



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:35 PM UTC

PDB ID : 7M7F / pdb\_00007m7f  
EMDB ID : EMD-23711  
Title : 6-Deoxyerythronolide B synthase (DEBS) module 1 in complex with antibody fragment 1B2: State 1  
Authors : Cogan, D.P.; Zhang, K.; Chiu, W.; Khosla, C.  
Deposited on : 2021-03-28  
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

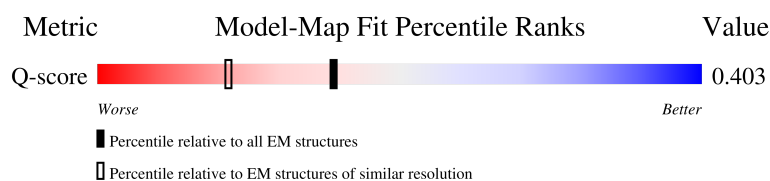
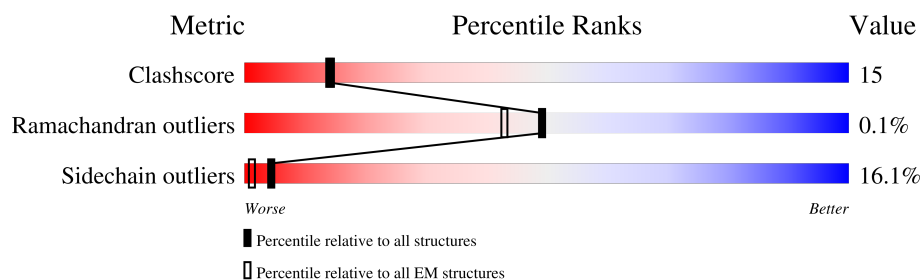
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 15020 ( 2.70 - 3.70 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 1   | A     | 1784   | <div> <div>11%</div> <div>46%</div> <div>26%</div> <div>• •</div> <div>22%</div> </div>           |
| 1   | B     | 1784   | <div> <div>6%</div> <div>33%</div> <div>20%</div> <div>•</div> <div>44%</div> </div>              |
| 2   | C     | 249    | <div> <div>•</div> <div>44%</div> <div>29%</div> <div>8%</div> <div>•</div> <div>18%</div> </div> |
| 2   | E     | 249    | <div> <div>•</div> <div>43%</div> <div>31%</div> <div>8%</div> <div>•</div> <div>18%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                              |
|-----|-------|--------|-------------------------------------------------------------------------------|
| 3   | D     | 236    | <div><div></div><div>43%</div><div>40%</div><div>•</div><div>13%</div></div>  |
| 3   | F     | 236    | <div><div></div><div>42%</div><div>40%</div><div>5%</div><div>13%</div></div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23971 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | B     | 999      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7417  | 4613 | 1363 | 1414 | 27 |         |       |
| 1   | A     | 1390     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 10319 | 6413 | 1899 | 1972 | 35 |         |       |

There are 106 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 1       | MET      | -      | expression tag | UNP Q5UNP6 |
| B     | 2       | ALA      | -      | expression tag | UNP Q5UNP6 |
| B     | 3       | SER      | -      | expression tag | UNP Q5UNP6 |
| B     | 4       | THR      | -      | expression tag | UNP Q5UNP6 |
| B     | 5       | ASP      | -      | expression tag | UNP Q5UNP6 |
| B     | 6       | SER      | -      | expression tag | UNP Q5UNP6 |
| B     | 7       | GLU      | -      | expression tag | UNP Q5UNP6 |
| B     | 8       | LYS      | -      | expression tag | UNP Q5UNP6 |
| B     | 9       | VAL      | -      | expression tag | UNP Q5UNP6 |
| B     | 10      | ALA      | -      | expression tag | UNP Q5UNP6 |
| B     | 11      | GLU      | -      | expression tag | UNP Q5UNP6 |
| B     | 12      | TYR      | -      | expression tag | UNP Q5UNP6 |
| B     | 13      | LEU      | -      | expression tag | UNP Q5UNP6 |
| B     | 14      | ARG      | -      | expression tag | UNP Q5UNP6 |
| B     | 15      | ARG      | -      | expression tag | UNP Q5UNP6 |
| B     | 16      | ALA      | -      | expression tag | UNP Q5UNP6 |
| B     | 17      | THR      | -      | expression tag | UNP Q5UNP6 |
| B     | 18      | LEU      | -      | expression tag | UNP Q5UNP6 |
| B     | 19      | ASP      | -      | expression tag | UNP Q5UNP6 |
| B     | 20      | LEU      | -      | expression tag | UNP Q5UNP6 |
| B     | 21      | ARG      | -      | expression tag | UNP Q5UNP6 |
| B     | 22      | ALA      | -      | expression tag | UNP Q5UNP6 |
| B     | 23      | ALA      | -      | expression tag | UNP Q5UNP6 |
| B     | 24      | ARG      | -      | expression tag | UNP Q5UNP6 |
| B     | 25      | GLN      | -      | expression tag | UNP Q5UNP6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 26      | ARG      | -      | expression tag | UNP Q5UNP6 |
| B     | 27      | ILE      | -      | expression tag | UNP Q5UNP6 |
| B     | 28      | ARG      | -      | expression tag | UNP Q5UNP6 |
| B     | 29      | GLU      | -      | expression tag | UNP Q5UNP6 |
| B     | 30      | LEU      | -      | expression tag | UNP Q5UNP6 |
| B     | 31      | GLU      | -      | expression tag | UNP Q5UNP6 |
| B     | 1486    | THR      | -      | linker         | UNP Q5UNP6 |
| B     | 1487    | SER      | -      | linker         | UNP Q5UNP6 |
| B     | 1488    | GLU      | -      | linker         | UNP Q5UNP6 |
| B     | 1489    | LEU      | -      | linker         | UNP Q5UNP6 |
| B     | 1490    | GLY      | -      | linker         | UNP Q5UNP6 |
| B     | 1768    | SER      | -      | expression tag | UNP Q03133 |
| B     | 1769    | SER      | -      | expression tag | UNP Q03133 |
| B     | 1770    | VAL      | -      | expression tag | UNP Q03133 |
| B     | 1771    | ASP      | -      | expression tag | UNP Q03133 |
| B     | 1772    | LYS      | -      | expression tag | UNP Q03133 |
| B     | 1773    | LEU      | -      | expression tag | UNP Q03133 |
| B     | 1774    | ALA      | -      | expression tag | UNP Q03133 |
| B     | 1775    | ALA      | -      | expression tag | UNP Q03133 |
| B     | 1776    | ALA      | -      | expression tag | UNP Q03133 |
| B     | 1777    | LEU      | -      | expression tag | UNP Q03133 |
| B     | 1778    | GLU      | -      | expression tag | UNP Q03133 |
| B     | 1779    | HIS      | -      | expression tag | UNP Q03133 |
| B     | 1780    | HIS      | -      | expression tag | UNP Q03133 |
| B     | 1781    | HIS      | -      | expression tag | UNP Q03133 |
| B     | 1782    | HIS      | -      | expression tag | UNP Q03133 |
| B     | 1783    | HIS      | -      | expression tag | UNP Q03133 |
| B     | 1784    | HIS      | -      | expression tag | UNP Q03133 |
| A     | 1       | MET      | -      | expression tag | UNP Q5UNP6 |
| A     | 2       | ALA      | -      | expression tag | UNP Q5UNP6 |
| A     | 3       | SER      | -      | expression tag | UNP Q5UNP6 |
| A     | 4       | THR      | -      | expression tag | UNP Q5UNP6 |
| A     | 5       | ASP      | -      | expression tag | UNP Q5UNP6 |
| A     | 6       | SER      | -      | expression tag | UNP Q5UNP6 |
| A     | 7       | GLU      | -      | expression tag | UNP Q5UNP6 |
| A     | 8       | LYS      | -      | expression tag | UNP Q5UNP6 |
| A     | 9       | VAL      | -      | expression tag | UNP Q5UNP6 |
| A     | 10      | ALA      | -      | expression tag | UNP Q5UNP6 |
| A     | 11      | GLU      | -      | expression tag | UNP Q5UNP6 |
| A     | 12      | TYR      | -      | expression tag | UNP Q5UNP6 |
| A     | 13      | LEU      | -      | expression tag | UNP Q5UNP6 |
| A     | 14      | ARG      | -      | expression tag | UNP Q5UNP6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 15      | ARG      | -      | expression tag | UNP Q5UNP6 |
| A     | 16      | ALA      | -      | expression tag | UNP Q5UNP6 |
| A     | 17      | THR      | -      | expression tag | UNP Q5UNP6 |
| A     | 18      | LEU      | -      | expression tag | UNP Q5UNP6 |
| A     | 19      | ASP      | -      | expression tag | UNP Q5UNP6 |
| A     | 20      | LEU      | -      | expression tag | UNP Q5UNP6 |
| A     | 21      | ARG      | -      | expression tag | UNP Q5UNP6 |
| A     | 22      | ALA      | -      | expression tag | UNP Q5UNP6 |
| A     | 23      | ALA      | -      | expression tag | UNP Q5UNP6 |
| A     | 24      | ARG      | -      | expression tag | UNP Q5UNP6 |
| A     | 25      | GLN      | -      | expression tag | UNP Q5UNP6 |
| A     | 26      | ARG      | -      | expression tag | UNP Q5UNP6 |
| A     | 27      | ILE      | -      | expression tag | UNP Q5UNP6 |
| A     | 28      | ARG      | -      | expression tag | UNP Q5UNP6 |
| A     | 29      | GLU      | -      | expression tag | UNP Q5UNP6 |
| A     | 30      | LEU      | -      | expression tag | UNP Q5UNP6 |
| A     | 31      | GLU      | -      | expression tag | UNP Q5UNP6 |
| A     | 1486    | THR      | -      | linker         | UNP Q5UNP6 |
| A     | 1487    | SER      | -      | linker         | UNP Q5UNP6 |
| A     | 1488    | GLU      | -      | linker         | UNP Q5UNP6 |
| A     | 1489    | LEU      | -      | linker         | UNP Q5UNP6 |
| A     | 1490    | GLY      | -      | linker         | UNP Q5UNP6 |
| A     | 1768    | SER      | -      | expression tag | UNP Q03133 |
| A     | 1769    | SER      | -      | expression tag | UNP Q03133 |
| A     | 1770    | VAL      | -      | expression tag | UNP Q03133 |
| A     | 1771    | ASP      | -      | expression tag | UNP Q03133 |
| A     | 1772    | LYS      | -      | expression tag | UNP Q03133 |
| A     | 1773    | LEU      | -      | expression tag | UNP Q03133 |
| A     | 1774    | ALA      | -      | expression tag | UNP Q03133 |
| A     | 1775    | ALA      | -      | expression tag | UNP Q03133 |
| A     | 1776    | ALA      | -      | expression tag | UNP Q03133 |
| A     | 1777    | LEU      | -      | expression tag | UNP Q03133 |
| A     | 1778    | GLU      | -      | expression tag | UNP Q03133 |
| A     | 1779    | HIS      | -      | expression tag | UNP Q03133 |
| A     | 1780    | HIS      | -      | expression tag | UNP Q03133 |
| A     | 1781    | HIS      | -      | expression tag | UNP Q03133 |
| A     | 1782    | HIS      | -      | expression tag | UNP Q03133 |
| A     | 1783    | HIS      | -      | expression tag | UNP Q03133 |
| A     | 1784    | HIS      | -      | expression tag | UNP Q03133 |

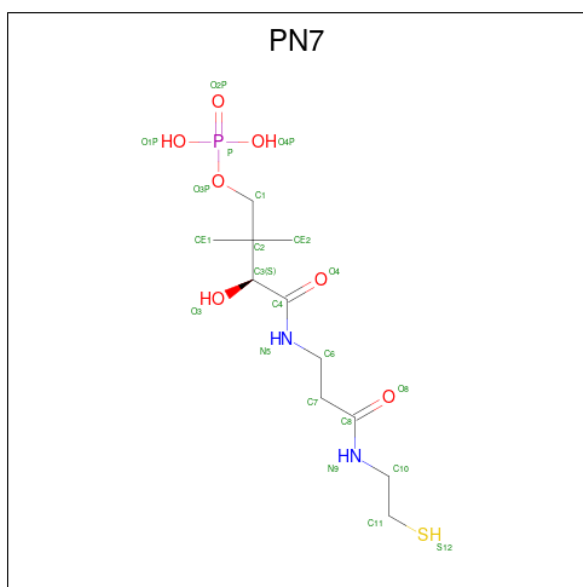
- Molecule 2 is a protein called 1B2 (heavy chain).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | C     | 205      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1539  | 978 | 257 | 298 | 6 |         |       |
| 2   | E     | 205      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1539  | 978 | 257 | 298 | 6 |         |       |

- Molecule 3 is a protein called 1B2 (light chain).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | D     | 206      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1568  | 983 | 262 | 317 | 6 |         |       |
| 3   | F     | 206      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1568  | 984 | 262 | 316 | 6 |         |       |

- Molecule 4 is N 3 -[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-(2-sulfanylet hyl)-beta-alaninamide (CCD ID: PN7) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 4   | B     | 1        | Total | C  | N | O | P | S       |
|     |       |          | 21    | 11 | 2 | 6 | 1 | 1       |
|     |       |          |       |    |   |   |   | 0       |



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
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| ASP | ALA | TRP | LEU | GLY | GLY | ASN | SER | SER | VAL | LYS | LEU | ALA | ALA | ALA | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | HIS | 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● Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

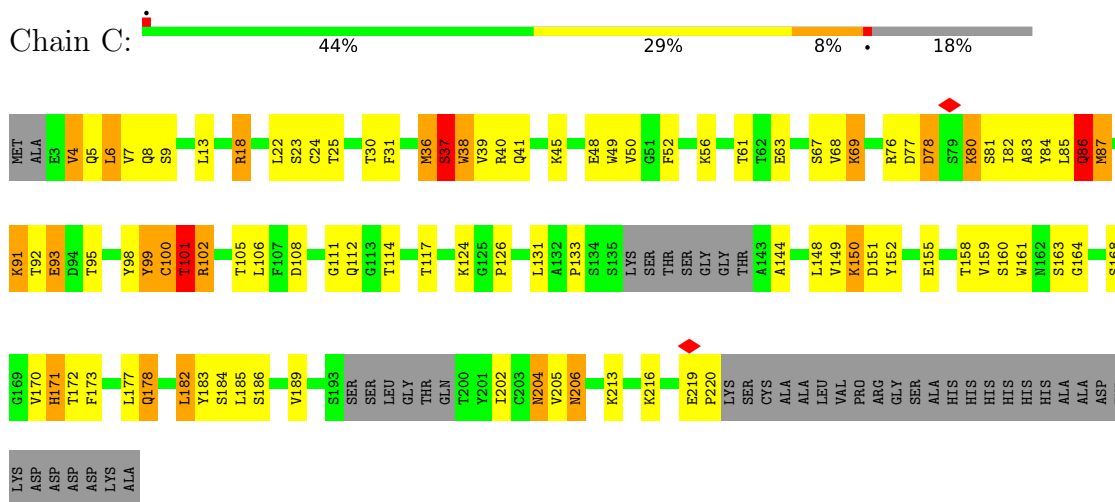


|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| M1   | A2   | S3   | T4   | D5   | S6   | E7   | K8   | V9   | Y12  | L13  | E14  | R15  | A16  | T17  | R24  | E29  | E33  | V38  | A39  | M40  | A41  | C42  | R43  | I44  | E52  | E53  | F54  | W55  | E56  | L57  | R62  | D63  | A64  | V65  | P68  | T70  | D71  | R86  | S87  | H91  | Q92  | R93  | G94  | F97  | L98  | A103 |
| F108 | A116 | I117 | A118 | V119 | D120 | Q123 | R124 | L125 | M126 | L129 | S130 | A131 | E132 | V133 | A137 | G138 | I139 | P140 | P141 | T149 | V153 | G154 | L155 | I156 | P157 | Q158 | E159 | P162 | R163 | V171 | E172 | G173 | Y174 | L175 | M176 | T177 | G178 | T180 | V183 | A184 | I188 | R189 | L194 | P197 | S200 | V201 |

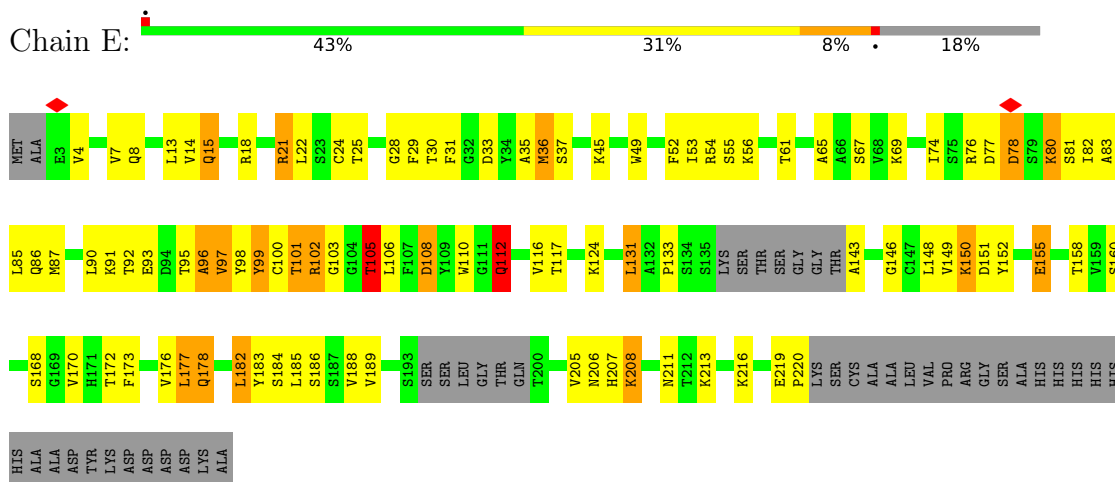
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| G1325 | F1326 | V1327 | R1330 | F1331 | R1332 | R1333 | H1334 | V1335 | V1336 | I1337 | E1338 | M1339 | P1340 | P1341 | E1342 | V1357 | T1360 | V1361 | D1362 | D1363 | V1364 | R1365 | W1366 | D1367 | F1368 | F1369 | L1370 | L1371 | Q1376 | R1377 | F1378 | L1379 | R1380 | D1383 | E1384 | I1385 | R1389 | R1390 | ALA   | ALA   | PRO   | GLN   | ALA   | ALA   | GLU   | PRO   | ARG   | VAL   | GLY   | ALA   | LEU   | ALA   |       |       |       |       |       |
| H1242 | R1243 | I1244 | A1247 | S1248 | R1249 | A1250 | K1251 | V1252 | L1253 | L1258 | H1259 | E1260 | L1261 | T1262 | K1263 | F1264 | L1265 | D1266 | L1267 | T1268 | D1269 | V1270 | F1271 | L1272 | S1278 | Y1288 | A1289 | L1295 | D1296 | G1297 | L1298 | A1299 | Q1300 | Q1301 | R1302 | S1303 | S1304 | D1305 | G1306 | L1307 | P1308 | A1309 | T1310 | A1311 | V1312 | A1313 | W1317 | A1318 | G1321 | M1322 | A1323 | E1324 |       |       |       |       |       |
| G1164 | A1165 | P1166 | H1167 | L1168 | L1169 | L1170 | V1171 | S1172 | R1173 | P1176 | D1177 | A1178 | D1179 | E1183 | L1184 | L1188 | E1189 | A1190 | R1194 | T1195 | V1196 | L1197 | A1198 | A1199 | C1200 | D1201 | V1202 | E1206 | R1209 | E1210 | L1211 | D1217 | D1218 | V1219 | S1222 | A1223 | V1224 | F1225 | H1226 | A1229 | T1230 | L1231 | T1235 | V1236 | D1237 | M1238 | L1239 | T1240 | G1241 |       |       |       |       |       |       |       |       |
| H1068 | G1069 | V1070 | G1071 | R1072 | V1073 | I1074 | A1075 | M1078 | P1079 | A1080 | V1081 | W1082 | L1085 | V1086 | D1087 | V1088 | F1089 | A1090 | V1093 | L1096 | L1100 | S1105 | E1110 | Q1111 | Q1112 | L1113 | A1114 | W1125 | A1129 | D1135 | E1136 | W1137 | P1138 | V1139 | V1143 | L1144 | V1145 | V1152 | Q1155 | A1156 | R1157 | M1158 | V1159 | L1160 | R1163 |       |       |       |       |       |       |       |       |       |       |       |       |
| G0969 | E0970 | V0976 | R0977 | E0978 | V0979 | D0980 | V0981 | D0982 | L0990 | G0998 | E0999 | V1000 | A1001 | G1002 | V1003 | L1004 | L1007 | D1010 | E1013 | P1014 | E1015 | L1019 | A1025 | L1028 | S1029 | L1030 | V1031 | Q1032 | A1033 | M1034 | A1037 | E1038 | L1039 | L1043 | W1044 | E1048 | S1049 | G1054 | P1055 | F1056 | R1060 | M1061 | V1062 | A1063 | A1066 | L1067 |       |       |       |       |       |       |       |       |       |       |       |
| G0869 | E0870 | V0880 | A0881 | V0882 | D0883 | V0884 | R0894 | R0895 | V0896 | P0897 | L0898 | P0899 | R0905 | E0906 | R0907 | V0908 | W0909 | E0911 | K0912 | K0913 | V0914 | V0915 | A0916 | R0917 | R0918 | S0919 | L0928 | R0929 | Y0930 | R0931 | Y0932 | A0943 | R0944 | L0945 | L0946 | G0947 | T0948 | W0949 | L0950 | A0955 | G0956 | T0957 | A0958 | D0959 | E0960 | T0961 | R0966 | L0969 | A0972 |       |       |       |       |       |       |       |       |
| L0798 | D0799 | A0800 | G0801 | Y0802 | W0803 | Y0804 | R0805 | R0806 | L0807 | R0808 | R0809 | T0810 | V0811 | R0812 | F0813 | A0814 | D0815 | A0816 | V0817 | L0820 | A0821 | E0822 | R0826 | L0829 | E0830 | V0831 | L0837 | T0838 | A0839 | A0840 | T0841 | E0842 | E0843 | I0844 | G0845 | D0846 | G0847 | S0848 | G0849 | A0850 | D0851 | L0852 | S0853 | A0854 | I0855 | H0856 | R0859 | R0860 | G0861 | L0865 | A0866 | D0867 | F0868 |       |       |       |       |
| R0734 | L0735 | V0736 | A0737 | S0738 | C0739 | T0740 | T0741 | E0742 | C0743 | I0744 | R0745 | A0746 | K0747 | R0748 | L0749 | A0750 | V0751 | D0752 | A0754 | S0755 | H0756 | S0757 | S0758 | H0759 | V0760 | T0761 | T0762 | I0763 | R0764 | D0765 | A0766 | L0767 | H0768 | A0769 | E0770 | L0771 | G0772 | E0773 | D0774 | H0775 | H0776 | P0777 | L0778 | P0779 | G0780 | F0781 | V0782 | P0783 | F0784 | H0785 | S0786 | W0792 | T0793 | Q0794 | P0795 | E0796 | E0797 |
| D0673 | A0674 | A0675 | R0676 | A0679 | L0680 | R0681 | S0682 | R0683 | V0684 | R0685 | A0686 | T0687 | M0688 | G0689 | N0691 | K0692 | G0693 | M0694 | A0695 | S0696 | I0697 | A0698 | A0699 | T0700 | G0701 | A0702 | E0703 | D0704 | R0705 | A0706 | S0707 | I0708 | G0709 | D0710 | R0711 | V0712 | E0713 | I0714 | A0715 | A0716 | H0717 | W0718 | G0719 | P0720 | R0721 | S0722 | V0723 | T0724 | V0725 | A0726 | G0727 | D0728 | S0729 | D0730 | E0731 | L0732 | D0733 |
| E0601 | V0602 | I0603 | P0604 | F0605 | L0606 | R0607 | A0608 | E0609 | A0610 | A0611 | R0612 | R0613 | E0614 | Q0615 | D0616 | A0617 | A0618 | L0619 | S0620 | T0621 | E0622 | R0623 | V0624 | D0625 | V0626 | G0627 | A0628 | S0629 | M0630 | M0631 | M0635 | L0638 | A0639 | S0640 | M0641 | W0642 | R0643 | G0646 | V0647 | E0648 | V0652 | I0653 | G0654 | H0655 | S0656 | Q0657 | G0658 | E0659 | I0660 | A0666 | G0667 | A0668 | D0672 |       |       |       |       |
| L0518 | A0522 | A0523 | F0524 | P0525 | P0526 | V0527 | D0528 | E0529 | S0530 | A0531 | A0532 | L0533 | R0534 | V0535 | L0536 | L0539 | Q0555 | Q0556 | R0557 | A0558 | V0561 | F0562 | Q0565 | Q0568 | V0569 | A0570 | G0571 | M0572 | A0573 | V0574 | L0576 | L0577 | L0585 | D0578 | T0579 | S0580 | A0584 | A0585 | R0588 | E0589 | C0590 | A0591 | D0592 | A0593 | L0594 | L0595 | P0596 | H0597 | L0598 | D0599 | F0600 |       |       |       |       |       |       |
| I0413 | I0420 | S0421 | L0422 | R0437 | A0438 | G0439 | V0440 | A0441 | S0442 | F0443 | N0449 | I0453 | I0454 | A0455 | V0460 | E0462 | G0463 | E0464 | R0465 | V0466 | E0467 | V0471 | V0476 | L0477 | S0478 | A0479 | S0480 | L0485 | Q0488 | L0492 | A0493 | A0494 | H0495 | R0497 | E0498 | R0505 | D0506 | S0510 | L0511 | L0512 | R0515 | A0516 | A0517 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| N0312 | A0315 | Q0316 | V0317 | R0318 | V0319 | L0329 | G0330 | P0331 | L0334 | V0337 | E0338 | A0339 | H0340 | G0341 | T0342 | T0344 | P0349 | I0350 | A0358 | Y0359 | R0363 | L0367 | H0368 | L0369 | G0372 | S0374 | N0375 | L0376 | Q0380 | A0381 | V0385 | V0388 | I0389 | K0390 | M0391 | V0392 | L0393 | P0401 | R0402 | T0403 | L0404 | H0405 | A0406 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| D0202 | T0203 | S0207 | S0208 | L0209 | R0220 | R0221 | G0222 | G0223 | S0224 | S0225 | L0226 | A0227 | M0228 | V0232 | T0233 | V0234 | M0235 | P0236 | M0240 | L0241 | V0242 | D0243 | F0244 | M0247 | L0260 | D0253 | G0254 | R0255 | G0256 | F0266 | M0268 | A0269 | E0270 | G0271 | A0272 | L0276 | L0277 | E0278 | V0283 | D0302 | S0305 | W0306 | G0307 | L0308 | P0311 |       |       |       |       |       |       |       |       |       |       |       |       |

|     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASN | SER | SER | GLY | PRO | PRO | GLN | SER | ARG | SER |
| SER | SER | GLY | LEU | ARG | GLN | GLY | ASP | LEU | PRO |
| SER | PRO | GLY | THR | PRO | PRO | PRO | PHE | PRO | ALA |
| VAL | VAL | VAL | LEU | VAL | TYR | TYR | GLU | THR | THR |
| ASP | ASP | LEU | LEU | LEU | GLU | GLU | HIS | THR | GLU |
| LYS | VAL | VAL | VAL | ILE | GLY | GLY | PHE | VAL | ARG |
| LEU | SER | SER | SER | ASP | GLY | GLY | ASP | PHE | GLU |
| ALA | ALA | ALA | ALA | VAL | GLU | GLU | GLY | ASP | LYS |
| ALA | ALA | GLY | GLY | TYR | PRO | PRO | SER | HIS | LEU |
| ALA | GLU | GLU | GLU | PRO | PRO | PRO | GLY | PRO | ASP |
| LEU | LEU | PRO | PRO | PRO | SER | SER | PHE | VAL | GLU |
| GLU | GLU | MET | GLY | GLY | GLY | GLY | GLY | VAL | ASP |
| HIS | HIS | GLY | HIS | HIS | SER | SER | LEU | ARG | VAL |
| HIS | HIS | PRO | THR | ASP | ALA | ASP | LEU | LEU | SER |
| HIS | HIS | PRO | PRO | ALA | VAL | VAL | VAL | ALA | HIS |
| HIS | ASP | ASP | MET | MET | VAL | ALA | ASP | HIS | ALA |
|     | SER | SER | SER | ALA | ALA | ALA | MET | LEU | ALA |
|     | THR | THR | THR | LEU | VAL | GLN | ASP | THR | ALA |
|     | LYS | LYS | LEU | LEU | GLN | ASP | GLY | GLU | VAL |
|     | PRO | PRO | GLU | GLU | ALA | ASP | GLY | LEU | LEU |
|     | THR | THR | THR | GLU | ASP | PRO | PRO | LEU | GLY |
|     | THR | THR | LEU | LEU | ALA | ALA | GLY | GLY | HIS |
|     | ASP | ASP | PHE | PHE | THR | ILE | ILE | ALA | ALA |
|     | THR | THR | VAL | ARG | GLY | GLY | CYS | ARG | VAL |
|     | VAL | VAL | ALA | ALA | LYS | VAL | CYS | GLU | PRO |
|     | VAL | VAL | VAL | THR | PRO | PRO | GLY | ALA | ALA |
|     | PRO | PRO | VAL | VAL | PHE | PHE | THR | SER | GLN |
|     | GLY | GLY | ARG | VAL | VAL | ALA | ALA | ALA | ALA |
|     | ASP | ASP | MET | MET | VAL | VAL | ALA | LEU | PHE |
|     | HIS | HIS | PHE | ASP | ALA | ASP | ILE | ARG | ALA |
|     | PHE | PHE | ASP | ASP | GLY | GLY | SER | ASP | GLU |
|     | THR | THR | THR | THR | HIS | HIS | GLY | GLY | LEU |
|     | MET | MET | MET | ARG | SER | SER | PRO | TYR | GLY |
|     | VAL | VAL | VAL | LEU | ALA | ALA | HIS | ARG | VAL |
|     | GLN | GLN | THR | THR | GLY | GLY | GLY | GLN | ASP |
|     | GLU | GLU | GLU | ALA | ALA | ALA | PHE | ALA | SER |
|     | HIS | HIS | LEU | LEU | LEU | LEU | THR | VAL | GLY |
|     | ALA | ALA | ALA | GLY | MET | ALA | ARG | GLY | LEU |
|     | ASP | ASP | ALA | TYR | TYR | ALA | LEU | SER | ALA |
|     | ILE | ILE | ILE | ASP | ALA | ALA | ALA | GLY | LEU |
|     | ARG | ARG | ARG | ARG | LEU | LEU | LEU | VAL | GLU |
|     | HIS | HIS | THR | THR | THR | THR | ARG | ARG | ARG |
|     | THR | THR | THR | THR | GLU | GLU | GLY | SER | ASN |
|     | ILE | ILE | ILE | GLY | GLY | LEU | ILE | TYR | LEU |
|     | ASP | ASP | ASP | GLN | LEU | LEU | GLY | LEU | GLY |
|     | ALA | ALA | ALA | TRP | LEU | LEU | ASP | ASP | GLY |
|     | THR | THR | THR | ARG | ASP | ASP | PRO | LEU | ALA |
|     | LEU | LEU | GLY | PRO | ARG | GLY | VAL | LEU | ALA |
|     | GLY | GLY | GLY | GLY | HIS | ALA | ARG | ALA | THR |
|     | GLY | GLY | GLY | THR | PRO | PRO | ALA | GLY | VAL |

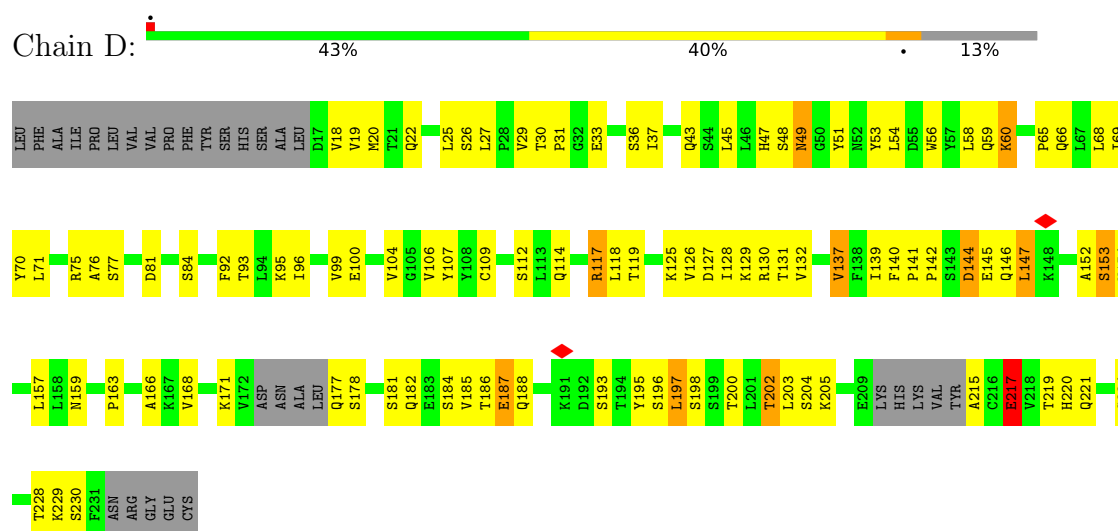
- Molecule 2: 1B2 (heavy chain)



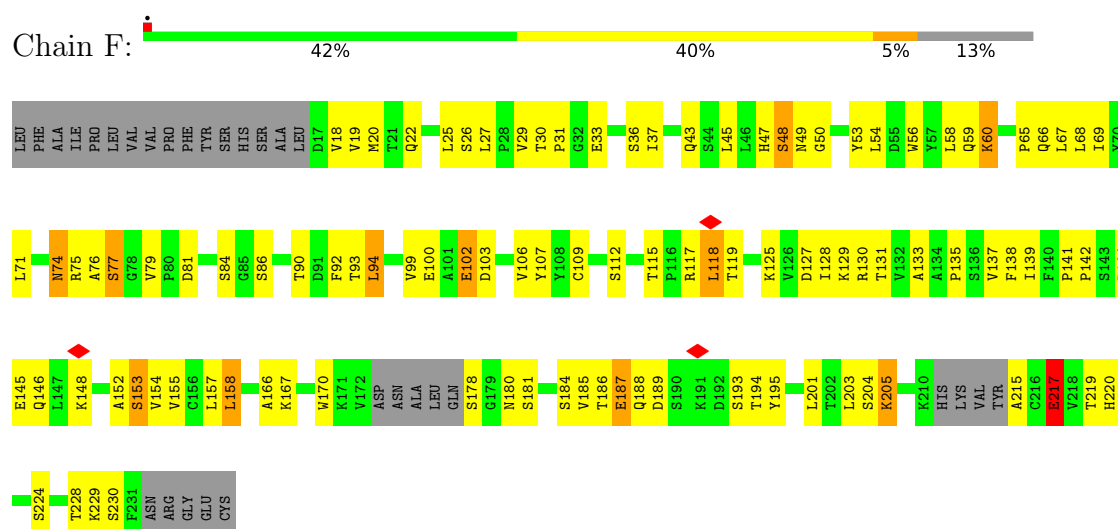
- Molecule 2: 1B2 (heavy chain)



- Molecule 3: 1B2 (light chain)



- Molecule 3: 1B2 (light chain)



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 172352                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 7.734                                   | Depositor |
| Minimum map value                    | -4.602                                  | Depositor |
| Average map value                    | 0.005                                   | Depositor |
| Map value standard deviation         | 0.138                                   | Depositor |
| Recommended contour level            | 0.53                                    | Depositor |
| Map size (Å)                         | 336.0, 336.0, 336.0                     | wwPDB     |
| Map dimensions                       | 336, 336, 336                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.0, 1.0, 1.0                           | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PN7

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$      | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.94         | 64/10522 (0.6%)  | 1.20        | 101/14323 (0.7%) |
| 1   | B     | 0.93         | 50/7566 (0.7%)   | 1.18        | 84/10293 (0.8%)  |
| 2   | C     | 0.86         | 9/1575 (0.6%)    | 1.12        | 12/2141 (0.6%)   |
| 2   | E     | 0.81         | 5/1575 (0.3%)    | 1.18        | 10/2141 (0.5%)   |
| 3   | D     | 0.58         | 0/1601           | 0.97        | 7/2175 (0.3%)    |
| 3   | F     | 0.70         | 5/1601 (0.3%)    | 1.05        | 12/2174 (0.6%)   |
| All | All   | 0.89         | 133/24440 (0.5%) | 1.17        | 226/33247 (0.7%) |

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                   |
| 2   | C     | 0                   | 1                   |
| 2   | E     | 0                   | 3                   |
| 3   | F     | 0                   | 1                   |
| All | All   | 0                   | 6                   |

All (133) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | A     | 442 | SER  | CA-CB | -14.41 | 1.30        | 1.53     |
| 1   | A     | 43  | ARG  | C-O   | -14.33 | 1.07        | 1.24     |
| 1   | A     | 207 | SER  | CA-CB | -14.15 | 1.28        | 1.53     |
| 1   | B     | 197 | PRO  | C-O   | -13.30 | 1.06        | 1.24     |
| 1   | B     | 908 | VAL  | C-O   | -12.62 | 1.08        | 1.23     |
| 1   | A     | 442 | SER  | C-O   | -12.62 | 1.09        | 1.24     |
| 1   | A     | 440 | VAL  | C-O   | -12.41 | 1.10        | 1.24     |
| 1   | B     | 399 | THR  | C-O   | -12.12 | 1.08        | 1.23     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 1   | A     | 120 | ASP  | C-O   | -11.26 | 1.09        | 1.23     |
| 1   | B     | 43  | ARG  | C-O   | -11.12 | 1.11        | 1.23     |
| 1   | A     | 524 | PHE  | C-O   | -10.91 | 1.11        | 1.23     |
| 1   | B     | 54  | PHE  | C-O   | -10.90 | 1.10        | 1.24     |
| 1   | B     | 388 | VAL  | C-O   | -10.32 | 1.10        | 1.24     |
| 1   | B     | 234 | VAL  | C-O   | -9.90  | 1.12        | 1.24     |
| 1   | A     | 234 | VAL  | C-O   | -9.82  | 1.13        | 1.24     |
| 1   | B     | 384 | GLY  | C-N   | -9.69  | 1.22        | 1.33     |
| 1   | A     | 374 | SER  | CA-CB | -9.43  | 1.38        | 1.53     |
| 1   | B     | 230 | GLY  | C-O   | -9.42  | 1.09        | 1.23     |
| 1   | A     | 243 | ASP  | C-O   | -9.22  | 1.12        | 1.24     |
| 1   | A     | 233 | THR  | C-O   | -8.99  | 1.13        | 1.24     |
| 1   | B     | 475 | TRP  | C-O   | -8.91  | 1.12        | 1.23     |
| 1   | A     | 441 | SER  | CA-CB | -8.90  | 1.36        | 1.53     |
| 1   | A     | 270 | GLU  | C-O   | -8.90  | 1.12        | 1.23     |
| 1   | A     | 162 | PRO  | C-O   | -8.89  | 1.12        | 1.23     |
| 1   | B     | 454 | ILE  | C-O   | -8.88  | 1.13        | 1.24     |
| 1   | A     | 116 | ALA  | C-O   | -8.84  | 1.12        | 1.24     |
| 1   | B     | 507 | ILE  | C-O   | -8.77  | 1.14        | 1.24     |
| 1   | B     | 385 | VAL  | C-O   | -8.76  | 1.14        | 1.24     |
| 1   | A     | 94  | GLY  | C-O   | -8.72  | 1.17        | 1.24     |
| 1   | B     | 439 | GLY  | C-O   | -8.54  | 1.12        | 1.23     |
| 1   | B     | 59  | SER  | CA-CB | -8.41  | 1.40        | 1.53     |
| 1   | A     | 236 | PRO  | C-O   | -8.35  | 1.12        | 1.24     |
| 1   | A     | 155 | LEU  | C-O   | -8.31  | 1.14        | 1.23     |
| 1   | B     | 57  | LEU  | C-O   | -8.27  | 1.11        | 1.23     |
| 1   | A     | 117 | LEU  | C-O   | -8.26  | 1.13        | 1.24     |
| 1   | A     | 232 | VAL  | C-O   | -8.20  | 1.15        | 1.24     |
| 3   | F     | 74  | ASN  | C-O   | -8.19  | 1.13        | 1.23     |
| 2   | C     | 101 | THR  | C-O   | -8.16  | 1.13        | 1.23     |
| 2   | E     | 97  | VAL  | C-O   | -8.14  | 1.14        | 1.24     |
| 1   | A     | 441 | SER  | C-O   | -8.07  | 1.14        | 1.24     |
| 1   | A     | 120 | ASP  | CA-C  | -8.04  | 1.44        | 1.53     |
| 1   | A     | 156 | ILE  | C-O   | -8.00  | 1.14        | 1.24     |
| 1   | A     | 172 | GLU  | C-O   | -7.99  | 1.14        | 1.24     |
| 1   | B     | 492 | LEU  | C-O   | -7.97  | 1.13        | 1.24     |
| 2   | C     | 99  | TYR  | C-O   | -7.95  | 1.13        | 1.23     |
| 1   | B     | 266 | PHE  | C-O   | -7.87  | 1.13        | 1.24     |
| 1   | A     | 207 | SER  | C-O   | -7.84  | 1.13        | 1.24     |
| 1   | A     | 42  | CYS  | C-O   | -7.81  | 1.14        | 1.23     |
| 1   | A     | 163 | ARG  | C-O   | -7.77  | 1.14        | 1.23     |
| 1   | B     | 162 | PRO  | C-O   | -7.74  | 1.15        | 1.23     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 64  | ALA  | CA-CB | -7.72 | 1.42        | 1.53     |
| 1   | A     | 183 | VAL  | C-O   | -7.59 | 1.11        | 1.23     |
| 1   | A     | 62  | ARG  | C-O   | -7.54 | 1.14        | 1.24     |
| 1   | B     | 8   | LYS  | C-O   | -7.53 | 1.14        | 1.24     |
| 1   | B     | 198 | ALA  | CA-CB | -7.53 | 1.41        | 1.52     |
| 2   | E     | 101 | THR  | C-O   | -7.52 | 1.14        | 1.23     |
| 1   | B     | 493 | ALA  | CA-CB | -7.51 | 1.41        | 1.53     |
| 1   | A     | 118 | ALA  | CA-CB | -7.51 | 1.40        | 1.53     |
| 1   | A     | 65  | VAL  | C-O   | -7.47 | 1.15        | 1.24     |
| 1   | B     | 338 | GLU  | C-O   | -7.46 | 1.11        | 1.23     |
| 1   | B     | 495 | HIS  | C-O   | -7.38 | 1.14        | 1.24     |
| 2   | C     | 98  | TYR  | C-O   | -7.29 | 1.15        | 1.24     |
| 3   | F     | 76  | ALA  | CA-CB | -7.24 | 1.43        | 1.53     |
| 2   | C     | 102 | ARG  | C-O   | -7.24 | 1.14        | 1.24     |
| 1   | A     | 443 | PHE  | C-O   | -7.20 | 1.14        | 1.24     |
| 1   | A     | 116 | ALA  | CA-CB | -7.09 | 1.41        | 1.53     |
| 3   | F     | 76  | ALA  | C-O   | -7.07 | 1.15        | 1.24     |
| 1   | A     | 162 | PRO  | N-CA  | -7.02 | 1.38        | 1.47     |
| 1   | A     | 175 | LEU  | C-O   | -6.98 | 1.14        | 1.24     |
| 1   | A     | 157 | PRO  | N-CA  | -6.93 | 1.38        | 1.47     |
| 3   | F     | 75  | ARG  | C-O   | -6.90 | 1.15        | 1.23     |
| 1   | A     | 243 | ASP  | CA-C  | -6.80 | 1.46        | 1.52     |
| 1   | A     | 202 | ASP  | C-O   | -6.79 | 1.15        | 1.23     |
| 2   | E     | 103 | GLY  | C-O   | -6.78 | 1.14        | 1.23     |
| 2   | C     | 39  | VAL  | C-O   | -6.77 | 1.16        | 1.24     |
| 2   | E     | 102 | ARG  | C-O   | -6.70 | 1.14        | 1.23     |
| 1   | B     | 392 | VAL  | C-O   | -6.64 | 1.15        | 1.24     |
| 1   | B     | 162 | PRO  | N-CA  | -6.62 | 1.39        | 1.46     |
| 1   | B     | 902 | PRO  | C-O   | -6.58 | 1.15        | 1.24     |
| 1   | A     | 266 | PHE  | C-O   | -6.57 | 1.15        | 1.23     |
| 1   | A     | 159 | GLU  | C-O   | -6.55 | 1.16        | 1.24     |
| 1   | B     | 438 | ALA  | C-N   | -6.51 | 1.24        | 1.33     |
| 1   | B     | 197 | PRO  | N-CA  | -6.45 | 1.39        | 1.47     |
| 1   | B     | 401 | PRO  | N-CA  | -6.30 | 1.39        | 1.47     |
| 1   | B     | 494 | ALA  | C-O   | -6.29 | 1.16        | 1.24     |
| 1   | B     | 491 | ARG  | C-O   | -6.29 | 1.16        | 1.24     |
| 1   | B     | 402 | ARG  | C-O   | -6.27 | 1.15        | 1.23     |
| 1   | A     | 236 | PRO  | N-CA  | -6.24 | 1.39        | 1.47     |
| 1   | B     | 401 | PRO  | C-O   | -6.22 | 1.13        | 1.23     |
| 2   | C     | 6   | LEU  | C-O   | -6.21 | 1.15        | 1.23     |
| 2   | E     | 102 | ARG  | CA-C  | -6.20 | 1.46        | 1.53     |
| 1   | B     | 390 | LYS  | C-O   | -6.18 | 1.16        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 177 | THR  | C-O   | -6.15 | 1.15        | 1.24     |
| 1   | B     | 43  | ARG  | CA-C  | -6.13 | 1.45        | 1.53     |
| 1   | A     | 234 | VAL  | CA-C  | -6.10 | 1.45        | 1.52     |
| 1   | A     | 440 | VAL  | CA-C  | -6.07 | 1.45        | 1.52     |
| 1   | A     | 244 | PHE  | C-O   | -5.93 | 1.16        | 1.24     |
| 1   | A     | 909 | TRP  | C-O   | -5.92 | 1.17        | 1.24     |
| 1   | B     | 58  | LEU  | C-O   | -5.88 | 1.16        | 1.24     |
| 1   | B     | 266 | PHE  | C-N   | -5.87 | 1.23        | 1.33     |
| 1   | B     | 493 | ALA  | C-O   | -5.87 | 1.17        | 1.24     |
| 1   | A     | 91  | HIS  | C-O   | -5.86 | 1.16        | 1.24     |
| 1   | A     | 422 | LEU  | C-O   | -5.83 | 1.17        | 1.23     |
| 1   | A     | 92  | GLN  | C-O   | -5.79 | 1.17        | 1.24     |
| 1   | A     | 908 | VAL  | C-O   | -5.76 | 1.16        | 1.23     |
| 1   | B     | 235 | MET  | C-O   | -5.74 | 1.17        | 1.24     |
| 1   | A     | 62  | ARG  | CA-C  | -5.70 | 1.46        | 1.52     |
| 1   | B     | 511 | LEU  | C-O   | -5.70 | 1.16        | 1.24     |
| 1   | B     | 234 | VAL  | CA-CB | -5.68 | 1.47        | 1.54     |
| 1   | B     | 400 | LEU  | C-O   | -5.62 | 1.17        | 1.24     |
| 1   | A     | 43  | ARG  | CA-CB | -5.60 | 1.44        | 1.53     |
| 1   | B     | 234 | VAL  | CA-C  | -5.51 | 1.46        | 1.52     |
| 1   | A     | 207 | SER  | CA-C  | -5.49 | 1.45        | 1.52     |
| 1   | A     | 910 | LEU  | C-O   | -5.46 | 1.17        | 1.24     |
| 1   | A     | 176 | MET  | C-O   | -5.40 | 1.15        | 1.23     |
| 1   | A     | 183 | VAL  | CA-C  | -5.32 | 1.47        | 1.53     |
| 1   | B     | 502 | GLN  | C-O   | -5.30 | 1.17        | 1.24     |
| 1   | A     | 124 | ARG  | C-O   | -5.30 | 1.17        | 1.24     |
| 1   | B     | 57  | LEU  | CA-C  | -5.29 | 1.45        | 1.52     |
| 1   | A     | 63  | ASP  | C-O   | -5.28 | 1.17        | 1.23     |
| 2   | C     | 38  | TRP  | C-O   | -5.22 | 1.18        | 1.24     |
| 1   | B     | 338 | GLU  | C-N   | -5.19 | 1.26        | 1.33     |
| 1   | A     | 174 | TYR  | C-O   | -5.15 | 1.17        | 1.24     |
| 3   | F     | 48  | SER  | CA-CB | -5.15 | 1.44        | 1.53     |
| 1   | B     | 266 | PHE  | N-CA  | 5.14  | 1.52        | 1.46     |
| 1   | A     | 24  | ARG  | C-O   | -5.14 | 1.17        | 1.24     |
| 1   | A     | 157 | PRO  | C-O   | -5.13 | 1.17        | 1.24     |
| 1   | B     | 230 | GLY  | CA-C  | -5.10 | 1.45        | 1.51     |
| 1   | B     | 475 | TRP  | CA-CB | -5.10 | 1.46        | 1.52     |
| 1   | A     | 118 | ALA  | C-O   | -5.09 | 1.17        | 1.24     |
| 2   | C     | 101 | THR  | CA-C  | -5.08 | 1.46        | 1.52     |
| 2   | C     | 37  | SER  | CA-CB | -5.08 | 1.43        | 1.54     |
| 1   | A     | 242 | VAL  | C-O   | -5.04 | 1.16        | 1.24     |

All (226) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1   | A     | 162 | PRO  | N-CA-CB   | -23.65 | 83.45       | 103.32   |
| 1   | A     | 159 | GLU  | CB-CA-C   | -19.80 | 78.12       | 110.19   |
| 1   | B     | 883 | ASP  | CB-CA-C   | -18.93 | 78.51       | 109.75   |
| 1   | B     | 266 | PHE  | CA-CB-CG  | 17.75  | 131.55      | 113.80   |
| 1   | A     | 43  | ARG  | CB-CA-C   | -17.11 | 83.20       | 110.74   |
| 1   | A     | 914 | PRO  | N-CA-C    | 15.18  | 134.18      | 111.41   |
| 1   | B     | 902 | PRO  | CB-CA-C   | -15.13 | 86.60       | 111.56   |
| 2   | E     | 102 | ARG  | CB-CA-C   | -14.79 | 89.93       | 112.12   |
| 1   | A     | 233 | THR  | CA-CB-OG1 | -14.71 | 87.54       | 109.60   |
| 1   | A     | 157 | PRO  | N-CA-CB   | -14.12 | 88.43       | 103.25   |
| 1   | A     | 233 | THR  | CB-CA-C   | -13.75 | 90.54       | 110.62   |
| 1   | A     | 162 | PRO  | CB-CA-C   | -13.62 | 93.95       | 111.39   |
| 1   | B     | 493 | ALA  | N-CA-C    | -12.45 | 97.70       | 111.14   |
| 1   | B     | 385 | VAL  | N-CA-C    | -12.10 | 101.67      | 113.53   |
| 1   | A     | 175 | LEU  | N-CA-C    | -11.19 | 99.17       | 113.72   |
| 1   | A     | 43  | ARG  | CA-C-O    | -11.12 | 108.72      | 120.40   |
| 1   | B     | 197 | PRO  | CB-CA-C   | -11.08 | 93.27       | 111.56   |
| 1   | A     | 120 | ASP  | CA-CB-CG  | 11.07  | 123.67      | 112.60   |
| 1   | A     | 234 | VAL  | N-CA-C    | -10.88 | 92.88       | 108.11   |
| 1   | A     | 270 | GLU  | CB-CG-CD  | -10.80 | 94.24       | 112.60   |
| 1   | B     | 54  | PHE  | CA-CB-CG  | 10.76  | 124.56      | 113.80   |
| 1   | A     | 266 | PHE  | CA-CB-CG  | 10.73  | 124.53      | 113.80   |
| 1   | A     | 243 | ASP  | CB-CA-C   | -10.53 | 93.78       | 111.26   |
| 1   | A     | 236 | PRO  | N-CA-CB   | -10.51 | 91.98       | 103.23   |
| 1   | A     | 43  | ARG  | N-CA-CB   | -10.50 | 94.06       | 110.65   |
| 2   | C     | 102 | ARG  | CB-CA-C   | -10.33 | 89.87       | 110.42   |
| 1   | A     | 155 | LEU  | CA-C-N    | -10.07 | 115.75      | 122.60   |
| 1   | A     | 155 | LEU  | C-N-CA    | -10.07 | 115.75      | 122.60   |
| 1   | A     | 403 | THR  | N-CA-C    | -9.72  | 90.79       | 107.99   |
| 1   | B     | 57  | LEU  | N-CA-C    | -9.71  | 102.00      | 114.04   |
| 1   | A     | 174 | TYR  | CB-CA-C   | -9.71  | 96.01       | 111.06   |
| 2   | C     | 101 | THR  | N-CA-CB   | -9.66  | 95.50       | 110.56   |
| 1   | A     | 63  | ASP  | CB-CA-C   | -9.63  | 93.22       | 109.50   |
| 1   | B     | 72  | ARG  | CB-CG-CD  | -9.55  | 89.33       | 111.30   |
| 2   | E     | 99  | TYR  | CA-C-O    | -9.44  | 110.07      | 121.11   |
| 1   | A     | 738 | SER  | N-CA-C    | -9.40  | 101.96      | 113.15   |
| 1   | B     | 401 | PRO  | N-CD-CG   | -9.34  | 89.19       | 103.20   |
| 1   | A     | 156 | ILE  | N-CA-C    | -9.20  | 99.19       | 107.56   |
| 1   | B     | 401 | PRO  | N-CA-CB   | -8.92  | 91.89       | 102.86   |
| 1   | A     | 92  | GLN  | CB-CG-CD  | -8.68  | 97.84       | 112.60   |
| 1   | B     | 234 | VAL  | CA-C-O    | -8.50  | 111.47      | 120.57   |
| 1   | A     | 126 | MET  | N-CA-C    | -8.41  | 103.61      | 114.04   |
| 1   | A     | 234 | VAL  | CA-C-O    | -8.26  | 111.72      | 120.39   |

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| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | B     | 234  | VAL  | N-CA-C    | -8.21 | 96.61       | 108.36   |
| 2   | E     | 100  | CYS  | CB-CA-C   | -8.21 | 97.53       | 110.74   |
| 1   | B     | 230  | GLY  | CA-C-O    | -8.17 | 112.17      | 122.39   |
| 2   | C     | 100  | CYS  | CB-CA-C   | -8.15 | 98.72       | 110.62   |
| 1   | A     | 440  | VAL  | CA-C-O    | -8.08 | 111.92      | 120.48   |
| 2   | E     | 101  | THR  | N-CA-CB   | -7.85 | 98.29       | 110.85   |
| 1   | A     | 176  | MET  | N-CA-C    | -7.83 | 103.56      | 113.43   |
| 2   | C     | 101  | THR  | CA-CB-OG1 | -7.75 | 97.98       | 109.60   |
| 3   | F     | 180  | ASN  | CB-CA-C   | -7.75 | 96.58       | 110.37   |
| 1   | A     | 914  | PRO  | CB-CA-C   | -7.72 | 100.84      | 110.95   |
| 1   | B     | 14   | ARG  | N-CA-C    | -7.71 | 103.45      | 113.17   |
| 2   | C     | 101  | THR  | CA-C-O    | -7.70 | 112.27      | 121.66   |
| 1   | A     | 120  | ASP  | CA-C-O    | -7.62 | 112.08      | 120.69   |
| 1   | B     | 511  | LEU  | N-CA-C    | -7.59 | 102.66      | 112.23   |
| 1   | A     | 233  | THR  | CA-C-O    | -7.59 | 110.69      | 120.25   |
| 1   | B     | 54   | PHE  | CB-CA-C   | -7.58 | 95.79       | 110.11   |
| 1   | B     | 266  | PHE  | CB-CA-C   | -7.55 | 94.22       | 109.55   |
| 2   | C     | 41   | GLN  | CB-CA-C   | -7.53 | 99.58       | 111.17   |
| 1   | A     | 912  | PRO  | N-CA-C    | -7.48 | 99.34       | 111.15   |
| 1   | B     | 266  | PHE  | N-CA-CB   | 7.44  | 122.05      | 110.44   |
| 1   | B     | 198  | ALA  | CA-C-O    | -7.44 | 113.06      | 121.39   |
| 3   | F     | 50   | GLY  | N-CA-C    | -7.44 | 104.31      | 115.32   |
| 1   | A     | 1014 | PRO  | N-CA-C    | -7.39 | 99.63       | 110.80   |
| 1   | A     | 156  | ILE  | CA-C-O    | -7.38 | 114.98      | 119.12   |
| 1   | B     | 26   | ARG  | N-CA-C    | -7.33 | 104.47      | 113.41   |
| 1   | A     | 737  | ALA  | N-CA-C    | -7.30 | 104.17      | 113.23   |
| 1   | A     | 731  | GLU  | N-CA-C    | -7.29 | 106.31      | 114.62   |
| 1   | B     | 230  | GLY  | CA-C-N    | 7.25  | 128.34      | 121.46   |
| 1   | B     | 230  | GLY  | C-N-CA    | 7.25  | 128.34      | 121.46   |
| 2   | E     | 86   | GLN  | CA-C-N    | -7.24 | 113.02      | 123.00   |
| 2   | E     | 86   | GLN  | C-N-CA    | -7.24 | 113.02      | 123.00   |
| 1   | A     | 183  | VAL  | CA-C-O    | -7.17 | 112.97      | 120.14   |
| 1   | A     | 162  | PRO  | CA-N-CD   | -7.13 | 102.01      | 112.00   |
| 1   | B     | 387  | GLY  | O-C-N     | -7.09 | 114.55      | 122.28   |
| 1   | A     | 243  | ASP  | CA-CB-CG  | -7.09 | 105.51      | 112.60   |
| 1   | A     | 42   | CYS  | CA-C-O    | -7.00 | 111.60      | 120.14   |
| 1   | A     | 1303 | ARG  | CB-CA-C   | 6.99  | 123.15      | 109.72   |
| 1   | A     | 524  | PHE  | CA-C-O    | -6.98 | 113.81      | 121.28   |
| 1   | B     | 54   | PHE  | N-CA-C    | -6.95 | 102.79      | 112.45   |
| 1   | A     | 911  | GLU  | CB-CA-C   | 6.95  | 118.86      | 108.86   |
| 1   | B     | 7    | GLU  | N-CA-C    | -6.94 | 102.86      | 112.30   |
| 1   | B     | 491  | ARG  | CG-CD-NE  | -6.87 | 96.88       | 112.00   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | B     | 5    | ASP  | CB-CA-C  | 6.87  | 124.05      | 110.65   |
| 1   | B     | 399  | THR  | CA-C-O   | -6.85 | 113.35      | 120.89   |
| 1   | A     | 223  | GLU  | N-CA-C   | -6.79 | 106.20      | 114.75   |
| 1   | B     | 72   | ARG  | N-CA-CB  | -6.76 | 100.05      | 110.46   |
| 2   | C     | 101  | THR  | CB-CA-C  | -6.76 | 98.65       | 109.80   |
| 1   | B     | 389  | ILE  | O-C-N    | -6.72 | 114.20      | 121.80   |
| 1   | A     | 159  | GLU  | CA-C-O   | -6.71 | 113.18      | 120.36   |
| 1   | A     | 524  | PHE  | CA-CB-CG | 6.68  | 120.48      | 113.80   |
| 1   | B     | 496  | LEU  | N-CA-C   | -6.67 | 104.27      | 112.88   |
| 1   | B     | 198  | ALA  | N-CA-CB  | -6.67 | 99.45       | 110.53   |
| 1   | A     | 52   | GLU  | N-CA-C   | -6.66 | 106.35      | 114.75   |
| 1   | B     | 631  | MET  | N-CA-C   | -6.66 | 103.71      | 110.97   |
| 1   | B     | 197  | PRO  | N-CA-CB  | -6.65 | 96.27       | 103.25   |
| 1   | B     | 399  | THR  | CB-CA-C  | -6.64 | 98.01       | 110.16   |
| 1   | A     | 158  | GLN  | CB-CG-CD | -6.62 | 101.34      | 112.60   |
| 1   | B     | 241  | LEU  | N-CA-C   | -6.61 | 104.69      | 112.89   |
| 3   | F     | 60   | LYS  | CA-C-N   | 6.59  | 127.62      | 119.98   |
| 3   | F     | 60   | LYS  | C-N-CA   | 6.59  | 127.62      | 119.98   |
| 1   | A     | 243  | ASP  | N-CA-C   | -6.58 | 103.30      | 112.12   |
| 1   | A     | 62   | ARG  | CB-CA-C  | -6.58 | 97.54       | 109.38   |
| 2   | C     | 4    | VAL  | N-CA-C   | -6.55 | 100.31      | 109.21   |
| 1   | B     | 198  | ALA  | CB-CA-C  | -6.52 | 100.80      | 111.68   |
| 3   | D     | 60   | LYS  | CB-CA-C  | 6.51  | 118.87      | 109.11   |
| 1   | A     | 236  | PRO  | N-CD-CG  | -6.37 | 93.65       | 103.20   |
| 1   | A     | 524  | PHE  | CB-CA-C  | -6.34 | 99.53       | 110.95   |
| 3   | D     | 202  | THR  | CA-C-N   | -6.30 | 111.24      | 122.45   |
| 3   | D     | 202  | THR  | C-N-CA   | -6.30 | 111.24      | 122.45   |
| 1   | A     | 242  | VAL  | N-CA-C   | -6.27 | 107.02      | 113.10   |
| 1   | A     | 740  | THR  | N-CA-C   | -6.27 | 105.95      | 113.97   |
| 1   | A     | 441  | SER  | CB-CA-C  | -6.26 | 98.37       | 109.70   |
| 1   | A     | 57   | LEU  | N-CA-C   | -6.25 | 105.55      | 113.43   |
| 1   | B     | 75   | ASP  | CB-CA-C  | -6.25 | 101.06      | 110.88   |
| 1   | B     | 1411 | GLU  | N-CA-C   | -6.24 | 104.58      | 111.82   |
| 1   | A     | 497  | ARG  | N-CA-C   | -6.24 | 105.49      | 113.23   |
| 1   | A     | 441  | SER  | CA-C-O   | -6.24 | 113.39      | 120.32   |
| 1   | A     | 392  | VAL  | N-CA-C   | -6.23 | 107.79      | 113.71   |
| 1   | A     | 741  | THR  | N-CA-C   | -6.22 | 105.17      | 112.89   |
| 1   | A     | 120  | ASP  | CA-C-N   | 6.19  | 125.81      | 119.56   |
| 1   | A     | 120  | ASP  | C-N-CA   | 6.19  | 125.81      | 119.56   |
| 1   | B     | 337  | VAL  | O-C-N    | -6.18 | 114.88      | 122.61   |
| 1   | A     | 760  | VAL  | N-CA-C   | -6.17 | 107.48      | 113.53   |
| 1   | A     | 443  | PHE  | CA-C-O   | -6.12 | 114.08      | 120.70   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 735  | LEU  | N-CA-C   | -6.12 | 105.95      | 113.41   |
| 1   | B     | 390  | LYS  | CB-CA-C  | -6.11 | 97.92       | 110.38   |
| 1   | A     | 120  | ASP  | N-CA-C   | -6.06 | 101.41      | 109.84   |
| 1   | B     | 498  | GLU  | N-CA-C   | -6.03 | 105.74      | 114.12   |
| 1   | A     | 162  | PRO  | CA-C-O   | -6.02 | 114.69      | 121.43   |
| 2   | C     | 99   | TYR  | CA-C-O   | -5.96 | 114.64      | 121.68   |
| 1   | B     | 827  | THR  | CB-CA-C  | 5.96  | 120.49      | 109.70   |
| 1   | B     | 489  | ALA  | N-CA-C   | -5.95 | 106.15      | 113.41   |
| 3   | F     | 217  | GLU  | CA-CB-CG | 5.92  | 125.94      | 114.10   |
| 3   | D     | 217  | GLU  | CA-CB-CG | 5.91  | 125.92      | 114.10   |
| 1   | A     | 1380 | ARG  | CB-CA-C  | 5.90  | 121.32      | 110.11   |
| 1   | B     | 439  | GLY  | CA-C-N   | 5.90  | 130.95      | 123.10   |
| 1   | B     | 439  | GLY  | C-N-CA   | 5.90  | 130.95      | 123.10   |
| 1   | B     | 265  | GLY  | CA-C-O   | -5.90 | 117.55      | 122.33   |
| 1   | A     | 124  | ARG  | N-CA-CB  | -5.90 | 100.50      | 110.41   |
| 1   | B     | 387  | GLY  | CA-C-N   | 5.89  | 130.43      | 120.29   |
| 1   | B     | 387  | GLY  | C-N-CA   | 5.89  | 130.43      | 120.29   |
| 1   | B     | 15   | ARG  | N-CA-C   | -5.86 | 104.89      | 112.68   |
| 1   | B     | 902  | PRO  | CA-N-CD  | -5.85 | 103.81      | 112.00   |
| 1   | B     | 403  | THR  | N-CA-C   | -5.84 | 98.21       | 108.20   |
| 1   | A     | 838  | THR  | N-CA-C   | -5.81 | 105.03      | 111.36   |
| 1   | A     | 909  | TRP  | CA-C-O   | -5.75 | 113.94      | 120.32   |
| 1   | A     | 117  | LEU  | N-CA-C   | -5.74 | 105.11      | 111.71   |
| 1   | B     | 198  | ALA  | O-C-N    | 5.70  | 129.58      | 122.63   |
| 1   | B     | 494  | ALA  | CA-C-O   | -5.69 | 114.48      | 120.63   |
| 1   | B     | 495  | HIS  | N-CA-C   | -5.68 | 106.30      | 113.18   |
| 2   | E     | 98   | TYR  | CA-C-O   | -5.67 | 114.91      | 121.15   |
| 1   | B     | 57   | LEU  | CB-CA-C  | -5.66 | 99.07       | 109.15   |
| 3   | D     | 47   | HIS  | CA-CB-CG | 5.66  | 119.46      | 113.80   |
| 1   | A     | 93   | ARG  | N-CA-C   | -5.66 | 105.58      | 112.88   |
| 1   | A     | 176  | MET  | CB-CG-SD | -5.65 | 95.76       | 112.70   |
| 1   | A     | 736  | VAL  | N-CA-C   | -5.63 | 105.41      | 113.07   |
| 1   | B     | 390  | LYS  | N-CA-C   | -5.63 | 105.13      | 112.23   |
| 3   | F     | 75   | ARG  | CA-C-O   | -5.62 | 114.81      | 121.16   |
| 1   | A     | 930  | TYR  | CA-C-O   | -5.62 | 115.07      | 121.58   |
| 1   | A     | 1325 | GLY  | O-C-N    | -5.60 | 116.17      | 121.77   |
| 1   | B     | 162  | PRO  | CB-CA-C  | 5.59  | 118.99      | 110.21   |
| 1   | A     | 158  | GLN  | CA-C-O   | -5.57 | 114.82      | 121.11   |
| 3   | D     | 49   | ASN  | CA-CB-CG | 5.54  | 118.14      | 112.60   |
| 1   | B     | 400  | LEU  | N-CA-C   | -5.52 | 101.02      | 109.64   |
| 1   | B     | 401  | PRO  | CA-N-CD  | 5.52  | 119.73      | 112.00   |
| 1   | B     | 511  | LEU  | CA-C-O   | -5.51 | 113.29      | 119.79   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | A     | 511  | LEU  | N-CA-C   | -5.49 | 107.12      | 113.88   |
| 2   | C     | 38   | TRP  | CA-C-O   | -5.49 | 114.40      | 120.33   |
| 1   | B     | 43   | ARG  | N-CA-C   | -5.48 | 96.26       | 107.70   |
| 1   | A     | 340  | HIS  | N-CA-C   | -5.47 | 105.00      | 110.97   |
| 1   | A     | 174  | TYR  | CA-C-O   | -5.46 | 113.10      | 120.15   |
| 1   | A     | 492  | LEU  | N-CA-C   | -5.45 | 104.99      | 111.69   |
| 1   | A     | 1304 | SER  | N-CA-C   | -5.44 | 106.83      | 112.93   |
| 1   | A     | 266  | PHE  | CA-C-N   | 5.44  | 132.07      | 121.41   |
| 1   | A     | 266  | PHE  | C-N-CA   | 5.44  | 132.07      | 121.41   |
| 1   | A     | 908  | VAL  | N-CA-CB  | -5.43 | 105.08      | 111.60   |
| 1   | A     | 913  | LYS  | N-CA-C   | 5.43  | 119.56      | 112.17   |
| 2   | E     | 96   | ALA  | O-C-N    | -5.43 | 117.39      | 123.04   |
| 1   | B     | 833  | ALA  | N-CA-C   | -5.40 | 105.83      | 112.90   |
| 1   | B     | 218  | SER  | N-CA-C   | -5.39 | 106.66      | 113.18   |
| 1   | B     | 270  | GLU  | CB-CA-C  | 5.38  | 119.92      | 109.33   |
| 1   | A     | 124  | ARG  | CA-C-O   | -5.37 | 112.23      | 119.11   |
| 3   | F     | 60   | LYS  | CA-C-O   | -5.37 | 114.62      | 120.69   |
| 1   | B     | 43   | ARG  | CA-C-O   | -5.34 | 113.09      | 120.52   |
| 1   | B     | 902  | PRO  | N-CD-CG  | -5.34 | 95.19       | 103.20   |
| 1   | B     | 605  | PHE  | N-CA-C   | -5.34 | 106.60      | 113.01   |
| 1   | B     | 454  | ILE  | CA-C-O   | -5.32 | 113.78      | 120.69   |
| 1   | A     | 176  | MET  | CB-CA-C  | -5.31 | 100.73      | 109.65   |
| 1   | A     | 24   | ARG  | N-CA-C   | -5.30 | 106.86      | 113.38   |
| 1   | B     | 385  | VAL  | CA-C-O   | -5.30 | 113.52      | 118.98   |
| 1   | A     | 913  | LYS  | CB-CA-C  | -5.30 | 105.25      | 113.57   |
| 1   | A     | 389  | ILE  | N-CA-C   | -5.29 | 107.23      | 113.42   |
| 1   | A     | 527  | VAL  | N-CA-C   | -5.29 | 105.97      | 111.58   |
| 1   | A     | 43   | ARG  | N-CA-C   | -5.27 | 98.80       | 108.02   |
| 1   | B     | 611  | ALA  | N-CA-C   | -5.27 | 105.95      | 112.38   |
| 1   | A     | 960  | GLU  | N-CA-C   | -5.26 | 106.12      | 112.54   |
| 2   | E     | 105  | THR  | N-CA-C   | -5.25 | 106.20      | 113.18   |
| 2   | E     | 112  | GLN  | N-CA-CB  | -5.25 | 101.85      | 110.40   |
| 1   | B     | 475  | TRP  | CA-C-O   | -5.24 | 115.47      | 120.92   |
| 3   | D     | 147  | LEU  | N-CA-C   | -5.21 | 105.77      | 111.82   |
| 1   | B     | 500  | PRO  | N-CA-C   | 5.18  | 120.33      | 111.68   |
| 2   | C     | 102  | ARG  | CB-CG-CD | -5.17 | 99.40       | 111.30   |
| 1   | B     | 882  | VAL  | CA-C-O   | -5.17 | 116.26      | 121.59   |
| 3   | F     | 166  | ALA  | N-CA-CB  | -5.16 | 102.47      | 110.57   |
| 1   | B     | 402  | ARG  | CB-CA-C  | -5.15 | 99.51       | 109.76   |
| 3   | F     | 76   | ALA  | CA-C-O   | -5.15 | 114.72      | 120.54   |
| 1   | B     | 265  | GLY  | O-C-N    | -5.13 | 119.07      | 123.43   |
| 1   | B     | 792  | TRP  | N-CA-C   | -5.13 | 102.27      | 109.96   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | B     | 388  | VAL  | N-CA-C   | -5.12 | 104.58      | 111.44   |
| 3   | F     | 47   | HIS  | CA-C-O   | -5.11 | 116.06      | 121.94   |
| 3   | F     | 60   | LYS  | CB-CA-C  | 5.11  | 117.84      | 109.46   |
| 1   | A     | 233  | THR  | N-CA-C   | -5.10 | 98.98       | 107.80   |
| 1   | A     | 1377 | ARG  | CA-C-O   | -5.09 | 115.28      | 120.63   |
| 1   | A     | 1202 | VAL  | N-CA-C   | -5.06 | 108.57      | 113.53   |
| 2   | C     | 86   | GLN  | CA-CB-CG | 5.06  | 124.22      | 114.10   |
| 1   | B     | 266  | PHE  | N-CA-C   | 5.05  | 119.49      | 113.23   |
| 1   | B     | 1427 | VAL  | N-CA-C   | -5.04 | 107.02      | 113.22   |
| 1   | B     | 497  | ARG  | N-CA-C   | -5.01 | 107.15      | 114.12   |
| 1   | A     | 171  | VAL  | N-CA-CB  | -5.01 | 105.94      | 111.66   |
| 3   | F     | 205  | LYS  | N-CA-C   | 5.01  | 116.56      | 111.14   |
| 1   | B     | 163  | ARG  | N-CA-C   | -5.01 | 102.78      | 110.30   |
| 1   | A     | 201  | VAL  | O-C-N    | -5.01 | 116.31      | 122.57   |
| 1   | B     | 58   | LEU  | N-CA-C   | -5.00 | 107.35      | 113.50   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1301 | GLN  | Mainchain |
| 2   | C     | 155  | GLU  | Peptide   |
| 2   | E     | 155  | GLU  | Peptide   |
| 2   | E     | 21   | ARG  | Sidechain |
| 2   | E     | 96   | ALA  | Mainchain |
| 3   | F     | 115  | THR  | 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   | A     | 10319 | 0        | 10164    | 317     | 0            |
| 1   | B     | 7417  | 0        | 7306     | 220     | 0            |
| 2   | C     | 1539  | 0        | 1511     | 61      | 0            |
| 2   | E     | 1539  | 0        | 1511     | 62      | 0            |
| 3   | D     | 1568  | 0        | 1528     | 55      | 0            |
| 3   | F     | 1568  | 0        | 1533     | 62      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | B     | 21    | 0        | 22       | 2       | 0            |
| All | All   | 23971 | 0        | 23575    | 736     | 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 15.

All (736) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:777:PRO:HB3   | 1:A:796:ASP:HA    | 1.54                     | 0.88              |
| 2:C:86:GLN:HA     | 2:C:86:GLN:HE21   | 1.38                     | 0.87              |
| 2:E:108:ASP:CG    | 3:F:67:LEU:CD2    | 2.60                     | 0.75              |
| 2:E:108:ASP:CG    | 3:F:67:LEU:HD23   | 2.11                     | 0.75              |
| 1:B:567:TRP:HB3   | 1:B:834:HIS:HB3   | 1.68                     | 0.74              |
| 1:A:1019:LEU:HD13 | 1:A:1244:ILE:HG22 | 1.70                     | 0.73              |
| 1:A:1249:ARG:HB2  | 1:A:1253:LEU:HD13 | 1.74                     | 0.69              |
| 1:A:526:PRO:HG3   | 1:A:532:ALA:HB2   | 1.74                     | 0.69              |
| 1:B:528:ASP:OD1   | 1:B:530:SER:N     | 2.24                     | 0.69              |
| 1:A:43:ARG:HG2    | 1:A:129:LEU:HD11  | 1.75                     | 0.69              |
| 2:E:108:ASP:OD1   | 3:F:67:LEU:HD23   | 1.93                     | 0.69              |
| 1:A:1157:ALA:HA   | 1:A:1160:LEU:HD12 | 1.75                     | 0.68              |
| 1:A:120:ASP:HB3   | 1:A:123:GLN:HG3   | 1.76                     | 0.67              |
| 1:A:739:CYS:HB3   | 1:A:744:ILE:HG22  | 1.77                     | 0.66              |
| 1:A:54:PHE:HE1    | 1:A:376:LEU:HD21  | 1.61                     | 0.66              |
| 1:A:981:VAL:HB    | 1:A:990:LEU:HD21  | 1.78                     | 0.66              |
| 1:A:734:ARG:HA    | 1:A:737:ALA:HB3   | 1.77                     | 0.65              |
| 1:A:126:MET:HB3   | 1:A:188:ILE:HD11  | 1.79                     | 0.65              |
| 1:A:1171:VAL:HG21 | 1:A:1211:LEU:HD21 | 1.77                     | 0.65              |
| 2:C:86:GLN:HA     | 2:C:86:GLN:NE2    | 2.10                     | 0.65              |
| 2:E:8:GLN:HE22    | 2:E:99:TYR:HA     | 1.62                     | 0.65              |
| 1:B:14:ARG:HG2    | 3:D:51:TYR:HE2    | 1.62                     | 0.64              |
| 2:C:144:ALA:HB3   | 3:D:140:PHE:HZ    | 1.63                     | 0.64              |
| 1:A:1000:VAL:HB   | 1:A:1039:LEU:HD21 | 1.81                     | 0.63              |
| 1:B:561:VAL:HG13  | 1:B:828:PHE:HB2   | 1.81                     | 0.62              |
| 1:A:817:VAL:HA    | 1:A:820:LEU:HD12  | 1.81                     | 0.62              |
| 2:E:87:MET:HB3    | 2:E:90:LEU:HD21   | 1.81                     | 0.62              |
| 1:B:122:GLN:HB3   | 1:B:155:LEU:HD23  | 1.81                     | 0.62              |
| 1:A:117:LEU:HA    | 1:A:908:VAL:CG1   | 2.29                     | 0.62              |
| 1:B:1416:LEU:HD21 | 1:B:1485:LEU:HB3  | 1.79                     | 0.62              |
| 2:E:146:GLY:HA3   | 2:E:188:VAL:HG22  | 1.81                     | 0.62              |
| 1:A:1239:LEU:HD23 | 1:A:1243:ARG:HD3  | 1.81                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:99:VAL:HG13   | 3:F:103:ASP:HB2   | 1.82                     | 0.62              |
| 2:C:163:SER:HA    | 2:C:204:ASN:HD21  | 1.65                     | 0.61              |
| 1:A:704:VAL:HG11  | 1:A:723:VAL:HG21  | 1.81                     | 0.61              |
| 1:B:1428:LEU:HD21 | 1:B:1447:VAL:HG22 | 1.82                     | 0.61              |
| 1:A:721:ARG:HB2   | 1:A:843:GLU:HB3   | 1.82                     | 0.61              |
| 1:A:562:PHE:HB2   | 1:A:654:GLY:HA2   | 1.82                     | 0.61              |
| 1:B:76:LEU:H      | 1:B:79:LEU:HD13   | 1.65                     | 0.61              |
| 1:A:13:LEU:HD21   | 3:F:71:LEU:HD11   | 1.81                     | 0.61              |
| 1:A:1075:ALA:HB2  | 1:A:1082:TRP:HD1  | 1.66                     | 0.61              |
| 1:A:1231:LEU:HD13 | 1:A:1288:TYR:HB2  | 1.83                     | 0.61              |
| 3:D:188:GLN:NE2   | 3:D:193:SER:HB2   | 2.16                     | 0.61              |
| 3:F:188:GLN:NE2   | 3:F:193:SER:HB2   | 2.16                     | 0.61              |
| 1:A:149:THR:HB    | 1:A:194:LEU:HD22  | 1.83                     | 0.60              |
| 1:A:155:LEU:HD11  | 1:A:184:ALA:HB3   | 1.83                     | 0.60              |
| 1:A:766:ALA:HA    | 1:A:770:GLU:HB3   | 1.83                     | 0.60              |
| 1:A:642:TRP:HB3   | 1:A:647:VAL:HB    | 1.83                     | 0.60              |
| 1:A:126:MET:HE3   | 1:A:232:VAL:HB    | 1.83                     | 0.60              |
| 3:D:203:LEU:HG    | 3:D:204:SER:H     | 1.66                     | 0.60              |
| 3:F:68:LEU:HA     | 3:F:79:VAL:HG21   | 1.83                     | 0.60              |
| 2:E:4:VAL:HA      | 2:E:28:GLY:HA3    | 1.83                     | 0.60              |
| 3:F:69:ILE:HD12   | 3:F:94:LEU:HD12   | 1.83                     | 0.60              |
| 1:A:118:ALA:HB2   | 1:A:171:VAL:HG12  | 1.84                     | 0.60              |
| 1:A:737:ALA:C     | 1:A:739:CYS:H     | 2.09                     | 0.60              |
| 1:B:205:CYS:HB2   | 1:B:444:GLY:HA2   | 1.84                     | 0.60              |
| 1:A:117:LEU:HA    | 1:A:908:VAL:HG13  | 1.84                     | 0.60              |
| 3:F:203:LEU:HG    | 3:F:204:SER:H     | 1.66                     | 0.60              |
| 1:B:624:VAL:HA    | 1:B:627:VAL:HG12  | 1.84                     | 0.60              |
| 1:B:855:ILE:HG23  | 1:B:874:ARG:HG3   | 1.83                     | 0.60              |
| 1:B:1427:VAL:HG22 | 1:B:1451:SER:HA   | 1.84                     | 0.60              |
| 1:A:830:GLU:HB2   | 1:A:838:THR:HG23  | 1.83                     | 0.60              |
| 3:F:152:ALA:HB3   | 3:F:203:LEU:HB3   | 1.84                     | 0.60              |
| 1:B:35:VAL:HA     | 1:B:279:ARG:HA    | 1.84                     | 0.60              |
| 1:B:609:GLU:H     | 1:B:612:ARG:HG3   | 1.66                     | 0.60              |
| 1:B:577:LEU:HD12  | 1:B:584:ALA:HA    | 1.84                     | 0.59              |
| 1:B:783:PRO:HB3   | 1:B:792:TRP:HE1   | 1.67                     | 0.59              |
| 1:A:629:PRO:HG3   | 1:A:679:ALA:HA    | 1.84                     | 0.59              |
| 1:B:82:PRO:HB3    | 1:A:1306:GLY:HA2  | 1.83                     | 0.59              |
| 2:C:9:SER:HG      | 2:C:23:SER:HG     | 1.50                     | 0.59              |
| 3:D:29:VAL:O      | 3:D:129:LYS:N     | 2.36                     | 0.59              |
| 2:E:87:MET:HE1    | 2:E:116:VAL:HG11  | 1.84                     | 0.59              |
| 2:E:149:VAL:O     | 2:E:152:TYR:HD1   | 1.85                     | 0.59              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:F:135:PRO:HB2  | 3:F:158:LEU:HD12  | 1.85                     | 0.59              |
| 3:F:137:VAL:HG22 | 3:F:158:LEU:HD11  | 1.84                     | 0.59              |
| 1:B:1:MET:O      | 2:E:54:ARG:NH2    | 2.35                     | 0.59              |
| 1:B:692:LYS:HB3  | 1:B:754:ALA:HB2   | 1.84                     | 0.59              |
| 1:A:493:ALA:HB2  | 1:A:536:LEU:HB3   | 1.83                     | 0.59              |
| 1:B:13:LEU:HD21  | 3:D:71:LEU:HD11   | 1.84                     | 0.59              |
| 1:B:700:PRO:HB2  | 1:B:703:GLU:HB3   | 1.85                     | 0.59              |
| 1:A:1230:THR:OG1 | 1:A:1247:ALA:O    | 2.16                     | 0.59              |
| 1:B:395:MET:O    | 1:B:436:ARG:NH2   | 2.35                     | 0.59              |
| 1:A:610:ALA:HB2  | 1:A:613:ARG:HH21  | 1.68                     | 0.59              |
| 1:B:296:GLY:HA3  | 1:B:327:SER:HB3   | 1.84                     | 0.58              |
| 1:B:692:LYS:HE2  | 1:B:728:ASP:HB3   | 1.85                     | 0.58              |
| 1:B:162:PRO:HG2  | 1:B:175:LEU:HD11  | 1.86                     | 0.58              |
| 1:A:1070:VAL:O   | 1:A:1074:ILE:HG13 | 2.01                     | 0.58              |
| 3:D:152:ALA:HB3  | 3:D:203:LEU:HB3   | 1.84                     | 0.58              |
| 1:B:835:PRO:HD3  | 1:B:858:LEU:O     | 2.03                     | 0.58              |
| 1:A:928:LEU:HB3  | 1:A:1361:VAL:HG13 | 1.85                     | 0.58              |
| 2:E:4:VAL:HG23   | 2:E:29:PHE:HD1    | 1.68                     | 0.58              |
| 1:A:720:PRO:HB2  | 1:A:721:ARG:HH11  | 1.69                     | 0.58              |
| 1:A:1222:SER:HA  | 1:A:1267:LEU:HA   | 1.86                     | 0.58              |
| 2:E:65:ALA:HB1   | 3:F:118:LEU:HD11  | 1.85                     | 0.58              |
| 3:F:29:VAL:O     | 3:F:129:LYS:N     | 2.36                     | 0.58              |
| 1:A:1025:ALA:HB2 | 1:A:1241:GLY:HA3  | 1.86                     | 0.57              |
| 1:B:711:ARG:NH1  | 1:B:758:SER:OG    | 2.37                     | 0.57              |
| 1:B:787:THR:HB   | 1:B:811:VAL:HG13  | 1.84                     | 0.57              |
| 1:A:966:ARG:HA   | 1:A:969:LEU:HB2   | 1.86                     | 0.57              |
| 1:B:828:PHE:CZ   | 1:B:841:ILE:HB    | 2.40                     | 0.57              |
| 1:A:316:GLN:HA   | 1:A:319:VAL:HG12  | 1.86                     | 0.57              |
| 1:A:331:PRO:O    | 1:A:363:ARG:NH1   | 2.38                     | 0.57              |
| 1:A:929:ARG:NH2  | 1:A:1129:ALA:O    | 2.38                     | 0.57              |
| 1:A:1125:TRP:HH2 | 1:A:1362:ILE:HG13 | 1.70                     | 0.57              |
| 1:A:608:ALA:HB1  | 1:A:612:ARG:HG3   | 1.86                     | 0.57              |
| 1:B:29:GLU:HA    | 1:B:33:GLU:HB2    | 1.86                     | 0.57              |
| 1:B:316:GLN:O    | 1:B:320:ILE:HG13  | 2.05                     | 0.57              |
| 1:A:580:SER:HB3  | 1:A:865:LEU:HD22  | 1.87                     | 0.57              |
| 1:A:561:VAL:HG23 | 1:A:813:PHE:HZ    | 1.69                     | 0.56              |
| 1:A:966:ARG:HB2  | 1:A:976:VAL:HG21  | 1.86                     | 0.56              |
| 3:D:188:GLN:HE21 | 3:D:193:SER:HB2   | 1.71                     | 0.56              |
| 3:F:188:GLN:HE21 | 3:F:193:SER:HB2   | 1.70                     | 0.56              |
| 1:A:1060:ARG:HG3 | 1:A:1061:ASN:N    | 2.21                     | 0.56              |
| 1:B:55:TRP:CH2   | 1:B:401:PRO:HG3   | 2.41                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:302:ASP:OD1   | 1:A:449:ASN:ND2   | 2.34                     | 0.56              |
| 2:C:149:VAL:O     | 2:C:152:TYR:HD1   | 1.89                     | 0.56              |
| 1:A:945:LEU:N     | 1:A:972:ALA:O     | 2.37                     | 0.56              |
| 2:C:6:LEU:O       | 2:C:111:GLY:HA2   | 2.04                     | 0.56              |
| 2:E:95:THR:HG23   | 2:E:117:THR:HG23  | 1.86                     | 0.56              |
| 2:E:155:GLU:HG2   | 2:E:183:TYR:CE2   | 2.41                     | 0.56              |
| 1:B:395:MET:HE1   | 1:B:454:ILE:O     | 2.06                     | 0.56              |
| 1:A:334:ILE:HD13  | 1:A:359:TYR:HE1   | 1.70                     | 0.56              |
| 1:B:649:PRO:HB2   | 1:B:782:VAL:HG11  | 1.87                     | 0.56              |
| 1:B:729:SER:HA    | 1:B:732:LEU:HB2   | 1.88                     | 0.56              |
| 1:A:1226:HIS:HD2  | 1:A:1258:LEU:HD12 | 1.71                     | 0.56              |
| 1:A:715:ALA:HB3   | 1:A:724:VAL:HG12  | 1.88                     | 0.55              |
| 1:A:1031:VAL:HG13 | 1:A:1078:ASN:HD21 | 1.71                     | 0.55              |
| 1:B:476:VAL:HG11  | 1:B:884:TRP:CZ2   | 2.41                     | 0.55              |
| 1:B:624:VAL:HG11  | 1:B:685:ILE:HG22  | 1.89                     | 0.55              |
| 1:A:1301:GLN:C    | 1:A:1304:SER:H    | 2.15                     | 0.55              |
| 1:A:1063:ALA:O    | 1:A:1066:ALA:HB3  | 2.07                     | 0.55              |
| 1:A:565:GLN:OE1   | 1:A:657:GLN:NE2   | 2.40                     | 0.55              |
| 1:A:1048:GLU:HG3  | 1:A:1090:ALA:HA   | 1.87                     | 0.55              |
| 1:A:1236:VAL:HA   | 1:A:1239:LEU:HB2  | 1.89                     | 0.55              |
| 2:E:150:LYS:NZ    | 3:F:146:GLN:OE1   | 2.35                     | 0.55              |
| 1:B:241:LEU:HA    | 1:B:250:LEU:HD11  | 1.88                     | 0.55              |
| 3:D:58:LEU:HB2    | 3:D:68:LEU:HD11   | 1.89                     | 0.55              |
| 2:E:15:GLN:HB2    | 2:E:18:ARG:HE     | 1.71                     | 0.55              |
| 3:F:54:LEU:HD11   | 3:F:109:CYS:SG    | 2.47                     | 0.55              |
| 1:B:232:VAL:HG23  | 1:B:272:ALA:HB2   | 1.89                     | 0.55              |
| 1:A:1222:SER:HB3  | 1:A:1268:THR:HG22 | 1.88                     | 0.55              |
| 1:A:209:LEU:HD12  | 1:A:442:SER:OG    | 2.06                     | 0.55              |
| 1:B:60:GLU:HG3    | 1:B:62:ARG:HG3    | 1.89                     | 0.54              |
| 3:D:54:LEU:HD11   | 3:D:109:CYS:SG    | 2.47                     | 0.54              |
| 1:A:8:LYS:HB2     | 2:C:105:THR:HG21  | 1.88                     | 0.54              |
| 3:F:58:LEU:HB2    | 3:F:68:LEU:HD11   | 1.89                     | 0.54              |
| 1:A:65:VAL:HG21   | 1:A:255:ARG:HG3   | 1.89                     | 0.54              |
| 2:C:22:LEU:HB2    | 2:C:85:LEU:HB3    | 1.90                     | 0.54              |
| 1:B:126:MET:HB3   | 1:B:188:ILE:HD11  | 1.88                     | 0.54              |
| 1:B:199:ILE:HG23  | 1:A:201:VAL:HG23  | 1.88                     | 0.54              |
| 1:B:301:SER:HA    | 1:B:448:THR:HA    | 1.89                     | 0.54              |
| 2:E:22:LEU:HB2    | 2:E:85:LEU:HB3    | 1.90                     | 0.54              |
| 1:B:716:ALA:HB3   | 1:B:724:VAL:HB    | 1.90                     | 0.54              |
| 1:B:104:PHE:HB3   | 1:B:908:VAL:HG21  | 1.90                     | 0.54              |
| 1:B:778:LEU:HD12  | 1:B:779:PRO:HD2   | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1262:THR:HA   | 1:A:1265:LEU:HD13 | 1.88                     | 0.53              |
| 2:E:77:ASP:O      | 2:E:81:SER:HA     | 2.08                     | 0.53              |
| 3:F:130:ARG:NH1   | 3:F:133:ALA:HB2   | 2.23                     | 0.53              |
| 1:A:156:ILE:O     | 1:A:157:PRO:C     | 2.51                     | 0.53              |
| 3:D:171:LYS:HD3   | 3:D:177:GLN:HB3   | 1.90                     | 0.53              |
| 1:A:340:HIS:CD2   | 1:A:442:SER:HA    | 2.44                     | 0.53              |
| 2:E:149:VAL:HG13  | 2:E:205:VAL:HG11  | 1.89                     | 0.53              |
| 1:A:945:LEU:HD21  | 1:A:1105:SER:HB3  | 1.90                     | 0.53              |
| 2:C:40:ARG:HH22   | 2:C:68:VAL:HG11   | 1.73                     | 0.53              |
| 3:F:30:THR:HB     | 3:F:129:LYS:HB3   | 1.91                     | 0.53              |
| 1:B:287:GLY:O     | 1:B:895:ARG:NH1   | 2.42                     | 0.53              |
| 1:A:646:GLY:HA3   | 1:A:883:ASP:HB3   | 1.90                     | 0.53              |
| 3:F:19:VAL:HG11   | 3:F:45:LEU:HD21   | 1.90                     | 0.53              |
| 3:F:56:TRP:HB2    | 3:F:69:ILE:HB     | 1.90                     | 0.53              |
| 1:B:528:ASP:OD1   | 1:B:529:GLU:N     | 2.42                     | 0.53              |
| 2:C:173:PHE:CZ    | 3:D:196:SER:HB3   | 2.43                     | 0.53              |
| 1:A:162:PRO:HB2   | 1:A:175:LEU:HD21  | 1.90                     | 0.53              |
| 1:A:1272:LEU:HD23 | 1:A:1295:LEU:HD22 | 1.91                     | 0.53              |
| 1:B:187:ARG:HA    | 1:A:308:LEU:HD11  | 1.90                     | 0.53              |
| 1:B:712:VAL:HA    | 1:B:727:GLY:HA3   | 1.90                     | 0.53              |
| 1:A:233:THR:HG21  | 1:A:380:GLN:NE2   | 2.23                     | 0.53              |
| 1:A:368:HIS:HB3   | 1:A:423:LEU:HD21  | 1.90                     | 0.53              |
| 1:A:642:TRP:HZ3   | 1:A:831:VAL:HG13  | 1.72                     | 0.53              |
| 1:A:1072:ARG:HG2  | 1:A:1112:GLN:HE21 | 1.74                     | 0.53              |
| 1:B:103:ALA:HB1   | 1:B:905:ARG:HB3   | 1.90                     | 0.53              |
| 1:A:613:ARG:NH2   | 1:A:620:SER:OG    | 2.42                     | 0.53              |
| 1:A:692:LYS:HG3   | 1:A:728:ASP:HA    | 1.91                     | 0.53              |
| 1:A:1028:LEU:HD11 | 1:A:1244:ILE:HD11 | 1.91                     | 0.53              |
| 2:C:8:GLN:HE22    | 2:C:99:TYR:HA     | 1.74                     | 0.53              |
| 3:F:142:PRO:HD3   | 3:F:154:VAL:HB    | 1.91                     | 0.53              |
| 3:D:56:TRP:HB2    | 3:D:69:ILE:HB     | 1.90                     | 0.53              |
| 1:B:591:ALA:HB2   | 1:B:602:VAL:HG22  | 1.91                     | 0.52              |
| 1:B:680:LEU:HA    | 1:B:683:ARG:HE    | 1.73                     | 0.52              |
| 3:D:142:PRO:HD3   | 3:D:154:VAL:HB    | 1.91                     | 0.52              |
| 3:F:19:VAL:HG22   | 3:F:43:GLN:HB2    | 1.91                     | 0.52              |
| 1:B:14:ARG:HG2    | 3:D:51:TYR:CE2    | 2.42                     | 0.52              |
| 1:A:86:ARG:HG3    | 1:A:87:SER:H      | 1.73                     | 0.52              |
| 1:A:950:LEU:HB2   | 1:A:1003:VAL:HG22 | 1.91                     | 0.52              |
| 1:A:1313:ALA:HB3  | 1:A:1360:ILE:HG23 | 1.91                     | 0.52              |
| 3:D:19:VAL:HG11   | 3:D:45:LEU:HD21   | 1.90                     | 0.52              |
| 2:C:77:ASP:O      | 2:C:81:SER:HA     | 2.08                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:19:VAL:HG22   | 3:D:43:GLN:HB2    | 1.91                     | 0.52              |
| 3:D:30:THR:HB     | 3:D:129:LYS:HB3   | 1.91                     | 0.52              |
| 1:B:339:ALA:HB1   | 1:B:351:GLU:OE2   | 2.10                     | 0.52              |
| 1:A:1074:ILE:HG22 | 1:A:1082:TRP:HB2  | 1.91                     | 0.52              |
| 3:D:27:LEU:HD13   | 3:D:37:ILE:HG13   | 1.92                     | 0.52              |
| 2:E:206:ASN:HB3   | 2:E:213:LYS:HG3   | 1.89                     | 0.52              |
| 1:A:1259:HIS:CE1  | 1:A:1302:ARG:HG3  | 2.44                     | 0.52              |
| 1:B:609:GLU:O     | 1:B:613:ARG:HB2   | 2.10                     | 0.52              |
| 1:A:153:VAL:HG12  | 1:A:155:LEU:HG    | 1.92                     | 0.52              |
| 1:A:906:GLU:HG2   | 1:A:907:ARG:H     | 1.75                     | 0.52              |
| 1:B:562:PHE:HB3   | 1:B:635:MET:HE1   | 1.90                     | 0.52              |
| 2:C:177:LEU:HD13  | 2:C:183:TYR:CE1   | 2.44                     | 0.52              |
| 3:D:127:ASP:OD1   | 3:D:195:TYR:OH    | 2.28                     | 0.52              |
| 1:A:208:SER:HB2   | 1:A:385:VAL:HB    | 1.92                     | 0.52              |
| 1:A:1170:LEU:H    | 1:A:1170:LEU:HD12 | 1.74                     | 0.52              |
| 3:D:130:ARG:HG3   | 3:D:131:THR:O     | 2.11                     | 0.52              |
| 1:B:817:VAL:O     | 1:B:820:LEU:HB3   | 2.09                     | 0.51              |
| 1:A:154:GLY:HA3   | 1:A:207:SER:HB3   | 1.91                     | 0.51              |
| 1:B:133:VAL:HG22  | 1:B:276:LEU:HB2   | 1.91                     | 0.51              |
| 1:B:519:PRO:O     | 1:B:520:HIS:ND1   | 2.44                     | 0.51              |
| 1:A:43:ARG:HB2    | 1:A:272:ALA:HB3   | 1.92                     | 0.51              |
| 1:B:558:ALA:HB2   | 1:B:880:VAL:HG13  | 1.91                     | 0.51              |
| 2:C:171:HIS:CE1   | 3:D:159:ASN:HD21  | 2.28                     | 0.51              |
| 1:B:788:VAL:HB    | 1:B:806:ASN:HA    | 1.93                     | 0.51              |
| 3:F:27:LEU:HD13   | 3:F:37:ILE:HG13   | 1.92                     | 0.51              |
| 1:A:1068:TRP:HZ2  | 1:A:1087:ASP:HB2  | 1.76                     | 0.51              |
| 1:B:8:LYS:HG2     | 2:E:105:THR:HG21  | 1.92                     | 0.51              |
| 1:B:605:PHE:CD2   | 1:B:630:VAL:HG11  | 2.46                     | 0.51              |
| 1:B:605:PHE:HD2   | 1:B:630:VAL:HG11  | 1.74                     | 0.51              |
| 1:A:511:LEU:HD13  | 1:A:898:LEU:HD13  | 1.93                     | 0.51              |
| 1:A:571:GLY:O     | 1:A:574:VAL:HG13  | 2.10                     | 0.51              |
| 2:E:101:THR:HG22  | 2:E:110:TRP:CD2   | 2.46                     | 0.51              |
| 3:F:130:ARG:HG3   | 3:F:131:THR:O     | 2.10                     | 0.51              |
| 1:B:1427:VAL:HG11 | 1:B:1455:LEU:HB2  | 1.93                     | 0.51              |
| 1:A:293:VAL:HG23  | 1:A:455:GLU:HB3   | 1.93                     | 0.51              |
| 1:A:619:LEU:HB2   | 1:A:623:ARG:HG3   | 1.91                     | 0.51              |
| 1:A:1278:SER:OG   | 1:A:1289:ALA:O    | 2.29                     | 0.51              |
| 2:C:150:LYS:NZ    | 3:D:146:GLN:OE1   | 2.39                     | 0.51              |
| 1:B:149:THR:HB    | 1:B:194:LEU:HD22  | 1.92                     | 0.51              |
| 1:A:38:VAL:N      | 1:A:276:LEU:O     | 2.40                     | 0.51              |
| 1:A:155:LEU:HD23  | 1:A:232:VAL:HG13  | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:602:VAL:HG12  | 1:B:630:VAL:HG12  | 1.93                     | 0.51              |
| 1:A:92:GLN:HE21   | 1:A:254:GLY:HA2   | 1.75                     | 0.51              |
| 1:A:269:ALA:O     | 1:A:380:GLN:NE2   | 2.44                     | 0.51              |
| 1:A:390:LYS:HE3   | 1:A:401:PRO:HG2   | 1.92                     | 0.51              |
| 1:A:1087:ASP:HB3  | 1:A:1114:ALA:HA   | 1.93                     | 0.51              |
| 3:F:127:ASP:OD1   | 3:F:195:TYR:OH    | 2.28                     | 0.51              |
| 1:A:558:ALA:HB2   | 1:A:880:VAL:HG13  | 1.92                     | 0.51              |
| 1:A:1209:ARG:HA   | 1:A:1261:LEU:HD21 | 1.92                     | 0.51              |
| 2:E:24:CYS:HB3    | 2:E:83:ALA:HB3    | 1.92                     | 0.51              |
| 1:B:688:MET:HE1   | 1:B:760:VAL:HA    | 1.91                     | 0.50              |
| 1:B:828:PHE:HE1   | 1:B:852:LEU:HB3   | 1.76                     | 0.50              |
| 1:A:367:LEU:HB3   | 1:A:420:ILE:HG12  | 1.92                     | 0.50              |
| 1:A:471:VAL:HG11  | 1:A:865:LEU:HD23  | 1.93                     | 0.50              |
| 1:A:577:LEU:HB2   | 1:A:584:ALA:HB2   | 1.93                     | 0.50              |
| 1:A:692:LYS:HE3   | 1:A:754:ALA:HA    | 1.91                     | 0.50              |
| 1:A:797:GLU:HB2   | 1:A:805:ARG:HH22  | 1.76                     | 0.50              |
| 2:C:24:CYS:HB3    | 2:C:83:ALA:HB3    | 1.92                     | 0.50              |
| 1:B:623:ARG:O     | 1:B:627:VAL:N     | 2.33                     | 0.50              |
| 1:B:683:ARG:HD2   | 1:B:770:GLU:HG2   | 1.92                     | 0.50              |
| 1:A:158:GLN:NE2   | 1:A:240:MET:HE2   | 2.26                     | 0.50              |
| 2:C:105:THR:HA    | 3:D:117:ARG:HH22  | 1.75                     | 0.50              |
| 1:B:576:LEU:HD22  | 1:B:858:LEU:HD11  | 1.94                     | 0.50              |
| 1:A:54:PHE:HZ     | 1:A:372:VAL:HG21  | 1.77                     | 0.50              |
| 1:A:171:VAL:HG21  | 1:A:910:LEU:HD11  | 1.94                     | 0.50              |
| 1:A:339:ALA:HB2   | 1:A:369:LEU:HD11  | 1.93                     | 0.50              |
| 3:F:130:ARG:HD2   | 3:F:193:SER:OG    | 2.11                     | 0.50              |
| 1:A:1302:ARG:HA   | 1:A:1305:ASP:OD2  | 2.12                     | 0.50              |
| 3:F:170:TRP:CD2   | 3:F:201:LEU:HD13  | 2.47                     | 0.50              |
| 1:A:1337:ILE:HG22 | 1:A:1363:ASP:HB3  | 1.94                     | 0.50              |
| 3:F:69:ILE:HG23   | 3:F:74:ASN:O      | 2.11                     | 0.50              |
| 1:B:141:PRO:HD2   | 1:B:516:ALA:HB2   | 1.93                     | 0.50              |
| 1:A:329:LEU:HD13  | 1:A:437:ARG:HD3   | 1.93                     | 0.50              |
| 1:A:627:VAL:O     | 1:A:631:MET:HG2   | 2.12                     | 0.50              |
| 2:C:91:LYS:HE3    | 2:C:93:GLU:HB3    | 1.94                     | 0.50              |
| 2:C:178:GLN:OE1   | 2:C:184:SER:OG    | 2.15                     | 0.50              |
| 2:E:178:GLN:OE1   | 2:E:184:SER:OG    | 2.15                     | 0.50              |
| 1:B:292:ALA:HB3   | 1:B:392:VAL:HG22  | 1.94                     | 0.50              |
| 1:B:666:ALA:O     | 1:B:781:PHE:N     | 2.29                     | 0.50              |
| 1:B:701:ALA:HA    | 1:B:704:VAL:HG22  | 1.94                     | 0.50              |
| 1:A:1302:ARG:HD3  | 1:A:1309:ALA:HB2  | 1.94                     | 0.50              |
| 2:E:170:VAL:HG22  | 2:E:189:VAL:HG12  | 1.94                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:C:170:VAL:HG22 | 2:C:189:VAL:HG12  | 1.94                     | 0.50              |
| 2:E:177:LEU:HB2  | 2:E:183:TYR:HE1   | 1.77                     | 0.50              |
| 1:B:93:ARG:NH2   | 1:A:1055:PRO:O    | 2.27                     | 0.49              |
| 1:B:595:GLU:HA   | 1:B:598:LEU:O     | 2.12                     | 0.49              |
| 1:A:597:HIS:CE1  | 1:A:676:ARG:HB2   | 2.47                     | 0.49              |
| 1:A:776:HIS:HB2  | 2:C:213:LYS:NZ    | 2.27                     | 0.49              |
| 1:B:736:VAL:HG22 | 1:B:746:ALA:HB3   | 1.94                     | 0.49              |
| 1:A:698:ALA:HA   | 1:A:722:SER:HA    | 1.94                     | 0.49              |
| 1:A:837:LEU:O    | 1:A:841:ILE:N     | 2.45                     | 0.49              |
| 1:A:800:ALA:HA   | 1:A:803:TRP:CD1   | 2.48                     | 0.49              |
| 3:D:130:ARG:HD2  | 3:D:193:SER:OG    | 2.11                     | 0.49              |
| 1:A:38:VAL:HG12  | 1:A:137:ALA:HB1   | 1.93                     | 0.49              |
| 1:A:108:PHE:HZ   | 1:A:131:TRP:CE2   | 2.30                     | 0.49              |
| 1:A:642:TRP:CD1  | 1:A:829:LEU:HD21  | 2.47                     | 0.49              |
| 2:C:133:PRO:HG2  | 2:C:220:PRO:HB3   | 1.94                     | 0.49              |
| 3:D:217:GLU:HB3  | 3:D:228:THR:HA    | 1.95                     | 0.49              |
| 1:B:300:ASN:O    | 1:B:449:ASN:N     | 2.45                     | 0.49              |
| 1:A:840:ALA:HA   | 1:A:843:GLU:OE1   | 2.13                     | 0.49              |
| 1:B:77:ASP:OD2   | 1:A:931:ARG:NE    | 2.46                     | 0.49              |
| 1:A:40:MET:HE1   | 1:A:393:LEU:HD21  | 1.95                     | 0.49              |
| 1:A:932:ILE:HD11 | 1:A:1125:TRP:CD1  | 2.47                     | 0.49              |
| 2:E:177:LEU:HB2  | 2:E:183:TYR:CE1   | 2.47                     | 0.49              |
| 1:A:103:ALA:HB1  | 1:A:905:ARG:HB3   | 1.95                     | 0.49              |
| 1:A:841:ILE:O    | 1:A:844:ILE:HB    | 2.13                     | 0.49              |
| 1:A:1068:TRP:CZ2 | 1:A:1087:ASP:HB2  | 2.48                     | 0.49              |
| 1:B:162:PRO:HD2  | 1:B:175:LEU:HD21  | 1.94                     | 0.49              |
| 1:A:737:ALA:C    | 1:A:739:CYS:N     | 2.70                     | 0.49              |
| 1:A:1019:LEU:HG  | 1:A:1252:VAL:HG21 | 1.94                     | 0.49              |
| 1:A:243:ASP:O    | 1:A:244:PHE:C     | 2.52                     | 0.49              |
| 1:A:1383:ASP:OD1 | 1:A:1389:ARG:NH2  | 2.46                     | 0.49              |
| 1:A:305:SER:OG   | 1:A:307:GLY:O     | 2.29                     | 0.48              |
| 2:C:160:SER:HB3  | 2:C:164:GLY:H     | 1.78                     | 0.48              |
| 2:C:177:LEU:HD13 | 2:C:183:TYR:HE1   | 1.76                     | 0.48              |
| 3:D:25:LEU:O     | 3:D:125:LYS:N     | 2.41                     | 0.48              |
| 2:E:133:PRO:HG2  | 2:E:220:PRO:HB3   | 1.95                     | 0.48              |
| 1:A:704:VAL:HG22 | 1:A:714:ILE:HD11  | 1.95                     | 0.48              |
| 1:A:1270:PHE:O   | 1:A:1272:LEU:HD12 | 2.13                     | 0.48              |
| 2:C:6:LEU:HD11   | 2:C:102:ARG:HG3   | 1.95                     | 0.48              |
| 1:A:838:THR:HA   | 1:A:841:ILE:HB    | 1.96                     | 0.48              |
| 2:C:151:ASP:HA   | 2:C:182:LEU:HB3   | 1.95                     | 0.48              |
| 1:B:98:LEU:HD12  | 1:B:234:VAL:HG22  | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:688:MET:N     | 1:B:689:PRO:HD3   | 2.28                     | 0.48              |
| 1:B:712:VAL:HG12  | 1:B:725:VAL:HG22  | 1.95                     | 0.48              |
| 1:B:718:ASN:O     | 1:B:840:ALA:HB1   | 2.13                     | 0.48              |
| 3:F:217:GLU:HB3   | 3:F:228:THR:HA    | 1.95                     | 0.48              |
| 1:B:622:GLU:OE1   | 1:B:623:ARG:NH1   | 2.46                     | 0.48              |
| 1:A:162:PRO:HD2   | 1:A:910:LEU:HG    | 1.95                     | 0.48              |
| 1:A:1096:LEU:HA   | 1:A:1100:LEU:HG   | 1.94                     | 0.48              |
| 2:C:131:LEU:HD11  | 2:C:148:LEU:HG    | 1.94                     | 0.48              |
| 2:C:177:LEU:O     | 3:D:182:GLN:NE2   | 2.24                     | 0.48              |
| 3:D:187:GLU:OE1   | 3:D:187:GLU:N     | 2.47                     | 0.48              |
| 1:B:302:ASP:N     | 1:B:447:GLY:O     | 2.46                     | 0.48              |
| 1:B:764:ARG:HE    | 1:B:768:HIS:CD2   | 2.32                     | 0.48              |
| 1:A:71:ASP:O      | 1:A:907:ARG:NH2   | 2.46                     | 0.48              |
| 1:A:156:ILE:HG13  | 1:A:381:ALA:HB2   | 1.95                     | 0.48              |
| 1:A:385:VAL:O     | 1:A:389:ILE:HG13  | 2.13                     | 0.48              |
| 1:A:1143:VAL:HG11 | 1:A:1160:LEU:HD13 | 1.94                     | 0.48              |
| 3:F:187:GLU:N     | 3:F:187:GLU:OE1   | 2.47                     | 0.48              |
| 1:B:257:LYS:HG3   | 1:B:405:HIS:HB3   | 1.96                     | 0.48              |
| 1:B:491:ARG:HD3   | 1:B:902:PRO:HD3   | 1.96                     | 0.48              |
| 2:C:149:VAL:CG1   | 2:C:205:VAL:HG11  | 2.43                     | 0.48              |
| 1:B:391:MET:HE1   | 1:B:400:LEU:HD21  | 1.95                     | 0.48              |
| 1:B:562:PHE:HB2   | 1:B:654:GLY:HA2   | 1.96                     | 0.48              |
| 1:B:663:ALA:HB1   | 1:B:669:LEU:HB2   | 1.96                     | 0.48              |
| 1:B:680:LEU:HD23  | 1:B:771:LEU:HA    | 1.95                     | 0.48              |
| 1:B:814:ALA:HB1   | 1:B:844:ILE:HD11  | 1.96                     | 0.48              |
| 1:A:15:ARG:HH21   | 3:D:76:ALA:HB1    | 1.79                     | 0.48              |
| 2:C:95:THR:HG23   | 2:C:117:THR:HG23  | 1.95                     | 0.48              |
| 3:D:58:LEU:HD13   | 3:D:107:TYR:CZ    | 2.49                     | 0.48              |
| 1:B:475:TRP:CD1   | 1:B:508:ALA:HB2   | 2.48                     | 0.48              |
| 1:A:736:VAL:HA    | 1:A:739:CYS:HB2   | 1.96                     | 0.48              |
| 1:A:784:PHE:O     | 1:A:792:TRP:HD1   | 1.96                     | 0.47              |
| 1:B:19:ASP:OD1    | 3:F:77:SER:HB3    | 2.13                     | 0.47              |
| 1:B:241:LEU:HD23  | 1:B:268:MET:HE2   | 1.94                     | 0.47              |
| 1:A:568:GLN:OE1   | 1:A:568:GLN:N     | 2.36                     | 0.47              |
| 1:A:1171:VAL:HG22 | 1:A:1198:ALA:HB3  | 1.96                     | 0.47              |
| 1:B:429:TRP:HH2   | 1:B:438:ALA:HB2   | 1.79                     | 0.47              |
| 1:B:783:PRO:HB3   | 1:B:792:TRP:NE1   | 2.28                     | 0.47              |
| 1:B:819:ALA:O     | 1:B:823:GLN:HB2   | 2.15                     | 0.47              |
| 1:A:197:PRO:HD2   | 1:A:224:SER:HB3   | 1.96                     | 0.47              |
| 1:A:1158:ARG:HG2  | 1:A:1188:LEU:HD23 | 1.96                     | 0.47              |
| 1:A:1313:ALA:HB3  | 1:A:1360:ILE:HA   | 1.95                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:E:108:ASP:CG    | 3:F:67:LEU:HD22  | 2.37                     | 0.47              |
| 2:E:155:GLU:HG2   | 2:E:183:TYR:CD2  | 2.49                     | 0.47              |
| 2:E:185:LEU:HD23  | 2:E:186:SER:N    | 2.29                     | 0.47              |
| 1:B:273:GLY:HA3   | 1:B:385:VAL:HG13 | 1.97                     | 0.47              |
| 1:B:329:LEU:HD13  | 1:B:437:ARG:HD3  | 1.97                     | 0.47              |
| 2:E:151:ASP:HA    | 2:E:182:LEU:HB3  | 1.95                     | 0.47              |
| 1:B:12:TYR:CD1    | 2:E:106:LEU:HD22 | 2.49                     | 0.47              |
| 1:B:159:GLU:HG2   | 1:A:163:ARG:HE   | 1.79                     | 0.47              |
| 2:C:36:MET:HB3    | 2:C:36:MET:HE3   | 1.23                     | 0.47              |
| 3:D:184:SER:HB3   | 3:D:198:SER:HB3  | 1.96                     | 0.47              |
| 3:F:58:LEU:HD13   | 3:F:107:TYR:CZ   | 2.49                     | 0.47              |
| 1:B:502:GLN:HB2   | 1:B:507:ILE:HD11 | 1.96                     | 0.47              |
| 1:A:652:VAL:HG21  | 1:A:666:ALA:HB2  | 1.96                     | 0.47              |
| 1:B:242:VAL:O     | 1:B:246:ARG:HG2  | 2.14                     | 0.47              |
| 1:B:308:LEU:HD21  | 1:A:183:VAL:HB   | 1.97                     | 0.47              |
| 1:B:391:MET:O     | 1:B:395:MET:HG3  | 2.14                     | 0.47              |
| 1:B:753:TYR:HE2   | 1:B:755:SER:HB2  | 1.79                     | 0.47              |
| 4:B:1801:PN7:O2P  | 4:B:1801:PN7:O3  | 2.32                     | 0.47              |
| 1:A:683:ARG:HA    | 1:A:683:ARG:HD3  | 1.69                     | 0.47              |
| 1:A:688:MET:N     | 1:A:689:PRO:HD2  | 2.30                     | 0.47              |
| 1:A:802:TYR:HA    | 1:A:805:ARG:HE   | 1.80                     | 0.47              |
| 1:A:1152:VAL:HG22 | 1:A:1317:TRP:CD1 | 2.49                     | 0.47              |
| 1:A:1301:GLN:C    | 1:A:1303:ARG:N   | 2.70                     | 0.47              |
| 1:A:226:LEU:HD12  | 1:A:278:GLU:HB2  | 1.96                     | 0.47              |
| 1:A:1000:VAL:HG12 | 1:A:1002:GLY:H   | 1.78                     | 0.47              |
| 1:B:28:ARG:HH21   | 3:D:75:ARG:HH21  | 1.63                     | 0.47              |
| 1:B:118:ALA:O     | 1:B:178:GLY:HA3  | 2.15                     | 0.47              |
| 1:B:154:GLY:HA3   | 1:B:207:SER:HB3  | 1.97                     | 0.47              |
| 1:A:312:ASN:HD22  | 1:A:315:ALA:HB2  | 1.80                     | 0.47              |
| 1:A:340:HIS:HD2   | 1:A:442:SER:HA   | 1.80                     | 0.47              |
| 1:A:478:SER:O     | 1:A:488:GLN:NE2  | 2.48                     | 0.47              |
| 1:A:524:PHE:HE2   | 1:A:532:ALA:HB1  | 1.80                     | 0.47              |
| 3:D:163:PRO:O     | 3:D:220:HIS:NE2  | 2.48                     | 0.47              |
| 1:B:472:VAL:HG21  | 1:B:866:ALA:HA   | 1.97                     | 0.47              |
| 1:A:555:GLN:O     | 1:A:557:ARG:HG2  | 2.15                     | 0.47              |
| 1:B:652:VAL:C     | 1:B:653:ILE:HG12 | 2.40                     | 0.46              |
| 1:B:835:PRO:HB3   | 1:B:856:HIS:HB2  | 1.96                     | 0.46              |
| 1:A:856:HIS:CE1   | 1:A:859:ARG:HG2  | 2.50                     | 0.46              |
| 1:B:680:LEU:HG    | 1:B:770:GLU:HG3  | 1.98                     | 0.46              |
| 1:B:476:VAL:HB    | 1:B:876:PHE:CE2  | 2.51                     | 0.46              |
| 2:E:7:VAL:HG23    | 2:E:25:THR:HB    | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:36:MET:HE3    | 2:E:36:MET:HB3    | 1.58                     | 0.46              |
| 1:B:680:LEU:O     | 1:B:684:VAL:HG13  | 2.16                     | 0.46              |
| 1:B:855:ILE:HG12  | 1:B:875:ALA:HA    | 1.97                     | 0.46              |
| 1:A:638:LEU:HB3   | 1:A:642:TRP:CZ3   | 2.51                     | 0.46              |
| 1:A:1079:PRO:HB3  | 1:A:1377:ARG:HG2  | 1.98                     | 0.46              |
| 2:C:87:MET:HE2    | 2:C:87:MET:HB3    | 1.78                     | 0.46              |
| 1:B:69:PRO:CG     | 1:B:72:ARG:HD2    | 2.45                     | 0.46              |
| 1:A:485:LEU:HD21  | 1:A:522:ALA:HB2   | 1.95                     | 0.46              |
| 1:A:495:HIS:NE2   | 1:A:897:PRO:O     | 2.47                     | 0.46              |
| 1:A:756:HIS:H     | 1:A:807:LEU:HA    | 1.81                     | 0.46              |
| 3:D:166:ALA:HB2   | 3:D:220:HIS:HB2   | 1.97                     | 0.46              |
| 2:E:208:LYS:HA    | 2:E:208:LYS:HD2   | 1.70                     | 0.46              |
| 1:B:562:PHE:CE1   | 1:B:652:VAL:HG13  | 2.51                     | 0.46              |
| 1:B:632:PHE:CE1   | 1:B:660:ILE:HB    | 2.50                     | 0.46              |
| 1:A:317:VAL:HG13  | 1:A:358:ALA:HB2   | 1.98                     | 0.46              |
| 1:A:660:ILE:HG22  | 1:A:674:ALA:HB1   | 1.96                     | 0.46              |
| 2:E:152:TYR:HB2   | 2:E:207:HIS:CD2   | 2.50                     | 0.46              |
| 1:B:121:PRO:HG2   | 1:B:236:PRO:HB3   | 1.97                     | 0.46              |
| 2:E:131:LEU:HB2   | 2:E:146:GLY:C     | 2.40                     | 0.46              |
| 1:B:400:LEU:HD22  | 1:B:423:LEU:HD11  | 1.98                     | 0.46              |
| 1:A:476:VAL:O     | 1:A:511:LEU:HG    | 2.16                     | 0.46              |
| 1:A:1137:TRP:HE1  | 1:A:1268:THR:HG23 | 1.81                     | 0.46              |
| 1:A:1176:PRO:HD2  | 1:A:1199:ALA:HB2  | 1.97                     | 0.46              |
| 1:A:1272:LEU:HD23 | 1:A:1295:LEU:CD2  | 2.46                     | 0.46              |
| 1:B:121:PRO:HG3   | 1:B:909:TRP:CZ3   | 2.51                     | 0.46              |
| 1:B:336:ALA:HB2   | 1:B:400:LEU:HD11  | 1.98                     | 0.46              |
| 1:B:1421:ARG:NH1  | 1:B:1436:VAL:H    | 2.14                     | 0.46              |
| 2:E:13:LEU:HD13   | 2:E:117:THR:HB    | 1.98                     | 0.46              |
| 2:E:31:PHE:HB3    | 2:E:78:ASP:OD1    | 2.16                     | 0.46              |
| 1:B:207:SER:HB2   | 1:B:381:ALA:HB1   | 1.98                     | 0.46              |
| 1:B:521:ARG:HD3   | 1:B:876:PHE:O     | 2.16                     | 0.46              |
| 1:B:526:PRO:HB3   | 1:B:532:ALA:HB2   | 1.97                     | 0.46              |
| 1:B:731:GLU:O     | 1:B:735:LEU:HG    | 2.16                     | 0.46              |
| 1:A:349:PRO:HA    | 1:A:413:ILE:HG12  | 1.98                     | 0.46              |
| 1:A:1209:ARG:HD2  | 1:A:1261:LEU:HD11 | 1.98                     | 0.46              |
| 3:D:144:ASP:HA    | 3:D:147:LEU:HD12  | 1.98                     | 0.46              |
| 2:E:31:PHE:CE2    | 2:E:76:ARG:HB2    | 2.51                     | 0.46              |
| 1:B:521:ARG:NH1   | 1:B:552:SER:OG    | 2.49                     | 0.45              |
| 1:B:635:MET:HE2   | 1:B:635:MET:HB3   | 1.81                     | 0.45              |
| 1:A:241:LEU:HB3   | 1:A:268:MET:CE    | 2.47                     | 0.45              |
| 1:A:584:ALA:O     | 1:A:588:ARG:HG2   | 2.15                     | 0.45              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:692:LYS:NZ   | 1:A:726:ALA:HB1   | 2.31                     | 0.45              |
| 2:E:143:ALA:HA   | 3:F:138:PHE:HE2   | 1.81                     | 0.45              |
| 2:E:188:VAL:HG21 | 3:F:157:LEU:HD12  | 1.99                     | 0.45              |
| 1:B:339:ALA:HB2  | 1:B:355:LEU:HD11  | 1.99                     | 0.45              |
| 1:A:510:SER:HB3  | 1:A:895:ARG:HB2   | 1.98                     | 0.45              |
| 2:E:37:SER:HB2   | 2:E:101:THR:OG1   | 2.15                     | 0.45              |
| 3:F:58:LEU:O     | 3:F:66:GLN:N      | 2.40                     | 0.45              |
| 1:B:205:CYS:HB3  | 1:B:378:HIS:NE2   | 2.32                     | 0.45              |
| 1:B:165:ALA:O    | 1:A:242:VAL:HG11  | 2.15                     | 0.45              |
| 1:B:351:GLU:HG3  | 1:B:443:PHE:HE2   | 1.81                     | 0.45              |
| 1:B:443:PHE:CD1  | 1:B:449:ASN:HB3   | 2.50                     | 0.45              |
| 1:B:632:PHE:HE1  | 1:B:661:ALA:N     | 2.14                     | 0.45              |
| 1:A:194:LEU:HD11 | 1:A:228:MET:HE2   | 1.98                     | 0.45              |
| 1:A:388:VAL:HG22 | 1:A:440:VAL:HG21  | 1.99                     | 0.45              |
| 2:C:31:PHE:HB3   | 2:C:78:ASP:OD1    | 2.16                     | 0.45              |
| 1:B:2:ALA:HA     | 2:E:54:ARG:HH21   | 1.81                     | 0.45              |
| 1:B:765:ASP:OD1  | 1:B:766:ALA:N     | 2.49                     | 0.45              |
| 1:A:1229:ALA:HB1 | 1:A:1288:TYR:HE1  | 1.82                     | 0.45              |
| 1:A:1377:ARG:HA  | 1:A:1377:ARG:HD2  | 1.77                     | 0.45              |
| 2:C:31:PHE:CE2   | 2:C:76:ARG:HB2    | 2.51                     | 0.45              |
| 1:B:1448:ASP:O   | 1:B:1449:SER:C    | 2.59                     | 0.45              |
| 1:A:17:THR:HG23  | 3:F:74:ASN:HD21   | 1.81                     | 0.45              |
| 3:D:130:ARG:HD2  | 3:D:193:SER:HG    | 1.81                     | 0.45              |
| 2:E:77:ASP:O     | 2:E:81:SER:CA     | 2.64                     | 0.45              |
| 3:F:137:VAL:HB   | 3:F:229:LYS:NZ    | 2.32                     | 0.45              |
| 1:A:805:ARG:HD2  | 1:A:809:ARG:NH2   | 2.32                     | 0.45              |
| 2:C:77:ASP:O     | 2:C:81:SER:CA     | 2.64                     | 0.45              |
| 1:B:797:GLU:H    | 1:B:797:GLU:HG3   | 1.66                     | 0.45              |
| 1:A:539:LEU:HD22 | 1:A:539:LEU:HA    | 1.70                     | 0.45              |
| 1:A:826:ARG:HG3  | 1:A:852:LEU:HA    | 1.99                     | 0.45              |
| 2:C:7:VAL:HG23   | 2:C:25:THR:HB     | 1.98                     | 0.45              |
| 1:A:696:SER:HB2  | 1:A:747:LYS:HE2   | 1.99                     | 0.45              |
| 3:D:58:LEU:HD13  | 3:D:107:TYR:CE2   | 2.52                     | 0.45              |
| 2:E:176:VAL:CG2  | 3:F:184:SER:HB2   | 2.47                     | 0.45              |
| 1:B:561:VAL:CG1  | 1:B:828:PHE:HB2   | 2.47                     | 0.45              |
| 1:B:565:GLN:HG2  | 1:B:657:GLN:HE22  | 1.82                     | 0.45              |
| 1:B:782:VAL:HG12 | 1:B:783:PRO:O     | 2.17                     | 0.45              |
| 1:A:103:ALA:HA   | 1:A:906:GLU:O     | 2.17                     | 0.45              |
| 1:A:1034:MET:SD  | 1:A:1081:VAL:HG13 | 2.57                     | 0.45              |
| 3:F:137:VAL:HG22 | 3:F:158:LEU:CD1   | 2.46                     | 0.45              |
| 1:B:79:LEU:HD21  | 1:B:238:PRO:HB3   | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:131:LEU:HD12  | 2:E:131:LEU:HA    | 1.81                     | 0.44              |
| 1:B:8:LYS:C       | 1:B:10:ALA:H      | 2.25                     | 0.44              |
| 1:B:661:ALA:O     | 1:B:665:VAL:HG22  | 2.18                     | 0.44              |
| 1:A:1043:LEU:N    | 1:A:1081:VAL:O    | 2.48                     | 0.44              |
| 1:A:1139:PRO:HB2  | 1:A:1165:ALA:HA   | 1.99                     | 0.44              |
| 1:A:1310:THR:HG22 | 1:A:1312:VAL:HG13 | 1.98                     | 0.44              |
| 1:A:1362:ILE:HB   | 1:A:1364:VAL:HG12 | 2.00                     | 0.44              |
| 2:E:148:LEU:HD21  | 3:F:155:VAL:HG21  | 2.00                     | 0.44              |
| 3:F:58:LEU:HD13   | 3:F:107:TYR:CE2   | 2.52                     | 0.44              |
| 1:A:176:MET:HB3   | 1:A:176:MET:HE3   | 1.00                     | 0.44              |
| 1:A:763:ILE:HB    | 1:A:767:LEU:HB2   | 1.99                     | 0.44              |
| 1:A:784:PHE:CE2   | 1:A:798:LEU:HD11  | 2.52                     | 0.44              |
| 1:A:1068:TRP:O    | 1:A:1072:ARG:HG3  | 2.16                     | 0.44              |
| 1:A:1188:LEU:H    | 1:A:1188:LEU:HG   | 1.50                     | 0.44              |
| 2:E:207:HIS:O     | 2:E:211:ASN:N     | 2.49                     | 0.44              |
| 1:B:483:GLU:OE1   | 1:B:486:ARG:NH2   | 2.49                     | 0.44              |
| 1:B:813:PHE:CE2   | 1:B:841:ILE:HD11  | 2.52                     | 0.44              |
| 1:A:329:LEU:HD12  | 1:A:453:ILE:HG21  | 1.99                     | 0.44              |
| 1:A:528:ASP:H     | 1:A:531:ALA:HB3   | 1.83                     | 0.44              |
| 2:C:52:PHE:CE1    | 2:C:63:GLU:HB3    | 2.53                     | 0.44              |
| 3:D:58:LEU:O      | 3:D:66:GLN:N      | 2.40                     | 0.44              |
| 1:B:349:PRO:HA    | 1:B:413:ILE:HG12  | 1.99                     | 0.44              |
| 1:A:480:SER:HB2   | 1:A:518:LEU:HD22  | 2.00                     | 0.44              |
| 1:A:619:LEU:HD12  | 1:A:619:LEU:HA    | 1.71                     | 0.44              |
| 1:A:720:PRO:HB2   | 1:A:721:ARG:HD2   | 1.99                     | 0.44              |
| 3:F:158:LEU:HD13  | 3:F:158:LEU:HA    | 1.82                     | 0.44              |
| 1:B:44:LEU:HD22   | 1:B:376:LEU:HD13  | 2.00                     | 0.44              |
| 1:B:1459:LEU:HD12 | 1:B:1459:LEU:HA   | 1.82                     | 0.44              |
| 1:A:302:ASP:HB3   | 1:A:312:ASN:HB2   | 2.00                     | 0.44              |
| 1:A:568:GLN:HE21  | 1:A:621:THR:HG21  | 1.82                     | 0.44              |
| 1:A:655:HIS:NE2   | 1:A:724:VAL:HG21  | 2.33                     | 0.44              |
| 1:B:317:VAL:HG13  | 1:B:358:ALA:HB2   | 1.99                     | 0.44              |
| 1:B:529:GLU:O     | 1:B:533:LEU:HD13  | 2.16                     | 0.44              |
| 1:B:710:ASP:HB2   | 1:B:731:GLU:HG3   | 1.98                     | 0.44              |
| 2:E:35:ALA:CB     | 2:E:54:ARG:HA     | 2.48                     | 0.44              |
| 1:B:234:VAL:HA    | 1:B:270:GLU:HG3   | 2.00                     | 0.44              |
| 1:A:682:SER:HA    | 1:A:685:ILE:HG22  | 2.00                     | 0.44              |
| 1:A:1093:VAL:HB   | 1:A:1096:LEU:HD12 | 1.98                     | 0.44              |
| 1:A:1143:VAL:HG21 | 1:A:1160:LEU:HD22 | 2.00                     | 0.44              |
| 1:A:1224:VAL:HB   | 1:A:1270:PHE:HD1  | 1.83                     | 0.44              |
| 2:C:37:SER:O      | 2:C:101:THR:OG1   | 2.36                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:F:25:LEU:O      | 3:F:125:LYS:N     | 2.41                     | 0.44              |
| 1:B:512:ALA:HB1   | 1:B:884:TRP:HB3   | 2.00                     | 0.43              |
| 1:B:588:ARG:HD2   | 1:B:603:ILE:HG13  | 2.00                     | 0.43              |
| 1:A:69:PRO:HG3    | 1:A:97:PHE:HB3    | 2.00                     | 0.43              |
| 1:A:778:LEU:HD22  | 1:A:778:LEU:HA    | 1.81                     | 0.43              |
| 1:B:8:LYS:C       | 1:B:10:ALA:N      | 2.75                     | 0.43              |
| 1:B:34:PRO:HB2    | 1:B:293:VAL:HG11  | 1.99                     | 0.43              |
| 1:A:1028:LEU:HD21 | 1:A:1070:VAL:HG21 | 1.99                     | 0.43              |
| 1:A:1096:LEU:HD22 | 1:A:1100:LEU:HD11 | 2.00                     | 0.43              |
| 1:A:1110:GLU:HB2  | 1:A:1113:LEU:HD21 | 1.99                     | 0.43              |
| 1:A:1298:LEU:O    | 1:A:1302:ARG:HB2  | 2.18                     | 0.43              |
| 3:F:22:GLN:N      | 3:F:22:GLN:OE1    | 2.51                     | 0.43              |
| 1:B:171:VAL:HG21  | 1:B:910:LEU:HD21  | 1.99                     | 0.43              |
| 1:B:379:THR:HB    | 1:B:382:ALA:HB3   | 2.00                     | 0.43              |
| 1:A:573:ALA:HB1   | 1:A:576:LEU:HB3   | 2.00                     | 0.43              |
| 1:A:1071:GLY:HA3  | 1:A:1085:LEU:HD11 | 2.00                     | 0.43              |
| 1:A:1167:HIS:CD2  | 1:A:1219:VAL:HG11 | 2.53                     | 0.43              |
| 3:D:128:ILE:HB    | 3:D:188:GLN:NE2   | 2.34                     | 0.43              |
| 1:A:177:THR:O     | 1:A:183:VAL:HG21  | 2.19                     | 0.43              |
| 1:A:703:GLU:HG2   | 1:A:704:VAL:N     | 2.34                     | 0.43              |
| 1:B:492:LEU:HD21  | 1:B:511:LEU:HD11  | 2.01                     | 0.43              |
| 1:A:149:THR:HA    | 1:A:226:LEU:O     | 2.19                     | 0.43              |
| 1:A:705:ARG:HG2   | 1:A:714:ILE:HG13  | 2.00                     | 0.43              |
| 1:A:949:TRP:HZ3   | 1:A:1044:TRP:HD1  | 1.65                     | 0.43              |
| 3:F:31:PRO:HA     | 3:F:99:VAL:O      | 2.19                     | 0.43              |
| 1:B:80:PHE:CE1    | 1:B:93:ARG:HD2    | 2.53                     | 0.43              |
| 1:B:338:GLU:O     | 1:B:338:GLU:HG3   | 2.18                     | 0.43              |
| 1:A:641:MET:HG2   | 1:A:868:PHE:CZ    | 2.53                     | 0.43              |
| 3:D:22:GLN:OE1    | 3:D:22:GLN:N      | 2.51                     | 0.43              |
| 1:B:697:ILE:HG12  | 1:B:699:ALA:H     | 1.84                     | 0.43              |
| 2:C:8:GLN:HE21    | 2:C:100:CYS:HB2   | 1.83                     | 0.43              |
| 1:A:155:LEU:HD12  | 1:A:200:SER:OG    | 2.19                     | 0.43              |
| 1:A:610:ALA:HA    | 1:A:613:ARG:HE    | 1.83                     | 0.43              |
| 1:A:1088:VAL:HG11 | 1:A:1096:LEU:HD23 | 2.00                     | 0.43              |
| 3:D:31:PRO:HA     | 3:D:99:VAL:O      | 2.19                     | 0.43              |
| 3:D:137:VAL:HB    | 3:D:229:LYS:NZ    | 2.34                     | 0.43              |
| 2:E:80:LYS:O      | 2:E:82:ILE:HG12   | 2.18                     | 0.43              |
| 2:E:205:VAL:O     | 2:E:213:LYS:HA    | 2.19                     | 0.43              |
| 1:B:632:PHE:O     | 1:B:636:VAL:HG12  | 2.19                     | 0.43              |
| 1:A:39:ALA:HB2    | 1:A:137:ALA:HB2   | 2.00                     | 0.43              |
| 1:A:593:ALA:HB1   | 1:A:672:ASP:HA    | 2.00                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:E:53:ILE:HB     | 2:E:74:ILE:HG22  | 2.01                     | 0.43              |
| 2:E:112:GLN:H     | 2:E:112:GLN:HG3  | 1.17                     | 0.43              |
| 3:F:29:VAL:HB     | 3:F:99:VAL:HG11  | 2.00                     | 0.43              |
| 3:F:106:VAL:HG22  | 3:F:125:LYS:HD2  | 2.01                     | 0.43              |
| 1:B:739:CYS:SG    | 1:B:740:THR:N    | 2.91                     | 0.43              |
| 1:B:836:ILE:H     | 1:B:836:ILE:HG13 | 1.36                     | 0.43              |
| 1:A:406:ALA:HB1   | 1:A:422:LEU:HD13 | 2.01                     | 0.43              |
| 1:A:512:ALA:HB1   | 1:A:884:TRP:CG   | 2.54                     | 0.43              |
| 1:A:1155:GLN:HG3  | 1:A:1158:ARG:NH1 | 2.34                     | 0.43              |
| 1:A:1173:ARG:HD2  | 1:A:1201:ASP:HA  | 2.00                     | 0.43              |
| 3:F:58:LEU:HD21   | 3:F:60:LYS:HG3   | 2.01                     | 0.43              |
| 1:A:64:ALA:N      | 1:A:375:ASN:O    | 2.45                     | 0.42              |
| 1:A:235:MET:HA    | 1:A:236:PRO:HD2  | 1.83                     | 0.42              |
| 1:A:367:LEU:O     | 1:A:421:SER:N    | 2.39                     | 0.42              |
| 1:A:1033:ALA:O    | 1:A:1037:ALA:N   | 2.50                     | 0.42              |
| 1:A:1143:VAL:HG11 | 1:A:1160:LEU:CD1 | 2.49                     | 0.42              |
| 1:B:349:PRO:O     | 1:B:353:ARG:HG3  | 2.18                     | 0.42              |
| 1:B:805:ARG:HG2   | 1:B:809:ARG:HH12 | 1.84                     | 0.42              |
| 1:A:29:GLU:HA     | 1:A:33:GLU:HB2   | 2.01                     | 0.42              |
| 1:A:532:ALA:HA    | 1:A:535:VAL:HG23 | 2.01                     | 0.42              |
| 1:A:608:ALA:HA    | 1:A:612:ARG:HE   | 1.85                     | 0.42              |
| 2:C:49:TRP:HZ2    | 2:C:52:PHE:HD1   | 1.66                     | 0.42              |
| 2:C:80:LYS:O      | 2:C:82:ILE:HG12  | 2.19                     | 0.42              |
| 2:C:185:LEU:HD23  | 2:C:186:SER:N    | 2.34                     | 0.42              |
| 3:D:141:PRO:HA    | 3:D:154:VAL:HG23 | 2.01                     | 0.42              |
| 3:F:215:ALA:HA    | 3:F:230:SER:HA   | 2.01                     | 0.42              |
| 1:B:334:ILE:O     | 1:B:363:ARG:NH1  | 2.33                     | 0.42              |
| 1:B:719:GLY:H     | 1:B:814:ALA:HB2  | 1.83                     | 0.42              |
| 1:B:35:VAL:HG23   | 1:B:294:LEU:HB2  | 2.01                     | 0.42              |
| 1:B:36:ALA:HB1    | 1:B:290:VAL:HG13 | 2.02                     | 0.42              |
| 1:B:731:GLU:HA    | 1:B:734:ARG:HG2  | 2.00                     | 0.42              |
| 4:B:1801:PN7:H15  | 1:A:311:PRO:HD3  | 2.01                     | 0.42              |
| 1:A:337:VAL:HG23  | 1:A:367:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:668:ALA:HB2   | 1:A:795:PRO:HB2  | 2.01                     | 0.42              |
| 1:A:1159:TRP:HE1  | 1:A:1163:ARG:CZ  | 2.32                     | 0.42              |
| 1:B:774:ASP:OD1   | 1:B:774:ASP:N    | 2.52                     | 0.42              |
| 1:A:495:HIS:CG    | 1:A:899:PRO:HD3  | 2.55                     | 0.42              |
| 1:A:739:CYS:HA    | 1:A:742:GLU:HG2  | 2.02                     | 0.42              |
| 1:A:1007:LEU:H    | 1:A:1007:LEU:HG  | 1.42                     | 0.42              |
| 1:A:1339:MET:H    | 1:A:1339:MET:HG3 | 1.56                     | 0.42              |
| 3:D:29:VAL:HB     | 3:D:99:VAL:HG11  | 2.00                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:D:54:LEU:HD13   | 3:D:92:PHE:CG     | 2.54                     | 0.42              |
| 1:B:228:MET:HG2   | 1:B:276:LEU:HD13  | 2.02                     | 0.42              |
| 1:B:410:SER:HB3   | 1:B:413:ILE:HD12  | 2.02                     | 0.42              |
| 1:B:731:GLU:HG2   | 1:B:734:ARG:HH11  | 1.84                     | 0.42              |
| 1:A:40:MET:HE1    | 1:A:393:LEU:CD2   | 2.49                     | 0.42              |
| 1:A:944:ARG:HD3   | 1:A:944:ARG:HA    | 1.92                     | 0.42              |
| 2:C:69:LYS:HA     | 2:C:69:LYS:HD3    | 1.84                     | 0.42              |
| 2:C:206:ASN:HD22  | 2:C:213:LYS:HG3   | 1.85                     | 0.42              |
| 1:B:269:ALA:HB2   | 1:B:377:GLY:HA3   | 2.01                     | 0.42              |
| 1:B:434:ARG:HE    | 1:B:434:ARG:HB3   | 1.61                     | 0.42              |
| 1:B:1465:VAL:HG21 | 1:B:1485:LEU:HD11 | 2.02                     | 0.42              |
| 1:A:1049:SER:N    | 1:A:1088:VAL:O    | 2.50                     | 0.42              |
| 1:A:1331:PHE:HB3  | 1:A:1336:VAL:HG13 | 2.02                     | 0.42              |
| 3:F:128:ILE:HB    | 3:F:188:GLN:NE2   | 2.34                     | 0.42              |
| 1:B:378:HIS:CD2   | 1:B:380:GLN:H     | 2.38                     | 0.42              |
| 1:A:265:GLY:HA2   | 1:A:344:THR:HA    | 2.02                     | 0.42              |
| 1:A:338:GLU:N     | 1:A:439:GLY:O     | 2.46                     | 0.42              |
| 1:A:556:GLN:HG3   | 1:A:881:ALA:HB2   | 2.02                     | 0.42              |
| 1:A:628:GLN:HB2   | 1:A:682:SER:HB2   | 2.02                     | 0.42              |
| 3:F:102:GLU:H     | 3:F:102:GLU:HG2   | 1.66                     | 0.42              |
| 1:A:506:ASP:OD2   | 1:A:894:ARG:NH1   | 2.53                     | 0.42              |
| 1:A:577:LEU:HD23  | 1:A:577:LEU:H     | 1.85                     | 0.42              |
| 1:A:589:GLU:HG2   | 1:A:590:CYS:N     | 2.35                     | 0.42              |
| 1:A:1222:SER:HB3  | 1:A:1268:THR:H    | 1.85                     | 0.42              |
| 3:D:168:VAL:HG21  | 3:D:197:LEU:HD22  | 2.02                     | 0.42              |
| 1:A:465:ARG:HD2   | 1:A:465:ARG:HA    | 1.39                     | 0.42              |
| 2:C:149:VAL:HG13  | 2:C:205:VAL:HG11  | 2.01                     | 0.42              |
| 3:F:118:LEU:HD13  | 3:F:118:LEU:HA    | 1.83                     | 0.42              |
| 1:B:400:LEU:HA    | 1:B:401:PRO:HD3   | 1.88                     | 0.41              |
| 1:B:695:ALA:O     | 1:B:725:VAL:HG12  | 2.20                     | 0.41              |
| 1:A:311:PRO:HG2   | 1:A:350:ILE:HD12  | 2.01                     | 0.41              |
| 2:C:18:ARG:HA     | 2:C:18:ARG:HD3    | 1.74                     | 0.41              |
| 2:C:38:TRP:O      | 2:C:50:VAL:HB     | 2.19                     | 0.41              |
| 1:B:1409:ALA:C    | 1:B:1411:GLU:N    | 2.78                     | 0.41              |
| 1:A:253:ASP:OD2   | 1:A:255:ARG:HD3   | 2.20                     | 0.41              |
| 1:A:811:VAL:HG12  | 1:A:813:PHE:HB2   | 2.01                     | 0.41              |
| 2:C:171:HIS:CE1   | 3:D:159:ASN:ND2   | 2.88                     | 0.41              |
| 3:D:215:ALA:HA    | 3:D:230:SER:HA    | 2.01                     | 0.41              |
| 2:E:49:TRP:HZ2    | 2:E:52:PHE:HD1    | 1.66                     | 0.41              |
| 1:B:34:PRO:HB2    | 1:B:293:VAL:CG1   | 2.50                     | 0.41              |
| 1:B:39:ALA:HB2    | 1:B:137:ALA:HB2   | 2.01                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:B:221:ARG:HD2   | 1:B:223:GLU:HB2  | 2.03                     | 0.41              |
| 1:B:244:PHE:HD2   | 1:B:268:MET:HE1  | 1.85                     | 0.41              |
| 1:A:12:TYR:CE1    | 3:D:70:TYR:HB2   | 2.55                     | 0.41              |
| 1:A:802:TYR:HD1   | 1:A:805:ARG:HH21 | 1.68                     | 0.41              |
| 3:D:106:VAL:HG22  | 3:D:125:LYS:HD2  | 2.01                     | 0.41              |
| 1:B:55:TRP:O      | 1:B:59:SER:HB3   | 2.20                     | 0.41              |
| 1:B:650:ALA:HB1   | 1:B:825:TYR:CZ   | 2.56                     | 0.41              |
| 1:B:1437:PRO:HB2  | 1:B:1440:GLN:HB2 | 2.02                     | 0.41              |
| 1:A:604:PRO:HB3   | 1:A:607:ARG:HH21 | 1.86                     | 0.41              |
| 2:E:21:ARG:NH1    | 2:E:84:TYR:CD2   | 2.88                     | 0.41              |
| 2:E:53:ILE:HG23   | 2:E:76:ARG:HH11  | 1.84                     | 0.41              |
| 2:E:80:LYS:NZ     | 2:E:82:ILE:HG13  | 2.36                     | 0.41              |
| 1:B:227:ALA:O     | 1:B:276:LEU:HD12 | 2.21                     | 0.41              |
| 1:B:1409:ALA:HB3  | 1:B:1411:GLU:CG  | 2.51                     | 0.41              |
| 1:A:139:ILE:HD12  | 1:A:139:ILE:H    | 1.85                     | 0.41              |
| 1:A:171:VAL:HG21  | 1:A:910:LEU:CD1  | 2.50                     | 0.41              |
| 1:A:625:ASP:HB3   | 1:A:686:ALA:HB2  | 2.01                     | 0.41              |
| 2:C:6:LEU:HD22    | 2:C:24:CYS:SG    | 2.61                     | 0.41              |
| 3:D:146:GLN:OE1   | 3:D:153:SER:HB2  | 2.20                     | 0.41              |
| 3:F:59:GLN:OE1    | 3:F:65:PRO:HG3   | 2.20                     | 0.41              |
| 1:B:140:PRO:HA    | 1:B:141:PRO:HD3  | 1.96                     | 0.41              |
| 1:B:1471:THR:HG23 | 1:B:1475:HIS:HD2 | 1.85                     | 0.41              |
| 1:A:562:PHE:HB3   | 1:A:635:MET:HE1  | 2.03                     | 0.41              |
| 1:A:1030:LEU:O    | 1:A:1034:MET:HG3 | 2.21                     | 0.41              |
| 2:E:77:ASP:O      | 2:E:81:SER:N     | 2.54                     | 0.41              |
| 3:F:141:PRO:HA    | 3:F:154:VAL:HG23 | 2.01                     | 0.41              |
| 3:F:146:GLN:OE1   | 3:F:153:SER:HB2  | 2.20                     | 0.41              |
| 1:B:329:LEU:HD12  | 1:B:453:ILE:HG21 | 2.03                     | 0.41              |
| 1:B:512:ALA:HB1   | 1:B:884:TRP:CG   | 2.56                     | 0.41              |
| 2:C:80:LYS:NZ     | 2:C:82:ILE:HG13  | 2.36                     | 0.41              |
| 1:B:130:SER:HB2   | 1:B:228:MET:HE1  | 2.02                     | 0.41              |
| 1:A:92:GLN:HB2    | 1:A:250:LEU:HD23 | 2.01                     | 0.41              |
| 1:A:865:LEU:HD12  | 1:A:865:LEU:HA   | 1.86                     | 0.41              |
| 2:C:126:PRO:HB3   | 2:C:149:VAL:CG1  | 2.51                     | 0.41              |
| 3:D:59:GLN:OE1    | 3:D:65:PRO:HG3   | 2.20                     | 0.41              |
| 3:F:189:ASP:OD1   | 3:F:194:THR:N    | 2.49                     | 0.41              |
| 1:B:115:GLU:O     | 1:B:119:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:357:GLU:HA    | 1:B:361:ARG:HG2  | 2.02                     | 0.41              |
| 1:A:141:PRO:HG2   | 1:A:516:ALA:HB2  | 2.03                     | 0.41              |
| 1:A:911:GLU:O     | 1:A:912:PRO:C    | 2.64                     | 0.41              |
| 1:A:1054:GLY:HA3  | 1:A:1056:PHE:CE1 | 2.56                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:C:31:PHE:HE2    | 2:C:76:ARG:HB2   | 1.86                     | 0.41              |
| 2:C:37:SER:HB3    | 2:C:52:PHE:HB3   | 2.03                     | 0.41              |
| 2:C:149:VAL:HG12  | 2:C:152:TYR:CD1  | 2.55                     | 0.41              |
| 2:C:161:TRP:HD1   | 2:C:170:VAL:HG13 | 1.85                     | 0.41              |
| 1:B:465:ARG:HH12  | 1:B:467:GLU:CD   | 2.29                     | 0.41              |
| 1:B:511:LEU:O     | 1:B:515:ARG:HB2  | 2.20                     | 0.41              |
| 1:B:839:ALA:HA    | 1:B:842:GLU:HB2  | 2.03                     | 0.41              |
| 1:B:1409:ALA:C    | 1:B:1411:GLU:H   | 2.28                     | 0.41              |
| 1:A:773:GLU:H     | 1:A:773:GLU:HG3  | 1.47                     | 0.41              |
| 1:A:911:GLU:HA    | 1:A:912:PRO:HD2  | 1.86                     | 0.41              |
| 1:A:1206:GLU:HA   | 1:A:1209:ARG:HB3 | 2.03                     | 0.41              |
| 1:A:1318:ALA:HB3  | 1:A:1341:PRO:HD3 | 2.03                     | 0.41              |
| 3:F:53:TYR:O      | 3:F:112:SER:N    | 2.54                     | 0.41              |
| 3:F:130:ARG:HH12  | 3:F:133:ALA:HB2  | 1.85                     | 0.41              |
| 1:B:689:PRO:HG3   | 1:B:753:TYR:HB3  | 2.02                     | 0.40              |
| 1:B:692:LYS:HG3   | 1:B:759:HIS:CD2  | 2.56                     | 0.40              |
| 1:B:712:VAL:HG22  | 1:B:727:GLY:HA3  | 2.02                     | 0.40              |
| 1:A:692:LYS:HE2   | 1:A:757:SER:OG   | 2.20                     | 0.40              |
| 1:A:1229:ALA:H    | 1:A:1322:MET:HE2 | 1.87                     | 0.40              |
| 1:A:1334:HIS:HA   | 1:A:1368:ARG:HB3 | 2.03                     | 0.40              |
| 2:C:77:ASP:O      | 2:C:81:SER:N     | 2.54                     | 0.40              |
| 2:C:159:VAL:HG22  | 2:C:205:VAL:HG13 | 2.03                     | 0.40              |
| 1:A:533:LEU:HD13  | 1:A:533:LEU:HA   | 1.75                     | 0.40              |
| 1:A:805:ARG:HD2   | 1:A:809:ARG:HH21 | 1.85                     | 0.40              |
| 1:A:1078:ASN:CG   | 1:A:1081:VAL:HB  | 2.46                     | 0.40              |
| 2:C:13:LEU:HD13   | 2:C:117:THR:HB   | 2.03                     | 0.40              |
| 3:D:104:VAL:HG23  | 3:D:126:VAL:HG12 | 2.03                     | 0.40              |
| 2:E:173:PHE:O     | 2:E:185:LEU:HG   | 2.21                     | 0.40              |
| 3:F:135:PRO:HG3   | 3:F:220:HIS:HB3  | 2.04                     | 0.40              |
| 1:B:506:ASP:HB3   | 1:B:896:VAL:HG21 | 2.03                     | 0.40              |
| 1:A:443:PHE:HA    | 1:A:449:ASN:HA   | 2.04                     | 0.40              |
| 1:A:1239:LEU:HD23 | 1:A:1239:LEU:HA  | 1.95                     | 0.40              |
| 2:E:31:PHE:O      | 2:E:76:ARG:NH2   | 2.54                     | 0.40              |
| 1:A:133:VAL:HG22  | 1:A:276:LEU:HB2  | 2.04                     | 0.40              |
| 1:A:609:GLU:O     | 1:A:613:ARG:N    | 2.54                     | 0.40              |
| 1:A:1321:GLY:HA2  | 1:A:1324:GLU:HB3 | 2.04                     | 0.40              |
| 1:A:1366:TRP:HA   | 1:A:1369:PHE:HB3 | 2.02                     | 0.40              |
| 3:D:53:TYR:O      | 3:D:112:SER:N    | 2.54                     | 0.40              |
| 1:B:163:ARG:HE    | 1:A:159:GLU:HG2  | 1.86                     | 0.40              |
| 1:B:217:GLN:HG3   | 1:A:221:ARG:NH1  | 2.37                     | 0.40              |
| 1:B:659:GLU:HG3   | 1:B:806:ASN:ND2  | 2.37                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:680:LEU:HD12 | 1:B:683:ARG:NH2  | 2.36                     | 0.40              |
| 1:A:93:ARG:HE    | 1:A:93:ARG:HB3   | 1.42                     | 0.40              |
| 1:A:562:PHE:HD2  | 1:A:635:MET:HE2  | 1.87                     | 0.40              |
| 1:A:640:SER:HA   | 1:A:643:ARG:HD3  | 2.04                     | 0.40              |
| 1:A:682:SER:O    | 1:A:685:ILE:HG22 | 2.21                     | 0.40              |
| 2:C:6:LEU:HD23   | 2:C:6:LEU:HA     | 1.93                     | 0.40              |
| 2:C:40:ARG:N     | 2:C:48:GLU:O     | 2.46                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 1388/1784 (78%) | 1264 (91%) | 123 (9%) | 1 (0%)   | 48          | 79  |
| 1   | B     | 995/1784 (56%)  | 915 (92%)  | 78 (8%)  | 2 (0%)   | 43          | 73  |
| 2   | C     | 199/249 (80%)   | 179 (90%)  | 20 (10%) | 0        | 100         | 100 |
| 2   | E     | 199/249 (80%)   | 176 (88%)  | 23 (12%) | 0        | 100         | 100 |
| 3   | D     | 200/236 (85%)   | 184 (92%)  | 16 (8%)  | 0        | 100         | 100 |
| 3   | F     | 200/236 (85%)   | 187 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| All | All   | 3181/4538 (70%) | 2905 (91%) | 273 (9%) | 3 (0%)   | 49          | 79  |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 1449 | SER  |
| 1   | B     | 720  | PRO  |
| 1   | A     | 779  | 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 PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |    |
|-----|-------|-----------------|------------|-----------|-------------|----|
| 1   | A     | 1028/1325 (78%) | 873 (85%)  | 155 (15%) | 3           | 14 |
| 1   | B     | 746/1325 (56%)  | 651 (87%)  | 95 (13%)  | 4           | 20 |
| 2   | C     | 170/203 (84%)   | 133 (78%)  | 37 (22%)  | 1           | 6  |
| 2   | E     | 170/203 (84%)   | 135 (79%)  | 35 (21%)  | 1           | 7  |
| 3   | D     | 182/208 (88%)   | 143 (79%)  | 39 (21%)  | 1           | 6  |
| 3   | F     | 182/208 (88%)   | 145 (80%)  | 37 (20%)  | 1           | 7  |
| All | All   | 2478/3472 (71%) | 2080 (84%) | 398 (16%) | 4           | 13 |

All (398) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 7   | GLU  |
| 1   | B     | 9   | VAL  |
| 1   | B     | 31  | GLU  |
| 1   | B     | 52  | GLU  |
| 1   | B     | 57  | LEU  |
| 1   | B     | 75  | ASP  |
| 1   | B     | 100 | GLU  |
| 1   | B     | 111 | MET  |
| 1   | B     | 112 | SER  |
| 1   | B     | 114 | ARG  |
| 1   | B     | 123 | GLN  |
| 1   | B     | 124 | ARG  |
| 1   | B     | 126 | MET  |
| 1   | B     | 129 | LEU  |
| 1   | B     | 156 | ILE  |
| 1   | B     | 159 | GLU  |
| 1   | B     | 162 | PRO  |
| 1   | B     | 163 | ARG  |
| 1   | B     | 164 | LEU  |
| 1   | B     | 175 | LEU  |
| 1   | B     | 180 | THR  |
| 1   | B     | 181 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 182 | SER  |
| 1   | B     | 197 | PRO  |
| 1   | B     | 199 | ILE  |
| 1   | B     | 205 | CYS  |
| 1   | B     | 209 | LEU  |
| 1   | B     | 212 | VAL  |
| 1   | B     | 214 | LEU  |
| 1   | B     | 220 | ARG  |
| 1   | B     | 221 | ARG  |
| 1   | B     | 237 | THR  |
| 1   | B     | 240 | MET  |
| 1   | B     | 241 | LEU  |
| 1   | B     | 264 | ASN  |
| 1   | B     | 268 | MET  |
| 1   | B     | 270 | GLU  |
| 1   | B     | 342 | THR  |
| 1   | B     | 344 | THR  |
| 1   | B     | 345 | ARG  |
| 1   | B     | 400 | LEU  |
| 1   | B     | 402 | ARG  |
| 1   | B     | 553 | ARG  |
| 1   | B     | 556 | GLN  |
| 1   | B     | 567 | TRP  |
| 1   | B     | 572 | MET  |
| 1   | B     | 574 | VAL  |
| 1   | B     | 575 | ASP  |
| 1   | B     | 577 | LEU  |
| 1   | B     | 579 | THR  |
| 1   | B     | 581 | PRO  |
| 1   | B     | 606 | LEU  |
| 1   | B     | 607 | ARG  |
| 1   | B     | 612 | ARG  |
| 1   | B     | 631 | MET  |
| 1   | B     | 653 | ILE  |
| 1   | B     | 660 | ILE  |
| 1   | B     | 682 | SER  |
| 1   | B     | 684 | VAL  |
| 1   | B     | 703 | GLU  |
| 1   | B     | 705 | ARG  |
| 1   | B     | 721 | ARG  |
| 1   | B     | 751 | VAL  |
| 1   | B     | 752 | ASP  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 788  | VAL  |
| 1   | B     | 797  | GLU  |
| 1   | B     | 799  | ASP  |
| 1   | B     | 827  | THR  |
| 1   | B     | 831  | VAL  |
| 1   | B     | 836  | ILE  |
| 1   | B     | 837  | LEU  |
| 1   | B     | 852  | LEU  |
| 1   | B     | 853  | SER  |
| 1   | B     | 859  | ARG  |
| 1   | B     | 865  | LEU  |
| 1   | B     | 870  | GLU  |
| 1   | B     | 872  | LEU  |
| 1   | B     | 873  | SER  |
| 1   | B     | 908  | VAL  |
| 1   | B     | 1407 | LEU  |
| 1   | B     | 1411 | GLU  |
| 1   | B     | 1412 | ARG  |
| 1   | B     | 1414 | LYS  |
| 1   | B     | 1435 | ARG  |
| 1   | B     | 1436 | VAL  |
| 1   | B     | 1447 | VAL  |
| 1   | B     | 1448 | ASP  |
| 1   | B     | 1453 | LEU  |
| 1   | B     | 1455 | LEU  |
| 1   | B     | 1456 | ARG  |
| 1   | B     | 1458 | ARG  |
| 1   | B     | 1459 | LEU  |
| 1   | B     | 1463 | THR  |
| 1   | B     | 1466 | ARG  |
| 1   | B     | 1485 | LEU  |
| 1   | A     | 1    | MET  |
| 1   | A     | 3    | SER  |
| 1   | A     | 5    | ASP  |
| 1   | A     | 7    | GLU  |
| 1   | A     | 8    | LYS  |
| 1   | A     | 9    | VAL  |
| 1   | A     | 42   | CYS  |
| 1   | A     | 43   | ARG  |
| 1   | A     | 44   | LEU  |
| 1   | A     | 56   | GLU  |
| 1   | A     | 57   | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 62  | ARG  |
| 1   | A     | 65  | VAL  |
| 1   | A     | 92  | GLN  |
| 1   | A     | 93  | ARG  |
| 1   | A     | 98  | LEU  |
| 1   | A     | 117 | LEU  |
| 1   | A     | 124 | ARG  |
| 1   | A     | 157 | PRO  |
| 1   | A     | 158 | GLN  |
| 1   | A     | 159 | GLU  |
| 1   | A     | 162 | PRO  |
| 1   | A     | 163 | ARG  |
| 1   | A     | 171 | VAL  |
| 1   | A     | 176 | MET  |
| 1   | A     | 179 | THR  |
| 1   | A     | 180 | THR  |
| 1   | A     | 203 | THR  |
| 1   | A     | 207 | SER  |
| 1   | A     | 220 | ARG  |
| 1   | A     | 232 | VAL  |
| 1   | A     | 233 | THR  |
| 1   | A     | 243 | ASP  |
| 1   | A     | 247 | MET  |
| 1   | A     | 250 | LEU  |
| 1   | A     | 266 | PHE  |
| 1   | A     | 342 | THR  |
| 1   | A     | 376 | LEU  |
| 1   | A     | 404 | LEU  |
| 1   | A     | 422 | LEU  |
| 1   | A     | 460 | VAL  |
| 1   | A     | 461 | VAL  |
| 1   | A     | 462 | GLU  |
| 1   | A     | 464 | GLU  |
| 1   | A     | 465 | ARG  |
| 1   | A     | 467 | GLU  |
| 1   | A     | 498 | GLU  |
| 1   | A     | 505 | ARG  |
| 1   | A     | 515 | ARG  |
| 1   | A     | 524 | PHE  |
| 1   | A     | 527 | VAL  |
| 1   | A     | 530 | SER  |
| 1   | A     | 533 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 534 | ARG  |
| 1   | A     | 535 | VAL  |
| 1   | A     | 539 | LEU  |
| 1   | A     | 599 | ASP  |
| 1   | A     | 601 | GLU  |
| 1   | A     | 619 | LEU  |
| 1   | A     | 623 | ARG  |
| 1   | A     | 627 | VAL  |
| 1   | A     | 683 | ARG  |
| 1   | A     | 703 | GLU  |
| 1   | A     | 704 | VAL  |
| 1   | A     | 711 | ARG  |
| 1   | A     | 717 | VAL  |
| 1   | A     | 722 | SER  |
| 1   | A     | 723 | VAL  |
| 1   | A     | 731 | GLU  |
| 1   | A     | 732 | LEU  |
| 1   | A     | 735 | LEU  |
| 1   | A     | 736 | VAL  |
| 1   | A     | 745 | ARG  |
| 1   | A     | 748 | ARG  |
| 1   | A     | 759 | HIS  |
| 1   | A     | 762 | THR  |
| 1   | A     | 763 | ILE  |
| 1   | A     | 765 | ASP  |
| 1   | A     | 767 | LEU  |
| 1   | A     | 770 | GLU  |
| 1   | A     | 771 | LEU  |
| 1   | A     | 773 | GLU  |
| 1   | A     | 775 | PHE  |
| 1   | A     | 777 | PRO  |
| 1   | A     | 778 | LEU  |
| 1   | A     | 782 | VAL  |
| 1   | A     | 784 | PHE  |
| 1   | A     | 785 | PHE  |
| 1   | A     | 786 | SER  |
| 1   | A     | 797 | GLU  |
| 1   | A     | 799 | ASP  |
| 1   | A     | 826 | ARG  |
| 1   | A     | 841 | ILE  |
| 1   | A     | 853 | SER  |
| 1   | A     | 855 | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 859  | ARG  |
| 1   | A     | 867  | ASP  |
| 1   | A     | 870  | GLU  |
| 1   | A     | 911  | GLU  |
| 1   | A     | 913  | LYS  |
| 1   | A     | 918  | ARG  |
| 1   | A     | 948  | THR  |
| 1   | A     | 950  | LEU  |
| 1   | A     | 961  | THR  |
| 1   | A     | 977  | ARG  |
| 1   | A     | 978  | GLU  |
| 1   | A     | 980  | VAL  |
| 1   | A     | 981  | VAL  |
| 1   | A     | 982  | ASP  |
| 1   | A     | 1004 | LEU  |
| 1   | A     | 1007 | LEU  |
| 1   | A     | 1010 | ASP  |
| 1   | A     | 1015 | GLU  |
| 1   | A     | 1125 | TRP  |
| 1   | A     | 1144 | LEU  |
| 1   | A     | 1145 | VAL  |
| 1   | A     | 1168 | LEU  |
| 1   | A     | 1169 | LEU  |
| 1   | A     | 1171 | VAL  |
| 1   | A     | 1179 | ASP  |
| 1   | A     | 1184 | LEU  |
| 1   | A     | 1188 | LEU  |
| 1   | A     | 1194 | ARG  |
| 1   | A     | 1195 | THR  |
| 1   | A     | 1196 | THR  |
| 1   | A     | 1235 | THR  |
| 1   | A     | 1237 | ASP  |
| 1   | A     | 1238 | THR  |
| 1   | A     | 1244 | ILE  |
| 1   | A     | 1249 | ARG  |
| 1   | A     | 1251 | LYS  |
| 1   | A     | 1253 | LEU  |
| 1   | A     | 1263 | ARG  |
| 1   | A     | 1296 | ASP  |
| 1   | A     | 1300 | GLN  |
| 1   | A     | 1303 | ARG  |
| 1   | A     | 1307 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1327 | VAL  |
| 1   | A     | 1330 | ARG  |
| 1   | A     | 1333 | ARG  |
| 1   | A     | 1336 | VAL  |
| 1   | A     | 1339 | MET  |
| 1   | A     | 1342 | GLU  |
| 1   | A     | 1357 | VAL  |
| 1   | A     | 1360 | ILE  |
| 1   | A     | 1362 | ILE  |
| 1   | A     | 1363 | ASP  |
| 1   | A     | 1364 | VAL  |
| 1   | A     | 1367 | ASP  |
| 1   | A     | 1371 | LEU  |
| 1   | A     | 1376 | GLN  |
| 1   | A     | 1377 | ARG  |
| 1   | A     | 1379 | THR  |
| 1   | A     | 1380 | ARG  |
| 1   | A     | 1385 | ILE  |
| 2   | C     | 4    | VAL  |
| 2   | C     | 5    | GLN  |
| 2   | C     | 18   | ARG  |
| 2   | C     | 30   | THR  |
| 2   | C     | 36   | MET  |
| 2   | C     | 37   | SER  |
| 2   | C     | 45   | LYS  |
| 2   | C     | 56   | LYS  |
| 2   | C     | 61   | THR  |
| 2   | C     | 67   | SER  |
| 2   | C     | 69   | LYS  |
| 2   | C     | 78   | ASP  |
| 2   | C     | 80   | LYS  |
| 2   | C     | 84   | TYR  |
| 2   | C     | 86   | GLN  |
| 2   | C     | 87   | MET  |
| 2   | C     | 91   | LYS  |
| 2   | C     | 92   | THR  |
| 2   | C     | 93   | GLU  |
| 2   | C     | 101  | THR  |
| 2   | C     | 106  | LEU  |
| 2   | C     | 108  | ASP  |
| 2   | C     | 112  | GLN  |
| 2   | C     | 114  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | C     | 124 | LYS  |
| 2   | C     | 150 | LYS  |
| 2   | C     | 158 | THR  |
| 2   | C     | 168 | SER  |
| 2   | C     | 171 | HIS  |
| 2   | C     | 172 | THR  |
| 2   | C     | 178 | GLN  |
| 2   | C     | 182 | LEU  |
| 2   | C     | 202 | ILE  |
| 2   | C     | 204 | ASN  |
| 2   | C     | 206 | ASN  |
| 2   | C     | 216 | LYS  |
| 2   | C     | 219 | GLU  |
| 3   | D     | 18  | VAL  |
| 3   | D     | 20  | MET  |
| 3   | D     | 26  | SER  |
| 3   | D     | 33  | GLU  |
| 3   | D     | 36  | SER  |
| 3   | D     | 48  | SER  |
| 3   | D     | 49  | ASN  |
| 3   | D     | 60  | LYS  |
| 3   | D     | 77  | SER  |
| 3   | D     | 81  | ASP  |
| 3   | D     | 84  | SER  |
| 3   | D     | 93  | THR  |
| 3   | D     | 95  | LYS  |
| 3   | D     | 96  | ILE  |
| 3   | D     | 100 | GLU  |
| 3   | D     | 114 | GLN  |
| 3   | D     | 117 | ARG  |
| 3   | D     | 118 | LEU  |
| 3   | D     | 119 | THR  |
| 3   | D     | 132 | VAL  |
| 3   | D     | 137 | VAL  |
| 3   | D     | 139 | ILE  |
| 3   | D     | 144 | ASP  |
| 3   | D     | 145 | GLU  |
| 3   | D     | 153 | SER  |
| 3   | D     | 157 | LEU  |
| 3   | D     | 178 | SER  |
| 3   | D     | 181 | SER  |
| 3   | D     | 185 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 186 | THR  |
| 3   | D     | 187 | GLU  |
| 3   | D     | 197 | LEU  |
| 3   | D     | 200 | THR  |
| 3   | D     | 202 | THR  |
| 3   | D     | 205 | LYS  |
| 3   | D     | 217 | GLU  |
| 3   | D     | 219 | THR  |
| 3   | D     | 221 | GLN  |
| 3   | D     | 224 | SER  |
| 2   | E     | 14  | VAL  |
| 2   | E     | 15  | GLN  |
| 2   | E     | 30  | THR  |
| 2   | E     | 33  | ASP  |
| 2   | E     | 36  | MET  |
| 2   | E     | 45  | LYS  |
| 2   | E     | 55  | SER  |
| 2   | E     | 56  | LYS  |
| 2   | E     | 61  | THR  |
| 2   | E     | 67  | SER  |
| 2   | E     | 69  | LYS  |
| 2   | E     | 78  | ASP  |
| 2   | E     | 80  | LYS  |
| 2   | E     | 84  | TYR  |
| 2   | E     | 91  | LYS  |
| 2   | E     | 92  | THR  |
| 2   | E     | 93  | GLU  |
| 2   | E     | 97  | VAL  |
| 2   | E     | 102 | ARG  |
| 2   | E     | 105 | THR  |
| 2   | E     | 108 | ASP  |
| 2   | E     | 112 | GLN  |
| 2   | E     | 124 | LYS  |
| 2   | E     | 131 | LEU  |
| 2   | E     | 150 | LYS  |
| 2   | E     | 158 | THR  |
| 2   | E     | 160 | SER  |
| 2   | E     | 168 | SER  |
| 2   | E     | 172 | THR  |
| 2   | E     | 177 | LEU  |
| 2   | E     | 178 | GLN  |
| 2   | E     | 182 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 208 | LYS  |
| 2   | E     | 216 | LYS  |
| 2   | E     | 219 | GLU  |
| 3   | F     | 18  | VAL  |
| 3   | F     | 20  | MET  |
| 3   | F     | 26  | SER  |
| 3   | F     | 33  | GLU  |
| 3   | F     | 36  | SER  |
| 3   | F     | 48  | SER  |
| 3   | F     | 49  | ASN  |
| 3   | F     | 77  | SER  |
| 3   | F     | 81  | ASP  |
| 3   | F     | 84  | SER  |
| 3   | F     | 86  | SER  |
| 3   | F     | 90  | THR  |
| 3   | F     | 92  | PHE  |
| 3   | F     | 93  | THR  |
| 3   | F     | 94  | LEU  |
| 3   | F     | 100 | GLU  |
| 3   | F     | 102 | GLU  |
| 3   | F     | 117 | ARG  |
| 3   | F     | 118 | LEU  |
| 3   | F     | 119 | THR  |
| 3   | F     | 139 | ILE  |
| 3   | F     | 144 | ASP  |
| 3   | F     | 145 | GLU  |
| 3   | F     | 148 | LYS  |
| 3   | F     | 153 | SER  |
| 3   | F     | 158 | LEU  |
| 3   | F     | 167 | LYS  |
| 3   | F     | 178 | SER  |
| 3   | F     | 181 | SER  |
| 3   | F     | 185 | VAL  |
| 3   | F     | 186 | THR  |
| 3   | F     | 187 | GLU  |
| 3   | F     | 205 | LYS  |
| 3   | F     | 217 | GLU  |
| 3   | F     | 219 | THR  |
| 3   | F     | 221 | GLN  |
| 3   | F     | 224 | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 213  | HIS  |
| 1   | B     | 217  | GLN  |
| 1   | B     | 449  | ASN  |
| 1   | B     | 556  | GLN  |
| 1   | B     | 615  | GLN  |
| 1   | B     | 657  | GLN  |
| 1   | B     | 806  | ASN  |
| 1   | B     | 904  | GLN  |
| 1   | A     | 81   | HIS  |
| 1   | A     | 158  | GLN  |
| 1   | A     | 217  | GLN  |
| 1   | A     | 312  | ASN  |
| 1   | A     | 340  | HIS  |
| 1   | A     | 378  | HIS  |
| 1   | A     | 597  | HIS  |
| 1   | A     | 776  | HIS  |
| 1   | A     | 1112 | GLN  |
| 1   | A     | 1226 | HIS  |
| 1   | A     | 1334 | HIS  |
| 1   | A     | 1349 | GLN  |
| 2   | C     | 8    | GLN  |
| 2   | C     | 41   | GLN  |
| 2   | C     | 86   | GLN  |
| 2   | C     | 112  | GLN  |
| 2   | C     | 171  | HIS  |
| 2   | C     | 178  | GLN  |
| 2   | C     | 204  | ASN  |
| 2   | C     | 206  | ASN  |
| 3   | D     | 52   | ASN  |
| 3   | D     | 111  | GLN  |
| 3   | D     | 159  | ASN  |
| 3   | D     | 180  | ASN  |
| 3   | D     | 188  | GLN  |
| 2   | E     | 178  | GLN  |
| 2   | E     | 207  | HIS  |
| 3   | F     | 52   | ASN  |
| 3   | F     | 66   | GLN  |
| 3   | F     | 111  | GLN  |
| 3   | F     | 169  | GLN  |
| 3   | F     | 188  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | PN7  | B     | 1801 | 1    | 14,20,21     | 2.13 | 4 (28%)     | 18,26,29    | 1.42 | 5 (27%)     |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings |
|-----|------|-------|------|------|---------|-------------|-------|
| 4   | PN7  | B     | 1801 | 1    | -       | 12/24/26/27 | -     |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4   | B     | 1801 | PN7  | C8-N9 | 4.99  | 1.45        | 1.33     |
| 4   | B     | 1801 | PN7  | C4-N5 | 4.97  | 1.45        | 1.33     |
| 4   | B     | 1801 | PN7  | O4-C4 | -2.36 | 1.18        | 1.23     |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 4   | B     | 1801 | PN7  | O8-C8 | -2.15 | 1.19        | 1.23     |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 4   | B     | 1801 | PN7  | C6-C7-C8   | 2.43  | 116.44      | 112.39   |
| 4   | B     | 1801 | PN7  | C6-N5-C4   | -2.25 | 118.50      | 122.55   |
| 4   | B     | 1801 | PN7  | CE2-C2-C3  | 2.20  | 112.52      | 108.77   |
| 4   | B     | 1801 | PN7  | C11-C10-N9 | -2.04 | 107.68      | 112.31   |
| 4   | B     | 1801 | PN7  | C3-C4-N5   | 2.03  | 120.34      | 116.48   |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 4   | B     | 1801 | PN7  | C1-C2-C3-O3    |
| 4   | B     | 1801 | PN7  | C1-C2-C3-C4    |
| 4   | B     | 1801 | PN7  | CE1-C2-C3-O3   |
| 4   | B     | 1801 | PN7  | CE1-C2-C3-C4   |
| 4   | B     | 1801 | PN7  | CE2-C2-C3-O3   |
| 4   | B     | 1801 | PN7  | CE2-C2-C3-C4   |
| 4   | B     | 1801 | PN7  | N9-C10-C11-S12 |
| 4   | B     | 1801 | PN7  | N5-C6-C7-C8    |
| 4   | B     | 1801 | PN7  | O3P-C1-C2-CE1  |
| 4   | B     | 1801 | PN7  | O3P-C1-C2-CE2  |
| 4   | B     | 1801 | PN7  | O3-C3-C4-N5    |
| 4   | B     | 1801 | PN7  | O3P-C1-C2-C3   |

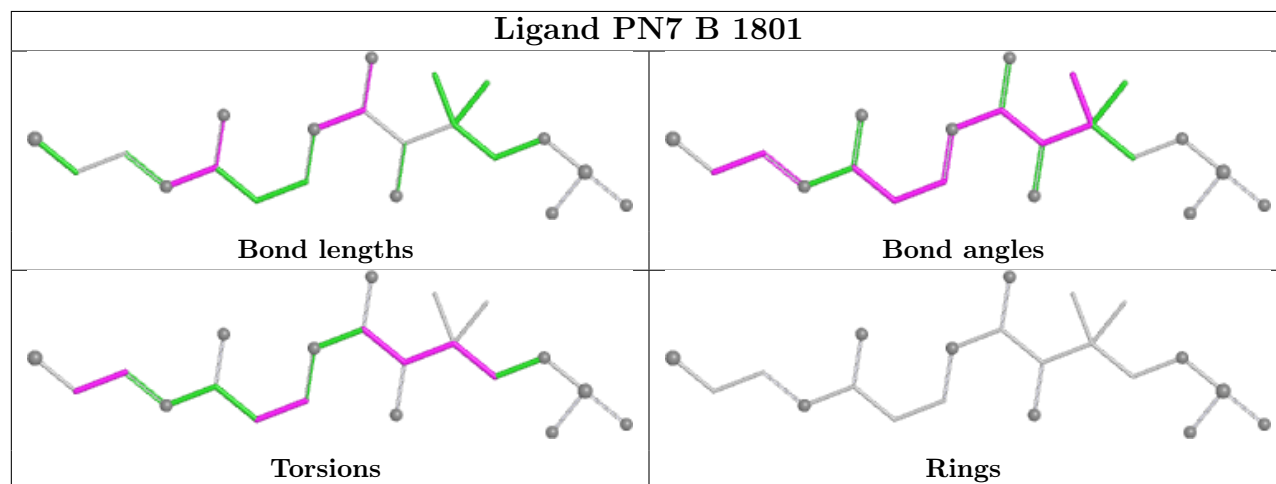
There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | B     | 1801 | PN7  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

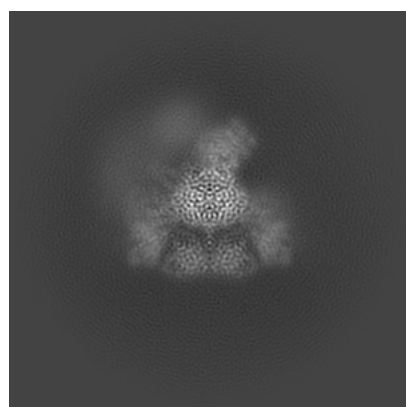
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23711. These allow visual inspection of the internal detail of the map and identification of artifacts.

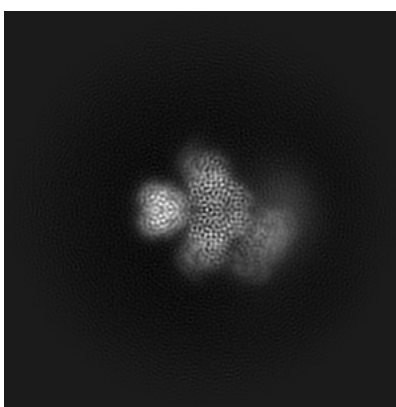
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

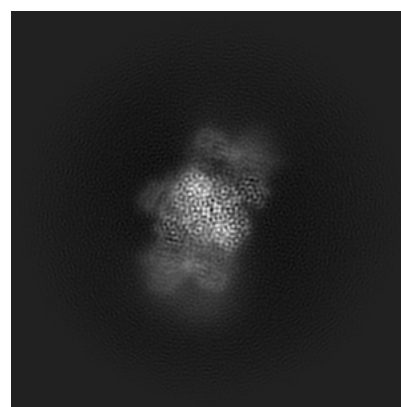
#### 6.1.1 Primary map



X



Y

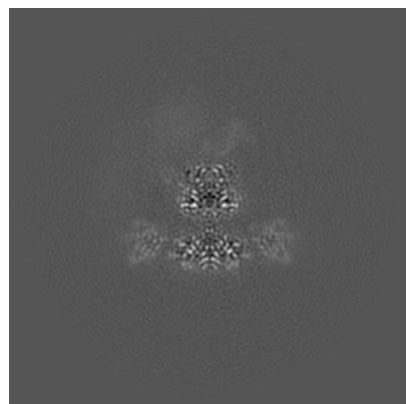


Z

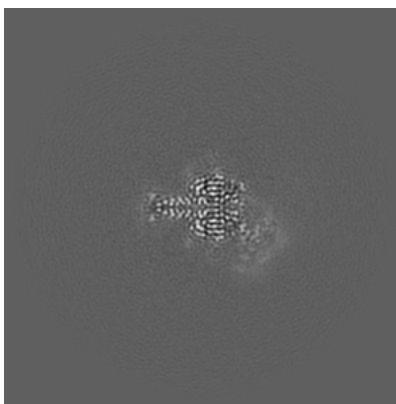
The images above show the map projected in three orthogonal directions.

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

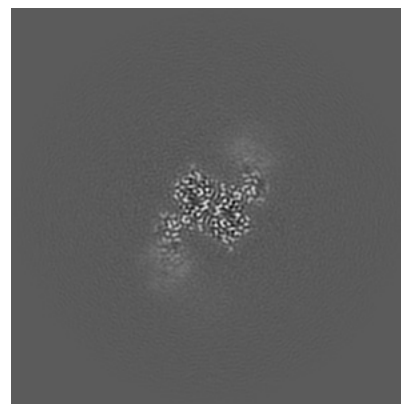
#### 6.2.1 Primary map



X Index: 168



Y Index: 168

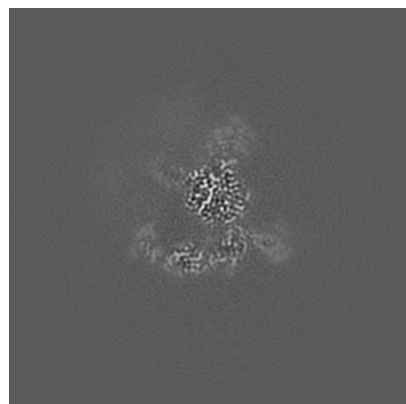


Z Index: 168

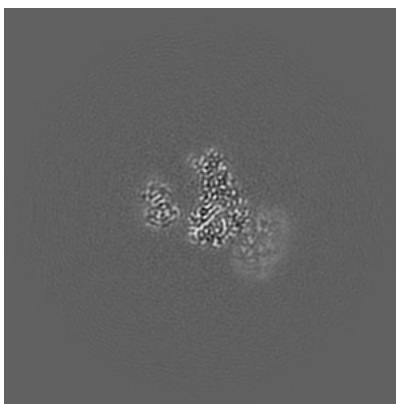
The images above show central slices of the map in three orthogonal directions.

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

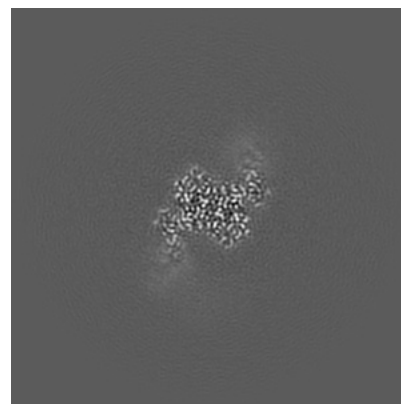
### 6.3.1 Primary map



X Index: 157



Y Index: 181

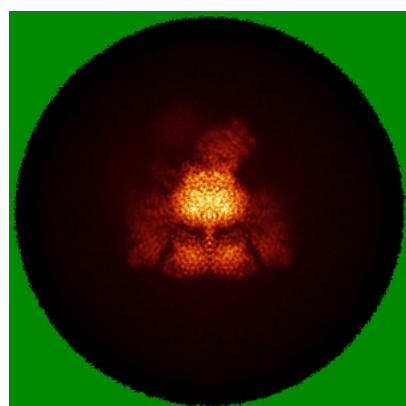


Z Index: 173

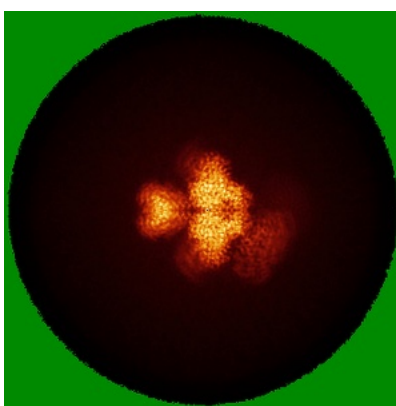
The images above show the largest variance slices of the map in three orthogonal directions.

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

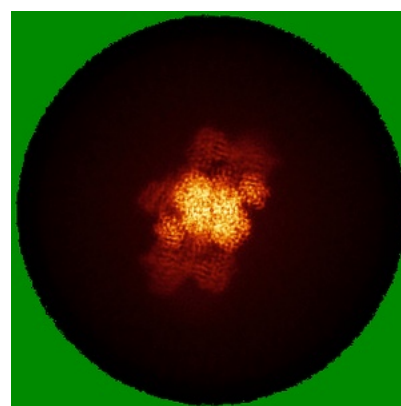
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.53. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

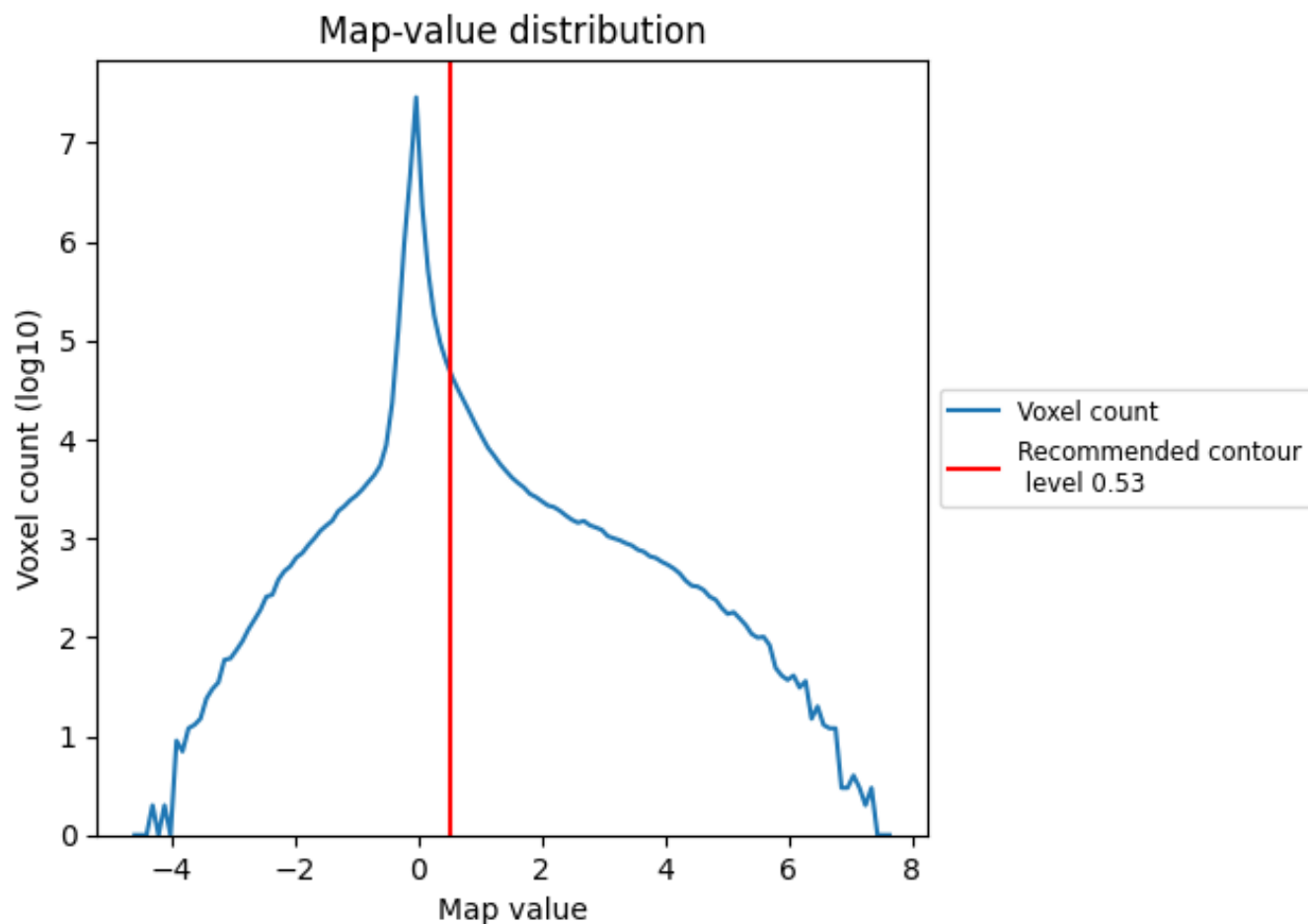
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

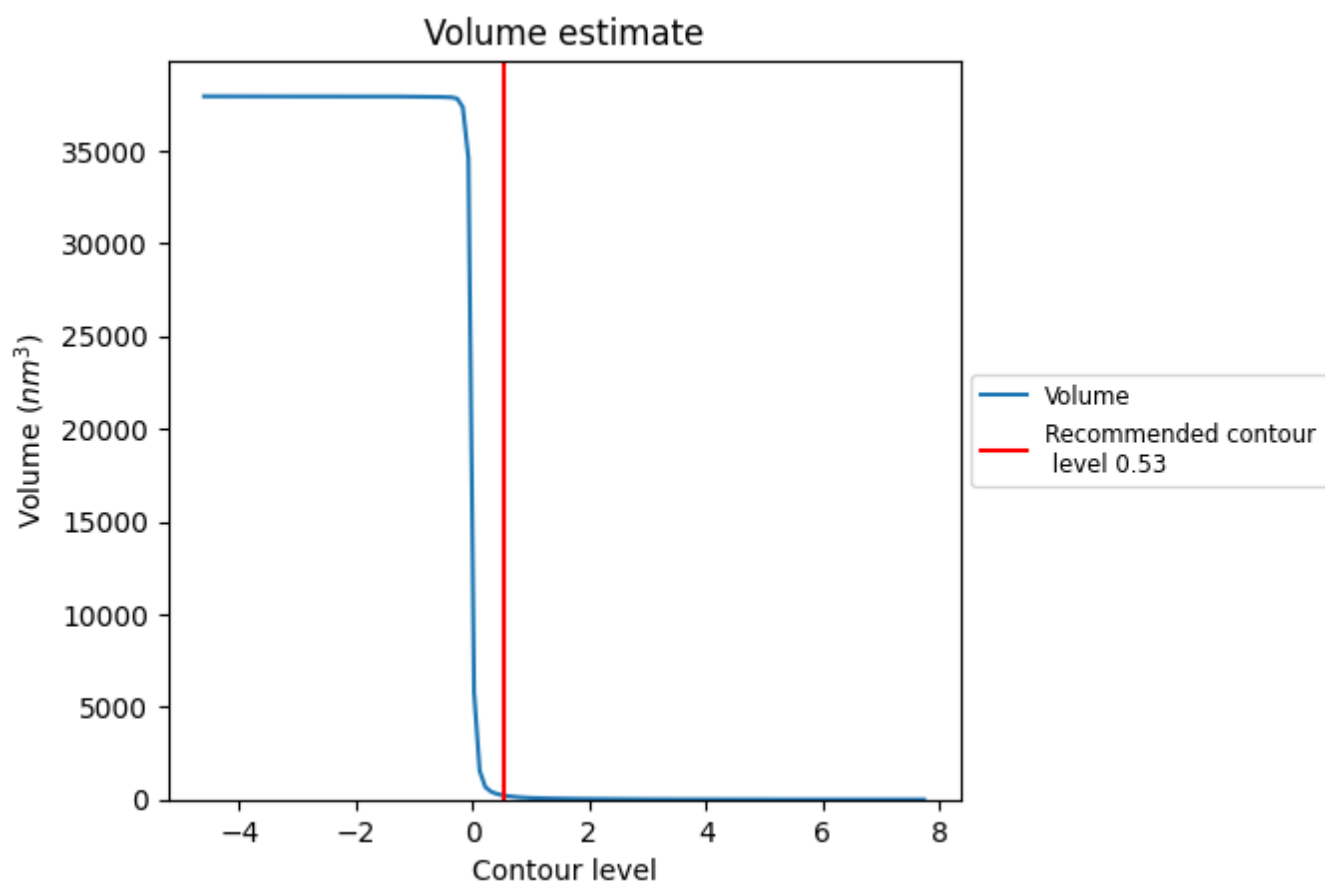
This section contains the results of statistical analysis of the map.

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



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

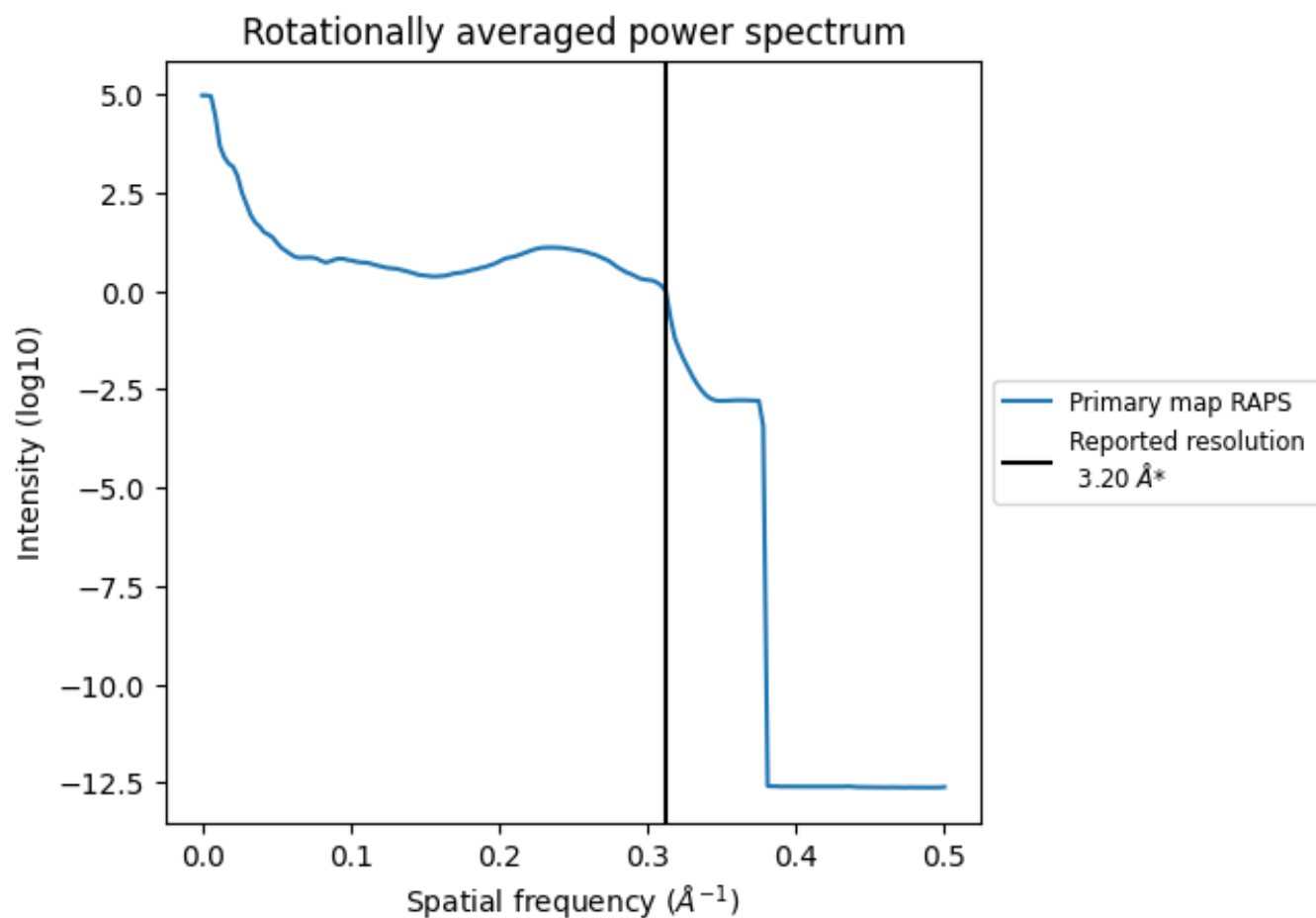
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 226 nm<sup>3</sup>; this corresponds to an approximate mass of 204 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

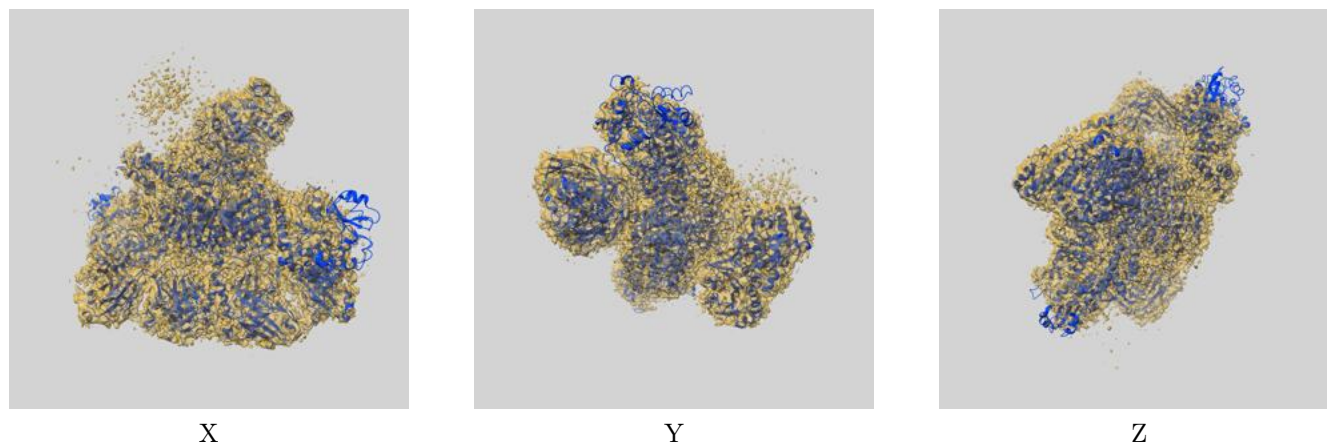
## 8 Fourier-Shell correlation ⓘ

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

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

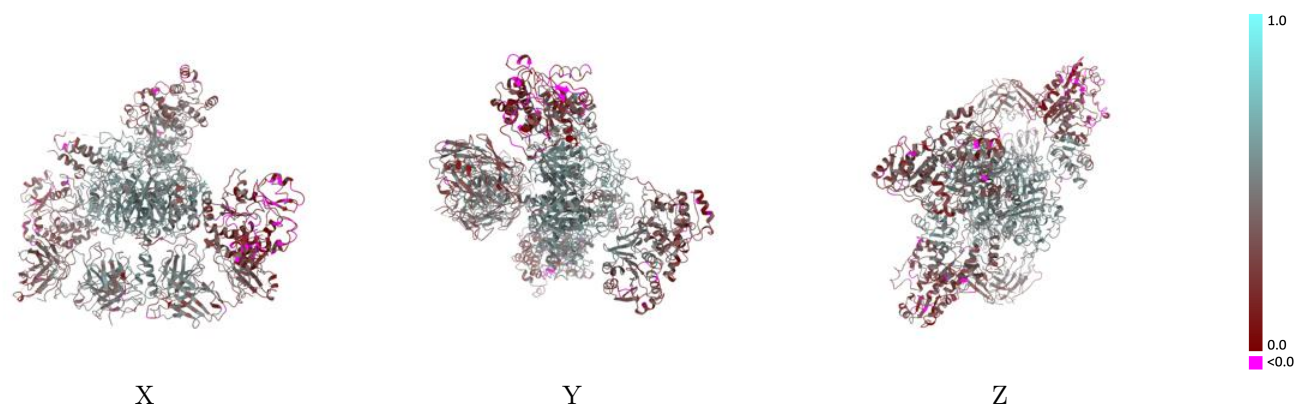
This section contains information regarding the fit between EMDB map EMD-23711 and PDB model 7M7F. Per-residue inclusion information can be found in section 3 on page 8.

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



The images above show the 3D surface view of the map at the recommended contour level 0.53 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

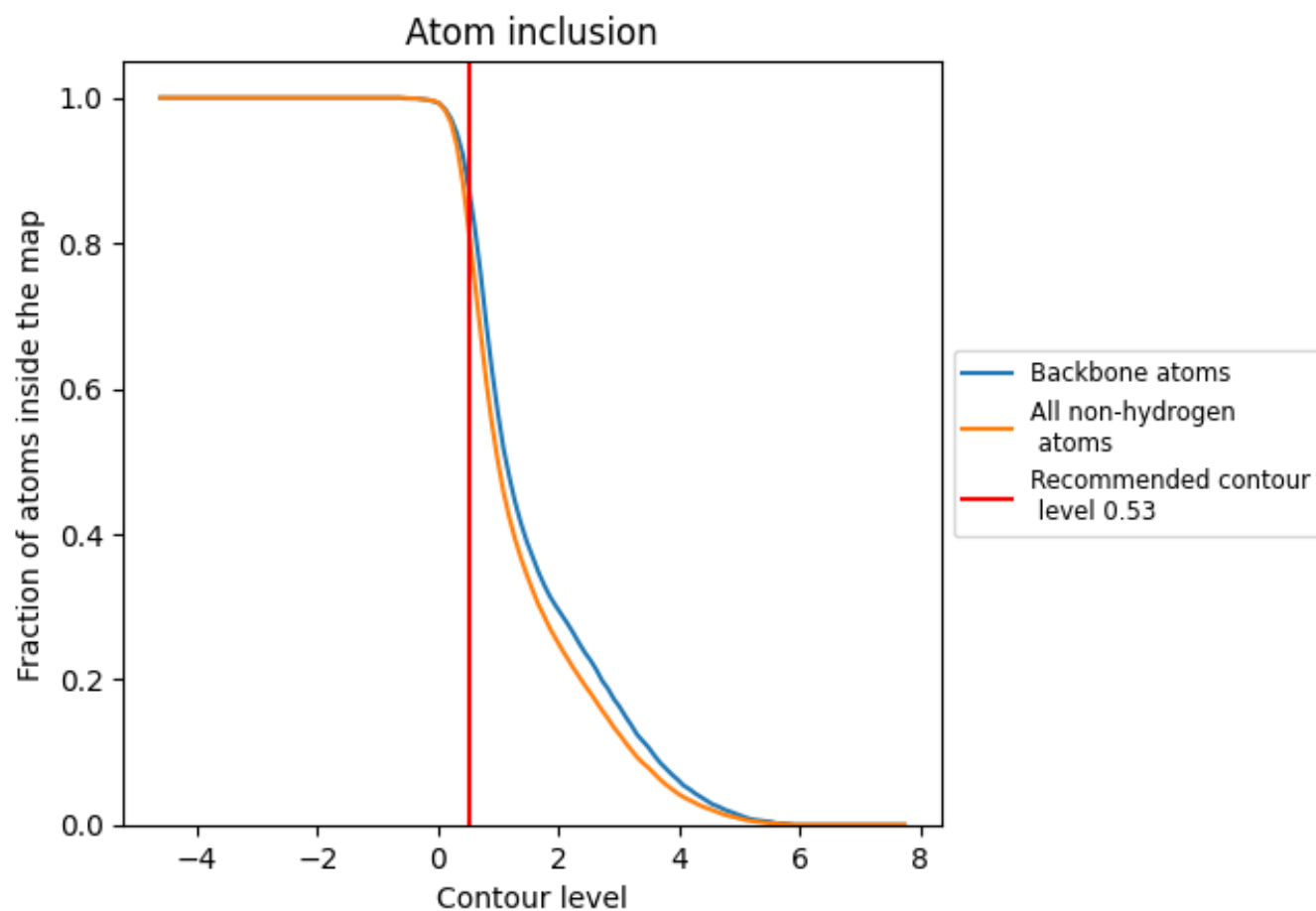


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.53) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.8030 | <div><div></div></div> 0.4030 |
| A     | <div><div></div></div> 0.7710 | <div><div></div></div> 0.3800 |
| B     | <div><div></div></div> 0.8070 | <div><div></div></div> 0.4320 |
| C     | <div><div></div></div> 0.8310 | <div><div></div></div> 0.3850 |
| D     | <div><div></div></div> 0.8630 | <div><div></div></div> 0.4110 |
| E     | <div><div></div></div> 0.8640 | <div><div></div></div> 0.4200 |
| F     | <div><div></div></div> 0.8520 | <div><div></div></div> 0.4070 |

1.0

0.0

<0.0