 143/147 (97%)   | 137 (96%)  | 6 (4%)   | 30          | 63 |
| 1   | X     | 142/147 (97%)   | 136 (96%)  | 6 (4%)   | 30          | 63 |
| 1   | Y     | 142/147 (97%)   | 136 (96%)  | 6 (4%)   | 30          | 63 |
| 1   | Z     | 142/147 (97%)   | 136 (96%)  | 6 (4%)   | 30          | 63 |
| All | All   | 5115/5292 (97%) | 4833 (94%) | 282 (6%) | 21          | 52 |

All (282) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 1   | MET  |
| 1   | 0     | 4   | GLU  |
| 1   | 0     | 5   | ARG  |
| 1   | 0     | 6   | MET  |
| 1   | 0     | 8   | LYS  |
| 1   | 0     | 22  | TYR  |
| 1   | 0     | 72  | GLU  |
| 1   | 0     | 79  | GLU  |
| 1   | 0     | 85  | LYS  |
| 1   | 0     | 96  | PHE  |
| 1   | 0     | 100 | SER  |
| 1   | 0     | 110 | GLU  |
| 1   | 0     | 133 | SER  |
| 1   | 0     | 154 | LEU  |
| 1   | 1     | 1   | MET  |
| 1   | 1     | 5   | ARG  |
| 1   | 1     | 6   | MET  |
| 1   | 1     | 22  | TYR  |
| 1   | 1     | 32  | GLU  |
| 1   | 1     | 72  | GLU  |
| 1   | 1     | 100 | SER  |
| 1   | 1     | 149 | GLN  |
| 1   | 1     | 154 | LEU  |
| 1   | 2     | 15  | ASN  |
| 1   | 2     | 22  | TYR  |
| 1   | 2     | 65  | ASN  |
| 1   | 2     | 98  | SER  |
| 1   | 2     | 100 | SER  |
| 1   | 2     | 133 | SER  |
| 1   | 2     | 149 | GLN  |
| 1   | 2     | 156 | LYS  |
| 1   | 3     | 1   | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 3     | 5   | ARG  |
| 1   | 3     | 15  | ASN  |
| 1   | 3     | 22  | TYR  |
| 1   | 3     | 72  | GLU  |
| 1   | 3     | 136 | LYS  |
| 1   | 3     | 143 | PHE  |
| 1   | 3     | 146 | ASP  |
| 1   | 3     | 149 | GLN  |
| 1   | 3     | 165 | LEU  |
| 1   | 4     | 1   | MET  |
| 1   | 4     | 6   | MET  |
| 1   | 4     | 15  | ASN  |
| 1   | 4     | 72  | GLU  |
| 1   | 4     | 96  | PHE  |
| 1   | 4     | 104 | LEU  |
| 1   | 4     | 109 | GLU  |
| 1   | 5     | 22  | TYR  |
| 1   | 5     | 72  | GLU  |
| 1   | 5     | 100 | SER  |
| 1   | 5     | 104 | LEU  |
| 1   | 6     | 6   | MET  |
| 1   | 6     | 22  | TYR  |
| 1   | 6     | 72  | GLU  |
| 1   | 6     | 78  | LYS  |
| 1   | 6     | 88  | GLU  |
| 1   | 6     | 149 | GLN  |
| 1   | 7     | 4   | GLU  |
| 1   | 7     | 22  | TYR  |
| 1   | 7     | 58  | TYR  |
| 1   | 7     | 65  | ASN  |
| 1   | 7     | 98  | SER  |
| 1   | 7     | 100 | SER  |
| 1   | 7     | 104 | LEU  |
| 1   | 7     | 109 | GLU  |
| 1   | 7     | 117 | ARG  |
| 1   | 7     | 119 | PHE  |
| 1   | 7     | 133 | SER  |
| 1   | 7     | 146 | ASP  |
| 1   | 7     | 154 | LEU  |
| 1   | 7     | 164 | LYS  |
| 1   | 8     | 1   | MET  |
| 1   | 8     | 5   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 8     | 6   | MET  |
| 1   | 8     | 20  | SER  |
| 1   | 8     | 22  | TYR  |
| 1   | 8     | 85  | LYS  |
| 1   | 8     | 104 | LEU  |
| 1   | 8     | 133 | SER  |
| 1   | 8     | 154 | LEU  |
| 1   | 8     | 165 | LEU  |
| 1   | 9     | 5   | ARG  |
| 1   | 9     | 15  | ASN  |
| 1   | 9     | 22  | TYR  |
| 1   | 9     | 65  | ASN  |
| 1   | 9     | 133 | SER  |
| 1   | 9     | 136 | LYS  |
| 1   | 9     | 143 | PHE  |
| 1   | 9     | 149 | GLN  |
| 1   | 9     | 165 | LEU  |
| 1   | A     | 1   | MET  |
| 1   | A     | 3   | SER  |
| 1   | A     | 22  | TYR  |
| 1   | A     | 72  | GLU  |
| 1   | A     | 110 | GLU  |
| 1   | A     | 135 | LYS  |
| 1   | A     | 149 | GLN  |
| 1   | B     | 5   | ARG  |
| 1   | B     | 20  | SER  |
| 1   | B     | 22  | TYR  |
| 1   | B     | 34  | LEU  |
| 1   | B     | 67  | ARG  |
| 1   | B     | 72  | GLU  |
| 1   | B     | 149 | GLN  |
| 1   | B     | 154 | LEU  |
| 1   | C     | 1   | MET  |
| 1   | C     | 5   | ARG  |
| 1   | C     | 6   | MET  |
| 1   | C     | 34  | LEU  |
| 1   | C     | 72  | GLU  |
| 1   | C     | 149 | GLN  |
| 1   | D     | 1   | MET  |
| 1   | D     | 6   | MET  |
| 1   | D     | 22  | TYR  |
| 1   | D     | 72  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 92  | GLU  |
| 1   | D     | 104 | LEU  |
| 1   | D     | 145 | LYS  |
| 1   | D     | 149 | GLN  |
| 1   | E     | 6   | MET  |
| 1   | E     | 22  | TYR  |
| 1   | E     | 67  | ARG  |
| 1   | E     | 92  | GLU  |
| 1   | E     | 104 | LEU  |
| 1   | E     | 110 | GLU  |
| 1   | E     | 149 | GLN  |
| 1   | F     | 1   | MET  |
| 1   | F     | 6   | MET  |
| 1   | F     | 15  | ASN  |
| 1   | F     | 22  | TYR  |
| 1   | F     | 72  | GLU  |
| 1   | F     | 100 | SER  |
| 1   | F     | 119 | PHE  |
| 1   | F     | 146 | ASP  |
| 1   | F     | 152 | PHE  |
| 1   | F     | 165 | LEU  |
| 1   | G     | 1   | MET  |
| 1   | G     | 67  | ARG  |
| 1   | G     | 78  | LYS  |
| 1   | G     | 81  | GLU  |
| 1   | G     | 100 | SER  |
| 1   | G     | 149 | GLN  |
| 1   | H     | 1   | MET  |
| 1   | H     | 6   | MET  |
| 1   | H     | 22  | TYR  |
| 1   | H     | 58  | TYR  |
| 1   | H     | 67  | ARG  |
| 1   | H     | 110 | GLU  |
| 1   | H     | 119 | PHE  |
| 1   | H     | 147 | SER  |
| 1   | I     | 5   | ARG  |
| 1   | I     | 72  | GLU  |
| 1   | I     | 104 | LEU  |
| 1   | I     | 119 | PHE  |
| 1   | I     | 136 | LYS  |
| 1   | I     | 143 | PHE  |
| 1   | I     | 145 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 22  | TYR  |
| 1   | J     | 33  | ASP  |
| 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     | 22  | TYR  |
| 1   | K     | 33  | ASP  |
| 1   | K     | 72  | GLU  |
| 1   | K     | 81  | GLU  |
| 1   | K     | 104 | LEU  |
| 1   | K     | 121 | GLU  |
| 1   | K     | 149 | GLN  |
| 1   | K     | 165 | LEU  |
| 1   | L     | 6   | MET  |
| 1   | L     | 22  | TYR  |
| 1   | L     | 69  | GLU  |
| 1   | L     | 92  | GLU  |
| 1   | L     | 133 | SER  |
| 1   | L     | 149 | GLN  |
| 1   | L     | 165 | LEU  |
| 1   | M     | 1   | MET  |
| 1   | M     | 6   | MET  |
| 1   | M     | 22  | TYR  |
| 1   | M     | 69  | GLU  |
| 1   | M     | 72  | GLU  |
| 1   | M     | 99  | LYS  |
| 1   | M     | 103 | GLU  |
| 1   | M     | 149 | GLN  |
| 1   | M     | 154 | LEU  |
| 1   | M     | 164 | LYS  |
| 1   | N     | 4   | GLU  |
| 1   | N     | 6   | MET  |
| 1   | N     | 22  | TYR  |
| 1   | N     | 56  | ARG  |
| 1   | N     | 149 | GLN  |
| 1   | O     | 1   | MET  |
| 1   | O     | 4   | GLU  |
| 1   | O     | 11  | ASN  |
| 1   | O     | 22  | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | O     | 72  | GLU  |
| 1   | O     | 83  | PRO  |
| 1   | O     | 85  | LYS  |
| 1   | O     | 92  | GLU  |
| 1   | O     | 98  | SER  |
| 1   | O     | 99  | LYS  |
| 1   | O     | 100 | SER  |
| 1   | O     | 133 | SER  |
| 1   | P     | 22  | TYR  |
| 1   | P     | 95  | LYS  |
| 1   | P     | 100 | SER  |
| 1   | P     | 133 | SER  |
| 1   | P     | 149 | GLN  |
| 1   | P     | 153 | MET  |
| 1   | P     | 164 | LYS  |
| 1   | Q     | 1   | MET  |
| 1   | Q     | 6   | MET  |
| 1   | Q     | 22  | TYR  |
| 1   | Q     | 75  | LYS  |
| 1   | Q     | 100 | SER  |
| 1   | Q     | 103 | GLU  |
| 1   | Q     | 145 | LYS  |
| 1   | Q     | 146 | ASP  |
| 1   | Q     | 156 | LYS  |
| 1   | R     | 1   | MET  |
| 1   | R     | 5   | ARG  |
| 1   | R     | 6   | MET  |
| 1   | R     | 15  | ASN  |
| 1   | R     | 22  | TYR  |
| 1   | R     | 72  | GLU  |
| 1   | R     | 110 | GLU  |
| 1   | R     | 165 | LEU  |
| 1   | S     | 1   | MET  |
| 1   | S     | 22  | TYR  |
| 1   | S     | 34  | LEU  |
| 1   | S     | 67  | ARG  |
| 1   | S     | 99  | LYS  |
| 1   | S     | 146 | ASP  |
| 1   | S     | 149 | GLN  |
| 1   | S     | 165 | LEU  |
| 1   | T     | 1   | MET  |
| 1   | T     | 22  | TYR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | T     | 34  | LEU  |
| 1   | T     | 72  | GLU  |
| 1   | T     | 154 | LEU  |
| 1   | U     | 1   | MET  |
| 1   | U     | 34  | LEU  |
| 1   | U     | 72  | GLU  |
| 1   | U     | 154 | LEU  |
| 1   | U     | 165 | LEU  |
| 1   | V     | 1   | MET  |
| 1   | V     | 6   | MET  |
| 1   | V     | 72  | GLU  |
| 1   | V     | 103 | GLU  |
| 1   | V     | 145 | LYS  |
| 1   | V     | 149 | GLN  |
| 1   | V     | 153 | MET  |
| 1   | V     | 154 | LEU  |
| 1   | W     | 34  | LEU  |
| 1   | W     | 81  | GLU  |
| 1   | W     | 119 | PHE  |
| 1   | W     | 135 | LYS  |
| 1   | W     | 149 | GLN  |
| 1   | W     | 154 | LEU  |
| 1   | X     | 5   | ARG  |
| 1   | X     | 22  | TYR  |
| 1   | X     | 65  | ASN  |
| 1   | X     | 104 | LEU  |
| 1   | X     | 149 | GLN  |
| 1   | X     | 157 | GLU  |
| 1   | Y     | 5   | ARG  |
| 1   | Y     | 67  | ARG  |
| 1   | Y     | 100 | SER  |
| 1   | Y     | 104 | LEU  |
| 1   | Y     | 149 | GLN  |
| 1   | Y     | 165 | LEU  |
| 1   | Z     | 6   | MET  |
| 1   | Z     | 11  | ASN  |
| 1   | Z     | 22  | TYR  |
| 1   | Z     | 72  | GLU  |
| 1   | Z     | 149 | GLN  |
| 1   | Z     | 165 | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 149 | GLN  |
| 1   | 2     | 15  | ASN  |
| 1   | 2     | 149 | GLN  |
| 1   | 3     | 15  | ASN  |
| 1   | 3     | 149 | GLN  |
| 1   | 6     | 149 | GLN  |
| 1   | 7     | 15  | ASN  |
| 1   | 7     | 65  | ASN  |
| 1   | 8     | 149 | GLN  |
| 1   | 9     | 15  | ASN  |
| 1   | 9     | 65  | ASN  |
| 1   | 9     | 149 | GLN  |
| 1   | B     | 149 | GLN  |
| 1   | F     | 15  | ASN  |
| 1   | G     | 149 | GLN  |
| 1   | I     | 11  | ASN  |
| 1   | I     | 149 | GLN  |
| 1   | J     | 149 | GLN  |
| 1   | K     | 149 | GLN  |
| 1   | M     | 13  | GLN  |
| 1   | M     | 15  | ASN  |
| 1   | N     | 65  | ASN  |
| 1   | N     | 149 | GLN  |
| 1   | O     | 149 | GLN  |
| 1   | Q     | 149 | GLN  |
| 1   | R     | 11  | ASN  |
| 1   | R     | 15  | ASN  |
| 1   | R     | 149 | GLN  |
| 1   | S     | 149 | GLN  |
| 1   | U     | 149 | GLN  |
| 1   | W     | 149 | GLN  |
| 1   | X     | 149 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 134 ligands modelled in this entry, 108 are monoatomic - leaving 26 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  | R     | 1168 | -    | 4,4,4        | 0.18 | 0           | 6,6,6       | 0.25 | 0           |
| 3   | SO4  | C     | 1169 | -    | 4,4,4        | 0.29 | 0           | 6,6,6       | 0.51 | 0           |
| 3   | SO4  | 2     | 1668 | -    | 4,4,4        | 0.16 | 0           | 6,6,6       | 0.25 | 0           |
| 3   | SO4  | O     | 1168 | -    | 4,4,4        | 0.12 | 0           | 6,6,6       | 0.48 | 0           |
| 3   | SO4  | I     | 1168 | -    | 4,4,4        | 0.38 | 0           | 6,6,6       | 0.51 | 0           |
| 3   | SO4  | G     | 1168 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.38 | 0           |
| 3   | SO4  | V     | 1669 | -    | 4,4,4        | 0.14 | 0           | 6,6,6       | 0.44 | 0           |
| 3   | SO4  | 1     | 1668 | -    | 4,4,4        | 0.18 | 0           | 6,6,6       | 0.18 | 0           |
| 3   | SO4  | G     | 1169 | -    | 4,4,4        | 0.18 | 0           | 6,6,6       | 0.27 | 0           |
| 3   | SO4  | B     | 1169 | -    | 4,4,4        | 0.15 | 0           | 6,6,6       | 0.50 | 0           |
| 3   | SO4  | W     | 1668 | -    | 4,4,4        | 0.20 | 0           | 6,6,6       | 0.40 | 0           |
| 3   | SO4  | B     | 1168 | -    | 4,4,4        | 0.20 | 0           | 6,6,6       | 0.23 | 0           |
| 3   | SO4  | C     | 1170 | -    | 4,4,4        | 0.15 | 0           | 6,6,6       | 0.30 | 0           |
| 3   | SO4  | Y     | 1669 | -    | 4,4,4        | 0.24 | 0           | 6,6,6       | 0.29 | 0           |
| 3   | SO4  | H     | 1168 | -    | 4,4,4        | 0.17 | 0           | 6,6,6       | 0.43 | 0           |
| 3   | SO4  | J     | 1168 | -    | 4,4,4        | 0.20 | 0           | 6,6,6       | 0.27 | 0           |
| 3   | SO4  | Y     | 1668 | -    | 4,4,4        | 0.19 | 0           | 6,6,6       | 0.30 | 0           |
| 3   | SO4  | V     | 1668 | -    | 4,4,4        | 0.17 | 0           | 6,6,6       | 0.44 | 0           |
| 3   | SO4  | 8     | 1668 | -    | 4,4,4        | 0.16 | 0           | 6,6,6       | 0.36 | 0           |
| 3   | SO4  | 3     | 1668 | -    | 4,4,4        | 0.12 | 0           | 6,6,6       | 0.53 | 0           |
| 3   | SO4  | C     | 1168 | -    | 4,4,4        | 0.13 | 0           | 6,6,6       | 0.26 | 0           |
| 3   | SO4  | A     | 1168 | -    | 4,4,4        | 0.17 | 0           | 6,6,6       | 0.44 | 0           |
| 3   | SO4  | T     | 1668 | -    | 4,4,4        | 0.21 | 0           | 6,6,6       | 0.37 | 0           |
| 3   | SO4  | I     | 1169 | -    | 4,4,4        | 0.17 | 0           | 6,6,6       | 0.68 | 0           |
| 3   | SO4  | 3     | 1669 | -    | 4,4,4        | 0.23 | 0           | 6,6,6       | 0.53 | 0           |
| 3   | SO4  | S     | 1668 | -    | 4,4,4        | 0.16 | 0           | 6,6,6       | 0.21 | 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.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | Y     | 1669 | SO4  | 1       | 0            |

## 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.