



## Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 11:00 PM UTC

PDB ID : 6WOV / pdb\_00006wov  
EMDB ID : EMD-21862  
Title : Cryo-EM structure of recombinant mouse Ryanodine Receptor type 2 wild type in complex with FKBP12.6  
Authors : Iyer, K.A.; Hu, Y.; Nayak, A.R.; Kurebayashi, N.; Murayama, T.; Samso, M.  
Deposited on : 2020-04-25  
Resolution : 5.10 Å(reported)  
Based on initial model : 5L1D

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  
MolProbity : 4-5-2 with Phenix2.0  
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

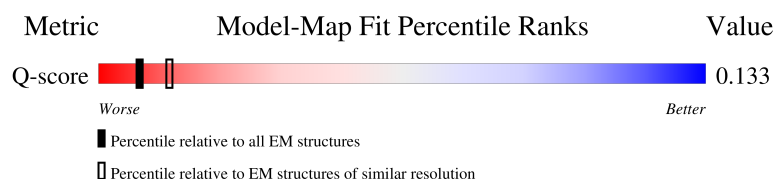
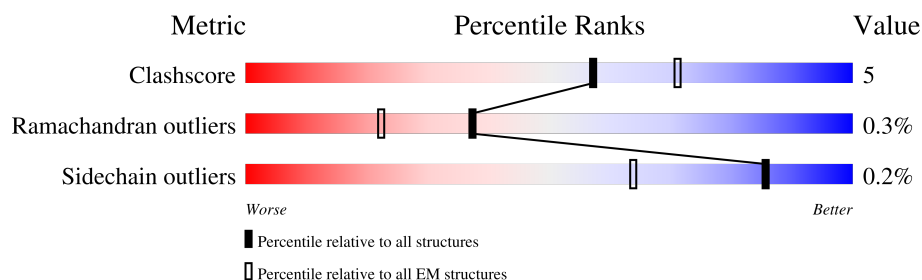
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.10 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                       | 844 ( 4.60 - 5.60 )                                      |

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     | 4966   | <br>13% 69% 10% 21% |
| 1   | B     | 4966   | <br>13% 69% 10% 21% |
| 1   | C     | 4966   | <br>13% 69% 10% 21% |
| 1   | D     | 4966   | <br>13% 69% 10% 21% |

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| Mol | Chain | Length | Quality of chain                             |     |         |
|-----|-------|--------|----------------------------------------------|-----|---------|
| 2   | E     | 107    | <div><div></div><div></div><div></div></div> | 18% | 79% 21% |
| 2   | F     | 107    | <div><div></div><div></div><div></div></div> | 16% | 79% 21% |
| 2   | G     | 107    | <div><div></div><div></div><div></div></div> | 18% | 81% 19% |
| 2   | H     | 107    | <div><div></div><div></div><div></div></div> | 17% | 79% 21% |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 245656 atoms, of which 120412 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 Ryanodine receptor 2.

| Mol | Chain | Residues | Atoms |       |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|------|------|-----|---------|-------|
| 1   | A     | 3921     | Total | C     | H     | N    | O    | S   | 0       | 0     |
|     |       |          | 59769 | 19350 | 29277 | 5253 | 5698 | 191 |         |       |
| 1   | B     | 3921     | Total | C     | H     | N    | O    | S   | 0       | 0     |
|     |       |          | 59772 | 19350 | 29280 | 5253 | 5698 | 191 |         |       |
| 1   | C     | 3921     | Total | C     | H     | N    | O    | S   | 0       | 0     |
|     |       |          | 59773 | 19350 | 29281 | 5253 | 5698 | 191 |         |       |
| 1   | D     | 3921     | Total | C     | H     | N    | O    | S   | 0       | 0     |
|     |       |          | 59770 | 19350 | 29278 | 5253 | 5698 | 191 |         |       |

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 2   | E     | 107      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 516 | 824 | 144 | 154 | 4 |         |       |
| 2   | F     | 107      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 516 | 824 | 144 | 154 | 4 |         |       |
| 2   | G     | 107      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 516 | 824 | 144 | 154 | 4 |         |       |
| 2   | H     | 107      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1642  | 516 | 824 | 144 | 154 | 4 |         |       |

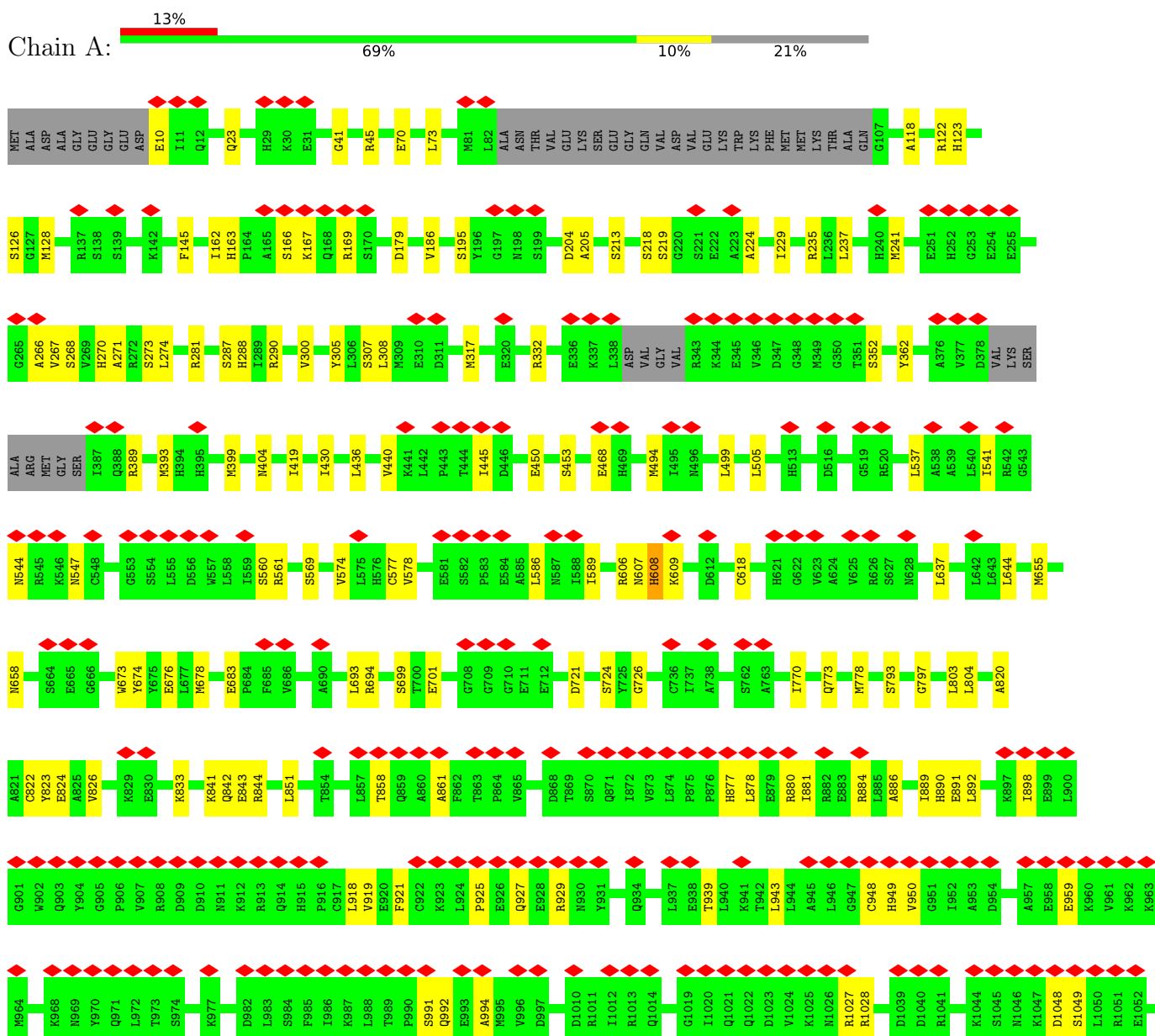
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 3   | A     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | C     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | D     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

### 3 Residue-property plots

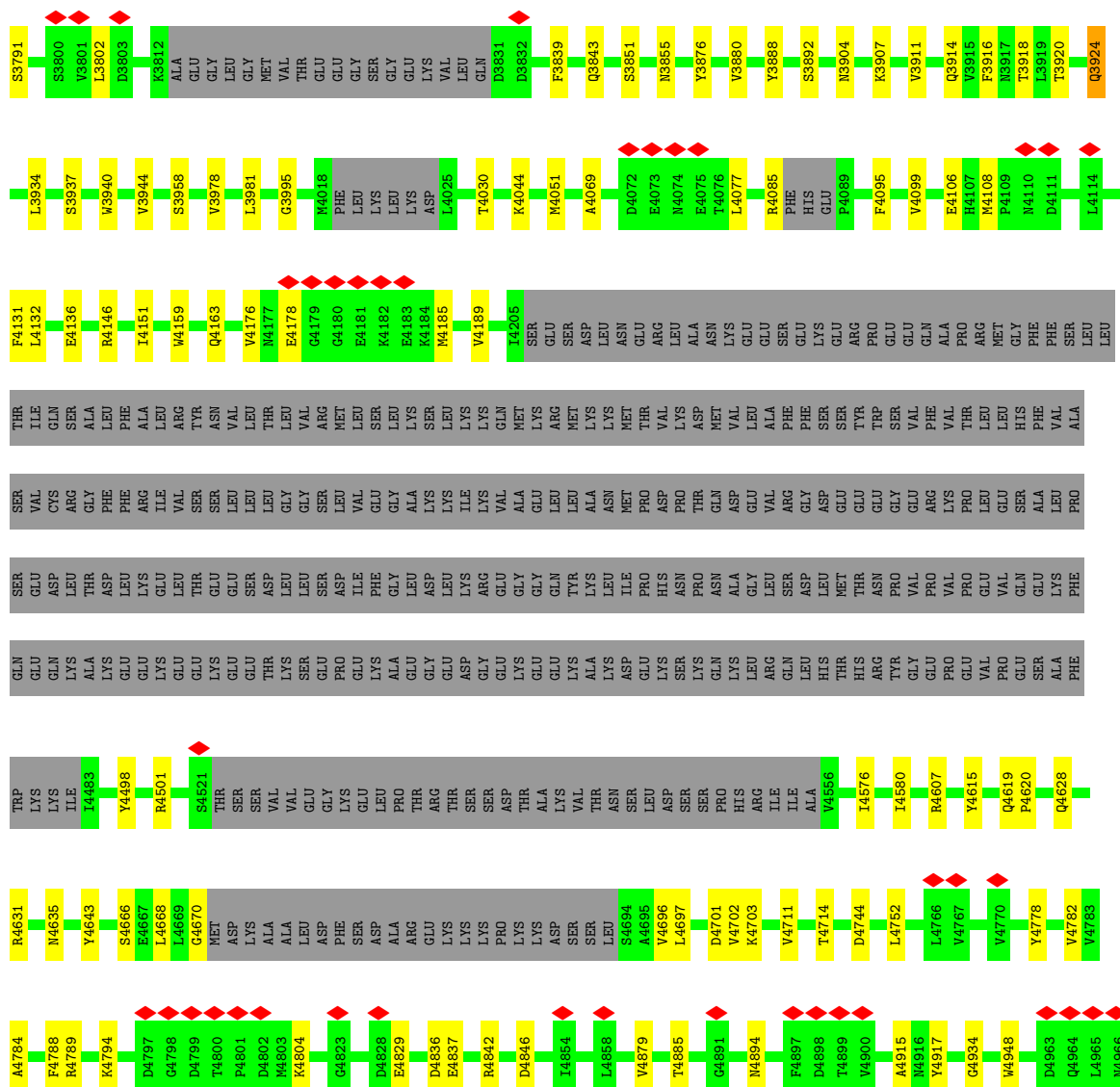
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Ryanodine receptor 2

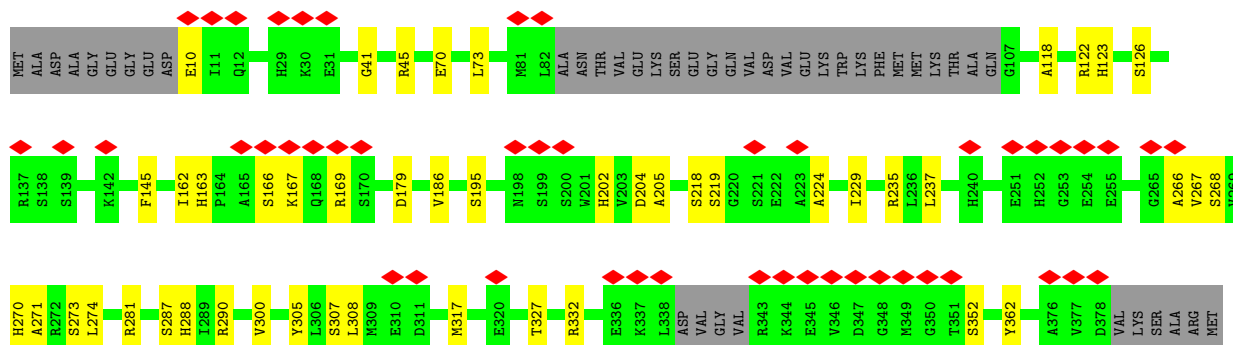








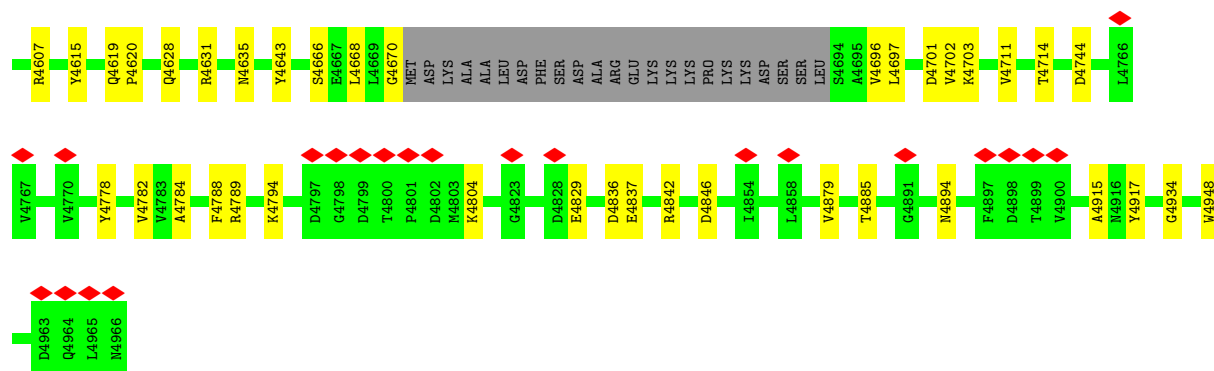
• Molecule 1: Ryanodine receptor 2



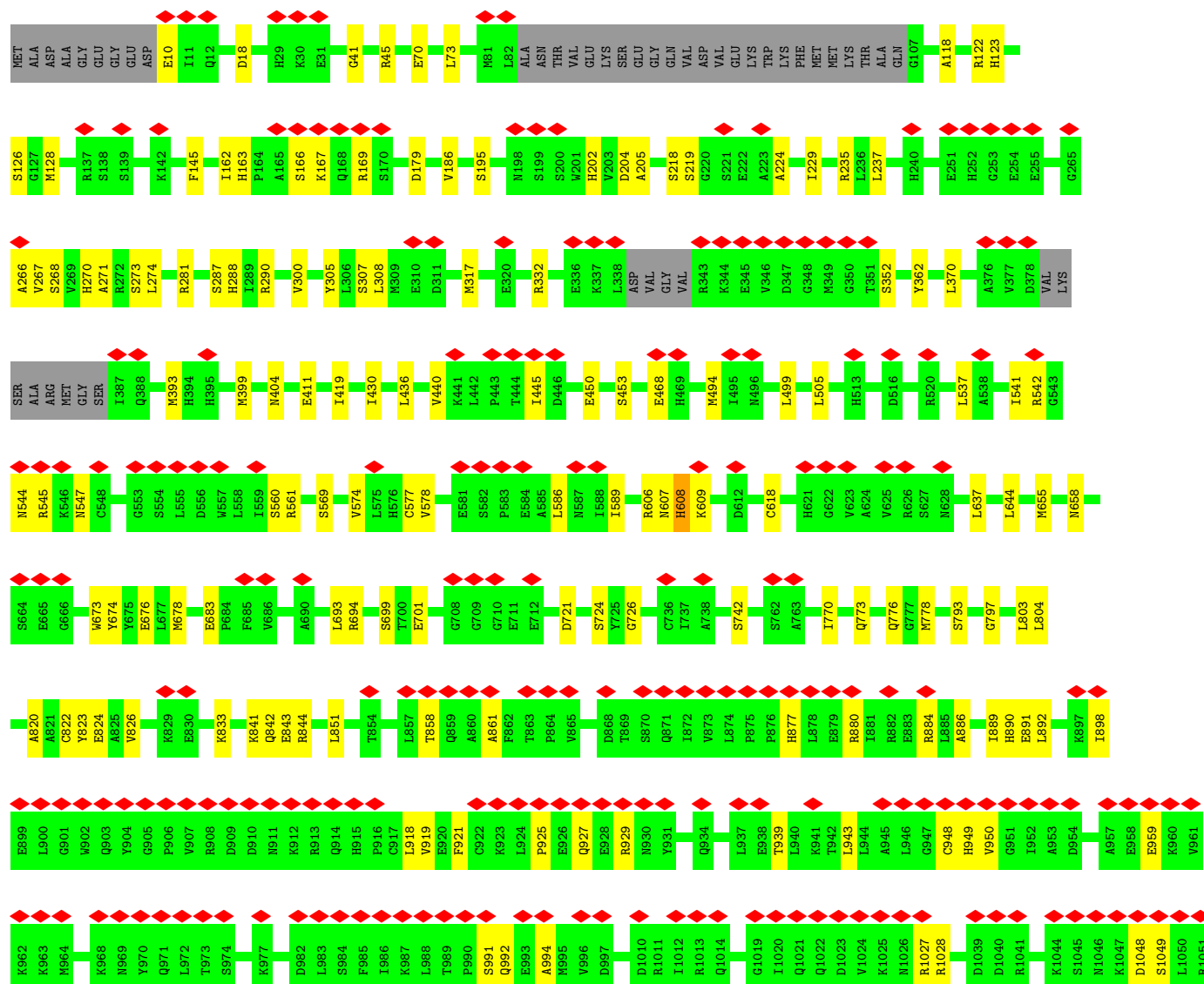






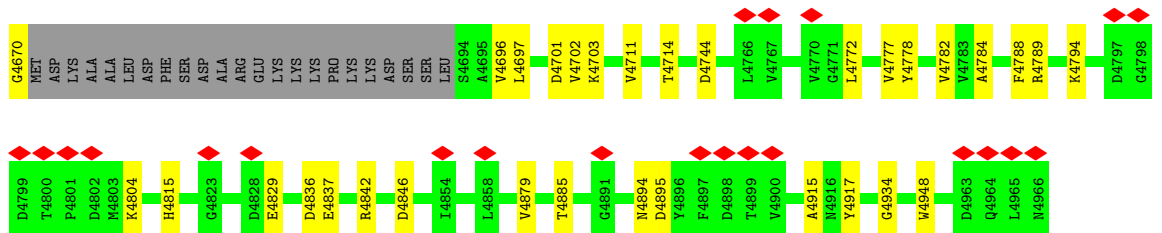


• Molecule 1: Ryanodine receptor 2

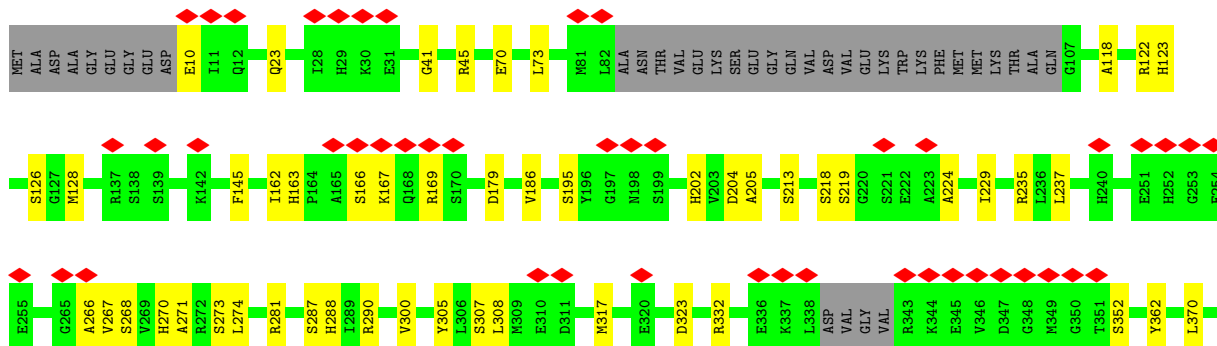


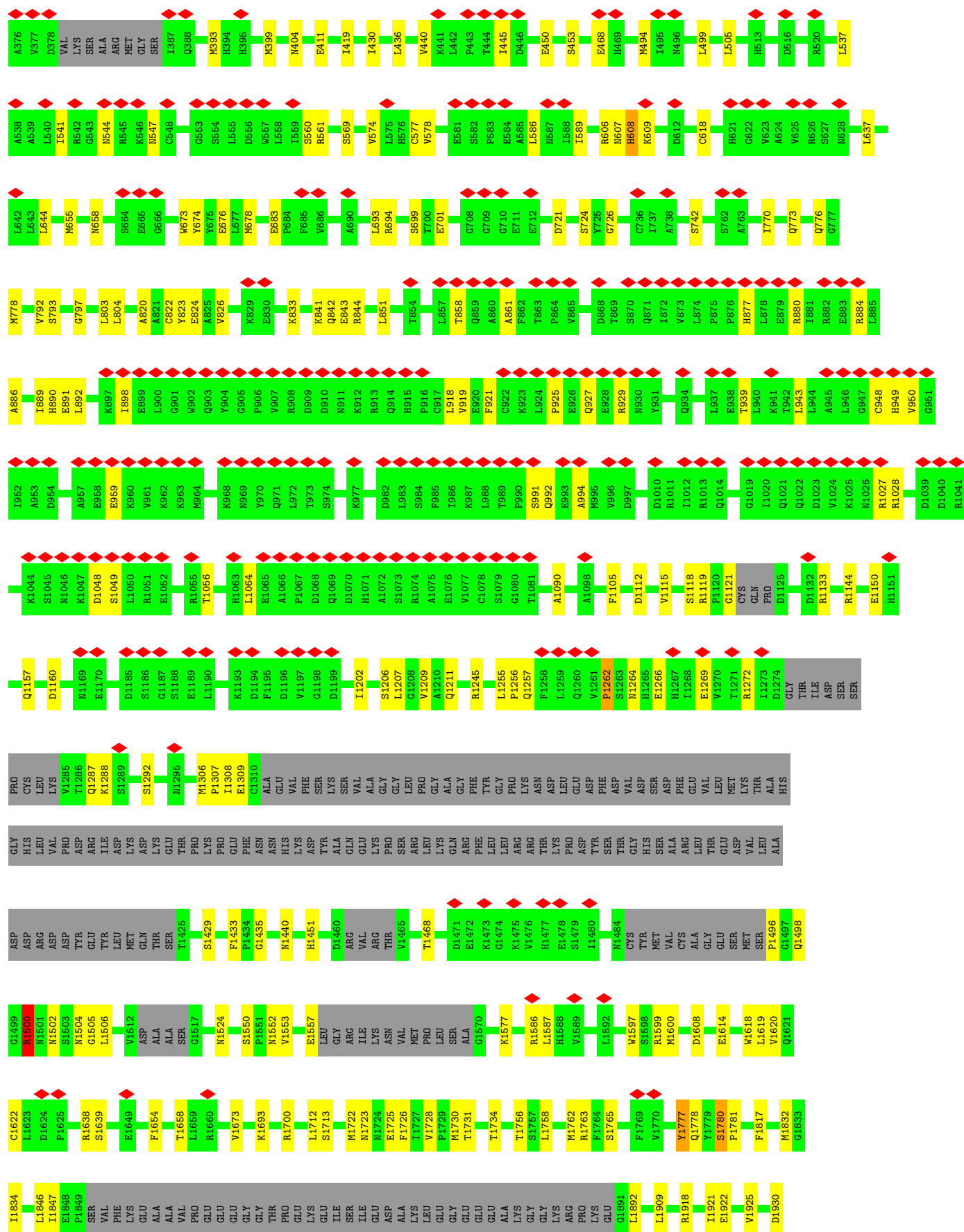






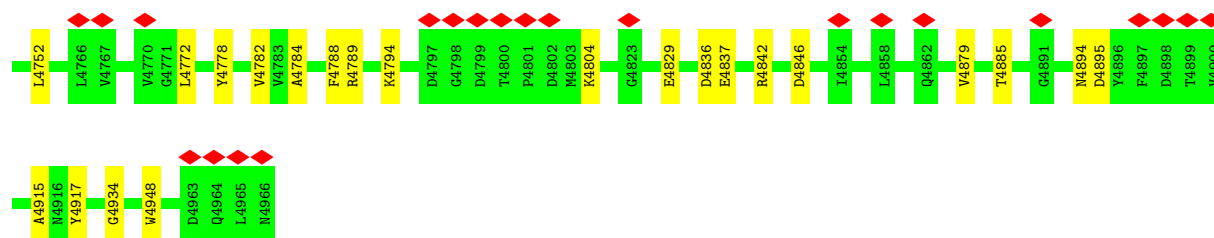
Chain D: 



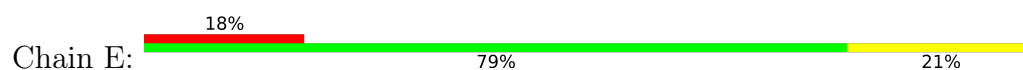




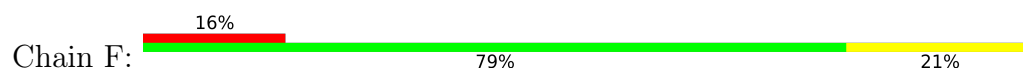




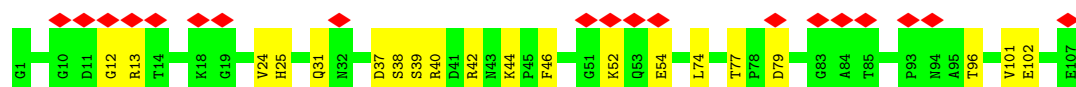
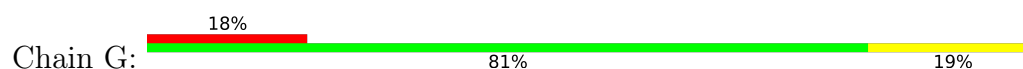
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



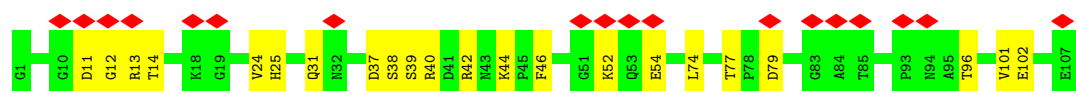
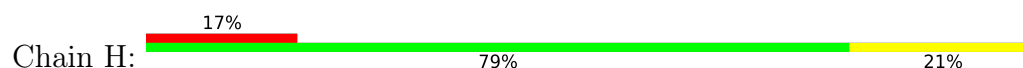
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, C4                       | Depositor |
| Number of particles used             | 103845                          | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                              | Depositor |
| Minimum defocus (nm)                 | 2000                            | Depositor |
| Maximum defocus (nm)                 | 4500                            | Depositor |
| Magnification                        | 105000                          | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)       | Depositor |
| Maximum map value                    | 24.070                          | Depositor |
| Minimum map value                    | -7.125                          | Depositor |
| Average map value                    | -0.000                          | Depositor |
| Map value standard deviation         | 1.000                           | Depositor |
| Recommended contour level            | 3                               | Depositor |
| Map size ( $\text{\AA}$ )            | 484.70398, 484.70398, 484.70398 | wwPDB     |
| Map dimensions                       | 352, 352, 352                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.377, 1.377, 1.377             | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                  |
|-----|-------|--------------|-------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 0.29         | 0/31108     | 0.56        | 9/42056 (0.0%)   |
| 1   | B     | 0.29         | 0/31108     | 0.56        | 9/42056 (0.0%)   |
| 1   | C     | 0.29         | 0/31108     | 0.56        | 9/42056 (0.0%)   |
| 1   | D     | 0.29         | 0/31108     | 0.56        | 9/42056 (0.0%)   |
| 2   | E     | 0.26         | 0/834       | 0.51        | 0/1123           |
| 2   | F     | 0.26         | 0/834       | 0.51        | 0/1123           |
| 2   | G     | 0.26         | 0/834       | 0.51        | 0/1123           |
| 2   | H     | 0.26         | 0/834       | 0.51        | 0/1123           |
| All | All   | 0.29         | 0/127768    | 0.56        | 36/172716 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 15                  |
| 1   | B     | 0                   | 15                  |
| 1   | C     | 0                   | 15                  |
| 1   | D     | 0                   | 15                  |
| All | All   | 0                   | 60                  |

There are no bond length outliers.

All (36) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|------|-------------|----------|
| 1   | B     | 1500 | ARG  | N-CA-C | 9.55 | 131.14      | 110.80   |
| 1   | C     | 1500 | ARG  | N-CA-C | 9.55 | 131.14      | 110.80   |
| 1   | D     | 1500 | ARG  | N-CA-C | 9.54 | 131.12      | 110.80   |
| 1   | A     | 1500 | ARG  | N-CA-C | 9.54 | 131.12      | 110.80   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 1   | C     | 1496 | PRO  | N-CA-CB  | 6.87 | 110.55      | 103.00   |
| 1   | D     | 1496 | PRO  | N-CA-CB  | 6.85 | 110.54      | 103.00   |
| 1   | A     | 1496 | PRO  | N-CA-CB  | 6.83 | 110.51      | 103.00   |
| 1   | B     | 1496 | PRO  | N-CA-CB  | 6.83 | 110.51      | 103.00   |
| 1   | B     | 2657 | GLU  | N-CA-C   | 6.63 | 119.31      | 111.02   |
| 1   | A     | 2657 | GLU  | N-CA-C   | 6.62 | 119.29      | 111.02   |
| 1   | C     | 2657 | GLU  | N-CA-C   | 6.62 | 119.29      | 111.02   |
| 1   | D     | 2657 | GLU  | N-CA-C   | 6.60 | 119.27      | 111.02   |
| 1   | A     | 2133 | MET  | CA-C-N   | 5.84 | 132.86      | 121.41   |
| 1   | A     | 2133 | MET  | C-N-CA   | 5.84 | 132.86      | 121.41   |
| 1   | D     | 2133 | MET  | CA-C-N   | 5.84 | 132.86      | 121.41   |
| 1   | D     | 2133 | MET  | C-N-CA   | 5.84 | 132.86      | 121.41   |
| 1   | B     | 2133 | MET  | CA-C-N   | 5.83 | 132.84      | 121.41   |
| 1   | B     | 2133 | MET  | C-N-CA   | 5.83 | 132.84      | 121.41   |
| 1   | C     | 2133 | MET  | CA-C-N   | 5.83 | 132.83      | 121.41   |
| 1   | C     | 2133 | MET  | C-N-CA   | 5.83 | 132.83      | 121.41   |
| 1   | C     | 2660 | LEU  | CA-CB-CG | 5.81 | 136.63      | 116.30   |
| 1   | D     | 2660 | LEU  | CA-CB-CG | 5.81 | 136.63      | 116.30   |
| 1   | A     | 2660 | LEU  | CA-CB-CG | 5.80 | 136.62      | 116.30   |
| 1   | B     | 2660 | LEU  | CA-CB-CG | 5.79 | 136.57      | 116.30   |
| 1   | A     | 3653 | GLU  | CA-CB-CG | 5.21 | 124.53      | 114.10   |
| 1   | C     | 3653 | GLU  | CA-CB-CG | 5.21 | 124.53      | 114.10   |
| 1   | B     | 3653 | GLU  | CA-CB-CG | 5.20 | 124.51      | 114.10   |
| 1   | D     | 3653 | GLU  | CA-CB-CG | 5.20 | 124.50      | 114.10   |
| 1   | D     | 1504 | ASN  | CA-C-N   | 5.14 | 131.48      | 121.41   |
| 1   | D     | 1504 | ASN  | C-N-CA   | 5.14 | 131.48      | 121.41   |
| 1   | B     | 1504 | ASN  | CA-C-N   | 5.14 | 131.48      | 121.41   |
| 1   | B     | 1504 | ASN  | C-N-CA   | 5.14 | 131.48      | 121.41   |
| 1   | A     | 1504 | ASN  | CA-C-N   | 5.12 | 131.45      | 121.41   |
| 1   | A     | 1504 | ASN  | C-N-CA   | 5.12 | 131.45      | 121.41   |
| 1   | C     | 1504 | ASN  | CA-C-N   | 5.12 | 131.44      | 121.41   |
| 1   | C     | 1504 | ASN  | C-N-CA   | 5.12 | 131.44      | 121.41   |

There are no chirality outliers.

All (60) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1266 | GLU  | Peptide |
| 1   | A     | 1500 | ARG  | Peptide |
| 1   | A     | 1502 | ASN  | Peptide |
| 1   | A     | 1552 | ASN  | Peptide |
| 1   | A     | 1777 | TYR  | Peptide |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | A     | 1780 | SER  | Peptide |
| 1   | A     | 1947 | MET  | Peptide |
| 1   | A     | 2132 | ARG  | Peptide |
| 1   | A     | 2134 | GLY  | Peptide |
| 1   | A     | 2234 | ARG  | Peptide |
| 1   | A     | 2385 | ASN  | Peptide |
| 1   | A     | 3924 | GLN  | Peptide |
| 1   | A     | 544  | ASN  | Peptide |
| 1   | A     | 608  | HIS  | Peptide |
| 1   | A     | 618  | CYS  | Peptide |
| 1   | B     | 1266 | GLU  | Peptide |
| 1   | B     | 1500 | ARG  | Peptide |
| 1   | B     | 1502 | ASN  | Peptide |
| 1   | B     | 1552 | ASN  | Peptide |
| 1   | B     | 1777 | TYR  | Peptide |
| 1   | B     | 1780 | SER  | Peptide |
| 1   | B     | 1947 | MET  | Peptide |
| 1   | B     | 2132 | ARG  | Peptide |
| 1   | B     | 2134 | GLY  | Peptide |
| 1   | B     | 2234 | ARG  | Peptide |
| 1   | B     | 2385 | ASN  | Peptide |
| 1   | B     | 3924 | GLN  | Peptide |
| 1   | B     | 544  | ASN  | Peptide |
| 1   | B     | 608  | HIS  | Peptide |
| 1   | B     | 618  | CYS  | Peptide |
| 1   | C     | 1266 | GLU  | Peptide |
| 1   | C     | 1500 | ARG  | Peptide |
| 1   | C     | 1502 | ASN  | Peptide |
| 1   | C     | 1552 | ASN  | Peptide |
| 1   | C     | 1777 | TYR  | Peptide |
| 1   | C     | 1780 | SER  | Peptide |
| 1   | C     | 1947 | MET  | Peptide |
| 1   | C     | 2132 | ARG  | Peptide |
| 1   | C     | 2134 | GLY  | Peptide |
| 1   | C     | 2234 | ARG  | Peptide |
| 1   | C     | 2385 | ASN  | Peptide |
| 1   | C     | 3924 | GLN  | Peptide |
| 1   | C     | 544  | ASN  | Peptide |
| 1   | C     | 608  | HIS  | Peptide |
| 1   | C     | 618  | CYS  | Peptide |
| 1   | D     | 1266 | GLU  | Peptide |
| 1   | D     | 1500 | ARG  | Peptide |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 1   | D     | 1502 | ASN  | Peptide |
| 1   | D     | 1552 | ASN  | Peptide |
| 1   | D     | 1777 | TYR  | Peptide |
| 1   | D     | 1780 | SER  | Peptide |
| 1   | D     | 1947 | MET  | Peptide |
| 1   | D     | 2132 | ARG  | Peptide |
| 1   | D     | 2134 | GLY  | Peptide |
| 1   | D     | 2234 | ARG  | Peptide |
| 1   | D     | 2385 | ASN  | Peptide |
| 1   | D     | 3924 | GLN  | Peptide |
| 1   | D     | 544  | ASN  | Peptide |
| 1   | D     | 608  | HIS  | Peptide |
| 1   | D     | 618  | CYS  | 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     | 30492  | 29277    | 29270    | 281     | 0            |
| 1   | B     | 30492  | 29280    | 29270    | 287     | 0            |
| 1   | C     | 30492  | 29281    | 29270    | 284     | 0            |
| 1   | D     | 30492  | 29278    | 29270    | 286     | 0            |
| 2   | E     | 818    | 824      | 824      | 14      | 0            |
| 2   | F     | 818    | 824      | 824      | 14      | 0            |
| 2   | G     | 818    | 824      | 824      | 13      | 0            |
| 2   | H     | 818    | 824      | 824      | 14      | 0            |
| 3   | A     | 1      | 0        | 0        | 0       | 0            |
| 3   | B     | 1      | 0        | 0        | 0       | 0            |
| 3   | C     | 1      | 0        | 0        | 0       | 0            |
| 3   | D     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 125244 | 120412   | 120376   | 1187    | 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 5.

All (1187) 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:B:644:LEU:HD11 | 1:B:1658:THR:HG21 | 1.70                     | 0.74              |
| 1:C:644:LEU:HD11 | 1:C:1658:THR:HG21 | 1.69                     | 0.73              |
| 1:A:644:LEU:HD11 | 1:A:1658:THR:HG21 | 1.69                     | 0.73              |
| 1:C:2106:THR:OG1 | 1:C:3612:ARG:O    | 2.06                     | 0.73              |
| 1:B:288:HIS:O    | 1:B:290:ARG:NH1   | 2.22                     | 0.72              |
| 1:D:644:LEU:HD11 | 1:D:1658:THR:HG21 | 1.69                     | 0.72              |
| 1:D:288:HIS:O    | 1:D:290:ARG:NH1   | 2.22                     | 0.72              |
| 1:C:288:HIS:O    | 1:C:290:ARG:NH1   | 2.22                     | 0.72              |
| 1:A:288:HIS:O    | 1:A:290:ARG:NH1   | 2.22                     | 0.71              |
| 1:A:2106:THR:OG1 | 1:A:3612:ARG:O    | 2.06                     | 0.71              |
| 2:E:52:LYS:NZ    | 2:E:54:GLU:OE1    | 2.24                     | 0.71              |
| 1:D:2106:THR:OG1 | 1:D:3612:ARG:O    | 2.06                     | 0.71              |
| 1:A:778:MET:O    | 1:A:1468:THR:OG1  | 2.10                     | 0.70              |
| 1:D:1713:SER:HG  | 1:D:1777:TYR:HH   | 1.38                     | 0.70              |
| 2:F:52:LYS:NZ    | 2:F:54:GLU:OE1    | 2.24                     | 0.70              |
| 1:C:778:MET:O    | 1:C:1468:THR:OG1  | 2.10                     | 0.70              |
| 1:B:778:MET:O    | 1:B:1468:THR:OG1  | 2.10                     | 0.70              |
| 1:D:778:MET:O    | 1:D:1468:THR:OG1  | 2.10                     | 0.69              |
| 2:H:52:LYS:NZ    | 2:H:54:GLU:OE1    | 2.24                     | 0.69              |
| 1:A:2313:GLU:O   | 1:A:2317:ASN:ND2  | 2.26                     | 0.69              |
| 1:D:2313:GLU:O   | 1:D:2317:ASN:ND2  | 2.26                     | 0.69              |
| 1:B:1700:ARG:NH1 | 1:B:1817:PHE:O    | 2.26                     | 0.69              |
| 1:C:1700:ARG:NH1 | 1:C:1817:PHE:O    | 2.26                     | 0.69              |
| 1:B:890:HIS:NE2  | 1:B:919:VAL:O     | 2.26                     | 0.69              |
| 1:D:890:HIS:NE2  | 1:D:919:VAL:O     | 2.26                     | 0.69              |
| 2:G:52:LYS:NZ    | 2:G:54:GLU:OE1    | 2.24                     | 0.69              |
| 1:A:890:HIS:NE2  | 1:A:919:VAL:O     | 2.26                     | 0.68              |
| 1:B:2313:GLU:O   | 1:B:2317:ASN:ND2  | 2.26                     | 0.68              |
| 1:C:890:HIS:NE2  | 1:C:919:VAL:O     | 2.26                     | 0.68              |
| 1:D:4607:ARG:NE  | 1:D:4643:TYR:OH   | 2.27                     | 0.68              |
| 1:C:2313:GLU:O   | 1:C:2317:ASN:ND2  | 2.26                     | 0.68              |
| 1:D:1700:ARG:NH1 | 1:D:1817:PHE:O    | 2.26                     | 0.68              |
| 1:A:1700:ARG:NH1 | 1:A:1817:PHE:O    | 2.26                     | 0.68              |
| 1:A:721:ASP:O    | 1:A:724:SER:OG    | 2.12                     | 0.68              |
| 1:C:1112:ASP:OD2 | 1:C:1211:GLN:NE2  | 2.27                     | 0.68              |
| 1:B:858:THR:OG1  | 1:B:861:ALA:O     | 2.12                     | 0.68              |
| 1:B:1112:ASP:OD2 | 1:B:1211:GLN:NE2  | 2.27                     | 0.68              |
| 1:A:1112:ASP:OD2 | 1:A:1211:GLN:NE2  | 2.27                     | 0.67              |
| 1:A:4607:ARG:NE  | 1:A:4643:TYR:OH   | 2.27                     | 0.67              |
| 1:D:1756:THR:OG1 | 1:D:1922:GLU:OE2  | 2.12                     | 0.67              |
| 1:D:1112:ASP:OD2 | 1:D:1211:GLN:NE2  | 2.27                     | 0.67              |
| 1:B:721:ASP:O    | 1:B:724:SER:OG    | 2.12                     | 0.67              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:4607:ARG:NE  | 1:B:4643:TYR:OH  | 2.27                     | 0.67              |
| 1:C:2649:ASP:O   | 1:C:2653:GLN:NE2 | 2.28                     | 0.67              |
| 1:D:858:THR:OG1  | 1:D:861:ALA:O    | 2.12                     | 0.67              |
| 1:D:2004:THR:OG1 | 1:D:2012:GLU:OE1 | 2.13                     | 0.67              |
| 1:D:2649:ASP:O   | 1:D:2653:GLN:NE2 | 2.28                     | 0.67              |
| 1:B:1756:THR:OG1 | 1:B:1922:GLU:OE2 | 2.12                     | 0.67              |
| 1:C:721:ASP:O    | 1:C:724:SER:OG   | 2.12                     | 0.67              |
| 1:C:3101:LEU:O   | 1:C:3174:LEU:N   | 2.28                     | 0.67              |
| 2:F:37:ASP:OD1   | 2:F:42:ARG:NH2   | 2.28                     | 0.67              |
| 1:C:4607:ARG:NE  | 1:C:4643:TYR:OH  | 2.27                     | 0.67              |
| 1:B:770:ILE:O    | 1:B:773:GLN:NE2  | 2.28                     | 0.67              |
| 1:D:770:ILE:O    | 1:D:773:GLN:NE2  | 2.28                     | 0.67              |
| 1:D:3101:LEU:O   | 1:D:3174:LEU:N   | 2.28                     | 0.67              |
| 2:G:37:ASP:OD1   | 2:G:42:ARG:NH2   | 2.28                     | 0.67              |
| 1:A:1756:THR:OG1 | 1:A:1922:GLU:OE2 | 2.12                     | 0.66              |
| 1:B:2649:ASP:O   | 1:B:2653:GLN:NE2 | 2.28                     | 0.66              |
| 1:A:797:GLY:N    | 1:A:1622:CYS:O   | 2.29                     | 0.66              |
| 1:A:2649:ASP:O   | 1:A:2653:GLN:NE2 | 2.28                     | 0.66              |
| 1:B:2106:THR:OG1 | 1:B:3612:ARG:O   | 2.06                     | 0.66              |
| 1:D:721:ASP:O    | 1:D:724:SER:OG   | 2.12                     | 0.66              |
| 2:H:37:ASP:OD1   | 2:H:42:ARG:NH2   | 2.28                     | 0.66              |
| 1:C:1257:GLN:O   | 1:C:1597:TRP:N   | 2.29                     | 0.66              |
| 1:C:1287:GLN:NE2 | 1:C:1288:LYS:O   | 2.28                     | 0.66              |
| 1:B:797:GLY:N    | 1:B:1622:CYS:O   | 2.29                     | 0.66              |
| 1:B:1257:GLN:O   | 1:B:1597:TRP:N   | 2.29                     | 0.66              |
| 1:A:770:ILE:O    | 1:A:773:GLN:NE2  | 2.28                     | 0.66              |
| 1:C:4131:PHE:O   | 1:C:4151:ILE:N   | 2.28                     | 0.66              |
| 1:D:4131:PHE:O   | 1:D:4151:ILE:N   | 2.28                     | 0.66              |
| 2:E:37:ASP:OD1   | 2:E:42:ARG:NH2   | 2.28                     | 0.66              |
| 1:A:858:THR:OG1  | 1:A:861:ALA:O    | 2.12                     | 0.66              |
| 1:A:3851:SER:O   | 1:A:3855:ASN:ND2 | 2.29                     | 0.66              |
| 1:D:1257:GLN:O   | 1:D:1597:TRP:N   | 2.29                     | 0.66              |
| 1:A:1257:GLN:O   | 1:A:1597:TRP:N   | 2.29                     | 0.66              |
| 1:B:3101:LEU:O   | 1:B:3174:LEU:N   | 2.28                     | 0.66              |
| 1:C:1756:THR:OG1 | 1:C:1922:GLU:OE2 | 2.12                     | 0.66              |
| 1:D:3851:SER:O   | 1:D:3855:ASN:ND2 | 2.29                     | 0.66              |
| 1:C:797:GLY:N    | 1:C:1622:CYS:O   | 2.29                     | 0.66              |
| 1:C:2004:THR:OG1 | 1:C:2012:GLU:OE1 | 2.13                     | 0.66              |
| 1:A:4615:TYR:O   | 1:A:4619:GLN:NE2 | 2.29                     | 0.66              |
| 1:B:2004:THR:OG1 | 1:B:2012:GLU:OE1 | 2.13                     | 0.66              |
| 1:D:797:GLY:N    | 1:D:1622:CYS:O   | 2.29                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:24:VAL:O     | 2:F:46:PHE:N     | 2.29                     | 0.66              |
| 1:A:4131:PHE:O   | 1:A:4151:ILE:N   | 2.28                     | 0.66              |
| 1:B:4615:TYR:O   | 1:B:4619:GLN:NE2 | 2.29                     | 0.65              |
| 1:A:1287:GLN:NE2 | 1:A:1288:LYS:O   | 2.28                     | 0.65              |
| 1:A:2004:THR:OG1 | 1:A:2012:GLU:OE1 | 2.13                     | 0.65              |
| 1:B:4131:PHE:O   | 1:B:4151:ILE:N   | 2.28                     | 0.65              |
| 1:C:4615:TYR:O   | 1:C:4619:GLN:NE2 | 2.29                     | 0.65              |
| 1:C:4136:GLU:O   | 1:C:4917:TYR:OH  | 2.15                     | 0.65              |
| 1:D:4615:TYR:O   | 1:D:4619:GLN:NE2 | 2.29                     | 0.65              |
| 1:A:3101:LEU:O   | 1:A:3174:LEU:N   | 2.28                     | 0.65              |
| 1:C:3851:SER:O   | 1:C:3855:ASN:ND2 | 2.28                     | 0.65              |
| 1:D:1287:GLN:NE2 | 1:D:1288:LYS:O   | 2.28                     | 0.65              |
| 1:D:4136:GLU:O   | 1:D:4917:TYR:OH  | 2.15                     | 0.65              |
| 2:G:24:VAL:O     | 2:G:46:PHE:N     | 2.29                     | 0.65              |
| 2:H:24:VAL:O     | 2:H:46:PHE:N     | 2.29                     | 0.65              |
| 1:C:770:ILE:O    | 1:C:773:GLN:NE2  | 2.28                     | 0.65              |
| 2:E:77:THR:OG1   | 2:E:79:ASP:OD2   | 2.09                     | 0.65              |
| 1:A:2678:ASP:OD2 | 1:A:3043:THR:OG1 | 2.14                     | 0.65              |
| 1:B:4136:GLU:O   | 1:B:4917:TYR:OH  | 2.15                     | 0.65              |
| 2:E:24:VAL:O     | 2:E:46:PHE:N     | 2.29                     | 0.65              |
| 1:A:4136:GLU:O   | 1:A:4917:TYR:OH  | 2.15                     | 0.65              |
| 1:B:1287:GLN:NE2 | 1:B:1288:LYS:O   | 2.28                     | 0.65              |
| 1:B:3851:SER:O   | 1:B:3855:ASN:ND2 | 2.29                     | 0.65              |
| 1:D:2576:CYS:SG  | 1:D:2578:GLN:NE2 | 2.70                     | 0.65              |
| 1:A:2576:CYS:SG  | 1:A:2578:GLN:NE2 | 2.70                     | 0.65              |
| 1:C:2576:CYS:SG  | 1:C:2578:GLN:NE2 | 2.70                     | 0.64              |
| 2:F:77:THR:OG1   | 2:F:79:ASP:OD2   | 2.09                     | 0.64              |
| 1:B:2576:CYS:SG  | 1:B:2578:GLN:NE2 | 2.70                     | 0.64              |
| 1:C:948:CYS:SG   | 1:C:949:HIS:N    | 2.71                     | 0.64              |
| 1:C:300:VAL:HG21 | 1:C:419:ILE:HD12 | 1.80                     | 0.64              |
| 2:H:31:GLN:OE1   | 2:H:96:THR:OG1   | 2.15                     | 0.64              |
| 1:D:300:VAL:HG21 | 1:D:419:ILE:HD12 | 1.80                     | 0.64              |
| 2:F:31:GLN:OE1   | 2:F:96:THR:OG1   | 2.15                     | 0.64              |
| 1:A:948:CYS:SG   | 1:A:949:HIS:N    | 2.70                     | 0.64              |
| 1:B:948:CYS:SG   | 1:B:949:HIS:N    | 2.70                     | 0.64              |
| 2:G:31:GLN:OE1   | 2:G:96:THR:OG1   | 2.15                     | 0.64              |
| 1:B:300:VAL:HG21 | 1:B:419:ILE:HD12 | 1.80                     | 0.64              |
| 1:A:1309:GLU:OE1 | 1:A:1577:LYS:N   | 2.31                     | 0.64              |
| 1:C:858:THR:OG1  | 1:C:861:ALA:O    | 2.12                     | 0.64              |
| 1:A:1027:ARG:NH2 | 1:A:1028:ARG:O   | 2.31                     | 0.63              |
| 1:A:300:VAL:HG21 | 1:A:419:ILE:HD12 | 1.80                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:1027:ARG:NH2  | 1:B:1028:ARG:O    | 2.31                     | 0.63              |
| 1:B:3191:ARG:NE   | 1:B:3191:ARG:O    | 2.32                     | 0.63              |
| 1:D:1027:ARG:NH2  | 1:D:1028:ARG:O    | 2.31                     | 0.63              |
| 2:E:31:GLN:OE1    | 2:E:96:THR:OG1    | 2.15                     | 0.63              |
| 1:B:362:TYR:OH    | 1:B:399:MET:O     | 2.16                     | 0.63              |
| 1:D:1309:GLU:OE1  | 1:D:1577:LYS:N    | 2.31                     | 0.63              |
| 1:B:2215:ASP:O    | 1:B:2218:SER:OG   | 2.14                     | 0.63              |
| 1:C:4099:VAL:HG22 | 1:C:4132:LEU:HD13 | 1.80                     | 0.63              |
| 1:A:362:TYR:OH    | 1:A:399:MET:O     | 2.16                     | 0.63              |
| 1:C:1309:GLU:OE1  | 1:C:1577:LYS:N    | 2.31                     | 0.63              |
| 1:A:3191:ARG:O    | 1:A:3191:ARG:NE   | 2.32                     | 0.63              |
| 1:C:1500:ARG:O    | 1:C:1524:ASN:ND2  | 2.32                     | 0.63              |
| 1:C:1027:ARG:NH2  | 1:C:1028:ARG:O    | 2.31                     | 0.62              |
| 1:D:948:CYS:SG    | 1:D:949:HIS:N     | 2.70                     | 0.62              |
| 1:D:3191:ARG:O    | 1:D:3191:ARG:NE   | 2.32                     | 0.62              |
| 1:B:1500:ARG:O    | 1:B:1524:ASN:ND2  | 2.32                     | 0.62              |
| 1:B:4099:VAL:HG22 | 1:B:4132:LEU:HD13 | 1.80                     | 0.62              |
| 1:D:362:TYR:OH    | 1:D:399:MET:O     | 2.16                     | 0.62              |
| 1:D:1500:ARG:O    | 1:D:1524:ASN:ND2  | 2.32                     | 0.62              |
| 1:C:3191:ARG:O    | 1:C:3191:ARG:NE   | 2.32                     | 0.62              |
| 1:B:1309:GLU:OE1  | 1:B:1577:LYS:N    | 2.31                     | 0.62              |
| 1:C:3642:ASP:OD1  | 1:C:3729:ARG:NH1  | 2.33                     | 0.62              |
| 1:C:362:TYR:OH    | 1:C:399:MET:O     | 2.16                     | 0.62              |
| 1:A:1500:ARG:O    | 1:A:1524:ASN:ND2  | 2.32                     | 0.62              |
| 1:B:123:HIS:ND1   | 1:B:126:SER:OG    | 2.33                     | 0.62              |
| 1:D:4099:VAL:HG22 | 1:D:4132:LEU:HD13 | 1.80                     | 0.62              |
| 1:D:3642:ASP:OD1  | 1:D:3729:ARG:NH1  | 2.33                     | 0.62              |
| 1:A:4099:VAL:HG22 | 1:A:4132:LEU:HD13 | 1.80                     | 0.61              |
| 1:B:145:PHE:O     | 1:B:205:ALA:N     | 2.33                     | 0.61              |
| 1:B:3642:ASP:OD1  | 1:B:3729:ARG:NH1  | 2.33                     | 0.61              |
| 1:D:2358:ARG:NH1  | 1:D:2365:SER:O    | 2.33                     | 0.61              |
| 1:A:3642:ASP:OD1  | 1:A:3729:ARG:NH1  | 2.33                     | 0.61              |
| 1:C:123:HIS:ND1   | 1:C:126:SER:OG    | 2.33                     | 0.61              |
| 1:D:145:PHE:O     | 1:D:205:ALA:N     | 2.33                     | 0.61              |
| 1:D:3385:LYS:O    | 1:D:3453:ARG:NH1  | 2.34                     | 0.61              |
| 1:A:3360:THR:O    | 1:A:3404:TYR:OH   | 2.18                     | 0.61              |
| 1:A:3385:LYS:O    | 1:A:3453:ARG:NH1  | 2.34                     | 0.61              |
| 1:B:281:ARG:NH2   | 1:B:287:SER:OG    | 2.34                     | 0.61              |
| 1:C:2334:LEU:N    | 1:C:2338:GLY:O    | 2.34                     | 0.61              |
| 1:D:1209:VAL:O    | 1:D:1211:GLN:NE2  | 2.34                     | 0.61              |
| 2:G:77:THR:OG1    | 2:G:79:ASP:OD2    | 2.09                     | 0.61              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:123:HIS:ND1  | 1:A:126:SER:OG    | 2.33                     | 0.61              |
| 1:A:1209:VAL:O   | 1:A:1211:GLN:NE2  | 2.34                     | 0.61              |
| 1:A:2334:LEU:N   | 1:A:2338:GLY:O    | 2.34                     | 0.61              |
| 1:B:1209:VAL:O   | 1:B:1211:GLN:NE2  | 2.34                     | 0.61              |
| 1:C:2678:ASP:OD2 | 1:C:3043:THR:OG1  | 2.14                     | 0.61              |
| 1:D:2334:LEU:N   | 1:D:2338:GLY:O    | 2.34                     | 0.61              |
| 1:B:2334:LEU:N   | 1:B:2338:GLY:O    | 2.34                     | 0.61              |
| 1:C:2358:ARG:NH1 | 1:C:2365:SER:O    | 2.34                     | 0.61              |
| 1:D:1763:ARG:O   | 1:D:1778:GLN:N    | 2.34                     | 0.61              |
| 1:D:3360:THR:O   | 1:D:3404:TYR:OH   | 2.18                     | 0.61              |
| 1:B:1765:SER:OG  | 1:B:1780:SER:O    | 2.18                     | 0.61              |
| 1:B:2358:ARG:NH1 | 1:B:2365:SER:O    | 2.34                     | 0.61              |
| 1:A:145:PHE:O    | 1:A:205:ALA:N     | 2.33                     | 0.60              |
| 1:B:694:ARG:NH2  | 1:B:726:GLY:O     | 2.34                     | 0.60              |
| 1:C:145:PHE:O    | 1:C:205:ALA:N     | 2.33                     | 0.60              |
| 1:C:699:SER:OG   | 1:C:721:ASP:OD2   | 2.19                     | 0.60              |
| 1:C:3340:LYS:O   | 1:C:3344:ARG:CB   | 2.50                     | 0.60              |
| 1:C:3385:LYS:O   | 1:C:3453:ARG:NH1  | 2.34                     | 0.60              |
| 1:D:2588:LEU:O   | 1:D:2592:VAL:HG23 | 2.01                     | 0.60              |
| 1:A:281:ARG:NH2  | 1:A:287:SER:OG    | 2.33                     | 0.60              |
| 1:C:281:ARG:NH2  | 1:C:287:SER:OG    | 2.33                     | 0.60              |
| 1:A:2588:LEU:O   | 1:A:2592:VAL:HG23 | 2.02                     | 0.60              |
| 1:B:3385:LYS:O   | 1:B:3453:ARG:NH1  | 2.34                     | 0.60              |
| 1:C:1763:ARG:O   | 1:C:1778:GLN:N    | 2.34                     | 0.60              |
| 1:D:699:SER:OG   | 1:D:721:ASP:OD2   | 2.20                     | 0.60              |
| 1:D:1731:THR:O   | 1:D:1734:THR:OG1  | 2.19                     | 0.60              |
| 1:C:3360:THR:O   | 1:C:3404:TYR:OH   | 2.18                     | 0.60              |
| 1:D:281:ARG:NH2  | 1:D:287:SER:OG    | 2.33                     | 0.60              |
| 1:D:3340:LYS:O   | 1:D:3344:ARG:CB   | 2.50                     | 0.60              |
| 1:A:2358:ARG:NH1 | 1:A:2365:SER:O    | 2.34                     | 0.60              |
| 1:A:2797:MET:HE1 | 1:A:2894:PHE:HD1  | 1.66                     | 0.60              |
| 1:C:2588:LEU:O   | 1:C:2592:VAL:HG23 | 2.02                     | 0.60              |
| 1:A:637:LEU:HD13 | 1:A:1673:VAL:HG13 | 1.84                     | 0.60              |
| 1:B:2797:MET:HE1 | 1:B:2894:PHE:HD1  | 1.66                     | 0.60              |
| 1:C:694:ARG:NH2  | 1:C:726:GLY:O     | 2.35                     | 0.60              |
| 1:A:694:ARG:NH2  | 1:A:726:GLY:O     | 2.35                     | 0.60              |
| 1:B:2588:LEU:O   | 1:B:2592:VAL:HG23 | 2.02                     | 0.60              |
| 1:A:1121:GLY:O   | 1:A:1133:ARG:NH1  | 2.35                     | 0.60              |
| 1:C:1209:VAL:O   | 1:C:1211:GLN:NE2  | 2.34                     | 0.60              |
| 1:D:694:ARG:NH2  | 1:D:726:GLY:O     | 2.35                     | 0.60              |
| 1:D:1121:GLY:O   | 1:D:1133:ARG:NH1  | 2.35                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1731:THR:O    | 1:A:1734:THR:OG1  | 2.19                     | 0.60              |
| 1:A:3340:LYS:O    | 1:A:3344:ARG:CB   | 2.50                     | 0.60              |
| 1:D:1429:SER:OG   | 1:D:1557:GLU:OE1  | 2.15                     | 0.60              |
| 1:A:4163:GLN:OE1  | 1:A:4498:TYR:OH   | 2.12                     | 0.59              |
| 1:B:3340:LYS:O    | 1:B:3344:ARG:CB   | 2.50                     | 0.59              |
| 1:D:123:HIS:ND1   | 1:D:126:SER:OG    | 2.33                     | 0.59              |
| 1:B:637:LEU:HD13  | 1:B:1673:VAL:HG13 | 1.84                     | 0.59              |
| 1:C:2146:GLY:O    | 1:C:2150:ASN:ND2  | 2.36                     | 0.59              |
| 1:C:1722:MET:SD   | 1:C:2126:ARG:NH1  | 2.75                     | 0.59              |
| 1:A:1722:MET:SD   | 1:A:2126:ARG:NH1  | 2.75                     | 0.59              |
| 1:B:1763:ARG:O    | 1:B:1778:GLN:N    | 2.34                     | 0.59              |
| 1:B:2146:GLY:O    | 1:B:2150:ASN:ND2  | 2.36                     | 0.59              |
| 1:C:1121:GLY:O    | 1:C:1133:ARG:NH1  | 2.35                     | 0.59              |
| 1:C:1713:SER:OG   | 1:C:1777:TYR:OH   | 2.17                     | 0.59              |
| 1:A:1144:ARG:N    | 1:A:1150:GLU:O    | 2.35                     | 0.59              |
| 1:B:699:SER:OG    | 1:B:721:ASP:OD2   | 2.20                     | 0.59              |
| 1:B:1121:GLY:O    | 1:B:1133:ARG:NH1  | 2.35                     | 0.59              |
| 1:C:4711:VAL:O    | 1:C:4714:THR:OG1  | 2.21                     | 0.59              |
| 1:A:2146:GLY:O    | 1:A:2150:ASN:ND2  | 2.36                     | 0.59              |
| 1:B:3360:THR:O    | 1:B:3404:TYR:OH   | 2.18                     | 0.59              |
| 1:D:637:LEU:HD13  | 1:D:1673:VAL:HG13 | 1.84                     | 0.59              |
| 1:C:1144:ARG:N    | 1:C:1150:GLU:O    | 2.35                     | 0.59              |
| 1:D:2146:GLY:O    | 1:D:2150:ASN:ND2  | 2.36                     | 0.59              |
| 1:A:699:SER:OG    | 1:A:721:ASP:OD2   | 2.20                     | 0.59              |
| 1:B:305:TYR:O     | 1:B:317:MET:N     | 2.36                     | 0.59              |
| 1:D:1722:MET:SD   | 1:D:2126:ARG:NH1  | 2.75                     | 0.59              |
| 1:D:2660:LEU:O    | 1:D:2664:ALA:N    | 2.36                     | 0.59              |
| 1:B:1722:MET:SD   | 1:B:2126:ARG:NH1  | 2.75                     | 0.58              |
| 1:D:2797:MET:HE1  | 1:D:2894:PHE:HD1  | 1.66                     | 0.58              |
| 1:C:2017:ASP:OD1  | 1:C:2017:ASP:N    | 2.37                     | 0.58              |
| 1:D:1765:SER:OG   | 1:D:1780:SER:O    | 2.18                     | 0.58              |
| 1:A:305:TYR:O     | 1:A:317:MET:N     | 2.36                     | 0.58              |
| 1:B:1586:ARG:NH2  | 1:B:1587:LEU:O    | 2.37                     | 0.58              |
| 1:C:637:LEU:HD13  | 1:C:1673:VAL:HG13 | 1.84                     | 0.58              |
| 1:C:2797:MET:HE1  | 1:C:2894:PHE:HD1  | 1.66                     | 0.58              |
| 1:A:1586:ARG:NH2  | 1:A:1587:LEU:O    | 2.37                     | 0.58              |
| 1:D:2017:ASP:OD1  | 1:D:2017:ASP:N    | 2.37                     | 0.58              |
| 1:B:1144:ARG:N    | 1:B:1150:GLU:O    | 2.35                     | 0.58              |
| 1:D:1847:ILE:HG22 | 1:D:1892:LEU:HB3  | 1.86                     | 0.58              |
| 1:A:1763:ARG:O    | 1:A:1778:GLN:N    | 2.34                     | 0.58              |
| 1:A:4711:VAL:O    | 1:A:4714:THR:OG1  | 2.21                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:305:TYR:O     | 1:C:317:MET:N     | 2.36                     | 0.58              |
| 1:D:305:TYR:O     | 1:D:317:MET:N     | 2.36                     | 0.58              |
| 1:A:1847:ILE:HG22 | 1:A:1892:LEU:HB3  | 1.86                     | 0.58              |
| 1:C:1586:ARG:NH2  | 1:C:1587:LEU:O    | 2.37                     | 0.58              |
| 1:C:1765:SER:OG   | 1:C:1780:SER:O    | 2.18                     | 0.58              |
| 1:D:1144:ARG:N    | 1:D:1150:GLU:O    | 2.35                     | 0.58              |
| 1:C:950:VAL:CG1   | 1:C:1064:LEU:HD13 | 2.34                     | 0.57              |
| 1:D:1586:ARG:NH2  | 1:D:1587:LEU:O    | 2.37                     | 0.57              |
| 1:A:267:VAL:O     | 1:A:273:SER:OG    | 2.21                     | 0.57              |
| 1:B:1429:SER:OG   | 1:B:1557:GLU:OE1  | 2.15                     | 0.57              |
| 1:C:4163:GLN:OE1  | 1:C:4498:TYR:OH   | 2.12                     | 0.57              |
| 1:D:4666:SER:O    | 1:D:4670:GLY:N    | 2.38                     | 0.57              |
| 1:C:2660:LEU:O    | 1:C:2664:ALA:N    | 2.36                     | 0.57              |
| 1:D:4711:VAL:O    | 1:D:4714:THR:OG1  | 2.21                     | 0.57              |
| 1:B:2660:LEU:O    | 1:B:2664:ALA:N    | 2.36                     | 0.57              |
| 1:B:1847:ILE:HG22 | 1:B:1892:LEU:HB3  | 1.86                     | 0.57              |
| 2:E:38:SER:O      | 2:E:42:ARG:NE     | 2.37                     | 0.57              |
| 1:A:950:VAL:CG1   | 1:A:1064:LEU:HD13 | 2.34                     | 0.57              |
| 1:A:2228:LEU:HD12 | 1:A:2237:THR:HB   | 1.87                     | 0.57              |
| 1:B:1713:SER:OG   | 1:B:1777:TYR:OH   | 2.17                     | 0.57              |
| 1:B:4711:VAL:O    | 1:B:4714:THR:OG1  | 2.21                     | 0.57              |
| 1:D:950:VAL:CG1   | 1:D:1064:LEU:HD13 | 2.34                     | 0.57              |
| 1:B:950:VAL:CG1   | 1:B:1064:LEU:HD13 | 2.34                     | 0.57              |
| 1:C:1119:ARG:O    | 1:C:1133:ARG:NH2  | 2.37                     | 0.57              |
| 1:C:4666:SER:O    | 1:C:4670:GLY:N    | 2.38                     | 0.57              |
| 2:H:77:THR:OG1    | 2:H:79:ASP:OD2    | 2.09                     | 0.57              |
| 1:A:1119:ARG:O    | 1:A:1133:ARG:NH2  | 2.38                     | 0.57              |
| 1:B:2228:LEU:HD12 | 1:B:2237:THR:HB   | 1.87                     | 0.57              |
| 1:C:3269:SER:OG   | 1:C:3342:GLU:OE1  | 2.21                     | 0.57              |
| 1:D:2678:ASP:OD2  | 1:D:3043:THR:OG1  | 2.14                     | 0.57              |
| 1:D:4030:THR:HG21 | 1:D:4051:MET:SD   | 2.45                     | 0.57              |
| 1:A:1765:SER:OG   | 1:A:1780:SER:O    | 2.18                     | 0.57              |
| 1:B:1119:ARG:O    | 1:B:1133:ARG:NH2  | 2.38                     | 0.57              |
| 1:B:1597:TRP:NE1  | 1:B:1599:ARG:O    | 2.38                     | 0.57              |
| 1:B:2017:ASP:OD1  | 1:B:2017:ASP:N    | 2.37                     | 0.57              |
| 1:C:2228:LEU:HD12 | 1:C:2237:THR:HB   | 1.87                     | 0.57              |
| 1:D:2228:LEU:HD12 | 1:D:2237:THR:HB   | 1.87                     | 0.57              |
| 2:H:74:LEU:HD22   | 2:H:101:VAL:HG21  | 1.87                     | 0.57              |
| 1:A:2017:ASP:N    | 1:A:2017:ASP:OD1  | 2.37                     | 0.56              |
| 1:B:2404:GLU:H    | 1:B:2407:LEU:HD22 | 1.70                     | 0.56              |
| 1:C:842:GLN:OE1   | 1:C:844:ARG:NH2   | 2.38                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1731:THR:O    | 1:C:1734:THR:OG1  | 2.19                     | 0.56              |
| 1:B:4163:GLN:OE1  | 1:B:4498:TYR:OH   | 2.12                     | 0.56              |
| 1:D:4696:VAL:HG13 | 1:D:4697:LEU:HG   | 1.88                     | 0.56              |
| 1:A:1762:MET:SD   | 1:A:1778:GLN:NE2  | 2.78                     | 0.56              |
| 1:A:4030:THR:HG21 | 1:A:4051:MET:SD   | 2.45                     | 0.56              |
| 1:B:237:LEU:O     | 1:B:404:ASN:N     | 2.39                     | 0.56              |
| 1:B:4696:VAL:HG13 | 1:B:4697:LEU:HG   | 1.87                     | 0.56              |
| 1:C:1847:ILE:HG22 | 1:C:1892:LEU:HB3  | 1.86                     | 0.56              |
| 1:C:4030:THR:HG21 | 1:C:4051:MET:SD   | 2.45                     | 0.56              |
| 1:D:3076:GLN:O    | 1:D:3080:THR:HG23 | 2.06                     | 0.56              |
| 1:A:4666:SER:O    | 1:A:4670:GLY:N    | 2.38                     | 0.56              |
| 1:B:3269:SER:OG   | 1:B:3342:GLU:OE1  | 2.21                     | 0.56              |
| 1:B:4030:THR:HG21 | 1:B:4051:MET:SD   | 2.45                     | 0.56              |
| 1:C:274:LEU:HD13  | 1:C:419:ILE:HD13  | 1.87                     | 0.56              |
| 1:C:1762:MET:SD   | 1:C:1778:GLN:NE2  | 2.79                     | 0.56              |
| 1:C:3076:GLN:O    | 1:C:3080:THR:HG23 | 2.06                     | 0.56              |
| 1:A:1429:SER:OG   | 1:A:1557:GLU:OE1  | 2.15                     | 0.56              |
| 1:A:2172:GLU:O    | 1:A:2176:ASN:ND2  | 2.38                     | 0.56              |
| 1:B:842:GLN:OE1   | 1:B:844:ARG:NH2   | 2.38                     | 0.56              |
| 1:B:1206:SER:O    | 1:B:1207:LEU:HD23 | 2.06                     | 0.56              |
| 1:C:2172:GLU:O    | 1:C:2176:ASN:ND2  | 2.38                     | 0.56              |
| 1:D:842:GLN:OE1   | 1:D:844:ARG:NH2   | 2.38                     | 0.56              |
| 1:D:1119:ARG:O    | 1:D:1133:ARG:NH2  | 2.38                     | 0.56              |
| 1:A:274:LEU:HD13  | 1:A:419:ILE:HD13  | 1.87                     | 0.56              |
| 1:A:842:GLN:OE1   | 1:A:844:ARG:NH2   | 2.38                     | 0.56              |
| 1:A:2660:LEU:O    | 1:A:2664:ALA:N    | 2.36                     | 0.56              |
| 1:C:1206:SER:O    | 1:C:1207:LEU:HD23 | 2.06                     | 0.56              |
| 1:C:2404:GLU:H    | 1:C:2407:LEU:HD22 | 1.70                     | 0.56              |
| 1:D:1597:TRP:NE1  | 1:D:1599:ARG:O    | 2.38                     | 0.56              |
| 2:E:74:LEU:HD22   | 2:E:101:VAL:HG21  | 1.87                     | 0.56              |
| 2:F:40:ARG:NH2    | 2:F:102:GLU:OE1   | 2.39                     | 0.56              |
| 1:D:1712:LEU:HD22 | 1:D:1832:MET:SD   | 2.46                     | 0.56              |
| 1:A:1597:TRP:NE1  | 1:A:1599:ARG:O    | 2.38                     | 0.56              |
| 1:A:1712:LEU:HD22 | 1:A:1832:MET:SD   | 2.46                     | 0.56              |
| 1:A:3076:GLN:O    | 1:A:3080:THR:HG23 | 2.06                     | 0.56              |
| 1:D:237:LEU:O     | 1:D:404:ASN:N     | 2.39                     | 0.56              |
| 1:D:4163:GLN:OE1  | 1:D:4498:TYR:OH   | 2.12                     | 0.56              |
| 1:B:1712:LEU:HD22 | 1:B:1832:MET:SD   | 2.46                     | 0.56              |
| 1:B:1731:THR:O    | 1:B:1734:THR:OG1  | 2.19                     | 0.56              |
| 2:G:40:ARG:NH2    | 2:G:102:GLU:OE1   | 2.39                     | 0.56              |
| 1:B:4666:SER:O    | 1:B:4670:GLY:N    | 2.38                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:237:LEU:O     | 1:C:404:ASN:N     | 2.39                     | 0.55              |
| 1:D:2172:GLU:O    | 1:D:2176:ASN:ND2  | 2.38                     | 0.55              |
| 1:D:2404:GLU:H    | 1:D:2407:LEU:HD22 | 1.70                     | 0.55              |
| 2:E:40:ARG:NH2    | 2:E:102:GLU:OE1   | 2.39                     | 0.55              |
| 2:F:74:LEU:HD22   | 2:F:101:VAL:HG21  | 1.87                     | 0.55              |
| 1:A:237:LEU:O     | 1:A:404:ASN:N     | 2.39                     | 0.55              |
| 1:A:1206:SER:O    | 1:A:1207:LEU:HD23 | 2.06                     | 0.55              |
| 1:A:2404:GLU:H    | 1:A:2407:LEU:HD22 | 1.70                     | 0.55              |
| 1:B:1762:MET:SD   | 1:B:1778:GLN:NE2  | 2.78                     | 0.55              |
| 1:B:2172:GLU:O    | 1:B:2176:ASN:ND2  | 2.38                     | 0.55              |
| 1:C:1597:TRP:NE1  | 1:C:1599:ARG:O    | 2.38                     | 0.55              |
| 1:B:2071:GLU:O    | 1:B:3659:ARG:NH1  | 2.40                     | 0.55              |
| 1:C:267:VAL:O     | 1:C:273:SER:OG    | 2.22                     | 0.55              |
| 1:B:683:GLU:OE1   | 1:B:683:GLU:N     | 2.40                     | 0.55              |
| 1:C:1429:SER:OG   | 1:C:1557:GLU:OE1  | 2.15                     | 0.55              |
| 1:D:1730:MET:N    | 1:D:2107:ILE:O    | 2.40                     | 0.55              |
| 2:G:74:LEU:HD22   | 2:G:101:VAL:HG21  | 1.87                     | 0.55              |
| 1:C:169:ARG:NH1   | 1:C:179:ASP:OD2   | 2.40                     | 0.55              |
| 1:C:683:GLU:N     | 1:C:683:GLU:OE1   | 2.40                     | 0.55              |
| 1:D:169:ARG:NH1   | 1:D:179:ASP:OD2   | 2.40                     | 0.55              |
| 1:D:274:LEU:HD13  | 1:D:419:ILE:HD13  | 1.87                     | 0.55              |
| 1:A:2071:GLU:O    | 1:A:3659:ARG:NH1  | 2.40                     | 0.55              |
| 1:D:1550:SER:HA   | 1:D:1553:VAL:HG12 | 1.88                     | 0.55              |
| 1:D:1762:MET:SD   | 1:D:1778:GLN:NE2  | 2.79                     | 0.55              |
| 1:A:2215:ASP:O    | 1:A:2218:SER:OG   | 2.14                     | 0.55              |
| 1:B:1550:SER:HA   | 1:B:1553:VAL:HG12 | 1.88                     | 0.55              |
| 1:C:1550:SER:HA   | 1:C:1553:VAL:HG12 | 1.88                     | 0.55              |
| 1:D:1725:GLU:OE2  | 1:D:2126:ARG:NH1  | 2.40                     | 0.55              |
| 1:B:274:LEU:HD13  | 1:B:419:ILE:HD13  | 1.87                     | 0.55              |
| 1:B:569:SER:O     | 1:B:609:LYS:NZ    | 2.40                     | 0.55              |
| 1:B:1245:ARG:NH1  | 1:B:1693:LYS:O    | 2.40                     | 0.55              |
| 1:B:2678:ASP:OD2  | 1:B:3043:THR:OG1  | 2.14                     | 0.55              |
| 1:C:1245:ARG:NH1  | 1:C:1693:LYS:O    | 2.40                     | 0.55              |
| 1:C:1712:LEU:HD22 | 1:C:1832:MET:SD   | 2.46                     | 0.55              |
| 1:A:683:GLU:N     | 1:A:683:GLU:OE1   | 2.40                     | 0.55              |
| 1:A:4696:VAL:HG13 | 1:A:4697:LEU:HG   | 1.88                     | 0.55              |
| 1:B:3076:GLN:O    | 1:B:3080:THR:HG23 | 2.06                     | 0.55              |
| 1:C:2071:GLU:O    | 1:C:3659:ARG:NH1  | 2.40                     | 0.55              |
| 1:C:4696:VAL:HG13 | 1:C:4697:LEU:HG   | 1.88                     | 0.55              |
| 1:D:1206:SER:O    | 1:D:1207:LEU:HD23 | 2.06                     | 0.55              |
| 2:H:40:ARG:NH2    | 2:H:102:GLU:OE1   | 2.39                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1550:SER:HA   | 1:A:1553:VAL:HG12 | 1.88                     | 0.55              |
| 1:A:169:ARG:NH1   | 1:A:179:ASP:OD2   | 2.40                     | 0.54              |
| 1:A:693:LEU:HD12  | 1:A:793:SER:O     | 2.07                     | 0.54              |
| 1:A:1725:GLU:OE2  | 1:A:2126:ARG:NH1  | 2.40                     | 0.54              |
| 1:A:3786:VAL:HG12 | 1:A:3790:GLN:HG3  | 1.90                     | 0.54              |
| 1:C:4106:GLU:OE2  | 1:C:4146:ARG:NH1  | 2.41                     | 0.54              |
| 1:D:267:VAL:O     | 1:D:273:SER:OG    | 2.22                     | 0.54              |
| 1:D:2071:GLU:O    | 1:D:3659:ARG:NH1  | 2.40                     | 0.54              |
| 2:H:38:SER:O      | 2:H:42:ARG:NE     | 2.37                     | 0.54              |
| 1:D:1245:ARG:NH1  | 1:D:1693:LYS:O    | 2.40                     | 0.54              |
| 1:D:3786:VAL:HG12 | 1:D:3790:GLN:HG3  | 1.90                     | 0.54              |
| 1:A:889:ILE:HD12  | 1:A:892:LEU:HD12  | 1.90                     | 0.54              |
| 1:B:3786:VAL:HG12 | 1:B:3790:GLN:HG3  | 1.90                     | 0.54              |
| 1:B:4106:GLU:OE2  | 1:B:4146:ARG:NH1  | 2.41                     | 0.54              |
| 1:D:693:LEU:HD12  | 1:D:793:SER:O     | 2.07                     | 0.54              |
| 1:B:169:ARG:NH1   | 1:B:179:ASP:OD2   | 2.40                     | 0.54              |
| 1:D:1506:LEU:N    | 1:D:1524:ASN:OD1  | 2.41                     | 0.54              |
| 1:B:1730:MET:N    | 1:B:2107:ILE:O    | 2.40                     | 0.54              |
| 1:B:3958:SER:O    | 1:B:4085:ARG:NH2  | 2.41                     | 0.54              |
| 1:C:3786:VAL:HG12 | 1:C:3790:GLN:HG3  | 1.90                     | 0.54              |
| 1:A:3958:SER:O    | 1:A:4085:ARG:NH2  | 2.41                     | 0.54              |
| 1:B:693:LEU:HD12  | 1:B:793:SER:O     | 2.07                     | 0.54              |
| 1:B:823:TYR:O     | 1:B:826:VAL:HG23  | 2.08                     | 0.54              |
| 1:C:3958:SER:O    | 1:C:4085:ARG:NH2  | 2.41                     | 0.54              |
| 1:A:4106:GLU:OE2  | 1:A:4146:ARG:NH1  | 2.41                     | 0.54              |
| 1:C:823:TYR:O     | 1:C:826:VAL:HG23  | 2.08                     | 0.54              |
| 1:D:2215:ASP:O    | 1:D:2218:SER:OG   | 2.14                     | 0.54              |
| 1:D:4106:GLU:OE2  | 1:D:4146:ARG:NH1  | 2.41                     | 0.54              |
| 1:D:1269:GLU:N    | 1:D:1269:GLU:OE2  | 2.41                     | 0.54              |
| 1:D:1832:MET:HE2  | 1:D:1834:ILE:HD11 | 1.90                     | 0.54              |
| 1:D:3802:LEU:HD11 | 1:D:3904:ASN:HB3  | 1.90                     | 0.54              |
| 1:D:4784:ALA:O    | 1:D:4788:PHE:N    | 2.41                     | 0.54              |
| 1:A:430:ILE:HG23  | 1:A:505:LEU:HD22  | 1.91                     | 0.53              |
| 1:A:1245:ARG:NH1  | 1:A:1693:LYS:O    | 2.40                     | 0.53              |
| 1:A:1730:MET:N    | 1:A:2107:ILE:O    | 2.40                     | 0.53              |
| 1:A:1832:MET:HE2  | 1:A:1834:ILE:HD11 | 1.90                     | 0.53              |
| 1:A:3802:LEU:HD11 | 1:A:3904:ASN:HB3  | 1.90                     | 0.53              |
| 1:A:4842:ARG:NH1  | 1:A:4846:ASP:OD1  | 2.41                     | 0.53              |
| 1:B:889:ILE:HD12  | 1:B:892:LEU:HD12  | 1.90                     | 0.53              |
| 1:B:3802:LEU:HD11 | 1:B:3904:ASN:HB3  | 1.90                     | 0.53              |
| 1:C:3078:GLN:O    | 1:C:3082:THR:OG1  | 2.18                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3958:SER:O    | 1:D:4085:ARG:NH2  | 2.41                     | 0.53              |
| 1:C:1832:MET:HE2  | 1:C:1834:ILE:HD11 | 1.90                     | 0.53              |
| 1:C:4842:ARG:NH1  | 1:C:4846:ASP:OD1  | 2.41                     | 0.53              |
| 1:A:2576:CYS:SG   | 1:A:2577:GLY:N    | 2.82                     | 0.53              |
| 1:B:2125:ILE:HD11 | 1:B:2144:GLY:HA3  | 1.90                     | 0.53              |
| 1:B:4178:GLU:OE2  | 1:B:4178:GLU:N    | 2.42                     | 0.53              |
| 1:C:430:ILE:HG23  | 1:C:505:LEU:HD22  | 1.91                     | 0.53              |
| 1:D:655:MET:SD    | 1:D:1620:VAL:HG11 | 2.49                     | 0.53              |
| 1:D:4842:ARG:NH1  | 1:D:4846:ASP:OD1  | 2.41                     | 0.53              |
| 1:A:655:MET:SD    | 1:A:1620:VAL:HG11 | 2.49                     | 0.53              |
| 1:A:1269:GLU:N    | 1:A:1269:GLU:OE2  | 2.41                     | 0.53              |
| 1:B:70:GLU:OE2    | 1:B:122:ARG:NH2   | 2.42                     | 0.53              |
| 1:B:4784:ALA:O    | 1:B:4788:PHE:N    | 2.42                     | 0.53              |
| 1:C:693:LEU:HD12  | 1:C:793:SER:O     | 2.07                     | 0.53              |
| 1:C:3802:LEU:HD11 | 1:C:3904:ASN:HB3  | 1.90                     | 0.53              |
| 1:D:2125:ILE:HD11 | 1:D:2144:GLY:HA3  | 1.90                     | 0.53              |
| 1:D:4885:THR:O    | 1:D:4894:ASN:N    | 2.42                     | 0.53              |
| 2:E:39:SER:OG     | 2:E:44:LYS:O      | 2.26                     | 0.53              |
| 2:H:39:SER:OG     | 2:H:44:LYS:O      | 2.26                     | 0.53              |
| 1:A:823:TYR:O     | 1:A:826:VAL:HG23  | 2.08                     | 0.53              |
| 1:C:4885:THR:O    | 1:C:4894:ASN:N    | 2.42                     | 0.53              |
| 1:D:499:LEU:HD22  | 1:D:537:LEU:HD12  | 1.91                     | 0.53              |
| 1:D:683:GLU:OE1   | 1:D:683:GLU:N     | 2.40                     | 0.53              |
| 1:D:823:TYR:O     | 1:D:826:VAL:HG23  | 2.08                     | 0.53              |
| 1:D:4178:GLU:OE2  | 1:D:4178:GLU:N    | 2.42                     | 0.53              |
| 1:A:1118:SER:OG   | 1:A:1119:ARG:N    | 2.42                     | 0.53              |
| 1:A:4784:ALA:O    | 1:A:4788:PHE:N    | 2.41                     | 0.53              |
| 1:B:430:ILE:HG23  | 1:B:505:LEU:HD22  | 1.91                     | 0.53              |
| 1:B:1723:ASN:O    | 1:B:1918:ARG:NH2  | 2.41                     | 0.53              |
| 1:C:655:MET:SD    | 1:C:1620:VAL:HG11 | 2.49                     | 0.53              |
| 1:C:1723:ASN:O    | 1:C:1918:ARG:NH2  | 2.41                     | 0.53              |
| 2:G:39:SER:OG     | 2:G:44:LYS:O      | 2.26                     | 0.53              |
| 1:B:2576:CYS:SG   | 1:B:2577:GLY:N    | 2.82                     | 0.53              |
| 1:C:70:GLU:OE2    | 1:C:122:ARG:NH2   | 2.42                     | 0.53              |
| 1:C:2125:ILE:HD11 | 1:C:2144:GLY:HA3  | 1.90                     | 0.53              |
| 1:B:499:LEU:HD22  | 1:B:537:LEU:HD12  | 1.91                     | 0.53              |
| 1:B:2135:LYS:HE2  | 1:B:2186:ILE:HD11 | 1.91                     | 0.53              |
| 1:B:4842:ARG:NH1  | 1:B:4846:ASP:OD1  | 2.41                     | 0.53              |
| 1:C:889:ILE:HD12  | 1:C:892:LEU:HD12  | 1.90                     | 0.53              |
| 1:C:3788:PHE:O    | 1:C:3791:SER:OG   | 2.22                     | 0.53              |
| 1:D:70:GLU:OE2    | 1:D:122:ARG:NH2   | 2.42                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1118:SER:OG   | 1:D:1119:ARG:N    | 2.42                     | 0.53              |
| 1:D:3788:PHE:O    | 1:D:3791:SER:OG   | 2.22                     | 0.53              |
| 1:A:499:LEU:HD22  | 1:A:537:LEU:HD12  | 1.91                     | 0.53              |
| 1:A:892:LEU:HD13  | 1:A:1056:THR:HG21 | 1.91                     | 0.53              |
| 1:A:2135:LYS:HE2  | 1:A:2186:ILE:HD11 | 1.91                     | 0.53              |
| 1:A:3269:SER:OG   | 1:A:3342:GLU:OE1  | 2.21                     | 0.53              |
| 1:B:1269:GLU:N    | 1:B:1269:GLU:OE2  | 2.41                     | 0.53              |
| 1:B:4885:THR:O    | 1:B:4894:ASN:N    | 2.42                     | 0.53              |
| 1:C:2576:CYS:SG   | 1:C:2577:GLY:N    | 2.82                     | 0.53              |
| 1:C:4784:ALA:O    | 1:C:4788:PHE:N    | 2.41                     | 0.53              |
| 1:D:1723:ASN:O    | 1:D:1918:ARG:NH2  | 2.41                     | 0.53              |
| 1:B:267:VAL:O     | 1:B:273:SER:OG    | 2.21                     | 0.53              |
| 1:B:1725:GLU:OE2  | 1:B:2126:ARG:NH1  | 2.40                     | 0.53              |
| 1:C:499:LEU:HD22  | 1:C:537:LEU:HD12  | 1.91                     | 0.53              |
| 1:C:569:SER:O     | 1:C:609:LYS:NZ    | 2.40                     | 0.53              |
| 1:C:1730:MET:N    | 1:C:2107:ILE:O    | 2.40                     | 0.53              |
| 1:C:4178:GLU:N    | 1:C:4178:GLU:OE2  | 2.42                     | 0.53              |
| 1:D:676:GLU:HB3   | 1:D:803:LEU:HD12  | 1.91                     | 0.53              |
| 1:D:2576:CYS:SG   | 1:D:2577:GLY:N    | 2.82                     | 0.53              |
| 1:A:1255:LEU:HD12 | 1:A:1256:PRO:HD2  | 1.91                     | 0.52              |
| 1:A:1257:GLN:HB2  | 1:A:1600:MET:HE2  | 1.92                     | 0.52              |
| 1:A:1440:ASN:ND2  | 1:A:1498:GLN:O    | 2.42                     | 0.52              |
| 1:A:2125:ILE:HD11 | 1:A:2144:GLY:HA3  | 1.90                     | 0.52              |
| 1:A:4159:TRP:CH2  | 1:A:4915:ALA:HB2  | 2.45                     | 0.52              |
| 1:A:4178:GLU:N    | 1:A:4178:GLU:OE2  | 2.42                     | 0.52              |
| 1:A:4885:THR:O    | 1:A:4894:ASN:N    | 2.42                     | 0.52              |
| 1:C:1118:SER:OG   | 1:C:1119:ARG:N    | 2.42                     | 0.52              |
| 1:D:430:ILE:HG23  | 1:D:505:LEU:HD22  | 1.91                     | 0.52              |
| 1:D:892:LEU:HD13  | 1:D:1056:THR:HG21 | 1.91                     | 0.52              |
| 1:D:1255:LEU:HD12 | 1:D:1256:PRO:HD2  | 1.91                     | 0.52              |
| 1:C:1440:ASN:ND2  | 1:C:1498:GLN:O    | 2.42                     | 0.52              |
| 1:C:4159:TRP:CH2  | 1:C:4915:ALA:HB2  | 2.45                     | 0.52              |
| 1:C:1269:GLU:OE2  | 1:C:1269:GLU:N    | 2.41                     | 0.52              |
| 1:D:889:ILE:HD12  | 1:D:892:LEU:HD12  | 1.90                     | 0.52              |
| 1:A:1723:ASN:O    | 1:A:1918:ARG:NH2  | 2.41                     | 0.52              |
| 1:B:1832:MET:HE2  | 1:B:1834:ILE:HD11 | 1.90                     | 0.52              |
| 1:B:4159:TRP:CH2  | 1:B:4915:ALA:HB2  | 2.45                     | 0.52              |
| 1:D:1440:ASN:ND2  | 1:D:1498:GLN:O    | 2.42                     | 0.52              |
| 1:A:70:GLU:OE2    | 1:A:122:ARG:NH2   | 2.42                     | 0.52              |
| 1:B:655:MET:SD    | 1:B:1620:VAL:HG11 | 2.49                     | 0.52              |
| 1:A:676:GLU:HB3   | 1:A:803:LEU:HD12  | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2987:ARG:O    | 1:A:2994:HIS:NE2  | 2.43                     | 0.52              |
| 1:B:892:LEU:HD13  | 1:B:1056:THR:HG21 | 1.91                     | 0.52              |
| 1:C:1255:LEU:HD12 | 1:C:1256:PRO:HD2  | 1.91                     | 0.52              |
| 1:C:1257:GLN:HB2  | 1:C:1600:MET:HE2  | 1.92                     | 0.52              |
| 1:D:1272:ARG:HH12 | 1:D:1308:ILE:HD11 | 1.75                     | 0.52              |
| 1:D:4159:TRP:CH2  | 1:D:4915:ALA:HB2  | 2.45                     | 0.52              |
| 2:H:25:HIS:O      | 2:H:40:ARG:NE     | 2.38                     | 0.52              |
| 1:B:1118:SER:OG   | 1:B:1119:ARG:N    | 2.42                     | 0.52              |
| 1:C:1725:GLU:OE2  | 1:C:2126:ARG:NH1  | 2.40                     | 0.52              |
| 1:D:3269:SER:OG   | 1:D:3342:GLU:OE1  | 2.21                     | 0.52              |
| 1:B:676:GLU:HB3   | 1:B:803:LEU:HD12  | 1.91                     | 0.52              |
| 1:B:1255:LEU:HD12 | 1:B:1256:PRO:HD2  | 1.92                     | 0.52              |
| 1:C:676:GLU:HB3   | 1:C:803:LEU:HD12  | 1.91                     | 0.52              |
| 1:B:1440:ASN:ND2  | 1:B:1498:GLN:O    | 2.42                     | 0.52              |
| 1:C:2135:LYS:HE2  | 1:C:2186:ILE:HD11 | 1.91                     | 0.52              |
| 1:D:673:TRP:NE1   | 1:D:824:GLU:OE2   | 2.43                     | 0.52              |
| 1:D:2135:LYS:HE2  | 1:D:2186:ILE:HD11 | 1.91                     | 0.52              |
| 1:A:4620:PRO:O    | 1:A:4628:GLN:NE2  | 2.43                     | 0.52              |
| 1:B:1257:GLN:HB2  | 1:B:1600:MET:HE2  | 1.92                     | 0.52              |
| 1:B:3788:PHE:O    | 1:B:3791:SER:OG   | 2.22                     | 0.52              |
| 1:B:4620:PRO:O    | 1:B:4628:GLN:NE2  | 2.43                     | 0.52              |
| 1:B:673:TRP:NE1   | 1:B:824:GLU:OE2   | 2.43                     | 0.51              |
| 1:C:3269:SER:OG   | 1:C:3347:MET:SD   | 2.69                     | 0.51              |
| 1:C:4620:PRO:O    | 1:C:4628:GLN:NE2  | 2.43                     | 0.51              |
| 1:A:673:TRP:NE1   | 1:A:824:GLU:OE2   | 2.43                     | 0.51              |
| 1:B:1272:ARG:HH12 | 1:B:1308:ILE:HD11 | 1.75                     | 0.51              |
| 1:C:673:TRP:NE1   | 1:C:824:GLU:OE2   | 2.43                     | 0.51              |
| 1:D:1257:GLN:HB2  | 1:D:1600:MET:HE2  | 1.91                     | 0.51              |
| 1:D:2987:ARG:O    | 1:D:2994:HIS:NE2  | 2.43                     | 0.51              |
| 1:A:843:GLU:OE2   | 1:A:1608:ASP:N    | 2.43                     | 0.51              |
| 1:A:1723:ASN:OD1  | 1:A:1918:ARG:NH2  | 2.43                     | 0.51              |
| 1:A:2437:ILE:HG21 | 1:A:2467:MET:HE3  | 1.93                     | 0.51              |
| 1:B:2437:ILE:HG21 | 1:B:2467:MET:HE3  | 1.93                     | 0.51              |
| 1:B:3269:SER:OG   | 1:B:3347:MET:SD   | 2.69                     | 0.51              |
| 1:C:892:LEU:HD13  | 1:C:1056:THR:HG21 | 1.91                     | 0.51              |
| 1:D:4620:PRO:O    | 1:D:4628:GLN:NE2  | 2.43                     | 0.51              |
| 1:A:436:LEU:HD23  | 1:A:440:VAL:HB    | 1.93                     | 0.51              |
| 1:B:4189:VAL:HG21 | 1:B:4948:TRP:CZ3  | 2.46                     | 0.51              |
| 1:C:606:ARG:O     | 1:C:608:HIS:ND1   | 2.44                     | 0.51              |
| 1:D:3269:SER:OG   | 1:D:3347:MET:SD   | 2.69                     | 0.51              |
| 2:F:39:SER:OG     | 2:F:44:LYS:O      | 2.26                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:38:SER:O      | 2:G:42:ARG:NE     | 2.37                     | 0.51              |
| 1:D:925:PRO:O     | 1:D:929:ARG:N     | 2.44                     | 0.51              |
| 1:D:4189:VAL:HG21 | 1:D:4948:TRP:CZ3  | 2.46                     | 0.51              |
| 2:G:25:HIS:O      | 2:G:40:ARG:NE     | 2.38                     | 0.51              |
| 1:B:891:GLU:N     | 1:B:891:GLU:OE1   | 2.44                     | 0.51              |
| 1:B:1506:LEU:N    | 1:B:1524:ASN:OD1  | 2.41                     | 0.51              |
| 1:B:2422:LEU:O    | 1:B:2431:LEU:HD11 | 2.11                     | 0.51              |
| 1:C:843:GLU:OE2   | 1:C:1608:ASP:N    | 2.43                     | 0.51              |
| 1:D:891:GLU:N     | 1:D:891:GLU:OE1   | 2.44                     | 0.51              |
| 1:D:2422:LEU:O    | 1:D:2431:LEU:HD11 | 2.11                     | 0.51              |
| 1:A:674:TYR:N     | 1:A:820:ALA:O     | 2.44                     | 0.51              |
| 1:B:678:MET:SD    | 1:B:812:LYS:NZ    | 2.71                     | 0.51              |
| 1:B:2667:CYS:SG   | 1:B:2691:GLN:NE2  | 2.84                     | 0.51              |
| 1:B:2987:ARG:O    | 1:B:2994:HIS:NE2  | 2.43                     | 0.51              |
| 1:D:2667:CYS:SG   | 1:D:2691:GLN:NE2  | 2.84                     | 0.51              |
| 1:A:1272:ARG:HH12 | 1:A:1308:ILE:HD11 | 1.75                     | 0.51              |
| 1:A:2667:CYS:SG   | 1:A:2691:GLN:NE2  | 2.84                     | 0.51              |
| 1:A:4189:VAL:HG21 | 1:A:4948:TRP:CZ3  | 2.46                     | 0.51              |
| 1:B:436:LEU:HD23  | 1:B:440:VAL:HB    | 1.93                     | 0.51              |
| 1:B:843:GLU:OE2   | 1:B:1608:ASP:N    | 2.43                     | 0.51              |
| 1:C:891:GLU:OE1   | 1:C:891:GLU:N     | 2.44                     | 0.51              |
| 1:D:436:LEU:HD23  | 1:D:440:VAL:HB    | 1.93                     | 0.51              |
| 1:B:4635:ASN:ND2  | 1:B:4668:LEU:O    | 2.44                     | 0.50              |
| 1:A:2797:MET:HE1  | 1:A:2894:PHE:CD1  | 2.46                     | 0.50              |
| 1:A:3916:PHE:O    | 1:A:3920:THR:HG23 | 2.12                     | 0.50              |
| 1:D:162:ILE:O     | 1:D:163:HIS:ND1   | 2.45                     | 0.50              |
| 1:A:3269:SER:OG   | 1:A:3347:MET:SD   | 2.69                     | 0.50              |
| 1:A:4635:ASN:ND2  | 1:A:4668:LEU:O    | 2.44                     | 0.50              |
| 1:C:2667:CYS:SG   | 1:C:2691:GLN:NE2  | 2.84                     | 0.50              |
| 1:C:4189:VAL:HG21 | 1:C:4948:TRP:CZ3  | 2.46                     | 0.50              |
| 1:D:1723:ASN:OD1  | 1:D:1918:ARG:NH2  | 2.43                     | 0.50              |
| 1:B:674:TYR:N     | 1:B:820:ALA:O     | 2.44                     | 0.50              |
| 1:C:2040:LYS:O    | 1:C:2056:SER:N    | 2.45                     | 0.50              |
| 1:B:162:ILE:O     | 1:B:163:HIS:ND1   | 2.45                     | 0.50              |
| 1:C:674:TYR:N     | 1:C:820:ALA:O     | 2.44                     | 0.50              |
| 1:C:1272:ARG:HH12 | 1:C:1308:ILE:HD11 | 1.75                     | 0.50              |
| 1:C:1946:VAL:HG12 | 1:C:1947:MET:H    | 1.77                     | 0.50              |
| 1:C:3916:PHE:O    | 1:C:3920:THR:HG23 | 2.12                     | 0.50              |
| 1:A:3788:PHE:O    | 1:A:3791:SER:OG   | 2.22                     | 0.50              |
| 1:C:436:LEU:HD23  | 1:C:440:VAL:HB    | 1.93                     | 0.50              |
| 1:C:2437:ILE:HG21 | 1:C:2467:MET:HE3  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:674:TYR:N     | 1:D:820:ALA:O     | 2.44                     | 0.50              |
| 1:D:3916:PHE:O    | 1:D:3920:THR:HG23 | 2.12                     | 0.50              |
| 1:B:1723:ASN:OD1  | 1:B:1918:ARG:NH2  | 2.43                     | 0.50              |
| 1:B:2162:ARG:NH2  | 1:B:2206:SER:OG   | 2.45                     | 0.50              |
| 1:C:436:LEU:HD21  | 1:C:445:ILE:HG22  | 1.93                     | 0.50              |
| 1:C:1638:ARG:NH2  | 1:C:1639:SER:OG   | 2.45                     | 0.50              |
| 1:C:2129:LEU:HD12 | 1:C:2130:SER:H    | 1.76                     | 0.50              |
| 1:D:2129:LEU:HD12 | 1:D:2130:SER:H    | 1.76                     | 0.50              |
| 1:A:925:PRO:O     | 1:A:929:ARG:N     | 2.44                     | 0.50              |
| 1:A:2129:LEU:HD12 | 1:A:2130:SER:H    | 1.76                     | 0.50              |
| 1:C:2162:ARG:NH2  | 1:C:2206:SER:OG   | 2.45                     | 0.50              |
| 1:C:2422:LEU:O    | 1:C:2431:LEU:HD11 | 2.11                     | 0.50              |
| 1:D:843:GLU:OE2   | 1:D:1608:ASP:N    | 2.43                     | 0.50              |
| 1:D:2162:ARG:NH2  | 1:D:2206:SER:OG   | 2.45                     | 0.50              |
| 1:D:2431:LEU:O    | 1:D:2434:VAL:HG22 | 2.12                     | 0.50              |
| 1:D:2726:HIS:CD2  | 1:D:2797:MET:HE3  | 2.47                     | 0.50              |
| 1:A:162:ILE:O     | 1:A:163:HIS:ND1   | 2.45                     | 0.50              |
| 1:A:891:GLU:OE1   | 1:A:891:GLU:N     | 2.44                     | 0.50              |
| 1:A:2162:ARG:NH2  | 1:A:2206:SER:OG   | 2.45                     | 0.50              |
| 1:B:1946:VAL:HG12 | 1:B:1947:MET:H    | 1.76                     | 0.50              |
| 1:D:2040:LYS:O    | 1:D:2056:SER:N    | 2.45                     | 0.50              |
| 1:A:436:LEU:HD21  | 1:A:445:ILE:HG22  | 1.93                     | 0.49              |
| 1:A:2726:HIS:CD2  | 1:A:2797:MET:HE3  | 2.47                     | 0.49              |
| 1:B:166:SER:OG    | 1:B:167:LYS:N     | 2.45                     | 0.49              |
| 1:B:436:LEU:HD21  | 1:B:445:ILE:HG22  | 1.93                     | 0.49              |
| 1:B:2040:LYS:O    | 1:B:2056:SER:N    | 2.45                     | 0.49              |
| 1:C:925:PRO:O     | 1:C:929:ARG:N     | 2.44                     | 0.49              |
| 1:D:1946:VAL:HG12 | 1:D:1947:MET:H    | 1.77                     | 0.49              |
| 1:D:4635:ASN:ND2  | 1:D:4668:LEU:O    | 2.44                     | 0.49              |
| 1:A:606:ARG:O     | 1:A:608:HIS:ND1   | 2.44                     | 0.49              |
| 1:A:2431:LEU:O    | 1:A:2434:VAL:HG22 | 2.12                     | 0.49              |
| 1:B:3916:PHE:O    | 1:B:3920:THR:HG23 | 2.12                     | 0.49              |
| 1:A:2422:LEU:O    | 1:A:2431:LEU:HD11 | 2.11                     | 0.49              |
| 1:B:1638:ARG:NH2  | 1:B:1639:SER:OG   | 2.45                     | 0.49              |
| 1:B:2726:HIS:CD2  | 1:B:2797:MET:HE3  | 2.47                     | 0.49              |
| 1:C:162:ILE:O     | 1:C:163:HIS:ND1   | 2.45                     | 0.49              |
| 1:C:166:SER:OG    | 1:C:167:LYS:N     | 2.45                     | 0.49              |
| 1:C:235:ARG:NE    | 1:C:268:SER:O     | 2.42                     | 0.49              |
| 1:C:2987:ARG:O    | 1:C:2994:HIS:NE2  | 2.43                     | 0.49              |
| 1:C:4635:ASN:ND2  | 1:C:4668:LEU:O    | 2.44                     | 0.49              |
| 1:D:569:SER:O     | 1:D:609:LYS:NZ    | 2.40                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2437:ILE:HG21 | 1:D:2467:MET:HE3  | 1.93                     | 0.49              |
| 1:B:606:ARG:O     | 1:B:608:HIS:ND1   | 2.44                     | 0.49              |
| 1:B:1726:PHE:CD2  | 1:B:1921:ILE:HD11 | 2.48                     | 0.49              |
| 1:B:2797:MET:HE1  | 1:B:2894:PHE:CD1  | 2.46                     | 0.49              |
| 1:B:4619:GLN:OE1  | 1:B:4631:ARG:NH1  | 2.46                     | 0.49              |
| 1:C:266:ALA:O     | 1:C:270:HIS:ND1   | 2.45                     | 0.49              |
| 1:D:1105:PHE:CD2  | 1:D:1115:VAL:HG11 | 2.47                     | 0.49              |
| 1:A:2040:LYS:O    | 1:A:2056:SER:N    | 2.45                     | 0.49              |
| 1:B:300:VAL:CG2   | 1:B:419:ILE:HD12  | 2.43                     | 0.49              |
| 1:C:1105:PHE:CD2  | 1:C:1115:VAL:HG11 | 2.47                     | 0.49              |
| 1:D:1726:PHE:CD2  | 1:D:1921:ILE:HD11 | 2.48                     | 0.49              |
| 1:A:1105:PHE:CD2  | 1:A:1115:VAL:HG11 | 2.47                     | 0.49              |
| 1:B:2129:LEU:HD12 | 1:B:2130:SER:H    | 1.76                     | 0.49              |
| 1:C:2169:THR:O    | 1:C:2173:VAL:HG23 | 2.13                     | 0.49              |
| 1:C:4619:GLN:OE1  | 1:C:4631:ARG:NH1  | 2.46                     | 0.49              |
| 1:A:877:HIS:O     | 1:A:880:ARG:NH1   | 2.46                     | 0.49              |
| 1:C:2431:LEU:O    | 1:C:2434:VAL:HG22 | 2.12                     | 0.49              |
| 1:D:1638:ARG:NH2  | 1:D:1639:SER:OG   | 2.45                     | 0.49              |
| 1:A:166:SER:OG    | 1:A:167:LYS:N     | 2.46                     | 0.49              |
| 1:A:4501:ARG:NH2  | 1:A:4744:ASP:OD1  | 2.46                     | 0.49              |
| 1:B:3737:GLU:N    | 1:B:3737:GLU:OE2  | 2.46                     | 0.49              |
| 1:B:3924:GLN:O    | 1:B:4934:GLY:N    | 2.46                     | 0.49              |
| 1:C:841:LYS:HA    | 1:C:851:LEU:HD12  | 1.95                     | 0.49              |
| 1:C:877:HIS:O     | 1:C:880:ARG:NH1   | 2.46                     | 0.49              |
| 1:C:1723:ASN:OD1  | 1:C:1918:ARG:NH2  | 2.43                     | 0.49              |
| 1:D:300:VAL:CG2   | 1:D:419:ILE:HD12  | 2.43                     | 0.49              |
| 1:D:436:LEU:HD21  | 1:D:445:ILE:HG22  | 1.93                     | 0.49              |
| 1:D:841:LYS:HA    | 1:D:851:LEU:HD12  | 1.95                     | 0.49              |
| 1:D:877:HIS:O     | 1:D:880:ARG:NH1   | 2.46                     | 0.49              |
| 1:A:1506:LEU:N    | 1:A:1524:ASN:OD1  | 2.41                     | 0.49              |
| 1:A:1726:PHE:CD2  | 1:A:1921:ILE:HD11 | 2.48                     | 0.49              |
| 1:A:1946:VAL:HG12 | 1:A:1947:MET:H    | 1.76                     | 0.49              |
| 1:A:2169:THR:O    | 1:A:2173:VAL:HG23 | 2.13                     | 0.49              |
| 1:A:3737:GLU:OE2  | 1:A:3737:GLU:N    | 2.46                     | 0.49              |
| 1:B:678:MET:HB2   | 1:B:803:LEU:HD11  | 1.95                     | 0.49              |
| 1:B:2468:VAL:HG11 | 1:B:2521:THR:HG22 | 1.95                     | 0.49              |
| 1:D:166:SER:OG    | 1:D:167:LYS:N     | 2.45                     | 0.49              |
| 1:D:2169:THR:O    | 1:D:2173:VAL:HG23 | 2.13                     | 0.48              |
| 1:A:300:VAL:CG2   | 1:A:419:ILE:HD12  | 2.43                     | 0.48              |
| 1:A:678:MET:HB2   | 1:A:803:LEU:HD11  | 1.95                     | 0.48              |
| 1:B:877:HIS:O     | 1:B:880:ARG:NH1   | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:300:VAL:CG2   | 1:C:419:ILE:HD12  | 2.43                     | 0.48              |
| 1:C:2726:HIS:CD2  | 1:C:2797:MET:HE3  | 2.47                     | 0.48              |
| 1:B:1105:PHE:CD2  | 1:B:1115:VAL:HG11 | 2.47                     | 0.48              |
| 1:B:3040:ASP:O    | 1:B:3044:VAL:HG22 | 2.14                     | 0.48              |
| 1:D:606:ARG:O     | 1:D:608:HIS:ND1   | 2.44                     | 0.48              |
| 1:D:3040:ASP:O    | 1:D:3044:VAL:HG22 | 2.14                     | 0.48              |
| 2:F:38:SER:O      | 2:F:42:ARG:NE     | 2.37                     | 0.48              |
| 1:A:569:SER:O     | 1:A:609:LYS:NZ    | 2.40                     | 0.48              |
| 1:A:1638:ARG:NH2  | 1:A:1639:SER:OG   | 2.45                     | 0.48              |
| 1:B:804:LEU:HD12  | 1:B:1618:TRP:CZ3  | 2.49                     | 0.48              |
| 1:B:2431:LEU:O    | 1:B:2434:VAL:HG22 | 2.12                     | 0.48              |
| 1:C:1505:GLY:O    | 1:C:1506:LEU:HD23 | 2.14                     | 0.48              |
| 1:C:2780:THR:OG1  | 1:C:2846:ASN:ND2  | 2.47                     | 0.48              |
| 1:C:3040:ASP:O    | 1:C:3044:VAL:HG22 | 2.14                     | 0.48              |
| 1:C:3404:TYR:O    | 1:C:3408:SER:OG   | 2.21                     | 0.48              |
| 1:D:2797:MET:HE1  | 1:D:2894:PHE:CD1  | 2.46                     | 0.48              |
| 1:B:1505:GLY:O    | 1:B:1506:LEU:HD23 | 2.14                     | 0.48              |
| 1:B:2780:THR:OG1  | 1:B:2846:ASN:ND2  | 2.47                     | 0.48              |
| 1:C:2468:VAL:HG11 | 1:C:2521:THR:HG22 | 1.95                     | 0.48              |
| 1:C:3727:GLN:O    | 1:C:3731:HIS:ND1  | 2.46                     | 0.48              |
| 1:C:3920:THR:O    | 1:C:3924:GLN:N    | 2.46                     | 0.48              |
| 1:C:4501:ARG:NH2  | 1:C:4744:ASP:OD1  | 2.46                     | 0.48              |
| 1:D:678:MET:HB2   | 1:D:803:LEU:HD11  | 1.95                     | 0.48              |
| 1:D:3727:GLN:O    | 1:D:3731:HIS:ND1  | 2.46                     | 0.48              |
| 1:D:4501:ARG:NH2  | 1:D:4744:ASP:OD1  | 2.46                     | 0.48              |
| 1:A:186:VAL:O     | 1:B:2417:ARG:NH1  | 2.47                     | 0.48              |
| 1:B:2169:THR:O    | 1:B:2173:VAL:HG23 | 2.13                     | 0.48              |
| 1:B:3078:GLN:O    | 1:B:3082:THR:OG1  | 2.18                     | 0.48              |
| 1:B:3727:GLN:O    | 1:B:3731:HIS:ND1  | 2.46                     | 0.48              |
| 1:C:1726:PHE:CD2  | 1:C:1921:ILE:HD11 | 2.48                     | 0.48              |
| 1:C:3737:GLU:OE2  | 1:C:3737:GLU:N    | 2.45                     | 0.48              |
| 1:A:2357:SER:OG   | 1:A:2358:ARG:N    | 2.47                     | 0.48              |
| 1:B:841:LYS:HA    | 1:B:851:LEU:HD12  | 1.95                     | 0.48              |
| 1:C:1506:LEU:N    | 1:C:1524:ASN:OD1  | 2.41                     | 0.48              |
| 1:D:3920:THR:O    | 1:D:3924:GLN:N    | 2.46                     | 0.48              |
| 1:A:841:LYS:HA    | 1:A:851:LEU:HD12  | 1.95                     | 0.48              |
| 1:A:2468:VAL:HG11 | 1:A:2521:THR:HG22 | 1.95                     | 0.48              |
| 1:A:3040:ASP:O    | 1:A:3044:VAL:HG22 | 2.14                     | 0.48              |
| 1:A:3727:GLN:O    | 1:A:3731:HIS:ND1  | 2.46                     | 0.48              |
| 1:C:4044:LYS:NZ   | 1:C:4069:ALA:O    | 2.36                     | 0.48              |
| 1:A:1505:GLY:O    | 1:A:1506:LEU:HD23 | 2.14                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3737:GLU:OE2  | 1:D:3737:GLU:N    | 2.46                     | 0.48              |
| 1:A:2417:ARG:NH1  | 1:D:186:VAL:O     | 2.47                     | 0.47              |
| 1:C:2215:ASP:O    | 1:C:2218:SER:OG   | 2.14                     | 0.47              |
| 1:C:2357:SER:OG   | 1:C:2358:ARG:N    | 2.47                     | 0.47              |
| 1:C:2797:MET:HE1  | 1:C:2894:PHE:CD1  | 2.46                     | 0.47              |
| 1:B:4044:LYS:NZ   | 1:B:4069:ALA:O    | 2.36                     | 0.47              |
| 1:D:804:LEU:HD12  | 1:D:1618:TRP:CZ3  | 2.48                     | 0.47              |
| 1:A:266:ALA:O     | 1:A:270:HIS:ND1   | 2.46                     | 0.47              |
| 1:A:886:ALA:HA    | 1:A:889:ILE:HG22  | 1.96                     | 0.47              |
| 1:A:3920:THR:O    | 1:A:3924:GLN:N    | 2.46                     | 0.47              |
| 1:B:4501:ARG:NH2  | 1:B:4744:ASP:OD1  | 2.46                     | 0.47              |
| 1:D:2357:SER:OG   | 1:D:2358:ARG:N    | 2.47                     | 0.47              |
| 1:A:2780:THR:OG1  | 1:A:2846:ASN:ND2  | 2.47                     | 0.47              |
| 1:B:235:ARG:NE    | 1:B:268:SER:O     | 2.42                     | 0.47              |
| 1:B:2357:SER:OG   | 1:B:2358:ARG:N    | 2.47                     | 0.47              |
| 1:D:235:ARG:NE    | 1:D:268:SER:O     | 2.42                     | 0.47              |
| 1:A:804:LEU:HD12  | 1:A:1618:TRP:CZ3  | 2.48                     | 0.47              |
| 1:D:1614:GLU:N    | 1:D:1619:LEU:O    | 2.47                     | 0.47              |
| 1:A:1614:GLU:N    | 1:A:1619:LEU:O    | 2.47                     | 0.47              |
| 1:D:266:ALA:O     | 1:D:270:HIS:ND1   | 2.46                     | 0.47              |
| 1:D:927:GLN:N     | 1:D:927:GLN:OE1   | 2.48                     | 0.47              |
| 1:D:1306:MET:HE3  | 1:D:1307:PRO:O    | 2.15                     | 0.47              |
| 1:D:2780:THR:OG1  | 1:D:2846:ASN:ND2  | 2.46                     | 0.47              |
| 1:A:4619:GLN:OE1  | 1:A:4631:ARG:NH1  | 2.46                     | 0.47              |
| 1:B:186:VAL:O     | 1:C:2417:ARG:NH1  | 2.47                     | 0.47              |
| 1:C:678:MET:HB2   | 1:C:803:LEU:HD11  | 1.95                     | 0.47              |
| 1:C:886:ALA:HA    | 1:C:889:ILE:HG22  | 1.96                     | 0.47              |
| 1:D:2468:VAL:HG11 | 1:D:2521:THR:HG22 | 1.95                     | 0.47              |
| 1:B:4836:ASP:OD1  | 1:B:4837:GLU:N    | 2.48                     | 0.47              |
| 1:C:586:LEU:HD22  | 1:C:589:ILE:HD11  | 1.97                     | 0.47              |
| 1:C:1306:MET:HE3  | 1:C:1307:PRO:O    | 2.15                     | 0.47              |
| 1:D:1505:GLY:O    | 1:D:1506:LEU:HD23 | 2.14                     | 0.47              |
| 1:B:925:PRO:O     | 1:B:929:ARG:N     | 2.44                     | 0.47              |
| 1:C:804:LEU:HD12  | 1:C:1618:TRP:CZ3  | 2.49                     | 0.47              |
| 1:A:3934:LEU:O    | 1:A:3937:SER:OG   | 2.28                     | 0.47              |
| 1:C:1614:GLU:N    | 1:C:1619:LEU:O    | 2.47                     | 0.47              |
| 1:A:1306:MET:HE3  | 1:A:1307:PRO:O    | 2.15                     | 0.46              |
| 1:C:1909:LEU:HD22 | 1:C:2061:ILE:HD11 | 1.96                     | 0.46              |
| 1:B:886:ALA:HA    | 1:B:889:ILE:HG22  | 1.96                     | 0.46              |
| 1:B:2582:SER:HB2  | 1:B:2875:THR:HG22 | 1.97                     | 0.46              |
| 1:B:4794:LYS:NZ   | 1:B:4829:GLU:OE1  | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:186:VAL:O     | 1:D:2417:ARG:NH1  | 2.48                     | 0.46              |
| 1:C:2154:PHE:HB2  | 1:C:2161:MET:HE3  | 1.97                     | 0.46              |
| 1:D:886:ALA:HA    | 1:D:889:ILE:HG22  | 1.96                     | 0.46              |
| 1:A:1255:LEU:HD13 | 1:A:1451:HIS:ND1  | 2.31                     | 0.46              |
| 1:B:1255:LEU:HD13 | 1:B:1451:HIS:ND1  | 2.31                     | 0.46              |
| 1:D:3786:VAL:HG12 | 1:D:3790:GLN:CG   | 2.46                     | 0.46              |
| 1:A:2154:PHE:HB2  | 1:A:2161:MET:HE3  | 1.97                     | 0.46              |
| 1:B:307:SER:OG    | 1:B:308:LEU:N     | 2.49                     | 0.46              |
| 1:B:701:GLU:N     | 1:B:701:GLU:OE1   | 2.49                     | 0.46              |
| 1:C:4794:LYS:NZ   | 1:C:4829:GLU:OE1  | 2.48                     | 0.46              |
| 1:D:307:SER:OG    | 1:D:308:LEU:N     | 2.49                     | 0.46              |
| 1:D:586:LEU:HD22  | 1:D:589:ILE:HD11  | 1.97                     | 0.46              |
| 1:D:939:THR:O     | 1:D:943:LEU:HD13  | 2.16                     | 0.46              |
| 1:A:701:GLU:N     | 1:A:701:GLU:OE1   | 2.49                     | 0.46              |
| 1:A:2582:SER:HB2  | 1:A:2875:THR:HG22 | 1.97                     | 0.46              |
| 1:B:2275:SER:OG   | 1:B:2383:MET:HE3  | 2.16                     | 0.46              |
| 1:B:3786:VAL:HG12 | 1:B:3790:GLN:CG   | 2.46                     | 0.46              |
| 1:C:307:SER:OG    | 1:C:308:LEU:N     | 2.49                     | 0.46              |
| 1:C:701:GLU:OE1   | 1:C:701:GLU:N     | 2.49                     | 0.46              |
| 1:C:939:THR:O     | 1:C:943:LEU:HD13  | 2.16                     | 0.46              |
| 1:D:1909:LEU:HD22 | 1:D:2061:ILE:HD11 | 1.96                     | 0.46              |
| 1:A:4794:LYS:NZ   | 1:A:4829:GLU:OE1  | 2.49                     | 0.46              |
| 1:B:927:GLN:OE1   | 1:B:927:GLN:N     | 2.48                     | 0.46              |
| 1:B:1909:LEU:HD22 | 1:B:2061:ILE:HD11 | 1.96                     | 0.46              |
| 1:C:2275:SER:OG   | 1:C:2383:MET:HE3  | 2.16                     | 0.46              |
| 1:D:73:LEU:O      | 1:D:118:ALA:N     | 2.49                     | 0.46              |
| 1:A:3786:VAL:HG12 | 1:A:3790:GLN:CG   | 2.46                     | 0.46              |
| 1:A:4836:ASP:OD1  | 1:A:4837:GLU:N    | 2.48                     | 0.46              |
| 1:D:3924:GLN:O    | 1:D:4934:GLY:N    | 2.46                     | 0.46              |
| 1:A:1157:GLN:NE2  | 1:A:1160:ASP:OD2  | 2.49                     | 0.46              |
| 1:A:2275:SER:OG   | 1:A:2383:MET:HE3  | 2.16                     | 0.46              |
| 1:A:3888:TYR:O    | 1:A:3892:SER:N    | 2.49                     | 0.46              |
| 1:A:4136:GLU:OE2  | 1:A:4146:ARG:NH2  | 2.48                     | 0.46              |
| 1:B:560:SER:OG    | 1:B:561:ARG:NH2   | 2.49                     | 0.46              |
| 1:B:1306:MET:HE3  | 1:B:1307:PRO:O    | 2.15                     | 0.46              |
| 1:B:1614:GLU:N    | 1:B:1619:LEU:O    | 2.47                     | 0.46              |
| 1:C:1255:LEU:HD13 | 1:C:1451:HIS:ND1  | 2.31                     | 0.46              |
| 1:D:701:GLU:N     | 1:D:701:GLU:OE1   | 2.49                     | 0.46              |
| 1:B:586:LEU:HD22  | 1:B:589:ILE:HD11  | 1.97                     | 0.46              |
| 1:C:927:GLN:OE1   | 1:C:927:GLN:N     | 2.48                     | 0.46              |
| 1:C:3786:VAL:HG12 | 1:C:3790:GLN:CG   | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:F:25:HIS:O      | 2:F:40:ARG:NE     | 2.38                     | 0.46              |
| 1:A:939:THR:O     | 1:A:943:LEU:HD13  | 2.16                     | 0.45              |
| 1:B:450:GLU:O     | 1:B:453:SER:OG    | 2.32                     | 0.45              |
| 1:B:3920:THR:O    | 1:B:3924:GLN:N    | 2.46                     | 0.45              |
| 1:B:4136:GLU:OE2  | 1:B:4146:ARG:NH2  | 2.48                     | 0.45              |
| 1:D:4176:VAL:HG13 | 1:D:4879:VAL:HG12 | 1.98                     | 0.45              |
| 1:D:4836:ASP:OD1  | 1:D:4837:GLU:N    | 2.48                     | 0.45              |
| 1:A:307:SER:OG    | 1:A:308:LEU:N     | 2.49                     | 0.45              |
| 1:A:494:MET:CE    | 1:A:499:LEU:HD21  | 2.46                     | 0.45              |
| 1:A:1909:LEU:HD22 | 1:A:2061:ILE:HD11 | 1.96                     | 0.45              |
| 1:B:266:ALA:O     | 1:B:270:HIS:ND1   | 2.46                     | 0.45              |
| 1:C:494:MET:CE    | 1:C:499:LEU:HD21  | 2.46                     | 0.45              |
| 1:C:1157:GLN:NE2  | 1:C:1160:ASP:OD2  | 2.49                     | 0.45              |
| 1:C:4176:VAL:HG13 | 1:C:4879:VAL:HG12 | 1.98                     | 0.45              |
| 1:D:494:MET:CE    | 1:D:499:LEU:HD21  | 2.46                     | 0.45              |
| 1:D:898:ILE:HD11  | 1:D:918:LEU:HD22  | 1.99                     | 0.45              |
| 1:D:1157:GLN:NE2  | 1:D:1160:ASP:OD2  | 2.49                     | 0.45              |
| 1:D:1255:LEU:HD13 | 1:D:1451:HIS:ND1  | 2.31                     | 0.45              |
| 1:A:195:SER:OG    | 1:A:204:ASP:OD2   | 2.34                     | 0.45              |
| 1:A:898:ILE:HD11  | 1:A:918:LEU:HD22  | 1.99                     | 0.45              |
| 1:C:886:ALA:HB1   | 1:C:921:PHE:CE1   | 2.52                     | 0.45              |
| 1:D:560:SER:OG    | 1:D:561:ARG:NH2   | 2.49                     | 0.45              |
| 1:A:73:LEU:O      | 1:A:118:ALA:N     | 2.49                     | 0.45              |
| 1:A:450:GLU:O     | 1:A:453:SER:OG    | 2.32                     | 0.45              |
| 1:A:4176:VAL:HG13 | 1:A:4879:VAL:HG12 | 1.98                     | 0.45              |
| 1:B:939:THR:O     | 1:B:943:LEU:HD13  | 2.16                     | 0.45              |
| 1:B:2154:PHE:HB2  | 1:B:2161:MET:HE3  | 1.97                     | 0.45              |
| 1:C:73:LEU:O      | 1:C:118:ALA:N     | 2.49                     | 0.45              |
| 1:C:560:SER:OG    | 1:C:561:ARG:NH2   | 2.49                     | 0.45              |
| 1:B:1157:GLN:NE2  | 1:B:1160:ASP:OD2  | 2.49                     | 0.45              |
| 1:C:2582:SER:HB2  | 1:C:2875:THR:HG22 | 1.97                     | 0.45              |
| 1:C:4836:ASP:OD1  | 1:C:4837:GLU:N    | 2.48                     | 0.45              |
| 1:A:560:SER:OG    | 1:A:561:ARG:NH2   | 2.49                     | 0.45              |
| 1:A:586:LEU:HD22  | 1:A:589:ILE:HD11  | 1.97                     | 0.45              |
| 1:A:927:GLN:OE1   | 1:A:927:GLN:N     | 2.48                     | 0.45              |
| 1:B:886:ALA:HB1   | 1:B:921:PHE:CE1   | 2.52                     | 0.45              |
| 1:B:898:ILE:HD11  | 1:B:918:LEU:HD22  | 1.99                     | 0.45              |
| 1:C:674:TYR:O     | 1:C:822:CYS:N     | 2.48                     | 0.45              |
| 1:C:3978:VAL:HA   | 1:C:3981:LEU:HD12 | 1.99                     | 0.45              |
| 1:B:10:GLU:OE2    | 1:B:10:GLU:N      | 2.50                     | 0.45              |
| 1:B:4176:VAL:HG13 | 1:B:4879:VAL:HG12 | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1262:PRO:O    | 1:C:1264:ASN:ND2  | 2.49                     | 0.45              |
| 1:C:1930:ASP:OD1  | 1:C:2027:ARG:NH2  | 2.49                     | 0.45              |
| 1:D:2154:PHE:HB2  | 1:D:2161:MET:HE3  | 1.97                     | 0.45              |
| 1:D:3940:TRP:O    | 1:D:3944:VAL:HG13 | 2.17                     | 0.45              |
| 1:C:898:ILE:HD11  | 1:C:918:LEU:HD22  | 1.99                     | 0.45              |
| 1:D:2275:SER:OG   | 1:D:2383:MET:HE3  | 2.16                     | 0.45              |
| 1:D:3934:LEU:O    | 1:D:3937:SER:OG   | 2.28                     | 0.45              |
| 1:A:3940:TRP:O    | 1:A:3944:VAL:HG13 | 2.17                     | 0.45              |
| 1:B:1105:PHE:CE2  | 1:B:1115:VAL:HG11 | 2.52                     | 0.45              |
| 1:C:3940:TRP:O    | 1:C:3944:VAL:HG13 | 2.17                     | 0.45              |
| 1:D:886:ALA:HB1   | 1:D:921:PHE:CE1   | 2.52                     | 0.45              |
| 1:D:4185:MET:O    | 1:D:4189:VAL:HG23 | 2.17                     | 0.45              |
| 1:D:4794:LYS:NZ   | 1:D:4829:GLU:OE1  | 2.48                     | 0.45              |
| 1:A:235:ARG:NE    | 1:A:268:SER:O     | 2.42                     | 0.44              |
| 1:A:1105:PHE:CE2  | 1:A:1115:VAL:HG11 | 2.52                     | 0.44              |
| 1:A:4185:MET:O    | 1:A:4189:VAL:HG23 | 2.17                     | 0.44              |
| 1:B:1262:PRO:O    | 1:B:1264:ASN:ND2  | 2.49                     | 0.44              |
| 1:B:2129:LEU:HD12 | 1:B:2130:SER:N    | 2.32                     | 0.44              |
| 1:C:1105:PHE:CE2  | 1:C:1115:VAL:HG11 | 2.53                     | 0.44              |
| 1:C:4018:MET:O    | 1:C:4026:THR:OG1  | 2.29                     | 0.44              |
| 1:D:1930:ASP:OD1  | 1:D:2027:ARG:NH2  | 2.49                     | 0.44              |
| 1:D:2582:SER:HB2  | 1:D:2875:THR:HG22 | 1.97                     | 0.44              |
| 1:B:73:LEU:O      | 1:B:118:ALA:N     | 2.49                     | 0.44              |
| 1:B:494:MET:CE    | 1:B:499:LEU:HD21  | 2.46                     | 0.44              |
| 1:C:2183:SER:OG   | 1:C:2184:LYS:N    | 2.50                     | 0.44              |
| 1:C:3934:LEU:O    | 1:C:3937:SER:OG   | 2.28                     | 0.44              |
| 1:D:1105:PHE:CE2  | 1:D:1115:VAL:HG11 | 2.52                     | 0.44              |
| 1:D:3404:TYR:O    | 1:D:3408:SER:OG   | 2.21                     | 0.44              |
| 1:D:3888:TYR:O    | 1:D:3892:SER:N    | 2.49                     | 0.44              |
| 1:A:1262:PRO:O    | 1:A:1264:ASN:ND2  | 2.49                     | 0.44              |
| 1:B:3888:TYR:O    | 1:B:3892:SER:N    | 2.49                     | 0.44              |
| 1:B:3940:TRP:O    | 1:B:3944:VAL:HG13 | 2.17                     | 0.44              |
| 1:C:2129:LEU:HD12 | 1:C:2130:SER:N    | 2.32                     | 0.44              |
| 1:C:3924:GLN:O    | 1:C:4934:GLY:N    | 2.46                     | 0.44              |
| 1:D:674:TYR:O     | 1:D:822:CYS:N     | 2.48                     | 0.44              |
| 1:D:2290:ASN:OD1  | 1:D:2290:ASN:N    | 2.51                     | 0.44              |
| 1:D:4619:GLN:OE1  | 1:D:4631:ARG:NH1  | 2.46                     | 0.44              |
| 1:A:886:ALA:HB1   | 1:A:921:PHE:CE1   | 2.52                     | 0.44              |
| 1:A:2129:LEU:HD12 | 1:A:2130:SER:N    | 2.32                     | 0.44              |
| 1:C:10:GLU:N      | 1:C:10:GLU:OE2    | 2.50                     | 0.44              |
| 1:C:4069:ALA:HB1  | 1:C:4077:LEU:HD13 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:2129:LEU:HD12 | 1:D:2130:SER:N    | 2.32                     | 0.44              |
| 2:E:25:HIS:O      | 2:E:40:ARG:NE     | 2.38                     | 0.44              |
| 1:A:3924:GLN:O    | 1:A:4934:GLY:N    | 2.46                     | 0.44              |
| 1:B:1930:ASP:OD1  | 1:B:2027:ARG:NH2  | 2.49                     | 0.44              |
| 1:C:2584:MET:SD   | 1:C:2584:MET:N    | 2.91                     | 0.44              |
| 1:C:3888:TYR:O    | 1:C:3892:SER:N    | 2.49                     | 0.44              |
| 1:D:3978:VAL:HA   | 1:D:3981:LEU:HD12 | 1.99                     | 0.44              |
| 2:H:24:VAL:N      | 2:H:46:PHE:O      | 2.50                     | 0.44              |
| 1:A:10:GLU:N      | 1:A:10:GLU:OE2    | 2.50                     | 0.44              |
| 1:A:2592:VAL:HG22 | 1:A:2641:ARG:NH2  | 2.33                     | 0.44              |
| 1:A:4069:ALA:HB1  | 1:A:4077:LEU:HD13 | 1.99                     | 0.44              |
| 1:B:2584:MET:SD   | 1:B:2584:MET:N    | 2.91                     | 0.44              |
| 1:B:4069:ALA:HB1  | 1:B:4077:LEU:HD13 | 1.99                     | 0.44              |
| 1:C:195:SER:OG    | 1:C:204:ASP:OD2   | 2.34                     | 0.44              |
| 1:C:4185:MET:O    | 1:C:4189:VAL:HG23 | 2.17                     | 0.44              |
| 1:D:2183:SER:OG   | 1:D:2184:LYS:N    | 2.50                     | 0.44              |
| 1:B:1846:LEU:HB2  | 1:B:1847:ILE:HG23 | 2.00                     | 0.44              |
| 1:D:10:GLU:N      | 1:D:10:GLU:OE2    | 2.50                     | 0.44              |
| 1:B:271:ALA:HA    | 1:B:274:LEU:HD12  | 2.00                     | 0.44              |
| 1:B:2592:VAL:HG22 | 1:B:2641:ARG:NH2  | 2.33                     | 0.44              |
| 1:B:3978:VAL:HA   | 1:B:3981:LEU:HD12 | 1.99                     | 0.44              |
| 1:D:4069:ALA:HB1  | 1:D:4077:LEU:HD13 | 1.99                     | 0.44              |
| 1:A:1048:ASP:OD2  | 1:A:1049:SER:N    | 2.51                     | 0.44              |
| 1:A:224:ALA:HB2   | 1:A:229:ILE:HD12  | 2.00                     | 0.43              |
| 1:A:878:LEU:O     | 1:A:881:ILE:N     | 2.50                     | 0.43              |
| 1:B:2183:SER:OG   | 1:B:2184:LYS:N    | 2.50                     | 0.43              |
| 1:C:271:ALA:HA    | 1:C:274:LEU:HD12  | 2.00                     | 0.43              |
| 1:C:1846:LEU:HB2  | 1:C:1847:ILE:HG23 | 2.00                     | 0.43              |
| 1:C:4789:ARG:O    | 1:C:4804:LYS:NZ   | 2.50                     | 0.43              |
| 1:D:271:ALA:HA    | 1:D:274:LEU:HD12  | 2.00                     | 0.43              |
| 1:D:1048:ASP:OD2  | 1:D:1049:SER:N    | 2.51                     | 0.43              |
| 1:D:3078:GLN:O    | 1:D:3082:THR:OG1  | 2.18                     | 0.43              |
| 1:A:3978:VAL:HA   | 1:A:3981:LEU:HD12 | 1.99                     | 0.43              |
| 1:B:218:SER:OG    | 1:B:219:SER:N     | 2.51                     | 0.43              |
| 1:B:2290:ASN:OD1  | 1:B:2290:ASN:N    | 2.51                     | 0.43              |
| 1:D:308:LEU:HD22  | 1:D:393:MET:HG3   | 2.00                     | 0.43              |
| 1:D:2584:MET:SD   | 1:D:2584:MET:N    | 2.91                     | 0.43              |
| 1:D:2592:VAL:HG22 | 1:D:2641:ARG:NH2  | 2.33                     | 0.43              |
| 1:A:41:GLY:O      | 1:A:45:ARG:NH1    | 2.52                     | 0.43              |
| 1:A:271:ALA:HA    | 1:A:274:LEU:HD12  | 2.00                     | 0.43              |
| 1:D:1262:PRO:O    | 1:D:1264:ASN:ND2  | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:218:SER:OG    | 1:A:219:SER:N     | 2.51                     | 0.43              |
| 1:A:2996:SER:OG   | 1:A:3070:THR:HG21 | 2.19                     | 0.43              |
| 1:B:541:ILE:HG23  | 1:B:547:ASN:O     | 2.19                     | 0.43              |
| 1:C:2154:PHE:CB   | 1:C:2161:MET:HE3  | 2.48                     | 0.43              |
| 1:C:2275:SER:HB2  | 1:C:2383:MET:HE3  | 2.01                     | 0.43              |
| 1:C:2315:ASN:O    | 1:C:2319:VAL:HG23 | 2.19                     | 0.43              |
| 1:D:2154:PHE:CB   | 1:D:2161:MET:HE3  | 2.48                     | 0.43              |
| 1:B:41:GLY:O      | 1:B:45:ARG:NH1    | 2.52                     | 0.43              |
| 1:B:2154:PHE:CB   | 1:B:2161:MET:HE3  | 2.48                     | 0.43              |
| 1:B:4185:MET:O    | 1:B:4189:VAL:HG23 | 2.17                     | 0.43              |
| 1:C:2290:ASN:OD1  | 1:C:2290:ASN:N    | 2.51                     | 0.43              |
| 1:D:2122:LEU:CD2  | 1:D:2164:LEU:HD13 | 2.49                     | 0.43              |
| 1:A:1930:ASP:OD1  | 1:A:2027:ARG:NH2  | 2.49                     | 0.43              |
| 1:A:2154:PHE:CB   | 1:A:2161:MET:HE3  | 2.48                     | 0.43              |
| 1:A:4099:VAL:HG22 | 1:A:4132:LEU:CD1  | 2.47                     | 0.43              |
| 1:B:1048:ASP:OD2  | 1:B:1049:SER:N    | 2.51                     | 0.43              |
| 1:B:2122:LEU:CD2  | 1:B:2164:LEU:HD13 | 2.49                     | 0.43              |
| 1:B:2275:SER:HB2  | 1:B:2383:MET:HE3  | 2.01                     | 0.43              |
| 1:B:3839:PHE:HB3  | 1:B:3918:THR:HG21 | 2.00                     | 0.43              |
| 1:B:4701:ASP:OD1  | 1:B:4703:LYS:N    | 2.52                     | 0.43              |
| 1:C:2122:LEU:CD2  | 1:C:2164:LEU:HD13 | 2.49                     | 0.43              |
| 1:C:3056:LEU:O    | 1:C:3060:LEU:N    | 2.52                     | 0.43              |
| 1:C:4136:GLU:OE2  | 1:C:4146:ARG:NH2  | 2.48                     | 0.43              |
| 1:D:218:SER:OG    | 1:D:219:SER:N     | 2.51                     | 0.43              |
| 1:D:224:ALA:HB2   | 1:D:229:ILE:HD12  | 2.00                     | 0.43              |
| 2:E:12:GLY:O      | 2:E:13:ARG:NE     | 2.52                     | 0.43              |
| 2:H:12:GLY:O      | 2:H:13:ARG:NE     | 2.52                     | 0.43              |
| 1:A:290:ARG:NH2   | 1:A:352:SER:OG    | 2.52                     | 0.43              |
| 1:A:541:ILE:HG23  | 1:A:547:ASN:O     | 2.19                     | 0.43              |
| 1:A:991:SER:O     | 1:A:994:ALA:N     | 2.52                     | 0.43              |
| 1:A:1846:LEU:HB2  | 1:A:1847:ILE:HG23 | 2.00                     | 0.43              |
| 1:A:2183:SER:OG   | 1:A:2184:LYS:N    | 2.50                     | 0.43              |
| 1:A:4789:ARG:O    | 1:A:4804:LYS:NZ   | 2.50                     | 0.43              |
| 1:B:308:LEU:HD22  | 1:B:393:MET:HG3   | 2.01                     | 0.43              |
| 1:B:991:SER:O     | 1:B:994:ALA:N     | 2.52                     | 0.43              |
| 1:D:1758:LEU:HD22 | 1:D:2116:ILE:HD11 | 2.01                     | 0.43              |
| 1:D:2275:SER:HB2  | 1:D:2383:MET:HE3  | 2.01                     | 0.43              |
| 1:D:3694:MET:O    | 1:D:3697:SER:OG   | 2.36                     | 0.43              |
| 1:A:3056:LEU:O    | 1:A:3060:LEU:N    | 2.52                     | 0.43              |
| 1:C:41:GLY:O      | 1:C:45:ARG:NH1    | 2.51                     | 0.43              |
| 1:C:218:SER:OG    | 1:C:219:SER:N     | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:411:GLU:OE1   | 1:C:411:GLU:N     | 2.49                     | 0.43              |
| 1:C:1048:ASP:OD2  | 1:C:1049:SER:N    | 2.51                     | 0.43              |
| 1:C:2592:VAL:HG22 | 1:C:2641:ARG:NH2  | 2.33                     | 0.43              |
| 1:D:2461:PRO:O    | 1:D:2518:TYR:OH   | 2.28                     | 0.43              |
| 2:F:24:VAL:N      | 2:F:46:PHE:O      | 2.50                     | 0.43              |
| 1:B:2986:SER:OG   | 1:B:2987:ARG:N    | 2.52                     | 0.43              |
| 1:D:4701:ASP:OD1  | 1:D:4703:LYS:N    | 2.52                     | 0.43              |
| 2:F:12:GLY:O      | 2:F:13:ARG:NE     | 2.52                     | 0.43              |
| 1:A:2290:ASN:OD1  | 1:A:2290:ASN:N    | 2.51                     | 0.43              |
| 1:A:2584:MET:SD   | 1:A:2584:MET:N    | 2.91                     | 0.43              |
| 1:B:224:ALA:HB2   | 1:B:229:ILE:HD12  | 2.00                     | 0.43              |
| 1:B:2720:ILE:O    | 1:B:2771:ARG:NE   | 2.44                     | 0.43              |
| 1:B:2996:SER:OG   | 1:B:3070:THR:HG21 | 2.19                     | 0.43              |
| 1:C:541:ILE:HG23  | 1:C:547:ASN:O     | 2.19                     | 0.43              |
| 1:C:742:SER:O     | 1:C:776:GLN:N     | 2.51                     | 0.43              |
| 1:C:991:SER:O     | 1:C:994:ALA:N     | 2.52                     | 0.43              |
| 1:C:3839:PHE:HB3  | 1:C:3918:THR:HG21 | 2.00                     | 0.43              |
| 1:D:1846:LEU:HB2  | 1:D:1847:ILE:HG23 | 2.00                     | 0.43              |
| 1:D:4136:GLU:OE2  | 1:D:4146:ARG:NH2  | 2.48                     | 0.43              |
| 2:G:12:GLY:O      | 2:G:13:ARG:NE     | 2.52                     | 0.43              |
| 1:A:658:ASN:N     | 1:A:833:LYS:O     | 2.53                     | 0.42              |
| 1:A:2122:LEU:CD2  | 1:A:2164:LEU:HD13 | 2.49                     | 0.42              |
| 1:A:2315:ASN:O    | 1:A:2319:VAL:HG23 | 2.19                     | 0.42              |
| 1:B:290:ARG:NH2   | 1:B:352:SER:OG    | 2.52                     | 0.42              |
| 1:B:2315:ASN:O    | 1:B:2319:VAL:HG23 | 2.19                     | 0.42              |
| 1:C:2112:VAL:O    | 1:C:2116:ILE:HD12 | 2.19                     | 0.42              |
| 1:D:991:SER:O     | 1:D:994:ALA:N     | 2.52                     | 0.42              |
| 1:A:4701:ASP:OD1  | 1:A:4703:LYS:N    | 2.52                     | 0.42              |
| 1:A:4778:TYR:O    | 1:A:4782:VAL:HG23 | 2.19                     | 0.42              |
| 1:B:2112:VAL:O    | 1:B:2116:ILE:HD12 | 2.19                     | 0.42              |
| 1:B:2210:GLN:NE2  | 1:B:2244:ALA:O    | 2.52                     | 0.42              |
| 1:C:224:ALA:HB2   | 1:C:229:ILE:HD12  | 2.00                     | 0.42              |
| 1:C:290:ARG:NH2   | 1:C:352:SER:OG    | 2.52                     | 0.42              |
| 1:C:1523:ALA:O    | 1:C:1526:LYS:NZ   | 2.52                     | 0.42              |
| 1:D:450:GLU:O     | 1:D:453:SER:OG    | 2.33                     | 0.42              |
| 1:D:884:ARG:NH2   | 1:D:959:GLU:OE1   | 2.52                     | 0.42              |
| 1:D:1292:SER:H    | 1:D:1553:VAL:HG22 | 1.84                     | 0.42              |
| 1:D:2996:SER:OG   | 1:D:3070:THR:HG21 | 2.19                     | 0.42              |
| 1:A:2275:SER:HB2  | 1:A:2383:MET:HE3  | 2.01                     | 0.42              |
| 1:A:3661:ASP:OD2  | 1:A:3664:HIS:N    | 2.50                     | 0.42              |
| 1:B:3914:GLN:O    | 1:B:3918:THR:HG23 | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:4701:ASP:OD1  | 1:C:4703:LYS:N    | 2.52                     | 0.42              |
| 1:D:41:GLY:O      | 1:D:45:ARG:NH1    | 2.52                     | 0.42              |
| 2:F:37:ASP:OD1    | 2:F:38:SER:N      | 2.53                     | 0.42              |
| 1:A:1758:LEU:HD22 | 1:A:2116:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:2210:GLN:NE2  | 1:A:2244:ALA:O    | 2.52                     | 0.42              |
| 1:C:1758:LEU:HD22 | 1:C:2116:ILE:HD11 | 2.01                     | 0.42              |
| 1:C:2210:GLN:NE2  | 1:C:2244:ALA:O    | 2.52                     | 0.42              |
| 1:A:308:LEU:HD22  | 1:A:393:MET:HG3   | 2.01                     | 0.42              |
| 1:B:2633:SER:OG   | 1:B:2634:GLU:N    | 2.53                     | 0.42              |
| 1:C:2275:SER:CB   | 1:C:2383:MET:HE3  | 2.49                     | 0.42              |
| 1:C:2986:SER:OG   | 1:C:2987:ARG:N    | 2.52                     | 0.42              |
| 1:C:2996:SER:OG   | 1:C:3070:THR:HG21 | 2.19                     | 0.42              |
| 1:C:4778:TYR:O    | 1:C:4782:VAL:HG23 | 2.19                     | 0.42              |
| 1:D:411:GLU:OE1   | 1:D:411:GLU:N     | 2.49                     | 0.42              |
| 2:G:24:VAL:N      | 2:G:46:PHE:O      | 2.50                     | 0.42              |
| 1:A:1090:ALA:HB3  | 1:A:1202:ILE:HD11 | 2.02                     | 0.42              |
| 1:A:2986:SER:OG   | 1:A:2987:ARG:N    | 2.52                     | 0.42              |
| 1:A:3694:MET:O    | 1:A:3697:SER:OG   | 2.36                     | 0.42              |
| 1:A:3914:GLN:O    | 1:A:3918:THR:HG23 | 2.20                     | 0.42              |
| 1:B:4778:TYR:O    | 1:B:4782:VAL:HG23 | 2.19                     | 0.42              |
| 1:B:4789:ARG:O    | 1:B:4804:LYS:NZ   | 2.50                     | 0.42              |
| 1:C:3914:GLN:O    | 1:C:3918:THR:HG23 | 2.19                     | 0.42              |
| 1:C:4099:VAL:HG22 | 1:C:4132:LEU:CD1  | 2.47                     | 0.42              |
| 1:C:4576:ILE:HG22 | 1:C:4580:ILE:HD12 | 2.02                     | 0.42              |
| 1:D:541:ILE:HG23  | 1:D:547:ASN:O     | 2.19                     | 0.42              |
| 1:D:658:ASN:N     | 1:D:833:LYS:O     | 2.53                     | 0.42              |
| 1:A:2512:ALA:O    | 1:A:2516:ASN:ND2  | 2.53                     | 0.42              |
| 1:A:2594:ASP:OD2  | 1:A:2600:GLU:N    | 2.53                     | 0.42              |
| 1:A:3237:VAL:O    | 1:A:3242:CYS:N    | 2.51                     | 0.42              |
| 1:A:3839:PHE:HB3  | 1:A:3918:THR:HG21 | 2.00                     | 0.42              |
| 1:B:2275:SER:CB   | 1:B:2383:MET:HE3  | 2.49                     | 0.42              |
| 1:C:1292:SER:H    | 1:C:1553:VAL:HG22 | 1.84                     | 0.42              |
| 1:C:3995:GLY:C    | 1:C:4108:MET:HE1  | 2.45                     | 0.42              |
| 1:D:290:ARG:NH2   | 1:D:352:SER:OG    | 2.52                     | 0.42              |
| 1:D:3056:LEU:O    | 1:D:3060:LEU:N    | 2.52                     | 0.42              |
| 1:D:4778:TYR:O    | 1:D:4782:VAL:HG23 | 2.19                     | 0.42              |
| 1:B:195:SER:OG    | 1:B:204:ASP:OD2   | 2.34                     | 0.42              |
| 1:B:742:SER:O     | 1:B:776:GLN:N     | 2.51                     | 0.42              |
| 1:D:742:SER:O     | 1:D:776:GLN:N     | 2.51                     | 0.42              |
| 1:D:2112:VAL:O    | 1:D:2116:ILE:HD12 | 2.19                     | 0.42              |
| 1:D:2594:ASP:OD2  | 1:D:2600:GLU:N    | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3839:PHE:HB3  | 1:D:3918:THR:HG21 | 2.00                     | 0.42              |
| 1:A:541:ILE:HG22  | 1:A:577:CYS:SG    | 2.60                     | 0.42              |
| 1:B:658:ASN:N     | 1:B:833:LYS:O     | 2.53                     | 0.42              |
| 1:B:892:LEU:HD13  | 1:B:1056:THR:CG2  | 2.50                     | 0.42              |
| 1:B:4099:VAL:HG22 | 1:B:4132:LEU:CD1  | 2.47                     | 0.42              |
| 1:C:308:LEU:HD22  | 1:C:393:MET:HG3   | 2.01                     | 0.42              |
| 1:C:1090:ALA:HB3  | 1:C:1202:ILE:HD11 | 2.02                     | 0.42              |
| 1:C:2633:SER:OG   | 1:C:2634:GLU:N    | 2.53                     | 0.42              |
| 1:D:2275:SER:CB   | 1:D:2383:MET:HE3  | 2.49                     | 0.42              |
| 1:D:2315:ASN:O    | 1:D:2319:VAL:HG23 | 2.19                     | 0.42              |
| 1:D:3914:GLN:O    | 1:D:3918:THR:HG23 | 2.20                     | 0.42              |
| 2:E:37:ASP:OD1    | 2:E:38:SER:N      | 2.53                     | 0.42              |
| 1:A:1433:PHE:O    | 1:A:1435:GLY:N    | 2.53                     | 0.42              |
| 1:A:3876:TYR:O    | 1:A:3880:VAL:HG23 | 2.20                     | 0.42              |
| 1:A:3995:GLY:C    | 1:A:4108:MET:HE1  | 2.45                     | 0.42              |
| 1:B:3056:LEU:O    | 1:B:3060:LEU:N    | 2.52                     | 0.42              |
| 1:C:3876:TYR:O    | 1:C:3880:VAL:HG23 | 2.20                     | 0.42              |
| 1:D:3876:TYR:O    | 1:D:3880:VAL:HG23 | 2.20                     | 0.42              |
| 2:G:37:ASP:OD1    | 2:G:38:SER:N      | 2.53                     | 0.42              |
| 2:H:11:ASP:OD2    | 2:H:14:THR:OG1    | 2.28                     | 0.42              |
| 1:A:4576:ILE:HG22 | 1:A:4580:ILE:HD12 | 2.01                     | 0.41              |
| 1:B:550:GLN:O     | 1:B:554:SER:N     | 2.53                     | 0.41              |
| 1:B:674:TYR:O     | 1:B:822:CYS:N     | 2.48                     | 0.41              |
| 1:B:1090:ALA:HB3  | 1:B:1202:ILE:HD11 | 2.02                     | 0.41              |
| 1:C:1433:PHE:O    | 1:C:1435:GLY:N    | 2.53                     | 0.41              |
| 1:D:2210:GLN:NE2  | 1:D:2244:ALA:O    | 2.52                     | 0.41              |
| 1:D:3995:GLY:C    | 1:D:4108:MET:HE1  | 2.45                     | 0.41              |
| 1:A:2720:ILE:O    | 1:A:2771:ARG:NE   | 2.44                     | 0.41              |
| 1:B:195:SER:OG    | 1:B:202:HIS:O     | 2.38                     | 0.41              |
| 1:B:3995:GLY:C    | 1:B:4108:MET:HE1  | 2.45                     | 0.41              |
| 1:C:4895:ASP:OD1  | 1:C:4895:ASP:N    | 2.53                     | 0.41              |
| 1:D:892:LEU:HD13  | 1:D:1056:THR:CG2  | 2.50                     | 0.41              |
| 1:D:1433:PHE:O    | 1:D:1435:GLY:N    | 2.53                     | 0.41              |
| 1:D:2633:SER:OG   | 1:D:2634:GLU:N    | 2.53                     | 0.41              |
| 1:D:2986:SER:OG   | 1:D:2987:ARG:N    | 2.52                     | 0.41              |
| 1:D:3630:THR:OG1  | 1:D:3631:GLU:N    | 2.53                     | 0.41              |
| 1:A:2633:SER:OG   | 1:A:2634:GLU:N    | 2.53                     | 0.41              |
| 1:B:327:THR:O     | 1:B:327:THR:OG1   | 2.38                     | 0.41              |
| 1:B:878:LEU:O     | 1:B:881:ILE:N     | 2.50                     | 0.41              |
| 1:B:1433:PHE:O    | 1:B:1435:GLY:N    | 2.53                     | 0.41              |
| 1:B:1758:LEU:HD22 | 1:B:2116:ILE:HD11 | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:3237:VAL:O    | 1:B:3242:CYS:N    | 2.51                     | 0.41              |
| 1:B:3694:MET:O    | 1:B:3697:SER:OG   | 2.35                     | 0.41              |
| 1:C:195:SER:OG    | 1:C:202:HIS:O     | 2.38                     | 0.41              |
| 1:C:658:ASN:N     | 1:C:833:LYS:O     | 2.53                     | 0.41              |
| 1:D:4895:ASP:OD1  | 1:D:4895:ASP:N    | 2.53                     | 0.41              |
| 1:A:1292:SER:H    | 1:A:1553:VAL:HG22 | 1.84                     | 0.41              |
| 1:A:2112:VAL:O    | 1:A:2116:ILE:HD12 | 2.19                     | 0.41              |
| 1:A:2275:SER:CB   | 1:A:2383:MET:HE3  | 2.49                     | 0.41              |
| 1:B:541:ILE:HG22  | 1:B:577:CYS:SG    | 2.60                     | 0.41              |
| 1:B:1292:SER:H    | 1:B:1553:VAL:HG22 | 1.84                     | 0.41              |
| 1:B:2461:PRO:O    | 1:B:2518:TYR:OH   | 2.28                     | 0.41              |
| 1:B:4576:ILE:HG22 | 1:B:4580:ILE:HD12 | 2.02                     | 0.41              |
| 1:D:541:ILE:HG22  | 1:D:577:CYS:SG    | 2.60                     | 0.41              |
| 1:D:4789:ARG:O    | 1:D:4804:LYS:NZ   | 2.50                     | 0.41              |
| 2:H:37:ASP:OD1    | 2:H:38:SER:N      | 2.53                     | 0.41              |
| 1:A:674:TYR:O     | 1:A:822:CYS:N     | 2.48                     | 0.41              |
| 1:A:2405:MET:SD   | 1:A:2405:MET:N    | 2.89                     | 0.41              |
| 1:A:3078:GLN:O    | 1:A:3082:THR:OG1  | 2.18                     | 0.41              |
| 1:C:892:LEU:HD13  | 1:C:1056:THR:CG2  | 2.50                     | 0.41              |
| 1:C:2210:GLN:OE1  | 1:C:2249:ASN:ND2  | 2.54                     | 0.41              |
| 1:C:4701:ASP:OD1  | 1:C:4702:VAL:N    | 2.53                     | 0.41              |
| 1:D:195:SER:OG    | 1:D:202:HIS:O     | 2.38                     | 0.41              |
| 1:D:1090:ALA:HB3  | 1:D:1202:ILE:HD11 | 2.02                     | 0.41              |
| 1:A:2081:ARG:O    | 1:A:2085:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:2788:ILE:HD11 | 1:A:2895:LEU:HD11 | 2.03                     | 0.41              |
| 1:A:3907:LYS:O    | 1:A:3911:VAL:HG23 | 2.21                     | 0.41              |
| 1:B:332:ARG:N     | 1:B:362:TYR:O     | 2.54                     | 0.41              |
| 1:B:2512:ALA:O    | 1:B:2516:ASN:ND2  | 2.53                     | 0.41              |
| 1:C:332:ARG:N     | 1:C:362:TYR:O     | 2.54                     | 0.41              |
| 1:C:3843:GLN:HB2  | 1:C:3918:THR:HG22 | 2.03                     | 0.41              |
| 1:D:332:ARG:N     | 1:D:362:TYR:O     | 2.54                     | 0.41              |
| 1:D:2512:ALA:O    | 1:D:2516:ASN:ND2  | 2.53                     | 0.41              |
| 1:D:3843:GLN:HB2  | 1:D:3918:THR:HG22 | 2.03                     | 0.41              |
| 1:D:4701:ASP:OD1  | 1:D:4702:VAL:N    | 2.53                     | 0.41              |
| 1:A:332:ARG:N     | 1:A:362:TYR:O     | 2.54                     | 0.41              |
| 1:A:991:SER:OG    | 1:A:992:GLN:N     | 2.54                     | 0.41              |
| 1:A:4044:LYS:NZ   | 1:A:4069:ALA:O    | 2.36                     | 0.41              |
| 1:B:2081:ARG:O    | 1:B:2085:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:2512:ALA:O    | 1:C:2516:ASN:ND2  | 2.53                     | 0.41              |
| 1:D:991:SER:OG    | 1:D:992:GLN:N     | 2.54                     | 0.41              |
| 1:D:2210:GLN:OE1  | 1:D:2249:ASN:ND2  | 2.54                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:884:ARG:NH2   | 1:A:959:GLU:OE1   | 2.52                     | 0.41              |
| 1:A:2583:MET:HE3  | 1:A:2610:THR:HG21 | 2.03                     | 0.41              |
| 1:B:3907:LYS:O    | 1:B:3911:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:541:ILE:HG22  | 1:C:577:CYS:SG    | 2.60                     | 0.41              |
| 1:C:2788:ILE:HD11 | 1:C:2895:LEU:HD11 | 2.03                     | 0.41              |
| 1:A:1728:VAL:HG11 | 1:A:1925:VAL:HG11 | 2.03                     | 0.41              |
| 1:A:2210:GLN:OE1  | 1:A:2249:ASN:ND2  | 2.54                     | 0.41              |
| 1:A:2365:SER:O    | 1:A:2365:SER:OG   | 2.37                     | 0.41              |
| 1:A:4701:ASP:OD1  | 1:A:4702:VAL:N    | 2.53                     | 0.41              |
| 1:B:2210:GLN:OE1  | 1:B:2249:ASN:ND2  | 2.54                     | 0.41              |
| 1:B:2594:ASP:OD2  | 1:B:2600:GLU:N    | 2.53                     | 0.41              |
| 1:B:3876:TYR:O    | 1:B:3880:VAL:HG23 | 2.20                     | 0.41              |
| 1:C:1993:ASP:OD2  | 1:C:1994:GLN:N    | 2.54                     | 0.41              |
| 1:C:2594:ASP:OD2  | 1:C:2600:GLU:N    | 2.53                     | 0.41              |
| 1:C:3907:LYS:O    | 1:C:3911:VAL:HG23 | 2.21                     | 0.41              |
| 1:C:4095:PHE:O    | 1:C:4099:VAL:HG23 | 2.21                     | 0.41              |
| 1:D:45:ARG:NH1    | 1:D:128:MET:HE2   | 2.36                     | 0.41              |
| 1:D:2109:GLY:O    | 1:D:2112:VAL:HG22 | 2.21                     | 0.41              |
| 1:D:3907:LYS:O    | 1:D:3911:VAL:HG23 | 2.21                     | 0.41              |
| 1:D:4095:PHE:O    | 1:D:4099:VAL:HG23 | 2.21                     | 0.41              |
| 1:D:4576:ILE:HG22 | 1:D:4580:ILE:HD12 | 2.02                     | 0.41              |
| 1:B:237:LEU:N     | 1:B:404:ASN:O     | 2.52                     | 0.41              |
| 1:B:574:VAL:O     | 1:B:578:VAL:HG23  | 2.21                     | 0.41              |
| 1:B:2788:ILE:HD11 | 1:B:2895:LEU:HD11 | 2.03                     | 0.41              |
| 1:B:3404:TYR:O    | 1:B:3408:SER:OG   | 2.21                     | 0.41              |
| 1:B:4701:ASP:OD1  | 1:B:4702:VAL:N    | 2.53                     | 0.41              |
| 1:C:450:GLU:O     | 1:C:453:SER:OG    | 2.32                     | 0.41              |
| 1:D:655:MET:N     | 1:D:792:VAL:O     | 2.54                     | 0.41              |
| 1:A:1654:PHE:O    | 1:A:1658:THR:HG23 | 2.21                     | 0.40              |
| 1:A:3630:THR:OG1  | 1:A:3631:GLU:N    | 2.53                     | 0.40              |
| 1:B:991:SER:OG    | 1:B:992:GLN:N     | 2.54                     | 0.40              |
| 1:B:1728:VAL:HG11 | 1:B:1925:VAL:HG11 | 2.03                     | 0.40              |
| 1:B:3843:GLN:HB2  | 1:B:3918:THR:HG22 | 2.03                     | 0.40              |
| 1:C:1654:PHE:O    | 1:C:1658:THR:HG23 | 2.21                     | 0.40              |
| 1:C:4772:LEU:HD21 | 1:D:4752:LEU:CD1  | 2.51                     | 0.40              |
| 1:D:323:ASP:N     | 1:D:323:ASP:OD1   | 2.54                     | 0.40              |
| 1:A:574:VAL:O     | 1:A:578:VAL:HG23  | 2.22                     | 0.40              |
| 1:B:948:CYS:SG    | 1:B:1064:LEU:HD12 | 2.62                     | 0.40              |
| 1:B:2583:MET:HE3  | 1:B:2610:THR:HG21 | 2.03                     | 0.40              |
| 1:C:574:VAL:O     | 1:C:578:VAL:HG23  | 2.22                     | 0.40              |
| 1:C:884:ARG:NH2   | 1:C:959:GLU:OE1   | 2.51                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:991:SER:OG    | 1:C:992:GLN:N     | 2.54                     | 0.40              |
| 1:C:2109:GLY:O    | 1:C:2112:VAL:HG22 | 2.21                     | 0.40              |
| 1:C:3870:ILE:O    | 1:C:3874:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:23:GLN:O      | 1:A:213:SER:N     | 2.52                     | 0.40              |
| 1:A:45:ARG:NH1    | 1:A:128:MET:HE2   | 2.36                     | 0.40              |
| 1:A:4095:PHE:O    | 1:A:4099:VAL:HG23 | 2.21                     | 0.40              |
| 1:A:4752:LEU:CD1  | 1:D:4772:LEU:HD21 | 2.51                     | 0.40              |
| 1:B:1993:ASP:OD2  | 1:B:1994:GLN:N    | 2.54                     | 0.40              |
| 1:C:45:ARG:NH1    | 1:C:128:MET:HE2   | 2.36                     | 0.40              |
| 1:C:542:ARG:O     | 1:C:545:ARG:NH1   | 2.55                     | 0.40              |
| 1:C:2095:GLY:O    | 1:C:2099:ARG:NH1  | 2.55                     | 0.40              |
| 1:D:2268:LEU:HD21 | 1:D:2297:TYR:HB2  | 2.04                     | 0.40              |
| 1:D:3870:ILE:O    | 1:D:3874:VAL:HG23 | 2.22                     | 0.40              |
| 2:E:22:CYS:SG     | 2:E:50:ILE:HD11   | 2.62                     | 0.40              |
| 2:F:22:CYS:SG     | 2:F:50:ILE:HD11   | 2.62                     | 0.40              |
| 1:A:3843:GLN:HB2  | 1:A:3918:THR:HG22 | 2.03                     | 0.40              |
| 1:B:411:GLU:OE1   | 1:B:411:GLU:N     | 2.49                     | 0.40              |
| 1:B:1654:PHE:O    | 1:B:1658:THR:HG23 | 2.21                     | 0.40              |
| 1:B:2095:GLY:O    | 1:B:2099:ARG:NH1  | 2.55                     | 0.40              |
| 1:B:2109:GLY:O    | 1:B:2112:VAL:HG22 | 2.21                     | 0.40              |
| 1:B:4095:PHE:O    | 1:B:4099:VAL:HG23 | 2.21                     | 0.40              |
| 1:C:18:ASP:OD1    | 1:C:18:ASP:N      | 2.54                     | 0.40              |
| 1:D:23:GLN:N      | 1:D:213:SER:O     | 2.54                     | 0.40              |
| 1:D:308:LEU:HD21  | 1:D:370:LEU:HD12  | 2.04                     | 0.40              |
| 1:D:1654:PHE:O    | 1:D:1658:THR:HG23 | 2.21                     | 0.40              |
| 1:D:1993:ASP:OD2  | 1:D:1994:GLN:N    | 2.54                     | 0.40              |
| 1:D:2095:GLY:O    | 1:D:2099:ARG:NH1  | 2.55                     | 0.40              |
| 1:D:2788:ILE:HD11 | 1:D:2895:LEU:HD11 | 2.03                     | 0.40              |
| 2:E:24:VAL:N      | 2:E:46:PHE:O      | 2.50                     | 0.40              |
| 1:A:241:MET:HE1   | 1:A:389:ARG:HG3   | 2.03                     | 0.40              |
| 1:A:1993:ASP:OD2  | 1:A:1994:GLN:N    | 2.54                     | 0.40              |
| 1:B:3870:ILE:O    | 1:B:3874:VAL:HG23 | 2.21                     | 0.40              |
| 1:B:4018:MET:O    | 1:B:4026:THR:OG1  | 2.29                     | 0.40              |
| 1:C:308:LEU:HD21  | 1:C:370:LEU:HD12  | 2.03                     | 0.40              |
| 1:C:4777:VAL:HG13 | 1:C:4815:HIS:HB3  | 2.04                     | 0.40              |
| 1:D:195:SER:OG    | 1:D:204:ASP:OD2   | 2.34                     | 0.40              |
| 1:D:574:VAL:O     | 1:D:578:VAL:HG23  | 2.21                     | 0.40              |
| 1:D:1728:VAL:HG11 | 1:D:1925:VAL:HG11 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|------------|----------|-------------|-----|
| 1   | A     | 3849/4966 (78%)   | 3357 (87%)  | 482 (12%)  | 10 (0%)  | 36          | 72  |
| 1   | B     | 3849/4966 (78%)   | 3358 (87%)  | 481 (12%)  | 10 (0%)  | 36          | 72  |
| 1   | C     | 3849/4966 (78%)   | 3358 (87%)  | 481 (12%)  | 10 (0%)  | 36          | 72  |
| 1   | D     | 3849/4966 (78%)   | 3359 (87%)  | 480 (12%)  | 10 (0%)  | 36          | 72  |
| 2   | E     | 105/107 (98%)     | 96 (91%)    | 9 (9%)     | 0        | 100         | 100 |
| 2   | F     | 105/107 (98%)     | 96 (91%)    | 9 (9%)     | 0        | 100         | 100 |
| 2   | G     | 105/107 (98%)     | 96 (91%)    | 9 (9%)     | 0        | 100         | 100 |
| 2   | H     | 105/107 (98%)     | 96 (91%)    | 9 (9%)     | 0        | 100         | 100 |
| All | All   | 15816/20292 (78%) | 13816 (87%) | 1960 (12%) | 40 (0%)  | 37          | 72  |

All (40) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1500 | ARG  |
| 1   | B     | 1500 | ARG  |
| 1   | C     | 1500 | ARG  |
| 1   | D     | 1500 | ARG  |
| 1   | A     | 607  | ASN  |
| 1   | B     | 607  | ASN  |
| 1   | C     | 607  | ASN  |
| 1   | D     | 607  | ASN  |
| 1   | A     | 2677 | PRO  |
| 1   | B     | 2677 | PRO  |
| 1   | C     | 2677 | PRO  |
| 1   | D     | 2677 | PRO  |
| 1   | A     | 2230 | SER  |
| 1   | B     | 2230 | SER  |
| 1   | C     | 2230 | SER  |
| 1   | D     | 2230 | SER  |
| 1   | A     | 468  | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1947 | MET  |
| 1   | A     | 2676 | PRO  |
| 1   | B     | 468  | GLU  |
| 1   | B     | 1947 | MET  |
| 1   | B     | 2676 | PRO  |
| 1   | C     | 468  | GLU  |
| 1   | C     | 1947 | MET  |
| 1   | C     | 2676 | PRO  |
| 1   | D     | 468  | GLU  |
| 1   | D     | 1947 | MET  |
| 1   | D     | 2676 | PRO  |
| 1   | A     | 1781 | PRO  |
| 1   | B     | 1781 | PRO  |
| 1   | C     | 1781 | PRO  |
| 1   | D     | 1781 | PRO  |
| 1   | A     | 1262 | PRO  |
| 1   | A     | 2231 | PRO  |
| 1   | B     | 1262 | PRO  |
| 1   | B     | 2231 | PRO  |
| 1   | C     | 1262 | PRO  |
| 1   | C     | 2231 | PRO  |
| 1   | D     | 1262 | PRO  |
| 1   | D     | 2231 | 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     | 3178/4355 (73%) | 3172 (100%) | 6 (0%)   | 87          | 86  |
| 1   | B     | 3178/4355 (73%) | 3172 (100%) | 6 (0%)   | 87          | 86  |
| 1   | C     | 3178/4355 (73%) | 3172 (100%) | 6 (0%)   | 87          | 86  |
| 1   | D     | 3178/4355 (73%) | 3172 (100%) | 6 (0%)   | 87          | 86  |
| 2   | E     | 88/88 (100%)    | 88 (100%)   | 0        | 100         | 100 |
| 2   | F     | 88/88 (100%)    | 88 (100%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 2   | G     | 88/88 (100%)      | 88 (100%)    | 0        | 100         | 100 |
| 2   | H     | 88/88 (100%)      | 88 (100%)    | 0        | 100         | 100 |
| All | All   | 13064/17772 (74%) | 13040 (100%) | 24 (0%)  | 85          | 86  |

All (24) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2017 | ASP  |
| 1   | A     | 2072 | SER  |
| 1   | A     | 2744 | GLU  |
| 1   | A     | 2828 | SER  |
| 1   | A     | 3653 | GLU  |
| 1   | A     | 3654 | ASP  |
| 1   | B     | 2017 | ASP  |
| 1   | B     | 2072 | SER  |
| 1   | B     | 2744 | GLU  |
| 1   | B     | 2828 | SER  |
| 1   | B     | 3653 | GLU  |
| 1   | B     | 3654 | ASP  |
| 1   | C     | 2017 | ASP  |
| 1   | C     | 2072 | SER  |
| 1   | C     | 2744 | GLU  |
| 1   | C     | 2828 | SER  |
| 1   | C     | 3653 | GLU  |
| 1   | C     | 3654 | ASP  |
| 1   | D     | 2017 | ASP  |
| 1   | D     | 2072 | SER  |
| 1   | D     | 2744 | GLU  |
| 1   | D     | 2828 | SER  |
| 1   | D     | 3653 | GLU  |
| 1   | D     | 3654 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 903  | GLN  |
| 1   | A     | 1157 | GLN  |
| 1   | A     | 1242 | ASN  |
| 1   | A     | 1287 | GLN  |
| 1   | A     | 1648 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1845 | GLN  |
| 1   | A     | 2150 | ASN  |
| 1   | A     | 2249 | ASN  |
| 1   | A     | 2317 | ASN  |
| 1   | A     | 2578 | GLN  |
| 1   | A     | 2691 | GLN  |
| 1   | A     | 2818 | HIS  |
| 1   | A     | 2846 | ASN  |
| 1   | A     | 3850 | ASN  |
| 1   | A     | 3900 | GLN  |
| 1   | A     | 3991 | ASN  |
| 1   | A     | 4635 | ASN  |
| 1   | A     | 4705 | GLN  |
| 1   | A     | 4932 | HIS  |
| 1   | B     | 745  | ASN  |
| 1   | B     | 903  | GLN  |
| 1   | B     | 1157 | GLN  |
| 1   | B     | 1242 | ASN  |
| 1   | B     | 1648 | GLN  |
| 1   | B     | 1845 | GLN  |
| 1   | B     | 2150 | ASN  |
| 1   | B     | 2249 | ASN  |
| 1   | B     | 2317 | ASN  |
| 1   | B     | 2578 | GLN  |
| 1   | B     | 2691 | GLN  |
| 1   | B     | 2818 | HIS  |
| 1   | B     | 2846 | ASN  |
| 1   | B     | 3850 | ASN  |
| 1   | B     | 3900 | GLN  |
| 1   | B     | 3991 | ASN  |
| 1   | B     | 4635 | ASN  |
| 1   | B     | 4932 | HIS  |
| 1   | C     | 745  | ASN  |
| 1   | C     | 903  | GLN  |
| 1   | C     | 1157 | GLN  |
| 1   | C     | 1242 | ASN  |
| 1   | C     | 1845 | GLN  |
| 1   | C     | 2150 | ASN  |
| 1   | C     | 2176 | ASN  |
| 1   | C     | 2249 | ASN  |
| 1   | C     | 2317 | ASN  |
| 1   | C     | 2578 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 2691 | GLN  |
| 1   | C     | 2818 | HIS  |
| 1   | C     | 2846 | ASN  |
| 1   | C     | 3850 | ASN  |
| 1   | C     | 3900 | GLN  |
| 1   | C     | 3991 | ASN  |
| 1   | C     | 4048 | HIS  |
| 1   | C     | 4635 | ASN  |
| 1   | C     | 4932 | HIS  |
| 1   | D     | 240  | HIS  |
| 1   | D     | 484  | ASN  |
| 1   | D     | 745  | ASN  |
| 1   | D     | 903  | GLN  |
| 1   | D     | 1157 | GLN  |
| 1   | D     | 1242 | ASN  |
| 1   | D     | 1845 | GLN  |
| 1   | D     | 2150 | ASN  |
| 1   | D     | 2249 | ASN  |
| 1   | D     | 2317 | ASN  |
| 1   | D     | 2578 | GLN  |
| 1   | D     | 2691 | GLN  |
| 1   | D     | 2818 | HIS  |
| 1   | D     | 2846 | ASN  |
| 1   | D     | 3850 | ASN  |
| 1   | D     | 3900 | GLN  |
| 1   | D     | 3991 | ASN  |
| 1   | D     | 4048 | HIS  |
| 1   | D     | 4635 | ASN  |
| 1   | D     | 4932 | HIS  |
| 2   | E     | 65   | GLN  |
| 2   | F     | 65   | GLN  |
| 2   | G     | 65   | GLN  |
| 2   | H     | 25   | HIS  |
| 2   | H     | 65   | 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

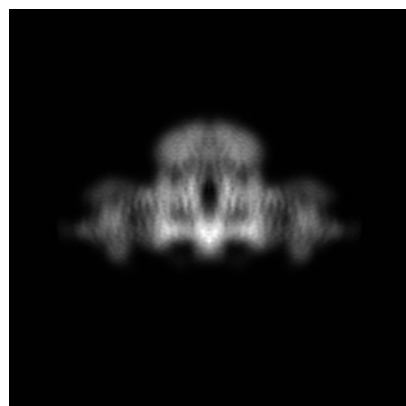
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21862. These allow visual inspection of the internal detail of the map and identification of artifacts.

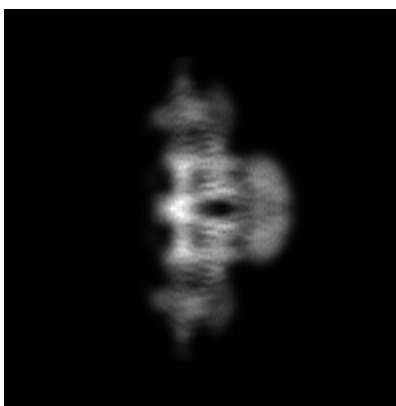
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

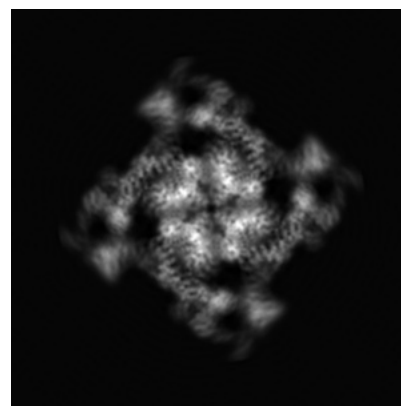
#### 6.1.1 Primary map



X

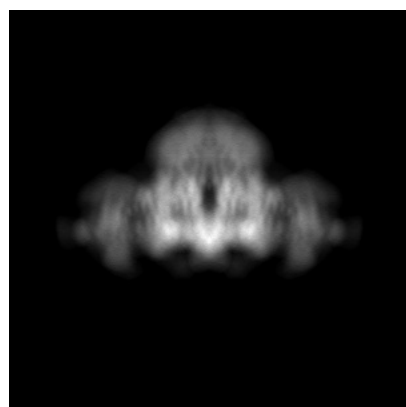


Y

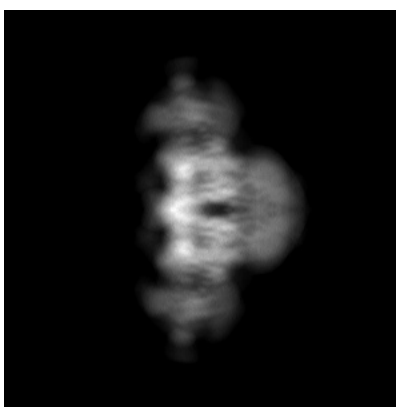


Z

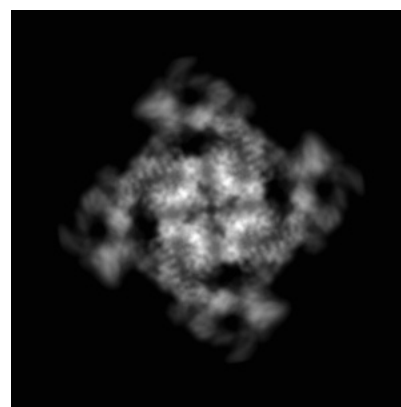
#### 6.1.2 Raw map



X



Y

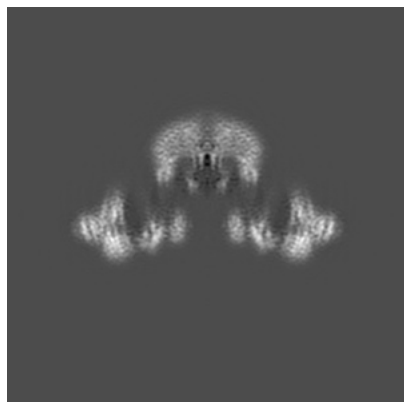


Z

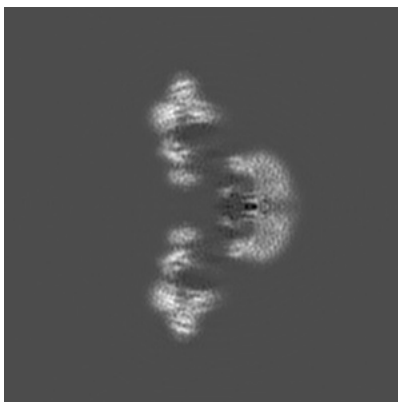
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

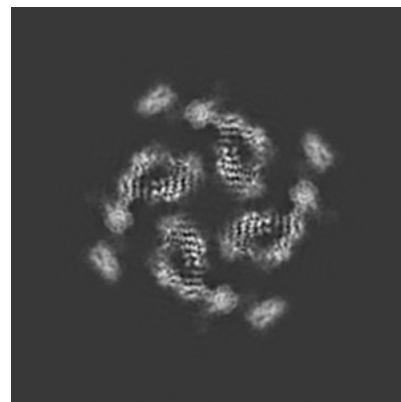
### 6.2.1 Primary map



X Index: 176

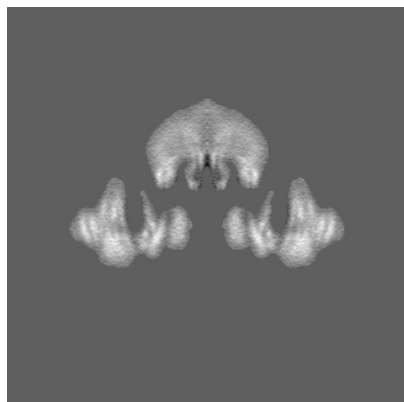


Y Index: 176

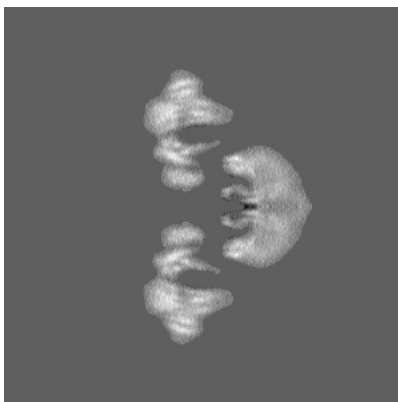


Z Index: 176

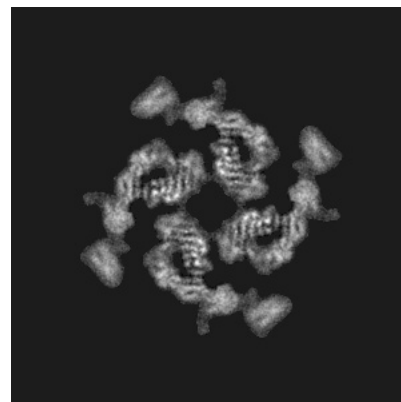
### 6.2.2 Raw map



X Index: 352



Y Index: 352

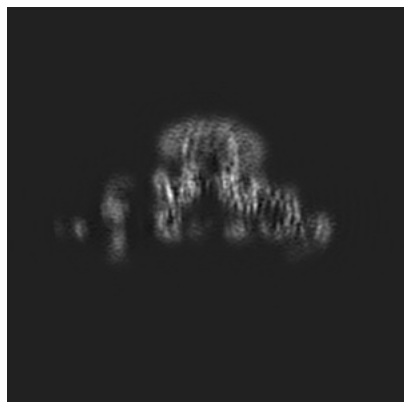


Z Index: 352

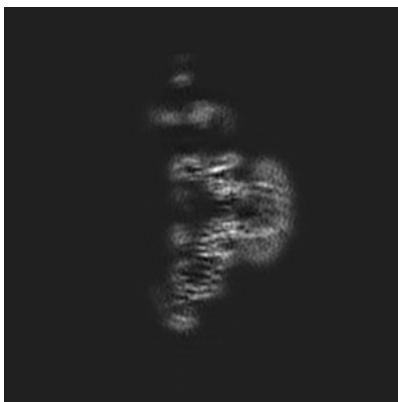
The images above show central slices of the map in three orthogonal directions.

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

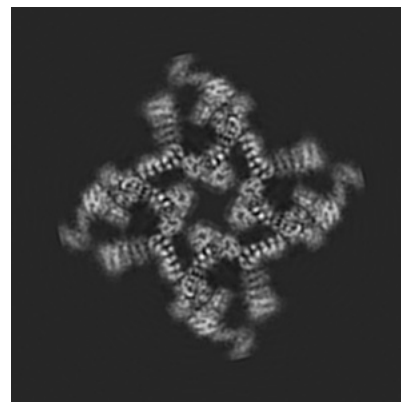
### 6.3.1 Primary map



X Index: 191

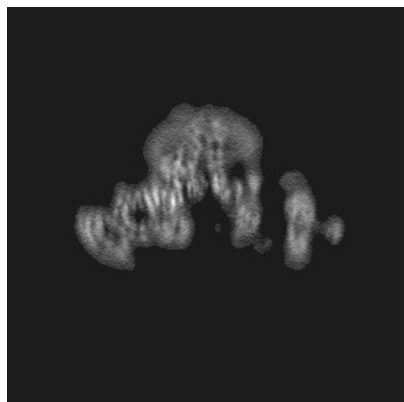


Y Index: 191



Z Index: 159

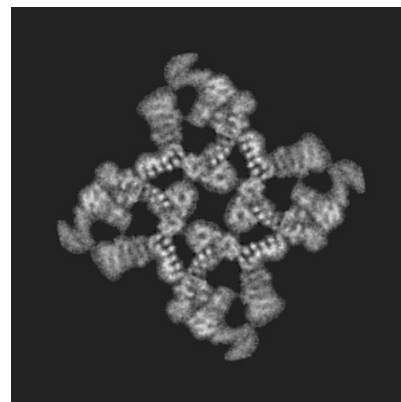
### 6.3.2 Raw map



X Index: 330



Y Index: 330

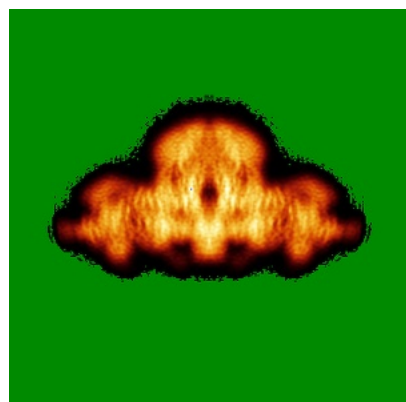


Z Index: 318

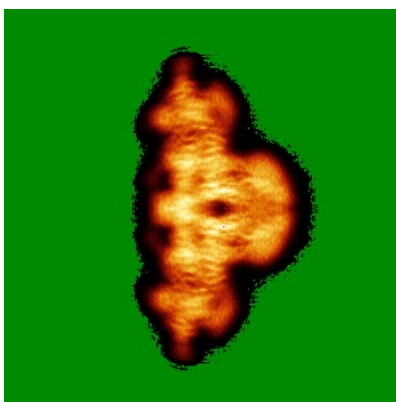
The images above show the largest variance slices of the map in three orthogonal directions.

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

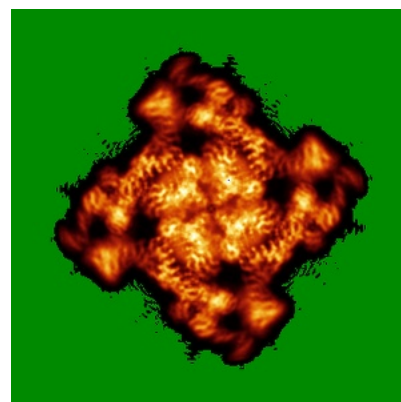
### 6.4.1 Primary map



X

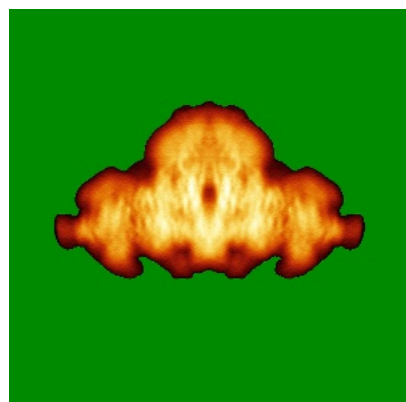


Y

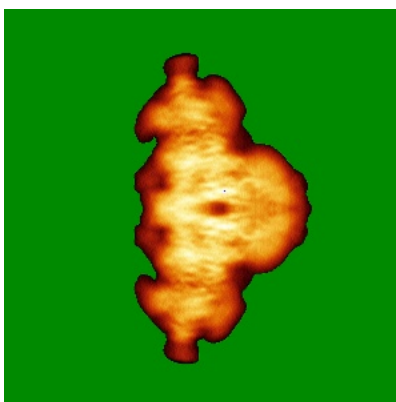


Z

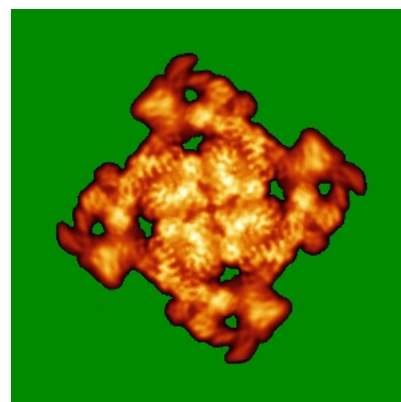
### 6.4.2 Raw map



X



Y

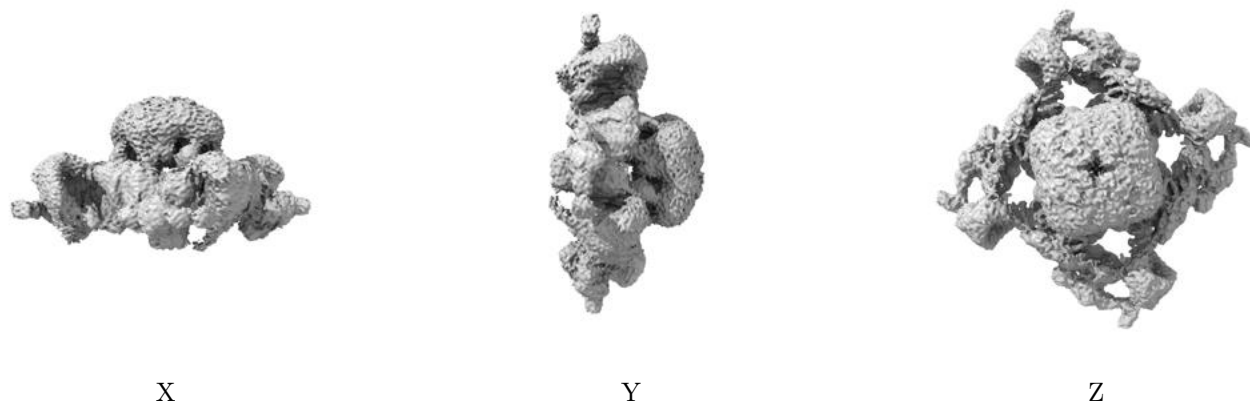


Z

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.

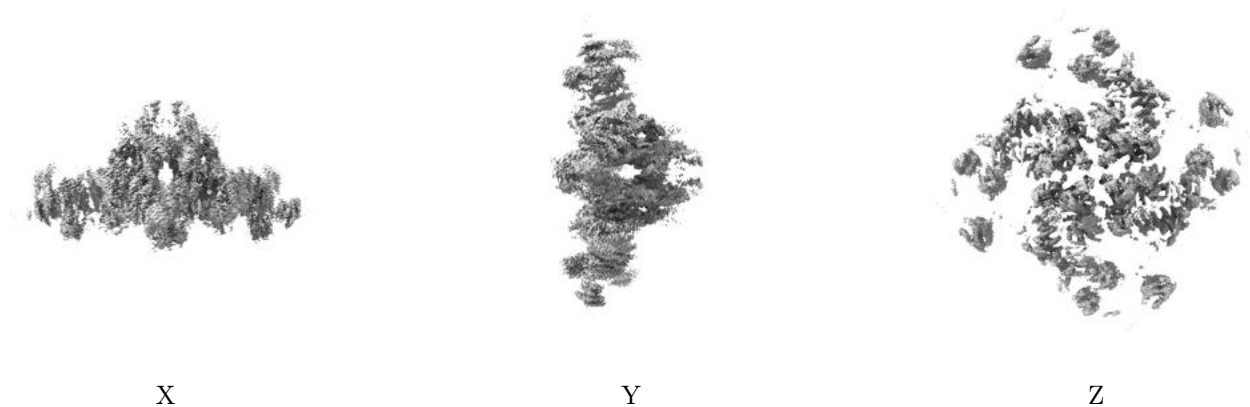
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

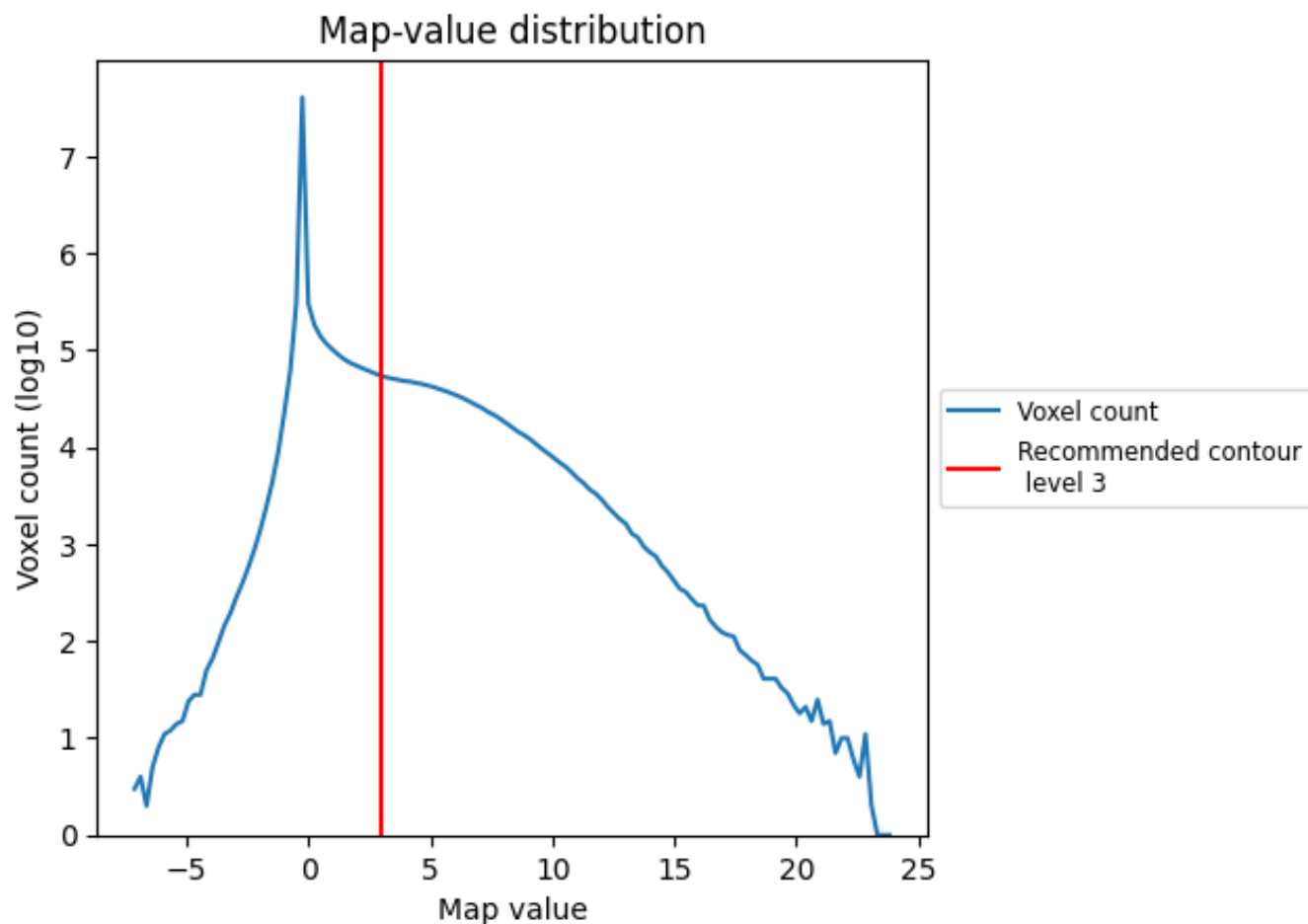
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

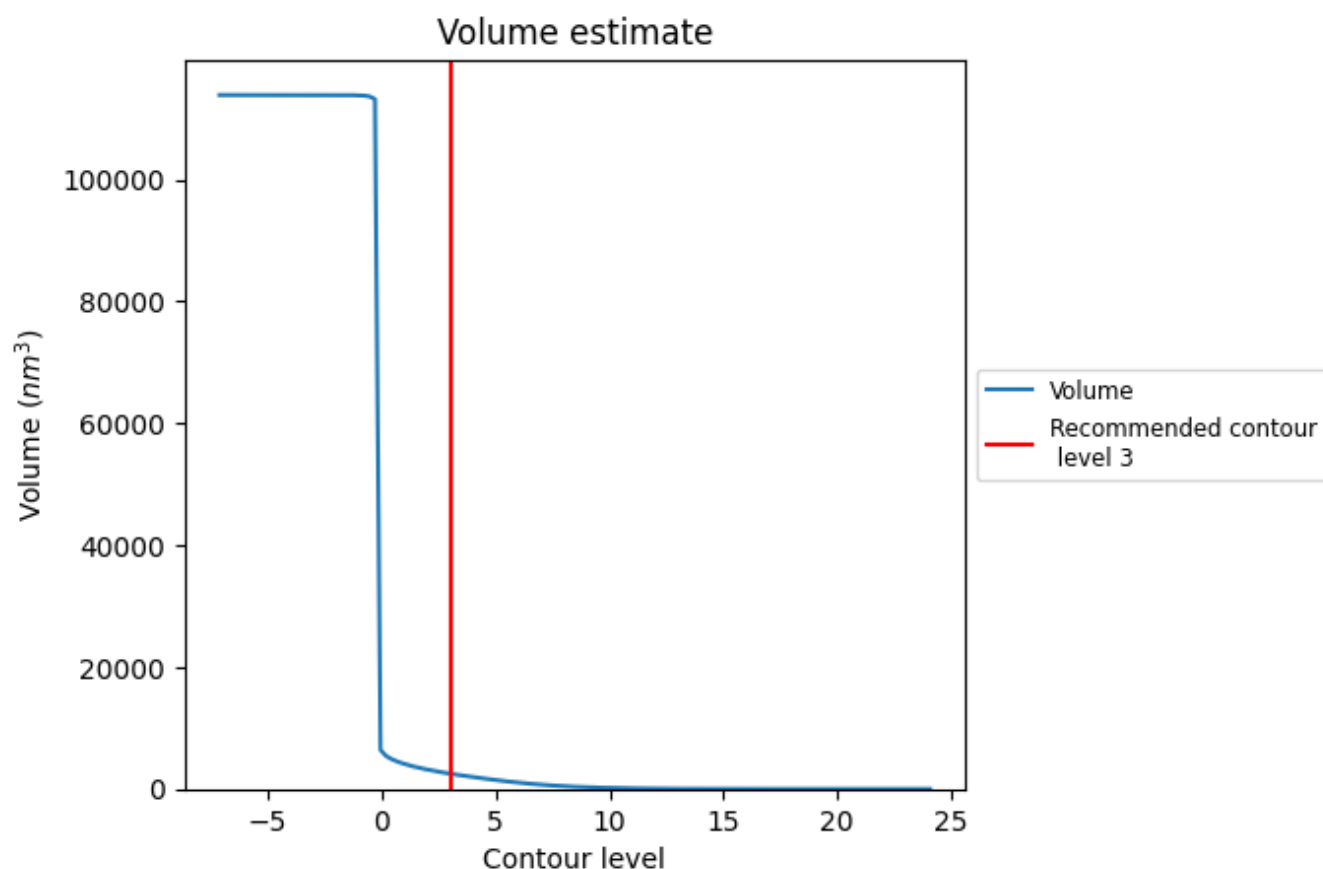
This section contains the results of statistical analysis of the map.

### 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.

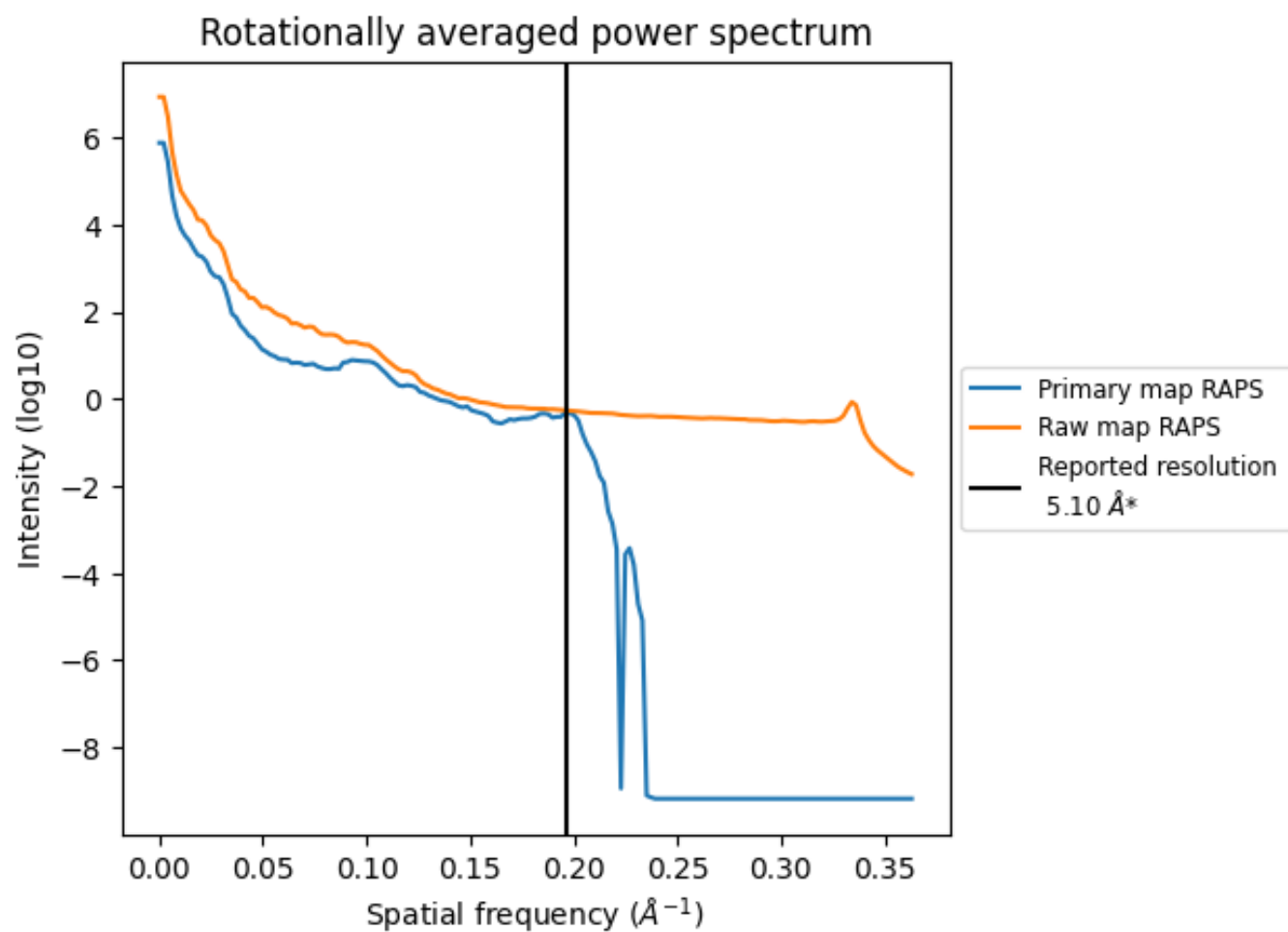
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2507  $\text{nm}^3$ ; this corresponds to an approximate mass of 2265 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 ⓘ

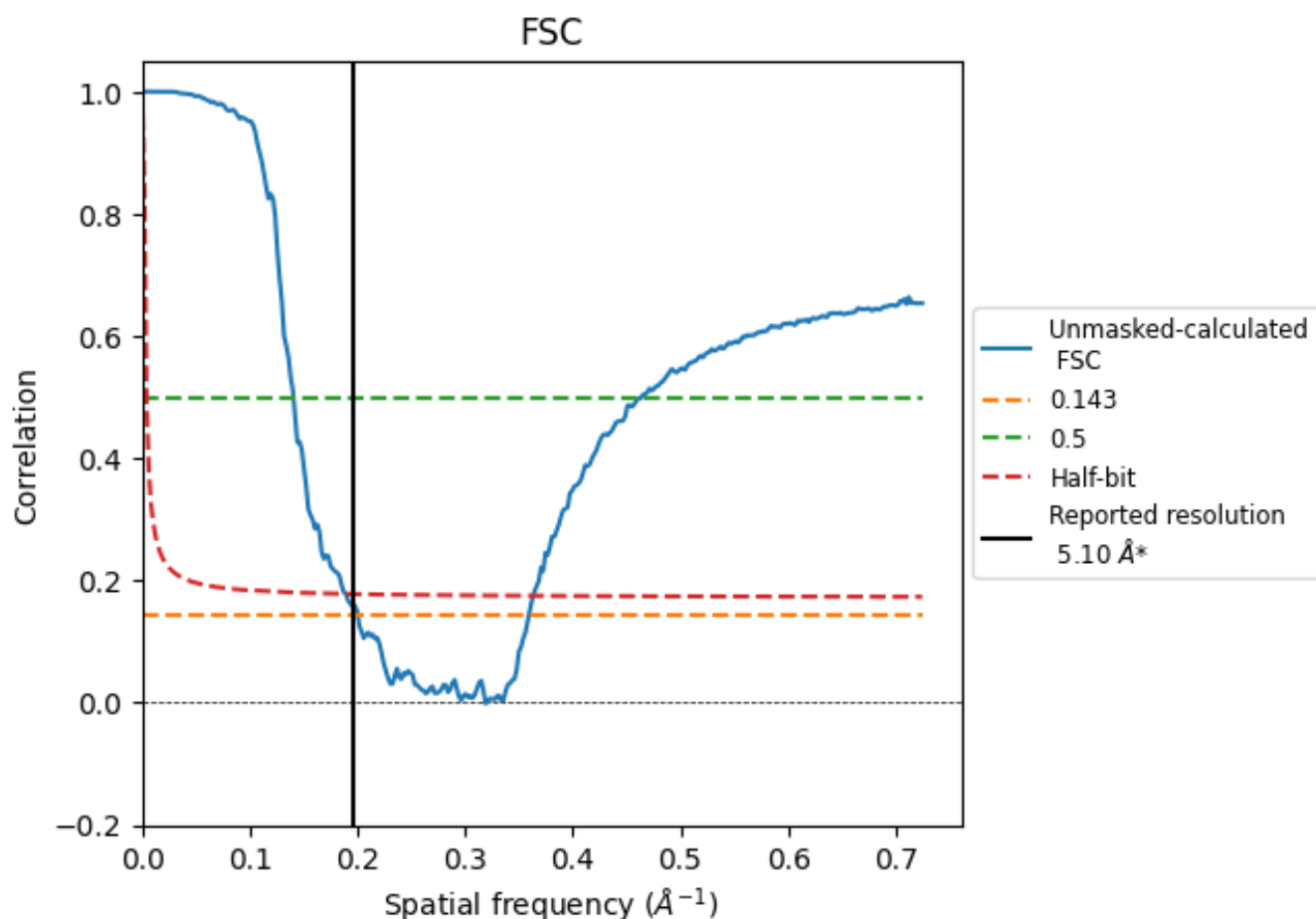


\*Reported resolution corresponds to spatial frequency of 0.196 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.196 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

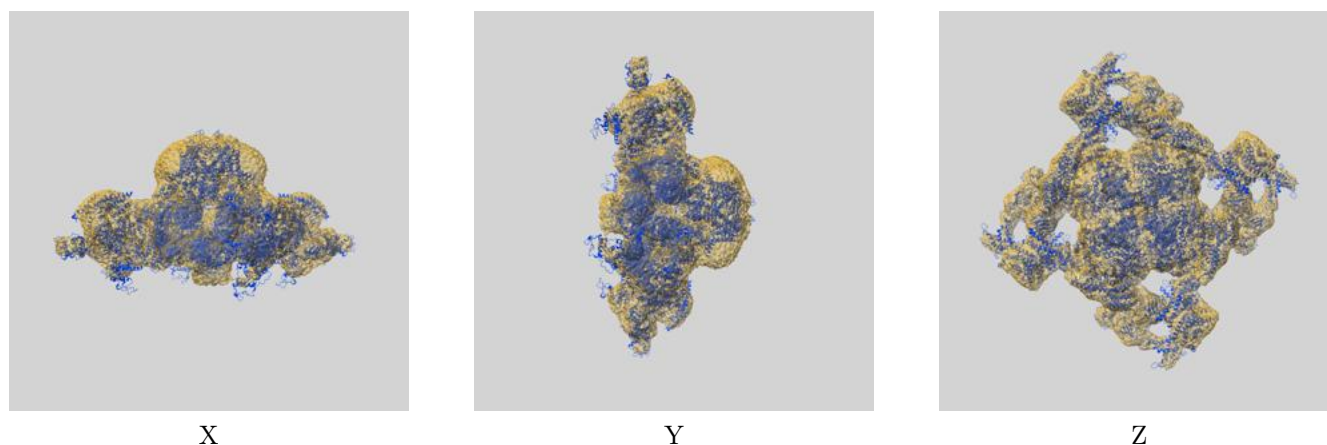
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 5.10                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.99                               | 7.12 | 5.28     |

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

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

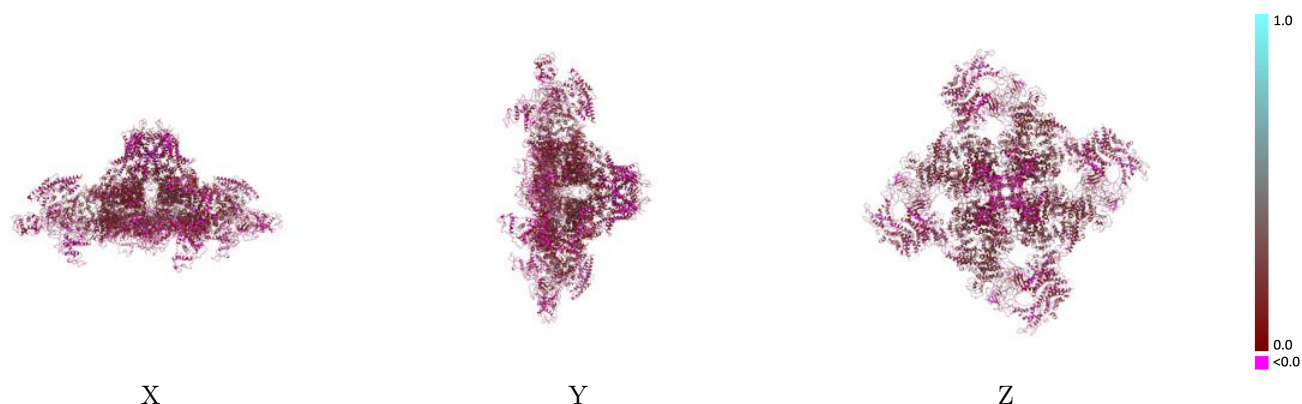
This section contains information regarding the fit between EMDB map EMD-21862 and PDB model 6WOV. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

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



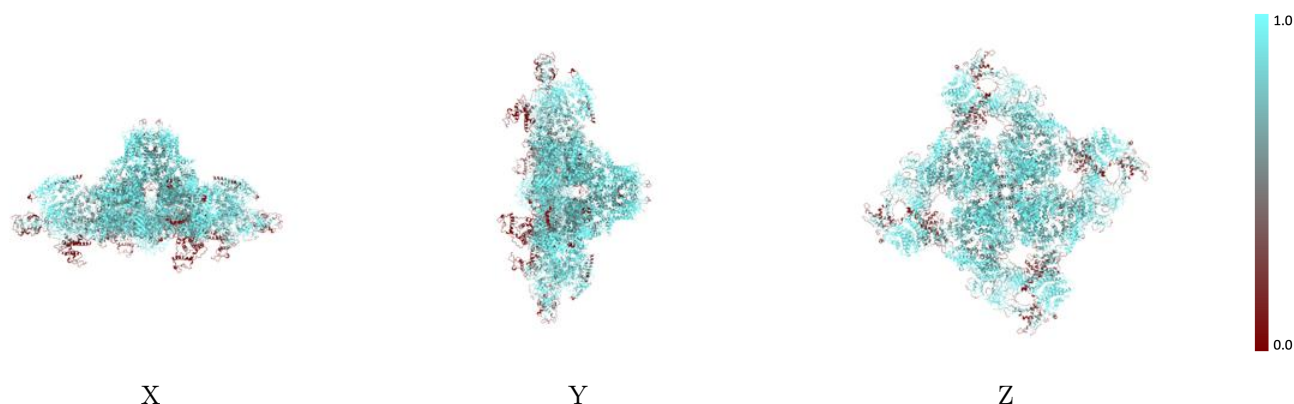
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



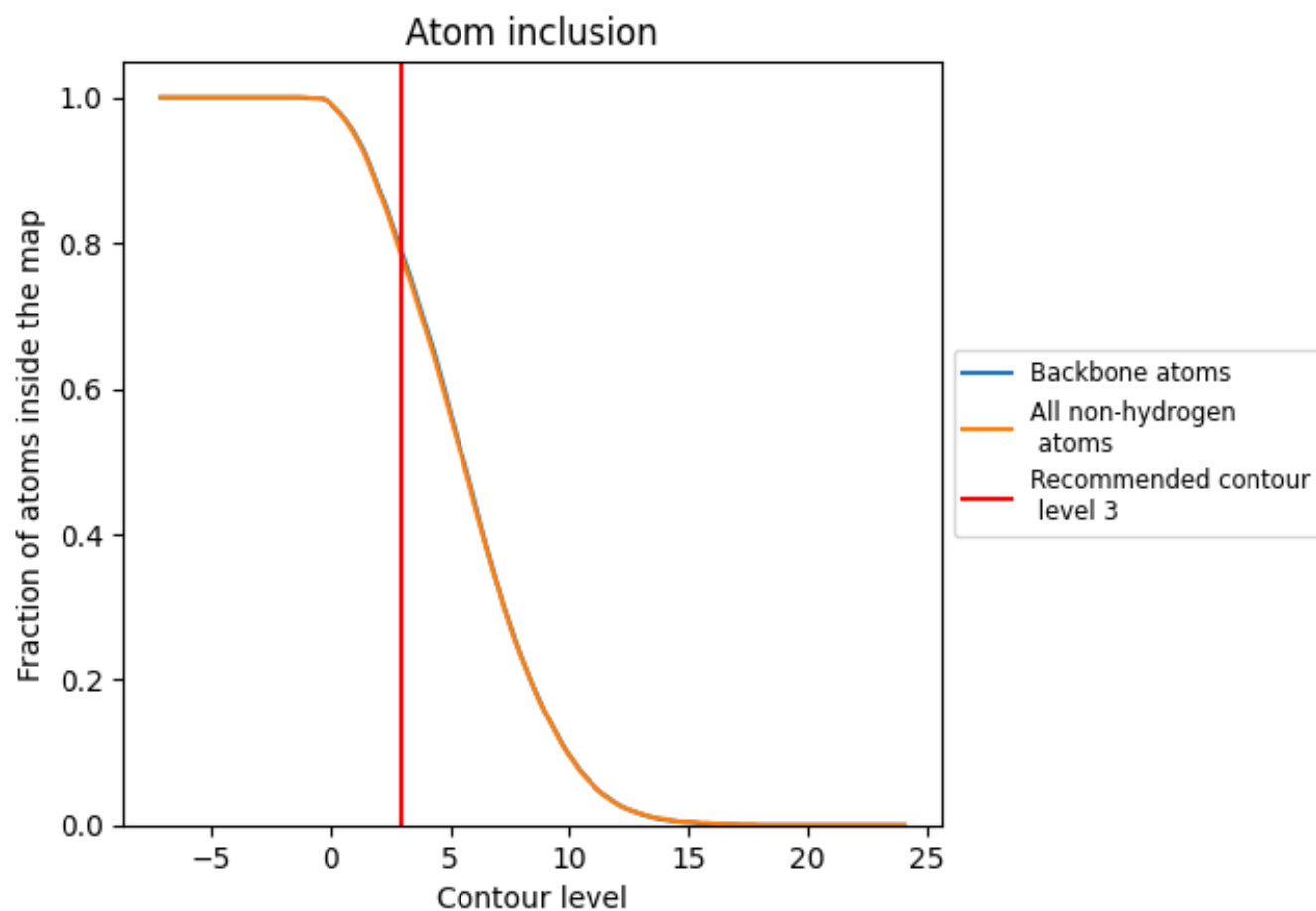
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                | Q-score                       |
|-------|-------------------------------|-------------------------------|
| All   | <div><div></div></div> 0.7800 | <div><div></div></div> 0.1330 |
| A     | <div><div></div></div> 0.7820 | <div><div></div></div> 0.1330 |
| B     | <div><div></div></div> 0.7810 | <div><div></div></div> 0.1330 |
| C     | <div><div></div></div> 0.7820 | <div><div></div></div> 0.1330 |
| D     | <div><div></div></div> 0.7820 | <div><div></div></div> 0.1330 |
| E     | <div><div></div></div> 0.7670 | <div><div></div></div> 0.1520 |
| F     | <div><div></div></div> 0.7720 | <div><div></div></div> 0.1540 |
| G     | <div><div></div></div> 0.7640 | <div><div></div></div> 0.1470 |
| H     | <div><div></div></div> 0.7640 | <div><div></div></div> 0.1430 |

1.0

0.0

<0.0