



## Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 02:54 AM UTC

PDB ID : 8CYE / pdb\_00008cye  
EMDB ID : EMD-27076  
Title : Cryo-EM asymmetric reconstruction of the EPEC H6 bacterial flagellar filament Normal Waveform  
Authors : Kreutzberger, M.A.B.; Chatterjee, S.; Frankel, G.; Egelman, E.H.  
Deposited on : 2022-05-23  
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

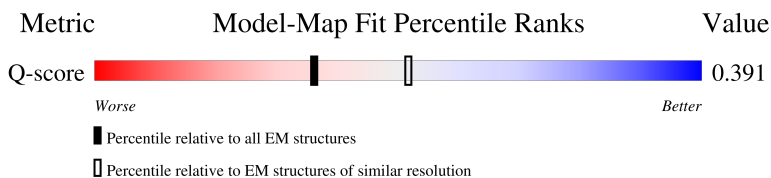
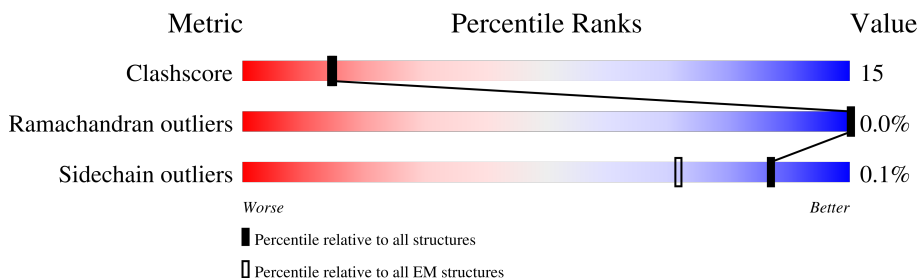
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.90 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.



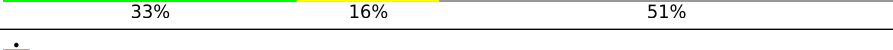
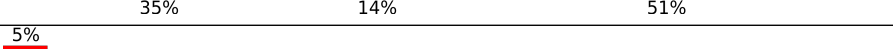
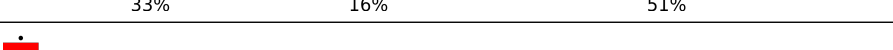
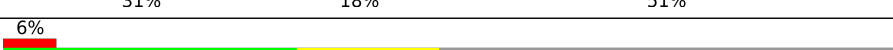
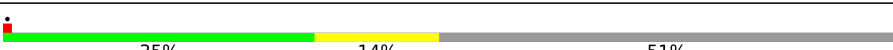
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 8855 ( 3.40 - 4.40 )                                     |

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     | 548    | <br>37% 12% 51%  |
| 1   | B     | 548    | <br>34% 15% 51%  |
| 1   | C     | 548    | <br>33% 16% 51%  |
| 1   | D     | 548    | <br>33% 16% 51%  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | E     | 548    |    |
| 1   | F     | 548    |    |
| 1   | G     | 548    |    |
| 1   | H     | 548    |    |
| 1   | I     | 548    |    |
| 1   | J     | 548    |    |
| 1   | K     | 548    |    |
| 1   | L     | 548    |    |
| 1   | M     | 548    |    |
| 1   | N     | 548    |    |
| 1   | O     | 548    |    |
| 1   | P     | 548    |  |
| 1   | Q     | 548    |  |
| 1   | R     | 548    |  |
| 1   | S     | 548    |  |
| 1   | T     | 548    |  |
| 1   | U     | 548    |  |
| 1   | V     | 548    |  |

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 44198 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Flagellin.

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | B     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | A     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | M     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | C     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | N     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | D     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | O     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | E     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | P     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | F     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | Q     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | G     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | R     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | H     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | S     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | I     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | T     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |

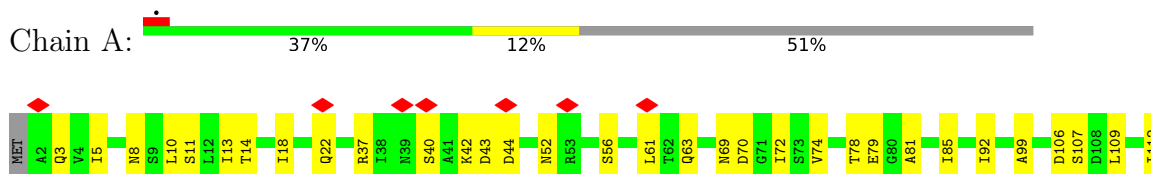
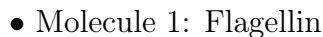
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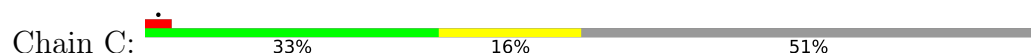
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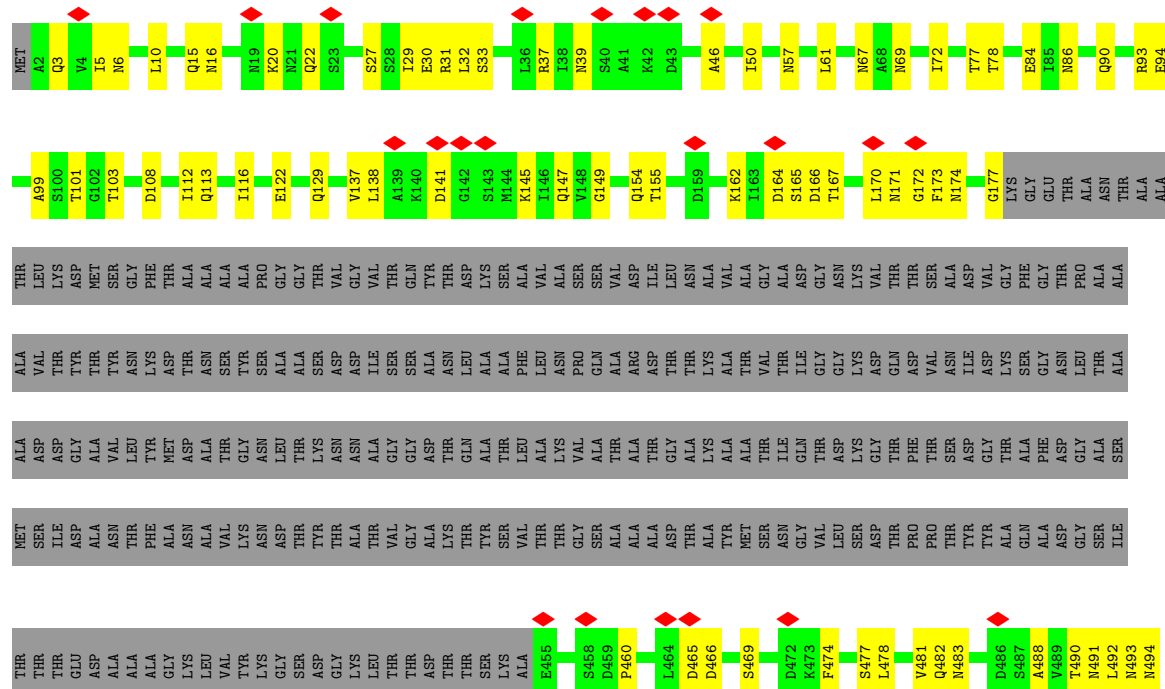
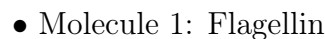
| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 1   | J     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | U     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | K     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | V     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |
| 1   | L     | 269      | Total<br>2009 | C<br>1205 | N<br>367 | O<br>435 | S<br>2 | 1       | 0     |



- Molecule 1: Flagellin



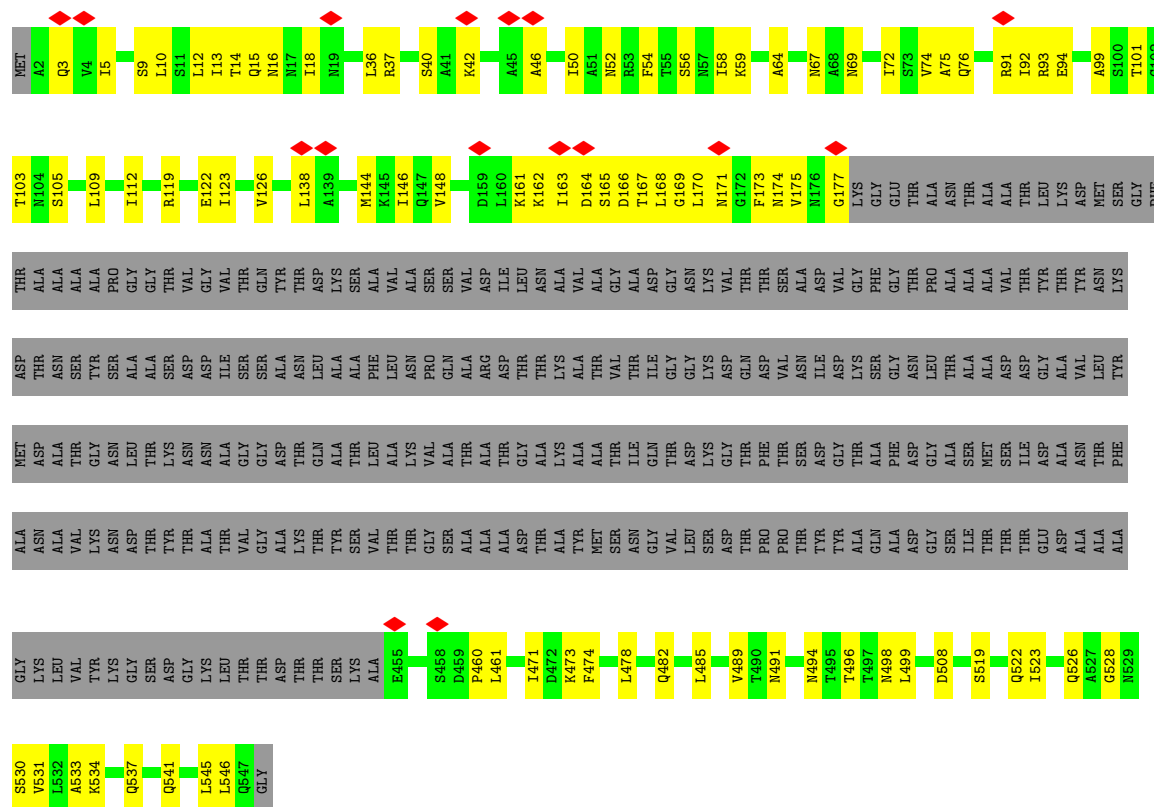
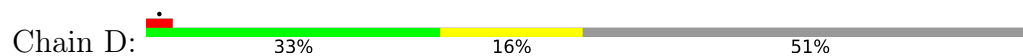




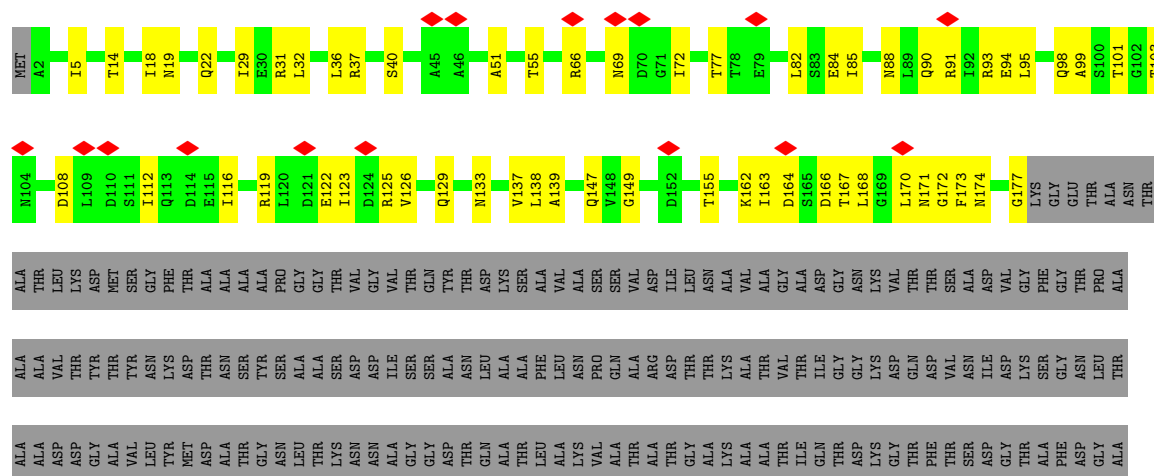
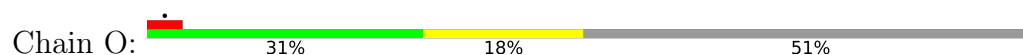




• Molecule 1: Flagellin

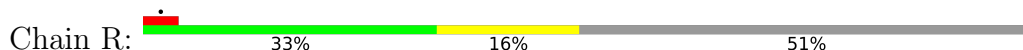


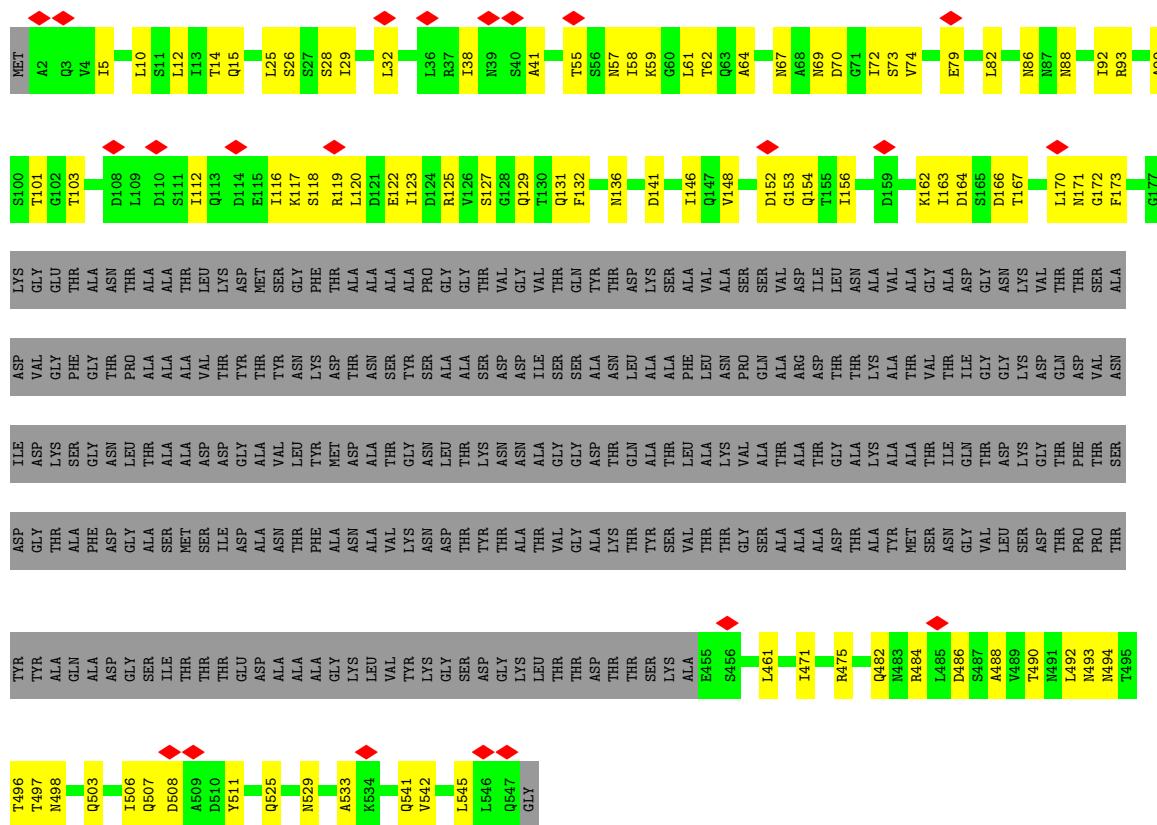
• Molecule 1: Flagellin



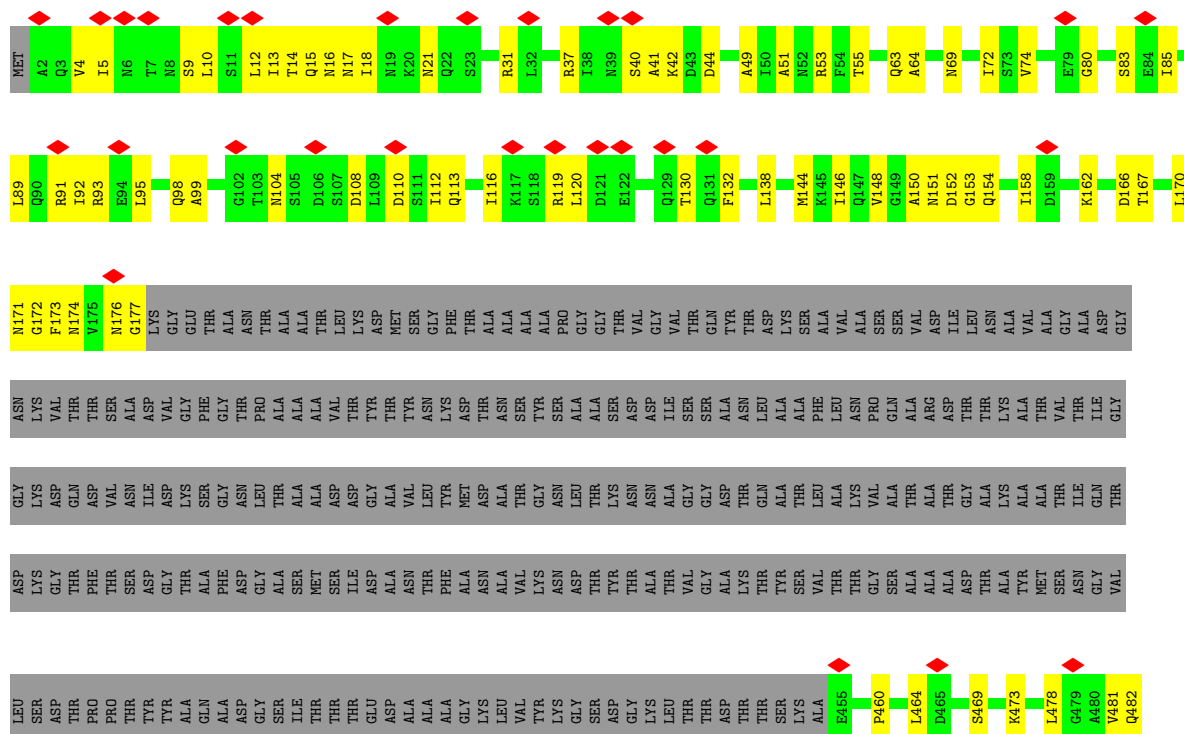
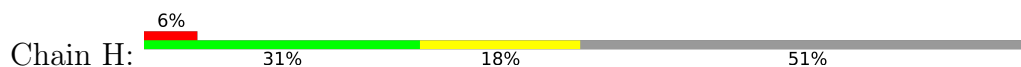


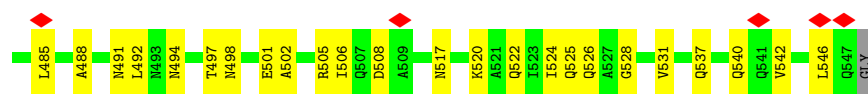




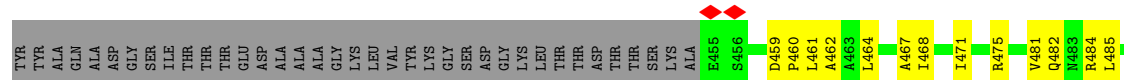
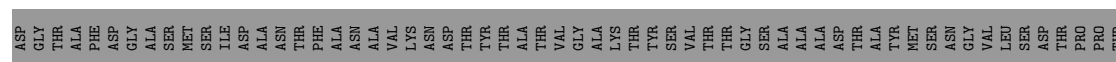
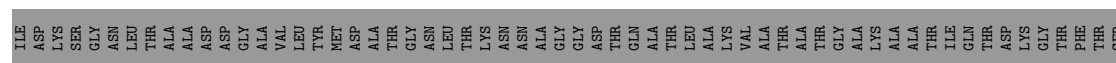
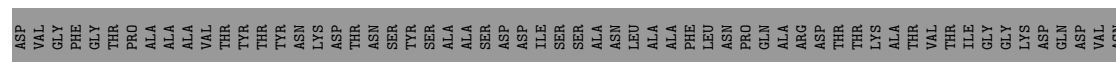
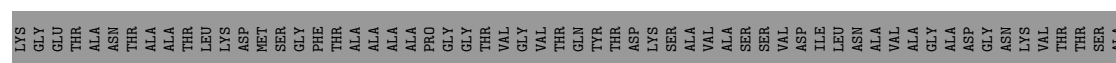
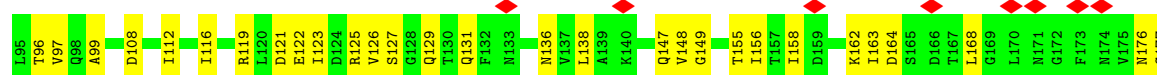
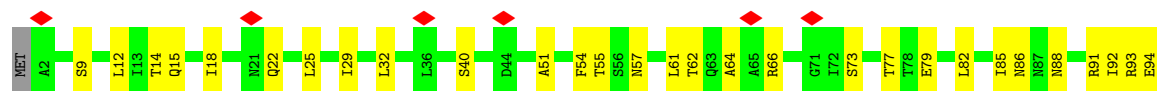
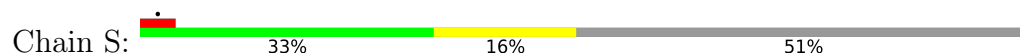


• Molecule 1: Flagellin

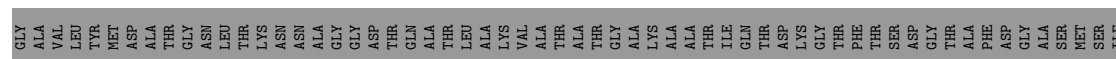
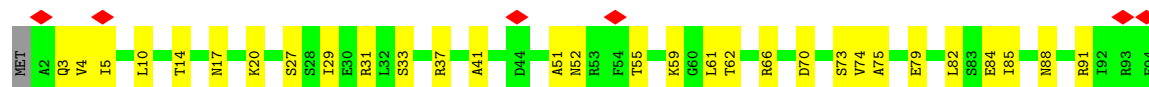
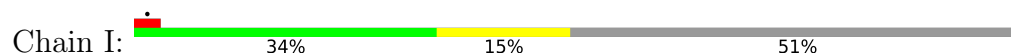




• Molecule 1: Flagellin

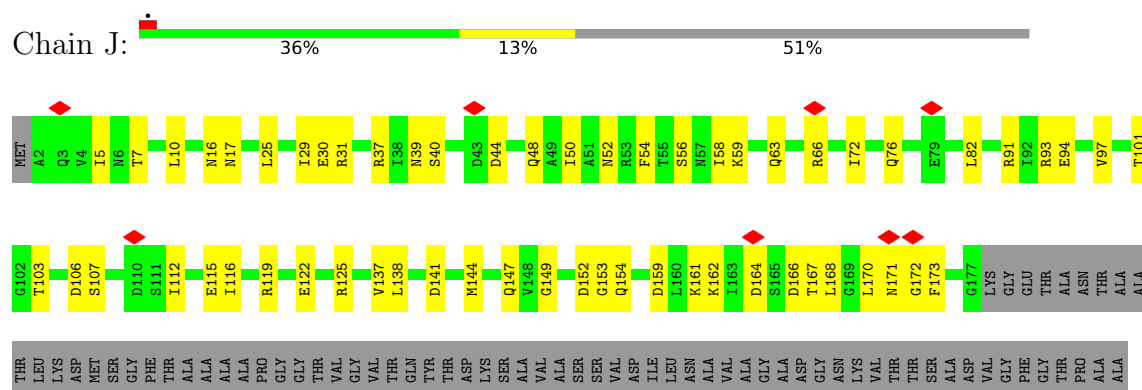


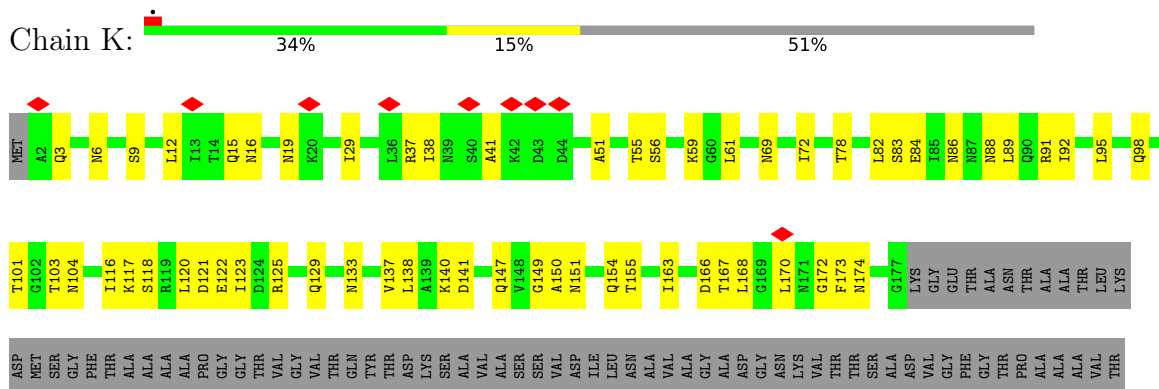
• Molecule 1: Flagellin



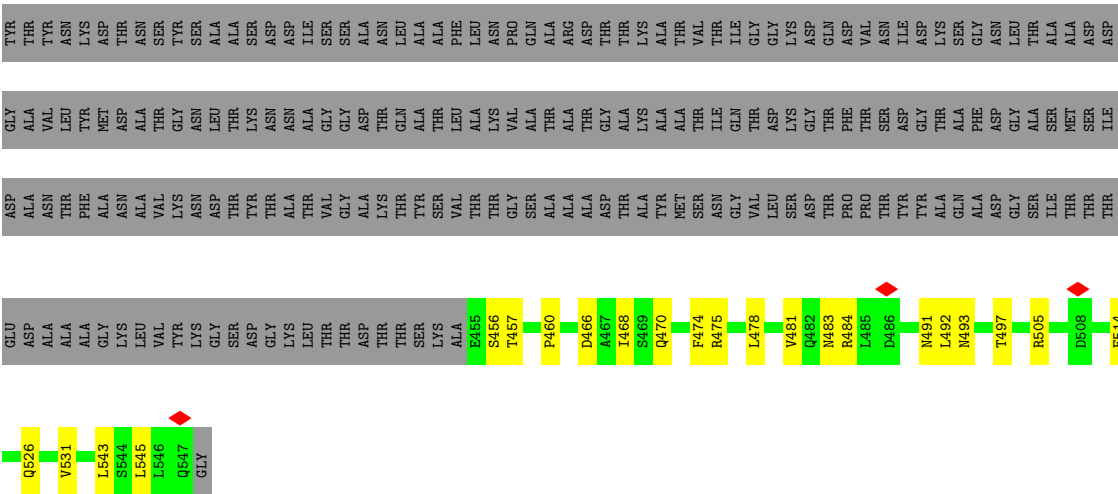
- Molecule 1: Flagellin

- Molecule 1: Flagellin

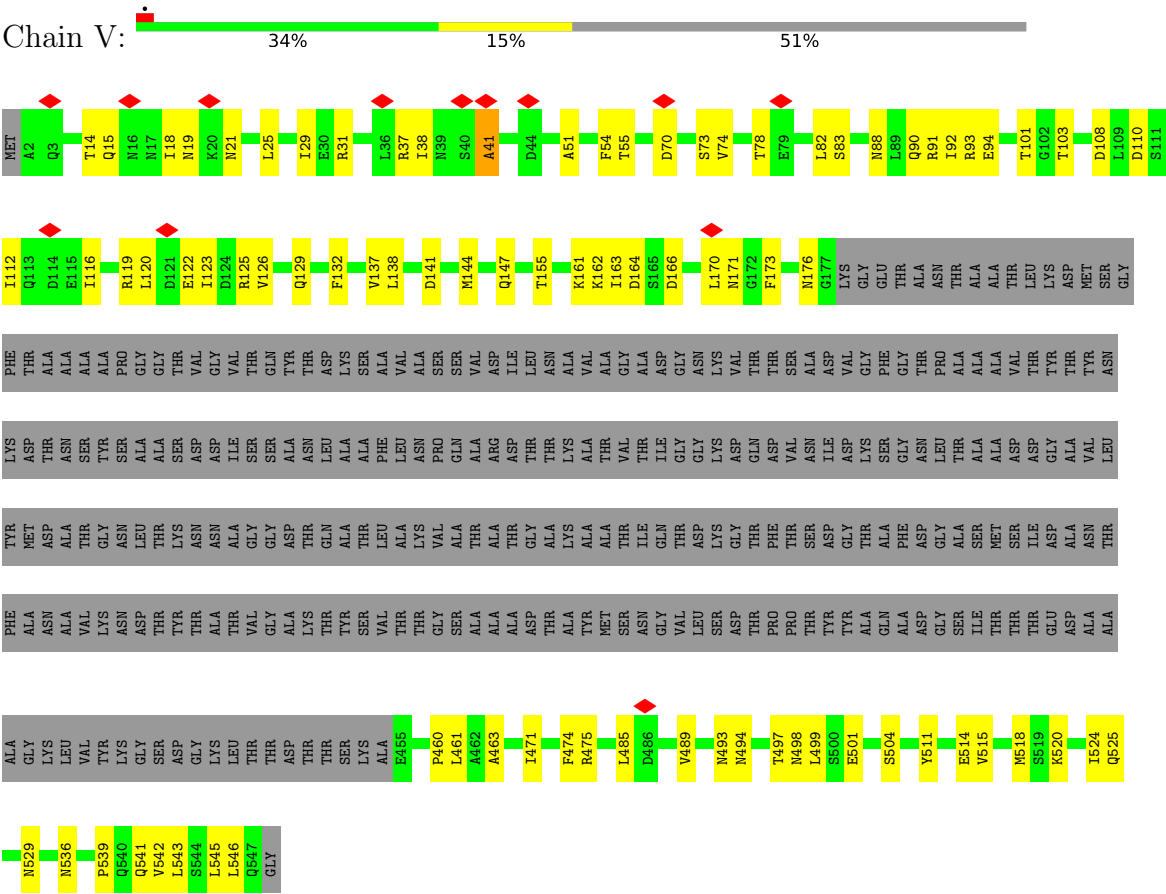




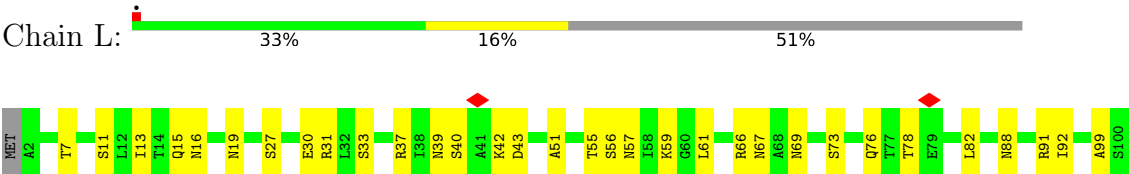




• Molecule 1: Flagellin



• Molecule 1: Flagellin



[illegible]

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 46895                                   | Depositor |
| Resolution determination method      | FSC 0.33 CUT-OFF                        | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.779                                   | Depositor |
| Minimum map value                    | -0.474                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.022                                   | Depositor |
| Recommended contour level            | 0.177                                   | Depositor |
| Map size (Å)                         | 673.92004, 673.92004, 673.92004         | wwPDB     |
| Map dimensions                       | 624, 624, 624                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.08, 1.08, 1.08                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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     | 0.14         | 0/2014  | 0.36        | 0/2724         |
| 1   | B     | 0.31         | 0/2014  | 0.58        | 5/2724 (0.2%)  |
| 1   | C     | 0.15         | 0/2014  | 0.44        | 1/2724 (0.0%)  |
| 1   | D     | 0.18         | 0/2014  | 0.41        | 0/2724         |
| 1   | E     | 0.16         | 0/2014  | 0.39        | 0/2724         |
| 1   | F     | 0.15         | 0/2014  | 0.37        | 0/2724         |
| 1   | G     | 0.16         | 0/2014  | 0.43        | 0/2724         |
| 1   | H     | 0.16         | 0/2014  | 0.42        | 0/2724         |
| 1   | I     | 0.16         | 0/2014  | 0.41        | 0/2724         |
| 1   | J     | 0.14         | 0/2014  | 0.36        | 0/2724         |
| 1   | K     | 0.16         | 0/2014  | 0.40        | 0/2724         |
| 1   | L     | 0.17         | 0/2014  | 0.41        | 0/2724         |
| 1   | M     | 0.17         | 0/2014  | 0.45        | 0/2724         |
| 1   | N     | 0.18         | 0/2014  | 0.45        | 0/2724         |
| 1   | O     | 0.17         | 0/2014  | 0.40        | 0/2724         |
| 1   | P     | 0.16         | 0/2014  | 0.41        | 0/2724         |
| 1   | Q     | 0.18         | 0/2014  | 0.46        | 0/2724         |
| 1   | R     | 0.14         | 0/2014  | 0.40        | 0/2724         |
| 1   | S     | 0.15         | 0/2014  | 0.37        | 0/2724         |
| 1   | T     | 0.14         | 0/2014  | 0.37        | 0/2724         |
| 1   | U     | 0.16         | 0/2014  | 0.38        | 0/2724         |
| 1   | V     | 0.17         | 0/2014  | 0.42        | 0/2724         |
| All | All   | 0.17         | 0/44308 | 0.42        | 6/59928 (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   | B     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | E     | 0                   | 2                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | H     | 0                   | 1                   |
| 1   | I     | 0                   | 1                   |
| 1   | J     | 0                   | 1                   |
| 1   | L     | 0                   | 1                   |
| 1   | O     | 0                   | 1                   |
| 1   | S     | 0                   | 1                   |
| 1   | T     | 0                   | 1                   |
| 1   | U     | 0                   | 1                   |
| 1   | V     | 0                   | 1                   |
| All | All   | 0                   | 13                  |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res   | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|---------|-------|-------------|----------|
| 1   | B     | 38[A] | ILE  | N-CA-C  | 7.15  | 117.91      | 110.62   |
| 1   | B     | 38[B] | ILE  | N-CA-C  | 7.15  | 117.91      | 110.62   |
| 1   | C     | 5     | ILE  | N-CA-C  | -5.84 | 107.81      | 113.53   |
| 1   | B     | 42    | LYS  | N-CA-C  | -5.47 | 105.42      | 111.71   |
| 1   | B     | 36    | LEU  | N-CA-C  | 5.14  | 118.32      | 110.20   |
| 1   | B     | 39    | ASN  | CB-CA-C | -5.01 | 110.42      | 117.23   |

There are no chirality outliers.

All (13) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | B     | 169 | GLY  | Peptide |
| 1   | D     | 169 | GLY  | Peptide |
| 1   | E     | 40  | SER  | Peptide |
| 1   | E     | 41  | ALA  | Peptide |
| 1   | H     | 40  | SER  | Peptide |
| 1   | I     | 41  | ALA  | Peptide |
| 1   | J     | 40  | SER  | Peptide |
| 1   | L     | 40  | SER  | Peptide |
| 1   | O     | 40  | SER  | Peptide |
| 1   | S     | 40  | SER  | Peptide |
| 1   | T     | 40  | SER  | Peptide |
| 1   | U     | 41  | ALA  | Peptide |
| 1   | V     | 41  | ALA  | 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     | 2009  | 0        | 1994     | 45      | 0            |
| 1   | B     | 2009  | 0        | 1994     | 95      | 0            |
| 1   | C     | 2009  | 0        | 1994     | 70      | 0            |
| 1   | D     | 2009  | 0        | 1994     | 67      | 0            |
| 1   | E     | 2009  | 0        | 1994     | 78      | 0            |
| 1   | F     | 2009  | 0        | 1994     | 55      | 0            |
| 1   | G     | 2009  | 0        | 1994     | 96      | 0            |
| 1   | H     | 2009  | 0        | 1994     | 82      | 0            |
| 1   | I     | 2009  | 0        | 1994     | 72      | 0            |
| 1   | J     | 2009  | 0        | 1994     | 58      | 0            |
| 1   | K     | 2009  | 0        | 1994     | 70      | 0            |
| 1   | L     | 2009  | 0        | 1994     | 81      | 0            |
| 1   | M     | 2009  | 0        | 1994     | 62      | 0            |
| 1   | N     | 2009  | 0        | 1994     | 81      | 0            |
| 1   | O     | 2009  | 0        | 1994     | 90      | 0            |
| 1   | P     | 2009  | 0        | 1994     | 71      | 0            |
| 1   | Q     | 2009  | 0        | 1994     | 75      | 0            |
| 1   | R     | 2009  | 0        | 1994     | 78      | 0            |
| 1   | S     | 2009  | 0        | 1994     | 67      | 0            |
| 1   | T     | 2009  | 0        | 1994     | 71      | 0            |
| 1   | U     | 2009  | 0        | 1994     | 59      | 0            |
| 1   | V     | 2009  | 0        | 1994     | 63      | 0            |
| All | All   | 44198 | 0        | 43868    | 1328    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1328) 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:32:LEU:HD22 | 1:L:531:VAL:CG2  | 1.66                     | 1.24              |
| 1:B:32:LEU:HD22 | 1:L:531:VAL:HG21 | 1.28                     | 1.14              |
| 1:K:83:SER:HA   | 1:K:475:ARG:HH22 | 1.35                     | 0.90              |
| 1:A:505:ARG:HD3 | 1:C:69:ASN:HB3   | 1.53                     | 0.88              |
| 1:B:32:LEU:CD2  | 1:L:531:VAL:HG21 | 2.04                     | 0.87              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:M:166:ASP:HB3    | 1:M:171:ASN:HD22 | 1.36                     | 0.87              |
| 1:B:42:LYS:O       | 1:B:42:LYS:NZ    | 2.08                     | 0.87              |
| 1:T:147:GLN:NE2    | 1:T:149:GLY:O    | 2.10                     | 0.85              |
| 1:G:31:ARG:HH21    | 1:G:37:ARG:HB2   | 1.42                     | 0.85              |
| 1:C:147:GLN:NE2    | 1:C:149:GLY:O    | 2.11                     | 0.84              |
| 1:B:32:LEU:CD2     | 1:L:531:VAL:CG2  | 2.53                     | 0.83              |
| 1:K:505:ARG:HH21   | 1:L:69:ASN:HD22  | 1.25                     | 0.83              |
| 1:N:99:ALA:HB2     | 1:N:112:ILE:HG21 | 1.62                     | 0.82              |
| 1:S:508:ASP:HB2    | 1:I:4:VAL:HG11   | 1.62                     | 0.81              |
| 1:K:484:ARG:HH12   | 1:L:121:ASP:HB3  | 1.45                     | 0.81              |
| 1:K:95:LEU:HD11    | 1:K:116:ILE:HD11 | 1.62                     | 0.81              |
| 1:M:520:LYS:NZ     | 1:N:6:ASN:O      | 2.12                     | 0.81              |
| 1:G:520:LYS:NZ     | 1:H:5:ILE:O      | 2.15                     | 0.80              |
| 1:V:497:THR:HG21   | 1:L:16:ASN:HD21  | 1.47                     | 0.80              |
| 1:M:518:MET:SD     | 1:M:522:GLN:NE2  | 2.56                     | 0.79              |
| 1:G:156:ILE:HD11   | 1:R:125:ARG:HH12 | 1.49                     | 0.78              |
| 1:I:95:LEU:HD11    | 1:I:116:ILE:HD11 | 1.65                     | 0.78              |
| 1:U:523:ILE:HD11   | 1:L:540:GLN:HG3  | 1.65                     | 0.78              |
| 1:I:147:GLN:NE2    | 1:I:149:GLY:O    | 2.16                     | 0.78              |
| 1:B:166:ASP:HB2    | 1:B:171:ASN:HD22 | 1.49                     | 0.77              |
| 1:B:32:LEU:HD22    | 1:L:531:VAL:HG23 | 1.62                     | 0.77              |
| 1:O:147:GLN:NE2    | 1:O:149:GLY:O    | 2.17                     | 0.77              |
| 1:R:482:GLN:OE1    | 1:H:42:LYS:NZ    | 2.17                     | 0.77              |
| 1:S:147:GLN:NE2    | 1:S:149:GLY:O    | 2.17                     | 0.77              |
| 1:B:36:LEU:O       | 1:B:36:LEU:HD12  | 1.85                     | 0.76              |
| 1:B:518:MET:SD     | 1:L:534:LYS:NZ   | 2.53                     | 0.76              |
| 1:E:10:LEU:HD21    | 1:P:29:ILE:HG21  | 1.68                     | 0.76              |
| 1:N:10:LEU:HD21    | 1:O:29:ILE:HG21  | 1.68                     | 0.76              |
| 1:H:506:ILE:O      | 1:I:66:ARG:NH2   | 2.19                     | 0.75              |
| 1:R:166:ASP:OD1    | 1:R:171:ASN:ND2  | 2.20                     | 0.75              |
| 1:E:147:GLN:NE2    | 1:E:149:GLY:O    | 2.19                     | 0.75              |
| 1:T:137:VAL:HG23   | 1:T:138:LEU:HG   | 1.69                     | 0.74              |
| 1:T:490:THR:O      | 1:T:494:ASN:ND2  | 2.19                     | 0.74              |
| 1:O:173:PHE:HE1    | 1:O:460:PRO:HB3  | 1.51                     | 0.74              |
| 1:V:162:LYS:NZ     | 1:V:164:ASP:OD2  | 2.21                     | 0.74              |
| 1:N:166:ASP:OD1    | 1:N:171:ASN:ND2  | 2.21                     | 0.74              |
| 1:S:511:TYR:HE2    | 1:I:5:ILE:H      | 1.36                     | 0.73              |
| 1:F:491:ASN:ND2    | 1:G:84:GLU:OE1   | 2.21                     | 0.73              |
| 1:N:164:ASP:OD1    | 1:N:165:SER:N    | 2.22                     | 0.73              |
| 1:M:38[B]:ILE:HG23 | 1:M:41:ALA:HB2   | 1.69                     | 0.73              |
| 1:L:147:GLN:NE2    | 1:L:149:GLY:O    | 2.22                     | 0.73              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:M:38[A]:ILE:HG23 | 1:M:41:ALA:HB2   | 1.70                     | 0.73              |
| 1:A:147:GLN:HG2    | 1:A:155:THR:HG22 | 1.69                     | 0.72              |
| 1:N:538:VAL:O      | 1:N:541:GLN:NE2  | 2.22                     | 0.72              |
| 1:F:147:GLN:NE2    | 1:F:149:GLY:O    | 2.22                     | 0.72              |
| 1:O:538:VAL:O      | 1:O:541:GLN:NE2  | 2.22                     | 0.72              |
| 1:A:501:GLU:OE2    | 1:A:505:ARG:NH2  | 2.20                     | 0.72              |
| 1:N:145:LYS:HB3    | 1:N:155:THR:HG21 | 1.71                     | 0.72              |
| 1:P:99:ALA:HB2     | 1:P:112:ILE:HG21 | 1.72                     | 0.71              |
| 1:E:162:LYS:NZ     | 1:E:164:ASP:OD2  | 2.23                     | 0.71              |
| 1:L:31:ARG:NH1     | 1:L:37:ARG:O     | 2.24                     | 0.71              |
| 1:B:99:ALA:HB2     | 1:B:112:ILE:HG21 | 1.72                     | 0.71              |
| 1:G:484:ARG:HD2    | 1:R:118:SER:HB2  | 1.72                     | 0.71              |
| 1:I:492:LEU:O      | 1:I:496:THR:HG23 | 1.91                     | 0.71              |
| 1:I:544:SER:HA     | 1:I:547:GLN:HE21 | 1.56                     | 0.71              |
| 1:U:116:ILE:HG21   | 1:U:173:PHE:HD2  | 1.55                     | 0.71              |
| 1:Q:101:THR:HG23   | 1:G:146:ILE:HA   | 1.72                     | 0.70              |
| 1:D:163:ILE:HG23   | 1:D:168:LEU:HD11 | 1.73                     | 0.70              |
| 1:B:162:LYS:NZ     | 1:B:164:ASP:OD2  | 2.25                     | 0.70              |
| 1:N:497:THR:HG21   | 1:D:16:ASN:HD22  | 1.57                     | 0.70              |
| 1:G:27:SER:O       | 1:G:31:ARG:HG3   | 1.90                     | 0.70              |
| 1:Q:9:SER:HA       | 1:Q:12:LEU:HD12  | 1.72                     | 0.70              |
| 1:D:162:LYS:NZ     | 1:D:167:THR:OG1  | 2.23                     | 0.70              |
| 1:B:129:GLN:OE1    | 1:L:151:ASN:ND2  | 2.25                     | 0.70              |
| 1:C:63:GLN:NE2     | 1:C:67:ASN:OD1   | 2.25                     | 0.69              |
| 1:Q:18:ILE:HG22    | 1:Q:22:GLN:HE22  | 1.56                     | 0.69              |
| 1:B:90:GLN:NE2     | 1:A:56:SER:OG    | 2.25                     | 0.69              |
| 1:P:137:VAL:HG23   | 1:P:138:LEU:HG   | 1.73                     | 0.69              |
| 1:J:31:ARG:NH1     | 1:J:37:ARG:O     | 2.25                     | 0.69              |
| 1:N:50:ILE:HD12    | 1:O:133:ASN:HD21 | 1.57                     | 0.69              |
| 1:D:164:ASP:OD1    | 1:D:165:SER:N    | 2.25                     | 0.69              |
| 1:O:90:GLN:NE2     | 1:E:55:THR:OG1   | 2.26                     | 0.69              |
| 1:C:115:GLU:OE2    | 1:C:119:ARG:NH2  | 2.26                     | 0.69              |
| 1:D:15:GLN:HA      | 1:D:18:ILE:HD12  | 1.75                     | 0.69              |
| 1:P:168:LEU:HD23   | 1:P:467:ALA:HB1  | 1.75                     | 0.69              |
| 1:V:497:THR:HG21   | 1:L:16:ASN:ND2   | 2.07                     | 0.69              |
| 1:G:58:ILE:HG23    | 1:G:496:THR:HG23 | 1.74                     | 0.69              |
| 1:I:3:GLN:HG3      | 1:I:4:VAL:H      | 1.58                     | 0.68              |
| 1:O:523:ILE:HG13   | 1:P:539:PRO:HB2  | 1.74                     | 0.68              |
| 1:G:18:ILE:HG22    | 1:G:22:GLN:HE22  | 1.58                     | 0.68              |
| 1:E:538:VAL:O      | 1:E:541:GLN:NE2  | 2.26                     | 0.68              |
| 1:D:58:ILE:HG23    | 1:D:496:THR:HG23 | 1.76                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:92:ILE:HG23  | 1:K:116:ILE:HD12 | 1.74                     | 0.68              |
| 1:P:95:LEU:HD11  | 1:P:112:ILE:HG12 | 1.76                     | 0.68              |
| 1:G:174:ASN:HB3  | 1:G:456:SER:HA   | 1.76                     | 0.68              |
| 1:T:94:GLU:OE2   | 1:J:63:GLN:NE2   | 2.26                     | 0.68              |
| 1:D:170:LEU:HD12 | 1:D:171:ASN:N    | 2.09                     | 0.67              |
| 1:Q:147:GLN:NE2  | 1:Q:149:GLY:O    | 2.28                     | 0.67              |
| 1:K:3:GLN:NE2    | 1:L:19:ASN:OD1   | 2.27                     | 0.67              |
| 1:K:15:GLN:O     | 1:K:19:ASN:ND2   | 2.26                     | 0.67              |
| 1:V:137:VAL:HG23 | 1:V:138:LEU:HG   | 1.75                     | 0.67              |
| 1:B:163:ILE:HG23 | 1:B:168:LEU:HD11 | 1.76                     | 0.67              |
| 1:P:162:LYS:NZ   | 1:P:167:THR:OG1  | 2.26                     | 0.67              |
| 1:B:37:ARG:HB2   | 1:B:508:ASP:O    | 1.95                     | 0.67              |
| 1:O:533:ALA:O    | 1:O:537:GLN:NE2  | 2.28                     | 0.67              |
| 1:I:505:ARG:NH2  | 1:T:76:GLN:OE1   | 2.27                     | 0.67              |
| 1:K:82:LEU:HD21  | 1:K:474:PHE:HD2  | 1.61                     | 0.66              |
| 1:O:163:ILE:HG23 | 1:O:168:LEU:HD21 | 1.78                     | 0.66              |
| 1:B:88:ASN:OD1   | 1:B:119:ARG:NH1  | 2.27                     | 0.66              |
| 1:R:525:GLN:NE2  | 1:R:529:ASN:OD1  | 2.28                     | 0.66              |
| 1:H:151:ASN:ND2  | 1:I:129:GLN:OE1  | 2.28                     | 0.66              |
| 1:J:542:VAL:HA   | 1:J:545:LEU:HD12 | 1.78                     | 0.66              |
| 1:B:44:ASP:OD2   | 1:B:44:ASP:N     | 2.27                     | 0.66              |
| 1:Q:93:ARG:HE    | 1:Q:461:LEU:HD22 | 1.61                     | 0.66              |
| 1:R:506:ILE:O    | 1:S:66:ARG:NH2   | 2.28                     | 0.66              |
| 1:V:543:LEU:HD23 | 1:V:546:LEU:HD12 | 1.78                     | 0.66              |
| 1:O:94:GLU:HB3   | 1:E:59:LYS:HZ2   | 1.60                     | 0.66              |
| 1:C:156:ILE:HG23 | 1:C:484:ARG:HD3  | 1.78                     | 0.65              |
| 1:P:88:ASN:OD1   | 1:P:119:ARG:NH1  | 2.29                     | 0.65              |
| 1:H:113:GLN:HE22 | 1:H:174:ASN:HA   | 1.61                     | 0.65              |
| 1:N:67:ASN:HD22  | 1:N:147:GLN:HB3  | 1.60                     | 0.65              |
| 1:A:505:ARG:NH1  | 1:C:73:SER:OG    | 2.30                     | 0.65              |
| 1:M:490:THR:O    | 1:M:494:ASN:ND2  | 2.28                     | 0.65              |
| 1:N:90:GLN:NE2   | 1:D:56:SER:OG    | 2.29                     | 0.65              |
| 1:G:505:ARG:NH1  | 1:R:73:SER:OG    | 2.30                     | 0.65              |
| 1:B:79:GLU:OE1   | 1:B:482:GLN:NE2  | 2.30                     | 0.65              |
| 1:S:88:ASN:OD1   | 1:S:119:ARG:NH1  | 2.30                     | 0.65              |
| 1:K:174:ASN:H    | 1:K:457:THR:HG23 | 1.62                     | 0.65              |
| 1:T:31:ARG:HH11  | 1:T:37:ARG:HB2   | 1.62                     | 0.64              |
| 1:N:490:THR:O    | 1:N:494:ASN:ND2  | 2.30                     | 0.64              |
| 1:P:523:ILE:HD12 | 1:G:543:LEU:HD21 | 1.78                     | 0.64              |
| 1:I:84:GLU:O     | 1:I:88:ASN:ND2   | 2.31                     | 0.64              |
| 1:T:94:GLU:HG3   | 1:J:59:LYS:HE2   | 1.79                     | 0.64              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:110:ASP:OD2    | 1:G:176:ASN:ND2  | 2.30                     | 0.64              |
| 1:H:80:GLY:O       | 1:H:83:SER:OG    | 2.11                     | 0.64              |
| 1:M:14:THR:O       | 1:M:18:ILE:HG13  | 1.98                     | 0.64              |
| 1:D:75:ALA:HB1     | 1:D:482:GLN:HE21 | 1.62                     | 0.64              |
| 1:G:92:ILE:O       | 1:G:96:THR:HG23  | 1.98                     | 0.64              |
| 1:H:505:ARG:NH1    | 1:I:73:SER:OG    | 2.31                     | 0.64              |
| 1:T:163:ILE:HG23   | 1:T:168:LEU:HD11 | 1.80                     | 0.64              |
| 1:V:120:LEU:HD11   | 1:V:173:PHE:HD2  | 1.61                     | 0.64              |
| 1:S:99:ALA:HB2     | 1:S:112:ILE:HG21 | 1.79                     | 0.64              |
| 1:S:168:LEU:HD23   | 1:S:467:ALA:HB1  | 1.79                     | 0.64              |
| 1:V:91:ARG:NH2     | 1:V:94:GLU:OE1   | 2.31                     | 0.64              |
| 1:V:74:VAL:HG11    | 1:V:144:MET:HE1  | 1.78                     | 0.63              |
| 1:V:101:THR:OG1    | 1:L:67:ASN:ND2   | 2.31                     | 0.63              |
| 1:P:101:THR:HB     | 1:F:67:ASN:HD21  | 1.64                     | 0.63              |
| 1:Q:140:LYS:HA     | 1:Q:162:LYS:HE3  | 1.80                     | 0.63              |
| 1:T:525:GLN:O      | 1:T:529:ASN:ND2  | 2.32                     | 0.63              |
| 1:P:497:THR:HG21   | 1:F:16:ASN:HD21  | 1.63                     | 0.63              |
| 1:T:64:ALA:HB1     | 1:T:148:VAL:HA   | 1.80                     | 0.63              |
| 1:T:88:ASN:ND2     | 1:T:122:GLU:OE1  | 2.31                     | 0.63              |
| 1:E:163:ILE:HG23   | 1:E:168:LEU:HD11 | 1.81                     | 0.63              |
| 1:S:79:GLU:OE1     | 1:S:482:GLN:NE2  | 2.32                     | 0.63              |
| 1:E:537:GLN:O      | 1:E:540:GLN:NE2  | 2.32                     | 0.63              |
| 1:G:82:LEU:HG      | 1:G:471:ILE:HD11 | 1.80                     | 0.63              |
| 1:H:170:LEU:HD13   | 1:H:173:PHE:HB2  | 1.81                     | 0.63              |
| 1:S:510:ASP:H      | 1:I:4:VAL:HG12   | 1.63                     | 0.63              |
| 1:V:14:THR:O       | 1:V:18:ILE:HG13  | 1.98                     | 0.63              |
| 1:J:491:ASN:C      | 1:J:491:ASN:HD22 | 2.06                     | 0.63              |
| 1:I:154:GLN:NE2    | 1:T:129:GLN:OE1  | 2.31                     | 0.63              |
| 1:N:173:PHE:HE1    | 1:N:460:PRO:HB3  | 1.63                     | 0.62              |
| 1:D:119:ARG:O      | 1:D:123:ILE:HG12 | 1.99                     | 0.62              |
| 1:V:38[A]:ILE:HG23 | 1:V:41:ALA:HB2   | 1.80                     | 0.62              |
| 1:V:38[B]:ILE:HG23 | 1:V:41:ALA:HB2   | 1.80                     | 0.62              |
| 1:B:32:LEU:CD2     | 1:L:531:VAL:HB   | 2.29                     | 0.62              |
| 1:K:86:ASN:HB2     | 1:K:475:ARG:HH21 | 1.64                     | 0.62              |
| 1:L:31:ARG:NH1     | 1:L:43:ASP:OD2   | 2.23                     | 0.62              |
| 1:R:101:THR:HG23   | 1:H:146:ILE:HA   | 1.81                     | 0.62              |
| 1:H:158:ILE:HG12   | 1:H:481:VAL:HG21 | 1.82                     | 0.62              |
| 1:M:98:GLN:NE2     | 1:C:63:GLN:OE1   | 2.28                     | 0.62              |
| 1:R:497:THR:HG21   | 1:H:16:ASN:HD21  | 1.65                     | 0.62              |
| 1:V:493:ASN:O      | 1:V:497:THR:HG23 | 2.00                     | 0.62              |
| 1:E:112:ILE:O      | 1:E:116:ILE:HG12 | 1.99                     | 0.62              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:P:138:LEU:HD22   | 1:P:163:ILE:HD12 | 1.81                     | 0.62              |
| 1:G:147:GLN:NE2    | 1:G:149:GLY:O    | 2.27                     | 0.62              |
| 1:J:44:ASP:OD1     | 1:U:91:ARG:NH2   | 2.32                     | 0.62              |
| 1:J:487:SER:OG     | 1:K:84:GLU:OE1   | 2.18                     | 0.62              |
| 1:N:101:THR:HG22   | 1:N:103:THR:H    | 1.65                     | 0.62              |
| 1:Q:497:THR:HG21   | 1:G:16:ASN:HD21  | 1.64                     | 0.62              |
| 1:J:137:VAL:HG23   | 1:J:138:LEU:HG   | 1.81                     | 0.62              |
| 1:K:483:ASN:HB3    | 1:L:119:ARG:HH12 | 1.65                     | 0.62              |
| 1:F:38[A]:ILE:HG23 | 1:F:41:ALA:HB2   | 1.82                     | 0.62              |
| 1:G:166:ASP:HA     | 1:G:171:ASN:HB2  | 1.81                     | 0.62              |
| 1:F:38[B]:ILE:HG23 | 1:F:41:ALA:HB2   | 1.82                     | 0.62              |
| 1:G:101:THR:O      | 1:G:104:ASN:ND2  | 2.33                     | 0.62              |
| 1:T:542:VAL:HA     | 1:T:545:LEU:HD12 | 1.82                     | 0.62              |
| 1:N:101:THR:OG1    | 1:D:67:ASN:ND2   | 2.26                     | 0.62              |
| 1:S:9:SER:HA       | 1:S:12:LEU:HD12  | 1.81                     | 0.62              |
| 1:J:106:ASP:OD1    | 1:J:107:SER:N    | 2.32                     | 0.62              |
| 1:V:110:ASP:OD1    | 1:V:176:ASN:ND2  | 2.32                     | 0.62              |
| 1:U:93:ARG:HE      | 1:K:56:SER:HG    | 1.48                     | 0.61              |
| 1:T:90:GLN:OE1     | 1:J:56:SER:OG    | 2.16                     | 0.61              |
| 1:N:94:GLU:OE1     | 1:D:59:LYS:HB3   | 2.01                     | 0.61              |
| 1:B:523:ILE:HG23   | 1:C:543:LEU:HD11 | 1.83                     | 0.61              |
| 1:M:89:LEU:HA      | 1:M:92:ILE:HD12  | 1.81                     | 0.61              |
| 1:O:531:VAL:HA     | 1:O:534:LYS:HE2  | 1.83                     | 0.61              |
| 1:U:35:GLY:C       | 1:K:6:ASN:HD21   | 2.08                     | 0.61              |
| 1:M:137:VAL:HG23   | 1:M:138:LEU:HG   | 1.81                     | 0.61              |
| 1:D:54:PHE:HE1     | 1:D:499:LEU:HD22 | 1.65                     | 0.61              |
| 1:H:170:LEU:HD12   | 1:H:171:ASN:N    | 2.15                     | 0.61              |
| 1:B:534:LYS:NZ     | 1:M:29:ILE:HG12  | 2.15                     | 0.61              |
| 1:V:92:ILE:HD12    | 1:V:116:ILE:HG23 | 1.82                     | 0.61              |
| 1:R:494:ASN:O      | 1:R:498:ASN:ND2  | 2.34                     | 0.61              |
| 1:H:170:LEU:HD12   | 1:H:171:ASN:H    | 1.65                     | 0.60              |
| 1:A:99:ALA:HB2     | 1:A:112:ILE:HG21 | 1.82                     | 0.60              |
| 1:M:90:GLN:OE1     | 1:C:56:SER:OG    | 2.19                     | 0.60              |
| 1:C:541:GLN:OE1    | 1:N:529:ASN:ND2  | 2.15                     | 0.60              |
| 1:I:159:ASP:OD2    | 1:I:161:LYS:NZ   | 2.34                     | 0.60              |
| 1:C:68:ALA:HB2     | 1:C:148:VAL:HG12 | 1.84                     | 0.60              |
| 1:G:480:ALA:O      | 1:G:484:ARG:HG3  | 2.01                     | 0.60              |
| 1:R:120:LEU:HD23   | 1:R:123:ILE:HD12 | 1.83                     | 0.60              |
| 1:B:166:ASP:HA     | 1:B:171:ASN:HB2  | 1.83                     | 0.60              |
| 1:E:154:GLN:HE22   | 1:P:125:ARG:HG3  | 1.65                     | 0.60              |
| 1:P:94:GLU:HB2     | 1:F:59:LYS:CE    | 2.31                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:91:ARG:HE    | 1:I:95:LEU:HD23  | 1.67                     | 0.60              |
| 1:V:101:THR:HG22 | 1:V:103:THR:H    | 1.66                     | 0.60              |
| 1:N:137:VAL:HG23 | 1:N:138:LEU:HD13 | 1.84                     | 0.60              |
| 1:U:112:ILE:O    | 1:U:116:ILE:HD12 | 2.02                     | 0.60              |
| 1:U:163:ILE:HG23 | 1:U:168:LEU:HD11 | 1.84                     | 0.60              |
| 1:M:119:ARG:O    | 1:M:123:ILE:HD12 | 2.00                     | 0.60              |
| 1:O:51:ALA:HB1   | 1:O:503:GLN:HE22 | 1.66                     | 0.60              |
| 1:I:31:ARG:NH2   | 1:I:37:ARG:HG3   | 2.17                     | 0.60              |
| 1:N:174:ASN:ND2  | 1:N:177:GLY:O    | 2.34                     | 0.60              |
| 1:P:163:ILE:HG23 | 1:P:168:LEU:HD11 | 1.83                     | 0.60              |
| 1:B:170:LEU:HD13 | 1:B:173:PHE:CD2  | 2.37                     | 0.60              |
| 1:I:31:ARG:HH22  | 1:I:37:ARG:HG3   | 1.66                     | 0.60              |
| 1:B:534:LYS:HZ2  | 1:M:29:ILE:HG12  | 1.67                     | 0.59              |
| 1:F:113:GLN:HE21 | 1:F:175:VAL:HG22 | 1.66                     | 0.59              |
| 1:L:88:ASN:HB3   | 1:L:123:ILE:HD11 | 1.84                     | 0.59              |
| 1:C:14:THR:O     | 1:C:18:ILE:HG12  | 2.02                     | 0.59              |
| 1:O:472:ASP:OD1  | 1:E:52:ASN:ND2   | 2.33                     | 0.59              |
| 1:S:86:ASN:HD21  | 1:I:52:ASN:ND2   | 2.00                     | 0.59              |
| 1:B:32:LEU:CD2   | 1:L:531:VAL:CB   | 2.80                     | 0.59              |
| 1:F:162:LYS:NZ   | 1:F:167:THR:OG1  | 2.35                     | 0.59              |
| 1:V:166:ASP:HA   | 1:V:171:ASN:HB2  | 1.83                     | 0.59              |
| 1:Q:63:GLN:NE2   | 1:Q:67:ASN:OD1   | 2.35                     | 0.59              |
| 1:G:68:ALA:HB1   | 1:G:485:LEU:HD12 | 1.84                     | 0.59              |
| 1:F:10:LEU:HD21  | 1:G:29:ILE:HD13  | 1.85                     | 0.59              |
| 1:J:93:ARG:HH12  | 1:J:461:LEU:HD13 | 1.67                     | 0.59              |
| 1:K:147:GLN:NE2  | 1:K:149:GLY:O    | 2.29                     | 0.59              |
| 1:C:166:ASP:OD1  | 1:C:171:ASN:ND2  | 2.36                     | 0.59              |
| 1:Q:37:ARG:NH2   | 1:Q:506:ILE:O    | 2.36                     | 0.59              |
| 1:K:151:ASN:H    | 1:K:154:GLN:NE2  | 2.00                     | 0.59              |
| 1:G:158:ILE:HG12 | 1:G:481:VAL:HG21 | 1.84                     | 0.59              |
| 1:H:95:LEU:HD11  | 1:H:116:ILE:HD11 | 1.85                     | 0.59              |
| 1:V:525:GLN:O    | 1:V:529:ASN:ND2  | 2.36                     | 0.59              |
| 1:S:85:ILE:HG23  | 1:S:123:ILE:HD12 | 1.85                     | 0.59              |
| 1:U:510:ASP:HA   | 1:K:3:GLN:HB3    | 1.85                     | 0.59              |
| 1:B:484:ARG:HG2  | 1:M:122:GLU:OE2  | 2.03                     | 0.58              |
| 1:Q:19:ASN:HA    | 1:Q:22:GLN:OE1   | 2.03                     | 0.58              |
| 1:K:82:LEU:HD21  | 1:K:474:PHE:CD2  | 2.38                     | 0.58              |
| 1:D:9:SER:O      | 1:D:13:ILE:HG13  | 2.02                     | 0.58              |
| 1:J:159:ASP:OD2  | 1:J:161:LYS:NZ   | 2.36                     | 0.58              |
| 1:B:493:ASN:HA   | 1:B:496:THR:HG22 | 1.85                     | 0.58              |
| 1:C:478:LEU:O    | 1:C:481:VAL:HG22 | 2.03                     | 0.58              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:Q:26:SER:O       | 1:Q:30:GLU:HG2   | 2.03                     | 0.58              |
| 1:Q:127:SER:OG     | 1:Q:163:ILE:O    | 2.18                     | 0.58              |
| 1:R:12:LEU:HA      | 1:R:15:GLN:HE21  | 1.68                     | 0.58              |
| 1:J:122:GLU:OE2    | 1:J:125:ARG:NH2  | 2.37                     | 0.58              |
| 1:U:534:LYS:HD2    | 1:V:518:MET:HE1  | 1.86                     | 0.58              |
| 1:L:91:ARG:HG2     | 1:L:119:ARG:HH21 | 1.67                     | 0.58              |
| 1:B:143:SER:OG     | 1:B:157:THR:OG1  | 2.22                     | 0.58              |
| 1:N:101:THR:HG23   | 1:D:146:ILE:HA   | 1.85                     | 0.58              |
| 1:G:170:LEU:HD12   | 1:G:170:LEU:H    | 1.68                     | 0.58              |
| 1:H:469:SER:O      | 1:H:473:LYS:HG3  | 2.03                     | 0.58              |
| 1:I:10:LEU:HD13    | 1:T:29:ILE:HG21  | 1.84                     | 0.58              |
| 1:N:170:LEU:HG     | 1:N:171:ASN:H    | 1.69                     | 0.58              |
| 1:D:138:LEU:HD22   | 1:D:163:ILE:HD13 | 1.85                     | 0.58              |
| 1:E:537:GLN:HA     | 1:E:540:GLN:HE22 | 1.67                     | 0.58              |
| 1:P:176:ASN:OD1    | 1:P:177:GLY:N    | 2.37                     | 0.58              |
| 1:S:92:ILE:HG23    | 1:S:116:ILE:HD12 | 1.84                     | 0.58              |
| 1:C:486:ASP:HA     | 1:C:489:VAL:HG12 | 1.86                     | 0.58              |
| 1:D:174:ASN:ND2    | 1:D:177:GLY:O    | 2.37                     | 0.58              |
| 1:R:162:LYS:NZ     | 1:R:167:THR:OG1  | 2.31                     | 0.58              |
| 1:K:505:ARG:HH21   | 1:L:69:ASN:ND2   | 1.99                     | 0.58              |
| 1:L:55:THR:O       | 1:L:59:LYS:HG3   | 2.03                     | 0.58              |
| 1:L:525:GLN:O      | 1:L:529:ASN:ND2  | 2.37                     | 0.58              |
| 1:N:86:ASN:O       | 1:N:90:GLN:HG2   | 2.03                     | 0.58              |
| 1:D:99:ALA:HB2     | 1:D:112:ILE:HG21 | 1.86                     | 0.58              |
| 1:I:27:SER:O       | 1:I:31:ARG:HG3   | 2.04                     | 0.57              |
| 1:I:505:ARG:HD2    | 1:T:69:ASN:HB3   | 1.86                     | 0.57              |
| 1:P:16:ASN:HB3     | 1:P:20:LYS:NZ    | 2.19                     | 0.57              |
| 1:V:504:SER:HB3    | 1:L:7:THR:HG21   | 1.86                     | 0.57              |
| 1:G:545:LEU:HD23   | 1:R:533:ALA:HB2  | 1.87                     | 0.57              |
| 1:S:131:GLN:HA     | 1:S:136:ASN:HA   | 1.86                     | 0.57              |
| 1:B:168:LEU:HD23   | 1:B:467:ALA:HB1  | 1.84                     | 0.57              |
| 1:M:91:ARG:NH1     | 1:M:94:GLU:OE1   | 2.38                     | 0.57              |
| 1:O:122:GLU:OE2    | 1:O:125:ARG:NH2  | 2.33                     | 0.57              |
| 1:M:113:GLN:NE2    | 1:M:173:PHE:O    | 2.28                     | 0.57              |
| 1:J:154:GLN:OE1    | 1:K:129:GLN:NE2  | 2.36                     | 0.57              |
| 1:U:101:THR:HG22   | 1:U:103:THR:H    | 1.69                     | 0.57              |
| 1:B:531:VAL:HG11   | 1:M:33:SER:HA    | 1.86                     | 0.57              |
| 1:J:10:LEU:HD23    | 1:K:29:ILE:HG21  | 1.87                     | 0.57              |
| 1:E:161:LYS:H      | 1:E:474:PHE:HE2  | 1.52                     | 0.57              |
| 1:P:38[B]:ILE:HG23 | 1:P:41:ALA:HB2   | 1.86                     | 0.57              |
| 1:V:93:ARG:NH1     | 1:L:56:SER:OG    | 2.38                     | 0.57              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:E:31:ARG:HD3     | 1:E:37:ARG:HG3   | 1.87                     | 0.57              |
| 1:Q:43:ASP:CG      | 1:Q:44:ASP:H     | 2.13                     | 0.57              |
| 1:V:88:ASN:OD1     | 1:V:119:ARG:NH1  | 2.38                     | 0.57              |
| 1:A:170:LEU:O      | 1:A:172:GLY:N    | 2.37                     | 0.57              |
| 1:P:94:GLU:HB2     | 1:F:59:LYS:HE2   | 1.87                     | 0.57              |
| 1:K:483:ASN:HB3    | 1:L:119:ARG:NH1  | 2.20                     | 0.57              |
| 1:V:520:LYS:O      | 1:V:524:ILE:HG12 | 2.04                     | 0.57              |
| 1:N:78:THR:HG23    | 1:N:138:LEU:HD11 | 1.87                     | 0.57              |
| 1:K:154:GLN:OE1    | 1:L:129:GLN:HB3  | 2.03                     | 0.57              |
| 1:C:148:VAL:HG11   | 1:C:156:ILE:HD12 | 1.85                     | 0.56              |
| 1:D:166:ASP:OD1    | 1:D:167:THR:N    | 2.38                     | 0.56              |
| 1:O:14:THR:O       | 1:O:18:ILE:HG13  | 2.05                     | 0.56              |
| 1:P:159:ASP:OD1    | 1:P:161:LYS:NZ   | 2.38                     | 0.56              |
| 1:J:63:GLN:OE1     | 1:J:66:ARG:NE    | 2.38                     | 0.56              |
| 1:V:83:SER:HB2     | 1:V:475:ARG:NH1  | 2.19                     | 0.56              |
| 1:Q:514:GLU:HA     | 1:Q:517:ASN:ND2  | 2.21                     | 0.56              |
| 1:G:141:ASP:OD1    | 1:G:142:GLY:N    | 2.39                     | 0.56              |
| 1:G:534:LYS:NZ     | 1:H:546:LEU:O    | 2.38                     | 0.56              |
| 1:E:516:SER:O      | 1:E:520:LYS:HG3  | 2.06                     | 0.56              |
| 1:Q:95:LEU:HD12    | 1:Q:112:ILE:HG23 | 1.88                     | 0.56              |
| 1:J:162:LYS:NZ     | 1:J:164:ASP:OD2  | 2.32                     | 0.56              |
| 1:P:38[A]:ILE:HG23 | 1:P:41:ALA:HB2   | 1.86                     | 0.56              |
| 1:F:144:MET:HB2    | 1:F:160:LEU:HD11 | 1.85                     | 0.56              |
| 1:G:168:LEU:HD12   | 1:G:467:ALA:HB1  | 1.86                     | 0.56              |
| 1:J:164:ASP:O      | 1:J:168:LEU:HD12 | 2.05                     | 0.56              |
| 1:P:156:ILE:HG13   | 1:P:484:ARG:NH2  | 2.21                     | 0.56              |
| 1:R:461:LEU:HB2    | 1:H:152:ASP:HB2  | 1.88                     | 0.56              |
| 1:J:147:GLN:NE2    | 1:J:149:GLY:O    | 2.36                     | 0.56              |
| 1:K:174:ASN:HB3    | 1:K:456:SER:HA   | 1.86                     | 0.56              |
| 1:O:69:ASN:O       | 1:O:72:ILE:HG22  | 2.05                     | 0.56              |
| 1:E:59:LYS:HA      | 1:E:62:THR:HG22  | 1.88                     | 0.56              |
| 1:E:18:ILE:O       | 1:E:22:GLN:HG3   | 2.05                     | 0.56              |
| 1:L:13:ILE:HA      | 1:L:16:ASN:ND2   | 2.20                     | 0.56              |
| 1:F:501:GLU:O      | 1:F:505:ARG:HG3  | 2.05                     | 0.56              |
| 1:E:69:ASN:HA      | 1:E:72:ILE:HG22  | 1.88                     | 0.56              |
| 1:Q:166:ASP:OD1    | 1:Q:167:THR:N    | 2.39                     | 0.56              |
| 1:G:55:THR:O       | 1:G:59:LYS:HG3   | 2.07                     | 0.56              |
| 1:Q:483:ASN:OD1    | 1:G:42:LYS:NZ    | 2.38                     | 0.55              |
| 1:P:170:LEU:C      | 1:P:172:GLY:H    | 2.13                     | 0.55              |
| 1:V:541:GLN:O      | 1:V:545:LEU:HG   | 2.06                     | 0.55              |
| 1:C:88:ASN:HB3     | 1:C:119:ARG:HG3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:O:164:ASP:OD1  | 1:O:167:THR:N    | 2.35                     | 0.55              |
| 1:T:50:ILE:HD13  | 1:T:53:ARG:HH21  | 1.70                     | 0.55              |
| 1:M:101:THR:OG1  | 1:C:67:ASN:ND2   | 2.37                     | 0.55              |
| 1:G:64:ALA:HB1   | 1:G:148:VAL:HA   | 1.87                     | 0.55              |
| 1:S:51:ALA:O     | 1:S:55:THR:HG23  | 2.06                     | 0.55              |
| 1:U:54:PHE:HB3   | 1:U:503:GLN:HE21 | 1.70                     | 0.55              |
| 1:A:8:ASN:HB2    | 1:L:520:LYS:NZ   | 2.22                     | 0.55              |
| 1:E:170:LEU:HG   | 1:E:171:ASN:H    | 1.71                     | 0.55              |
| 1:Q:516:SER:O    | 1:Q:520:LYS:HG3  | 2.07                     | 0.55              |
| 1:U:103:THR:O    | 1:K:133:ASN:ND2  | 2.40                     | 0.55              |
| 1:B:32:LEU:HD22  | 1:L:531:VAL:CB   | 2.34                     | 0.55              |
| 1:A:106:ASP:OD1  | 1:A:107:SER:N    | 2.40                     | 0.55              |
| 1:M:170:LEU:C    | 1:M:172:GLY:H    | 2.13                     | 0.55              |
| 1:O:98:GLN:HB3   | 1:E:63:GLN:CD    | 2.32                     | 0.55              |
| 1:G:9:SER:O      | 1:G:13:ILE:HG12  | 2.06                     | 0.55              |
| 1:S:461:LEU:HB2  | 1:I:152:ASP:HB2  | 1.89                     | 0.55              |
| 1:A:79:GLU:OE1   | 1:A:482:GLN:NE2  | 2.39                     | 0.55              |
| 1:C:51:ALA:O     | 1:C:55:THR:HG23  | 2.07                     | 0.55              |
| 1:N:483:ASN:ND2  | 1:D:42:LYS:O     | 2.39                     | 0.55              |
| 1:U:522:GLN:O    | 1:U:526:GLN:HG3  | 2.07                     | 0.55              |
| 1:N:154:GLN:NE2  | 1:O:129:GLN:HG3  | 2.22                     | 0.55              |
| 1:M:519:SER:O    | 1:M:523:ILE:HG12 | 2.07                     | 0.55              |
| 1:N:108:ASP:O    | 1:N:112:ILE:HG12 | 2.06                     | 0.55              |
| 1:E:88:ASN:OD1   | 1:E:119:ARG:NH1  | 2.40                     | 0.55              |
| 1:F:113:GLN:HE21 | 1:F:175:VAL:H    | 1.55                     | 0.55              |
| 1:G:542:VAL:HA   | 1:G:545:LEU:HD12 | 1.88                     | 0.55              |
| 1:R:86:ASN:C     | 1:R:86:ASN:HD22  | 2.13                     | 0.55              |
| 1:D:170:LEU:HD22 | 1:D:173:PHE:CD2  | 2.40                     | 0.55              |
| 1:E:37:ARG:NH2   | 1:E:506:ILE:O    | 2.39                     | 0.55              |
| 1:F:487:SER:OG   | 1:G:84:GLU:OE2   | 2.23                     | 0.55              |
| 1:O:534:LYS:O    | 1:O:538:VAL:HG23 | 2.07                     | 0.54              |
| 1:N:170:LEU:HD12 | 1:N:173:PHE:HB2  | 1.88                     | 0.54              |
| 1:P:491:ASN:HB2  | 1:Q:84:GLU:OE2   | 2.07                     | 0.54              |
| 1:Q:137:VAL:HG23 | 1:Q:138:LEU:HG   | 1.90                     | 0.54              |
| 1:V:494:ASN:O    | 1:V:498:ASN:ND2  | 2.41                     | 0.54              |
| 1:O:516:SER:O    | 1:O:520:LYS:HG2  | 2.07                     | 0.54              |
| 1:E:127:SER:OG   | 1:E:163:ILE:O    | 2.18                     | 0.54              |
| 1:R:99:ALA:HB2   | 1:R:112:ILE:HG21 | 1.88                     | 0.54              |
| 1:J:17:ASN:N     | 1:J:17:ASN:HD22  | 2.04                     | 0.54              |
| 1:P:497:THR:HG21 | 1:F:16:ASN:ND2   | 2.23                     | 0.54              |
| 1:S:490:THR:O    | 1:S:494:ASN:ND2  | 2.40                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:72:ILE:O     | 1:J:76:GLN:HG3   | 2.07                     | 0.54              |
| 1:V:112:ILE:O    | 1:V:116:ILE:HG13 | 2.08                     | 0.54              |
| 1:V:485:LEU:O    | 1:V:489:VAL:HG23 | 2.08                     | 0.54              |
| 1:L:546:LEU:HD22 | 1:L:547:GLN:NE2  | 2.22                     | 0.54              |
| 1:B:137:VAL:HG23 | 1:B:138:LEU:HG   | 1.88                     | 0.54              |
| 1:E:55:THR:O     | 1:E:59:LYS:HG2   | 2.07                     | 0.54              |
| 1:E:519:SER:O    | 1:E:523:ILE:HG12 | 2.08                     | 0.54              |
| 1:R:10:LEU:O     | 1:R:14:THR:HG23  | 2.08                     | 0.54              |
| 1:I:55:THR:O     | 1:I:59:LYS:HG2   | 2.07                     | 0.54              |
| 1:K:122:GLU:OE1  | 1:K:125:ARG:NH2  | 2.39                     | 0.54              |
| 1:C:541:GLN:NE2  | 1:C:544:SER:OG   | 2.41                     | 0.54              |
| 1:O:173:PHE:CE1  | 1:O:460:PRO:HB3  | 2.37                     | 0.54              |
| 1:Q:36:LEU:O     | 1:Q:39:ASN:ND2   | 2.41                     | 0.54              |
| 1:Q:93:ARG:NH2   | 1:G:150:ALA:O    | 2.41                     | 0.54              |
| 1:S:32:LEU:HD12  | 1:S:511:TYR:HD1  | 1.71                     | 0.54              |
| 1:O:170:LEU:HD13 | 1:O:173:PHE:CD1  | 2.43                     | 0.54              |
| 1:T:31:ARG:NH1   | 1:T:37:ARG:O     | 2.41                     | 0.54              |
| 1:J:152:ASP:OD1  | 1:J:153:GLY:N    | 2.40                     | 0.54              |
| 1:U:170:LEU:HD13 | 1:U:173:PHE:CD1  | 2.42                     | 0.54              |
| 1:N:491:ASN:HD21 | 1:O:126:VAL:HG23 | 1.73                     | 0.54              |
| 1:Q:97:VAL:HG13  | 1:G:147:GLN:HE22 | 1.73                     | 0.54              |
| 1:I:82:LEU:HD12  | 1:I:471:ILE:HG23 | 1.89                     | 0.54              |
| 1:B:102:GLY:HA3  | 1:A:145:LYS:HB3  | 1.89                     | 0.54              |
| 1:C:170:LEU:C    | 1:C:172:GLY:H    | 2.14                     | 0.54              |
| 1:G:484:ARG:NE   | 1:R:122:GLU:OE2  | 2.36                     | 0.54              |
| 1:H:130:THR:HG21 | 1:H:138:LEU:HD12 | 1.89                     | 0.54              |
| 1:S:158:ILE:HG12 | 1:S:481:VAL:HG21 | 1.89                     | 0.54              |
| 1:C:82:LEU:HD21  | 1:C:474:PHE:CD2  | 2.43                     | 0.53              |
| 1:C:145:LYS:HD2  | 1:C:155:THR:HG21 | 1.90                     | 0.53              |
| 1:O:99:ALA:HB2   | 1:O:112:ILE:HG21 | 1.90                     | 0.53              |
| 1:C:141:ASP:HB2  | 1:C:162:LYS:HG2  | 1.90                     | 0.53              |
| 1:N:57:ASN:O     | 1:N:61:LEU:HG    | 2.08                     | 0.53              |
| 1:F:113:GLN:NE2  | 1:F:175:VAL:HG22 | 2.23                     | 0.53              |
| 1:F:170:LEU:C    | 1:F:172:GLY:H    | 2.17                     | 0.53              |
| 1:Q:497:THR:HG22 | 1:G:12:LEU:HD21  | 1.89                     | 0.53              |
| 1:R:25:LEU:O     | 1:R:29:ILE:HD12  | 2.08                     | 0.53              |
| 1:H:491:ASN:HB2  | 1:I:84:GLU:OE1   | 2.08                     | 0.53              |
| 1:B:14:THR:O     | 1:B:18:ILE:HG13  | 2.09                     | 0.53              |
| 1:B:531:VAL:HG23 | 1:B:534:LYS:HE3  | 1.89                     | 0.53              |
| 1:P:154:GLN:HG2  | 1:Q:129:GLN:HG2  | 1.88                     | 0.53              |
| 1:Q:31:ARG:HG2   | 1:Q:39:ASN:HD22  | 1.73                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:37:ARG:NH1   | 1:U:66:ARG:HH12  | 2.07                     | 0.53              |
| 1:A:8:ASN:HB2    | 1:L:520:LYS:HZ1  | 1.72                     | 0.53              |
| 1:A:469:SER:HB3  | 1:A:473:LYS:NZ   | 2.24                     | 0.53              |
| 1:E:68:ALA:HB2   | 1:E:148:VAL:HG23 | 1.90                     | 0.53              |
| 1:P:79:GLU:OE1   | 1:P:482:GLN:NE2  | 2.31                     | 0.53              |
| 1:G:19:ASN:HA    | 1:G:22:GLN:OE1   | 2.08                     | 0.53              |
| 1:G:31:ARG:NH2   | 1:G:37:ARG:HB2   | 2.18                     | 0.53              |
| 1:S:530:SER:O    | 1:S:534:LYS:HG3  | 2.08                     | 0.53              |
| 1:M:534:LYS:O    | 1:M:538:VAL:HG23 | 2.09                     | 0.53              |
| 1:G:514:GLU:O    | 1:G:518:MET:HE3  | 2.09                     | 0.53              |
| 1:K:61:LEU:HD22  | 1:K:492:LEU:HD22 | 1.89                     | 0.53              |
| 1:L:101:THR:HG22 | 1:L:103:THR:H    | 1.73                     | 0.53              |
| 1:C:74:VAL:HG22  | 1:C:132:PHE:CD1  | 2.44                     | 0.53              |
| 1:Q:31:ARG:HH21  | 1:Q:37:ARG:HG2   | 1.74                     | 0.53              |
| 1:K:137:VAL:HG23 | 1:K:138:LEU:HG   | 1.90                     | 0.53              |
| 1:B:32:LEU:HD21  | 1:L:531:VAL:HB   | 1.90                     | 0.53              |
| 1:M:55:THR:HB    | 1:M:503:GLN:HE22 | 1.73                     | 0.53              |
| 1:E:82:LEU:HD11  | 1:E:474:PHE:HD1  | 1.74                     | 0.53              |
| 1:Q:35:GLY:O     | 1:G:6:ASN:ND2    | 2.41                     | 0.53              |
| 1:H:92:ILE:HD11  | 1:H:119:ARG:HB3  | 1.91                     | 0.53              |
| 1:B:112:ILE:O    | 1:B:116:ILE:HG12 | 2.09                     | 0.53              |
| 1:T:491:ASN:HB2  | 1:U:84:GLU:HG3   | 1.91                     | 0.53              |
| 1:H:478:LEU:O    | 1:H:482:GLN:HG3  | 2.08                     | 0.53              |
| 1:S:82:LEU:HD21  | 1:S:138:LEU:HD21 | 1.90                     | 0.53              |
| 1:B:36:LEU:HD12  | 1:B:36:LEU:C     | 2.33                     | 0.53              |
| 1:M:461:LEU:HD12 | 1:C:152:ASP:HA   | 1.91                     | 0.53              |
| 1:T:37:ARG:CZ    | 1:U:66:ARG:HH22  | 2.22                     | 0.53              |
| 1:Q:99:ALA:HB2   | 1:Q:112:ILE:HD13 | 1.91                     | 0.52              |
| 1:E:173:PHE:HE1  | 1:E:460:PRO:HB3  | 1.74                     | 0.52              |
| 1:G:50:ILE:HG22  | 1:G:54:PHE:CE2   | 2.44                     | 0.52              |
| 1:E:110:ASP:OD1  | 1:E:176:ASN:ND2  | 2.43                     | 0.52              |
| 1:M:513:THR:HA   | 1:N:15:GLN:HE22  | 1.74                     | 0.52              |
| 1:K:37:ARG:HD2   | 1:L:66:ARG:HH22  | 1.73                     | 0.52              |
| 1:K:98:GLN:O     | 1:K:104:ASN:ND2  | 2.42                     | 0.52              |
| 1:V:138:LEU:HB3  | 1:V:163:ILE:HG22 | 1.91                     | 0.52              |
| 1:F:514:GLU:HA   | 1:F:517:ASN:HD22 | 1.75                     | 0.52              |
| 1:K:493:ASN:O    | 1:K:497:THR:HG23 | 2.10                     | 0.52              |
| 1:B:488:ALA:O    | 1:B:492:LEU:HG   | 2.09                     | 0.52              |
| 1:N:3:GLN:OE1    | 1:O:19:ASN:ND2   | 2.42                     | 0.52              |
| 1:K:16:ASN:HA    | 1:K:19:ASN:HD22  | 1.75                     | 0.52              |
| 1:V:511:TYR:HA   | 1:V:514:GLU:HB3  | 1.90                     | 0.52              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:P:147:GLN:NE2    | 1:P:149:GLY:O    | 2.43                     | 0.52              |
| 1:F:82:LEU:HD12    | 1:F:471:ILE:HG23 | 1.91                     | 0.52              |
| 1:B:37:ARG:HE      | 1:M:66:ARG:HH12  | 1.56                     | 0.52              |
| 1:B:125:ARG:HH11   | 1:B:129:GLN:NE2  | 2.08                     | 0.52              |
| 1:M:465:ASP:HA     | 1:M:468:ILE:HD12 | 1.92                     | 0.52              |
| 1:F:13:ILE:HA      | 1:F:16:ASN:HD22  | 1.75                     | 0.52              |
| 1:G:38[A]:ILE:HG21 | 1:G:48:GLN:HB3   | 1.92                     | 0.52              |
| 1:B:511:TYR:HE2    | 1:A:5:ILE:HG21   | 1.75                     | 0.52              |
| 1:C:130:THR:HG21   | 1:C:138:LEU:HD12 | 1.92                     | 0.52              |
| 1:F:55:THR:O       | 1:F:59:LYS:HG2   | 2.09                     | 0.52              |
| 1:G:38[B]:ILE:HG21 | 1:G:48:GLN:HB3   | 1.92                     | 0.52              |
| 1:R:93:ARG:NH2     | 1:H:150:ALA:O    | 2.34                     | 0.52              |
| 1:I:543:LEU:HA     | 1:I:546:LEU:HD12 | 1.91                     | 0.52              |
| 1:U:166:ASP:HA     | 1:U:171:ASN:HB2  | 1.91                     | 0.52              |
| 1:K:51:ALA:O       | 1:K:55:THR:HG23  | 2.10                     | 0.52              |
| 1:P:119:ARG:O      | 1:P:123:ILE:HG13 | 2.10                     | 0.52              |
| 1:Q:479:GLY:O      | 1:Q:483:ASN:ND2  | 2.42                     | 0.52              |
| 1:J:164:ASP:H      | 1:J:167:THR:HB   | 1.74                     | 0.52              |
| 1:C:154:GLN:OE1    | 1:N:129:GLN:HG2  | 2.10                     | 0.51              |
| 1:E:161:LYS:HG2    | 1:E:474:PHE:HE2  | 1.75                     | 0.51              |
| 1:Q:520:LYS:O      | 1:Q:524:ILE:HG12 | 2.11                     | 0.51              |
| 1:H:10:LEU:HD11    | 1:I:29:ILE:HG21  | 1.91                     | 0.51              |
| 1:N:507:GLN:HG3    | 1:N:507:GLN:O    | 2.10                     | 0.51              |
| 1:E:170:LEU:C      | 1:E:172:GLY:H    | 2.18                     | 0.51              |
| 1:G:18:ILE:HG22    | 1:G:22:GLN:NE2   | 2.26                     | 0.51              |
| 1:H:10:LEU:HD21    | 1:I:29:ILE:HD13  | 1.91                     | 0.51              |
| 1:A:78:THR:HG22    | 1:A:137:VAL:HG21 | 1.92                     | 0.51              |
| 1:C:519:SER:O      | 1:C:523:ILE:HG12 | 2.10                     | 0.51              |
| 1:D:69:ASN:HA      | 1:D:72:ILE:HG12  | 1.92                     | 0.51              |
| 1:T:519:SER:O      | 1:T:523:ILE:HG12 | 2.11                     | 0.51              |
| 1:K:170:LEU:C      | 1:K:172:GLY:H    | 2.19                     | 0.51              |
| 1:Q:127:SER:OG     | 1:Q:164:ASP:OD1  | 2.28                     | 0.51              |
| 1:G:52:ASN:O       | 1:G:55:THR:OG1   | 2.23                     | 0.51              |
| 1:S:82:LEU:HD12    | 1:S:471:ILE:HG23 | 1.91                     | 0.51              |
| 1:J:141:ASP:HB2    | 1:J:162:LYS:H    | 1.75                     | 0.51              |
| 1:N:5:ILE:HG12     | 1:N:542:VAL:HG11 | 1.92                     | 0.51              |
| 1:N:32:LEU:HD12    | 1:N:511:TYR:CD1  | 2.45                     | 0.51              |
| 1:E:161:LYS:HG2    | 1:E:474:PHE:CE2  | 2.45                     | 0.51              |
| 1:P:31:ARG:HH22    | 1:P:37:ARG:HH21  | 1.58                     | 0.51              |
| 1:S:461:LEU:HD12   | 1:I:152:ASP:HA   | 1.93                     | 0.51              |
| 1:J:50:ILE:HD11    | 1:U:108:ASP:OD2  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:485:LEU:O    | 1:B:489:VAL:HG23 | 2.10                     | 0.51              |
| 1:C:34:SER:HB2   | 1:C:36:LEU:HD23  | 1.92                     | 0.51              |
| 1:C:498:ASN:HB3  | 1:N:77:THR:HG22  | 1.92                     | 0.51              |
| 1:C:534:LYS:O    | 1:C:538:VAL:HG23 | 2.11                     | 0.51              |
| 1:N:509:ALA:HB3  | 1:D:5:ILE:HD13   | 1.93                     | 0.51              |
| 1:D:522:GLN:O    | 1:D:526:GLN:HG2  | 2.11                     | 0.51              |
| 1:O:93:ARG:NH1   | 1:E:56:SER:OG    | 2.44                     | 0.51              |
| 1:O:480:ALA:O    | 1:O:484:ARG:HG3  | 2.11                     | 0.51              |
| 1:P:494:ASN:O    | 1:P:498:ASN:ND2  | 2.44                     | 0.51              |
| 1:K:163:ILE:HG23 | 1:K:168:LEU:HD11 | 1.92                     | 0.51              |
| 1:V:108:ASP:O    | 1:V:112:ILE:HG13 | 2.10                     | 0.51              |
| 1:E:91:ARG:HG2   | 1:E:119:ARG:HE   | 1.74                     | 0.51              |
| 1:G:145:LYS:HB3  | 1:G:155:THR:HB   | 1.92                     | 0.51              |
| 1:S:86:ASN:OD1   | 1:S:468:ILE:HD11 | 2.10                     | 0.51              |
| 1:T:541:GLN:N    | 1:T:541:GLN:OE1  | 2.44                     | 0.51              |
| 1:G:164:ASP:H    | 1:G:167:THR:HB   | 1.76                     | 0.51              |
| 1:S:62:THR:O     | 1:S:66:ARG:HG2   | 2.11                     | 0.51              |
| 1:S:93:ARG:NH1   | 1:S:461:LEU:HD22 | 2.26                     | 0.51              |
| 1:J:484:ARG:HH21 | 1:K:125:ARG:HH21 | 1.57                     | 0.51              |
| 1:P:501:GLU:O    | 1:P:505:ARG:HG3  | 2.10                     | 0.51              |
| 1:R:154:GLN:HE21 | 1:S:129:GLN:HE21 | 1.59                     | 0.51              |
| 1:I:116:ILE:HG21 | 1:I:173:PHE:HD2  | 1.76                     | 0.51              |
| 1:T:152:ASP:OD1  | 1:T:153:GLY:N    | 2.44                     | 0.51              |
| 1:L:125:ARG:O    | 1:L:129:GLN:HG2  | 2.11                     | 0.51              |
| 1:N:154:GLN:HE22 | 1:O:129:GLN:HG3  | 1.75                     | 0.51              |
| 1:D:170:LEU:HD22 | 1:D:173:PHE:CE2  | 2.45                     | 0.51              |
| 1:E:533:ALA:O    | 1:E:537:GLN:HG2  | 2.10                     | 0.51              |
| 1:R:5:ILE:HG23   | 1:R:542:VAL:HG21 | 1.93                     | 0.51              |
| 1:J:5:ILE:HD13   | 1:J:542:VAL:HG11 | 1.92                     | 0.51              |
| 1:J:491:ASN:HB2  | 1:K:84:GLU:HG3   | 1.92                     | 0.51              |
| 1:D:174:ASN:OD1  | 1:D:177:GLY:N    | 2.44                     | 0.50              |
| 1:O:464:LEU:O    | 1:O:468:ILE:HG13 | 2.11                     | 0.50              |
| 1:Q:174:ASN:OD1  | 1:Q:175:VAL:N    | 2.44                     | 0.50              |
| 1:G:504:SER:O    | 1:G:508:ASP:HB3  | 2.11                     | 0.50              |
| 1:H:31:ARG:HD3   | 1:H:37:ARG:HG3   | 1.93                     | 0.50              |
| 1:U:137:VAL:HG23 | 1:U:138:LEU:HG   | 1.92                     | 0.50              |
| 1:V:15:GLN:O     | 1:V:19:ASN:ND2   | 2.44                     | 0.50              |
| 1:B:528:GLY:HA2  | 1:B:531:VAL:HG12 | 1.92                     | 0.50              |
| 1:Q:79:GLU:HA    | 1:Q:82:LEU:HG    | 1.94                     | 0.50              |
| 1:R:497:THR:HG22 | 1:H:12:LEU:HD21  | 1.92                     | 0.50              |
| 1:T:481:VAL:HG12 | 1:T:484:ARG:HH12 | 1.76                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:U:491:ASN:HD22 | 1:V:125:ARG:HH22 | 1.59                     | 0.50              |
| 1:O:461:LEU:HD11 | 1:E:150:ALA:O    | 2.10                     | 0.50              |
| 1:E:116:ILE:HG21 | 1:E:173:PHE:CE2  | 2.46                     | 0.50              |
| 1:F:137:VAL:HG23 | 1:F:138:LEU:HG   | 1.92                     | 0.50              |
| 1:H:17:ASN:ND2   | 1:I:33:SER:OG    | 2.45                     | 0.50              |
| 1:S:86:ASN:HD22  | 1:S:475:ARG:NH2  | 2.09                     | 0.50              |
| 1:J:112:ILE:O    | 1:J:116:ILE:HG12 | 2.11                     | 0.50              |
| 1:B:37:ARG:NE    | 1:M:66:ARG:NH1   | 2.59                     | 0.50              |
| 1:B:541:GLN:NE2  | 1:M:525:GLN:OE1  | 2.30                     | 0.50              |
| 1:C:82:LEU:HA    | 1:C:85:ILE:HD12  | 1.94                     | 0.50              |
| 1:C:518:MET:HE2  | 1:C:522:GLN:HE22 | 1.76                     | 0.50              |
| 1:Q:494:ASN:O    | 1:Q:497:THR:OG1  | 2.27                     | 0.50              |
| 1:M:488:ALA:O    | 1:M:492:LEU:HG   | 2.11                     | 0.50              |
| 1:C:486:ASP:OD1  | 1:C:487:SER:N    | 2.44                     | 0.50              |
| 1:E:91:ARG:HG2   | 1:E:119:ARG:NE   | 2.26                     | 0.50              |
| 1:Q:170:LEU:C    | 1:Q:172:GLY:H    | 2.19                     | 0.50              |
| 1:Q:171:ASN:O    | 1:Q:171:ASN:ND2  | 2.44                     | 0.50              |
| 1:R:58:ILE:O     | 1:R:62:THR:HG23  | 2.11                     | 0.50              |
| 1:N:498:ASN:HB3  | 1:O:77:THR:HG22  | 1.94                     | 0.50              |
| 1:G:531:VAL:HG22 | 1:R:29:ILE:HG23  | 1.94                     | 0.50              |
| 1:R:88:ASN:HA    | 1:R:119:ARG:HH21 | 1.76                     | 0.50              |
| 1:N:46:ALA:O     | 1:N:50:ILE:HG12  | 2.11                     | 0.50              |
| 1:D:170:LEU:HD12 | 1:D:171:ASN:H    | 1.77                     | 0.50              |
| 1:D:494:ASN:OD1  | 1:D:498:ASN:ND2  | 2.44                     | 0.50              |
| 1:F:87:ASN:OD1   | 1:F:88:ASN:N     | 2.45                     | 0.50              |
| 1:P:163:ILE:HD11 | 1:P:474:PHE:CE1  | 2.46                     | 0.50              |
| 1:Q:511:TYR:O    | 1:Q:515:VAL:HG23 | 2.12                     | 0.50              |
| 1:I:106:ASP:HA   | 1:I:109:LEU:HD12 | 1.94                     | 0.50              |
| 1:T:162:LYS:NZ   | 1:T:167:THR:OG1  | 2.42                     | 0.50              |
| 1:J:82:LEU:HD12  | 1:J:471:ILE:HG23 | 1.94                     | 0.50              |
| 1:J:115:GLU:OE2  | 1:J:119:ARG:NH1  | 2.45                     | 0.50              |
| 1:A:501:GLU:OE2  | 1:C:76:GLN:NE2   | 2.45                     | 0.50              |
| 1:E:171:ASN:O    | 1:E:171:ASN:ND2  | 2.45                     | 0.50              |
| 1:Q:168:LEU:HD21 | 1:Q:471:ILE:HD11 | 1.92                     | 0.50              |
| 1:R:64:ALA:HB1   | 1:R:148:VAL:HA   | 1.93                     | 0.50              |
| 1:H:44:ASP:OD1   | 1:S:91:ARG:NH2   | 2.45                     | 0.50              |
| 1:S:94:GLU:OE1   | 1:I:59:LYS:HE2   | 2.12                     | 0.50              |
| 1:U:25:LEU:HB2   | 1:U:521:ALA:HB1  | 1.93                     | 0.50              |
| 1:L:69:ASN:OD1   | 1:L:489:VAL:HG21 | 2.12                     | 0.50              |
| 1:R:170:LEU:C    | 1:R:172:GLY:H    | 2.20                     | 0.49              |
| 1:H:21:ASN:ND2   | 1:H:524:ILE:HG23 | 2.27                     | 0.49              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:T:93:ARG:HH11    | 1:T:461:LEU:HD22 | 1.77                     | 0.49              |
| 1:T:168:LEU:HD23   | 1:T:467:ALA:HB1  | 1.94                     | 0.49              |
| 1:K:531:VAL:HG21   | 1:L:33:SER:HA    | 1.94                     | 0.49              |
| 1:B:478:LEU:O      | 1:B:481:VAL:HG12 | 2.13                     | 0.49              |
| 1:D:54:PHE:CE1     | 1:D:499:LEU:HD22 | 2.47                     | 0.49              |
| 1:F:508:ASP:OD1    | 1:F:509:ALA:N    | 2.45                     | 0.49              |
| 1:J:170:LEU:C      | 1:J:172:GLY:H    | 2.20                     | 0.49              |
| 1:D:541:GLN:O      | 1:D:545:LEU:HG   | 2.11                     | 0.49              |
| 1:G:27:SER:O       | 1:G:30:GLU:HG3   | 2.12                     | 0.49              |
| 1:H:173:PHE:HE1    | 1:H:460:PRO:HB3  | 1.77                     | 0.49              |
| 1:T:156:ILE:HD11   | 1:T:484:ARG:HD2  | 1.93                     | 0.49              |
| 1:U:82:LEU:HD12    | 1:U:471:ILE:HG23 | 1.93                     | 0.49              |
| 1:D:122:GLU:O      | 1:D:126:VAL:HG12 | 2.12                     | 0.49              |
| 1:R:79:GLU:OE2     | 1:R:475:ARG:NE   | 2.32                     | 0.49              |
| 1:I:85:ILE:HG23    | 1:I:123:ILE:HG23 | 1.94                     | 0.49              |
| 1:M:166:ASP:OD1    | 1:M:167:THR:N    | 2.46                     | 0.49              |
| 1:D:101:THR:HG22   | 1:D:103:THR:H    | 1.77                     | 0.49              |
| 1:F:38[A]:ILE:HG12 | 1:F:507:GLN:HG3  | 1.94                     | 0.49              |
| 1:R:493:ASN:O      | 1:R:497:THR:HG23 | 2.12                     | 0.49              |
| 1:K:505:ARG:HA     | 1:K:505:ARG:HH11 | 1.77                     | 0.49              |
| 1:N:32:LEU:HD12    | 1:N:511:TYR:HD1  | 1.78                     | 0.49              |
| 1:N:32:LEU:HD11    | 1:D:546:LEU:HD11 | 1.93                     | 0.49              |
| 1:O:82:LEU:HD13    | 1:O:85:ILE:HD12  | 1.94                     | 0.49              |
| 1:Q:101:THR:HB     | 1:G:67:ASN:HD22  | 1.76                     | 0.49              |
| 1:S:162:LYS:NZ     | 1:S:164:ASP:OD1  | 2.37                     | 0.49              |
| 1:N:3:GLN:HG2      | 1:O:22:GLN:HE22  | 1.77                     | 0.49              |
| 1:E:492:LEU:O      | 1:E:496:THR:HG23 | 2.13                     | 0.49              |
| 1:G:32:LEU:HB2     | 1:G:518:MET:HE1  | 1.94                     | 0.49              |
| 1:R:92:ILE:HG13    | 1:R:119:ARG:HD3  | 1.94                     | 0.49              |
| 1:H:69:ASN:O       | 1:H:72:ILE:HG22  | 2.12                     | 0.49              |
| 1:I:137:VAL:HG23   | 1:I:138:LEU:HD23 | 1.94                     | 0.49              |
| 1:U:86:ASN:HB2     | 1:U:475:ARG:HH22 | 1.77                     | 0.49              |
| 1:C:92:ILE:HD11    | 1:C:119:ARG:HB3  | 1.95                     | 0.49              |
| 1:O:506:ILE:HG23   | 1:O:507:GLN:OE1  | 2.12                     | 0.49              |
| 1:E:520:LYS:O      | 1:E:524:ILE:HG12 | 2.13                     | 0.49              |
| 1:F:11:SER:O       | 1:F:15:GLN:HG3   | 2.13                     | 0.49              |
| 1:A:162:LYS:O      | 1:A:163:ILE:HD13 | 2.12                     | 0.49              |
| 1:N:16:ASN:O       | 1:N:20:LYS:NZ    | 2.46                     | 0.49              |
| 1:D:491:ASN:ND2    | 1:E:126:VAL:HG23 | 2.28                     | 0.49              |
| 1:O:32:LEU:HD12    | 1:O:511:TYR:CD1  | 2.48                     | 0.49              |
| 1:R:162:LYS:HZ2    | 1:R:167:THR:HG1  | 1.56                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:70:ASP:O     | 1:I:74:VAL:HG23  | 2.13                     | 0.49              |
| 1:L:11:SER:O     | 1:L:15:GLN:HG3   | 2.13                     | 0.49              |
| 1:C:99:ALA:HB2   | 1:C:112:ILE:HG21 | 1.93                     | 0.49              |
| 1:P:120:LEU:HD23 | 1:P:123:ILE:HD12 | 1.95                     | 0.49              |
| 1:Q:18:ILE:HG22  | 1:Q:22:GLN:NE2   | 2.27                     | 0.49              |
| 1:G:15:GLN:HA    | 1:G:18:ILE:HD12  | 1.93                     | 0.49              |
| 1:S:539:PRO:O    | 1:S:542:VAL:HG12 | 2.13                     | 0.49              |
| 1:P:50:ILE:O     | 1:P:54:PHE:HD1   | 1.96                     | 0.48              |
| 1:F:149:GLY:N    | 1:F:154:GLN:HG2  | 2.28                     | 0.48              |
| 1:I:154:GLN:HG3  | 1:T:129:GLN:HE22 | 1.78                     | 0.48              |
| 1:A:151:ASN:ND2  | 1:C:129:GLN:OE1  | 2.47                     | 0.48              |
| 1:O:459:ASP:OD2  | 1:O:462:ALA:HB3  | 2.13                     | 0.48              |
| 1:P:513:THR:O    | 1:P:516:SER:OG   | 2.32                     | 0.48              |
| 1:Q:76:GLN:O     | 1:Q:79:GLU:HG2   | 2.13                     | 0.48              |
| 1:S:176:ASN:OD1  | 1:S:177:GLY:N    | 2.47                     | 0.48              |
| 1:N:170:LEU:C    | 1:N:172:GLY:H    | 2.21                     | 0.48              |
| 1:E:128:GLY:O    | 1:E:136:ASN:ND2  | 2.46                     | 0.48              |
| 1:T:475:ARG:HH22 | 1:J:48:GLN:NE2   | 2.12                     | 0.48              |
| 1:N:116:ILE:HG21 | 1:N:173:PHE:CD2  | 2.48                     | 0.48              |
| 1:N:519:SER:O    | 1:N:523:ILE:HG12 | 2.14                     | 0.48              |
| 1:D:519:SER:O    | 1:D:523:ILE:HG12 | 2.14                     | 0.48              |
| 1:E:174:ASN:OD1  | 1:E:177:GLY:N    | 2.45                     | 0.48              |
| 1:G:5:ILE:HD11   | 1:G:542:VAL:HG11 | 1.96                     | 0.48              |
| 1:R:503:GLN:HE22 | 1:R:507:GLN:HE21 | 1.61                     | 0.48              |
| 1:D:474:PHE:O    | 1:D:478:LEU:HG   | 2.13                     | 0.48              |
| 1:A:534:LYS:O    | 1:A:538:VAL:HG23 | 2.13                     | 0.48              |
| 1:E:174:ASN:ND2  | 1:E:177:GLY:O    | 2.45                     | 0.48              |
| 1:R:497:THR:HG21 | 1:H:16:ASN:ND2   | 2.27                     | 0.48              |
| 1:V:120:LEU:HD11 | 1:V:173:PHE:CD2  | 2.44                     | 0.48              |
| 1:B:493:ASN:OD1  | 1:B:494:ASN:N    | 2.46                     | 0.48              |
| 1:O:88:ASN:OD1   | 1:O:119:ARG:NH1  | 2.47                     | 0.48              |
| 1:O:482:GLN:HG2  | 1:E:42:LYS:HZ3   | 1.79                     | 0.48              |
| 1:F:99:ALA:HB2   | 1:F:112:ILE:HG21 | 1.96                     | 0.48              |
| 1:F:166:ASP:OD1  | 1:F:167:THR:N    | 2.45                     | 0.48              |
| 1:R:74:VAL:HG22  | 1:R:132:PHE:CD2  | 2.49                     | 0.48              |
| 1:S:147:GLN:HA   | 1:S:155:THR:HG22 | 1.95                     | 0.48              |
| 1:G:136:ASN:HB3  | 1:G:139:ALA:HB3  | 1.95                     | 0.48              |
| 1:R:503:GLN:HA   | 1:R:506:ILE:HD12 | 1.95                     | 0.48              |
| 1:T:93:ARG:NH1   | 1:T:461:LEU:HD22 | 2.29                     | 0.48              |
| 1:L:11:SER:HB2   | 1:L:532:LEU:HD12 | 1.96                     | 0.48              |
| 1:B:37:ARG:HE    | 1:M:66:ARG:NH1   | 2.12                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:145:LYS:NZ   | 1:B:155:THR:HG21 | 2.28                     | 0.48              |
| 1:O:471:ILE:HG22 | 1:O:475:ARG:NE   | 2.29                     | 0.48              |
| 1:O:494:ASN:OD1  | 1:O:498:ASN:ND2  | 2.46                     | 0.48              |
| 1:F:502:ALA:HA   | 1:F:505:ARG:HD2  | 1.96                     | 0.48              |
| 1:R:541:GLN:O    | 1:R:545:LEU:HG   | 2.14                     | 0.48              |
| 1:H:91:ARG:HG3   | 1:H:95:LEU:HD23  | 1.95                     | 0.48              |
| 1:H:170:LEU:HD13 | 1:H:173:PHE:CB   | 2.44                     | 0.48              |
| 1:U:545:LEU:HD21 | 1:V:529:ASN:HB3  | 1.95                     | 0.48              |
| 1:V:21:ASN:ND2   | 1:V:21:ASN:O     | 2.46                     | 0.48              |
| 1:B:85:ILE:HG23  | 1:B:123:ILE:HG23 | 1.96                     | 0.48              |
| 1:Q:168:LEU:HD23 | 1:Q:467:ALA:HB1  | 1.96                     | 0.48              |
| 1:R:88:ASN:HA    | 1:R:119:ARG:HE   | 1.79                     | 0.48              |
| 1:H:9:SER:O      | 1:H:13:ILE:HG13  | 2.14                     | 0.48              |
| 1:S:14:THR:O     | 1:S:18:ILE:HG13  | 2.14                     | 0.48              |
| 1:T:37:ARG:NE    | 1:U:66:ARG:HH22  | 2.11                     | 0.48              |
| 1:J:166:ASP:HA   | 1:J:171:ASN:HB2  | 1.96                     | 0.48              |
| 1:V:54:PHE:HE1   | 1:V:499:LEU:HD22 | 1.78                     | 0.48              |
| 1:V:501:GLU:O    | 1:V:504:SER:OG   | 2.23                     | 0.48              |
| 1:Q:55:THR:O     | 1:Q:59:LYS:HG3   | 2.14                     | 0.47              |
| 1:R:127:SER:OG   | 1:R:163:ILE:O    | 2.21                     | 0.47              |
| 1:H:517:ASN:HA   | 1:H:520:LYS:NZ   | 2.29                     | 0.47              |
| 1:S:88:ASN:HB2   | 1:S:123:ILE:HD11 | 1.96                     | 0.47              |
| 1:R:488:ALA:O    | 1:R:492:LEU:HD23 | 2.14                     | 0.47              |
| 1:H:162:LYS:NZ   | 1:H:167:THR:OG1  | 2.47                     | 0.47              |
| 1:U:91:ARG:HG2   | 1:U:119:ARG:CZ   | 2.44                     | 0.47              |
| 1:U:501:GLU:OE2  | 1:U:505:ARG:NE   | 2.44                     | 0.47              |
| 1:K:89:LEU:HD22  | 1:K:468:ILE:HG13 | 1.96                     | 0.47              |
| 1:B:37:ARG:NE    | 1:M:66:ARG:HH12  | 2.13                     | 0.47              |
| 1:B:491:ASN:C    | 1:B:491:ASN:HD22 | 2.20                     | 0.47              |
| 1:A:8:ASN:OD1    | 1:A:11:SER:N     | 2.43                     | 0.47              |
| 1:C:488:ALA:O    | 1:C:492:LEU:HG   | 2.14                     | 0.47              |
| 1:R:154:GLN:HB2  | 1:S:129:GLN:NE2  | 2.30                     | 0.47              |
| 1:H:93:ARG:HH11  | 1:H:93:ARG:HG2   | 1.80                     | 0.47              |
| 1:N:31:ARG:HD3   | 1:N:37:ARG:HA    | 1.96                     | 0.47              |
| 1:D:161:LYS:HE3  | 1:D:162:LYS:H    | 1.79                     | 0.47              |
| 1:Q:511:TYR:HA   | 1:Q:514:GLU:HG3  | 1.97                     | 0.47              |
| 1:Q:516:SER:O    | 1:Q:519:SER:OG   | 2.28                     | 0.47              |
| 1:C:149:GLY:HA3  | 1:C:154:GLN:HG3  | 1.96                     | 0.47              |
| 1:O:116:ILE:HG21 | 1:O:173:PHE:HD2  | 1.79                     | 0.47              |
| 1:F:70:ASP:O     | 1:F:73:SER:OG    | 2.25                     | 0.47              |
| 1:Q:173:PHE:HE1  | 1:Q:460:PRO:HB3  | 1.80                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:511:TYR:O    | 1:G:515:VAL:HG23 | 2.14                     | 0.47              |
| 1:I:3:GLN:HB2    | 1:T:22:GLN:OE1   | 2.14                     | 0.47              |
| 1:I:62:THR:O     | 1:I:66:ARG:HG2   | 2.13                     | 0.47              |
| 1:J:25:LEU:O     | 1:J:29:ILE:HG12  | 2.15                     | 0.47              |
| 1:Q:461:LEU:HB2  | 1:G:152:ASP:OD2  | 2.14                     | 0.47              |
| 1:R:10:LEU:HD11  | 1:S:29:ILE:HG21  | 1.95                     | 0.47              |
| 1:R:82:LEU:HD12  | 1:R:471:ILE:HG23 | 1.96                     | 0.47              |
| 1:T:534:LYS:O    | 1:T:538:VAL:HG23 | 2.15                     | 0.47              |
| 1:J:17:ASN:N     | 1:J:17:ASN:ND2   | 2.62                     | 0.47              |
| 1:K:78:THR:HG23  | 1:K:138:LEU:HD21 | 1.96                     | 0.47              |
| 1:B:92:ILE:O     | 1:B:96:THR:HG23  | 2.15                     | 0.47              |
| 1:B:119:ARG:HH21 | 1:L:483:ASN:HD21 | 1.62                     | 0.47              |
| 1:B:534:LYS:O    | 1:B:538:VAL:HG23 | 2.15                     | 0.47              |
| 1:N:477:SER:O    | 1:N:481:VAL:HG23 | 2.15                     | 0.47              |
| 1:O:5:ILE:HB     | 1:O:542:VAL:HG21 | 1.96                     | 0.47              |
| 1:P:127:SER:HB3  | 1:P:163:ILE:O    | 2.15                     | 0.47              |
| 1:G:488:ALA:HB2  | 1:R:125:ARG:HH22 | 1.80                     | 0.47              |
| 1:H:537:GLN:HA   | 1:H:540:GLN:HE22 | 1.79                     | 0.47              |
| 1:B:21:ASN:ND2   | 1:B:524:ILE:HG22 | 2.30                     | 0.47              |
| 1:B:86:ASN:HD21  | 1:A:52:ASN:ND2   | 2.12                     | 0.47              |
| 1:C:477:SER:O    | 1:C:481:VAL:HG13 | 2.15                     | 0.47              |
| 1:C:484:ARG:HH12 | 1:N:122:GLU:N    | 2.12                     | 0.47              |
| 1:N:508:ASP:OD1  | 1:D:5:ILE:HD12   | 2.15                     | 0.47              |
| 1:H:37:ARG:NH2   | 1:I:66:ARG:HH22  | 2.13                     | 0.47              |
| 1:H:49:ALA:HB1   | 1:H:53:ARG:HH12  | 1.79                     | 0.47              |
| 1:T:170:LEU:C    | 1:T:172:GLY:H    | 2.22                     | 0.47              |
| 1:L:119:ARG:O    | 1:L:123:ILE:HG12 | 2.15                     | 0.47              |
| 1:B:29:ILE:O     | 1:B:32:LEU:HB3   | 2.15                     | 0.47              |
| 1:A:525:GLN:HE22 | 1:A:529:ASN:HD21 | 1.62                     | 0.47              |
| 1:C:70:ASP:O     | 1:C:74:VAL:HG23  | 2.15                     | 0.47              |
| 1:C:93:ARG:HA    | 1:C:464:LEU:HD13 | 1.97                     | 0.47              |
| 1:N:488:ALA:O    | 1:N:492:LEU:HG   | 2.15                     | 0.47              |
| 1:Q:68:ALA:HA    | 1:Q:146:ILE:HG21 | 1.96                     | 0.47              |
| 1:Q:504:SER:HB3  | 1:G:7:THR:HB     | 1.96                     | 0.47              |
| 1:H:14:THR:O     | 1:H:18:ILE:HG13  | 2.15                     | 0.47              |
| 1:K:116:ILE:HG21 | 1:K:173:PHE:CD2  | 2.49                     | 0.47              |
| 1:A:92:ILE:HG22  | 1:A:464:LEU:HD21 | 1.97                     | 0.47              |
| 1:D:37:ARG:HG2   | 1:D:508:ASP:H    | 1.80                     | 0.47              |
| 1:O:95:LEU:O     | 1:O:98:GLN:HG3   | 2.15                     | 0.47              |
| 1:O:166:ASP:HA   | 1:O:171:ASN:HB2  | 1.97                     | 0.47              |
| 1:F:28:SER:HA    | 1:F:514:GLU:OE1  | 2.14                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:70:ASP:O     | 1:R:74:VAL:HG23  | 2.15                     | 0.47              |
| 1:J:541:GLN:HE21 | 1:K:526:GLN:NE2  | 2.12                     | 0.47              |
| 1:U:113:GLN:HE22 | 1:U:174:ASN:HA   | 1.79                     | 0.47              |
| 1:V:119:ARG:O    | 1:V:123:ILE:HG13 | 2.15                     | 0.47              |
| 1:Q:101:THR:HG22 | 1:Q:103:THR:H    | 1.80                     | 0.46              |
| 1:G:46:ALA:O     | 1:G:50:ILE:HG13  | 2.15                     | 0.46              |
| 1:U:170:LEU:C    | 1:U:172:GLY:H    | 2.22                     | 0.46              |
| 1:K:120:LEU:HA   | 1:K:123:ILE:HG12 | 1.98                     | 0.46              |
| 1:O:101:THR:HG22 | 1:O:103:THR:H    | 1.79                     | 0.46              |
| 1:P:85:ILE:HG23  | 1:P:123:ILE:HG23 | 1.97                     | 0.46              |
| 1:G:10:LEU:HD11  | 1:R:26:SER:HA    | 1.97                     | 0.46              |
| 1:G:170:LEU:C    | 1:G:172:GLY:H    | 2.23                     | 0.46              |
| 1:H:53:ARG:NH2   | 1:S:108:ASP:OD1  | 2.48                     | 0.46              |
| 1:H:64:ALA:HB1   | 1:H:148:VAL:HA   | 1.98                     | 0.46              |
| 1:H:502:ALA:O    | 1:H:506:ILE:HG13 | 2.15                     | 0.46              |
| 1:S:54:PHE:HB3   | 1:S:503:GLN:HE21 | 1.80                     | 0.46              |
| 1:S:57:ASN:O     | 1:S:61:LEU:HG    | 2.15                     | 0.46              |
| 1:T:485:LEU:O    | 1:T:489:VAL:HG23 | 2.15                     | 0.46              |
| 1:U:170:LEU:HD13 | 1:U:173:PHE:HD1  | 1.80                     | 0.46              |
| 1:P:495:THR:O    | 1:P:499:LEU:HD23 | 2.15                     | 0.46              |
| 1:H:116:ILE:HG21 | 1:H:173:PHE:HD2  | 1.81                     | 0.46              |
| 1:I:163:ILE:HG23 | 1:I:168:LEU:HD21 | 1.97                     | 0.46              |
| 1:J:170:LEU:HB3  | 1:J:173:PHE:HB2  | 1.96                     | 0.46              |
| 1:U:484:ARG:HE   | 1:V:122:GLU:HB2  | 1.80                     | 0.46              |
| 1:N:27:SER:O     | 1:N:30:GLU:HG3   | 2.14                     | 0.46              |
| 1:D:46:ALA:O     | 1:D:50:ILE:HG12  | 2.14                     | 0.46              |
| 1:D:168:LEU:HD21 | 1:D:471:ILE:HD11 | 1.96                     | 0.46              |
| 1:G:478:LEU:O    | 1:G:482:GLN:HG3  | 2.15                     | 0.46              |
| 1:S:127:SER:OG   | 1:S:163:ILE:O    | 2.32                     | 0.46              |
| 1:I:85:ILE:HA    | 1:I:88:ASN:HD22  | 1.80                     | 0.46              |
| 1:I:485:LEU:O    | 1:I:489:VAL:HG23 | 2.15                     | 0.46              |
| 1:K:9:SER:HA     | 1:K:12:LEU:HB3   | 1.97                     | 0.46              |
| 1:B:94:GLU:OE1   | 1:B:95:LEU:HD12  | 2.16                     | 0.46              |
| 1:A:170:LEU:C    | 1:A:172:GLY:H    | 2.23                     | 0.46              |
| 1:N:69:ASN:HA    | 1:N:72:ILE:HG12  | 1.97                     | 0.46              |
| 1:R:162:LYS:NZ   | 1:R:164:ASP:OD2  | 2.45                     | 0.46              |
| 1:R:508:ASP:HB2  | 1:H:4:VAL:HG22   | 1.97                     | 0.46              |
| 1:I:117:LYS:O    | 1:I:117:LYS:HD3  | 2.15                     | 0.46              |
| 1:U:154:GLN:OE1  | 1:V:129:GLN:NE2  | 2.49                     | 0.46              |
| 1:L:27:SER:HA    | 1:L:30:GLU:HG2   | 1.98                     | 0.46              |
| 1:M:78:THR:HG22  | 1:M:478:LEU:HD11 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:125:ARG:NH1  | 1:C:125:ARG:HG2  | 2.31                     | 0.46              |
| 1:N:478:LEU:O    | 1:N:482:GLN:OE1  | 2.32                     | 0.46              |
| 1:D:109:LEU:HA   | 1:D:112:ILE:HD12 | 1.97                     | 0.46              |
| 1:O:95:LEU:HA    | 1:O:98:GLN:HG3   | 1.96                     | 0.46              |
| 1:P:93:ARG:O     | 1:P:97:VAL:HG23  | 2.16                     | 0.46              |
| 1:G:512:ALA:O    | 1:H:15:GLN:NE2   | 2.49                     | 0.46              |
| 1:U:78:THR:HG23  | 1:U:138:LEU:HD21 | 1.97                     | 0.46              |
| 1:U:94:GLU:OE2   | 1:K:59:LYS:HB3   | 2.15                     | 0.46              |
| 1:L:533:ALA:O    | 1:L:537:GLN:HG2  | 2.16                     | 0.46              |
| 1:B:170:LEU:C    | 1:B:172:GLY:H    | 2.23                     | 0.46              |
| 1:N:164:ASP:H    | 1:N:167:THR:HG22 | 1.80                     | 0.46              |
| 1:D:533:ALA:O    | 1:D:537:GLN:HG2  | 2.16                     | 0.46              |
| 1:R:116:ILE:HG21 | 1:R:173:PHE:CD2  | 2.51                     | 0.46              |
| 1:T:475:ARG:HH12 | 1:J:48:GLN:HE22  | 1.63                     | 0.46              |
| 1:U:93:ARG:NH1   | 1:K:150:ALA:O    | 2.40                     | 0.46              |
| 1:C:10:LEU:HD21  | 1:N:29:ILE:HG21  | 1.98                     | 0.46              |
| 1:C:25:LEU:HB2   | 1:C:521:ALA:HB1  | 1.97                     | 0.46              |
| 1:P:50:ILE:HG22  | 1:P:54:PHE:CE1   | 2.51                     | 0.46              |
| 1:R:156:ILE:HD11 | 1:R:484:ARG:HB3  | 1.98                     | 0.46              |
| 1:O:166:ASP:OD1  | 1:O:171:ASN:ND2  | 2.47                     | 0.46              |
| 1:O:524:ILE:HG22 | 1:P:5:ILE:HD12   | 1.97                     | 0.46              |
| 1:E:101:THR:HG22 | 1:E:103:THR:H    | 1.81                     | 0.46              |
| 1:F:12:LEU:O     | 1:F:16:ASN:ND2   | 2.49                     | 0.46              |
| 1:H:154:GLN:HG2  | 1:I:129:GLN:HE21 | 1.80                     | 0.46              |
| 1:U:113:GLN:NE2  | 1:U:174:ASN:HA   | 2.31                     | 0.46              |
| 1:C:125:ARG:HG2  | 1:C:125:ARG:HH11 | 1.81                     | 0.46              |
| 1:N:497:THR:HG22 | 1:D:12:LEU:HD21  | 1.97                     | 0.46              |
| 1:O:478:LEU:HA   | 1:O:481:VAL:HG22 | 1.98                     | 0.46              |
| 1:P:170:LEU:HD13 | 1:P:173:PHE:CD1  | 2.51                     | 0.46              |
| 1:R:131:GLN:HB3  | 1:R:136:ASN:ND2  | 2.32                     | 0.46              |
| 1:R:154:GLN:NE2  | 1:S:129:GLN:HE21 | 2.14                     | 0.46              |
| 1:R:484:ARG:NE   | 1:S:122:GLU:OE1  | 2.49                     | 0.46              |
| 1:T:72:ILE:HG13  | 1:T:482:GLN:HG3  | 1.97                     | 0.46              |
| 1:T:82:LEU:HD13  | 1:T:475:ARG:HG3  | 1.97                     | 0.46              |
| 1:U:158:ILE:HD11 | 1:U:485:LEU:HD11 | 1.97                     | 0.46              |
| 1:B:37:ARG:CZ    | 1:M:66:ARG:CZ    | 2.94                     | 0.45              |
| 1:B:502:ALA:O    | 1:B:506:ILE:HG12 | 2.16                     | 0.45              |
| 1:N:466:ASP:O    | 1:N:469:SER:OG   | 2.27                     | 0.45              |
| 1:E:76:GLN:HA    | 1:E:79:GLU:HG2   | 1.98                     | 0.45              |
| 1:E:174:ASN:OD1  | 1:E:176:ASN:N    | 2.49                     | 0.45              |
| 1:E:503:GLN:HG2  | 1:E:507:GLN:HE22 | 1.81                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:507:GLN:HG2  | 1:E:507:GLN:O    | 2.16                     | 0.45              |
| 1:P:90:GLN:NE2   | 1:F:56:SER:OG    | 2.41                     | 0.45              |
| 1:H:5:ILE:HD11   | 1:H:542:VAL:HG21 | 1.98                     | 0.45              |
| 1:C:491:ASN:HD22 | 1:N:84:GLU:HG2   | 1.81                     | 0.45              |
| 1:I:519:SER:O    | 1:I:523:ILE:HG12 | 2.16                     | 0.45              |
| 1:T:164:ASP:OD1  | 1:T:167:THR:N    | 2.40                     | 0.45              |
| 1:V:51:ALA:O     | 1:V:55:THR:HG23  | 2.15                     | 0.45              |
| 1:L:492:LEU:HA   | 1:L:495:THR:HG22 | 1.98                     | 0.45              |
| 1:L:494:ASN:O    | 1:L:498:ASN:ND2  | 2.49                     | 0.45              |
| 1:B:164:ASP:H    | 1:B:167:THR:HB   | 1.81                     | 0.45              |
| 1:B:512:ALA:HA   | 1:A:545:LEU:HD21 | 1.99                     | 0.45              |
| 1:O:164:ASP:O    | 1:O:168:LEU:HG   | 2.17                     | 0.45              |
| 1:E:141:ASP:HA   | 1:E:161:LYS:HA   | 1.98                     | 0.45              |
| 1:E:144:MET:HB3  | 1:E:158:ILE:HB   | 1.98                     | 0.45              |
| 1:Q:164:ASP:H    | 1:Q:167:THR:HB   | 1.81                     | 0.45              |
| 1:Q:485:LEU:O    | 1:Q:489:VAL:HG23 | 2.16                     | 0.45              |
| 1:I:17:ASN:HA    | 1:I:20:LYS:HD2   | 1.97                     | 0.45              |
| 1:B:70:ASP:O     | 1:B:74:VAL:HG23  | 2.16                     | 0.45              |
| 1:B:125:ARG:CG   | 1:B:129:GLN:HE21 | 2.30                     | 0.45              |
| 1:M:116:ILE:HG21 | 1:M:173:PHE:HD2  | 1.81                     | 0.45              |
| 1:C:531:VAL:HG11 | 1:N:32:LEU:HG    | 1.98                     | 0.45              |
| 1:F:70:ASP:O     | 1:F:74:VAL:HG23  | 2.16                     | 0.45              |
| 1:I:488:ALA:O    | 1:I:492:LEU:HD23 | 2.17                     | 0.45              |
| 1:J:170:LEU:HD13 | 1:J:173:PHE:HB2  | 1.97                     | 0.45              |
| 1:J:484:ARG:NH2  | 1:K:122:GLU:OE1  | 2.49                     | 0.45              |
| 1:V:170:LEU:HD11 | 1:V:463:ALA:HB3  | 1.98                     | 0.45              |
| 1:L:481:VAL:O    | 1:L:485:LEU:HD23 | 2.16                     | 0.45              |
| 1:B:3:GLN:OE1    | 1:M:22:GLN:HG2   | 2.17                     | 0.45              |
| 1:M:74:VAL:HG22  | 1:M:132:PHE:CD2  | 2.51                     | 0.45              |
| 1:O:31:ARG:HD3   | 1:O:37:ARG:HG3   | 1.99                     | 0.45              |
| 1:Q:505:ARG:HB2  | 1:Q:505:ARG:NH1  | 2.32                     | 0.45              |
| 1:Q:518:MET:O    | 1:Q:522:GLN:HG3  | 2.16                     | 0.45              |
| 1:R:103:THR:HA   | 1:H:144:MET:HE1  | 1.99                     | 0.45              |
| 1:M:8:ASN:O      | 1:M:11:SER:OG    | 2.27                     | 0.45              |
| 1:C:479:GLY:HA2  | 1:C:482:GLN:OE1  | 2.17                     | 0.45              |
| 1:C:498:ASN:HD22 | 1:N:77:THR:HA    | 1.81                     | 0.45              |
| 1:D:92:ILE:HD11  | 1:D:119:ARG:HB3  | 1.98                     | 0.45              |
| 1:P:16:ASN:HB3   | 1:P:20:LYS:HZ3   | 1.80                     | 0.45              |
| 1:P:27:SER:O     | 1:P:31:ARG:HG3   | 2.17                     | 0.45              |
| 1:P:503:GLN:OE1  | 1:P:507:GLN:NE2  | 2.50                     | 0.45              |
| 1:R:69:ASN:O     | 1:R:72:ILE:HG12  | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:486:ASP:OD2  | 1:H:42:LYS:HE3   | 2.15                     | 0.45              |
| 1:K:140:LYS:NZ   | 1:K:141:ASP:O    | 2.50                     | 0.45              |
| 1:V:92:ILE:HD11  | 1:V:119:ARG:CB   | 2.46                     | 0.45              |
| 1:B:146:ILE:HD13 | 1:B:485:LEU:HD21 | 1.98                     | 0.45              |
| 1:M:45:ALA:HB1   | 1:M:48:GLN:HE21  | 1.82                     | 0.45              |
| 1:N:112:ILE:O    | 1:N:116:ILE:HG12 | 2.17                     | 0.45              |
| 1:O:69:ASN:HA    | 1:O:72:ILE:HG22  | 1.98                     | 0.45              |
| 1:F:10:LEU:HD11  | 1:G:29:ILE:HG21  | 1.99                     | 0.45              |
| 1:H:170:LEU:C    | 1:H:172:GLY:H    | 2.25                     | 0.45              |
| 1:U:520:LYS:O    | 1:U:524:ILE:HG12 | 2.17                     | 0.45              |
| 1:L:174:ASN:ND2  | 1:L:177:GLY:O    | 2.50                     | 0.45              |
| 1:L:502:ALA:O    | 1:L:506:ILE:HG12 | 2.17                     | 0.45              |
| 1:B:31:ARG:HA    | 1:B:39:ASN:HD21  | 1.80                     | 0.45              |
| 1:M:511:TYR:O    | 1:M:515:VAL:HG12 | 2.16                     | 0.45              |
| 1:G:176:ASN:OD1  | 1:G:176:ASN:N    | 2.49                     | 0.45              |
| 1:G:512:ALA:C    | 1:H:15:GLN:HE22  | 2.25                     | 0.45              |
| 1:H:152:ASP:OD1  | 1:H:153:GLY:N    | 2.50                     | 0.45              |
| 1:C:116:ILE:HG21 | 1:C:173:PHE:HD2  | 1.81                     | 0.45              |
| 1:O:147:GLN:HA   | 1:O:155:THR:HG22 | 1.99                     | 0.45              |
| 1:P:50:ILE:HG22  | 1:P:54:PHE:HE1   | 1.81                     | 0.45              |
| 1:K:91:ARG:HD3   | 1:K:95:LEU:HD23  | 1.98                     | 0.45              |
| 1:L:493:ASN:O    | 1:L:497:THR:HG23 | 2.16                     | 0.45              |
| 1:B:154:GLN:HE21 | 1:B:155:THR:H    | 1.63                     | 0.45              |
| 1:M:82:LEU:HD12  | 1:M:471:ILE:HG23 | 1.99                     | 0.45              |
| 1:O:85:ILE:HG23  | 1:O:123:ILE:HG23 | 1.99                     | 0.45              |
| 1:E:537:GLN:CA   | 1:E:540:GLN:HE22 | 2.30                     | 0.45              |
| 1:P:163:ILE:HD11 | 1:P:474:PHE:CD1  | 2.52                     | 0.45              |
| 1:F:69:ASN:O     | 1:F:72:ILE:HG22  | 2.16                     | 0.45              |
| 1:Q:521:ALA:O    | 1:Q:524:ILE:N    | 2.50                     | 0.45              |
| 1:T:113:GLN:OE1  | 1:T:174:ASN:HA   | 2.17                     | 0.45              |
| 1:N:474:PHE:CE2  | 1:N:478:LEU:HD11 | 2.52                     | 0.44              |
| 1:D:485:LEU:O    | 1:D:489:VAL:HG23 | 2.17                     | 0.44              |
| 1:P:152:ASP:OD1  | 1:P:153:GLY:N    | 2.49                     | 0.44              |
| 1:S:97:VAL:HG13  | 1:I:147:GLN:OE1  | 2.17                     | 0.44              |
| 1:I:122:GLU:OE2  | 1:I:125:ARG:NE   | 2.48                     | 0.44              |
| 1:J:485:LEU:O    | 1:J:489:VAL:HG23 | 2.18                     | 0.44              |
| 1:V:525:GLN:HG2  | 1:V:529:ASN:HD21 | 1.82                     | 0.44              |
| 1:L:514:GLU:HA   | 1:L:514:GLU:OE1  | 2.16                     | 0.44              |
| 1:C:10:LEU:HD11  | 1:N:29:ILE:HB    | 1.98                     | 0.44              |
| 1:D:105:SER:O    | 1:D:109:LEU:HD12 | 2.17                     | 0.44              |
| 1:P:516:SER:O    | 1:P:520:LYS:HG3  | 2.17                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:166:ASP:OD1  | 1:K:167:THR:N    | 2.50                     | 0.44              |
| 1:N:162:LYS:HG3  | 1:N:167:THR:HG21 | 2.00                     | 0.44              |
| 1:D:173:PHE:HE1  | 1:D:460:PRO:HA   | 1.83                     | 0.44              |
| 1:P:158:ILE:HG12 | 1:P:481:VAL:HG21 | 1.99                     | 0.44              |
| 1:P:168:LEU:HD21 | 1:P:471:ILE:HD11 | 1.99                     | 0.44              |
| 1:R:58:ILE:HG23  | 1:R:496:THR:HG23 | 1.99                     | 0.44              |
| 1:R:152:ASP:OD1  | 1:R:153:GLY:N    | 2.50                     | 0.44              |
| 1:R:486:ASP:O    | 1:R:490:THR:HG22 | 2.17                     | 0.44              |
| 1:T:162:LYS:NZ   | 1:T:167:THR:HG1  | 2.15                     | 0.44              |
| 1:J:101:THR:HG22 | 1:J:103:THR:H    | 1.81                     | 0.44              |
| 1:U:116:ILE:HG21 | 1:U:173:PHE:CD2  | 2.44                     | 0.44              |
| 1:L:486:ASP:O    | 1:L:490:THR:HG23 | 2.17                     | 0.44              |
| 1:L:522:GLN:O    | 1:L:526:GLN:HG3  | 2.17                     | 0.44              |
| 1:B:98:GLN:HB2   | 1:A:63:GLN:CD    | 2.43                     | 0.44              |
| 1:A:109:LEU:HB3  | 1:A:176:ASN:HB3  | 1.99                     | 0.44              |
| 1:M:125:ARG:NH1  | 1:M:125:ARG:HG2  | 2.33                     | 0.44              |
| 1:D:3:GLN:N      | 1:D:3:GLN:OE1    | 2.50                     | 0.44              |
| 1:E:52:ASN:O     | 1:E:55:THR:OG1   | 2.30                     | 0.44              |
| 1:P:37:ARG:NH1   | 1:Q:66:ARG:HH22  | 2.14                     | 0.44              |
| 1:P:148:VAL:HG22 | 1:Q:125:ARG:HH21 | 1.82                     | 0.44              |
| 1:R:55:THR:O     | 1:R:59:LYS:HG3   | 2.17                     | 0.44              |
| 1:R:170:LEU:HG   | 1:R:171:ASN:H    | 1.83                     | 0.44              |
| 1:S:112:ILE:O    | 1:S:116:ILE:HG12 | 2.17                     | 0.44              |
| 1:I:504:SER:OG   | 1:I:508:ASP:OD2  | 2.26                     | 0.44              |
| 1:U:520:LYS:HB2  | 1:U:520:LYS:HE2  | 1.70                     | 0.44              |
| 1:B:125:ARG:O    | 1:B:129:GLN:HG3  | 2.17                     | 0.44              |
| 1:H:85:ILE:O     | 1:H:89:LEU:HD13  | 2.17                     | 0.44              |
| 1:I:515:VAL:O    | 1:I:518:MET:HG3  | 2.16                     | 0.44              |
| 1:J:91:ARG:NH1   | 1:J:94:GLU:OE1   | 2.50                     | 0.44              |
| 1:D:530:SER:O    | 1:D:534:LYS:NZ   | 2.50                     | 0.44              |
| 1:E:170:LEU:HG   | 1:E:171:ASN:N    | 2.33                     | 0.44              |
| 1:P:32:LEU:HD12  | 1:P:511:TYR:CD1  | 2.52                     | 0.44              |
| 1:Q:32:LEU:HD13  | 1:Q:514:GLU:OE2  | 2.17                     | 0.44              |
| 1:H:63:GLN:OE1   | 1:H:63:GLN:HA    | 2.16                     | 0.44              |
| 1:T:13:ILE:O     | 1:T:17:ASN:ND2   | 2.51                     | 0.44              |
| 1:B:526:GLN:HG2  | 1:L:541:GLN:OE1  | 2.18                     | 0.44              |
| 1:C:531:VAL:HG21 | 1:N:33:SER:HA    | 1.98                     | 0.44              |
| 1:E:168:LEU:HD21 | 1:E:471:ILE:HD11 | 2.00                     | 0.44              |
| 1:F:109:LEU:HA   | 1:F:112:ILE:HD12 | 1.99                     | 0.44              |
| 1:S:96:THR:HG21  | 1:S:460:PRO:HB2  | 1.98                     | 0.44              |
| 1:I:61:LEU:HD11  | 1:I:499:LEU:HD12 | 2.00                     | 0.44              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:T:491:ASN:C      | 1:T:491:ASN:HD22 | 2.26                     | 0.44              |
| 1:J:484:ARG:NE     | 1:K:122:GLU:HB2  | 2.33                     | 0.44              |
| 1:U:9:SER:HA       | 1:U:12:LEU:HB3   | 2.00                     | 0.44              |
| 1:K:101:THR:HG22   | 1:K:103:THR:H    | 1.82                     | 0.44              |
| 1:L:122:GLU:HA     | 1:L:122:GLU:OE2  | 2.17                     | 0.44              |
| 1:M:69:ASN:HA      | 1:M:72:ILE:HG12  | 2.00                     | 0.44              |
| 1:O:72:ILE:HD11    | 1:O:482:GLN:HG2  | 2.00                     | 0.44              |
| 1:O:474:PHE:O      | 1:O:478:LEU:HD23 | 2.18                     | 0.44              |
| 1:F:38[B]:ILE:HG12 | 1:F:507:GLN:HG3  | 2.00                     | 0.44              |
| 1:F:71:GLY:HA3     | 1:F:146:ILE:HD13 | 2.00                     | 0.44              |
| 1:V:147:GLN:HA     | 1:V:155:THR:HG22 | 2.00                     | 0.44              |
| 1:V:460:PRO:HG2    | 1:V:461:LEU:HD12 | 1.99                     | 0.44              |
| 1:B:48:GLN:OE1     | 1:B:48:GLN:HA    | 2.18                     | 0.44              |
| 1:A:43:ASP:CG      | 1:A:44:ASP:H     | 2.25                     | 0.44              |
| 1:F:51:ALA:O       | 1:F:55:THR:HG23  | 2.16                     | 0.44              |
| 1:F:72:ILE:HD11    | 1:F:482:GLN:HG3  | 2.00                     | 0.44              |
| 1:G:518:MET:HE2    | 1:G:518:MET:HB3  | 1.84                     | 0.44              |
| 1:U:92:ILE:HD11    | 1:U:119:ARG:HB2  | 2.00                     | 0.44              |
| 1:U:534:LYS:O      | 1:U:538:VAL:HG23 | 2.17                     | 0.44              |
| 1:B:78:THR:OG1     | 1:B:478:LEU:HD11 | 2.18                     | 0.43              |
| 1:B:92:ILE:HG23    | 1:B:116:ILE:HG23 | 1.99                     | 0.43              |
| 1:O:82:LEU:HG      | 1:O:474:PHE:CD2  | 2.53                     | 0.43              |
| 1:P:5:ILE:HG22     | 1:P:542:VAL:HG21 | 1.99                     | 0.43              |
| 1:F:498:ASN:HA     | 1:F:501:GLU:HG2  | 1.99                     | 0.43              |
| 1:R:484:ARG:HD2    | 1:S:122:GLU:HB2  | 2.00                     | 0.43              |
| 1:H:517:ASN:HA     | 1:H:520:LYS:HZ3  | 1.83                     | 0.43              |
| 1:I:82:LEU:HD13    | 1:I:85:ILE:HD12  | 2.00                     | 0.43              |
| 1:I:147:GLN:HA     | 1:I:155:THR:HG22 | 2.00                     | 0.43              |
| 1:J:162:LYS:O      | 1:J:167:THR:HG21 | 2.18                     | 0.43              |
| 1:J:484:ARG:HD3    | 1:K:118:SER:O    | 2.18                     | 0.43              |
| 1:U:10:LEU:HD21    | 1:V:29:ILE:HG21  | 2.00                     | 0.43              |
| 1:A:145:LYS:NZ     | 1:A:155:THR:HG21 | 2.33                     | 0.43              |
| 1:M:92:ILE:HG23    | 1:M:116:ILE:HD12 | 1.99                     | 0.43              |
| 1:Q:43:ASP:CG      | 1:Q:44:ASP:N     | 2.76                     | 0.43              |
| 1:G:455:GLU:OE2    | 1:G:456:SER:N    | 2.48                     | 0.43              |
| 1:S:518:MET:SD     | 1:S:522:GLN:NE2  | 2.91                     | 0.43              |
| 1:T:541:GLN:NE2    | 1:U:526:GLN:HE21 | 2.15                     | 0.43              |
| 1:L:73:SER:O       | 1:L:76:GLN:HG2   | 2.18                     | 0.43              |
| 1:L:78:THR:O       | 1:L:82:LEU:HD23  | 2.17                     | 0.43              |
| 1:B:478:LEU:O      | 1:B:482:GLN:HG3  | 2.18                     | 0.43              |
| 1:C:152:ASP:OD1    | 1:C:153:GLY:N    | 2.50                     | 0.43              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:P:71:GLY:HA3     | 1:P:146:ILE:HD13 | 2.00                     | 0.43              |
| 1:I:164:ASP:O      | 1:I:168:LEU:HG   | 2.19                     | 0.43              |
| 1:T:90:GLN:NE2     | 1:J:52:ASN:OD1   | 2.52                     | 0.43              |
| 1:L:478:LEU:O      | 1:L:482:GLN:HG3  | 2.18                     | 0.43              |
| 1:E:152:ASP:OD1    | 1:E:153:GLY:N    | 2.52                     | 0.43              |
| 1:T:170:LEU:HD13   | 1:T:173:PHE:CD1  | 2.53                     | 0.43              |
| 1:V:122:GLU:O      | 1:V:126:VAL:HG12 | 2.17                     | 0.43              |
| 1:M:59:LYS:HB2     | 1:M:59:LYS:HE2   | 1.78                     | 0.43              |
| 1:C:38[A]:ILE:HG22 | 1:C:41:ALA:H     | 1.83                     | 0.43              |
| 1:E:71:GLY:HA2     | 1:E:74:VAL:HG12  | 1.99                     | 0.43              |
| 1:Q:497:THR:HG21   | 1:G:16:ASN:ND2   | 2.32                     | 0.43              |
| 1:H:488:ALA:O      | 1:H:492:LEU:HD23 | 2.18                     | 0.43              |
| 1:I:75:ALA:HA      | 1:I:478:LEU:HD11 | 2.01                     | 0.43              |
| 1:T:170:LEU:HD13   | 1:T:173:PHE:HB2  | 2.01                     | 0.43              |
| 1:A:37:ARG:HB2     | 1:A:508:ASP:O    | 2.19                     | 0.43              |
| 1:A:538:VAL:HB     | 1:A:539:PRO:HD3  | 2.01                     | 0.43              |
| 1:M:99:ALA:HB1     | 1:M:175:VAL:HB   | 2.00                     | 0.43              |
| 1:F:546:LEU:HD23   | 1:F:546:LEU:HA   | 1.92                     | 0.43              |
| 1:G:520:LYS:O      | 1:G:524:ILE:HG12 | 2.18                     | 0.43              |
| 1:V:141:ASP:HB2    | 1:V:162:LYS:HB2  | 2.01                     | 0.43              |
| 1:B:119:ARG:NH2    | 1:L:483:ASN:HD21 | 2.16                     | 0.43              |
| 1:O:51:ALA:O       | 1:O:55:THR:HG23  | 2.19                     | 0.43              |
| 1:E:82:LEU:HD13    | 1:E:475:ARG:HG2  | 1.99                     | 0.43              |
| 1:P:147:GLN:NE2    | 1:P:149:GLY:H    | 2.16                     | 0.43              |
| 1:P:523:ILE:HG23   | 1:G:543:LEU:HD21 | 2.01                     | 0.43              |
| 1:F:460:PRO:O      | 1:F:464:LEU:HD13 | 2.19                     | 0.43              |
| 1:G:76:GLN:HA      | 1:G:79:GLU:HG3   | 2.00                     | 0.43              |
| 1:G:141:ASP:N      | 1:G:162:LYS:HB3  | 2.33                     | 0.43              |
| 1:G:156:ILE:HG23   | 1:G:484:ARG:NH2  | 2.33                     | 0.43              |
| 1:H:69:ASN:HA      | 1:H:72:ILE:HG22  | 2.01                     | 0.43              |
| 1:A:14:THR:O       | 1:A:18:ILE:HG13  | 2.19                     | 0.43              |
| 1:C:163:ILE:HG23   | 1:C:168:LEU:HD21 | 2.01                     | 0.43              |
| 1:C:515:VAL:O      | 1:C:518:MET:HG3  | 2.19                     | 0.43              |
| 1:D:72:ILE:O       | 1:D:76:GLN:HG2   | 2.18                     | 0.43              |
| 1:E:537:GLN:C      | 1:E:540:GLN:HE22 | 2.26                     | 0.43              |
| 1:G:170:LEU:HD22   | 1:G:173:PHE:CE1  | 2.53                     | 0.43              |
| 1:R:28:SER:O       | 1:R:32:LEU:HD23  | 2.18                     | 0.43              |
| 1:H:37:ARG:HB2     | 1:H:508:ASP:O    | 2.19                     | 0.43              |
| 1:H:93:ARG:HA      | 1:H:464:LEU:HD13 | 2.01                     | 0.43              |
| 1:V:31:ARG:HD2     | 1:V:37:ARG:HA    | 2.01                     | 0.43              |
| 1:L:526:GLN:HA     | 1:L:529:ASN:HD22 | 1.84                     | 0.43              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:A:70:ASP:O       | 1:A:74:VAL:HG23  | 2.19                     | 0.43              |
| 1:N:505:ARG:O      | 1:O:66:ARG:NH2   | 2.52                     | 0.43              |
| 1:P:469:SER:O      | 1:P:473:LYS:HG2  | 2.19                     | 0.43              |
| 1:G:518:MET:O      | 1:G:522:GLN:HG3  | 2.19                     | 0.43              |
| 1:G:537:GLN:OE1    | 1:G:541:GLN:NE2  | 2.51                     | 0.43              |
| 1:H:174:ASN:OD1    | 1:H:177:GLY:N    | 2.52                     | 0.43              |
| 1:H:498:ASN:HA     | 1:H:501:GLU:OE1  | 2.19                     | 0.43              |
| 1:S:156:ILE:HD13   | 1:S:485:LEU:HD22 | 2.01                     | 0.43              |
| 1:I:79:GLU:OE1     | 1:I:482:GLN:NE2  | 2.51                     | 0.43              |
| 1:K:38[B]:ILE:HG23 | 1:K:41:ALA:HB2   | 2.00                     | 0.43              |
| 1:K:491:ASN:C      | 1:K:491:ASN:HD22 | 2.27                     | 0.43              |
| 1:V:25:LEU:HD22    | 1:V:525:GLN:OE1  | 2.19                     | 0.43              |
| 1:A:61:LEU:O       | 1:A:492:LEU:HD23 | 2.19                     | 0.43              |
| 1:A:469:SER:HB3    | 1:A:473:LYS:HZ1  | 1.84                     | 0.43              |
| 1:M:174:ASN:ND2    | 1:M:177:GLY:O    | 2.48                     | 0.43              |
| 1:E:536:ASN:O      | 1:E:539:PRO:HD2  | 2.18                     | 0.43              |
| 1:P:5:ILE:HG21     | 1:P:542:VAL:HG11 | 2.00                     | 0.43              |
| 1:S:86:ASN:HD21    | 1:I:52:ASN:HD21  | 1.66                     | 0.43              |
| 1:A:493:ASN:O      | 1:A:497:THR:HG23 | 2.19                     | 0.42              |
| 1:N:149:GLY:HA3    | 1:N:154:GLN:OE1  | 2.19                     | 0.42              |
| 1:N:494:ASN:ND2    | 1:O:84:GLU:OE2   | 2.33                     | 0.42              |
| 1:N:506:ILE:HA     | 1:O:66:ARG:HH21  | 1.84                     | 0.42              |
| 1:R:141:ASP:N      | 1:R:162:LYS:HB3  | 2.34                     | 0.42              |
| 1:R:484:ARG:HH12   | 1:S:121:ASP:HB3  | 1.83                     | 0.42              |
| 1:H:108:ASP:O      | 1:H:112:ILE:HD12 | 2.19                     | 0.42              |
| 1:T:69:ASN:HA      | 1:T:72:ILE:HG22  | 2.00                     | 0.42              |
| 1:J:58:ILE:HG13    | 1:J:496:THR:HG23 | 2.00                     | 0.42              |
| 1:V:70:ASP:O       | 1:V:73:SER:OG    | 2.31                     | 0.42              |
| 1:V:94:GLU:OE2     | 1:L:59:LYS:HB3   | 2.19                     | 0.42              |
| 1:B:74:VAL:HG22    | 1:B:132:PHE:CD2  | 2.54                     | 0.42              |
| 1:M:74:VAL:HG22    | 1:M:132:PHE:HD2  | 1.83                     | 0.42              |
| 1:D:91:ARG:HD2     | 1:D:94:GLU:OE2   | 2.18                     | 0.42              |
| 1:O:66:ARG:HA      | 1:O:66:ARG:HD2   | 1.76                     | 0.42              |
| 1:O:98:GLN:HB3     | 1:E:63:GLN:CG    | 2.49                     | 0.42              |
| 1:P:41:ALA:HB1     | 1:P:43:ASP:OD1   | 2.20                     | 0.42              |
| 1:F:38[B]:ILE:HB   | 1:F:507:GLN:HE21 | 1.84                     | 0.42              |
| 1:T:74:VAL:HG21    | 1:T:144:MET:HE1  | 2.01                     | 0.42              |
| 1:T:478:LEU:HA     | 1:T:481:VAL:HG22 | 2.01                     | 0.42              |
| 1:U:173:PHE:HE1    | 1:U:460:PRO:HB3  | 1.84                     | 0.42              |
| 1:B:541:GLN:HB3    | 1:M:529:ASN:ND2  | 2.34                     | 0.42              |
| 1:D:14:THR:O       | 1:D:18:ILE:HG13  | 2.20                     | 0.42              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:O:492:LEU:O      | 1:O:496:THR:HG23 | 2.18                     | 0.42              |
| 1:T:170:LEU:HB3    | 1:T:173:PHE:HB2  | 2.02                     | 0.42              |
| 1:A:81:ALA:O       | 1:A:85:ILE:HG13  | 2.20                     | 0.42              |
| 1:C:38[B]:ILE:HG22 | 1:C:41:ALA:H     | 1.83                     | 0.42              |
| 1:C:501:GLU:O      | 1:C:505:ARG:HG3  | 2.20                     | 0.42              |
| 1:O:37:ARG:HB3     | 1:O:507:GLN:HB2  | 2.01                     | 0.42              |
| 1:O:90:GLN:OE1     | 1:E:59:LYS:HE3   | 2.18                     | 0.42              |
| 1:E:478:LEU:HA     | 1:E:481:VAL:HG22 | 2.01                     | 0.42              |
| 1:F:164:ASP:N      | 1:F:164:ASP:OD2  | 2.52                     | 0.42              |
| 1:G:82:LEU:HD21    | 1:G:474:PHE:CD1  | 2.54                     | 0.42              |
| 1:H:116:ILE:HG21   | 1:H:173:PHE:CD2  | 2.54                     | 0.42              |
| 1:S:459:ASP:HB3    | 1:S:462:ALA:HB3  | 2.00                     | 0.42              |
| 1:I:14:THR:HG21    | 1:I:531:VAL:HG13 | 2.02                     | 0.42              |
| 1:I:531:VAL:HG11   | 1:T:33:SER:HA    | 2.00                     | 0.42              |
| 1:T:82:LEU:HD11    | 1:T:474:PHE:CD2  | 2.55                     | 0.42              |
| 1:T:481:VAL:HA     | 1:T:484:ARG:HH12 | 1.84                     | 0.42              |
| 1:A:40:SER:O       | 1:A:42:LYS:N     | 2.52                     | 0.42              |
| 1:M:520:LYS:HZ2    | 1:M:520:LYS:HG3  | 1.57                     | 0.42              |
| 1:O:511:TYR:CD2    | 1:E:5:ILE:HD13   | 2.54                     | 0.42              |
| 1:P:519:SER:O      | 1:P:523:ILE:HG12 | 2.19                     | 0.42              |
| 1:S:536:ASN:O      | 1:S:539:PRO:HD2  | 2.19                     | 0.42              |
| 1:I:120:LEU:HD23   | 1:I:123:ILE:HD12 | 2.02                     | 0.42              |
| 1:I:141:ASP:HB2    | 1:I:162:LYS:H    | 1.85                     | 0.42              |
| 1:T:481:VAL:HA     | 1:T:484:ARG:NH1  | 2.34                     | 0.42              |
| 1:K:514:GLU:OE1    | 1:K:514:GLU:HA   | 2.20                     | 0.42              |
| 1:V:110:ASP:HA     | 1:V:176:ASN:HD22 | 1.83                     | 0.42              |
| 1:L:51:ALA:O       | 1:L:55:THR:HG23  | 2.20                     | 0.42              |
| 1:A:10:LEU:HA      | 1:A:13:ILE:HG22  | 2.01                     | 0.42              |
| 1:C:164:ASP:OD1    | 1:C:167:THR:HG23 | 2.20                     | 0.42              |
| 1:O:94:GLU:HB3     | 1:E:59:LYS:NZ    | 2.31                     | 0.42              |
| 1:F:93:ARG:O       | 1:F:97:VAL:HG13  | 2.19                     | 0.42              |
| 1:H:99:ALA:HB2     | 1:H:112:ILE:HG21 | 2.02                     | 0.42              |
| 1:S:85:ILE:HG23    | 1:S:123:ILE:HG23 | 2.01                     | 0.42              |
| 1:S:93:ARG:HA      | 1:S:464:LEU:HD13 | 2.02                     | 0.42              |
| 1:I:82:LEU:HD21    | 1:I:138:LEU:HD11 | 2.01                     | 0.42              |
| 1:K:478:LEU:HA     | 1:K:481:VAL:HG22 | 2.02                     | 0.42              |
| 1:L:30:GLU:OE1     | 1:L:39:ASN:ND2   | 2.53                     | 0.42              |
| 1:L:113:GLN:HA     | 1:L:116:ILE:HG12 | 2.01                     | 0.42              |
| 1:M:61:LEU:CD1     | 1:M:492:LEU:HD22 | 2.50                     | 0.42              |
| 1:N:141:ASP:N      | 1:N:162:LYS:HB3  | 2.35                     | 0.42              |
| 1:F:38[A]:ILE:HB   | 1:F:507:GLN:HE21 | 1.85                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:166:ASP:HA   | 1:H:171:ASN:HB3  | 2.01                     | 0.42              |
| 1:K:147:GLN:HA   | 1:K:155:THR:HG22 | 2.02                     | 0.42              |
| 1:K:505:ARG:NH2  | 1:L:69:ASN:HD22  | 2.04                     | 0.42              |
| 1:V:161:LYS:HE2  | 1:V:474:PHE:CD1  | 2.55                     | 0.42              |
| 1:C:75:ALA:HB1   | 1:C:482:GLN:NE2  | 2.35                     | 0.42              |
| 1:P:69:ASN:O     | 1:P:72:ILE:HG22  | 2.19                     | 0.42              |
| 1:Q:480:ALA:HA   | 1:Q:483:ASN:HD22 | 1.84                     | 0.42              |
| 1:R:101:THR:HG22 | 1:R:103:THR:H    | 1.85                     | 0.42              |
| 1:H:74:VAL:HG22  | 1:H:132:PHE:CD2  | 2.54                     | 0.42              |
| 1:I:138:LEU:HD12 | 1:I:163:ILE:HB   | 2.01                     | 0.42              |
| 1:I:139:ALA:O    | 1:I:162:LYS:HG3  | 2.19                     | 0.42              |
| 1:T:15:GLN:HA    | 1:T:18:ILE:HG22  | 2.01                     | 0.42              |
| 1:T:520:LYS:O    | 1:T:524:ILE:HG13 | 2.20                     | 0.42              |
| 1:U:162:LYS:NZ   | 1:U:164:ASP:OD2  | 2.53                     | 0.42              |
| 1:L:170:LEU:HD12 | 1:L:173:PHE:CE1  | 2.55                     | 0.42              |
| 1:N:493:ASN:O    | 1:N:497:THR:HG23 | 2.20                     | 0.42              |
| 1:O:174:ASN:OD1  | 1:O:177:GLY:N    | 2.53                     | 0.42              |
| 1:U:117:LYS:O    | 1:U:117:LYS:HD3  | 2.20                     | 0.42              |
| 1:V:511:TYR:O    | 1:V:515:VAL:HG12 | 2.20                     | 0.42              |
| 1:V:536:ASN:O    | 1:V:539:PRO:HD2  | 2.19                     | 0.42              |
| 1:V:542:VAL:O    | 1:V:546:LEU:HG   | 2.19                     | 0.42              |
| 1:L:170:LEU:C    | 1:L:172:GLY:H    | 2.27                     | 0.42              |
| 1:B:154:GLN:HE21 | 1:B:155:THR:N    | 2.17                     | 0.42              |
| 1:A:156:ILE:HD11 | 1:A:484:ARG:HG2  | 2.01                     | 0.42              |
| 1:M:485:LEU:O    | 1:M:489:VAL:HG23 | 2.20                     | 0.42              |
| 1:Q:86:ASN:C     | 1:Q:86:ASN:HD22  | 2.28                     | 0.42              |
| 1:Q:493:ASN:O    | 1:Q:497:THR:HG23 | 2.20                     | 0.42              |
| 1:G:69:ASN:HA    | 1:G:72:ILE:HG12  | 2.01                     | 0.42              |
| 1:S:119:ARG:O    | 1:S:123:ILE:HG12 | 2.20                     | 0.42              |
| 1:S:519:SER:O    | 1:S:523:ILE:HG12 | 2.19                     | 0.42              |
| 1:T:103:THR:HG22 | 1:J:144:MET:HE2  | 2.01                     | 0.42              |
| 1:K:84:GLU:OE1   | 1:K:88:ASN:ND2   | 2.53                     | 0.42              |
| 1:V:90:GLN:NE2   | 1:L:55:THR:OG1   | 2.52                     | 0.42              |
| 1:B:78:THR:O     | 1:B:82:LEU:HD23  | 2.19                     | 0.41              |
| 1:N:116:ILE:HG21 | 1:N:173:PHE:HD2  | 1.84                     | 0.41              |
| 1:D:64:ALA:HB1   | 1:D:148:VAL:C    | 2.44                     | 0.41              |
| 1:O:170:LEU:C    | 1:O:172:GLY:H    | 2.28                     | 0.41              |
| 1:O:537:GLN:O    | 1:O:540:GLN:HG2  | 2.20                     | 0.41              |
| 1:F:93:ARG:NH1   | 1:F:465:ASP:OD1  | 2.53                     | 0.41              |
| 1:Q:91:ARG:O     | 1:Q:94:GLU:HB3   | 2.20                     | 0.41              |
| 1:H:494:ASN:O    | 1:H:497:THR:OG1  | 2.33                     | 0.41              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:H:522:GLN:O    | 1:H:526:GLN:OE1    | 2.38                     | 0.41              |
| 1:T:92:ILE:HG23  | 1:T:116:ILE:HD12   | 2.01                     | 0.41              |
| 1:J:50:ILE:HG22  | 1:J:54:PHE:CE2     | 2.55                     | 0.41              |
| 1:U:78:THR:O     | 1:U:82:LEU:HD23    | 2.19                     | 0.41              |
| 1:K:116:ILE:HG21 | 1:K:173:PHE:CE2    | 2.55                     | 0.41              |
| 1:K:173:PHE:HE1  | 1:K:460:PRO:HB3    | 1.85                     | 0.41              |
| 1:L:92:ILE:HD11  | 1:L:119:ARG:HG3    | 2.02                     | 0.41              |
| 1:B:38[A]:ILE:O  | 1:B:38[A]:ILE:HG22 | 2.19                     | 0.41              |
| 1:B:79:GLU:HB2   | 1:B:478:LEU:HD22   | 2.01                     | 0.41              |
| 1:B:129:GLN:HE22 | 1:L:154:GLN:HG2    | 1.85                     | 0.41              |
| 1:B:461:LEU:HB2  | 1:A:152:ASP:HB2    | 2.01                     | 0.41              |
| 1:M:170:LEU:C    | 1:M:172:GLY:N      | 2.79                     | 0.41              |
| 1:E:68:ALA:HB1   | 1:E:485:LEU:HD12   | 2.02                     | 0.41              |
| 1:G:101:THR:HG22 | 1:G:103:THR:HG22   | 2.01                     | 0.41              |
| 1:N:170:LEU:HG   | 1:N:171:ASN:N      | 2.33                     | 0.41              |
| 1:D:40:SER:O     | 1:D:40:SER:OG      | 2.38                     | 0.41              |
| 1:O:137:VAL:HG23 | 1:O:138:LEU:HG     | 2.03                     | 0.41              |
| 1:G:505:ARG:CZ   | 1:R:69:ASN:HB3     | 2.50                     | 0.41              |
| 1:T:18:ILE:HD12  | 1:T:18:ILE:HA      | 1.91                     | 0.41              |
| 1:T:523:ILE:HD12 | 1:K:543:LEU:HD11   | 2.01                     | 0.41              |
| 1:V:82:LEU:HD12  | 1:V:471:ILE:HG23   | 2.02                     | 0.41              |
| 1:L:57:ASN:OD1   | 1:L:61:LEU:HD13    | 2.21                     | 0.41              |
| 1:B:36:LEU:C     | 1:B:36:LEU:CD1     | 2.93                     | 0.41              |
| 1:B:37:ARG:HB2   | 1:B:508:ASP:C      | 2.46                     | 0.41              |
| 1:M:91:ARG:HD2   | 1:M:91:ARG:HA      | 1.89                     | 0.41              |
| 1:D:50:ILE:HD11  | 1:O:108:ASP:OD2    | 2.21                     | 0.41              |
| 1:E:530:SER:HB2  | 1:F:546:LEU:HD13   | 2.02                     | 0.41              |
| 1:P:498:ASN:O    | 1:P:501:GLU:HG2    | 2.21                     | 0.41              |
| 1:G:511:TYR:HA   | 1:G:514:GLU:OE2    | 2.20                     | 0.41              |
| 1:R:25:LEU:O     | 1:R:28:SER:OG      | 2.30                     | 0.41              |
| 1:R:57:ASN:O     | 1:R:61:LEU:HG      | 2.21                     | 0.41              |
| 1:R:125:ARG:HD2  | 1:R:125:ARG:C      | 2.46                     | 0.41              |
| 1:L:474:PHE:CE2  | 1:L:478:LEU:HD21   | 2.56                     | 0.41              |
| 1:M:101:THR:HG22 | 1:M:103:THR:H      | 1.85                     | 0.41              |
| 1:N:93:ARG:NH1   | 1:N:465:ASP:OD2    | 2.53                     | 0.41              |
| 1:O:170:LEU:HD13 | 1:O:173:PHE:HD1    | 1.85                     | 0.41              |
| 1:O:481:VAL:O    | 1:O:485:LEU:HD23   | 2.20                     | 0.41              |
| 1:O:485:LEU:O    | 1:O:489:VAL:HG23   | 2.20                     | 0.41              |
| 1:H:120:LEU:HD11 | 1:H:170:LEU:HD11   | 2.03                     | 0.41              |
| 1:A:528:GLY:HA2  | 1:A:531:VAL:HG12   | 2.02                     | 0.41              |
| 1:N:86:ASN:HD21  | 1:D:52:ASN:ND2     | 2.17                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:112:ILE:HG22 | 1:D:175:VAL:HG21 | 2.02                     | 0.41              |
| 1:E:534:LYS:O    | 1:E:538:VAL:HG23 | 2.20                     | 0.41              |
| 1:Q:32:LEU:HD22  | 1:Q:518:MET:HE1  | 2.02                     | 0.41              |
| 1:G:34:SER:OG    | 1:G:39:ASN:OD1   | 2.32                     | 0.41              |
| 1:R:67:ASN:OD1   | 1:R:146:ILE:HG23 | 2.21                     | 0.41              |
| 1:H:113:GLN:NE2  | 1:H:174:ASN:HA   | 2.32                     | 0.41              |
| 1:U:92:ILE:HA    | 1:U:95:LEU:HD23  | 2.03                     | 0.41              |
| 1:K:474:PHE:O    | 1:K:478:LEU:HD23 | 2.21                     | 0.41              |
| 1:B:32:LEU:C     | 1:B:32:LEU:HD23  | 2.45                     | 0.41              |
| 1:O:482:GLN:OE1  | 1:E:42:LYS:HD3   | 2.19                     | 0.41              |
| 1:P:485:LEU:O    | 1:P:489:VAL:HG23 | 2.20                     | 0.41              |
| 1:Q:170:LEU:HG   | 1:Q:171:ASN:H    | 1.85                     | 0.41              |
| 1:Q:541:GLN:O    | 1:Q:545:LEU:HG   | 2.20                     | 0.41              |
| 1:G:170:LEU:HD22 | 1:G:173:PHE:CZ   | 2.56                     | 0.41              |
| 1:R:484:ARG:NH2  | 1:S:125:ARG:HD3  | 2.36                     | 0.41              |
| 1:S:122:GLU:O    | 1:S:126:VAL:HG12 | 2.21                     | 0.41              |
| 1:T:10:LEU:HD21  | 1:U:26:SER:HA    | 2.03                     | 0.41              |
| 1:T:80:GLY:O     | 1:T:84:GLU:HG3   | 2.20                     | 0.41              |
| 1:J:30:GLU:O     | 1:J:39:ASN:ND2   | 2.53                     | 0.41              |
| 1:K:545:LEU:HD21 | 1:L:529:ASN:HB3  | 2.03                     | 0.41              |
| 1:M:163:ILE:O    | 1:M:163:ILE:HG23 | 2.20                     | 0.41              |
| 1:E:49:ALA:O     | 1:E:53:ARG:HG3   | 2.21                     | 0.41              |
| 1:H:154:GLN:HG2  | 1:I:129:GLN:NE2  | 2.36                     | 0.41              |
| 1:T:497:THR:HG21 | 1:J:16:ASN:OD1   | 2.21                     | 0.41              |
| 1:J:93:ARG:O     | 1:J:97:VAL:HG23  | 2.21                     | 0.41              |
| 1:M:94:GLU:O     | 1:M:97:VAL:HG22  | 2.21                     | 0.41              |
| 1:N:30:GLU:OE1   | 1:N:39:ASN:ND2   | 2.53                     | 0.41              |
| 1:N:113:GLN:HE22 | 1:N:174:ASN:HA   | 1.86                     | 0.41              |
| 1:D:74:VAL:HG11  | 1:D:144:MET:HE1  | 2.02                     | 0.41              |
| 1:D:93:ARG:HH12  | 1:D:461:LEU:HB3  | 1.85                     | 0.41              |
| 1:O:82:LEU:HG    | 1:O:474:PHE:CE2  | 2.56                     | 0.41              |
| 1:O:168:LEU:HD22 | 1:O:471:ILE:HD11 | 2.02                     | 0.41              |
| 1:O:518:MET:O    | 1:O:522:GLN:HG3  | 2.21                     | 0.41              |
| 1:O:519:SER:O    | 1:O:523:ILE:HG12 | 2.21                     | 0.41              |
| 1:O:536:ASN:O    | 1:O:539:PRO:HD2  | 2.20                     | 0.41              |
| 1:E:37:ARG:HB2   | 1:E:508:ASP:O    | 2.21                     | 0.41              |
| 1:E:481:VAL:O    | 1:E:485:LEU:HD23 | 2.21                     | 0.41              |
| 1:P:95:LEU:HG    | 1:P:112:ILE:HG23 | 2.02                     | 0.41              |
| 1:F:170:LEU:HG   | 1:F:171:ASN:H    | 1.85                     | 0.41              |
| 1:F:469:SER:O    | 1:F:473:LYS:HG2  | 2.21                     | 0.41              |
| 1:Q:469:SER:O    | 1:Q:473:LYS:HG3  | 2.21                     | 0.41              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:Q:472:ASP:HA   | 1:Q:475:ARG:HG2    | 2.03                     | 0.41              |
| 1:G:515:VAL:O    | 1:G:518:MET:HG2    | 2.20                     | 0.41              |
| 1:G:528:GLY:HA2  | 1:G:531:VAL:HG12   | 2.03                     | 0.41              |
| 1:R:494:ASN:O    | 1:R:497:THR:OG1    | 2.33                     | 0.41              |
| 1:R:511:TYR:CE1  | 1:H:5:ILE:HD12     | 2.56                     | 0.41              |
| 1:H:51:ALA:O     | 1:H:55:THR:HG23    | 2.21                     | 0.41              |
| 1:H:481:VAL:O    | 1:H:485:LEU:HD23   | 2.21                     | 0.41              |
| 1:S:485:LEU:O    | 1:S:489:VAL:HG23   | 2.21                     | 0.41              |
| 1:T:95:LEU:HA    | 1:T:98:GLN:HG3     | 2.03                     | 0.41              |
| 1:T:511:TYR:HE1  | 1:J:5:ILE:HG21     | 1.85                     | 0.41              |
| 1:U:14:THR:O     | 1:U:18:ILE:HG12    | 2.21                     | 0.41              |
| 1:L:42:LYS:HE2   | 1:L:42:LYS:HB3     | 1.86                     | 0.41              |
| 1:L:460:PRO:O    | 1:L:464:LEU:HG     | 2.21                     | 0.41              |
| 1:A:18:ILE:O     | 1:A:22:GLN:HG3     | 2.21                     | 0.41              |
| 1:D:50:ILE:HD12  | 1:E:133:ASN:OD1    | 2.21                     | 0.41              |
| 1:G:26:SER:HA    | 1:G:29:ILE:HG22    | 2.01                     | 0.41              |
| 1:G:151:ASN:HD21 | 1:R:129:GLN:NE2    | 2.18                     | 0.41              |
| 1:S:538:VAL:HB   | 1:S:539:PRO:HD3    | 2.03                     | 0.41              |
| 1:I:493:ASN:O    | 1:I:497:THR:HG23   | 2.20                     | 0.41              |
| 1:V:78:THR:O     | 1:V:82:LEU:HD23    | 2.20                     | 0.41              |
| 1:B:38[B]:ILE:O  | 1:B:38[B]:ILE:HG22 | 2.20                     | 0.40              |
| 1:B:511:TYR:HA   | 1:B:514:GLU:HB2    | 2.02                     | 0.40              |
| 1:A:3:GLN:HG2    | 1:C:22:GLN:OE1     | 2.21                     | 0.40              |
| 1:M:71:GLY:HA3   | 1:M:146:ILE:HD13   | 2.03                     | 0.40              |
| 1:M:89:LEU:HD11  | 1:M:467:ALA:HB1    | 2.02                     | 0.40              |
| 1:C:73:SER:O     | 1:C:76:GLN:HG2     | 2.22                     | 0.40              |
| 1:G:3:GLN:HG2    | 1:G:4:VAL:HG13     | 2.02                     | 0.40              |
| 1:T:101:THR:HG22 | 1:T:103:THR:H      | 1.86                     | 0.40              |
| 1:K:69:ASN:O     | 1:K:72:ILE:HG22    | 2.21                     | 0.40              |
| 1:K:117:LYS:NZ   | 1:K:121:ASP:OD1    | 2.54                     | 0.40              |
| 1:L:520:LYS:HD3  | 1:L:520:LYS:HA     | 1.75                     | 0.40              |
| 1:O:139:ALA:O    | 1:O:162:LYS:HG3    | 2.20                     | 0.40              |
| 1:Q:503:GLN:O    | 1:Q:507:GLN:HG2    | 2.21                     | 0.40              |
| 1:R:117:LYS:HA   | 1:R:117:LYS:HD3    | 1.81                     | 0.40              |
| 1:H:98:GLN:O     | 1:H:104:ASN:ND2    | 2.54                     | 0.40              |
| 1:S:73:SER:O     | 1:S:77:THR:HG23    | 2.21                     | 0.40              |
| 1:S:484:ARG:HE   | 1:S:484:ARG:HB3    | 1.72                     | 0.40              |
| 1:I:51:ALA:HB1   | 1:I:507:GLN:NE2    | 2.37                     | 0.40              |
| 1:B:125:ARG:HD3  | 1:L:484:ARG:NH2    | 2.37                     | 0.40              |
| 1:A:69:ASN:O     | 1:A:72:ILE:HG22    | 2.20                     | 0.40              |
| 1:M:80:GLY:O     | 1:M:83:SER:HB3     | 2.21                     | 0.40              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:N:510:ASP:H      | 1:D:5:ILE:HD12   | 1.87                     | 0.40              |
| 1:O:472:ASP:OD1    | 1:O:475:ARG:NH2  | 2.49                     | 0.40              |
| 1:O:492:LEU:HD23   | 1:O:492:LEU:HA   | 1.95                     | 0.40              |
| 1:E:480:ALA:O      | 1:E:484:ARG:HG3  | 2.21                     | 0.40              |
| 1:P:506:ILE:O      | 1:Q:66:ARG:NH2   | 2.55                     | 0.40              |
| 1:R:38[B]:ILE:HG23 | 1:R:41:ALA:HB2   | 2.03                     | 0.40              |
| 1:H:112:ILE:O      | 1:H:116:ILE:HG12 | 2.21                     | 0.40              |
| 1:I:520:LYS:NZ     | 1:J:7:THR:HA     | 2.37                     | 0.40              |
| 1:T:98:GLN:HE21    | 1:J:63:GLN:CD    | 2.22                     | 0.40              |
| 1:T:511:TYR:CE1    | 1:J:5:ILE:HG21   | 2.55                     | 0.40              |
| 1:U:54:PHE:HZ      | 1:V:132:PHE:CZ   | 2.40                     | 0.40              |
| 1:M:512:ALA:O      | 1:N:15:GLN:NE2   | 2.54                     | 0.40              |
| 1:C:91:ARG:HD3     | 1:C:91:ARG:O     | 2.20                     | 0.40              |
| 1:C:93:ARG:HH11    | 1:C:93:ARG:HG3   | 1.85                     | 0.40              |
| 1:D:473:LYS:HA     | 1:D:473:LYS:HD3  | 1.85                     | 0.40              |
| 1:O:119:ARG:O      | 1:O:123:ILE:HG13 | 2.22                     | 0.40              |
| 1:E:86:ASN:HD22    | 1:E:86:ASN:C     | 2.28                     | 0.40              |
| 1:P:502:ALA:O      | 1:P:506:ILE:HG12 | 2.22                     | 0.40              |
| 1:Q:466:ASP:O      | 1:Q:470:GLN:OE1  | 2.38                     | 0.40              |
| 1:Q:475:ARG:NH2    | 1:G:40:SER:O     | 2.54                     | 0.40              |
| 1:G:125:ARG:NH1    | 1:G:129:GLN:OE1  | 2.52                     | 0.40              |
| 1:H:528:GLY:HA2    | 1:H:531:VAL:HG22 | 2.03                     | 0.40              |
| 1:I:538:VAL:HB     | 1:I:539:PRO:HD3  | 2.04                     | 0.40              |
| 1:U:51:ALA:O       | 1:U:55:THR:HG23  | 2.21                     | 0.40              |
| 1:U:99:ALA:HB2     | 1:U:112:ILE:HG21 | 2.03                     | 0.40              |
| 1:L:31:ARG:HH11    | 1:L:37:ARG:HG3   | 1.86                     | 0.40              |
| 1:D:10:LEU:HD21    | 1:E:29:ILE:HD12  | 2.03                     | 0.40              |
| 1:D:528:GLY:HA2    | 1:D:531:VAL:HG12 | 2.04                     | 0.40              |
| 1:O:91:ARG:HG2     | 1:O:119:ARG:NH2  | 2.36                     | 0.40              |
| 1:P:493:ASN:O      | 1:P:497:THR:HG23 | 2.22                     | 0.40              |
| 1:F:514:GLU:HA     | 1:F:517:ASN:ND2  | 2.36                     | 0.40              |
| 1:Q:103:THR:HA     | 1:G:144:MET:SD   | 2.61                     | 0.40              |
| 1:G:37:ARG:HB3     | 1:G:508:ASP:O    | 2.20                     | 0.40              |
| 1:H:110:ASP:OD1    | 1:H:176:ASN:ND2  | 2.50                     | 0.40              |
| 1:H:525:GLN:HE21   | 1:H:525:GLN:HB3  | 1.71                     | 0.40              |
| 1:S:15:GLN:HA      | 1:S:18:ILE:HD12  | 2.02                     | 0.40              |
| 1:S:25:LEU:HB2     | 1:S:521:ALA:HB1  | 2.04                     | 0.40              |
| 1:S:64:ALA:HB1     | 1:S:148:VAL:HA   | 2.03                     | 0.40              |
| 1:U:90:GLN:HE22    | 1:U:468:ILE:HD13 | 1.86                     | 0.40              |
| 1:K:38[A]:ILE:HG23 | 1:K:41:ALA:HB2   | 2.02                     | 0.40              |
| 1:K:466:ASP:O      | 1:K:470:GLN:HG2  | 2.21                     | 0.40              |

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| Atom-1         | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:L:99:ALA:HB2 | 1:L:112:ILE:HG21 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 266/548 (48%) | 255 (96%) | 10 (4%) | 1 (0%)   | 30          | 64  |
| 1   | B     | 266/548 (48%) | 256 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | C     | 266/548 (48%) | 256 (96%) | 10 (4%) | 0        | 100         | 100 |
| 1   | D     | 266/548 (48%) | 255 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | E     | 266/548 (48%) | 255 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | F     | 266/548 (48%) | 253 (95%) | 13 (5%) | 0        | 100         | 100 |
| 1   | G     | 266/548 (48%) | 254 (96%) | 12 (4%) | 0        | 100         | 100 |
| 1   | H     | 266/548 (48%) | 257 (97%) | 8 (3%)  | 1 (0%)   | 30          | 64  |
| 1   | I     | 266/548 (48%) | 255 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | J     | 266/548 (48%) | 253 (95%) | 13 (5%) | 0        | 100         | 100 |
| 1   | K     | 266/548 (48%) | 251 (94%) | 15 (6%) | 0        | 100         | 100 |
| 1   | L     | 266/548 (48%) | 255 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | M     | 266/548 (48%) | 254 (96%) | 12 (4%) | 0        | 100         | 100 |
| 1   | N     | 266/548 (48%) | 251 (94%) | 15 (6%) | 0        | 100         | 100 |
| 1   | O     | 266/548 (48%) | 255 (96%) | 11 (4%) | 0        | 100         | 100 |
| 1   | P     | 266/548 (48%) | 253 (95%) | 13 (5%) | 0        | 100         | 100 |
| 1   | Q     | 266/548 (48%) | 251 (94%) | 15 (6%) | 0        | 100         | 100 |
| 1   | R     | 266/548 (48%) | 253 (95%) | 13 (5%) | 0        | 100         | 100 |
| 1   | S     | 266/548 (48%) | 257 (97%) | 9 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 1   | T     | 266/548 (48%)    | 254 (96%)  | 12 (4%)  | 0        | 100         | 100 |
| 1   | U     | 266/548 (48%)    | 254 (96%)  | 12 (4%)  | 0        | 100         | 100 |
| 1   | V     | 266/548 (48%)    | 253 (95%)  | 13 (5%)  | 0        | 100         | 100 |
| All | All   | 5852/12056 (48%) | 5590 (96%) | 260 (4%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 171 | ASN  |
| 1   | H     | 41  | ALA  |

### 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     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | B     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | C     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | D     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | E     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | F     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | G     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | H     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | I     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | J     | 227/425 (53%) | 226 (100%) | 1 (0%)   | 84          | 83  |
| 1   | K     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | L     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | M     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |
| 1   | N     | 227/425 (53%) | 226 (100%) | 1 (0%)   | 84          | 83  |
| 1   | O     | 227/425 (53%) | 227 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | P     | 227/425 (53%)   | 226 (100%)  | 1 (0%)   | 84          | 83  |
| 1   | Q     | 227/425 (53%)   | 227 (100%)  | 0        | 100         | 100 |
| 1   | R     | 227/425 (53%)   | 227 (100%)  | 0        | 100         | 100 |
| 1   | S     | 227/425 (53%)   | 226 (100%)  | 1 (0%)   | 84          | 83  |
| 1   | T     | 227/425 (53%)   | 227 (100%)  | 0        | 100         | 100 |
| 1   | U     | 227/425 (53%)   | 226 (100%)  | 1 (0%)   | 84          | 83  |
| 1   | V     | 227/425 (53%)   | 227 (100%)  | 0        | 100         | 100 |
| All | All   | 4994/9350 (53%) | 4989 (100%) | 5 (0%)   | 87          | 89  |

All (5) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | N     | 22  | GLN  |
| 1   | P     | 21  | ASN  |
| 1   | S     | 22  | GLN  |
| 1   | J     | 491 | ASN  |
| 1   | U     | 525 | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 15  | GLN  |
| 1   | B     | 19  | ASN  |
| 1   | B     | 39  | ASN  |
| 1   | B     | 57  | ASN  |
| 1   | B     | 86  | ASN  |
| 1   | B     | 98  | GLN  |
| 1   | B     | 129 | GLN  |
| 1   | B     | 131 | GLN  |
| 1   | B     | 171 | ASN  |
| 1   | B     | 482 | GLN  |
| 1   | B     | 503 | GLN  |
| 1   | B     | 507 | GLN  |
| 1   | A     | 90  | GLN  |
| 1   | A     | 151 | ASN  |
| 1   | A     | 154 | GLN  |
| 1   | A     | 525 | GLN  |
| 1   | A     | 540 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 48  | GLN  |
| 1   | M     | 171 | ASN  |
| 1   | M     | 503 | GLN  |
| 1   | M     | 536 | ASN  |
| 1   | C     | 151 | ASN  |
| 1   | N     | 15  | GLN  |
| 1   | N     | 63  | GLN  |
| 1   | N     | 67  | ASN  |
| 1   | N     | 90  | GLN  |
| 1   | N     | 154 | GLN  |
| 1   | N     | 171 | ASN  |
| 1   | N     | 491 | ASN  |
| 1   | N     | 517 | ASN  |
| 1   | D     | 15  | GLN  |
| 1   | D     | 16  | ASN  |
| 1   | D     | 507 | GLN  |
| 1   | O     | 133 | ASN  |
| 1   | O     | 503 | GLN  |
| 1   | O     | 522 | GLN  |
| 1   | O     | 529 | ASN  |
| 1   | O     | 537 | GLN  |
| 1   | E     | 63  | GLN  |
| 1   | E     | 136 | ASN  |
| 1   | E     | 151 | ASN  |
| 1   | E     | 491 | ASN  |
| 1   | E     | 498 | ASN  |
| 1   | E     | 525 | GLN  |
| 1   | E     | 536 | ASN  |
| 1   | E     | 540 | GLN  |
| 1   | P     | 129 | GLN  |
| 1   | P     | 498 | ASN  |
| 1   | P     | 503 | GLN  |
| 1   | P     | 507 | GLN  |
| 1   | P     | 529 | ASN  |
| 1   | F     | 16  | ASN  |
| 1   | F     | 17  | ASN  |
| 1   | F     | 67  | ASN  |
| 1   | F     | 113 | GLN  |
| 1   | F     | 517 | ASN  |
| 1   | F     | 526 | GLN  |
| 1   | Q     | 6   | ASN  |
| 1   | Q     | 63  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Q     | 76  | GLN  |
| 1   | Q     | 86  | ASN  |
| 1   | Q     | 517 | ASN  |
| 1   | G     | 67  | ASN  |
| 1   | G     | 76  | GLN  |
| 1   | G     | 491 | ASN  |
| 1   | G     | 522 | GLN  |
| 1   | R     | 76  | GLN  |
| 1   | R     | 86  | ASN  |
| 1   | R     | 129 | GLN  |
| 1   | R     | 154 | GLN  |
| 1   | R     | 176 | ASN  |
| 1   | R     | 498 | ASN  |
| 1   | R     | 503 | GLN  |
| 1   | R     | 522 | GLN  |
| 1   | R     | 525 | GLN  |
| 1   | R     | 526 | GLN  |
| 1   | R     | 529 | ASN  |
| 1   | H     | 57  | ASN  |
| 1   | H     | 69  | ASN  |
| 1   | H     | 90  | GLN  |
| 1   | H     | 113 | GLN  |
| 1   | S     | 21  | ASN  |
| 1   | S     | 22  | GLN  |
| 1   | S     | 57  | ASN  |
| 1   | S     | 86  | ASN  |
| 1   | S     | 154 | GLN  |
| 1   | S     | 482 | GLN  |
| 1   | S     | 522 | GLN  |
| 1   | I     | 63  | GLN  |
| 1   | I     | 86  | ASN  |
| 1   | I     | 88  | ASN  |
| 1   | I     | 154 | GLN  |
| 1   | I     | 547 | GLN  |
| 1   | T     | 86  | ASN  |
| 1   | T     | 90  | GLN  |
| 1   | T     | 129 | GLN  |
| 1   | T     | 482 | GLN  |
| 1   | T     | 536 | ASN  |
| 1   | J     | 15  | GLN  |
| 1   | J     | 17  | ASN  |
| 1   | J     | 48  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 57  | ASN  |
| 1   | J     | 491 | ASN  |
| 1   | U     | 22  | GLN  |
| 1   | U     | 136 | ASN  |
| 1   | U     | 491 | ASN  |
| 1   | U     | 494 | ASN  |
| 1   | U     | 522 | GLN  |
| 1   | U     | 525 | GLN  |
| 1   | U     | 526 | GLN  |
| 1   | K     | 19  | ASN  |
| 1   | K     | 154 | GLN  |
| 1   | K     | 482 | GLN  |
| 1   | K     | 491 | ASN  |
| 1   | K     | 526 | GLN  |
| 1   | K     | 540 | GLN  |
| 1   | V     | 483 | ASN  |
| 1   | V     | 517 | ASN  |
| 1   | V     | 536 | ASN  |
| 1   | L     | 16  | ASN  |
| 1   | L     | 21  | ASN  |
| 1   | L     | 48  | GLN  |
| 1   | L     | 52  | ASN  |
| 1   | L     | 86  | ASN  |
| 1   | L     | 151 | ASN  |
| 1   | L     | 154 | GLN  |
| 1   | L     | 503 | GLN  |
| 1   | L     | 526 | GLN  |
| 1   | L     | 529 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

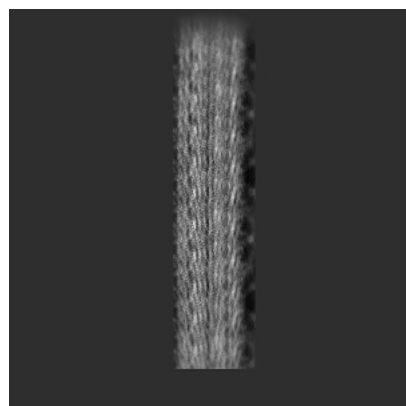
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27076. These allow visual inspection of the internal detail of the map and identification of artifacts.

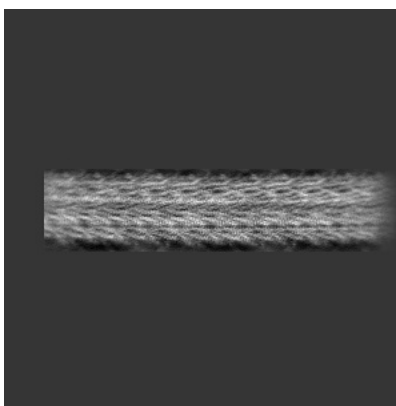
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

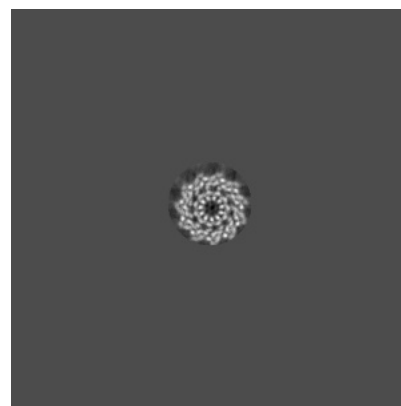
#### 6.1.1 Primary map



X

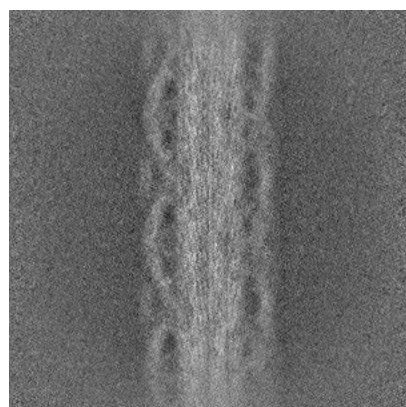


Y

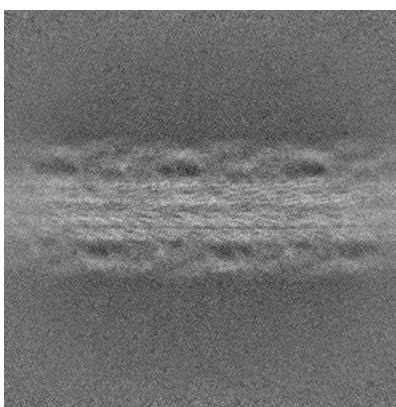


Z

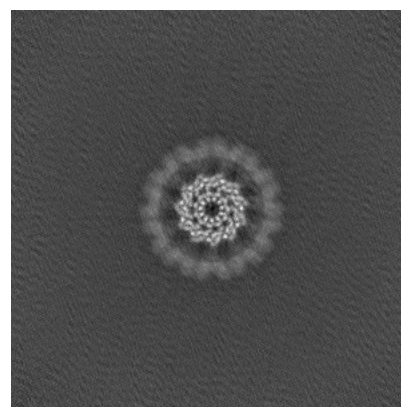
#### 6.1.2 Raw map



X



Y

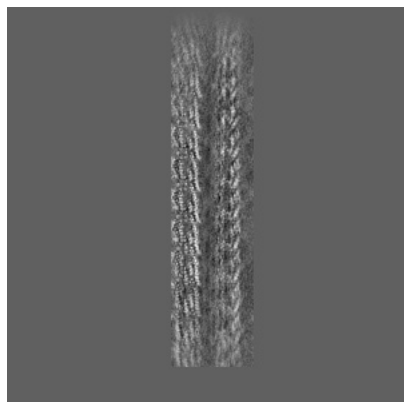


Z

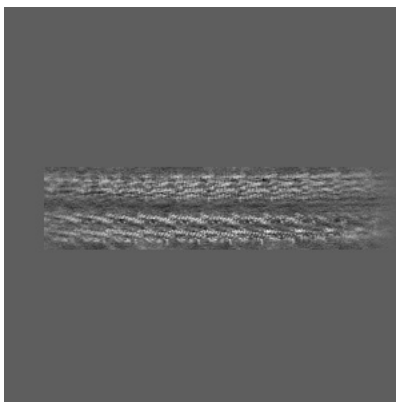
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

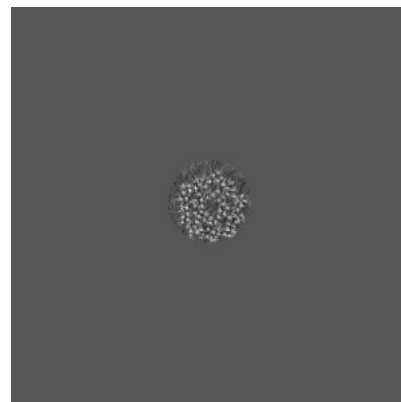
### 6.2.1 Primary map



X Index: 312

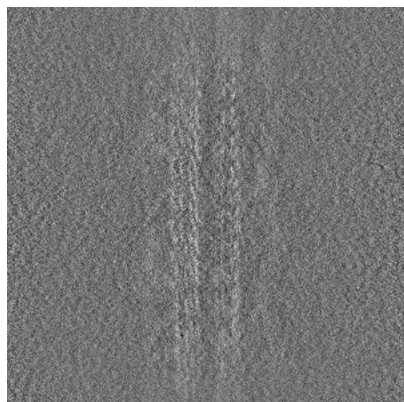


Y Index: 312

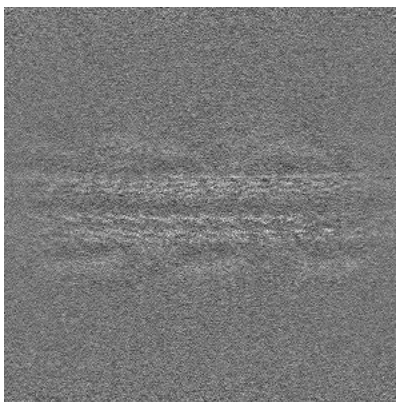


Z Index: 312

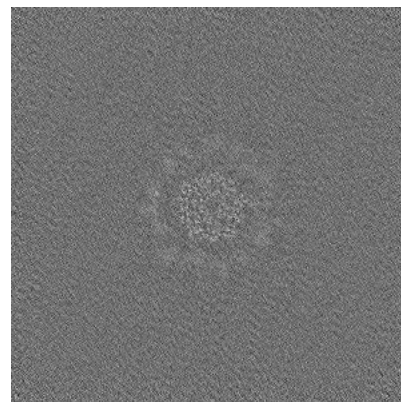
### 6.2.2 Raw map



X Index: 312



Y Index: 312



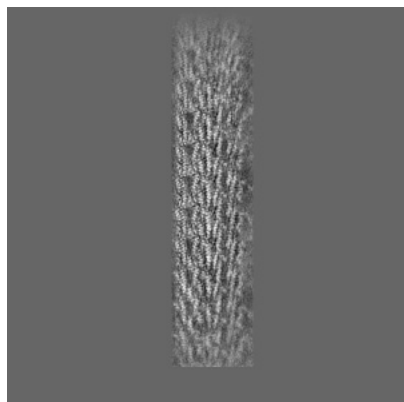
Z Index: 312

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

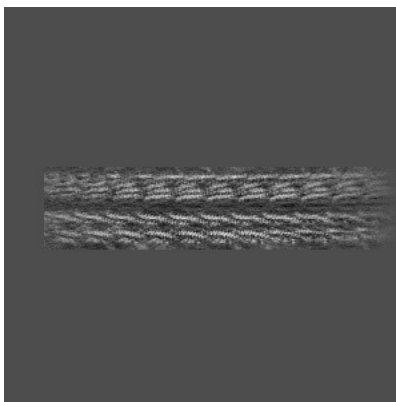


## 6.3 Largest variance slices [i](#)

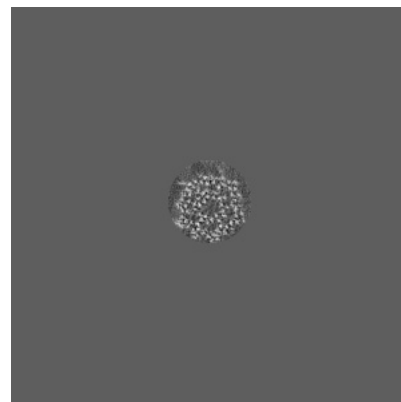
### 6.3.1 Primary map



X Index: 294

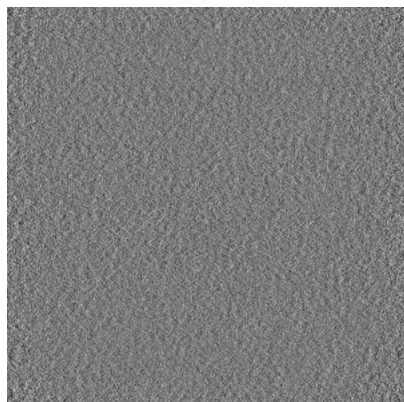


Y Index: 314

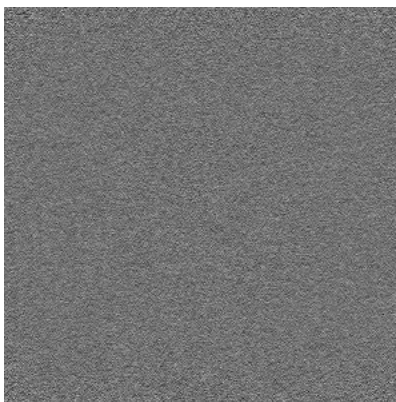


Z Index: 331

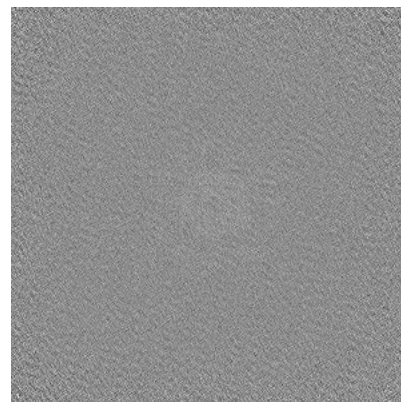
### 6.3.2 Raw map



X Index: 0



Y Index: 0



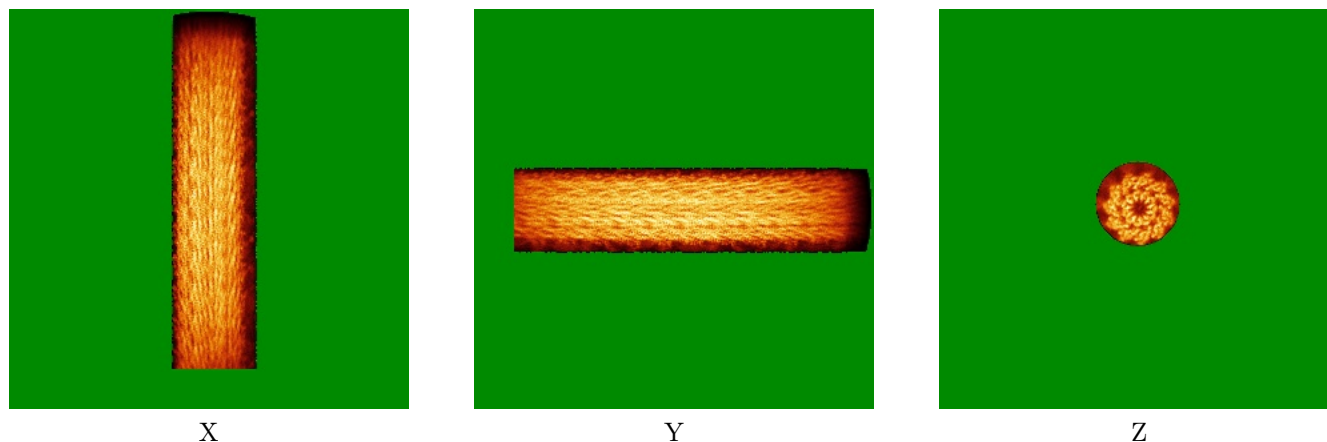
Z Index: 0

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

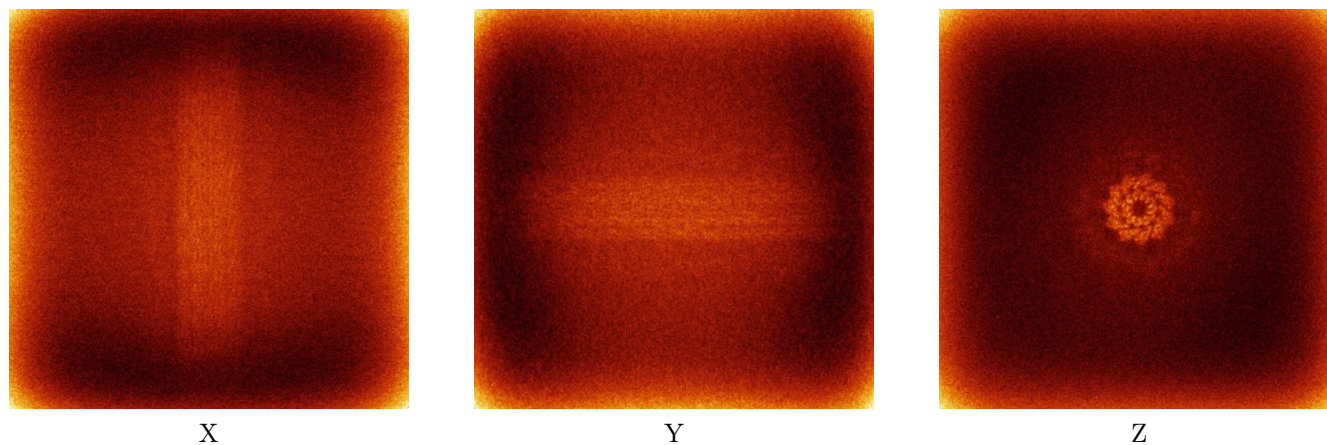


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

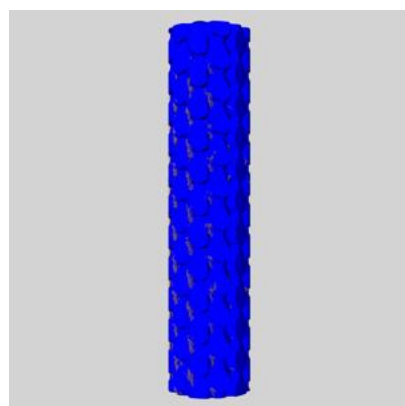
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

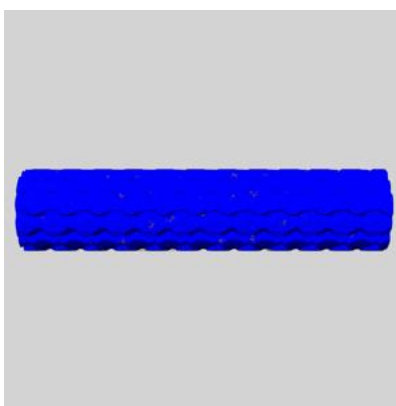
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

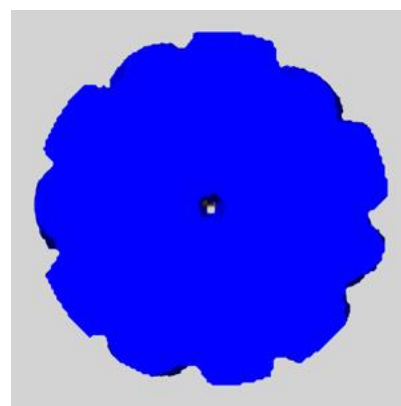
### 6.6.1 emd\_27076\_msk\_1.map [i](#)



X



Y

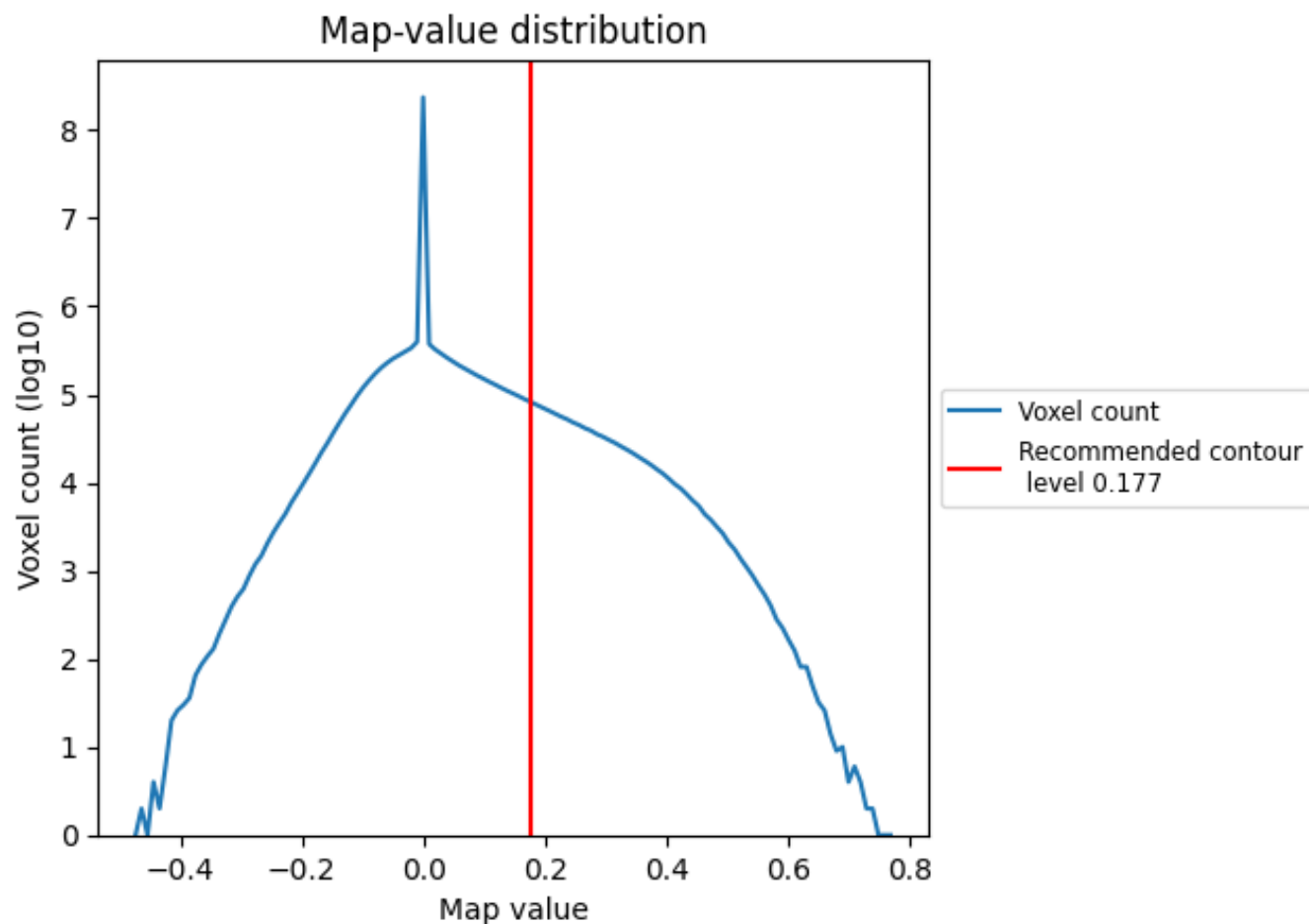


Z

## 7 Map analysis [i](#)

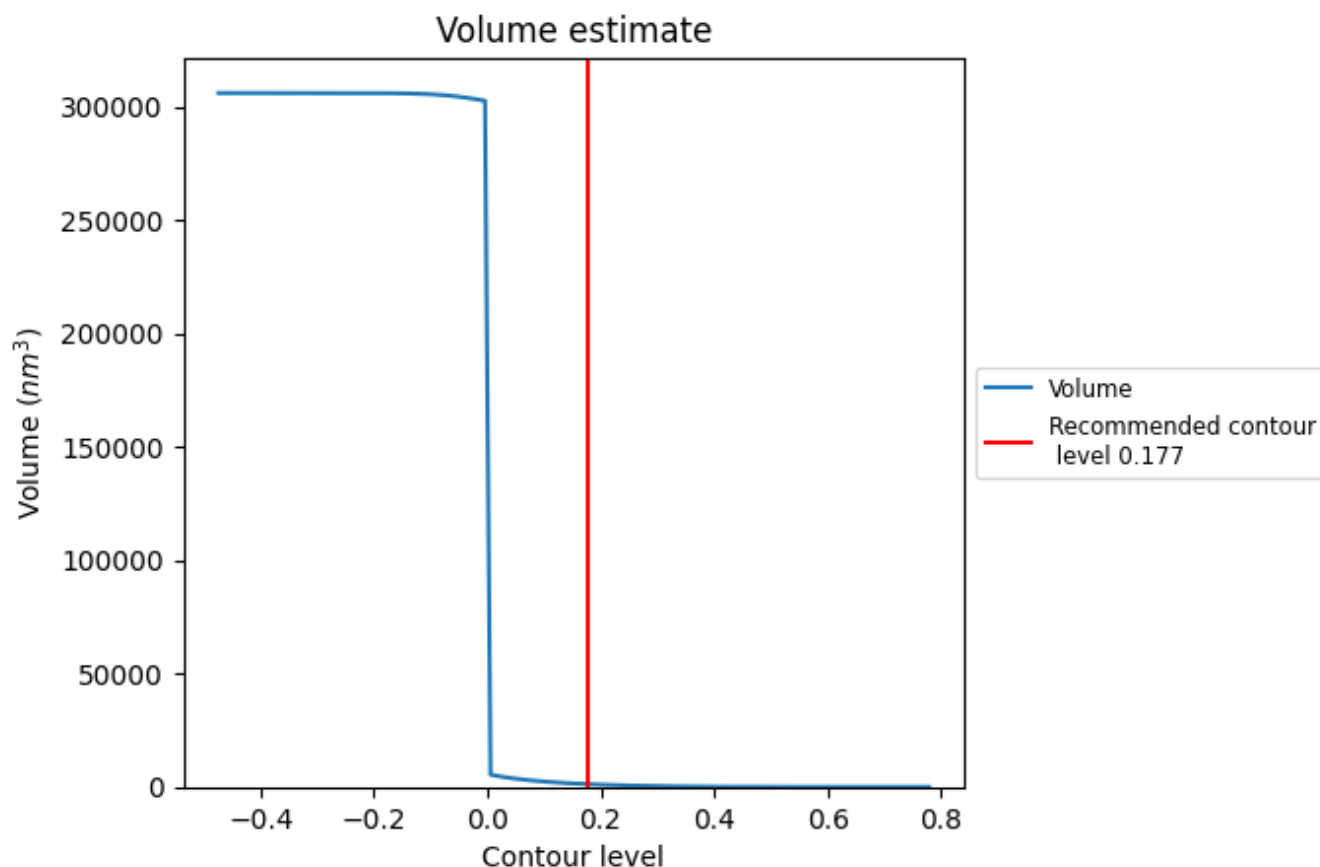
This section contains the results of statistical analysis of the map.

### 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.

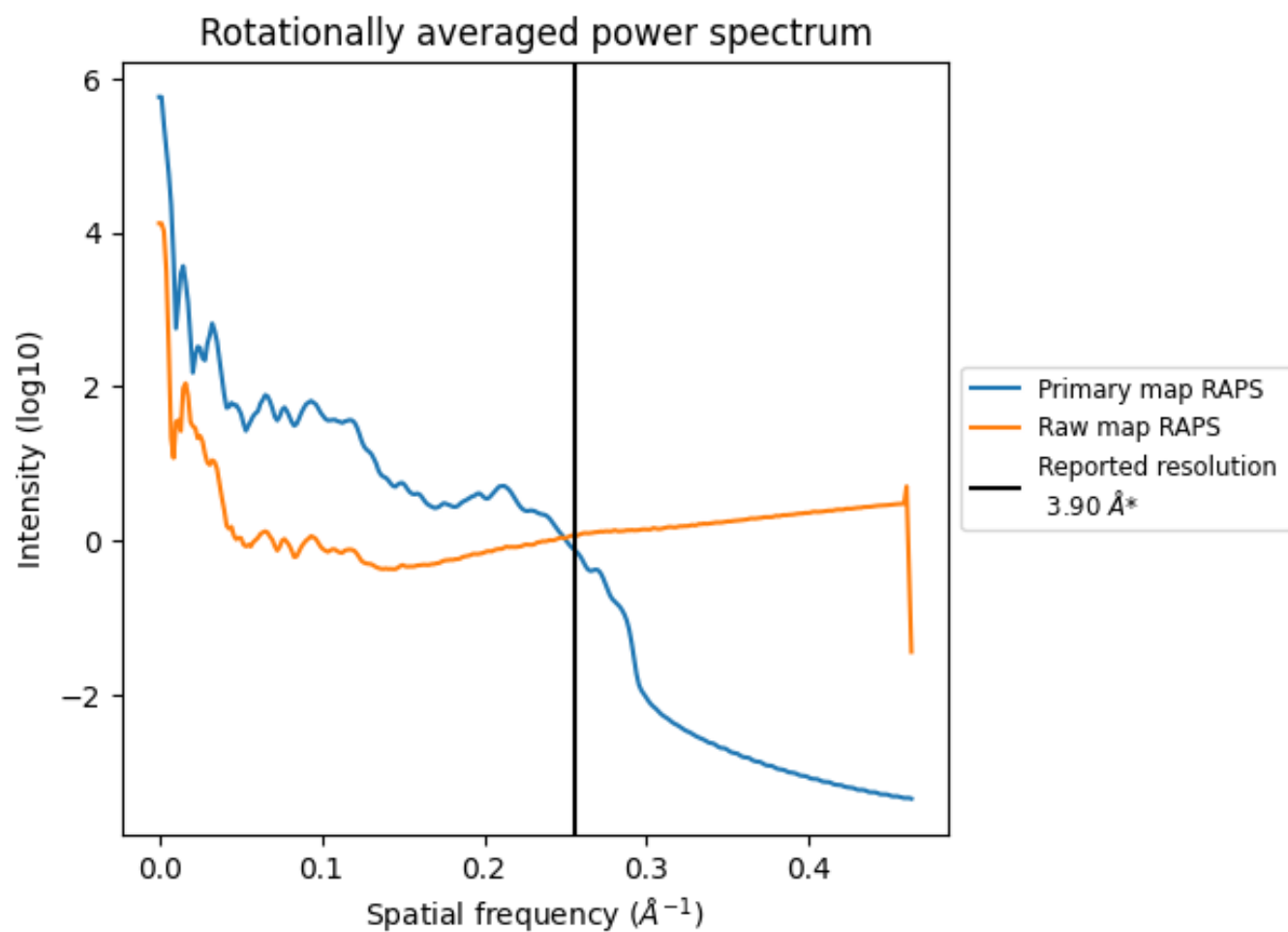
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1247 nm<sup>3</sup>; this corresponds to an approximate mass of 1126 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 ⓘ

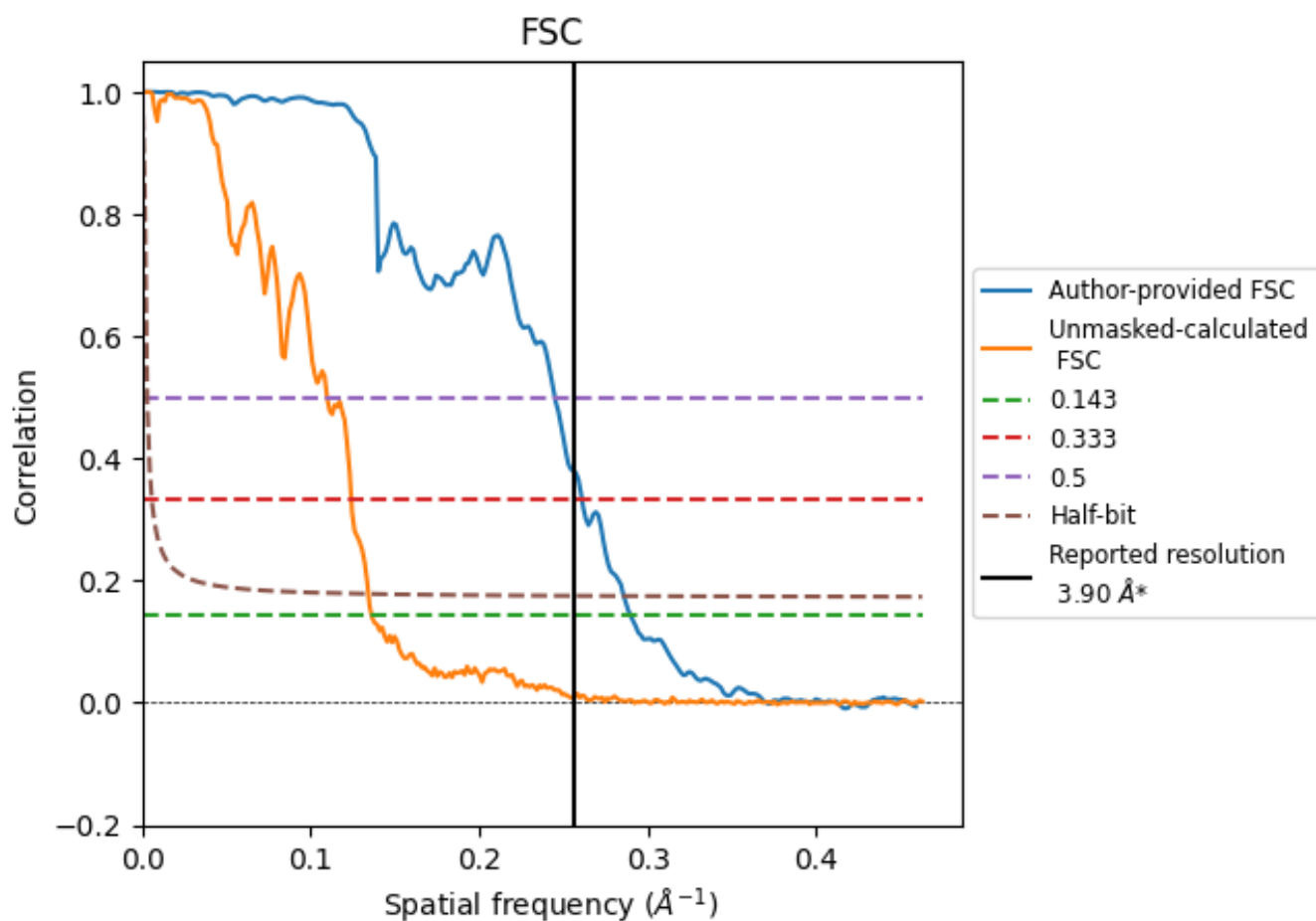


\*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

## 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 0.256 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

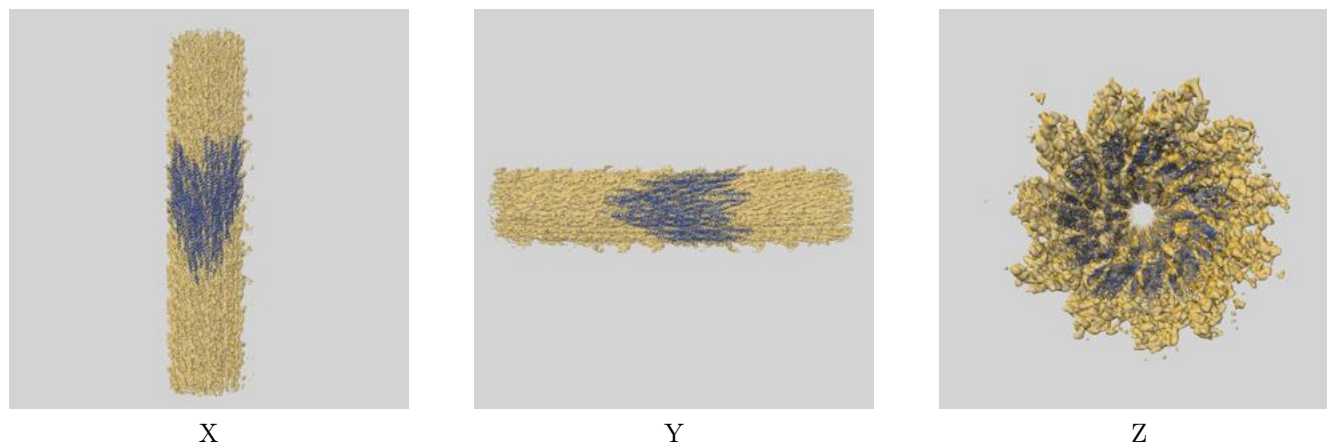
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |       |
|---------------------------|------------------------------------|------|----------|-------|
|                           | 0.143                              | 0.5  | Half-bit | 0.333 |
| Reported by author        | -                                  | -    | -        | 3.90  |
| Author-provided FSC curve | 3.45                               | 4.08 | 3.50     | 3.83  |
| Unmasked-calculated*      | 7.34                               | 9.11 | 7.45     | 8.06  |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.33 CUT-OFF 8.06 differs from the reported value 3.9 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-27076 and PDB model 8CYE. Per-residue inclusion information can be found in section 3 on page 6.

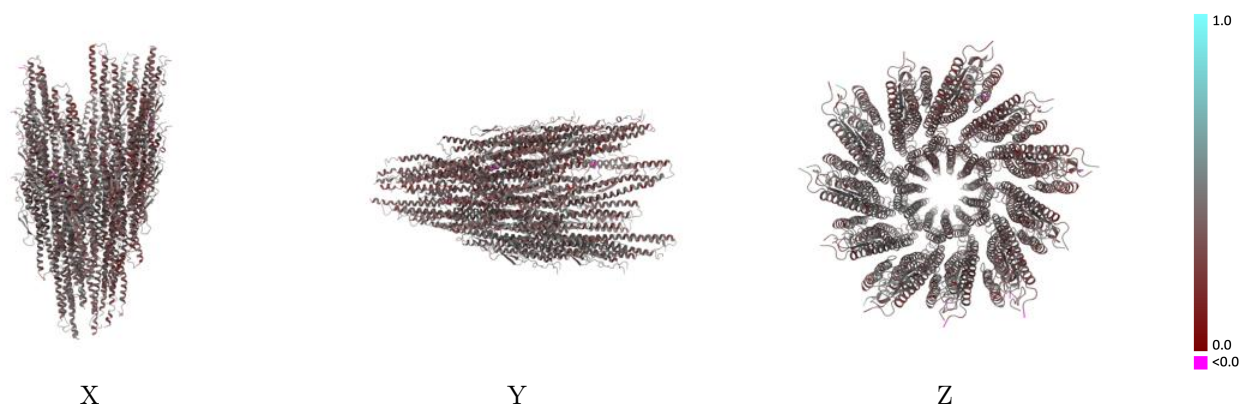
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.177 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.

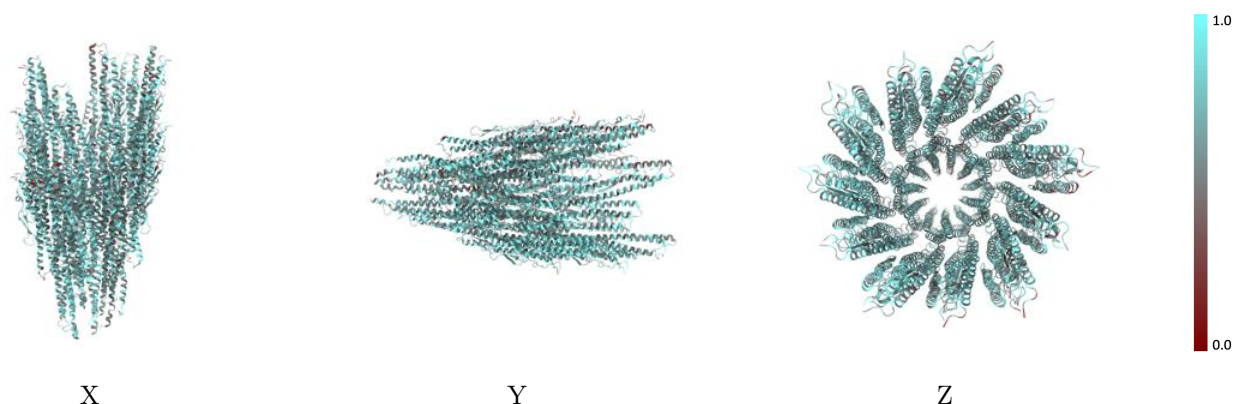


## 9.2 Q-score mapped to coordinate model [i](#)



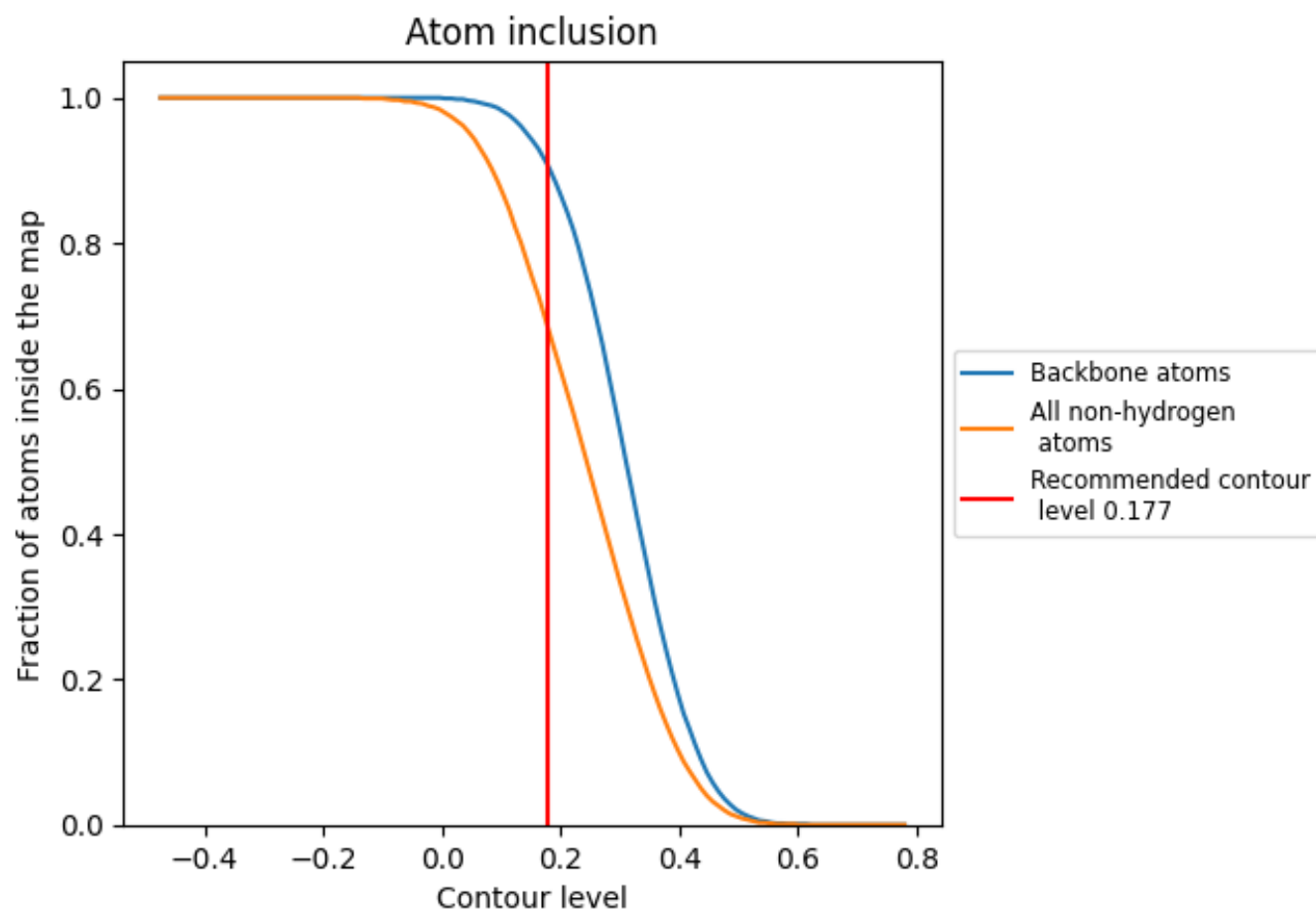
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.177).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.177) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6880   |  0.3910   |
| A     |  0.7110   |  0.4120   |
| B     |  0.7050   |  0.4150   |
| C     |  0.7150   |  0.4010   |
| D     |  0.6830   |  0.3870   |
| E     |  0.6680   |  0.3830   |
| F     |  0.6530   |  0.3610   |
| G     |  0.6530   |  0.3470   |
| H     |  0.6440   |  0.3620   |
| I     |  0.6810   |  0.3880   |
| J     |  0.7010   |  0.4250   |
| K     |  0.7180   |  0.4270   |
| L     |  0.7120   |  0.4120   |
| M     |  0.7210   |  0.4050   |
| N     |  0.6550  |  0.3960  |
| O     |  0.6820 |  0.3830 |
| P     |  0.6360 |  0.3660 |
| Q     |  0.6410 |  0.3400 |
| R     |  0.6770 |  0.3560 |
| S     |  0.6770 |  0.3840 |
| T     |  0.7600 |  0.4200 |
| U     |  0.7220 |  0.4260 |
| V     |  0.7120 |  0.4140 |

