



## Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 07:09 AM UTC

PDB ID : 5TAX / pdb\_00005tax  
EMDB ID : EMD-8388  
Title : Structure of rabbit RyR1 (ryanodine dataset, class 1)  
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;  
Frank, J.  
Deposited on : 2016-09-10  
Resolution : 6.60 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:

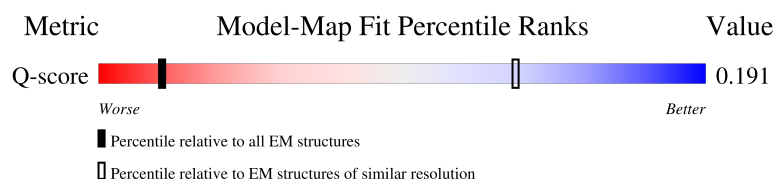
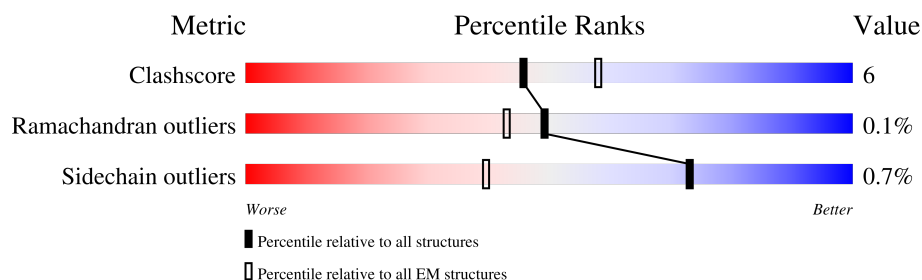
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 6.60 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.



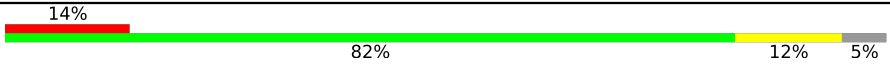
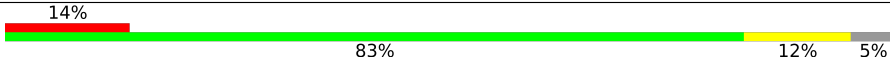
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 531 ( 6.10 - 7.10 )                                      |

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     | 108    |  |
| 1   | F     | 108    |  |
| 1   | H     | 108    |  |
| 1   | J     | 108    |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 2   | B     | 4416   |  |
| 2   | E     | 4416   |  |
| 2   | G     | 4416   |  |
| 2   | I     | 4416   |  |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | F     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 516 | 144 | 154 | 4 |         |       |
| 1   | A     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 516 | 144 | 154 | 4 |         |       |
| 1   | H     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 516 | 144 | 154 | 4 |         |       |
| 1   | J     | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 818   | 516 | 144 | 154 | 4 |         |       |

- Molecule 2 is a protein called Ryanodine receptor 1.

| Mol | Chain | Residues | Atoms |       |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|-------|------|------|-----|---------|-------|
| 2   | B     | 4194     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 29499 | 18686 | 5228 | 5428 | 157 |         |       |
| 2   | I     | 4194     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 29499 | 18686 | 5228 | 5428 | 157 |         |       |
| 2   | G     | 4194     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 29499 | 18686 | 5228 | 5428 | 157 |         |       |
| 2   | E     | 4194     | Total | C     | N    | O    | S   | 0       | 0     |
|     |       |          | 29499 | 18686 | 5228 | 5428 | 157 |         |       |

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

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 3   | B     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | I     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | G     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | E     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

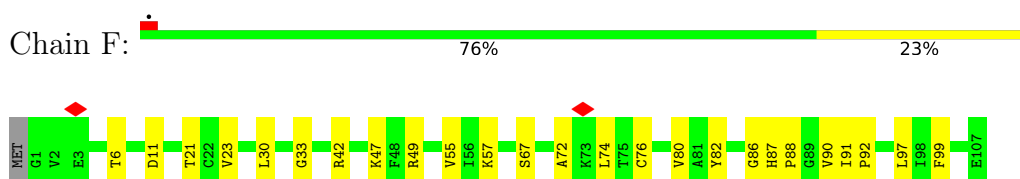
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 4   | B     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 4   | I     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 4   | G     | 1        | Total<br>1 | Ca<br>1 | 0       |
| 4   | E     | 1        | Total<br>1 | Ca<br>1 | 0       |

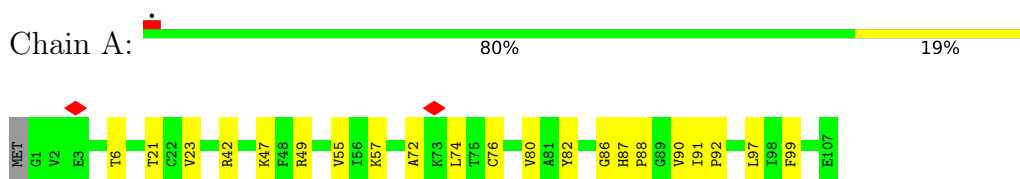
### 3 Residue-property plots

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

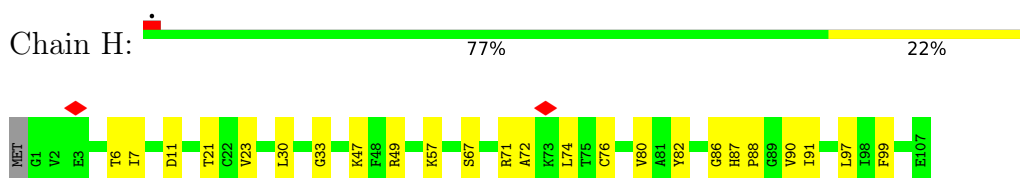
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



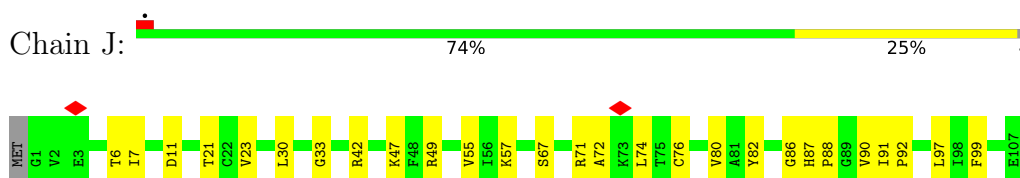
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



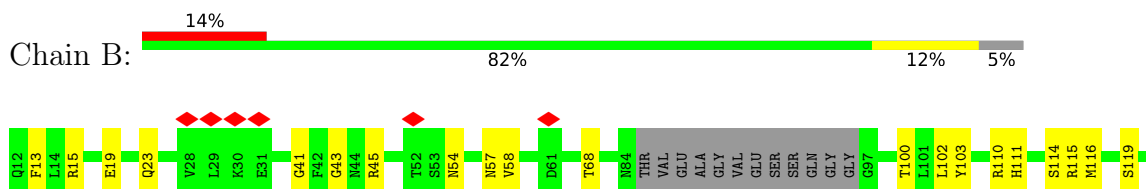
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

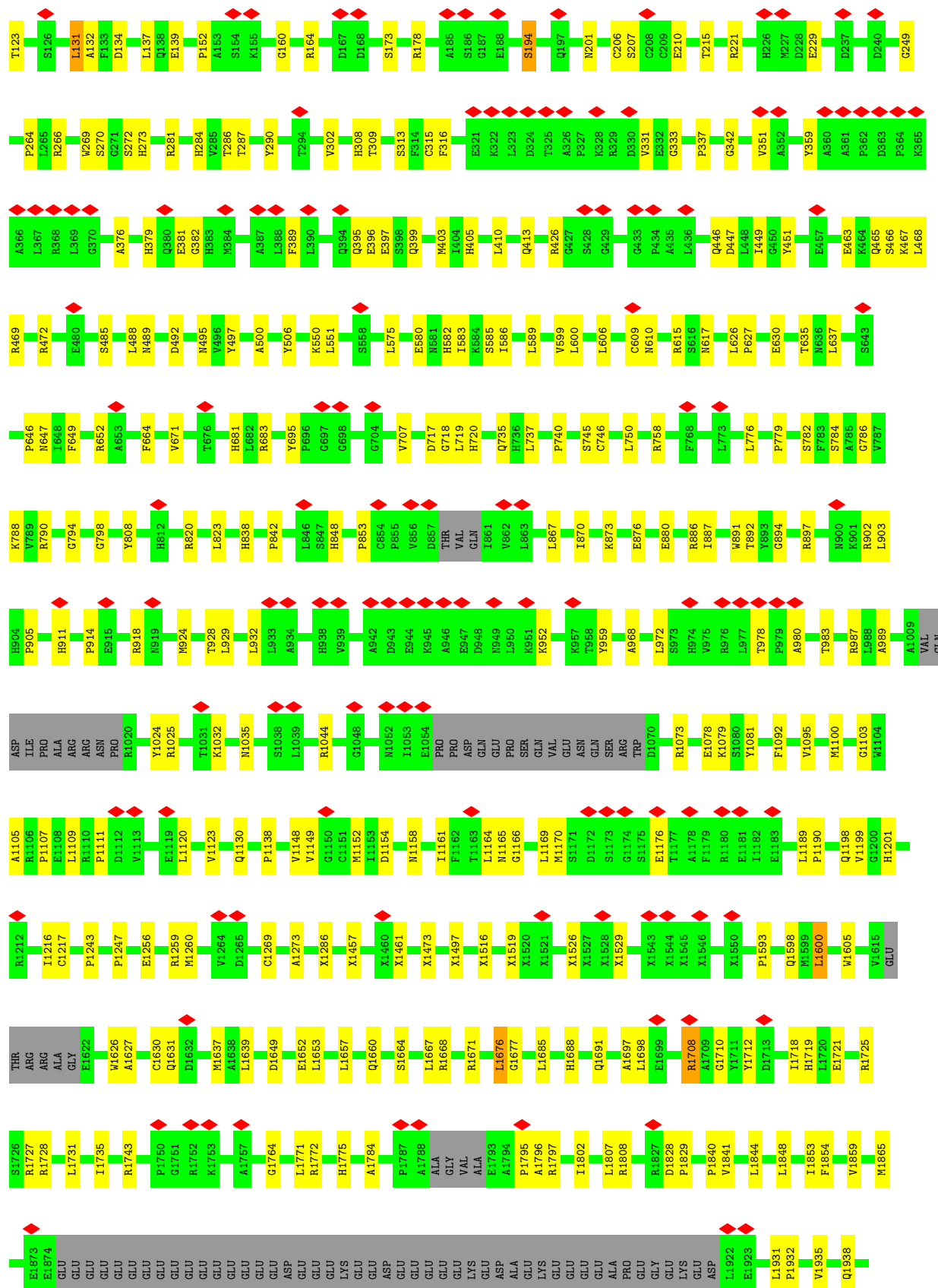


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

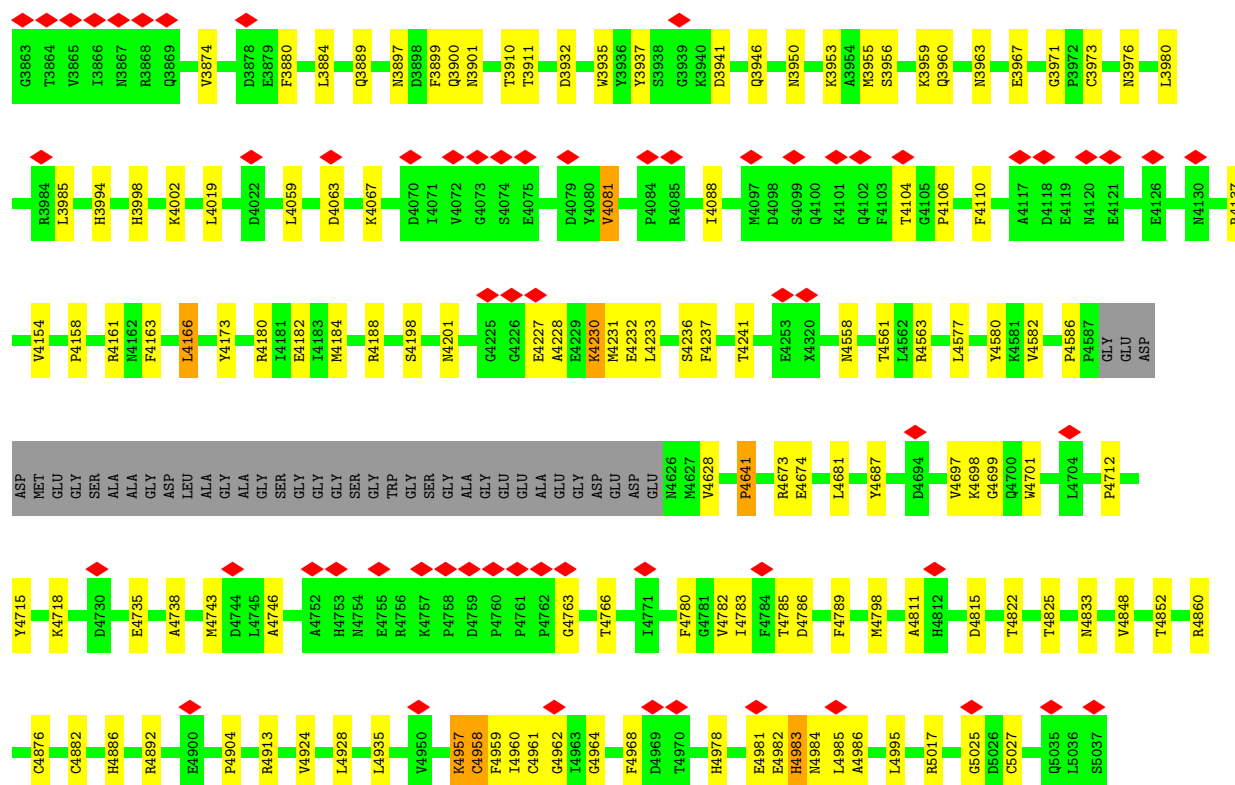


- Molecule 2: Ryanodine receptor 1

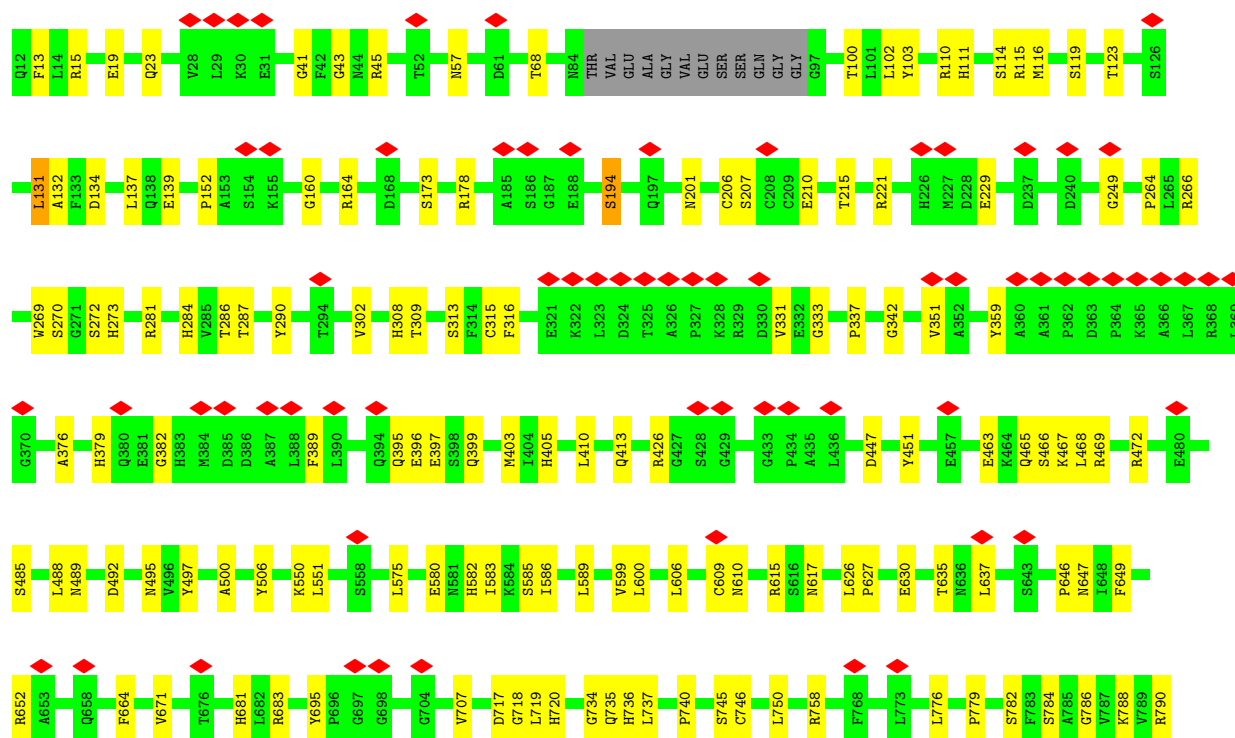
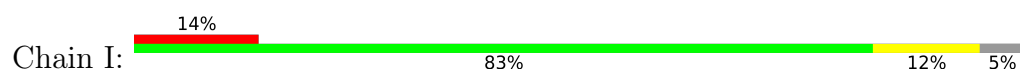


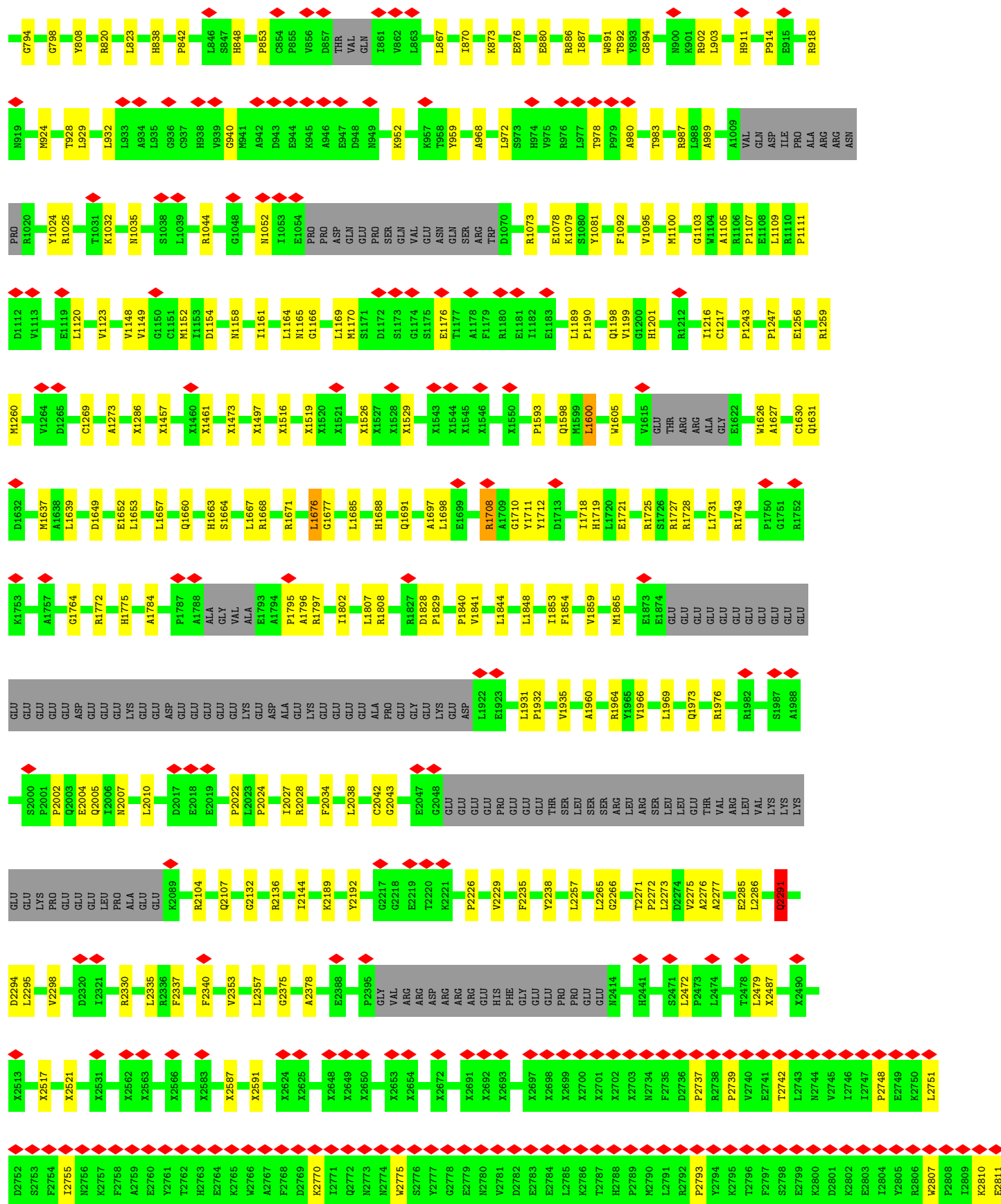






• Molecule 2: Ryanodine receptor 1

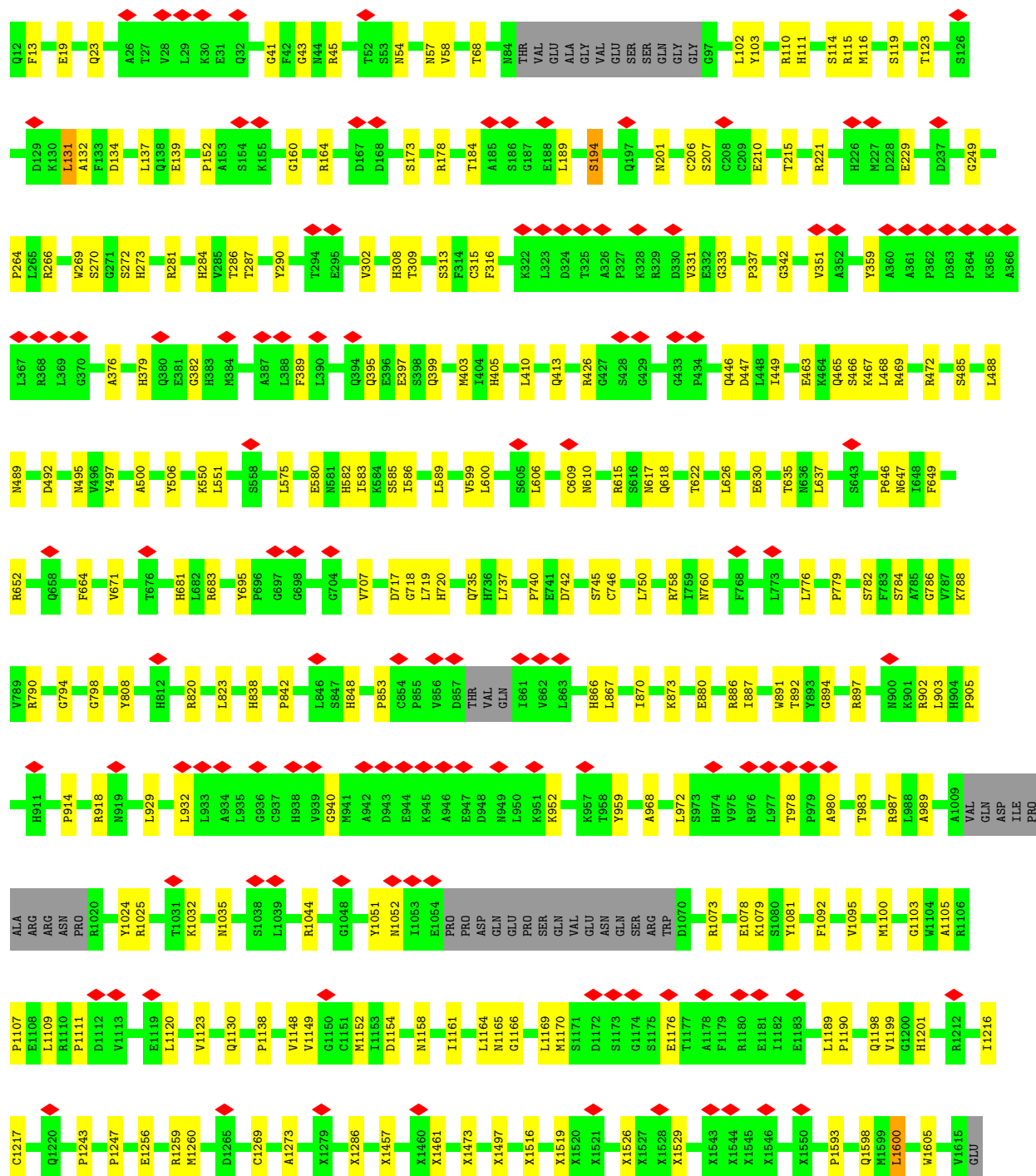
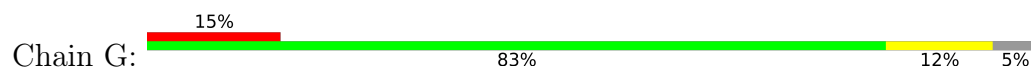




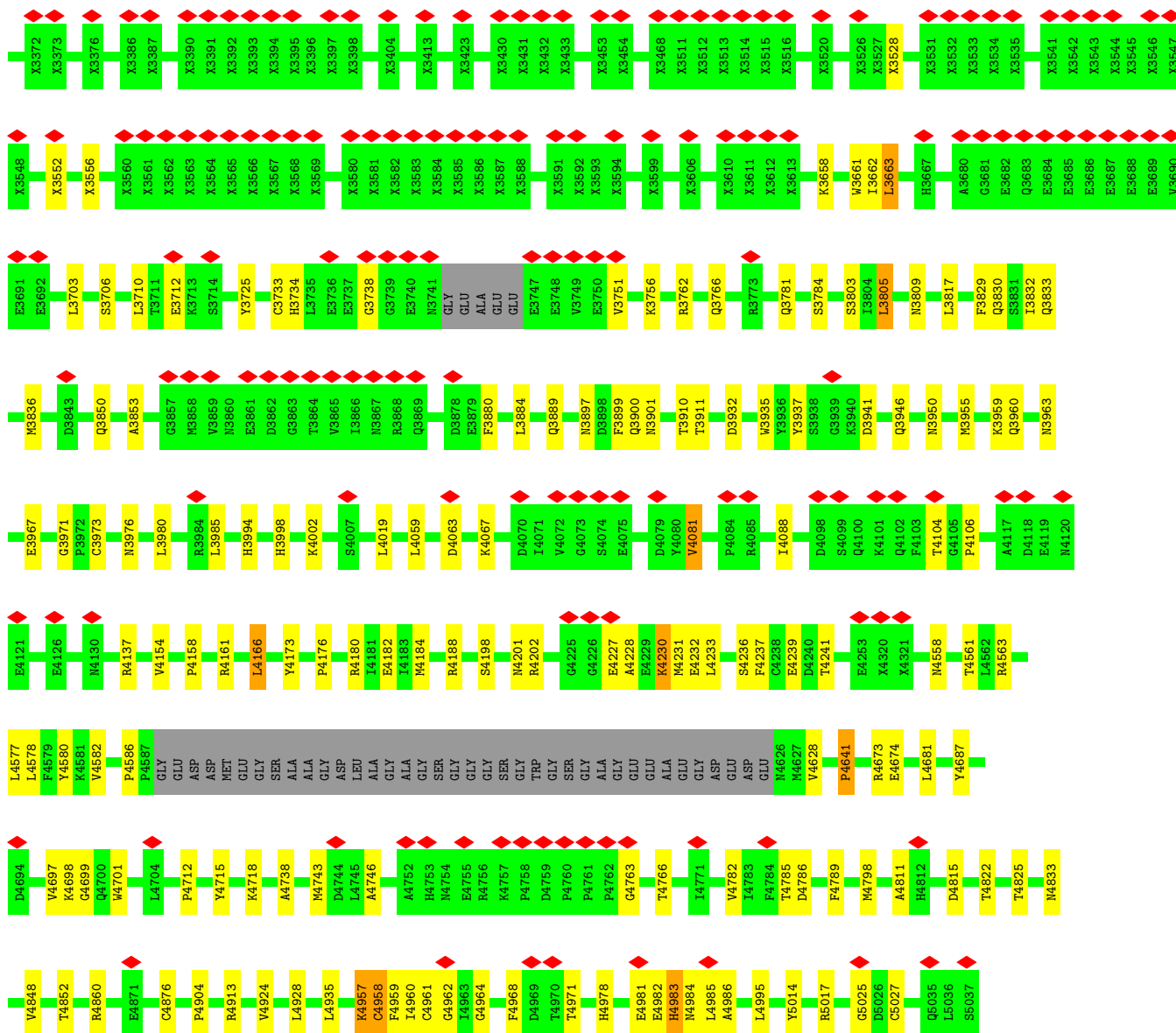




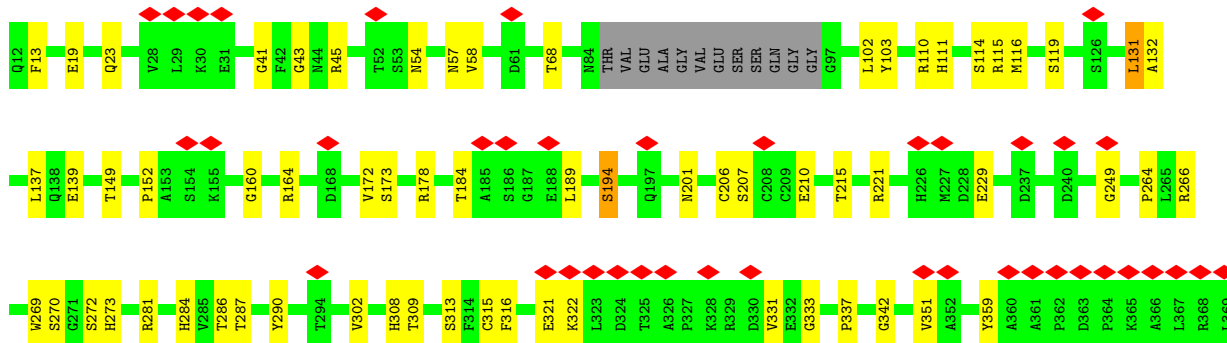
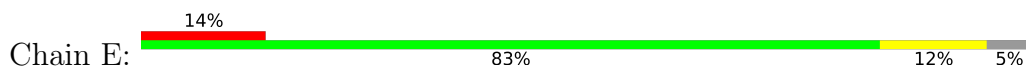
• Molecule 2: Ryanodine receptor 1





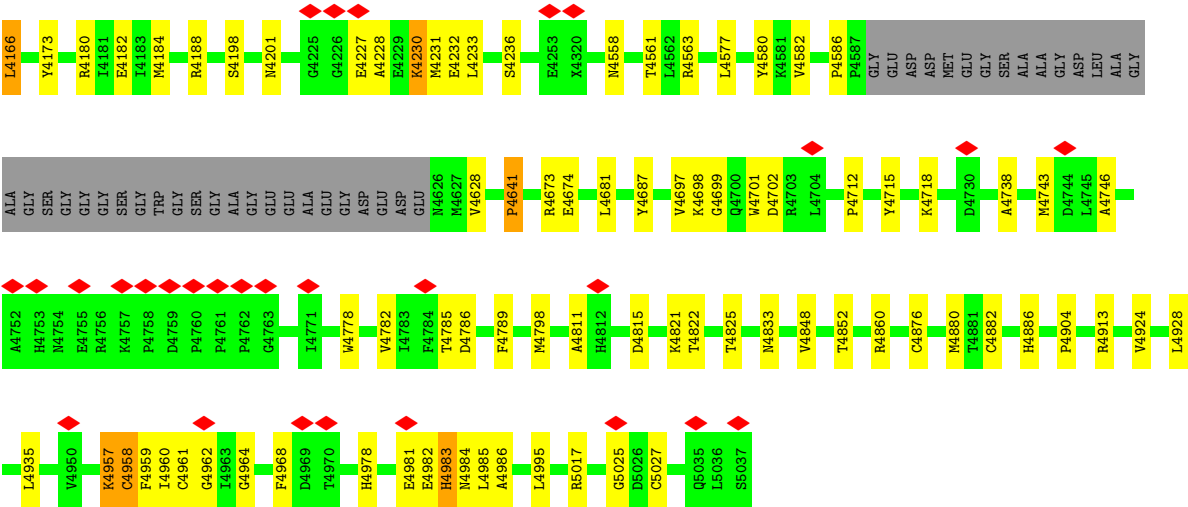


• Molecule 2: Ryanodine receptor 1









## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 55564                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI POLARA 300                          | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.100                                   | Depositor |
| Minimum map value                    | -0.044                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.025                                   | Depositor |
| Map size ( $\text{\AA}$ )            | 502.0, 502.0, 502.0                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.255, 1.255, 1.255                     | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

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     | 0.19         | 0/834       | 0.47        | 0/1123           |
| 1   | F     | 0.19         | 0/834       | 0.48        | 0/1123           |
| 1   | H     | 0.19         | 0/834       | 0.47        | 0/1123           |
| 1   | J     | 0.19         | 0/834       | 0.47        | 0/1123           |
| 2   | B     | 0.20         | 0/25428     | 0.52        | 4/34534 (0.0%)   |
| 2   | E     | 0.20         | 0/25428     | 0.52        | 4/34534 (0.0%)   |
| 2   | G     | 0.20         | 0/25428     | 0.52        | 4/34534 (0.0%)   |
| 2   | I     | 0.20         | 0/25428     | 0.52        | 4/34534 (0.0%)   |
| All | All   | 0.20         | 0/105048    | 0.52        | 16/142628 (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 |
|-----|-------|---------------------|---------------------|
| 2   | B     | 0                   | 11                  |
| 2   | E     | 0                   | 11                  |
| 2   | G     | 0                   | 11                  |
| 2   | I     | 0                   | 11                  |
| All | All   | 0                   | 44                  |

There are no bond length outliers.

All (16) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|------|-------------|----------|
| 2   | E     | 2291 | GLN  | CA-C-N | 5.85 | 132.72      | 121.54   |
| 2   | E     | 2291 | GLN  | C-N-CA | 5.85 | 132.72      | 121.54   |
| 2   | B     | 2291 | GLN  | CA-C-N | 5.84 | 132.70      | 121.54   |
| 2   | B     | 2291 | GLN  | C-N-CA | 5.84 | 132.70      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2   | G     | 2291 | GLN  | CA-C-N   | 5.84 | 132.70      | 121.54   |
| 2   | G     | 2291 | GLN  | C-N-CA   | 5.84 | 132.70      | 121.54   |
| 2   | I     | 2291 | GLN  | CA-C-N   | 5.84 | 132.69      | 121.54   |
| 2   | I     | 2291 | GLN  | C-N-CA   | 5.84 | 132.69      | 121.54   |
| 2   | I     | 1829 | PRO  | N-CA-C   | 5.04 | 119.12      | 111.11   |
| 2   | E     | 131  | LEU  | CA-CB-CG | 5.04 | 133.93      | 116.30   |
| 2   | I     | 131  | LEU  | CA-CB-CG | 5.03 | 133.90      | 116.30   |
| 2   | B     | 131  | LEU  | CA-CB-CG | 5.02 | 133.88      | 116.30   |
| 2   | B     | 1829 | PRO  | N-CA-C   | 5.02 | 119.09      | 111.11   |
| 2   | G     | 131  | LEU  | CA-CB-CG | 5.02 | 133.87      | 116.30   |
| 2   | E     | 1829 | PRO  | N-CA-C   | 5.01 | 119.08      | 111.11   |
| 2   | G     | 1829 | PRO  | N-CA-C   | 5.00 | 119.07      | 111.11   |

There are no chirality outliers.

All (44) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | B     | 139  | GLU  | Peptide |
| 2   | B     | 1676 | LEU  | Peptide |
| 2   | B     | 1795 | PRO  | Peptide |
| 2   | B     | 1828 | ASP  | Peptide |
| 2   | B     | 194  | SER  | Peptide |
| 2   | B     | 2291 | GLN  | Peptide |
| 2   | B     | 2472 | LEU  | Peptide |
| 2   | B     | 2807 | TRP  | Peptide |
| 2   | B     | 3971 | GLY  | Peptide |
| 2   | B     | 4641 | PRO  | Peptide |
| 2   | B     | 808  | TYR  | Peptide |
| 2   | E     | 139  | GLU  | Peptide |
| 2   | E     | 1676 | LEU  | Peptide |
| 2   | E     | 1795 | PRO  | Peptide |
| 2   | E     | 1828 | ASP  | Peptide |
| 2   | E     | 194  | SER  | Peptide |
| 2   | E     | 2291 | GLN  | Peptide |
| 2   | E     | 2472 | LEU  | Peptide |
| 2   | E     | 2807 | TRP  | Peptide |
| 2   | E     | 3971 | GLY  | Peptide |
| 2   | E     | 4641 | PRO  | Peptide |
| 2   | E     | 808  | TYR  | Peptide |
| 2   | G     | 139  | GLU  | Peptide |
| 2   | G     | 1676 | LEU  | Peptide |
| 2   | G     | 1795 | PRO  | Peptide |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | G     | 1828 | ASP  | Peptide |
| 2   | G     | 194  | SER  | Peptide |
| 2   | G     | 2291 | GLN  | Peptide |
| 2   | G     | 2472 | LEU  | Peptide |
| 2   | G     | 2807 | TRP  | Peptide |
| 2   | G     | 3971 | GLY  | Peptide |
| 2   | G     | 4641 | PRO  | Peptide |
| 2   | G     | 808  | TYR  | Peptide |
| 2   | I     | 139  | GLU  | Peptide |
| 2   | I     | 1676 | LEU  | Peptide |
| 2   | I     | 1795 | PRO  | Peptide |
| 2   | I     | 1828 | ASP  | Peptide |
| 2   | I     | 194  | SER  | Peptide |
| 2   | I     | 2291 | GLN  | Peptide |
| 2   | I     | 2472 | LEU  | Peptide |
| 2   | I     | 2807 | TRP  | Peptide |
| 2   | I     | 3971 | GLY  | Peptide |
| 2   | I     | 4641 | PRO  | Peptide |
| 2   | I     | 808  | TYR  | 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     | 818   | 0        | 824      | 13      | 0            |
| 1   | F     | 818   | 0        | 824      | 15      | 0            |
| 1   | H     | 818   | 0        | 824      | 13      | 0            |
| 1   | J     | 818   | 0        | 824      | 16      | 0            |
| 2   | B     | 29499 | 0        | 24741    | 341     | 0            |
| 2   | E     | 29499 | 0        | 24742    | 336     | 0            |
| 2   | G     | 29499 | 0        | 24741    | 336     | 0            |
| 2   | I     | 29499 | 0        | 24742    | 334     | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | I     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 4   | G     | 1      | 0        | 0        | 0       | 0            |
| 4   | I     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 121276 | 0        | 102262   | 1388    | 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 6.

All (1388) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:4182:GLU:OE2 | 2:I:4983:HIS:NE2  | 1.64                     | 1.31              |
| 2:E:4182:GLU:OE2 | 2:E:4983:HIS:NE2  | 1.64                     | 1.29              |
| 2:G:4182:GLU:OE2 | 2:G:4983:HIS:NE2  | 1.64                     | 1.29              |
| 2:B:4182:GLU:OE2 | 2:B:4983:HIS:NE2  | 1.64                     | 1.27              |
| 2:G:4982:GLU:OE1 | 2:G:5027:CYS:SG   | 1.98                     | 1.22              |
| 2:B:4982:GLU:OE1 | 2:B:5027:CYS:SG   | 1.98                     | 1.21              |
| 2:I:4982:GLU:OE1 | 2:I:5027:CYS:SG   | 1.98                     | 1.21              |
| 2:E:4982:GLU:OE1 | 2:E:5027:CYS:SG   | 1.98                     | 1.20              |
| 2:E:4230:LYS:HG3 | 2:E:4959:PHE:CZ   | 1.89                     | 1.07              |
| 2:G:4230:LYS:HG3 | 2:G:4959:PHE:CZ   | 1.89                     | 1.06              |
| 2:B:4230:LYS:HG3 | 2:B:4959:PHE:CZ   | 1.89                     | 1.06              |
| 2:I:4230:LYS:HG3 | 2:I:4959:PHE:CZ   | 1.89                     | 1.06              |
| 2:I:4968:PHE:CZ  | 2:I:4978:HIS:CE1  | 2.50                     | 1.00              |
| 2:G:4968:PHE:CZ  | 2:G:4978:HIS:CE1  | 2.50                     | 1.00              |
| 2:E:4968:PHE:CZ  | 2:E:4978:HIS:CE1  | 2.50                     | 0.99              |
| 2:B:4968:PHE:CZ  | 2:B:4978:HIS:CE1  | 2.50                     | 0.99              |
| 2:I:4230:LYS:HG3 | 2:I:4959:PHE:HZ   | 1.30                     | 0.96              |
| 2:B:4230:LYS:HG3 | 2:B:4959:PHE:HZ   | 1.30                     | 0.94              |
| 2:G:4230:LYS:HG3 | 2:G:4959:PHE:HZ   | 1.30                     | 0.93              |
| 2:E:4230:LYS:HG3 | 2:E:4959:PHE:HZ   | 1.30                     | 0.92              |
| 2:B:4231:MET:HE1 | 2:B:4960:ILE:HG23 | 1.51                     | 0.91              |
| 2:G:4230:LYS:HD2 | 2:G:4959:PHE:CZ   | 2.06                     | 0.91              |
| 2:E:4231:MET:HE1 | 2:E:4960:ILE:HG23 | 1.51                     | 0.91              |
| 2:I:4230:LYS:HD2 | 2:I:4959:PHE:CZ   | 2.06                     | 0.90              |
| 2:I:4231:MET:HE1 | 2:I:4960:ILE:HG23 | 1.51                     | 0.90              |
| 2:G:4231:MET:HE1 | 2:G:4960:ILE:HG23 | 1.51                     | 0.90              |
| 2:E:4230:LYS:HD2 | 2:E:4959:PHE:CZ   | 2.06                     | 0.90              |
| 2:B:4230:LYS:HD2 | 2:B:4959:PHE:CZ   | 2.06                     | 0.89              |
| 2:B:4230:LYS:CG  | 2:B:4959:PHE:CZ   | 2.59                     | 0.85              |
| 2:I:4230:LYS:CG  | 2:I:4959:PHE:CZ   | 2.59                     | 0.85              |
| 2:G:4230:LYS:CG  | 2:G:4959:PHE:CZ   | 2.59                     | 0.84              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:E:4230:LYS:CG   | 2:E:4959:PHE:CZ  | 2.59                     | 0.84              |
| 2:E:4978:HIS:HA   | 2:E:4982:GLU:HB2 | 1.61                     | 0.83              |
| 2:B:4978:HIS:HA   | 2:B:4982:GLU:HB2 | 1.61                     | 0.82              |
| 2:G:4968:PHE:CZ   | 2:G:4978:HIS:ND1 | 2.48                     | 0.82              |
| 2:B:4968:PHE:CZ   | 2:B:4978:HIS:ND1 | 2.48                     | 0.82              |
| 2:I:4978:HIS:HA   | 2:I:4982:GLU:HB2 | 1.61                     | 0.82              |
| 2:I:4968:PHE:CZ   | 2:I:4978:HIS:ND1 | 2.48                     | 0.82              |
| 2:G:4978:HIS:HA   | 2:G:4982:GLU:HB2 | 1.61                     | 0.81              |
| 2:G:4230:LYS:CD   | 2:G:4959:PHE:CZ  | 2.63                     | 0.81              |
| 2:E:4230:LYS:CD   | 2:E:4959:PHE:CZ  | 2.63                     | 0.81              |
| 2:I:4230:LYS:CD   | 2:I:4959:PHE:CZ  | 2.63                     | 0.81              |
| 2:E:4968:PHE:CZ   | 2:E:4978:HIS:ND1 | 2.48                     | 0.81              |
| 2:B:4230:LYS:CD   | 2:B:4959:PHE:CZ  | 2.63                     | 0.81              |
| 2:G:4957:LYS:HZ3  | 2:G:4957:LYS:HB2 | 1.55                     | 0.72              |
| 2:E:1259:ARG:HH12 | 2:E:1593:PRO:HA  | 1.56                     | 0.71              |
| 2:G:1259:ARG:HH12 | 2:G:1593:PRO:HA  | 1.56                     | 0.71              |
| 2:G:4957:LYS:HG3  | 2:G:4964:GLY:CA  | 2.22                     | 0.70              |
| 2:I:1260:MET:HB2  | 2:I:1269:CYS:H   | 1.56                     | 0.70              |
| 2:B:1260:MET:HB2  | 2:B:1269:CYS:H   | 1.56                     | 0.70              |
| 2:B:4957:LYS:HG3  | 2:B:4964:GLY:CA  | 2.22                     | 0.70              |
| 2:G:1260:MET:HB2  | 2:G:1269:CYS:H   | 1.56                     | 0.70              |
| 2:B:1259:ARG:HH12 | 2:B:1593:PRO:HA  | 1.56                     | 0.69              |
| 2:I:4957:LYS:HG3  | 2:I:4964:GLY:CA  | 2.22                     | 0.69              |
| 2:E:4957:LYS:HG3  | 2:E:4964:GLY:CA  | 2.22                     | 0.69              |
| 2:E:1260:MET:HB2  | 2:E:1269:CYS:H   | 1.56                     | 0.69              |
| 2:I:788:LYS:HG2   | 2:I:1630:CYS:H   | 1.58                     | 0.69              |
| 2:G:788:LYS:HG2   | 2:G:1630:CYS:H   | 1.58                     | 0.69              |
| 2:I:1259:ARG:HH12 | 2:I:1593:PRO:HA  | 1.56                     | 0.69              |
| 2:B:4957:LYS:HG3  | 2:B:4964:GLY:HA2 | 1.75                     | 0.69              |
| 2:G:4957:LYS:HG3  | 2:G:4964:GLY:HA2 | 1.76                     | 0.68              |
| 2:B:788:LYS:HG2   | 2:B:1630:CYS:H   | 1.58                     | 0.68              |
| 2:I:4957:LYS:HG3  | 2:I:4964:GLY:HA2 | 1.75                     | 0.67              |
| 2:I:4968:PHE:CZ   | 2:I:4978:HIS:HE1 | 2.09                     | 0.67              |
| 2:E:788:LYS:HG2   | 2:E:1630:CYS:H   | 1.58                     | 0.67              |
| 2:G:2291:GLN:HB2  | 2:G:2295:LEU:HG  | 1.76                     | 0.67              |
| 2:E:2291:GLN:HB2  | 2:E:2295:LEU:HG  | 1.76                     | 0.67              |
| 2:B:2291:GLN:HB2  | 2:B:2295:LEU:HG  | 1.76                     | 0.66              |
| 2:I:2291:GLN:HB2  | 2:I:2295:LEU:HG  | 1.76                     | 0.66              |
| 2:G:4968:PHE:CZ   | 2:G:4978:HIS:HE1 | 2.09                     | 0.66              |
| 2:E:4968:PHE:CZ   | 2:E:4978:HIS:HE1 | 2.09                     | 0.66              |
| 2:I:2291:GLN:HB3  | 2:I:2294:ASP:H   | 1.60                     | 0.66              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:4957:LYS:HG3  | 2:E:4964:GLY:HA2  | 1.76                     | 0.66              |
| 2:B:646:PRO:HD2   | 2:B:779:PRO:HB2   | 1.77                     | 0.66              |
| 2:B:2291:GLN:HB3  | 2:B:2294:ASP:H    | 1.60                     | 0.66              |
| 2:B:4230:LYS:HD2  | 2:B:4959:PHE:CE1  | 2.31                     | 0.65              |
| 2:E:2291:GLN:HB3  | 2:E:2294:ASP:H    | 1.60                     | 0.65              |
| 2:G:379:HIS:HD2   | 2:G:382:GLY:H     | 1.44                     | 0.65              |
| 2:E:646:PRO:HD2   | 2:E:779:PRO:HB2   | 1.77                     | 0.65              |
| 2:E:379:HIS:HD2   | 2:E:382:GLY:H     | 1.44                     | 0.65              |
| 2:G:4230:LYS:HD2  | 2:G:4959:PHE:CE1  | 2.31                     | 0.65              |
| 2:G:2291:GLN:HB3  | 2:G:2294:ASP:H    | 1.60                     | 0.65              |
| 2:I:646:PRO:HD2   | 2:I:779:PRO:HB2   | 1.77                     | 0.65              |
| 2:I:4230:LYS:HD2  | 2:I:4959:PHE:CE1  | 2.31                     | 0.65              |
| 2:E:4230:LYS:HD2  | 2:E:4959:PHE:CE1  | 2.31                     | 0.65              |
| 2:B:626:LEU:HD23  | 2:B:630:GLU:H     | 1.62                     | 0.64              |
| 2:B:4968:PHE:CZ   | 2:B:4978:HIS:HE1  | 2.09                     | 0.64              |
| 2:G:626:LEU:HD23  | 2:G:630:GLU:H     | 1.62                     | 0.64              |
| 2:G:646:PRO:HD2   | 2:G:779:PRO:HB2   | 1.78                     | 0.64              |
| 2:E:626:LEU:HD23  | 2:E:630:GLU:H     | 1.62                     | 0.64              |
| 2:I:379:HIS:HD2   | 2:I:382:GLY:H     | 1.44                     | 0.64              |
| 2:B:379:HIS:HD2   | 2:B:382:GLY:H     | 1.44                     | 0.64              |
| 2:E:1667:LEU:HD23 | 2:E:1671:ARG:HH12 | 1.63                     | 0.64              |
| 2:G:1667:LEU:HD23 | 2:G:1671:ARG:HH12 | 1.63                     | 0.64              |
| 2:B:426:ARG:HB2   | 2:B:506:TYR:HA    | 1.80                     | 0.63              |
| 2:I:426:ARG:HB2   | 2:I:506:TYR:HA    | 1.80                     | 0.63              |
| 2:G:426:ARG:HB2   | 2:G:506:TYR:HA    | 1.80                     | 0.63              |
| 2:I:626:LEU:HD23  | 2:I:630:GLU:H     | 1.62                     | 0.63              |
| 2:E:4957:LYS:CG   | 2:E:4964:GLY:HA2  | 2.29                     | 0.63              |
| 2:B:4957:LYS:CG   | 2:B:4964:GLY:HA2  | 2.29                     | 0.62              |
| 2:G:745:SER:HB2   | 2:G:758:ARG:HB3   | 1.81                     | 0.62              |
| 2:I:331:VAL:HG12  | 2:I:333:GLY:H     | 1.64                     | 0.62              |
| 2:I:1667:LEU:HD23 | 2:I:1671:ARG:HH12 | 1.63                     | 0.62              |
| 2:E:111:HIS:HD2   | 2:E:114:SER:H     | 1.47                     | 0.62              |
| 2:E:426:ARG:HB2   | 2:E:506:TYR:HA    | 1.80                     | 0.62              |
| 2:E:745:SER:HB2   | 2:E:758:ARG:HB3   | 1.82                     | 0.62              |
| 2:B:497:TYR:HB3   | 2:B:500:ALA:HB2   | 1.82                     | 0.62              |
| 2:B:745:SER:HB2   | 2:B:758:ARG:HB3   | 1.82                     | 0.62              |
| 2:I:497:TYR:HB3   | 2:I:500:ALA:HB2   | 1.82                     | 0.62              |
| 2:I:745:SER:HB2   | 2:I:758:ARG:HB3   | 1.82                     | 0.62              |
| 2:I:4063:ASP:OD2  | 2:I:4067:LYS:NZ   | 2.33                     | 0.62              |
| 2:I:4957:LYS:CG   | 2:I:4964:GLY:HA2  | 2.29                     | 0.62              |
| 2:G:4957:LYS:CG   | 2:G:4964:GLY:HA2  | 2.29                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:4063:ASP:OD2  | 2:E:4067:LYS:NZ   | 2.33                     | 0.62              |
| 2:B:331:VAL:HG12  | 2:B:333:GLY:H     | 1.64                     | 0.62              |
| 2:I:1079:LYS:NZ   | 2:I:1107:PRO:O    | 2.33                     | 0.62              |
| 2:G:1653:LEU:HB3  | 2:G:1660:GLN:HB2  | 1.81                     | 0.62              |
| 2:B:1667:LEU:HD23 | 2:B:1671:ARG:HH12 | 1.63                     | 0.61              |
| 2:B:4063:ASP:OD2  | 2:B:4067:LYS:NZ   | 2.33                     | 0.61              |
| 2:G:497:TYR:HB3   | 2:G:500:ALA:HB2   | 1.82                     | 0.61              |
| 2:B:1653:LEU:HB3  | 2:B:1660:GLN:HB2  | 1.81                     | 0.61              |
| 2:E:1079:LYS:NZ   | 2:E:1107:PRO:O    | 2.33                     | 0.61              |
| 2:G:331:VAL:HG12  | 2:G:333:GLY:H     | 1.64                     | 0.61              |
| 1:F:87:HIS:H      | 1:F:91:ILE:HB     | 1.65                     | 0.61              |
| 2:B:111:HIS:HD2   | 2:B:114:SER:H     | 1.47                     | 0.61              |
| 2:B:1079:LYS:NZ   | 2:B:1107:PRO:O    | 2.33                     | 0.61              |
| 2:G:4063:ASP:OD2  | 2:G:4067:LYS:NZ   | 2.33                     | 0.61              |
| 2:E:497:TYR:HB3   | 2:E:500:ALA:HB2   | 1.82                     | 0.61              |
| 2:B:132:ALA:HA    | 2:B:194:SER:HB2   | 1.83                     | 0.61              |
| 2:G:1079:LYS:NZ   | 2:G:1107:PRO:O    | 2.33                     | 0.61              |
| 2:B:4198:SER:HB3  | 2:B:4201:ASN:HB2  | 1.83                     | 0.61              |
| 2:E:331:VAL:HG12  | 2:E:333:GLY:H     | 1.64                     | 0.61              |
| 1:A:87:HIS:H      | 1:A:91:ILE:HB     | 1.66                     | 0.61              |
| 1:H:87:HIS:H      | 1:H:91:ILE:HB     | 1.66                     | 0.61              |
| 2:I:1170:MET:HE1  | 2:I:1176:GLU:HG3  | 1.83                     | 0.61              |
| 2:E:132:ALA:HA    | 2:E:194:SER:HB2   | 1.83                     | 0.61              |
| 2:B:4957:LYS:HB2  | 2:B:4957:LYS:HZ3  | 1.65                     | 0.61              |
| 2:G:111:HIS:HD2   | 2:G:114:SER:H     | 1.47                     | 0.61              |
| 2:E:4198:SER:HB3  | 2:E:4201:ASN:HB2  | 1.83                     | 0.61              |
| 2:G:465:GLN:HG3   | 2:G:3710:LEU:HB3  | 1.83                     | 0.60              |
| 2:G:1170:MET:HE1  | 2:G:1176:GLU:HG3  | 1.83                     | 0.60              |
| 2:E:465:GLN:HG3   | 2:E:3710:LEU:HB3  | 1.83                     | 0.60              |
| 2:E:683:ARG:HB2   | 2:E:782:SER:HB3   | 1.83                     | 0.60              |
| 2:E:1170:MET:HE1  | 2:E:1176:GLU:HG3  | 1.83                     | 0.60              |
| 1:J:87:HIS:H      | 1:J:91:ILE:HB     | 1.66                     | 0.60              |
| 2:B:3937:TYR:O    | 2:B:4002:LYS:NZ   | 2.35                     | 0.60              |
| 2:I:111:HIS:HD2   | 2:I:114:SER:H     | 1.47                     | 0.60              |
| 2:I:1653:LEU:HB3  | 2:I:1660:GLN:HB2  | 1.81                     | 0.60              |
| 2:G:4198:SER:HB3  | 2:G:4201:ASN:HB2  | 1.83                     | 0.60              |
| 2:I:132:ALA:HA    | 2:I:194:SER:HB2   | 1.83                     | 0.60              |
| 2:I:3937:TYR:O    | 2:I:4002:LYS:NZ   | 2.35                     | 0.60              |
| 2:G:3937:TYR:O    | 2:G:4002:LYS:NZ   | 2.35                     | 0.60              |
| 2:B:683:ARG:HB2   | 2:B:782:SER:HB3   | 1.83                     | 0.60              |
| 2:I:469:ARG:HH21  | 2:I:3712:GLU:HB3  | 1.67                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:2755:ILE:HD13 | 2:I:2810:LYS:HG2  | 1.83                     | 0.60              |
| 2:I:4198:SER:HB3  | 2:I:4201:ASN:HB2  | 1.83                     | 0.60              |
| 2:G:132:ALA:HA    | 2:G:194:SER:HB2   | 1.83                     | 0.60              |
| 2:E:1653:LEU:HB3  | 2:E:1660:GLN:HB2  | 1.81                     | 0.60              |
| 2:E:3937:TYR:O    | 2:E:4002:LYS:NZ   | 2.35                     | 0.60              |
| 2:E:4957:LYS:HZ3  | 2:E:4957:LYS:HB2  | 1.66                     | 0.60              |
| 2:I:210:GLU:HG3   | 2:I:337:PRO:HG3   | 1.84                     | 0.60              |
| 2:G:210:GLU:HG3   | 2:G:337:PRO:HG3   | 1.84                     | 0.60              |
| 2:G:469:ARG:HH21  | 2:G:3712:GLU:HB3  | 1.67                     | 0.60              |
| 2:G:463:GLU:OE2   | 2:G:467:LYS:NZ    | 2.35                     | 0.60              |
| 2:E:210:GLU:HG3   | 2:E:337:PRO:HG3   | 1.84                     | 0.60              |
| 2:I:4674:GLU:HB3  | 2:I:4715:TYR:HB2  | 1.84                     | 0.60              |
| 2:G:683:ARG:HB2   | 2:G:782:SER:HB3   | 1.83                     | 0.60              |
| 2:E:463:GLU:OE2   | 2:E:467:LYS:NZ    | 2.35                     | 0.60              |
| 2:B:2755:ILE:HD13 | 2:B:2810:LYS:HG2  | 1.83                     | 0.59              |
| 2:E:2755:ILE:HD13 | 2:E:2810:LYS:HG2  | 1.83                     | 0.59              |
| 2:I:463:GLU:OE2   | 2:I:467:LYS:NZ    | 2.35                     | 0.59              |
| 2:I:683:ARG:NH1   | 2:I:707:VAL:O     | 2.36                     | 0.59              |
| 2:G:4674:GLU:HB3  | 2:G:4715:TYR:HB2  | 1.84                     | 0.59              |
| 2:B:210:GLU:HG3   | 2:B:337:PRO:HG3   | 1.84                     | 0.59              |
| 2:B:465:GLN:HG3   | 2:B:3710:LEU:HB3  | 1.83                     | 0.59              |
| 2:I:281:ARG:NH2   | 2:I:309:THR:OG1   | 2.36                     | 0.59              |
| 2:I:465:GLN:HG3   | 2:I:3710:LEU:HB3  | 1.83                     | 0.59              |
| 2:B:469:ARG:HH21  | 2:B:3712:GLU:HB3  | 1.67                     | 0.59              |
| 2:B:1671:ARG:NH2  | 2:B:1710:GLY:O    | 2.36                     | 0.59              |
| 2:B:4674:GLU:HB3  | 2:B:4715:TYR:HB2  | 1.84                     | 0.59              |
| 2:E:281:ARG:NH2   | 2:E:309:THR:OG1   | 2.36                     | 0.59              |
| 2:B:1170:MET:HE1  | 2:B:1176:GLU:HG3  | 1.83                     | 0.59              |
| 2:E:1671:ARG:NH2  | 2:E:1710:GLY:O    | 2.36                     | 0.59              |
| 2:I:1671:ARG:NH2  | 2:I:1710:GLY:O    | 2.36                     | 0.59              |
| 2:E:1685:LEU:HA   | 2:E:1688:HIS:HD2  | 1.68                     | 0.59              |
| 2:G:1685:LEU:HA   | 2:G:1688:HIS:HD2  | 1.68                     | 0.59              |
| 2:G:2755:ILE:HD13 | 2:G:2810:LYS:HG2  | 1.83                     | 0.59              |
| 2:E:315:CYS:SG    | 2:E:316:PHE:N     | 2.77                     | 0.58              |
| 2:E:469:ARG:HH21  | 2:E:3712:GLU:HB3  | 1.67                     | 0.58              |
| 2:E:683:ARG:NH1   | 2:E:707:VAL:O     | 2.36                     | 0.58              |
| 2:B:315:CYS:SG    | 2:B:316:PHE:N     | 2.77                     | 0.58              |
| 2:B:463:GLU:OE2   | 2:B:467:LYS:NZ    | 2.35                     | 0.58              |
| 2:I:683:ARG:HB2   | 2:I:782:SER:HB3   | 1.83                     | 0.58              |
| 2:B:683:ARG:NH1   | 2:B:707:VAL:O     | 2.36                     | 0.58              |
| 2:B:4860:ARG:HD2  | 2:E:4582:VAL:HG11 | 1.84                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:315:CYS:SG    | 2:I:316:PHE:N     | 2.77                     | 0.58              |
| 2:G:315:CYS:SG    | 2:G:316:PHE:N     | 2.77                     | 0.58              |
| 2:G:1671:ARG:NH2  | 2:G:1710:GLY:O    | 2.36                     | 0.58              |
| 2:E:1152:MET:HB2  | 2:E:1161:ILE:HB   | 1.85                     | 0.58              |
| 2:E:4674:GLU:HB3  | 2:E:4715:TYR:HB2  | 1.84                     | 0.58              |
| 2:I:1092:PHE:HB3  | 2:I:1149:VAL:HB   | 1.85                     | 0.58              |
| 2:I:1152:MET:HB2  | 2:I:1161:ILE:HB   | 1.85                     | 0.58              |
| 2:B:3889:GLN:OE1  | 2:B:3960:GLN:NE2  | 2.37                     | 0.58              |
| 2:B:3955:MET:HG3  | 2:B:4019:LEU:HD22 | 1.85                     | 0.58              |
| 2:B:1247:PRO:HA   | 2:B:1598:GLN:HA   | 1.86                     | 0.58              |
| 2:I:2911:LEU:HB2  | 2:I:2916:LYS:HE3  | 1.86                     | 0.58              |
| 2:I:3889:GLN:OE1  | 2:I:3960:GLN:NE2  | 2.37                     | 0.58              |
| 2:I:3955:MET:HG3  | 2:I:4019:LEU:HD22 | 1.85                     | 0.58              |
| 2:E:4983:HIS:CD2  | 2:E:4983:HIS:H    | 2.22                     | 0.58              |
| 2:B:609:CYS:SG    | 2:B:610:ASN:N     | 2.77                     | 0.58              |
| 2:B:1109:LEU:HA   | 2:B:1120:LEU:HD21 | 1.86                     | 0.58              |
| 2:I:119:SER:H     | 2:I:137:LEU:HA    | 1.69                     | 0.58              |
| 2:G:683:ARG:NH1   | 2:G:707:VAL:O     | 2.36                     | 0.58              |
| 2:E:2022:PRO:O    | 2:E:2028:ARG:NH2  | 2.37                     | 0.58              |
| 2:E:3889:GLN:OE1  | 2:E:3960:GLN:NE2  | 2.37                     | 0.58              |
| 2:B:1092:PHE:HB3  | 2:B:1149:VAL:HB   | 1.85                     | 0.58              |
| 2:G:1109:LEU:HA   | 2:G:1120:LEU:HD21 | 1.86                     | 0.58              |
| 2:B:2911:LEU:HB2  | 2:B:2916:LYS:HE3  | 1.86                     | 0.57              |
| 2:G:717:ASP:OD1   | 2:G:720:HIS:ND1   | 2.37                     | 0.57              |
| 2:G:3955:MET:HG3  | 2:G:4019:LEU:HD22 | 1.85                     | 0.57              |
| 2:I:2257:LEU:HD11 | 2:I:2276:ALA:HB2  | 1.86                     | 0.57              |
| 2:I:4738:ALA:HA   | 2:I:4743:MET:HE3  | 1.86                     | 0.57              |
| 2:G:1865:MET:SD   | 2:G:1865:MET:N    | 2.77                     | 0.57              |
| 2:G:3889:GLN:OE1  | 2:G:3960:GLN:NE2  | 2.37                     | 0.57              |
| 2:E:2911:LEU:HB2  | 2:E:2916:LYS:HE3  | 1.86                     | 0.57              |
| 2:B:119:SER:H     | 2:B:137:LEU:HA    | 1.69                     | 0.57              |
| 2:I:1685:LEU:HA   | 2:I:1688:HIS:HD2  | 1.68                     | 0.57              |
| 2:G:281:ARG:NH2   | 2:G:309:THR:OG1   | 2.36                     | 0.57              |
| 2:G:2022:PRO:O    | 2:G:2028:ARG:NH2  | 2.37                     | 0.57              |
| 2:E:1109:LEU:HA   | 2:E:1120:LEU:HD21 | 1.86                     | 0.57              |
| 2:E:1865:MET:SD   | 2:E:1865:MET:N    | 2.77                     | 0.57              |
| 2:B:717:ASP:OD1   | 2:B:720:HIS:ND1   | 2.37                     | 0.57              |
| 2:B:4738:ALA:HA   | 2:B:4743:MET:HE3  | 1.87                     | 0.57              |
| 2:I:23:GLN:HB3    | 2:I:201:ASN:HB2   | 1.86                     | 0.57              |
| 2:I:717:ASP:OD1   | 2:I:720:HIS:ND1   | 2.37                     | 0.57              |
| 2:I:4904:PRO:HB3  | 2:I:4913:ARG:HD3  | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:2911:LEU:HB2  | 2:G:2916:LYS:HE3  | 1.86                     | 0.57              |
| 2:E:3955:MET:HG3  | 2:E:4019:LEU:HD22 | 1.85                     | 0.57              |
| 2:E:4983:HIS:CD2  | 2:E:4983:HIS:N    | 2.73                     | 0.57              |
| 2:B:1152:MET:HB2  | 2:B:1161:ILE:HB   | 1.85                     | 0.57              |
| 2:B:1685:LEU:HA   | 2:B:1688:HIS:HD2  | 1.68                     | 0.57              |
| 2:B:4904:PRO:HB3  | 2:B:4913:ARG:HD3  | 1.86                     | 0.57              |
| 2:E:1247:PRO:HA   | 2:E:1598:GLN:HA   | 1.86                     | 0.57              |
| 2:B:281:ARG:NH2   | 2:B:309:THR:OG1   | 2.36                     | 0.57              |
| 2:B:2257:LEU:HD11 | 2:B:2276:ALA:HB2  | 1.87                     | 0.57              |
| 2:I:4978:HIS:CE1  | 2:I:5027:CYS:SG   | 2.98                     | 0.57              |
| 2:G:609:CYS:SG    | 2:G:610:ASN:N     | 2.77                     | 0.57              |
| 2:G:1152:MET:HB2  | 2:G:1161:ILE:HB   | 1.85                     | 0.57              |
| 2:E:1092:PHE:HB3  | 2:E:1149:VAL:HB   | 1.85                     | 0.57              |
| 2:E:4738:ALA:HA   | 2:E:4743:MET:HE3  | 1.86                     | 0.57              |
| 2:B:4582:VAL:HG11 | 2:I:4860:ARG:HD2  | 1.86                     | 0.57              |
| 2:E:609:CYS:SG    | 2:E:610:ASN:N     | 2.77                     | 0.57              |
| 2:B:1865:MET:SD   | 2:B:1865:MET:N    | 2.77                     | 0.57              |
| 2:I:1865:MET:SD   | 2:I:1865:MET:N    | 2.77                     | 0.57              |
| 2:I:3973:CYS:SG   | 2:I:3976:ASN:ND2  | 2.78                     | 0.57              |
| 2:G:4957:LYS:HB2  | 2:G:4957:LYS:NZ   | 2.20                     | 0.57              |
| 2:E:4978:HIS:CE1  | 2:E:5027:CYS:SG   | 2.98                     | 0.57              |
| 2:G:1092:PHE:HB3  | 2:G:1149:VAL:HB   | 1.85                     | 0.57              |
| 2:G:1247:PRO:HA   | 2:G:1598:GLN:HA   | 1.86                     | 0.57              |
| 2:G:4738:ALA:HA   | 2:G:4743:MET:HE3  | 1.86                     | 0.57              |
| 2:B:1152:MET:HE1  | 2:B:1217:CYS:HB3  | 1.87                     | 0.57              |
| 2:B:2022:PRO:O    | 2:B:2028:ARG:NH2  | 2.37                     | 0.57              |
| 2:I:110:ARG:HH21  | 2:I:115:ARG:HB3   | 1.70                     | 0.56              |
| 2:I:1109:LEU:HA   | 2:I:1120:LEU:HD21 | 1.86                     | 0.56              |
| 2:I:1152:MET:HE1  | 2:I:1217:CYS:HB3  | 1.87                     | 0.56              |
| 2:I:4582:VAL:HG11 | 2:G:4860:ARG:HD2  | 1.87                     | 0.56              |
| 2:G:4983:HIS:N    | 2:G:4983:HIS:CD2  | 2.73                     | 0.56              |
| 2:E:4904:PRO:HB3  | 2:E:4913:ARG:HD3  | 1.86                     | 0.56              |
| 2:E:4957:LYS:HB2  | 2:E:4957:LYS:NZ   | 2.20                     | 0.56              |
| 2:I:609:CYS:SG    | 2:I:610:ASN:N     | 2.77                     | 0.56              |
| 2:I:2022:PRO:O    | 2:I:2028:ARG:NH2  | 2.37                     | 0.56              |
| 2:G:23:GLN:HB3    | 2:G:201:ASN:HB2   | 1.86                     | 0.56              |
| 2:G:4180:ARG:HH22 | 2:G:4981:GLU:HA   | 1.71                     | 0.56              |
| 2:E:4180:ARG:HH22 | 2:E:4981:GLU:HA   | 1.71                     | 0.56              |
| 1:F:55:VAL:HA     | 2:E:1784:ALA:HA   | 1.87                     | 0.56              |
| 2:B:110:ARG:HH21  | 2:B:115:ARG:HB3   | 1.70                     | 0.56              |
| 2:G:119:SER:H     | 2:G:137:LEU:HA    | 1.69                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:2257:LEU:HD11 | 2:G:2276:ALA:HB2  | 1.86                     | 0.56              |
| 2:G:2748:PRO:HD2  | 2:G:2751:LEU:HD12 | 1.88                     | 0.56              |
| 2:G:3973:CYS:SG   | 2:G:3976:ASN:ND2  | 2.78                     | 0.56              |
| 2:G:4582:VAL:HG11 | 2:E:4860:ARG:HD2  | 1.87                     | 0.56              |
| 2:G:4904:PRO:HB3  | 2:G:4913:ARG:HD3  | 1.85                     | 0.56              |
| 2:G:4978:HIS:CE1  | 2:G:5027:CYS:SG   | 2.98                     | 0.56              |
| 2:E:23:GLN:HB3    | 2:E:201:ASN:HB2   | 1.86                     | 0.56              |
| 2:E:717:ASP:OD1   | 2:E:720:HIS:ND1   | 2.37                     | 0.56              |
| 2:E:3973:CYS:SG   | 2:E:3976:ASN:ND2  | 2.78                     | 0.56              |
| 2:I:1247:PRO:HA   | 2:I:1598:GLN:HA   | 1.86                     | 0.56              |
| 2:B:3973:CYS:SG   | 2:B:3976:ASN:ND2  | 2.78                     | 0.56              |
| 2:I:4957:LYS:HB2  | 2:I:4957:LYS:NZ   | 2.20                     | 0.56              |
| 2:G:4983:HIS:CD2  | 2:G:4983:HIS:H    | 2.22                     | 0.56              |
| 2:E:119:SER:H     | 2:E:137:LEU:HA    | 1.69                     | 0.56              |
| 2:B:952:LYS:HB3   | 2:B:968:ALA:HB1   | 1.88                     | 0.56              |
| 2:B:1721:GLU:OE2  | 2:B:1725:ARG:NH2  | 2.39                     | 0.56              |
| 2:B:4180:ARG:HH22 | 2:B:4981:GLU:HA   | 1.70                     | 0.56              |
| 2:B:4230:LYS:HE2  | 2:B:4231:MET:HE2  | 1.87                     | 0.56              |
| 2:I:1721:GLU:OE2  | 2:I:1725:ARG:NH2  | 2.39                     | 0.56              |
| 2:G:1721:GLU:OE2  | 2:G:1725:ARG:NH2  | 2.39                     | 0.56              |
| 2:G:4230:LYS:HE2  | 2:G:4231:MET:HE2  | 1.87                     | 0.56              |
| 2:E:110:ARG:HH21  | 2:E:115:ARG:HB3   | 1.70                     | 0.56              |
| 2:E:952:LYS:HB3   | 2:E:968:ALA:HB1   | 1.88                     | 0.56              |
| 2:E:1721:GLU:OE2  | 2:E:1725:ARG:NH2  | 2.39                     | 0.56              |
| 2:B:4978:HIS:CE1  | 2:B:5027:CYS:SG   | 2.98                     | 0.56              |
| 2:I:2748:PRO:HD2  | 2:I:2751:LEU:HD12 | 1.87                     | 0.56              |
| 2:B:23:GLN:HB3    | 2:B:201:ASN:HB2   | 1.86                     | 0.56              |
| 2:I:4983:HIS:H    | 2:I:4983:HIS:CD2  | 2.22                     | 0.56              |
| 2:G:4968:PHE:HZ   | 2:G:4978:HIS:HE1  | 1.54                     | 0.56              |
| 2:E:2257:LEU:HD11 | 2:E:2276:ALA:HB2  | 1.87                     | 0.56              |
| 2:I:4180:ARG:HH22 | 2:I:4981:GLU:HA   | 1.70                     | 0.56              |
| 2:G:110:ARG:HH21  | 2:G:115:ARG:HB3   | 1.71                     | 0.56              |
| 2:B:3932:ASP:HA   | 2:B:3935:TRP:HD1  | 1.71                     | 0.56              |
| 2:G:1152:MET:HE1  | 2:G:1217:CYS:HB3  | 1.87                     | 0.56              |
| 2:E:2479:LEU:O    | 2:E:2487:UNK:N    | 2.39                     | 0.56              |
| 2:E:2748:PRO:HD2  | 2:E:2751:LEU:HD12 | 1.88                     | 0.56              |
| 2:E:1764:GLY:HA3  | 2:E:1859:VAL:HG11 | 1.88                     | 0.55              |
| 2:I:3910:THR:HG23 | 2:I:3911:THR:HG23 | 1.89                     | 0.55              |
| 2:I:4968:PHE:HZ   | 2:I:4978:HIS:HE1  | 1.54                     | 0.55              |
| 2:G:3762:ARG:O    | 2:G:3766:GLN:NE2  | 2.38                     | 0.55              |
| 2:E:3932:ASP:HA   | 2:E:3935:TRP:HD1  | 1.71                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:4983:HIS:CD2  | 2:B:4983:HIS:H    | 2.22                     | 0.55              |
| 2:G:952:LYS:HB3   | 2:G:968:ALA:HB1   | 1.88                     | 0.55              |
| 2:G:2770:LYS:HB3  | 2:G:2775:TRP:HB2  | 1.89                     | 0.55              |
| 2:G:3932:ASP:HA   | 2:G:3935:TRP:HD1  | 1.71                     | 0.55              |
| 2:E:1152:MET:HE1  | 2:E:1217:CYS:HB3  | 1.87                     | 0.55              |
| 2:B:3910:THR:HG23 | 2:B:3911:THR:HG23 | 1.89                     | 0.55              |
| 2:I:2770:LYS:HB3  | 2:I:2775:TRP:HB2  | 1.89                     | 0.55              |
| 2:I:4983:HIS:CD2  | 2:I:4983:HIS:N    | 2.73                     | 0.55              |
| 2:G:1764:GLY:HA3  | 2:G:1859:VAL:HG11 | 1.88                     | 0.55              |
| 2:B:606:LEU:O     | 2:B:617:ASN:ND2   | 2.40                     | 0.55              |
| 2:B:4957:LYS:HB2  | 2:B:4957:LYS:NZ   | 2.20                     | 0.55              |
| 2:G:1243:PRO:HB2  | 2:G:1600:LEU:HD22 | 1.89                     | 0.55              |
| 2:E:1243:PRO:HB2  | 2:E:1600:LEU:HD22 | 1.89                     | 0.55              |
| 2:B:2479:LEU:O    | 2:B:2487:UNK:N    | 2.39                     | 0.55              |
| 2:I:4230:LYS:HE2  | 2:I:4231:MET:HE2  | 1.87                     | 0.55              |
| 2:G:1808:ARG:NH1  | 2:G:1853:ILE:O    | 2.38                     | 0.55              |
| 2:E:2002:PRO:HA   | 2:E:2005:GLN:HB3  | 1.89                     | 0.55              |
| 2:E:635:THR:HB    | 2:E:1639:LEU:HD23 | 1.89                     | 0.55              |
| 2:B:2748:PRO:HD2  | 2:B:2751:LEU:HD12 | 1.88                     | 0.55              |
| 2:B:1519:UNK:HA   | 2:B:1526:UNK:HA   | 1.89                     | 0.54              |
| 2:B:4983:HIS:CD2  | 2:B:4983:HIS:N    | 2.73                     | 0.54              |
| 2:I:952:LYS:HB3   | 2:I:968:ALA:HB1   | 1.88                     | 0.54              |
| 2:I:1667:LEU:O    | 2:I:1671:ARG:NH1  | 2.41                     | 0.54              |
| 2:I:1764:GLY:HA3  | 2:I:1859:VAL:HG11 | 1.88                     | 0.54              |
| 2:I:3932:ASP:HA   | 2:I:3935:TRP:HD1  | 1.71                     | 0.54              |
| 2:G:664:PHE:HB2   | 2:G:746:CYS:HB2   | 1.89                     | 0.54              |
| 2:B:664:PHE:HB2   | 2:B:746:CYS:HB2   | 1.89                     | 0.54              |
| 2:I:2479:LEU:O    | 2:I:2487:UNK:N    | 2.39                     | 0.54              |
| 2:G:19:GLU:HB2    | 2:G:206:CYS:HB3   | 1.90                     | 0.54              |
| 2:B:19:GLU:HB2    | 2:B:206:CYS:HB3   | 1.89                     | 0.54              |
| 2:B:635:THR:HB    | 2:B:1639:LEU:HD23 | 1.89                     | 0.54              |
| 2:B:2770:LYS:HB3  | 2:B:2775:TRP:HB2  | 1.89                     | 0.54              |
| 2:G:2479:LEU:O    | 2:G:2487:UNK:N    | 2.39                     | 0.54              |
| 2:E:19:GLU:HB2    | 2:E:206:CYS:HB3   | 1.89                     | 0.54              |
| 2:E:1519:UNK:HA   | 2:E:1526:UNK:HA   | 1.89                     | 0.54              |
| 2:E:4230:LYS:HE2  | 2:E:4231:MET:HE2  | 1.87                     | 0.54              |
| 2:B:1667:LEU:O    | 2:B:1671:ARG:NH1  | 2.41                     | 0.54              |
| 2:I:19:GLU:HB2    | 2:I:206:CYS:HB3   | 1.89                     | 0.54              |
| 2:I:4968:PHE:CE2  | 2:I:4978:HIS:CE1  | 2.96                     | 0.54              |
| 2:G:606:LEU:O     | 2:G:617:ASN:ND2   | 2.40                     | 0.54              |
| 2:E:606:LEU:O     | 2:E:617:ASN:ND2   | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:2298:VAL:HG21 | 2:E:2335:LEU:HD21 | 1.90                     | 0.54              |
| 2:B:1764:GLY:HA3  | 2:B:1859:VAL:HG11 | 1.88                     | 0.54              |
| 2:B:2002:PRO:HA   | 2:B:2005:GLN:HB3  | 1.89                     | 0.54              |
| 2:G:1667:LEU:O    | 2:G:1671:ARG:NH1  | 2.41                     | 0.54              |
| 2:G:2002:PRO:HA   | 2:G:2005:GLN:HB3  | 1.89                     | 0.54              |
| 2:G:3910:THR:HG23 | 2:G:3911:THR:HG23 | 1.89                     | 0.54              |
| 2:E:3897:ASN:O    | 2:E:3901:ASN:ND2  | 2.41                     | 0.54              |
| 2:I:2002:PRO:HA   | 2:I:2005:GLN:HB3  | 1.89                     | 0.54              |
| 2:I:3897:ASN:O    | 2:I:3901:ASN:ND2  | 2.41                     | 0.54              |
| 2:B:1100:MET:HE2  | 2:B:1198:GLN:HB3  | 1.89                     | 0.54              |
| 2:B:2266:GLY:O    | 2:B:2330:ARG:NH2  | 2.41                     | 0.54              |
| 2:I:606:LEU:O     | 2:I:617:ASN:ND2   | 2.40                     | 0.54              |
| 2:I:2266:GLY:O    | 2:I:2330:ARG:NH2  | 2.41                     | 0.54              |
| 2:I:3733:CYS:HB2  | 2:I:3803:SER:HB3  | 1.90                     | 0.54              |
| 2:E:1111:PRO:HD3  | 2:E:1605:TRP:HE1  | 1.73                     | 0.54              |
| 2:B:1808:ARG:NH1  | 2:B:1853:ILE:O    | 2.38                     | 0.54              |
| 2:I:4059:LEU:O    | 2:I:4063:ASP:N    | 2.36                     | 0.54              |
| 2:I:4957:LYS:HB2  | 2:I:4957:LYS:HZ3  | 1.72                     | 0.54              |
| 2:E:3910:THR:HG23 | 2:E:3911:THR:HG23 | 1.89                     | 0.54              |
| 2:G:989:ALA:O     | 2:G:1035:ASN:ND2  | 2.41                     | 0.54              |
| 2:E:2770:LYS:HB3  | 2:E:2775:TRP:HB2  | 1.89                     | 0.54              |
| 2:E:3733:CYS:HB2  | 2:E:3803:SER:HB3  | 1.90                     | 0.54              |
| 2:E:3762:ARG:O    | 2:E:3766:GLN:NE2  | 2.38                     | 0.54              |
| 2:E:4968:PHE:CE2  | 2:E:4978:HIS:CE1  | 2.96                     | 0.54              |
| 2:B:1243:PRO:HB2  | 2:B:1600:LEU:HD22 | 1.89                     | 0.53              |
| 2:I:1243:PRO:HB2  | 2:I:1600:LEU:HD22 | 1.89                     | 0.53              |
| 2:E:2739:PRO:HB3  | 2:E:2884:ASN:HB3  | 1.91                     | 0.53              |
| 2:B:3897:ASN:O    | 2:B:3901:ASN:ND2  | 2.41                     | 0.53              |
| 2:E:3733:CYS:HA   | 2:E:3766:GLN:HG2  | 1.90                     | 0.53              |
| 1:A:74:LEU:HB2    | 1:A:99:PHE:HB2    | 1.90                     | 0.53              |
| 1:H:74:LEU:HB2    | 1:H:99:PHE:HB2    | 1.90                     | 0.53              |
| 1:J:55:VAL:HA     | 2:I:1784:ALA:HA   | 1.90                     | 0.53              |
| 2:B:2739:PRO:HB3  | 2:B:2884:ASN:HB3  | 1.91                     | 0.53              |
| 2:I:2739:PRO:HB3  | 2:I:2884:ASN:HB3  | 1.90                     | 0.53              |
| 2:G:635:THR:HB    | 2:G:1639:LEU:HD23 | 1.89                     | 0.53              |
| 2:G:1100:MET:HE2  | 2:G:1198:GLN:HB3  | 1.89                     | 0.53              |
| 2:G:3897:ASN:O    | 2:G:3901:ASN:ND2  | 2.41                     | 0.53              |
| 2:E:664:PHE:HB2   | 2:E:746:CYS:HB2   | 1.89                     | 0.53              |
| 2:B:4137:ARG:NH1  | 2:B:4173:TYR:OH   | 2.42                     | 0.53              |
| 2:I:2298:VAL:HG21 | 2:I:2335:LEU:HD21 | 1.90                     | 0.53              |
| 2:G:3733:CYS:HA   | 2:G:3766:GLN:HG2  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:6:THR:HA      | 1:J:72:ALA:HA     | 1.91                     | 0.53              |
| 2:B:1111:PRO:HD3  | 2:B:1605:TRP:HE1  | 1.73                     | 0.53              |
| 2:I:2737:PRO:O    | 2:I:2888:ARG:NH2  | 2.42                     | 0.53              |
| 2:G:1111:PRO:HD3  | 2:G:1605:TRP:HE1  | 1.73                     | 0.53              |
| 2:G:2298:VAL:HG21 | 2:G:2335:LEU:HD21 | 1.90                     | 0.53              |
| 1:F:6:THR:HA      | 1:F:72:ALA:HA     | 1.91                     | 0.53              |
| 2:B:989:ALA:O     | 2:B:1035:ASN:ND2  | 2.41                     | 0.53              |
| 2:B:2298:VAL:HG21 | 2:B:2335:LEU:HD21 | 1.90                     | 0.53              |
| 2:I:635:THR:HB    | 2:I:1639:LEU:HD23 | 1.89                     | 0.53              |
| 2:I:1519:UNK:HA   | 2:I:1526:UNK:HA   | 1.89                     | 0.53              |
| 2:G:2739:PRO:HB3  | 2:G:2884:ASN:HB3  | 1.91                     | 0.53              |
| 2:G:3733:CYS:HB2  | 2:G:3803:SER:HB3  | 1.90                     | 0.53              |
| 2:E:1667:LEU:O    | 2:E:1671:ARG:NH1  | 2.41                     | 0.53              |
| 2:E:2266:GLY:O    | 2:E:2330:ARG:NH2  | 2.41                     | 0.53              |
| 2:E:2737:PRO:O    | 2:E:2888:ARG:NH2  | 2.42                     | 0.53              |
| 1:H:6:THR:HA      | 1:H:72:ALA:HA     | 1.91                     | 0.53              |
| 2:B:4968:PHE:HZ   | 2:B:4978:HIS:HE1  | 1.54                     | 0.53              |
| 2:I:3830:GLN:HA   | 2:I:3833:GLN:HG2  | 1.91                     | 0.53              |
| 2:G:41:GLY:O      | 2:G:45:ARG:NH1    | 2.42                     | 0.53              |
| 1:F:74:LEU:HB2    | 1:F:99:PHE:HB2    | 1.90                     | 0.53              |
| 1:A:6:THR:HA      | 1:A:72:ALA:HA     | 1.91                     | 0.53              |
| 2:B:3830:GLN:HA   | 2:B:3833:GLN:HG2  | 1.91                     | 0.53              |
| 2:B:4968:PHE:CE2  | 2:B:4978:HIS:CE1  | 2.96                     | 0.53              |
| 2:I:266:ARG:NH2   | 2:I:272:SER:OG    | 2.42                     | 0.53              |
| 2:I:1111:PRO:HD3  | 2:I:1605:TRP:HE1  | 1.73                     | 0.53              |
| 2:G:2737:PRO:O    | 2:G:2888:ARG:NH2  | 2.42                     | 0.53              |
| 2:B:2042:CYS:SG   | 2:B:2043:GLY:N    | 2.82                     | 0.53              |
| 2:I:4786:ASP:OD2  | 2:I:4789:PHE:N    | 2.42                     | 0.53              |
| 1:A:55:VAL:HA     | 2:B:1784:ALA:HA   | 1.90                     | 0.53              |
| 2:B:3733:CYS:HB2  | 2:B:3803:SER:HB3  | 1.90                     | 0.53              |
| 2:B:4681:LEU:HD21 | 2:B:4687:TYR:HD2  | 1.74                     | 0.53              |
| 2:I:173:SER:HB3   | 2:I:178:ARG:H     | 1.74                     | 0.53              |
| 2:I:647:ASN:ND2   | 2:I:820:ARG:O     | 2.42                     | 0.53              |
| 2:I:989:ALA:O     | 2:I:1035:ASN:ND2  | 2.41                     | 0.53              |
| 2:G:173:SER:HB3   | 2:G:178:ARG:H     | 1.74                     | 0.53              |
| 2:G:1519:UNK:HA   | 2:G:1526:UNK:HA   | 1.90                     | 0.53              |
| 2:E:718:GLY:HA3   | 2:E:737:LEU:HA    | 1.91                     | 0.53              |
| 2:G:2266:GLY:O    | 2:G:2330:ARG:NH2  | 2.41                     | 0.52              |
| 2:E:989:ALA:O     | 2:E:1035:ASN:ND2  | 2.41                     | 0.52              |
| 2:E:1100:MET:HE2  | 2:E:1198:GLN:HB3  | 1.89                     | 0.52              |
| 2:I:664:PHE:HB2   | 2:I:746:CYS:HB2   | 1.89                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:3734:HIS:O    | 2:I:3738:GLY:N    | 2.43                     | 0.52              |
| 2:I:4137:ARG:NH1  | 2:I:4173:TYR:OH   | 2.42                     | 0.52              |
| 2:G:718:GLY:HA3   | 2:G:737:LEU:HA    | 1.91                     | 0.52              |
| 2:G:4968:PHE:CE2  | 2:G:4978:HIS:CE1  | 2.96                     | 0.52              |
| 2:E:41:GLY:O      | 2:E:45:ARG:NH1    | 2.42                     | 0.52              |
| 2:E:4137:ARG:NH1  | 2:E:4173:TYR:OH   | 2.42                     | 0.52              |
| 2:B:2737:PRO:O    | 2:B:2888:ARG:NH2  | 2.42                     | 0.52              |
| 2:G:3830:GLN:HA   | 2:G:3833:GLN:HG2  | 1.91                     | 0.52              |
| 2:E:3734:HIS:O    | 2:E:3738:GLY:N    | 2.43                     | 0.52              |
| 1:J:74:LEU:HB2    | 1:J:99:PHE:HB2    | 1.90                     | 0.52              |
| 2:G:1808:ARG:HD3  | 2:G:1853:ILE:HG22 | 1.91                     | 0.52              |
| 2:E:1166:GLY:HA3  | 2:E:1216:ILE:HD13 | 1.92                     | 0.52              |
| 2:E:3830:GLN:HA   | 2:E:3833:GLN:HG2  | 1.91                     | 0.52              |
| 2:E:4184:MET:HE2  | 2:E:4188:ARG:HA   | 1.91                     | 0.52              |
| 2:B:173:SER:HB3   | 2:B:178:ARG:H     | 1.74                     | 0.52              |
| 2:B:1808:ARG:HD3  | 2:B:1853:ILE:HG22 | 1.91                     | 0.52              |
| 2:G:13:PHE:HA     | 2:G:164:ARG:HA    | 1.92                     | 0.52              |
| 2:B:313:SER:HB3   | 2:B:351:VAL:HB    | 1.92                     | 0.52              |
| 2:I:1100:MET:HE2  | 2:I:1198:GLN:HB3  | 1.89                     | 0.52              |
| 2:G:1166:GLY:HA3  | 2:G:1216:ILE:HD13 | 1.92                     | 0.52              |
| 2:B:4786:ASP:OD2  | 2:B:4789:PHE:N    | 2.42                     | 0.52              |
| 2:G:4137:ARG:NH1  | 2:G:4173:TYR:OH   | 2.42                     | 0.52              |
| 2:E:1649:ASP:HB3  | 2:E:1652:GLU:HG2  | 1.92                     | 0.52              |
| 2:E:4232:GLU:OE2  | 2:E:5017:ARG:NH1  | 2.39                     | 0.52              |
| 2:B:266:ARG:NH2   | 2:B:272:SER:OG    | 2.42                     | 0.52              |
| 2:I:718:GLY:HA3   | 2:I:737:LEU:HA    | 1.91                     | 0.52              |
| 2:I:1025:ARG:O    | 2:I:1032:LYS:NZ   | 2.39                     | 0.52              |
| 2:I:3733:CYS:HA   | 2:I:3766:GLN:HG2  | 1.90                     | 0.52              |
| 2:I:4681:LEU:HD21 | 2:I:4687:TYR:HD2  | 1.74                     | 0.52              |
| 2:G:266:ARG:NH2   | 2:G:272:SER:OG    | 2.42                     | 0.52              |
| 2:G:2042:CYS:SG   | 2:G:2043:GLY:N    | 2.82                     | 0.52              |
| 2:E:13:PHE:HA     | 2:E:164:ARG:HA    | 1.92                     | 0.52              |
| 2:B:718:GLY:HA3   | 2:B:737:LEU:HA    | 1.91                     | 0.52              |
| 2:B:1166:GLY:HA3  | 2:B:1216:ILE:HD13 | 1.92                     | 0.52              |
| 2:B:3733:CYS:HA   | 2:B:3766:GLN:HG2  | 1.90                     | 0.52              |
| 2:I:4232:GLU:OE2  | 2:I:5017:ARG:NH1  | 2.39                     | 0.52              |
| 2:G:3734:HIS:O    | 2:G:3738:GLY:N    | 2.43                     | 0.52              |
| 2:G:4184:MET:HE2  | 2:G:4188:ARG:HA   | 1.91                     | 0.52              |
| 2:E:4681:LEU:HD21 | 2:E:4687:TYR:HD2  | 1.74                     | 0.52              |
| 2:E:173:SER:HB3   | 2:E:178:ARG:H     | 1.74                     | 0.52              |
| 2:B:41:GLY:O      | 2:B:45:ARG:NH1    | 2.42                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:4184:MET:HE2  | 2:B:4188:ARG:HA   | 1.91                     | 0.51              |
| 2:I:13:PHE:HA     | 2:I:164:ARG:HA    | 1.92                     | 0.51              |
| 2:I:4833:ASN:ND2  | 2:I:4935:LEU:O    | 2.44                     | 0.51              |
| 2:I:4958:CYS:SG   | 2:I:4961:CYS:N    | 2.84                     | 0.51              |
| 2:G:111:HIS:CD2   | 2:G:114:SER:H     | 2.26                     | 0.51              |
| 2:E:266:ARG:NH2   | 2:E:272:SER:OG    | 2.42                     | 0.51              |
| 1:A:82:TYR:O      | 1:A:86:GLY:N      | 2.44                     | 0.51              |
| 2:I:1808:ARG:HD3  | 2:I:1853:ILE:HG22 | 1.91                     | 0.51              |
| 2:G:264:PRO:HG2   | 2:G:270:SER:HB2   | 1.92                     | 0.51              |
| 2:E:671:VAL:HG22  | 2:E:740:PRO:HG3   | 1.92                     | 0.51              |
| 2:E:4833:ASN:ND2  | 2:E:4935:LEU:O    | 2.44                     | 0.51              |
| 2:B:13:PHE:HA     | 2:B:164:ARG:HA    | 1.92                     | 0.51              |
| 2:B:1649:ASP:HB3  | 2:B:1652:GLU:HG2  | 1.92                     | 0.51              |
| 2:I:41:GLY:O      | 2:I:45:ARG:NH1    | 2.42                     | 0.51              |
| 2:I:1166:GLY:HA3  | 2:I:1216:ILE:HD13 | 1.92                     | 0.51              |
| 2:G:313:SER:HB3   | 2:G:351:VAL:HB    | 1.92                     | 0.51              |
| 2:G:671:VAL:HG22  | 2:G:740:PRO:HG3   | 1.92                     | 0.51              |
| 2:G:4232:GLU:OE2  | 2:G:5017:ARG:NH1  | 2.39                     | 0.51              |
| 2:E:264:PRO:HG2   | 2:E:270:SER:HB2   | 1.92                     | 0.51              |
| 2:E:1808:ARG:HD3  | 2:E:1853:ILE:HG22 | 1.91                     | 0.51              |
| 2:E:4968:PHE:HZ   | 2:E:4978:HIS:HE1  | 1.54                     | 0.51              |
| 2:I:111:HIS:CD2   | 2:I:114:SER:H     | 2.26                     | 0.51              |
| 2:G:1649:ASP:HB3  | 2:G:1652:GLU:HG2  | 1.92                     | 0.51              |
| 2:G:4681:LEU:HD21 | 2:G:4687:TYR:HD2  | 1.74                     | 0.51              |
| 2:E:111:HIS:CD2   | 2:E:114:SER:H     | 2.26                     | 0.51              |
| 2:I:649:PHE:HB3   | 2:I:776:LEU:HD13  | 1.93                     | 0.51              |
| 2:G:647:ASN:ND2   | 2:G:820:ARG:O     | 2.42                     | 0.51              |
| 2:G:4786:ASP:OD2  | 2:G:4789:PHE:N    | 2.42                     | 0.51              |
| 2:I:1808:ARG:NH1  | 2:I:1853:ILE:O    | 2.38                     | 0.51              |
| 2:B:264:PRO:HG2   | 2:B:270:SER:HB2   | 1.92                     | 0.51              |
| 2:B:4860:ARG:HG3  | 2:B:4876:CYS:HB3  | 1.93                     | 0.51              |
| 1:F:82:TYR:O      | 1:F:86:GLY:N      | 2.44                     | 0.51              |
| 2:B:4833:ASN:ND2  | 2:B:4935:LEU:O    | 2.44                     | 0.51              |
| 2:I:1649:ASP:HB3  | 2:I:1652:GLU:HG2  | 1.92                     | 0.51              |
| 2:I:4184:MET:HE2  | 2:I:4188:ARG:HA   | 1.91                     | 0.51              |
| 2:I:4860:ARG:HG3  | 2:I:4876:CYS:HB3  | 1.93                     | 0.51              |
| 2:I:264:PRO:HG2   | 2:I:270:SER:HB2   | 1.92                     | 0.51              |
| 2:I:4673:ARG:HH22 | 2:I:4698:LYS:HB2  | 1.76                     | 0.51              |
| 2:G:4860:ARG:HG3  | 2:G:4876:CYS:HB3  | 1.93                     | 0.51              |
| 2:G:4958:CYS:SG   | 2:G:4961:CYS:N    | 2.84                     | 0.51              |
| 1:H:82:TYR:O      | 1:H:86:GLY:N      | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:82:TYR:O      | 1:J:86:GLY:N      | 2.44                     | 0.51              |
| 2:B:671:VAL:HG22  | 2:B:740:PRO:HG3   | 1.92                     | 0.51              |
| 2:B:4958:CYS:SG   | 2:B:4961:CYS:N    | 2.84                     | 0.51              |
| 2:I:313:SER:HB3   | 2:I:351:VAL:HB    | 1.92                     | 0.51              |
| 2:G:649:PHE:HB3   | 2:G:776:LEU:HD13  | 1.93                     | 0.51              |
| 2:E:313:SER:HB3   | 2:E:351:VAL:HB    | 1.92                     | 0.51              |
| 2:E:2337:PHE:HA   | 2:E:2340:PHE:HB2  | 1.93                     | 0.51              |
| 2:B:111:HIS:CD2   | 2:B:114:SER:H     | 2.26                     | 0.50              |
| 2:G:4833:ASN:ND2  | 2:G:4935:LEU:O    | 2.44                     | 0.50              |
| 2:E:4673:ARG:HH22 | 2:E:4698:LYS:HB2  | 1.76                     | 0.50              |
| 2:B:3734:HIS:O    | 2:B:3738:GLY:N    | 2.43                     | 0.50              |
| 2:B:3980:LEU:HD22 | 2:B:3985:LEU:HD22 | 1.92                     | 0.50              |
| 2:I:68:THR:N      | 2:I:110:ARG:O     | 2.44                     | 0.50              |
| 2:E:4958:CYS:SG   | 2:E:4961:CYS:N    | 2.84                     | 0.50              |
| 2:G:3980:LEU:HD22 | 2:G:3985:LEU:HD22 | 1.92                     | 0.50              |
| 2:G:4230:LYS:HG3  | 2:G:4959:PHE:CE2  | 2.44                     | 0.50              |
| 2:G:4673:ARG:HH22 | 2:G:4698:LYS:HB2  | 1.76                     | 0.50              |
| 2:E:68:THR:N      | 2:E:110:ARG:O     | 2.44                     | 0.50              |
| 2:E:1725:ARG:HA   | 2:E:1728:ARG:HG2  | 1.94                     | 0.50              |
| 2:E:3980:LEU:HD22 | 2:E:3985:LEU:HD22 | 1.92                     | 0.50              |
| 2:B:68:THR:N      | 2:B:110:ARG:O     | 2.44                     | 0.50              |
| 1:H:76:CYS:HB2    | 1:H:97:LEU:HB2    | 1.94                     | 0.50              |
| 2:B:2337:PHE:HA   | 2:B:2340:PHE:HB2  | 1.93                     | 0.50              |
| 2:B:4232:GLU:OE2  | 2:B:5017:ARG:NH1  | 2.39                     | 0.50              |
| 2:I:4182:GLU:OE2  | 2:I:4983:HIS:CD2  | 2.57                     | 0.50              |
| 2:E:647:ASN:ND2   | 2:E:820:ARG:O     | 2.42                     | 0.50              |
| 1:F:42:ARG:HG2    | 2:E:1691:GLN:HG2  | 1.93                     | 0.50              |
| 2:E:4786:ASP:OD2  | 2:E:4789:PHE:N    | 2.42                     | 0.50              |
| 1:J:76:CYS:HB2    | 1:J:97:LEU:HB2    | 1.94                     | 0.50              |
| 2:B:1725:ARG:HA   | 2:B:1728:ARG:HG2  | 1.94                     | 0.50              |
| 2:B:2927:LEU:HD23 | 2:B:2930:LEU:HD12 | 1.94                     | 0.50              |
| 2:I:2337:PHE:HA   | 2:I:2340:PHE:HB2  | 1.93                     | 0.50              |
| 2:E:4860:ARG:HG3  | 2:E:4876:CYS:HB3  | 1.93                     | 0.50              |
| 2:B:978:THR:HB    | 2:B:980:ALA:H     | 1.77                     | 0.50              |
| 2:B:3751:VAL:O    | 2:B:3756:LYS:NZ   | 2.45                     | 0.50              |
| 2:I:978:THR:HB    | 2:I:980:ALA:H     | 1.77                     | 0.50              |
| 2:G:3805:LEU:HA   | 2:G:3809:ASN:HD22 | 1.77                     | 0.50              |
| 2:E:2927:LEU:HD23 | 2:E:2930:LEU:HD12 | 1.94                     | 0.50              |
| 2:B:649:PHE:HB3   | 2:B:776:LEU:HD13  | 1.93                     | 0.50              |
| 2:I:3751:VAL:O    | 2:I:3756:LYS:NZ   | 2.45                     | 0.50              |
| 2:I:4978:HIS:HE1  | 2:I:5027:CYS:SG   | 2.35                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:3751:VAL:O    | 2:E:3756:LYS:NZ   | 2.45                     | 0.50              |
| 2:B:647:ASN:ND2   | 2:B:820:ARG:O     | 2.42                     | 0.49              |
| 2:B:886:ARG:HB3   | 2:B:891:TRP:HB2   | 1.94                     | 0.49              |
| 2:B:3959:LYS:O    | 2:B:3963:ASN:ND2  | 2.45                     | 0.49              |
| 2:I:671:VAL:HG22  | 2:I:740:PRO:HG3   | 1.92                     | 0.49              |
| 2:E:359:TYR:HA    | 2:E:376:ALA:HA    | 1.94                     | 0.49              |
| 2:E:886:ARG:HB3   | 2:E:891:TRP:HB2   | 1.94                     | 0.49              |
| 2:I:3762:ARG:O    | 2:I:3766:GLN:NE2  | 2.38                     | 0.49              |
| 2:I:3980:LEU:HD22 | 2:I:3985:LEU:HD22 | 1.92                     | 0.49              |
| 2:G:221:ARG:NH2   | 2:G:397:GLU:OE2   | 2.45                     | 0.49              |
| 2:G:3941:ASP:HA   | 2:G:4002:LYS:HE3  | 1.94                     | 0.49              |
| 2:B:3941:ASP:HA   | 2:B:4002:LYS:HE3  | 1.94                     | 0.49              |
| 2:B:4978:HIS:HE1  | 2:B:5027:CYS:SG   | 2.35                     | 0.49              |
| 2:I:3959:LYS:O    | 2:I:3963:ASN:ND2  | 2.45                     | 0.49              |
| 2:G:399:GLN:HG2   | 2:G:403:MET:HE3   | 1.94                     | 0.49              |
| 2:E:3941:ASP:HA   | 2:E:4002:LYS:HE3  | 1.94                     | 0.49              |
| 1:A:76:CYS:HB2    | 1:A:97:LEU:HB2    | 1.94                     | 0.49              |
| 2:B:4962:GLY:HA3  | 2:B:5025:GLY:HA2  | 1.95                     | 0.49              |
| 2:I:3805:LEU:HA   | 2:I:3809:ASN:HD22 | 1.77                     | 0.49              |
| 2:G:68:THR:N      | 2:G:110:ARG:O     | 2.44                     | 0.49              |
| 2:E:649:PHE:HB3   | 2:E:776:LEU:HD13  | 1.93                     | 0.49              |
| 2:E:4978:HIS:HE1  | 2:E:5027:CYS:SG   | 2.35                     | 0.49              |
| 2:G:359:TYR:HA    | 2:G:376:ALA:HA    | 1.94                     | 0.49              |
| 2:G:4782:VAL:O    | 2:G:4785:THR:OG1  | 2.30                     | 0.49              |
| 2:E:221:ARG:NH2   | 2:E:397:GLU:OE2   | 2.45                     | 0.49              |
| 2:E:1663:HIS:NE2  | 2:E:1711:TYR:OH   | 2.42                     | 0.49              |
| 2:E:1808:ARG:NH1  | 2:E:1853:ILE:O    | 2.38                     | 0.49              |
| 2:E:4230:LYS:HG3  | 2:E:4959:PHE:CE2  | 2.44                     | 0.49              |
| 2:E:4962:GLY:HA3  | 2:E:5025:GLY:HA2  | 1.95                     | 0.49              |
| 2:B:284:HIS:HB3   | 2:B:287:THR:HB    | 1.94                     | 0.49              |
| 2:B:4059:LEU:O    | 2:B:4063:ASP:N    | 2.36                     | 0.49              |
| 2:G:2337:PHE:HA   | 2:G:2340:PHE:HB2  | 1.93                     | 0.49              |
| 2:G:3959:LYS:O    | 2:G:3963:ASN:ND2  | 2.45                     | 0.49              |
| 2:E:395:GLN:HG3   | 2:E:397:GLU:H     | 1.78                     | 0.49              |
| 1:F:76:CYS:HB2    | 1:F:97:LEU:HB2    | 1.94                     | 0.49              |
| 2:B:485:SER:O     | 2:B:489:ASN:N     | 2.40                     | 0.49              |
| 2:I:399:GLN:HG2   | 2:I:403:MET:HE3   | 1.94                     | 0.49              |
| 2:I:2042:CYS:SG   | 2:I:2043:GLY:N    | 2.82                     | 0.49              |
| 2:G:395:GLN:HG3   | 2:G:397:GLU:H     | 1.78                     | 0.49              |
| 2:G:3751:VAL:O    | 2:G:3756:LYS:NZ   | 2.45                     | 0.49              |
| 2:E:838:HIS:HA    | 2:E:1201:HIS:HB3  | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:838:HIS:HA    | 2:B:1201:HIS:HB3  | 1.95                     | 0.49              |
| 2:I:1725:ARG:HA   | 2:I:1728:ARG:HG2  | 1.94                     | 0.49              |
| 2:I:2869:ARG:HA   | 2:I:2872:GLN:HB3  | 1.95                     | 0.49              |
| 2:I:2927:LEU:HD23 | 2:I:2930:LEU:HD12 | 1.94                     | 0.49              |
| 2:G:1725:ARG:HA   | 2:G:1728:ARG:HG2  | 1.94                     | 0.49              |
| 2:G:2927:LEU:HD23 | 2:G:2930:LEU:HD12 | 1.94                     | 0.49              |
| 2:E:776:LEU:HG    | 2:E:848:HIS:HA    | 1.95                     | 0.49              |
| 2:E:1848:LEU:HD22 | 2:E:1853:ILE:HG13 | 1.95                     | 0.49              |
| 2:B:972:LEU:O     | 2:B:1044:ARG:NH2  | 2.46                     | 0.49              |
| 2:B:4673:ARG:HH22 | 2:B:4698:LYS:HB2  | 1.76                     | 0.49              |
| 2:I:229:GLU:HA    | 2:I:249:GLY:HA2   | 1.95                     | 0.49              |
| 2:I:972:LEU:O     | 2:I:1044:ARG:NH2  | 2.46                     | 0.49              |
| 2:E:3805:LEU:HA   | 2:E:3809:ASN:HD22 | 1.77                     | 0.49              |
| 1:H:23:VAL:HG22   | 1:H:47:LYS:HG2    | 1.95                     | 0.49              |
| 2:B:615:ARG:NH2   | 2:B:1677:GLY:O    | 2.43                     | 0.49              |
| 2:B:4782:VAL:O    | 2:B:4785:THR:OG1  | 2.30                     | 0.49              |
| 2:G:229:GLU:HA    | 2:G:249:GLY:HA2   | 1.95                     | 0.49              |
| 1:F:23:VAL:HG22   | 1:F:47:LYS:HG2    | 1.95                     | 0.48              |
| 2:B:4230:LYS:HG3  | 2:B:4959:PHE:CE2  | 2.44                     | 0.48              |
| 2:I:4833:ASN:HD21 | 2:I:4935:LEU:HG   | 1.78                     | 0.48              |
| 2:G:284:HIS:HB3   | 2:G:287:THR:HB    | 1.94                     | 0.48              |
| 2:G:4978:HIS:HE1  | 2:G:5027:CYS:SG   | 2.35                     | 0.48              |
| 2:E:3959:LYS:O    | 2:E:3963:ASN:ND2  | 2.45                     | 0.48              |
| 2:B:43:GLY:N      | 2:B:447:ASP:OD2   | 2.43                     | 0.48              |
| 2:B:359:TYR:HA    | 2:B:376:ALA:HA    | 1.94                     | 0.48              |
| 2:B:399:GLN:HG2   | 2:B:403:MET:HE3   | 1.94                     | 0.48              |
| 2:B:776:LEU:HG    | 2:B:848:HIS:HA    | 1.95                     | 0.48              |
| 2:G:978:THR:HB    | 2:G:980:ALA:H     | 1.77                     | 0.48              |
| 2:E:867:LEU:HB3   | 2:E:929:LEU:HD13  | 1.95                     | 0.48              |
| 2:B:4230:LYS:HD2  | 2:B:4959:PHE:CE2  | 2.48                     | 0.48              |
| 2:B:4833:ASN:HD21 | 2:B:4935:LEU:HG   | 1.78                     | 0.48              |
| 2:I:3941:ASP:HA   | 2:I:4002:LYS:HE3  | 1.94                     | 0.48              |
| 2:I:4962:GLY:H    | 2:I:5025:GLY:N    | 2.12                     | 0.48              |
| 2:G:2869:ARG:HA   | 2:G:2872:GLN:HB3  | 1.95                     | 0.48              |
| 2:G:4577:LEU:HG   | 2:G:4580:TYR:HE2  | 1.79                     | 0.48              |
| 2:E:4962:GLY:H    | 2:E:5025:GLY:N    | 2.12                     | 0.48              |
| 2:B:1516:UNK:N    | 2:B:1529:UNK:O    | 2.47                     | 0.48              |
| 2:B:1743:ARG:O    | 2:B:1964:ARG:NH2  | 2.43                     | 0.48              |
| 2:I:4962:GLY:HA3  | 2:I:5025:GLY:HA2  | 1.95                     | 0.48              |
| 2:G:1743:ARG:O    | 2:G:1964:ARG:NH2  | 2.43                     | 0.48              |
| 2:E:2869:ARG:HA   | 2:E:2872:GLN:HB3  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:4833:ASN:HD21 | 2:E:4935:LEU:HG   | 1.78                     | 0.48              |
| 2:B:1105:ALA:HB1  | 2:B:1109:LEU:HD21 | 1.96                     | 0.48              |
| 2:I:359:TYR:HA    | 2:I:376:ALA:HA    | 1.94                     | 0.48              |
| 2:I:1660:GLN:O    | 2:I:1664:SER:N    | 2.47                     | 0.48              |
| 2:I:1848:LEU:HD22 | 2:I:1853:ILE:HG13 | 1.94                     | 0.48              |
| 2:I:4577:LEU:HG   | 2:I:4580:TYR:HE2  | 1.79                     | 0.48              |
| 2:G:867:LEU:HB3   | 2:G:929:LEU:HD13  | 1.95                     | 0.48              |
| 2:G:1516:UNK:N    | 2:G:1529:UNK:O    | 2.47                     | 0.48              |
| 2:G:4962:GLY:HA3  | 2:G:5025:GLY:HA2  | 1.95                     | 0.48              |
| 2:E:43:GLY:N      | 2:E:447:ASP:OD2   | 2.43                     | 0.48              |
| 2:E:972:LEU:O     | 2:E:1044:ARG:NH2  | 2.46                     | 0.48              |
| 2:E:978:THR:HB    | 2:E:980:ALA:H     | 1.77                     | 0.48              |
| 2:B:3762:ARG:O    | 2:B:3766:GLN:NE2  | 2.38                     | 0.48              |
| 2:B:3805:LEU:HA   | 2:B:3809:ASN:HD22 | 1.77                     | 0.48              |
| 2:I:886:ARG:HB3   | 2:I:891:TRP:HB2   | 1.94                     | 0.48              |
| 2:G:886:ARG:HB3   | 2:G:891:TRP:HB2   | 1.94                     | 0.48              |
| 2:G:972:LEU:O     | 2:G:1044:ARG:NH2  | 2.46                     | 0.48              |
| 2:G:1848:LEU:HD22 | 2:G:1853:ILE:HG13 | 1.94                     | 0.48              |
| 2:G:4962:GLY:H    | 2:G:5025:GLY:N    | 2.12                     | 0.48              |
| 2:E:399:GLN:HG2   | 2:E:403:MET:HE3   | 1.94                     | 0.48              |
| 2:E:1105:ALA:HB1  | 2:E:1109:LEU:HD21 | 1.96                     | 0.48              |
| 2:E:4233:LEU:HA   | 2:E:4236:SER:HB3  | 1.95                     | 0.48              |
| 1:J:23:VAL:HG22   | 1:J:47:LYS:HG2    | 1.95                     | 0.48              |
| 2:I:615:ARG:NH2   | 2:I:1677:GLY:O    | 2.43                     | 0.48              |
| 2:I:776:LEU:HG    | 2:I:848:HIS:HA    | 1.95                     | 0.48              |
| 2:I:838:HIS:HA    | 2:I:1201:HIS:HB3  | 1.95                     | 0.48              |
| 2:G:838:HIS:HA    | 2:G:1201:HIS:HB3  | 1.95                     | 0.48              |
| 2:G:4059:LEU:O    | 2:G:4063:ASP:N    | 2.36                     | 0.48              |
| 2:G:4833:ASN:HD21 | 2:G:4935:LEU:HG   | 1.78                     | 0.48              |
| 2:E:284:HIS:HB3   | 2:E:287:THR:HB    | 1.94                     | 0.48              |
| 2:E:1516:UNK:N    | 2:E:1529:UNK:O    | 2.47                     | 0.48              |
| 2:E:2285:GLU:HG3  | 2:E:2286:LEU:HG   | 1.96                     | 0.48              |
| 2:E:4059:LEU:O    | 2:E:4063:ASP:N    | 2.36                     | 0.48              |
| 2:I:284:HIS:HB3   | 2:I:287:THR:HB    | 1.94                     | 0.48              |
| 2:I:719:LEU:HD22  | 2:I:735:GLN:HG2   | 1.95                     | 0.48              |
| 2:I:1516:UNK:N    | 2:I:1529:UNK:O    | 2.47                     | 0.48              |
| 2:E:580:GLU:HG2   | 2:E:583:ILE:HD11  | 1.96                     | 0.48              |
| 2:E:4577:LEU:HG   | 2:E:4580:TYR:HE2  | 1.79                     | 0.48              |
| 1:A:42:ARG:HG2    | 2:B:1691:GLN:HG2  | 1.94                     | 0.48              |
| 2:B:395:GLN:HG3   | 2:B:397:GLU:H     | 1.78                     | 0.48              |
| 2:B:867:LEU:HB3   | 2:B:929:LEU:HD13  | 1.95                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:395:GLN:HG3   | 2:I:397:GLU:H     | 1.78                     | 0.48              |
| 2:E:719:LEU:HD22  | 2:E:735:GLN:HG2   | 1.95                     | 0.48              |
| 2:E:3900:GLN:NE2  | 2:E:3967:GLU:O    | 2.47                     | 0.48              |
| 2:E:4563:ARG:NH1  | 2:E:4815:ASP:OD1  | 2.47                     | 0.48              |
| 1:J:57:LYS:HB2    | 1:J:80:VAL:HB     | 1.96                     | 0.48              |
| 2:B:2869:ARG:HA   | 2:B:2872:GLN:HB3  | 1.95                     | 0.48              |
| 2:B:4577:LEU:HG   | 2:B:4580:TYR:HE2  | 1.79                     | 0.48              |
| 2:G:2285:GLU:HG3  | 2:G:2286:LEU:HG   | 1.96                     | 0.48              |
| 2:E:396:GLU:OE2   | 2:E:451:TYR:OH    | 2.32                     | 0.48              |
| 1:F:57:LYS:HB2    | 1:F:80:VAL:HB     | 1.96                     | 0.47              |
| 2:B:2285:GLU:HG3  | 2:B:2286:LEU:HG   | 1.96                     | 0.47              |
| 2:I:580:GLU:HG2   | 2:I:583:ILE:HD11  | 1.96                     | 0.47              |
| 2:I:1685:LEU:HD22 | 2:I:1718:ILE:HG21 | 1.96                     | 0.47              |
| 2:G:719:LEU:HD22  | 2:G:735:GLN:HG2   | 1.95                     | 0.47              |
| 2:G:776:LEU:HG    | 2:G:848:HIS:HA    | 1.95                     | 0.47              |
| 2:E:4230:LYS:HD2  | 2:E:4959:PHE:CE2  | 2.49                     | 0.47              |
| 1:A:23:VAL:HG22   | 1:A:47:LYS:HG2    | 1.95                     | 0.47              |
| 2:B:1685:LEU:HD22 | 2:B:1718:ILE:HG21 | 1.96                     | 0.47              |
| 2:B:4233:LEU:HA   | 2:B:4236:SER:HB3  | 1.95                     | 0.47              |
| 2:G:4563:ARG:NH1  | 2:G:4815:ASP:OD1  | 2.47                     | 0.47              |
| 2:E:983:THR:O     | 2:E:987:ARG:N     | 2.47                     | 0.47              |
| 2:B:3946:GLN:OE1  | 2:B:3950:ASN:ND2  | 2.47                     | 0.47              |
| 2:I:116:MET:HB2   | 2:I:137:LEU:HD12  | 1.96                     | 0.47              |
| 2:I:1960:ALA:O    | 2:I:1964:ARG:NE   | 2.47                     | 0.47              |
| 2:I:4563:ARG:NH1  | 2:I:4815:ASP:OD1  | 2.47                     | 0.47              |
| 2:G:1960:ALA:O    | 2:G:1964:ARG:NE   | 2.47                     | 0.47              |
| 2:G:3900:GLN:NE2  | 2:G:3967:GLU:O    | 2.47                     | 0.47              |
| 2:G:4230:LYS:HD2  | 2:G:4959:PHE:CE2  | 2.48                     | 0.47              |
| 2:E:229:GLU:HA    | 2:E:249:GLY:HA2   | 1.95                     | 0.47              |
| 1:A:57:LYS:HB2    | 1:A:80:VAL:HB     | 1.96                     | 0.47              |
| 2:B:229:GLU:HA    | 2:B:249:GLY:HA2   | 1.95                     | 0.47              |
| 2:B:3850:GLN:HA   | 2:B:3853:ALA:HB3  | 1.97                     | 0.47              |
| 2:G:116:MET:HB2   | 2:G:137:LEU:HD12  | 1.96                     | 0.47              |
| 2:G:615:ARG:NH2   | 2:G:1677:GLY:O    | 2.43                     | 0.47              |
| 2:G:3946:GLN:OE1  | 2:G:3950:ASN:ND2  | 2.48                     | 0.47              |
| 2:E:3946:GLN:OE1  | 2:E:3950:ASN:ND2  | 2.47                     | 0.47              |
| 2:E:4782:VAL:O    | 2:E:4785:THR:OG1  | 2.30                     | 0.47              |
| 2:I:983:THR:O     | 2:I:987:ARG:N     | 2.47                     | 0.47              |
| 2:I:2285:GLU:HG3  | 2:I:2286:LEU:HG   | 1.96                     | 0.47              |
| 2:I:4586:PRO:HB3  | 2:I:4628:VAL:HG21 | 1.97                     | 0.47              |
| 2:G:1685:LEU:HD22 | 2:G:1718:ILE:HG21 | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:221:ARG:NH2   | 2:B:397:GLU:OE2   | 2.45                     | 0.47              |
| 2:B:1848:LEU:HD22 | 2:B:1853:ILE:HG13 | 1.94                     | 0.47              |
| 2:G:580:GLU:HG2   | 2:G:583:ILE:HD11  | 1.96                     | 0.47              |
| 2:G:983:THR:O     | 2:G:987:ARG:N     | 2.47                     | 0.47              |
| 2:G:4239:GLU:OE2  | 2:G:5014:TYR:OH   | 2.30                     | 0.47              |
| 2:E:1685:LEU:HD22 | 2:E:1718:ILE:HG21 | 1.96                     | 0.47              |
| 2:B:2196:ASN:OD1  | 2:B:2199:ARG:NH1  | 2.38                     | 0.47              |
| 2:B:3900:GLN:NE2  | 2:B:3967:GLU:O    | 2.47                     | 0.47              |
| 2:B:4182:GLU:OE2  | 2:B:4983:HIS:CD2  | 2.57                     | 0.47              |
| 2:B:4822:THR:O    | 2:B:4825:THR:OG1  | 2.32                     | 0.47              |
| 2:I:103:TYR:HB3   | 2:I:152:PRO:HD3   | 1.97                     | 0.47              |
| 2:I:3900:GLN:NE2  | 2:I:3967:GLU:O    | 2.47                     | 0.47              |
| 2:I:4822:THR:O    | 2:I:4825:THR:OG1  | 2.32                     | 0.47              |
| 2:G:3850:GLN:HA   | 2:G:3853:ALA:HB3  | 1.97                     | 0.47              |
| 2:G:4233:LEU:HA   | 2:G:4236:SER:HB3  | 1.96                     | 0.47              |
| 2:E:3850:GLN:HA   | 2:E:3853:ALA:HB3  | 1.97                     | 0.47              |
| 2:E:4104:THR:HG22 | 2:E:4106:PRO:HD2  | 1.97                     | 0.47              |
| 2:I:894:GLY:HA3   | 2:I:903:LEU:HD22  | 1.97                     | 0.47              |
| 2:I:3850:GLN:HA   | 2:I:3853:ALA:HB3  | 1.97                     | 0.47              |
| 2:I:4104:THR:HG22 | 2:I:4106:PRO:HD2  | 1.97                     | 0.47              |
| 2:G:1660:GLN:O    | 2:G:1664:SER:N    | 2.47                     | 0.47              |
| 2:E:4558:ASN:HB2  | 2:E:4561:THR:HB   | 1.97                     | 0.47              |
| 1:H:57:LYS:HB2    | 1:H:80:VAL:HB     | 1.96                     | 0.47              |
| 2:B:103:TYR:HB3   | 2:B:152:PRO:HD3   | 1.97                     | 0.47              |
| 2:B:719:LEU:HD22  | 2:B:735:GLN:HG2   | 1.95                     | 0.47              |
| 2:B:2024:PRO:HB2  | 2:B:2027:ILE:HG12 | 1.97                     | 0.47              |
| 2:B:4563:ARG:NH1  | 2:B:4815:ASP:OD1  | 2.47                     | 0.47              |
| 2:B:4586:PRO:HB3  | 2:B:4628:VAL:HG21 | 1.97                     | 0.47              |
| 2:I:468:LEU:HB3   | 2:I:472:ARG:HH12  | 1.80                     | 0.47              |
| 2:G:853:PRO:HB3   | 2:G:1024:TYR:H    | 1.80                     | 0.47              |
| 2:G:1105:ALA:HB1  | 2:G:1109:LEU:HD21 | 1.96                     | 0.47              |
| 2:G:4586:PRO:HB3  | 2:G:4628:VAL:HG21 | 1.97                     | 0.47              |
| 2:B:1960:ALA:O    | 2:B:1964:ARG:NE   | 2.47                     | 0.47              |
| 2:B:4962:GLY:H    | 2:B:5025:GLY:N    | 2.12                     | 0.47              |
| 2:I:2024:PRO:HB2  | 2:I:2027:ILE:HG12 | 1.97                     | 0.47              |
| 2:E:2189:LYS:HA   | 2:E:2192:TYR:HD2  | 1.80                     | 0.47              |
| 2:E:4158:PRO:HA   | 2:E:4161:ARG:HB2  | 1.97                     | 0.47              |
| 2:E:4822:THR:O    | 2:E:4825:THR:OG1  | 2.32                     | 0.47              |
| 2:B:853:PRO:HB3   | 2:B:1024:TYR:H    | 1.80                     | 0.46              |
| 2:I:488:LEU:O     | 2:I:492:ASP:N     | 2.45                     | 0.46              |
| 2:I:867:LEU:HB3   | 2:I:929:LEU:HD13  | 1.95                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:4233:LEU:HA   | 2:I:4236:SER:HB3  | 1.95                     | 0.46              |
| 2:G:2751:LEU:HD11 | 2:G:2823:ILE:HG21 | 1.97                     | 0.46              |
| 2:G:4158:PRO:HA   | 2:G:4161:ARG:HB2  | 1.97                     | 0.46              |
| 2:E:2751:LEU:HD11 | 2:E:2823:ILE:HG21 | 1.97                     | 0.46              |
| 1:J:42:ARG:HG2    | 2:I:1691:GLN:HG2  | 1.97                     | 0.46              |
| 1:J:92:PRO:HD3    | 2:I:627:PRO:HB2   | 1.98                     | 0.46              |
| 2:B:580:GLU:HG2   | 2:B:583:ILE:HD11  | 1.96                     | 0.46              |
| 2:I:1105:ALA:HB1  | 2:I:1109:LEU:HD21 | 1.96                     | 0.46              |
| 2:G:103:TYR:HB3   | 2:G:152:PRO:HD3   | 1.97                     | 0.46              |
| 2:G:1025:ARG:O    | 2:G:1032:LYS:NZ   | 2.39                     | 0.46              |
| 2:E:468:LEU:HB3   | 2:E:472:ARG:HH12  | 1.80                     | 0.46              |
| 2:E:853:PRO:HB3   | 2:E:1024:TYR:H    | 1.80                     | 0.46              |
| 2:E:1743:ARG:O    | 2:E:1964:ARG:NH2  | 2.43                     | 0.46              |
| 2:I:1743:ARG:O    | 2:I:1964:ARG:NH2  | 2.43                     | 0.46              |
| 2:G:894:GLY:HA3   | 2:G:903:LEU:HD22  | 1.97                     | 0.46              |
| 2:G:2024:PRO:HB2  | 2:G:2027:ILE:HG12 | 1.97                     | 0.46              |
| 2:G:3528:UNK:HA   | 2:E:1220:GLN:NE2  | 2.30                     | 0.46              |
| 2:G:4697:VAL:O    | 2:G:4701:TRP:N    | 2.47                     | 0.46              |
| 2:E:615:ARG:NH2   | 2:E:1677:GLY:O    | 2.43                     | 0.46              |
| 2:E:1660:GLN:O    | 2:E:1664:SER:N    | 2.47                     | 0.46              |
| 1:J:21:THR:HA     | 1:J:49:ARG:HA     | 1.98                     | 0.46              |
| 2:B:116:MET:HB2   | 2:B:137:LEU:HD12  | 1.96                     | 0.46              |
| 2:B:4104:THR:HG22 | 2:B:4106:PRO:HD2  | 1.96                     | 0.46              |
| 2:G:887:ILE:HG21  | 2:G:959:TYR:HA    | 1.98                     | 0.46              |
| 2:G:4822:THR:O    | 2:G:4825:THR:OG1  | 2.32                     | 0.46              |
| 2:E:1796:ALA:HB1  | 2:E:1797:ARG:HH21 | 1.81                     | 0.46              |
| 2:E:1960:ALA:O    | 2:E:1964:ARG:NE   | 2.47                     | 0.46              |
| 2:B:2189:LYS:HA   | 2:B:2192:TYR:HD2  | 1.80                     | 0.46              |
| 2:B:4558:ASN:HB2  | 2:B:4561:THR:HB   | 1.97                     | 0.46              |
| 2:I:1931:LEU:HB3  | 2:I:1935:VAL:HB   | 1.98                     | 0.46              |
| 2:I:2189:LYS:HA   | 2:I:2192:TYR:HD2  | 1.80                     | 0.46              |
| 2:I:4558:ASN:HB2  | 2:I:4561:THR:HB   | 1.97                     | 0.46              |
| 2:G:4182:GLU:OE2  | 2:G:4983:HIS:CD2  | 2.57                     | 0.46              |
| 2:E:116:MET:HB2   | 2:E:137:LEU:HD12  | 1.96                     | 0.46              |
| 2:E:286:THR:HA    | 2:E:405:HIS:HB2   | 1.98                     | 0.46              |
| 2:E:4882:CYS:SG   | 2:E:4886:HIS:NE2  | 2.89                     | 0.46              |
| 1:H:21:THR:HA     | 1:H:49:ARG:HA     | 1.98                     | 0.46              |
| 2:B:468:LEU:HB3   | 2:B:472:ARG:HH12  | 1.80                     | 0.46              |
| 2:B:870:ILE:HD12  | 2:B:873:LYS:HB2   | 1.98                     | 0.46              |
| 2:I:786:GLY:HA2   | 2:I:1631:GLN:HA   | 1.98                     | 0.46              |
| 2:I:853:PRO:HB3   | 2:I:1024:TYR:H    | 1.80                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:870:ILE:HD12  | 2:I:873:LYS:HB2   | 1.98                     | 0.46              |
| 2:I:924:MET:O     | 2:I:928:THR:OG1   | 2.32                     | 0.46              |
| 2:I:3696:ASP:O    | 2:I:3700:GLN:N    | 2.46                     | 0.46              |
| 2:G:4957:LYS:HG3  | 2:G:4964:GLY:HA3  | 1.97                     | 0.46              |
| 2:E:870:ILE:HD12  | 2:E:873:LYS:HB2   | 1.98                     | 0.46              |
| 2:E:2024:PRO:HB2  | 2:E:2027:ILE:HG12 | 1.97                     | 0.46              |
| 2:E:4957:LYS:HG3  | 2:E:4964:GLY:HA3  | 1.96                     | 0.46              |
| 2:B:786:GLY:HA2   | 2:B:1631:GLN:HA   | 1.98                     | 0.46              |
| 2:B:983:THR:O     | 2:B:987:ARG:N     | 2.47                     | 0.46              |
| 2:I:57:ASN:HD22   | 2:I:308:HIS:HB2   | 1.81                     | 0.46              |
| 2:G:286:THR:HA    | 2:G:405:HIS:HB2   | 1.98                     | 0.46              |
| 2:G:870:ILE:HD12  | 2:G:873:LYS:HB2   | 1.98                     | 0.46              |
| 2:G:2189:LYS:HA   | 2:G:2192:TYR:HD2  | 1.80                     | 0.46              |
| 2:G:4960:ILE:HG22 | 2:G:4960:ILE:O    | 2.16                     | 0.46              |
| 2:E:4924:VAL:HG12 | 2:E:4928:LEU:HD12 | 1.98                     | 0.46              |
| 2:B:4882:CYS:SG   | 2:B:4886:HIS:NE2  | 2.89                     | 0.46              |
| 2:I:3946:GLN:OE1  | 2:I:3950:ASN:ND2  | 2.47                     | 0.46              |
| 2:I:4230:LYS:HG3  | 2:I:4959:PHE:CE2  | 2.44                     | 0.46              |
| 2:I:4782:VAL:O    | 2:I:4785:THR:OG1  | 2.30                     | 0.46              |
| 2:G:786:GLY:HA2   | 2:G:1631:GLN:HA   | 1.98                     | 0.46              |
| 2:G:1848:LEU:HB3  | 2:G:1853:ILE:HB   | 1.98                     | 0.46              |
| 2:E:786:GLY:HA2   | 2:E:1631:GLN:HA   | 1.98                     | 0.46              |
| 2:E:887:ILE:HG21  | 2:E:959:TYR:HA    | 1.97                     | 0.46              |
| 2:B:57:ASN:HD22   | 2:B:308:HIS:HB2   | 1.81                     | 0.46              |
| 2:B:894:GLY:HA3   | 2:B:903:LEU:HD22  | 1.97                     | 0.46              |
| 2:B:2751:LEU:HD11 | 2:B:2823:ILE:HG21 | 1.97                     | 0.46              |
| 2:I:2104:ARG:HA   | 2:I:2107:GLN:HB3  | 1.98                     | 0.46              |
| 2:I:4697:VAL:O    | 2:I:4701:TRP:N    | 2.47                     | 0.46              |
| 2:I:4882:CYS:SG   | 2:I:4886:HIS:NE2  | 2.89                     | 0.46              |
| 2:E:2375:GLY:HA3  | 2:E:2378:ALA:HB3  | 1.98                     | 0.46              |
| 2:E:4586:PRO:HB3  | 2:E:4628:VAL:HG21 | 1.97                     | 0.46              |
| 1:F:21:THR:HA     | 1:F:49:ARG:HA     | 1.98                     | 0.46              |
| 2:B:1848:LEU:HB3  | 2:B:1853:ILE:HB   | 1.98                     | 0.46              |
| 2:B:1931:LEU:HB3  | 2:B:1935:VAL:HB   | 1.98                     | 0.46              |
| 2:B:4924:VAL:HG12 | 2:B:4928:LEU:HD12 | 1.98                     | 0.46              |
| 2:I:823:LEU:HD23  | 2:I:1626:TRP:HB3  | 1.98                     | 0.46              |
| 2:I:2517:UNK:O    | 2:I:2521:UNK:N    | 2.49                     | 0.46              |
| 2:G:57:ASN:HD22   | 2:G:308:HIS:HB2   | 1.81                     | 0.46              |
| 2:G:1796:ALA:HB1  | 2:G:1797:ARG:HH21 | 1.81                     | 0.46              |
| 2:G:4104:THR:HG22 | 2:G:4106:PRO:HD2  | 1.96                     | 0.46              |
| 2:E:57:ASN:HD22   | 2:E:308:HIS:HB2   | 1.81                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:103:TYR:HB3   | 2:E:152:PRO:HD3   | 1.97                     | 0.46              |
| 2:E:695:TYR:OH    | 2:E:1073:ARG:NH1  | 2.48                     | 0.46              |
| 2:B:1078:GLU:HB3  | 2:B:1081:TYR:HD2  | 1.82                     | 0.45              |
| 2:B:3953:LYS:O    | 2:B:3956:SER:OG   | 2.32                     | 0.45              |
| 2:I:880:GLU:OE1   | 2:I:968:ALA:N     | 2.47                     | 0.45              |
| 2:I:887:ILE:HG21  | 2:I:959:TYR:HA    | 1.97                     | 0.45              |
| 2:I:1848:LEU:HB3  | 2:I:1853:ILE:HB   | 1.98                     | 0.45              |
| 2:I:4960:ILE:O    | 2:I:4960:ILE:HG22 | 2.16                     | 0.45              |
| 2:G:823:LEU:HD23  | 2:G:1626:TRP:HB3  | 1.99                     | 0.45              |
| 2:G:4081:VAL:HB   | 2:G:4088:ILE:HD12 | 1.98                     | 0.45              |
| 2:E:1848:LEU:HB3  | 2:E:1853:ILE:HB   | 1.98                     | 0.45              |
| 2:E:1931:LEU:HB3  | 2:E:1935:VAL:HB   | 1.98                     | 0.45              |
| 2:E:2277:ALA:HB1  | 2:E:2337:PHE:HD2  | 1.81                     | 0.45              |
| 2:B:4158:PRO:HA   | 2:B:4161:ARG:HB2  | 1.97                     | 0.45              |
| 2:I:790:ARG:HG2   | 2:I:1627:ALA:HA   | 1.98                     | 0.45              |
| 2:I:794:GLY:H     | 2:I:798:GLY:HA3   | 1.82                     | 0.45              |
| 2:G:468:LEU:HB3   | 2:G:472:ARG:HH12  | 1.80                     | 0.45              |
| 2:G:2277:ALA:HB1  | 2:G:2337:PHE:HD2  | 1.81                     | 0.45              |
| 2:B:2517:UNK:O    | 2:B:2521:UNK:N    | 2.49                     | 0.45              |
| 2:I:582:HIS:O     | 2:I:585:SER:OG    | 2.29                     | 0.45              |
| 2:I:2751:LEU:HD11 | 2:I:2823:ILE:HG21 | 1.97                     | 0.45              |
| 2:G:2104:ARG:HA   | 2:G:2107:GLN:HB3  | 1.98                     | 0.45              |
| 2:E:823:LEU:HD23  | 2:E:1626:TRP:HB3  | 1.98                     | 0.45              |
| 2:E:1078:GLU:HB3  | 2:E:1081:TYR:HD2  | 1.82                     | 0.45              |
| 1:A:21:THR:HA     | 1:A:49:ARG:HA     | 1.98                     | 0.45              |
| 2:B:823:LEU:HD23  | 2:B:1626:TRP:HB3  | 1.98                     | 0.45              |
| 2:B:2375:GLY:HA3  | 2:B:2378:ALA:HB3  | 1.98                     | 0.45              |
| 2:I:1148:VAL:HB   | 2:I:1165:ASN:HA   | 1.98                     | 0.45              |
| 2:I:1718:ILE:HG13 | 2:I:1719:HIS:CD2  | 2.52                     | 0.45              |
| 2:I:2277:ALA:HB1  | 2:I:2337:PHE:HD2  | 1.81                     | 0.45              |
| 2:I:4059:LEU:HD13 | 2:I:4166:LEU:HB3  | 1.99                     | 0.45              |
| 2:G:485:SER:HA    | 2:G:488:LEU:HB2   | 1.99                     | 0.45              |
| 2:G:794:GLY:H     | 2:G:798:GLY:HA3   | 1.82                     | 0.45              |
| 2:G:2517:UNK:O    | 2:G:2521:UNK:N    | 2.49                     | 0.45              |
| 2:E:894:GLY:HA3   | 2:E:903:LEU:HD22  | 1.97                     | 0.45              |
| 2:E:1148:VAL:HB   | 2:E:1165:ASN:HA   | 1.98                     | 0.45              |
| 2:E:2517:UNK:O    | 2:E:2521:UNK:N    | 2.49                     | 0.45              |
| 2:B:266:ARG:NH2   | 2:B:269:TRP:O     | 2.50                     | 0.45              |
| 2:B:396:GLU:OE2   | 2:B:451:TYR:OH    | 2.32                     | 0.45              |
| 2:B:1660:GLN:O    | 2:B:1664:SER:N    | 2.47                     | 0.45              |
| 2:B:1796:ALA:HB1  | 2:B:1797:ARG:HH21 | 1.81                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2874:MET:O    | 2:B:2878:LEU:N    | 2.42                     | 0.45              |
| 2:I:2375:GLY:HA3  | 2:I:2378:ALA:HB3  | 1.98                     | 0.45              |
| 2:I:3994:HIS:O    | 2:I:3998:HIS:ND1  | 2.46                     | 0.45              |
| 2:G:266:ARG:NH2   | 2:G:269:TRP:O     | 2.50                     | 0.45              |
| 2:G:4059:LEU:HD13 | 2:G:4166:LEU:HB3  | 1.99                     | 0.45              |
| 2:B:887:ILE:HG21  | 2:B:959:TYR:HA    | 1.97                     | 0.45              |
| 2:B:4957:LYS:HG3  | 2:B:4964:GLY:HA3  | 1.96                     | 0.45              |
| 2:I:637:LEU:HD23  | 2:I:1637:MET:HB3  | 1.99                     | 0.45              |
| 2:I:4158:PRO:HA   | 2:I:4161:ARG:HB2  | 1.97                     | 0.45              |
| 2:I:4957:LYS:HG3  | 2:I:4964:GLY:HA3  | 1.96                     | 0.45              |
| 2:E:866:HIS:O     | 2:E:1051:TYR:OH   | 2.34                     | 0.45              |
| 2:E:4059:LEU:HD13 | 2:E:4166:LEU:HB3  | 1.99                     | 0.45              |
| 2:B:286:THR:HA    | 2:B:405:HIS:HB2   | 1.98                     | 0.45              |
| 2:B:794:GLY:H     | 2:B:798:GLY:HA3   | 1.82                     | 0.45              |
| 2:B:2587:UNK:O    | 2:B:2591:UNK:N    | 2.50                     | 0.45              |
| 2:B:2742:THR:OG1  | 2:B:2811:GLU:OE1  | 2.32                     | 0.45              |
| 2:B:4059:LEU:HD13 | 2:B:4166:LEU:HB3  | 1.99                     | 0.45              |
| 2:I:221:ARG:NH2   | 2:I:397:GLU:OE2   | 2.45                     | 0.45              |
| 2:I:495:ASN:HD21  | 2:I:550:LYS:HE3   | 1.82                     | 0.45              |
| 2:G:3658:LYS:HA   | 2:G:3661:TRP:CE2  | 2.52                     | 0.45              |
| 2:E:485:SER:HA    | 2:E:488:LEU:HB2   | 1.99                     | 0.45              |
| 2:E:892:THR:N     | 2:E:902:ARG:O     | 2.48                     | 0.45              |
| 2:B:1718:ILE:HG13 | 2:B:1719:HIS:CD2  | 2.52                     | 0.45              |
| 2:B:3658:LYS:HA   | 2:B:3661:TRP:CE2  | 2.52                     | 0.45              |
| 2:B:3829:PHE:HA   | 2:B:3832:ILE:HD12 | 1.99                     | 0.45              |
| 2:B:4081:VAL:HB   | 2:B:4088:ILE:HD12 | 1.98                     | 0.45              |
| 2:B:4697:VAL:O    | 2:B:4701:TRP:N    | 2.47                     | 0.45              |
| 2:I:1802:ILE:HG21 | 2:I:1807:LEU:HD22 | 1.99                     | 0.45              |
| 2:G:495:ASN:HD21  | 2:G:550:LYS:HE3   | 1.82                     | 0.45              |
| 2:G:1802:ILE:HG21 | 2:G:1807:LEU:HD22 | 1.99                     | 0.45              |
| 2:G:1931:LEU:HB3  | 2:G:1935:VAL:HB   | 1.98                     | 0.45              |
| 2:G:4687:TYR:OH   | 2:G:4699:GLY:O    | 2.34                     | 0.45              |
| 2:G:4924:VAL:HG12 | 2:G:4928:LEU:HD12 | 1.98                     | 0.45              |
| 2:E:637:LEU:HD23  | 2:E:1637:MET:HB3  | 1.99                     | 0.45              |
| 2:E:4960:ILE:HG22 | 2:E:4960:ILE:O    | 2.16                     | 0.45              |
| 1:F:87:HIS:HD2    | 1:F:90:VAL:HB     | 1.82                     | 0.45              |
| 1:F:92:PRO:HD3    | 2:E:627:PRO:HB2   | 1.98                     | 0.45              |
| 1:A:87:HIS:HD2    | 1:A:90:VAL:HB     | 1.82                     | 0.45              |
| 2:B:1025:ARG:O    | 2:B:1032:LYS:NZ   | 2.39                     | 0.45              |
| 2:I:286:THR:HA    | 2:I:405:HIS:HB2   | 1.98                     | 0.45              |
| 2:I:3658:LYS:HA   | 2:I:3661:TRP:CE2  | 2.52                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:637:LEU:HD23  | 2:G:1637:MET:HB3  | 1.99                     | 0.45              |
| 2:G:1095:VAL:HB   | 2:G:1199:VAL:HG23 | 1.99                     | 0.45              |
| 2:E:2235:PHE:HA   | 2:E:2238:TYR:HD2  | 1.82                     | 0.45              |
| 2:I:43:GLY:N      | 2:I:447:ASP:OD2   | 2.43                     | 0.45              |
| 2:I:4924:VAL:HG12 | 2:I:4928:LEU:HD12 | 1.98                     | 0.45              |
| 2:G:652:ARG:HB2   | 2:G:750:LEU:HD13  | 1.99                     | 0.45              |
| 2:G:790:ARG:HG2   | 2:G:1627:ALA:HA   | 1.98                     | 0.45              |
| 2:G:1078:GLU:HB3  | 2:G:1081:TYR:HD2  | 1.82                     | 0.45              |
| 2:G:1718:ILE:HG13 | 2:G:1719:HIS:CD2  | 2.52                     | 0.45              |
| 2:G:2235:PHE:HA   | 2:G:2238:TYR:HD2  | 1.82                     | 0.45              |
| 2:G:2375:GLY:HA3  | 2:G:2378:ALA:HB3  | 1.98                     | 0.45              |
| 2:G:4558:ASN:HB2  | 2:G:4561:THR:HB   | 1.97                     | 0.45              |
| 2:E:794:GLY:H     | 2:E:798:GLY:HA3   | 1.82                     | 0.45              |
| 2:E:2004:GLU:HA   | 2:E:2007:ASN:HD22 | 1.82                     | 0.45              |
| 2:E:2874:MET:O    | 2:E:2878:LEU:N    | 2.42                     | 0.45              |
| 1:H:87:HIS:HD2    | 1:H:90:VAL:HB     | 1.82                     | 0.44              |
| 2:B:637:LEU:HD23  | 2:B:1637:MET:HB3  | 1.99                     | 0.44              |
| 2:B:2104:ARG:HA   | 2:B:2107:GLN:HB3  | 1.98                     | 0.44              |
| 2:I:1457:UNK:N    | 2:I:1497:UNK:O    | 2.50                     | 0.44              |
| 2:G:1148:VAL:HB   | 2:G:1165:ASN:HA   | 1.98                     | 0.44              |
| 2:G:2034:PHE:O    | 2:G:2038:LEU:N    | 2.50                     | 0.44              |
| 2:G:4798:MET:HG3  | 2:G:4811:ALA:HB3  | 1.99                     | 0.44              |
| 2:G:4848:VAL:O    | 2:G:4852:THR:N    | 2.50                     | 0.44              |
| 2:E:2042:CYS:SG   | 2:E:2043:GLY:N    | 2.82                     | 0.44              |
| 2:E:2104:ARG:HA   | 2:E:2107:GLN:HB3  | 1.98                     | 0.44              |
| 2:B:495:ASN:HD21  | 2:B:550:LYS:HE3   | 1.82                     | 0.44              |
| 2:B:1105:ALA:O    | 2:B:1189:LEU:N    | 2.51                     | 0.44              |
| 2:B:2862:LEU:HB3  | 2:B:2928:LYS:HB3  | 1.99                     | 0.44              |
| 2:B:4848:VAL:O    | 2:B:4852:THR:N    | 2.50                     | 0.44              |
| 2:B:4959:PHE:CG   | 2:B:4959:PHE:O    | 2.70                     | 0.44              |
| 2:B:4960:ILE:HG22 | 2:B:4960:ILE:O    | 2.16                     | 0.44              |
| 2:I:695:TYR:OH    | 2:I:1073:ARG:NH1  | 2.48                     | 0.44              |
| 2:I:1095:VAL:HB   | 2:I:1199:VAL:HG23 | 1.99                     | 0.44              |
| 2:I:2265:LEU:O    | 2:I:2330:ARG:NH1  | 2.51                     | 0.44              |
| 2:I:2587:UNK:O    | 2:I:2591:UNK:N    | 2.50                     | 0.44              |
| 2:E:2034:PHE:O    | 2:E:2038:LEU:N    | 2.50                     | 0.44              |
| 2:B:2235:PHE:HA   | 2:B:2238:TYR:HD2  | 1.82                     | 0.44              |
| 2:I:485:SER:HA    | 2:I:488:LEU:HB2   | 1.99                     | 0.44              |
| 2:I:1796:ALA:HB1  | 2:I:1797:ARG:HH21 | 1.81                     | 0.44              |
| 2:I:4798:MET:HG3  | 2:I:4811:ALA:HB3  | 2.00                     | 0.44              |
| 2:G:1105:ALA:N    | 2:G:1189:LEU:O    | 2.50                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:4959:PHE:O    | 2:G:4959:PHE:CD2  | 2.70                     | 0.44              |
| 2:E:54:ASN:O      | 2:E:58:VAL:N      | 2.47                     | 0.44              |
| 2:E:206:CYS:SG    | 2:E:207:SER:N     | 2.90                     | 0.44              |
| 2:E:2587:UNK:O    | 2:E:2591:UNK:N    | 2.50                     | 0.44              |
| 2:E:2862:LEU:HB3  | 2:E:2928:LYS:HB3  | 1.99                     | 0.44              |
| 2:B:290:TYR:O     | 2:B:302:VAL:N     | 2.51                     | 0.44              |
| 2:B:1457:UNK:N    | 2:B:1497:UNK:O    | 2.50                     | 0.44              |
| 2:B:2034:PHE:O    | 2:B:2038:LEU:N    | 2.50                     | 0.44              |
| 2:B:2265:LEU:O    | 2:B:2330:ARG:NH1  | 2.51                     | 0.44              |
| 2:I:4081:VAL:HB   | 2:I:4088:ILE:HD12 | 1.98                     | 0.44              |
| 2:I:4959:PHE:CD2  | 2:I:4959:PHE:O    | 2.70                     | 0.44              |
| 2:G:2265:LEU:O    | 2:G:2330:ARG:NH1  | 2.51                     | 0.44              |
| 2:G:2862:LEU:HB3  | 2:G:2928:LYS:HB3  | 1.99                     | 0.44              |
| 2:E:266:ARG:NH2   | 2:E:269:TRP:O     | 2.49                     | 0.44              |
| 2:E:495:ASN:HD21  | 2:E:550:LYS:HE3   | 1.82                     | 0.44              |
| 2:E:652:ARG:HB2   | 2:E:750:LEU:HD13  | 1.99                     | 0.44              |
| 2:E:790:ARG:HG2   | 2:E:1627:ALA:HA   | 1.98                     | 0.44              |
| 2:E:4848:VAL:O    | 2:E:4852:THR:N    | 2.50                     | 0.44              |
| 2:B:215:THR:HG22  | 2:B:273:HIS:HA    | 2.00                     | 0.44              |
| 2:I:206:CYS:SG    | 2:I:207:SER:N     | 2.90                     | 0.44              |
| 2:I:652:ARG:HB2   | 2:I:750:LEU:HD13  | 1.99                     | 0.44              |
| 2:I:2235:PHE:HA   | 2:I:2238:TYR:HD2  | 1.82                     | 0.44              |
| 2:G:2004:GLU:HA   | 2:G:2007:ASN:HD22 | 1.82                     | 0.44              |
| 2:E:290:TYR:O     | 2:E:302:VAL:N     | 2.51                     | 0.44              |
| 2:E:551:LEU:HD11  | 2:E:589:LEU:HD13  | 2.00                     | 0.44              |
| 1:J:87:HIS:HD2    | 1:J:90:VAL:HB     | 1.82                     | 0.44              |
| 2:B:652:ARG:HB2   | 2:B:750:LEU:HD13  | 1.99                     | 0.44              |
| 2:B:1148:VAL:HB   | 2:B:1165:ASN:HA   | 1.98                     | 0.44              |
| 2:B:2022:PRO:HB2  | 2:B:2024:PRO:HD2  | 1.99                     | 0.44              |
| 2:B:2226:PRO:HA   | 2:B:2229:VAL:HG12 | 2.00                     | 0.44              |
| 2:I:266:ARG:NH2   | 2:I:269:TRP:O     | 2.50                     | 0.44              |
| 2:G:206:CYS:SG    | 2:G:207:SER:N     | 2.90                     | 0.44              |
| 2:G:914:PRO:O     | 2:G:918:ARG:N     | 2.48                     | 0.44              |
| 2:G:2742:THR:OG1  | 2:G:2811:GLU:OE1  | 2.32                     | 0.44              |
| 2:E:488:LEU:O     | 2:E:492:ASP:N     | 2.45                     | 0.44              |
| 2:E:924:MET:O     | 2:E:928:THR:OG1   | 2.32                     | 0.44              |
| 2:E:1718:ILE:HG13 | 2:E:1719:HIS:CD2  | 2.51                     | 0.44              |
| 2:E:3658:LYS:HA   | 2:E:3661:TRP:CE2  | 2.52                     | 0.44              |
| 2:E:4081:VAL:HB   | 2:E:4088:ILE:HD12 | 1.98                     | 0.44              |
| 2:E:4798:MET:HG3  | 2:E:4811:ALA:HB3  | 1.99                     | 0.44              |
| 2:E:4959:PHE:O    | 2:E:4959:PHE:CD2  | 2.70                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:4959:PHE:O    | 2:E:4959:PHE:CG   | 2.70                     | 0.44              |
| 2:B:790:ARG:HG2   | 2:B:1627:ALA:HA   | 1.98                     | 0.44              |
| 2:I:681:HIS:O     | 2:I:784:SER:N     | 2.45                     | 0.44              |
| 2:I:1078:GLU:HB3  | 2:I:1081:TYR:HD2  | 1.81                     | 0.44              |
| 2:I:2004:GLU:HA   | 2:I:2007:ASN:HD22 | 1.82                     | 0.44              |
| 2:I:4848:VAL:O    | 2:I:4852:THR:N    | 2.51                     | 0.44              |
| 2:G:4959:PHE:O    | 2:G:4959:PHE:CG   | 2.70                     | 0.44              |
| 2:E:2226:PRO:HA   | 2:E:2229:VAL:HG12 | 2.00                     | 0.44              |
| 2:B:485:SER:HA    | 2:B:488:LEU:HB2   | 1.99                     | 0.44              |
| 2:B:582:HIS:O     | 2:B:585:SER:OG    | 2.29                     | 0.44              |
| 2:B:1103:GLY:HA3  | 2:B:1123:VAL:HA   | 2.00                     | 0.44              |
| 2:B:2277:ALA:HB1  | 2:B:2337:PHE:HD2  | 1.81                     | 0.44              |
| 2:B:4959:PHE:O    | 2:B:4959:PHE:CD2  | 2.70                     | 0.44              |
| 2:I:485:SER:O     | 2:I:489:ASN:N     | 2.40                     | 0.44              |
| 2:I:1103:GLY:HA3  | 2:I:1123:VAL:HA   | 2.00                     | 0.44              |
| 2:I:2034:PHE:O    | 2:I:2038:LEU:N    | 2.50                     | 0.44              |
| 2:G:43:GLY:N      | 2:G:447:ASP:OD2   | 2.43                     | 0.44              |
| 2:G:695:TYR:OH    | 2:G:1073:ARG:NH1  | 2.48                     | 0.44              |
| 2:G:1973:GLN:HA   | 2:G:1976:ARG:HB3  | 2.00                     | 0.44              |
| 2:E:1095:VAL:HB   | 2:E:1199:VAL:HG23 | 1.99                     | 0.44              |
| 2:B:924:MET:O     | 2:B:928:THR:OG1   | 2.32                     | 0.44              |
| 2:B:1802:ILE:HG21 | 2:B:1807:LEU:HD22 | 1.99                     | 0.44              |
| 2:I:583:ILE:HA    | 2:I:586:ILE:HD12  | 2.00                     | 0.44              |
| 2:I:1841:VAL:HG13 | 2:I:1844:LEU:HD23 | 2.00                     | 0.44              |
| 2:I:4743:MET:HB3  | 2:I:4746:ALA:HB3  | 2.00                     | 0.44              |
| 2:I:4959:PHE:O    | 2:I:4959:PHE:CG   | 2.70                     | 0.44              |
| 2:G:2353:VAL:O    | 2:G:2357:LEU:N    | 2.51                     | 0.44              |
| 2:G:2587:UNK:O    | 2:G:2591:UNK:N    | 2.50                     | 0.44              |
| 2:G:3829:PHE:HA   | 2:G:3832:ILE:HD12 | 1.99                     | 0.44              |
| 2:E:1841:VAL:HG13 | 2:E:1844:LEU:HD23 | 2.00                     | 0.44              |
| 2:E:3829:PHE:HA   | 2:E:3832:ILE:HD12 | 1.99                     | 0.44              |
| 2:B:4673:ARG:HH12 | 2:B:4698:LYS:HE3  | 1.83                     | 0.43              |
| 2:I:914:PRO:O     | 2:I:918:ARG:N     | 2.48                     | 0.43              |
| 2:I:2226:PRO:HA   | 2:I:2229:VAL:HG12 | 2.00                     | 0.43              |
| 2:I:3829:PHE:HA   | 2:I:3832:ILE:HD12 | 1.99                     | 0.43              |
| 2:G:215:THR:HG22  | 2:G:273:HIS:HA    | 2.00                     | 0.43              |
| 2:G:583:ILE:HA    | 2:G:586:ILE:HD12  | 2.00                     | 0.43              |
| 2:G:892:THR:N     | 2:G:902:ARG:O     | 2.48                     | 0.43              |
| 2:E:1105:ALA:O    | 2:E:1189:LEU:N    | 2.51                     | 0.43              |
| 2:E:1105:ALA:N    | 2:E:1189:LEU:O    | 2.50                     | 0.43              |
| 2:E:1457:UNK:N    | 2:E:1497:UNK:O    | 2.50                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:206:CYS:SG    | 2:B:207:SER:N     | 2.90                     | 0.43              |
| 2:B:1841:VAL:HG13 | 2:B:1844:LEU:HD23 | 2.00                     | 0.43              |
| 2:I:551:LEU:HD11  | 2:I:589:LEU:HD13  | 2.00                     | 0.43              |
| 2:I:1663:HIS:NE2  | 2:I:1711:TYR:OH   | 2.42                     | 0.43              |
| 2:I:2022:PRO:HB2  | 2:I:2024:PRO:HD2  | 1.99                     | 0.43              |
| 2:G:488:LEU:O     | 2:G:492:ASP:N     | 2.45                     | 0.43              |
| 2:G:551:LEU:HD11  | 2:G:589:LEU:HD13  | 2.00                     | 0.43              |
| 2:G:2226:PRO:HA   | 2:G:2229:VAL:HG12 | 2.00                     | 0.43              |
| 2:G:2271:THR:HG22 | 2:G:2273:LEU:H    | 1.83                     | 0.43              |
| 2:E:575:LEU:HD22  | 2:E:609:CYS:HB3   | 2.00                     | 0.43              |
| 2:E:1802:ILE:HG21 | 2:E:1807:LEU:HD22 | 1.99                     | 0.43              |
| 2:E:4697:VAL:O    | 2:E:4701:TRP:N    | 2.47                     | 0.43              |
| 2:B:2004:GLU:HA   | 2:B:2007:ASN:HD22 | 1.82                     | 0.43              |
| 2:B:4798:MET:HG3  | 2:B:4811:ALA:HB3  | 1.99                     | 0.43              |
| 2:G:1103:GLY:HA3  | 2:G:1123:VAL:HA   | 2.00                     | 0.43              |
| 2:G:1154:ASP:O    | 2:G:1158:ASN:N    | 2.52                     | 0.43              |
| 2:G:3805:LEU:H    | 2:G:3805:LEU:HG   | 1.74                     | 0.43              |
| 2:E:880:GLU:OE1   | 2:E:968:ALA:N     | 2.48                     | 0.43              |
| 2:E:1973:GLN:HA   | 2:E:1976:ARG:HB3  | 2.00                     | 0.43              |
| 2:E:4743:MET:HB3  | 2:E:4746:ALA:HB3  | 2.00                     | 0.43              |
| 1:H:87:HIS:HA     | 1:H:88:PRO:HD3    | 1.88                     | 0.43              |
| 2:B:583:ILE:HA    | 2:B:586:ILE:HD12  | 2.00                     | 0.43              |
| 2:B:1973:GLN:HA   | 2:B:1976:ARG:HB3  | 2.00                     | 0.43              |
| 2:I:2271:THR:HG22 | 2:I:2273:LEU:H    | 1.83                     | 0.43              |
| 2:G:1457:UNK:N    | 2:G:1497:UNK:O    | 2.50                     | 0.43              |
| 2:E:2022:PRO:HB2  | 2:E:2024:PRO:HD2  | 1.99                     | 0.43              |
| 2:E:4182:GLU:OE2  | 2:E:4983:HIS:CD2  | 2.57                     | 0.43              |
| 2:B:551:LEU:HD11  | 2:B:589:LEU:HD13  | 2.00                     | 0.43              |
| 2:I:290:TYR:O     | 2:I:302:VAL:N     | 2.51                     | 0.43              |
| 2:I:2862:LEU:HB3  | 2:I:2928:LYS:HB3  | 1.99                     | 0.43              |
| 2:I:4230:LYS:HD2  | 2:I:4959:PHE:CE2  | 2.48                     | 0.43              |
| 2:G:485:SER:O     | 2:G:489:ASN:N     | 2.40                     | 0.43              |
| 2:G:575:LEU:HD22  | 2:G:609:CYS:HB3   | 2.00                     | 0.43              |
| 2:G:2022:PRO:HB2  | 2:G:2024:PRO:HD2  | 1.99                     | 0.43              |
| 2:E:215:THR:HG22  | 2:E:273:HIS:HA    | 2.00                     | 0.43              |
| 2:B:2353:VAL:O    | 2:B:2357:LEU:N    | 2.51                     | 0.43              |
| 2:B:3552:UNK:O    | 2:B:3556:UNK:N    | 2.52                     | 0.43              |
| 2:I:2272:PRO:HA   | 2:I:2275:VAL:HG12 | 2.01                     | 0.43              |
| 2:G:683:ARG:HG2   | 2:G:717:ASP:HB3   | 2.01                     | 0.43              |
| 2:G:880:GLU:OE1   | 2:G:968:ALA:N     | 2.48                     | 0.43              |
| 2:G:1698:LEU:N    | 2:G:1712:TYR:OH   | 2.52                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:4984:ASN:ND2  | 2:G:4986:ALA:HB3  | 2.33                     | 0.43              |
| 2:E:1154:ASP:O    | 2:E:1158:ASN:N    | 2.52                     | 0.43              |
| 2:E:1698:LEU:N    | 2:E:1712:TYR:OH   | 2.52                     | 0.43              |
| 2:E:2265:LEU:O    | 2:E:2330:ARG:NH1  | 2.51                     | 0.43              |
| 2:E:4984:ASN:ND2  | 2:E:4986:ALA:HB3  | 2.33                     | 0.43              |
| 1:F:87:HIS:HA     | 1:F:88:PRO:HD3    | 1.89                     | 0.43              |
| 2:B:575:LEU:HD22  | 2:B:609:CYS:HB3   | 2.00                     | 0.43              |
| 2:B:3994:HIS:O    | 2:B:3998:HIS:ND1  | 2.46                     | 0.43              |
| 2:I:215:THR:HG22  | 2:I:273:HIS:HA    | 2.00                     | 0.43              |
| 2:I:929:LEU:HD23  | 2:I:932:LEU:HD12  | 2.01                     | 0.43              |
| 2:I:1269:CYS:HA   | 2:I:1473:UNK:HA   | 2.01                     | 0.43              |
| 2:I:2742:THR:OG1  | 2:I:2811:GLU:OE1  | 2.32                     | 0.43              |
| 2:I:4982:GLU:HB3  | 2:I:4983:HIS:H    | 1.71                     | 0.43              |
| 2:I:4984:ASN:ND2  | 2:I:4986:ALA:HB3  | 2.33                     | 0.43              |
| 2:G:1105:ALA:O    | 2:G:1189:LEU:N    | 2.51                     | 0.43              |
| 2:E:583:ILE:HA    | 2:E:586:ILE:HD12  | 2.00                     | 0.43              |
| 2:E:2271:THR:HG22 | 2:E:2273:LEU:H    | 1.83                     | 0.43              |
| 2:E:2353:VAL:O    | 2:E:2357:LEU:N    | 2.51                     | 0.43              |
| 2:B:683:ARG:HG2   | 2:B:717:ASP:HB3   | 2.01                     | 0.43              |
| 2:B:892:THR:N     | 2:B:902:ARG:O     | 2.48                     | 0.43              |
| 2:I:1154:ASP:O    | 2:I:1158:ASN:N    | 2.52                     | 0.43              |
| 2:I:3552:UNK:O    | 2:I:3556:UNK:N    | 2.52                     | 0.43              |
| 2:G:290:TYR:O     | 2:G:302:VAL:N     | 2.51                     | 0.43              |
| 2:G:1841:VAL:HG13 | 2:G:1844:LEU:HD23 | 2.00                     | 0.43              |
| 2:G:4673:ARG:HH12 | 2:G:4698:LYS:HE3  | 1.84                     | 0.43              |
| 2:E:929:LEU:HD23  | 2:E:932:LEU:HD12  | 2.01                     | 0.43              |
| 2:E:3781:GLN:HA   | 2:E:3784:SER:HB3  | 2.01                     | 0.43              |
| 1:H:11:ASP:OD1    | 1:H:67:SER:OG     | 2.34                     | 0.43              |
| 2:B:1095:VAL:HB   | 2:B:1199:VAL:HG23 | 1.99                     | 0.43              |
| 2:B:4743:MET:HB3  | 2:B:4746:ALA:HB3  | 2.00                     | 0.43              |
| 2:B:4984:ASN:ND2  | 2:B:4986:ALA:HB3  | 2.33                     | 0.43              |
| 2:I:4673:ARG:HH12 | 2:I:4698:LYS:HE3  | 1.83                     | 0.43              |
| 2:G:929:LEU:HD23  | 2:G:932:LEU:HD12  | 2.01                     | 0.43              |
| 2:B:463:GLU:O     | 2:B:466:SER:OG    | 2.35                     | 0.43              |
| 2:B:929:LEU:HD23  | 2:B:932:LEU:HD12  | 2.01                     | 0.43              |
| 2:B:1154:ASP:O    | 2:B:1158:ASN:N    | 2.52                     | 0.43              |
| 2:B:2271:THR:HG22 | 2:B:2273:LEU:H    | 1.83                     | 0.43              |
| 2:B:4962:GLY:H    | 2:B:5025:GLY:HA2  | 1.84                     | 0.43              |
| 2:I:683:ARG:HG2   | 2:I:717:ASP:HB3   | 2.01                     | 0.43              |
| 2:I:1698:LEU:N    | 2:I:1712:TYR:OH   | 2.52                     | 0.43              |
| 2:G:463:GLU:O     | 2:G:466:SER:OG    | 2.35                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1269:CYS:HA   | 2:E:1473:UNK:HA   | 2.01                     | 0.43              |
| 2:E:4673:ARG:HH12 | 2:E:4698:LYS:HE3  | 1.83                     | 0.43              |
| 2:B:695:TYR:OH    | 2:B:1073:ARG:NH1  | 2.48                     | 0.42              |
| 2:B:1731:LEU:HA   | 2:B:1772:ARG:HH12 | 1.84                     | 0.42              |
| 2:I:2874:MET:O    | 2:I:2878:LEU:N    | 2.42                     | 0.42              |
| 2:G:4237:PHE:O    | 2:G:4241:THR:OG1  | 2.32                     | 0.42              |
| 2:E:2272:PRO:HA   | 2:E:2275:VAL:HG12 | 2.01                     | 0.42              |
| 2:E:3552:UNK:O    | 2:E:3556:UNK:N    | 2.52                     | 0.42              |
| 1:F:11:ASP:OD1    | 1:F:67:SER:OG     | 2.34                     | 0.42              |
| 2:B:1105:ALA:N    | 2:B:1189:LEU:O    | 2.50                     | 0.42              |
| 2:B:3781:GLN:HA   | 2:B:3784:SER:HB3  | 2.01                     | 0.42              |
| 2:I:4962:GLY:H    | 2:I:5025:GLY:HA2  | 1.84                     | 0.42              |
| 2:E:379:HIS:CD2   | 2:E:382:GLY:H     | 2.32                     | 0.42              |
| 2:E:1103:GLY:HA3  | 2:E:1123:VAL:HA   | 2.00                     | 0.42              |
| 2:E:1691:GLN:HE22 | 2:E:1802:ILE:HG12 | 1.85                     | 0.42              |
| 2:E:2742:THR:OG1  | 2:E:2811:GLU:OE1  | 2.32                     | 0.42              |
| 2:E:4962:GLY:H    | 2:E:5025:GLY:HA2  | 1.84                     | 0.42              |
| 2:B:54:ASN:O      | 2:B:58:VAL:N      | 2.47                     | 0.42              |
| 2:B:3703:LEU:HA   | 2:B:3706:SER:HB3  | 2.01                     | 0.42              |
| 2:I:1973:GLN:HA   | 2:I:1976:ARG:HB3  | 2.00                     | 0.42              |
| 2:E:683:ARG:HG2   | 2:E:717:ASP:HB3   | 2.01                     | 0.42              |
| 2:E:3817:LEU:HD13 | 2:E:3899:PHE:HD1  | 1.84                     | 0.42              |
| 2:E:3832:ILE:O    | 2:E:3836:MET:N    | 2.50                     | 0.42              |
| 2:E:4968:PHE:CE1  | 2:E:4978:HIS:ND1  | 2.76                     | 0.42              |
| 2:B:842:PRO:HD3   | 2:B:1073:ARG:HG3  | 2.02                     | 0.42              |
| 2:B:1286:UNK:HA   | 2:B:1461:UNK:HA   | 2.02                     | 0.42              |
| 2:I:2132:GLY:O    | 2:I:2136:ARG:N    | 2.51                     | 0.42              |
| 2:I:4227:GLU:HG3  | 2:I:4228:ALA:H    | 1.84                     | 0.42              |
| 2:G:3552:UNK:O    | 2:G:3556:UNK:N    | 2.52                     | 0.42              |
| 2:B:1698:LEU:N    | 2:B:1712:TYR:OH   | 2.52                     | 0.42              |
| 2:I:575:LEU:HD22  | 2:I:609:CYS:HB3   | 2.00                     | 0.42              |
| 2:I:2265:LEU:HD22 | 2:I:2330:ARG:HB3  | 2.01                     | 0.42              |
| 2:I:3703:LEU:HA   | 2:I:3706:SER:HB3  | 2.01                     | 0.42              |
| 2:G:4227:GLU:HG3  | 2:G:4228:ALA:H    | 1.84                     | 0.42              |
| 2:G:4743:MET:HB3  | 2:G:4746:ALA:HB3  | 2.00                     | 0.42              |
| 2:E:681:HIS:HB3   | 2:E:784:SER:HB3   | 2.02                     | 0.42              |
| 2:E:914:PRO:O     | 2:E:918:ARG:N     | 2.48                     | 0.42              |
| 2:E:3696:ASP:O    | 2:E:3700:GLN:N    | 2.46                     | 0.42              |
| 1:J:7:ILE:N       | 1:J:71:ARG:O      | 2.48                     | 0.42              |
| 2:B:1164:LEU:HB3  | 2:B:1169:LEU:HD21 | 2.02                     | 0.42              |
| 2:B:3817:LEU:HD13 | 2:B:3899:PHE:HD1  | 1.85                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:842:PRO:HD3   | 2:I:1073:ARG:HG3  | 2.02                     | 0.42              |
| 2:I:1164:LEU:HB3  | 2:I:1169:LEU:HD21 | 2.02                     | 0.42              |
| 2:I:2810:LYS:O    | 2:I:2814:LYS:N    | 2.43                     | 0.42              |
| 2:I:4712:PRO:HB2  | 2:I:4718:LYS:HA   | 2.01                     | 0.42              |
| 2:G:1808:ARG:HD2  | 2:G:1854:PHE:HA   | 2.02                     | 0.42              |
| 2:E:1164:LEU:HB3  | 2:E:1169:LEU:HD21 | 2.02                     | 0.42              |
| 2:E:1808:ARG:HD2  | 2:E:1854:PHE:HA   | 2.02                     | 0.42              |
| 2:E:4712:PRO:HB2  | 2:E:4718:LYS:HA   | 2.01                     | 0.42              |
| 1:J:87:HIS:HA     | 1:J:88:PRO:HD3    | 1.88                     | 0.42              |
| 2:B:1189:LEU:HD12 | 2:B:1190:PRO:HD2  | 2.02                     | 0.42              |
| 2:B:2265:LEU:HD22 | 2:B:2330:ARG:HB3  | 2.01                     | 0.42              |
| 2:B:4687:TYR:OH   | 2:B:4699:GLY:O    | 2.34                     | 0.42              |
| 2:I:681:HIS:HB3   | 2:I:784:SER:HB3   | 2.02                     | 0.42              |
| 2:I:1668:ARG:HA   | 2:I:1671:ARG:HH11 | 1.85                     | 0.42              |
| 2:G:1164:LEU:HB3  | 2:G:1169:LEU:HD21 | 2.02                     | 0.42              |
| 2:G:1269:CYS:HA   | 2:G:1473:UNK:HA   | 2.01                     | 0.42              |
| 2:G:3832:ILE:O    | 2:G:3836:MET:N    | 2.50                     | 0.42              |
| 2:G:4962:GLY:H    | 2:G:5025:GLY:HA2  | 1.84                     | 0.42              |
| 2:G:4982:GLU:HB3  | 2:G:4983:HIS:H    | 1.71                     | 0.42              |
| 2:E:1668:ARG:HA   | 2:E:1671:ARG:HH11 | 1.85                     | 0.42              |
| 2:E:3361:UNK:O    | 2:E:3365:UNK:N    | 2.53                     | 0.42              |
| 2:B:488:LEU:O     | 2:B:492:ASP:N     | 2.45                     | 0.42              |
| 2:B:1668:ARG:HA   | 2:B:1671:ARG:HH11 | 1.85                     | 0.42              |
| 2:B:4227:GLU:HG3  | 2:B:4228:ALA:H    | 1.84                     | 0.42              |
| 2:B:4763:GLY:O    | 2:B:4766:THR:OG1  | 2.29                     | 0.42              |
| 2:B:4892:ARG:HD3  | 2:I:4918:ILE:HD13 | 2.02                     | 0.42              |
| 2:I:1189:LEU:HD12 | 2:I:1190:PRO:HD2  | 2.02                     | 0.42              |
| 2:G:582:HIS:O     | 2:G:585:SER:OG    | 2.29                     | 0.42              |
| 2:G:1286:UNK:HA   | 2:G:1461:UNK:HA   | 2.02                     | 0.42              |
| 2:G:1668:ARG:HA   | 2:G:1671:ARG:HH11 | 1.85                     | 0.42              |
| 2:E:1728:ARG:HA   | 2:E:1731:LEU:HB2  | 2.01                     | 0.42              |
| 2:B:2132:GLY:O    | 2:B:2136:ARG:N    | 2.51                     | 0.42              |
| 2:B:3696:ASP:O    | 2:B:3700:GLN:N    | 2.46                     | 0.42              |
| 2:I:892:THR:N     | 2:I:902:ARG:O     | 2.48                     | 0.42              |
| 2:I:1731:LEU:HA   | 2:I:1772:ARG:HH12 | 1.84                     | 0.42              |
| 2:G:681:HIS:HB3   | 2:G:784:SER:HB3   | 2.02                     | 0.42              |
| 2:G:3361:UNK:O    | 2:G:3365:UNK:N    | 2.53                     | 0.42              |
| 2:G:3781:GLN:HA   | 2:G:3784:SER:HB3  | 2.01                     | 0.42              |
| 2:E:2265:LEU:HD22 | 2:E:2330:ARG:HB3  | 2.01                     | 0.42              |
| 2:E:3994:HIS:O    | 2:E:3998:HIS:ND1  | 2.46                     | 0.42              |
| 2:E:4687:TYR:OH   | 2:E:4699:GLY:O    | 2.34                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:876:GLU:O     | 2:B:880:GLU:N     | 2.51                     | 0.42              |
| 2:B:2272:PRO:HA   | 2:B:2275:VAL:HG12 | 2.01                     | 0.42              |
| 2:G:1691:GLN:HE22 | 2:G:1802:ILE:HG12 | 1.84                     | 0.42              |
| 2:G:1697:ALA:HB1  | 2:G:1708:ARG:HB3  | 2.02                     | 0.42              |
| 2:G:1966:VAL:HA   | 2:G:1969:LEU:HB3  | 2.02                     | 0.42              |
| 2:G:2121:PHE:O    | 2:G:3725:TYR:OH   | 2.33                     | 0.42              |
| 2:G:3817:LEU:HD13 | 2:G:3899:PHE:HD1  | 1.84                     | 0.42              |
| 2:E:1966:VAL:HA   | 2:E:1969:LEU:HB3  | 2.02                     | 0.42              |
| 2:E:3703:LEU:HA   | 2:E:3706:SER:HB3  | 2.01                     | 0.42              |
| 1:H:7:ILE:N       | 1:H:71:ARG:O      | 2.48                     | 0.41              |
| 2:B:1697:ALA:HB1  | 2:B:1708:ARG:HB3  | 2.02                     | 0.41              |
| 2:B:1966:VAL:HA   | 2:B:1969:LEU:HB3  | 2.02                     | 0.41              |
| 2:B:3832:ILE:O    | 2:B:3836:MET:N    | 2.50                     | 0.41              |
| 2:I:599:VAL:HG23  | 2:I:600:LEU:HD12  | 2.02                     | 0.41              |
| 2:G:2265:LEU:HD22 | 2:G:2330:ARG:HB3  | 2.01                     | 0.41              |
| 2:G:3663:LEU:H    | 2:G:3663:LEU:HG   | 1.76                     | 0.41              |
| 2:E:463:GLU:O     | 2:E:466:SER:OG    | 2.35                     | 0.41              |
| 2:E:842:PRO:HD3   | 2:E:1073:ARG:HG3  | 2.02                     | 0.41              |
| 2:E:1731:LEU:HA   | 2:E:1772:ARG:HH12 | 1.84                     | 0.41              |
| 2:E:4227:GLU:HG3  | 2:E:4228:ALA:H    | 1.83                     | 0.41              |
| 1:A:92:PRO:HD3    | 2:B:627:PRO:HB2   | 2.01                     | 0.41              |
| 2:B:3361:UNK:O    | 2:B:3365:UNK:N    | 2.53                     | 0.41              |
| 2:B:4982:GLU:HB3  | 2:B:4983:HIS:H    | 1.71                     | 0.41              |
| 2:I:463:GLU:O     | 2:I:466:SER:OG    | 2.35                     | 0.41              |
| 2:I:3781:GLN:HA   | 2:I:3784:SER:HB3  | 2.01                     | 0.41              |
| 2:I:3817:LEU:HD13 | 2:I:3899:PHE:HD1  | 1.85                     | 0.41              |
| 2:G:866:HIS:O     | 2:G:1051:TYR:OH   | 2.34                     | 0.41              |
| 2:G:1728:ARG:HA   | 2:G:1731:LEU:HB2  | 2.01                     | 0.41              |
| 2:I:342:GLY:HA2   | 2:I:389:PHE:HB2   | 2.03                     | 0.41              |
| 2:I:940:GLY:O     | 2:I:1052:ASN:N    | 2.52                     | 0.41              |
| 2:I:1697:ALA:HB1  | 2:I:1708:ARG:HB3  | 2.02                     | 0.41              |
| 2:I:1728:ARG:HA   | 2:I:1731:LEU:HB2  | 2.01                     | 0.41              |
| 2:I:1966:VAL:HA   | 2:I:1969:LEU:HB3  | 2.02                     | 0.41              |
| 2:G:842:PRO:HD3   | 2:G:1073:ARG:HG3  | 2.02                     | 0.41              |
| 2:G:2272:PRO:HA   | 2:G:2275:VAL:HG12 | 2.01                     | 0.41              |
| 2:G:3703:LEU:HA   | 2:G:3706:SER:HB3  | 2.01                     | 0.41              |
| 2:E:1697:ALA:HB1  | 2:E:1708:ARG:HB3  | 2.02                     | 0.41              |
| 2:E:2196:ASN:OD1  | 2:E:2199:ARG:NH1  | 2.38                     | 0.41              |
| 2:E:4821:LYS:HE2  | 2:E:4821:LYS:HB3  | 1.96                     | 0.41              |
| 1:F:30:LEU:HD23   | 1:F:33:GLY:HA3    | 2.03                     | 0.41              |
| 2:B:1691:GLN:HE22 | 2:B:1802:ILE:HG12 | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1728:ARG:HA   | 2:B:1731:LEU:HB2  | 2.01                     | 0.41              |
| 2:B:3880:PHE:O    | 2:B:3884:LEU:N    | 2.54                     | 0.41              |
| 2:B:4712:PRO:HB2  | 2:B:4718:LYS:HA   | 2.01                     | 0.41              |
| 2:I:15:ARG:HG2    | 2:I:100:THR:HA    | 2.03                     | 0.41              |
| 2:I:1286:UNK:HA   | 2:I:1461:UNK:HA   | 2.02                     | 0.41              |
| 2:I:1808:ARG:HD2  | 2:I:1854:PHE:HA   | 2.02                     | 0.41              |
| 2:I:3361:UNK:O    | 2:I:3365:UNK:N    | 2.53                     | 0.41              |
| 2:I:4702:ASP:OD1  | 2:I:4778:TRP:NE1  | 2.48                     | 0.41              |
| 2:G:599:VAL:HG23  | 2:G:600:LEU:HD12  | 2.02                     | 0.41              |
| 2:G:2132:GLY:O    | 2:G:2136:ARG:N    | 2.51                     | 0.41              |
| 2:E:1189:LEU:HD12 | 2:E:1190:PRO:HD2  | 2.02                     | 0.41              |
| 1:H:30:LEU:HD23   | 1:H:33:GLY:HA3    | 2.03                     | 0.41              |
| 1:J:11:ASP:OD1    | 1:J:67:SER:OG     | 2.34                     | 0.41              |
| 2:B:914:PRO:O     | 2:B:918:ARG:N     | 2.48                     | 0.41              |
| 2:B:1808:ARG:HD2  | 2:B:1854:PHE:HA   | 2.02                     | 0.41              |
| 2:I:1691:GLN:HE22 | 2:I:1802:ILE:HG12 | 1.85                     | 0.41              |
| 2:I:2950:UNK:O    | 2:I:2954:UNK:N    | 2.54                     | 0.41              |
| 2:I:4163:PHE:HA   | 2:I:4166:LEU:HB2  | 2.02                     | 0.41              |
| 2:B:681:HIS:HB3   | 2:B:784:SER:HB3   | 2.02                     | 0.41              |
| 2:B:1269:CYS:HA   | 2:B:1473:UNK:HA   | 2.01                     | 0.41              |
| 2:I:379:HIS:CD2   | 2:I:382:GLY:H     | 2.32                     | 0.41              |
| 2:I:1256:GLU:HG2  | 2:I:1273:ALA:HB3  | 2.03                     | 0.41              |
| 2:G:1256:GLU:HG2  | 2:G:1273:ALA:HB3  | 2.03                     | 0.41              |
| 2:G:2810:LYS:O    | 2:G:2814:LYS:N    | 2.42                     | 0.41              |
| 2:G:3365:UNK:O    | 2:G:3369:UNK:N    | 2.54                     | 0.41              |
| 2:G:3994:HIS:O    | 2:G:3998:HIS:ND1  | 2.46                     | 0.41              |
| 2:E:4106:PRO:O    | 2:E:4110:PHE:N    | 2.53                     | 0.41              |
| 2:B:342:GLY:HA2   | 2:B:389:PHE:HB2   | 2.03                     | 0.41              |
| 2:B:599:VAL:HG23  | 2:B:600:LEU:HD12  | 2.02                     | 0.41              |
| 2:I:2353:VAL:O    | 2:I:2357:LEU:N    | 2.51                     | 0.41              |
| 2:I:3365:UNK:O    | 2:I:3369:UNK:N    | 2.54                     | 0.41              |
| 2:G:123:THR:OG1   | 2:G:134:ASP:OD1   | 2.39                     | 0.41              |
| 2:G:618:GLN:O     | 2:G:622:THR:OG1   | 2.35                     | 0.41              |
| 2:G:4763:GLY:O    | 2:G:4766:THR:OG1  | 2.29                     | 0.41              |
| 2:E:2950:UNK:O    | 2:E:2954:UNK:N    | 2.54                     | 0.41              |
| 2:E:3365:UNK:O    | 2:E:3369:UNK:N    | 2.54                     | 0.41              |
| 2:B:379:HIS:CD2   | 2:B:382:GLY:H     | 2.32                     | 0.41              |
| 2:B:1130:GLN:HG2  | 2:B:1138:PRO:HA   | 2.03                     | 0.41              |
| 2:G:1731:LEU:HA   | 2:G:1772:ARG:HH12 | 1.84                     | 0.41              |
| 2:G:3880:PHE:O    | 2:G:3884:LEU:N    | 2.54                     | 0.41              |
| 2:E:876:GLU:O     | 2:E:880:GLU:N     | 2.51                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:J:30:LEU:HD23   | 1:J:33:GLY:HA3    | 2.03                     | 0.41              |
| 2:B:15:ARG:HG2    | 2:B:100:THR:HA    | 2.03                     | 0.41              |
| 2:B:45:ARG:NH2    | 2:B:447:ASP:OD1   | 2.52                     | 0.41              |
| 2:B:102:LEU:HB3   | 2:B:160:GLY:HA2   | 2.03                     | 0.41              |
| 2:B:123:THR:OG1   | 2:B:134:ASP:OD1   | 2.39                     | 0.41              |
| 2:B:410:LEU:HD12  | 2:B:413:GLN:HE21  | 1.86                     | 0.41              |
| 2:B:911:HIS:O     | 2:B:918:ARG:NH2   | 2.52                     | 0.41              |
| 2:B:1256:GLU:HG2  | 2:B:1273:ALA:HB3  | 2.03                     | 0.41              |
| 2:B:1938:GLN:HA   | 2:B:1941:ASN:HD22 | 1.86                     | 0.41              |
| 2:B:4780:PHE:HA   | 2:B:4783:ILE:HD12 | 2.03                     | 0.41              |
| 2:I:734:GLY:O     | 2:I:736:HIS:ND1   | 2.54                     | 0.41              |
| 2:I:911:HIS:O     | 2:I:918:ARG:NH2   | 2.52                     | 0.41              |
| 2:I:4968:PHE:CE2  | 2:I:4978:HIS:ND1  | 2.89                     | 0.41              |
| 2:G:54:ASN:O      | 2:G:58:VAL:N      | 2.47                     | 0.41              |
| 2:G:102:LEU:HB3   | 2:G:160:GLY:HA2   | 2.03                     | 0.41              |
| 2:G:410:LEU:HD12  | 2:G:413:GLN:HE21  | 1.86                     | 0.41              |
| 2:G:1189:LEU:HD12 | 2:G:1190:PRO:HD2  | 2.02                     | 0.41              |
| 2:G:1938:GLN:HA   | 2:G:1941:ASN:HD22 | 1.86                     | 0.41              |
| 2:G:2874:MET:O    | 2:G:2878:LEU:N    | 2.42                     | 0.41              |
| 2:E:102:LEU:HB3   | 2:E:160:GLY:HA2   | 2.03                     | 0.41              |
| 2:E:379:HIS:CD2   | 2:E:381:GLU:H     | 2.39                     | 0.41              |
| 2:E:446:GLN:HA    | 2:E:449:ILE:HD12  | 2.03                     | 0.41              |
| 2:E:4163:PHE:HA   | 2:E:4166:LEU:HB2  | 2.02                     | 0.41              |
| 2:B:379:HIS:CD2   | 2:B:381:GLU:H     | 2.39                     | 0.41              |
| 2:B:2950:UNK:O    | 2:B:2954:UNK:N    | 2.54                     | 0.41              |
| 2:B:3365:UNK:O    | 2:B:3369:UNK:N    | 2.54                     | 0.41              |
| 2:B:4237:PHE:O    | 2:B:4241:THR:OG1  | 2.33                     | 0.41              |
| 2:I:410:LEU:HD12  | 2:I:413:GLN:HE21  | 1.86                     | 0.41              |
| 2:E:342:GLY:HA2   | 2:E:389:PHE:HB2   | 2.03                     | 0.41              |
| 2:E:485:SER:O     | 2:E:489:ASN:N     | 2.40                     | 0.41              |
| 2:E:3880:PHE:O    | 2:E:3884:LEU:N    | 2.53                     | 0.41              |
| 1:A:87:HIS:HA     | 1:A:88:PRO:HD3    | 1.88                     | 0.40              |
| 2:B:309:THR:O     | 2:B:313:SER:OG    | 2.39                     | 0.40              |
| 2:B:446:GLN:HA    | 2:B:449:ILE:HD12  | 2.03                     | 0.40              |
| 2:B:1727:ARG:HH21 | 2:B:1775:HIS:CE1  | 2.39                     | 0.40              |
| 2:B:4163:PHE:HA   | 2:B:4166:LEU:HB2  | 2.02                     | 0.40              |
| 2:I:4106:PRO:O    | 2:I:4110:PHE:N    | 2.53                     | 0.40              |
| 2:I:4780:PHE:HA   | 2:I:4783:ILE:HD12 | 2.03                     | 0.40              |
| 2:I:4962:GLY:H    | 2:I:5025:GLY:CA   | 2.34                     | 0.40              |
| 2:G:342:GLY:HA2   | 2:G:389:PHE:HB2   | 2.02                     | 0.40              |
| 2:G:742:ASP:HA    | 2:G:760:ASN:HD21  | 1.86                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:897:ARG:HD2   | 2:G:905:PRO:HG3   | 2.04                     | 0.40              |
| 2:G:1130:GLN:HG2  | 2:G:1138:PRO:HA   | 2.03                     | 0.40              |
| 2:G:4962:GLY:H    | 2:G:5025:GLY:CA   | 2.34                     | 0.40              |
| 2:E:410:LEU:HD12  | 2:E:413:GLN:HE21  | 1.86                     | 0.40              |
| 2:E:1256:GLU:HG2  | 2:E:1273:ALA:HB3  | 2.03                     | 0.40              |
| 2:E:1286:UNK:HA   | 2:E:1461:UNK:HA   | 2.02                     | 0.40              |
| 2:B:1735:ILE:HG23 | 2:B:1771:LEU:HD23 | 2.03                     | 0.40              |
| 2:I:102:LEU:HB3   | 2:I:160:GLY:HA2   | 2.03                     | 0.40              |
| 2:I:309:THR:O     | 2:I:313:SER:OG    | 2.39                     | 0.40              |
| 2:I:1105:ALA:O    | 2:I:1189:LEU:N    | 2.51                     | 0.40              |
| 2:I:3880:PHE:O    | 2:I:3884:LEU:N    | 2.54                     | 0.40              |
| 2:G:940:GLY:O     | 2:G:1052:ASN:N    | 2.52                     | 0.40              |
| 2:G:4712:PRO:HB2  | 2:G:4718:LYS:HA   | 2.01                     | 0.40              |
| 2:E:1141:ARG:HD2  | 2:E:1141:ARG:H    | 1.87                     | 0.40              |
| 2:B:4984:ASN:HD21 | 2:B:4986:ALA:HB3  | 1.86                     | 0.40              |
| 2:I:123:THR:OG1   | 2:I:134:ASP:OD1   | 2.39                     | 0.40              |
| 2:I:876:GLU:O     | 2:I:880:GLU:N     | 2.51                     | 0.40              |
| 2:I:1727:ARG:HH21 | 2:I:1775:HIS:CE1  | 2.39                     | 0.40              |
| 2:I:4957:LYS:NZ   | 2:I:4957:LYS:CB   | 2.83                     | 0.40              |
| 2:G:184:THR:HA    | 2:G:189:LEU:HA    | 2.03                     | 0.40              |
| 2:G:3662:ILE:H    | 2:G:3662:ILE:HG13 | 1.79                     | 0.40              |
| 2:G:4176:PRO:O    | 2:G:4202:ARG:NH2  | 2.55                     | 0.40              |
| 2:G:4984:ASN:HD21 | 2:G:4986:ALA:HB3  | 1.87                     | 0.40              |
| 2:E:184:THR:HA    | 2:E:189:LEU:HA    | 2.03                     | 0.40              |
| 2:E:599:VAL:HG23  | 2:E:600:LEU:HD12  | 2.02                     | 0.40              |
| 2:E:1735:ILE:HG23 | 2:E:1771:LEU:HD23 | 2.03                     | 0.40              |
| 2:B:897:ARG:HD2   | 2:B:905:PRO:HG3   | 2.04                     | 0.40              |
| 2:B:3843:ASP:H    | 2:B:3874:VAL:HG13 | 1.87                     | 0.40              |
| 2:B:4735:GLU:HA   | 2:B:4738:ALA:HB3  | 2.03                     | 0.40              |
| 2:I:2793:PRO:HG3  | 2:I:2855:TYR:CZ   | 2.57                     | 0.40              |
| 2:G:2950:UNK:O    | 2:G:2954:UNK:N    | 2.54                     | 0.40              |
| 2:G:4578:LEU:O    | 2:E:4880:MET:HG3  | 2.21                     | 0.40              |
| 2:E:321:GLU:HB3   | 2:E:322:LYS:H     | 1.73                     | 0.40              |
| 2:E:897:ARG:HD2   | 2:E:905:PRO:HG3   | 2.04                     | 0.40              |
| 2:E:4982:GLU:HB3  | 2:E:4983:HIS:H    | 1.71                     | 0.40              |
| 2:B:4106:PRO:O    | 2:B:4110:PHE:N    | 2.53                     | 0.40              |
| 2:I:396:GLU:OE2   | 2:I:451:TYR:OH    | 2.32                     | 0.40              |
| 2:G:446:GLN:HA    | 2:G:449:ILE:HD12  | 2.03                     | 0.40              |
| 2:G:2196:ASN:OD1  | 2:G:2199:ARG:NH1  | 2.38                     | 0.40              |
| 2:G:4968:PHE:CE2  | 2:G:4978:HIS:ND1  | 2.89                     | 0.40              |
| 2:G:4968:PHE:O    | 2:G:4971:THR:OG1  | 2.35                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:E:149:THR:N    | 2:E:172:VAL:O     | 2.54                     | 0.40              |
| 2:E:1090:PHE:HD2 | 2:E:1202:LEU:HD11 | 1.86                     | 0.40              |
| 2:E:4702:ASP:OD1 | 2:E:4778:TRP:NE1  | 2.48                     | 0.40              |
| 2:E:4962:GLY:H   | 2:E:5025:GLY:CA   | 2.34                     | 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     | 105/108 (97%)     | 92 (88%)    | 13 (12%)   | 0        | 100         | 100 |
| 1   | F     | 105/108 (97%)     | 92 (88%)    | 13 (12%)   | 0        | 100         | 100 |
| 1   | H     | 105/108 (97%)     | 92 (88%)    | 13 (12%)   | 0        | 100         | 100 |
| 1   | J     | 105/108 (97%)     | 92 (88%)    | 13 (12%)   | 0        | 100         | 100 |
| 2   | B     | 3235/4416 (73%)   | 2899 (90%)  | 332 (10%)  | 4 (0%)   | 48          | 83  |
| 2   | E     | 3235/4416 (73%)   | 2900 (90%)  | 331 (10%)  | 4 (0%)   | 48          | 83  |
| 2   | G     | 3235/4416 (73%)   | 2900 (90%)  | 331 (10%)  | 4 (0%)   | 48          | 83  |
| 2   | I     | 3235/4416 (73%)   | 2900 (90%)  | 331 (10%)  | 4 (0%)   | 48          | 83  |
| All | All   | 13360/18096 (74%) | 11967 (90%) | 1377 (10%) | 16 (0%)  | 49          | 83  |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 1708 | ARG  |
| 2   | I     | 1708 | ARG  |
| 2   | G     | 1708 | ARG  |
| 2   | E     | 1708 | ARG  |
| 2   | B     | 4641 | PRO  |
| 2   | I     | 4641 | PRO  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | G     | 4641 | PRO  |
| 2   | E     | 4641 | PRO  |
| 2   | B     | 1932 | PRO  |
| 2   | I     | 1932 | PRO  |
| 2   | G     | 1932 | PRO  |
| 2   | E     | 1932 | PRO  |
| 2   | B     | 1840 | PRO  |
| 2   | I     | 1840 | PRO  |
| 2   | G     | 1840 | PRO  |
| 2   | E     | 1840 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 1   | A     | 88/89 (99%)       | 88 (100%)   | 0        | 100         | 100 |
| 1   | F     | 88/89 (99%)       | 88 (100%)   | 0        | 100         | 100 |
| 1   | H     | 88/89 (99%)       | 88 (100%)   | 0        | 100         | 100 |
| 1   | J     | 88/89 (99%)       | 88 (100%)   | 0        | 100         | 100 |
| 2   | B     | 2493/3022 (82%)   | 2476 (99%)  | 17 (1%)  | 76          | 81  |
| 2   | E     | 2493/3022 (82%)   | 2476 (99%)  | 17 (1%)  | 76          | 81  |
| 2   | G     | 2493/3022 (82%)   | 2476 (99%)  | 17 (1%)  | 76          | 81  |
| 2   | I     | 2493/3022 (82%)   | 2476 (99%)  | 17 (1%)  | 76          | 81  |
| All | All   | 10324/12444 (83%) | 10256 (99%) | 68 (1%)  | 73          | 81  |

All (68) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 131  | LEU  |
| 2   | B     | 1600 | LEU  |
| 2   | B     | 1657 | LEU  |
| 2   | B     | 1676 | LEU  |
| 2   | B     | 2010 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 2144 | ILE  |
| 2   | B     | 3663 | LEU  |
| 2   | B     | 3805 | LEU  |
| 2   | B     | 4081 | VAL  |
| 2   | B     | 4154 | VAL  |
| 2   | B     | 4166 | LEU  |
| 2   | B     | 4230 | LYS  |
| 2   | B     | 4957 | LYS  |
| 2   | B     | 4958 | CYS  |
| 2   | B     | 4983 | HIS  |
| 2   | B     | 4985 | LEU  |
| 2   | B     | 4995 | LEU  |
| 2   | I     | 131  | LEU  |
| 2   | I     | 1600 | LEU  |
| 2   | I     | 1657 | LEU  |
| 2   | I     | 1676 | LEU  |
| 2   | I     | 2010 | LEU  |
| 2   | I     | 2144 | ILE  |
| 2   | I     | 3663 | LEU  |
| 2   | I     | 3805 | LEU  |
| 2   | I     | 4081 | VAL  |
| 2   | I     | 4154 | VAL  |
| 2   | I     | 4166 | LEU  |
| 2   | I     | 4230 | LYS  |
| 2   | I     | 4957 | LYS  |
| 2   | I     | 4958 | CYS  |
| 2   | I     | 4983 | HIS  |
| 2   | I     | 4985 | LEU  |
| 2   | I     | 4995 | LEU  |
| 2   | G     | 131  | LEU  |
| 2   | G     | 1600 | LEU  |
| 2   | G     | 1657 | LEU  |
| 2   | G     | 1676 | LEU  |
| 2   | G     | 2010 | LEU  |
| 2   | G     | 2144 | ILE  |
| 2   | G     | 3663 | LEU  |
| 2   | G     | 3805 | LEU  |
| 2   | G     | 4081 | VAL  |
| 2   | G     | 4154 | VAL  |
| 2   | G     | 4166 | LEU  |
| 2   | G     | 4230 | LYS  |
| 2   | G     | 4957 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | G     | 4958 | CYS  |
| 2   | G     | 4983 | HIS  |
| 2   | G     | 4985 | LEU  |
| 2   | G     | 4995 | LEU  |
| 2   | E     | 131  | LEU  |
| 2   | E     | 1600 | LEU  |
| 2   | E     | 1657 | LEU  |
| 2   | E     | 1676 | LEU  |
| 2   | E     | 2010 | LEU  |
| 2   | E     | 2144 | ILE  |
| 2   | E     | 3663 | LEU  |
| 2   | E     | 3805 | LEU  |
| 2   | E     | 4081 | VAL  |
| 2   | E     | 4154 | VAL  |
| 2   | E     | 4166 | LEU  |
| 2   | E     | 4230 | LYS  |
| 2   | E     | 4957 | LYS  |
| 2   | E     | 4958 | CYS  |
| 2   | E     | 4983 | HIS  |
| 2   | E     | 4985 | LEU  |
| 2   | E     | 4995 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (265) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 31  | GLN  |
| 1   | F     | 43  | ASN  |
| 1   | F     | 87  | HIS  |
| 1   | A     | 31  | GLN  |
| 1   | A     | 43  | ASN  |
| 1   | A     | 87  | HIS  |
| 1   | H     | 31  | GLN  |
| 1   | H     | 43  | ASN  |
| 1   | H     | 87  | HIS  |
| 1   | J     | 31  | GLN  |
| 1   | J     | 43  | ASN  |
| 1   | J     | 87  | HIS  |
| 2   | B     | 57  | ASN  |
| 2   | B     | 71  | GLN  |
| 2   | B     | 84  | ASN  |
| 2   | B     | 98  | HIS  |
| 2   | B     | 105 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 156  | GLN  |
| 2   | B     | 190  | GLN  |
| 2   | B     | 201  | ASN  |
| 2   | B     | 379  | HIS  |
| 2   | B     | 399  | GLN  |
| 2   | B     | 413  | GLN  |
| 2   | B     | 461  | HIS  |
| 2   | B     | 465  | GLN  |
| 2   | B     | 479  | GLN  |
| 2   | B     | 725  | HIS  |
| 2   | B     | 797  | HIS  |
| 2   | B     | 838  | HIS  |
| 2   | B     | 1198 | GLN  |
| 2   | B     | 1220 | GLN  |
| 2   | B     | 1598 | GLN  |
| 2   | B     | 1660 | GLN  |
| 2   | B     | 1679 | ASN  |
| 2   | B     | 1691 | GLN  |
| 2   | B     | 1693 | GLN  |
| 2   | B     | 1719 | HIS  |
| 2   | B     | 1775 | HIS  |
| 2   | B     | 1861 | GLN  |
| 2   | B     | 1928 | GLN  |
| 2   | B     | 1941 | ASN  |
| 2   | B     | 1949 | GLN  |
| 2   | B     | 1970 | GLN  |
| 2   | B     | 2007 | ASN  |
| 2   | B     | 2100 | HIS  |
| 2   | B     | 2127 | GLN  |
| 2   | B     | 2349 | ASN  |
| 2   | B     | 2772 | GLN  |
| 2   | B     | 2773 | ASN  |
| 2   | B     | 3809 | ASN  |
| 2   | B     | 3889 | GLN  |
| 2   | B     | 3896 | ASN  |
| 2   | B     | 3900 | GLN  |
| 2   | B     | 3946 | GLN  |
| 2   | B     | 3950 | ASN  |
| 2   | B     | 3960 | GLN  |
| 2   | B     | 3963 | ASN  |
| 2   | B     | 3976 | ASN  |
| 2   | B     | 3994 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 4034 | ASN  |
| 2   | B     | 4037 | ASN  |
| 2   | B     | 4054 | ASN  |
| 2   | B     | 4109 | GLN  |
| 2   | B     | 4120 | ASN  |
| 2   | B     | 4201 | ASN  |
| 2   | B     | 4209 | GLN  |
| 2   | B     | 4246 | GLN  |
| 2   | B     | 4806 | ASN  |
| 2   | B     | 4833 | ASN  |
| 2   | B     | 4946 | GLN  |
| 2   | B     | 4978 | HIS  |
| 2   | B     | 4987 | ASN  |
| 2   | I     | 57   | ASN  |
| 2   | I     | 71   | GLN  |
| 2   | I     | 84   | ASN  |
| 2   | I     | 98   | HIS  |
| 2   | I     | 105  | HIS  |
| 2   | I     | 111  | HIS  |
| 2   | I     | 156  | GLN  |
| 2   | I     | 190  | GLN  |
| 2   | I     | 273  | HIS  |
| 2   | I     | 379  | HIS  |
| 2   | I     | 413  | GLN  |
| 2   | I     | 461  | HIS  |
| 2   | I     | 465  | GLN  |
| 2   | I     | 479  | GLN  |
| 2   | I     | 725  | HIS  |
| 2   | I     | 797  | HIS  |
| 2   | I     | 838  | HIS  |
| 2   | I     | 1198 | GLN  |
| 2   | I     | 1220 | GLN  |
| 2   | I     | 1598 | GLN  |
| 2   | I     | 1660 | GLN  |
| 2   | I     | 1679 | ASN  |
| 2   | I     | 1691 | GLN  |
| 2   | I     | 1693 | GLN  |
| 2   | I     | 1719 | HIS  |
| 2   | I     | 1775 | HIS  |
| 2   | I     | 1861 | GLN  |
| 2   | I     | 1928 | GLN  |
| 2   | I     | 1941 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 1949 | GLN  |
| 2   | I     | 1970 | GLN  |
| 2   | I     | 2007 | ASN  |
| 2   | I     | 2100 | HIS  |
| 2   | I     | 2127 | GLN  |
| 2   | I     | 2349 | ASN  |
| 2   | I     | 2756 | ASN  |
| 2   | I     | 2772 | GLN  |
| 2   | I     | 2773 | ASN  |
| 2   | I     | 3809 | ASN  |
| 2   | I     | 3889 | GLN  |
| 2   | I     | 3896 | ASN  |
| 2   | I     | 3900 | GLN  |
| 2   | I     | 3946 | GLN  |
| 2   | I     | 3950 | ASN  |
| 2   | I     | 3960 | GLN  |
| 2   | I     | 3963 | ASN  |
| 2   | I     | 3976 | ASN  |
| 2   | I     | 3994 | HIS  |
| 2   | I     | 4034 | ASN  |
| 2   | I     | 4037 | ASN  |
| 2   | I     | 4054 | ASN  |
| 2   | I     | 4109 | GLN  |
| 2   | I     | 4120 | ASN  |
| 2   | I     | 4201 | ASN  |
| 2   | I     | 4209 | GLN  |
| 2   | I     | 4806 | ASN  |
| 2   | I     | 4833 | ASN  |
| 2   | I     | 4946 | GLN  |
| 2   | I     | 4978 | HIS  |
| 2   | I     | 4987 | ASN  |
| 2   | G     | 57   | ASN  |
| 2   | G     | 71   | GLN  |
| 2   | G     | 84   | ASN  |
| 2   | G     | 98   | HIS  |
| 2   | G     | 105  | HIS  |
| 2   | G     | 156  | GLN  |
| 2   | G     | 190  | GLN  |
| 2   | G     | 201  | ASN  |
| 2   | G     | 273  | HIS  |
| 2   | G     | 379  | HIS  |
| 2   | G     | 399  | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | G     | 413  | GLN  |
| 2   | G     | 461  | HIS  |
| 2   | G     | 465  | GLN  |
| 2   | G     | 479  | GLN  |
| 2   | G     | 725  | HIS  |
| 2   | G     | 797  | HIS  |
| 2   | G     | 838  | HIS  |
| 2   | G     | 1198 | GLN  |
| 2   | G     | 1220 | GLN  |
| 2   | G     | 1590 | GLN  |
| 2   | G     | 1598 | GLN  |
| 2   | G     | 1660 | GLN  |
| 2   | G     | 1679 | ASN  |
| 2   | G     | 1691 | GLN  |
| 2   | G     | 1693 | GLN  |
| 2   | G     | 1719 | HIS  |
| 2   | G     | 1775 | HIS  |
| 2   | G     | 1861 | GLN  |
| 2   | G     | 1928 | GLN  |
| 2   | G     | 1941 | ASN  |
| 2   | G     | 1949 | GLN  |
| 2   | G     | 1970 | GLN  |
| 2   | G     | 2005 | GLN  |
| 2   | G     | 2007 | ASN  |
| 2   | G     | 2100 | HIS  |
| 2   | G     | 2127 | GLN  |
| 2   | G     | 2349 | ASN  |
| 2   | G     | 2772 | GLN  |
| 2   | G     | 2773 | ASN  |
| 2   | G     | 3809 | ASN  |
| 2   | G     | 3889 | GLN  |
| 2   | G     | 3896 | ASN  |
| 2   | G     | 3900 | GLN  |
| 2   | G     | 3946 | GLN  |
| 2   | G     | 3950 | ASN  |
| 2   | G     | 3960 | GLN  |
| 2   | G     | 3963 | ASN  |
| 2   | G     | 3976 | ASN  |
| 2   | G     | 3994 | HIS  |
| 2   | G     | 4034 | ASN  |
| 2   | G     | 4037 | ASN  |
| 2   | G     | 4054 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | G     | 4109 | GLN  |
| 2   | G     | 4120 | ASN  |
| 2   | G     | 4201 | ASN  |
| 2   | G     | 4209 | GLN  |
| 2   | G     | 4246 | GLN  |
| 2   | G     | 4691 | GLN  |
| 2   | G     | 4806 | ASN  |
| 2   | G     | 4833 | ASN  |
| 2   | G     | 4946 | GLN  |
| 2   | G     | 4973 | HIS  |
| 2   | G     | 4978 | HIS  |
| 2   | G     | 4987 | ASN  |
| 2   | G     | 5031 | GLN  |
| 2   | E     | 57   | ASN  |
| 2   | E     | 71   | GLN  |
| 2   | E     | 84   | ASN  |
| 2   | E     | 98   | HIS  |
| 2   | E     | 105  | HIS  |
| 2   | E     | 111  | HIS  |
| 2   | E     | 156  | GLN  |
| 2   | E     | 190  | GLN  |
| 2   | E     | 201  | ASN  |
| 2   | E     | 273  | HIS  |
| 2   | E     | 379  | HIS  |
| 2   | E     | 399  | GLN  |
| 2   | E     | 413  | GLN  |
| 2   | E     | 461  | HIS  |
| 2   | E     | 465  | GLN  |
| 2   | E     | 479  | GLN  |
| 2   | E     | 495  | ASN  |
| 2   | E     | 725  | HIS  |
| 2   | E     | 797  | HIS  |
| 2   | E     | 838  | HIS  |
| 2   | E     | 1198 | GLN  |
| 2   | E     | 1220 | GLN  |
| 2   | E     | 1598 | GLN  |
| 2   | E     | 1660 | GLN  |
| 2   | E     | 1679 | ASN  |
| 2   | E     | 1691 | GLN  |
| 2   | E     | 1693 | GLN  |
| 2   | E     | 1719 | HIS  |
| 2   | E     | 1775 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 1861 | GLN  |
| 2   | E     | 1928 | GLN  |
| 2   | E     | 1941 | ASN  |
| 2   | E     | 1949 | GLN  |
| 2   | E     | 1970 | GLN  |
| 2   | E     | 2007 | ASN  |
| 2   | E     | 2100 | HIS  |
| 2   | E     | 2127 | GLN  |
| 2   | E     | 2349 | ASN  |
| 2   | E     | 2772 | GLN  |
| 2   | E     | 2773 | ASN  |
| 2   | E     | 3809 | ASN  |
| 2   | E     | 3889 | GLN  |
| 2   | E     | 3896 | ASN  |
| 2   | E     | 3900 | GLN  |
| 2   | E     | 3946 | GLN  |
| 2   | E     | 3950 | ASN  |
| 2   | E     | 3960 | GLN  |
| 2   | E     | 3963 | ASN  |
| 2   | E     | 3976 | ASN  |
| 2   | E     | 3994 | HIS  |
| 2   | E     | 4034 | ASN  |
| 2   | E     | 4037 | ASN  |
| 2   | E     | 4054 | ASN  |
| 2   | E     | 4109 | GLN  |
| 2   | E     | 4120 | ASN  |
| 2   | E     | 4201 | ASN  |
| 2   | E     | 4209 | GLN  |
| 2   | E     | 4246 | GLN  |
| 2   | E     | 4553 | ASN  |
| 2   | E     | 4691 | GLN  |
| 2   | E     | 4707 | ASN  |
| 2   | E     | 4806 | ASN  |
| 2   | E     | 4833 | ASN  |
| 2   | E     | 4946 | GLN  |
| 2   | E     | 4978 | HIS  |
| 2   | E     | 4987 | ASN  |
| 2   | E     | 5031 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 2   | B     | 14               |
| 2   | I     | 14               |
| 2   | G     | 14               |
| 2   | E     | 14               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 4345:UNK  | C      | 4540:PHE  | N      | 74.58        |
| 1     | I     | 4345:UNK  | C      | 4540:PHE  | N      | 74.58        |
| 1     | G     | 4345:UNK  | C      | 4540:PHE  | N      | 74.58        |
| 1     | E     | 4345:UNK  | C      | 4540:PHE  | N      | 74.58        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B     | 3613:UNK  | C      | 3639:THR  | N      | 46.52        |
| 1     | I     | 3613:UNK  | C      | 3639:THR  | N      | 46.52        |
| 1     | G     | 3613:UNK  | C      | 3639:THR  | N      | 46.52        |
| 1     | E     | 3613:UNK  | C      | 3639:THR  | N      | 46.52        |
| 1     | B     | 4253:GLU  | C      | 4320:UNK  | N      | 29.50        |
| 1     | I     | 4253:GLU  | C      | 4320:UNK  | N      | 29.50        |
| 1     | G     | 4253:GLU  | C      | 4320:UNK  | N      | 29.50        |
| 1     | E     | 4253:GLU  | C      | 4320:UNK  | N      | 29.50        |
| 1     | B     | 3163:UNK  | C      | 3170:UNK  | N      | 16.19        |
| 1     | I     | 3163:UNK  | C      | 3170:UNK  | N      | 16.19        |
| 1     | G     | 3163:UNK  | C      | 3170:UNK  | N      | 16.18        |
| 1     | E     | 3163:UNK  | C      | 3170:UNK  | N      | 16.18        |
| 1     | B     | 3063:UNK  | C      | 3134:UNK  | N      | 14.97        |
| 1     | I     | 3063:UNK  | C      | 3134:UNK  | N      | 14.97        |
| 1     | G     | 3063:UNK  | C      | 3134:UNK  | N      | 14.97        |
| 1     | E     | 3063:UNK  | C      | 3134:UNK  | N      | 14.97        |
| 1     | B     | 3468:UNK  | C      | 3511:UNK  | N      | 14.26        |
| 1     | I     | 3468:UNK  | C      | 3511:UNK  | N      | 14.26        |
| 1     | G     | 3468:UNK  | C      | 3511:UNK  | N      | 14.26        |
| 1     | E     | 3468:UNK  | C      | 3511:UNK  | N      | 14.26        |
| 1     | B     | 2703:UNK  | C      | 2734:ASN  | N      | 13.16        |
| 1     | I     | 2703:UNK  | C      | 2734:ASN  | N      | 13.16        |
| 1     | G     | 2703:UNK  | C      | 2734:ASN  | N      | 13.16        |
| 1     | E     | 2703:UNK  | C      | 2734:ASN  | N      | 13.16        |
| 1     | B     | 3236:UNK  | C      | 3241:UNK  | N      | 12.69        |
| 1     | I     | 3236:UNK  | C      | 3241:UNK  | N      | 12.69        |
| 1     | G     | 3236:UNK  | C      | 3241:UNK  | N      | 12.69        |
| 1     | E     | 3236:UNK  | C      | 3241:UNK  | N      | 12.69        |
| 1     | B     | 2976:UNK  | C      | 2995:UNK  | N      | 12.19        |
| 1     | I     | 2976:UNK  | C      | 2995:UNK  | N      | 12.19        |
| 1     | G     | 2976:UNK  | C      | 2995:UNK  | N      | 12.19        |
| 1     | E     | 2976:UNK  | C      | 2995:UNK  | N      | 12.19        |
| 1     | B     | 1564:UNK  | C      | 1573:MET  | N      | 12.11        |
| 1     | I     | 1564:UNK  | C      | 1573:MET  | N      | 12.11        |
| 1     | G     | 1564:UNK  | C      | 1573:MET  | N      | 12.11        |
| 1     | E     | 1564:UNK  | C      | 1573:MET  | N      | 12.11        |
| 1     | B     | 3254:UNK  | C      | 3261:UNK  | N      | 8.68         |
| 1     | I     | 3254:UNK  | C      | 3261:UNK  | N      | 8.68         |
| 1     | G     | 3254:UNK  | C      | 3261:UNK  | N      | 8.68         |
| 1     | E     | 3254:UNK  | C      | 3261:UNK  | N      | 8.68         |
| 1     | B     | 1297:UNK  | C      | 1430:UNK  | N      | 5.91         |
| 1     | I     | 1297:UNK  | C      | 1430:UNK  | N      | 5.91         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | G     | 1297:UNK  | C      | 1430:UNK  | N      | 5.91         |
| 1     | E     | 1297:UNK  | C      | 1430:UNK  | N      | 5.91         |
| 1     | B     | 2479:LEU  | C      | 2487:UNK  | N      | 3.40         |
| 1     | I     | 2479:LEU  | C      | 2487:UNK  | N      | 3.40         |
| 1     | G     | 2479:LEU  | C      | 2487:UNK  | N      | 3.40         |
| 1     | E     | 2479:LEU  | C      | 2487:UNK  | N      | 3.40         |
| 1     | B     | 2939:ARG  | C      | 2942:UNK  | N      | 3.21         |
| 1     | I     | 2939:ARG  | C      | 2942:UNK  | N      | 3.21         |
| 1     | G     | 2939:ARG  | C      | 2942:UNK  | N      | 3.21         |
| 1     | E     | 2939:ARG  | C      | 2942:UNK  | N      | 3.21         |

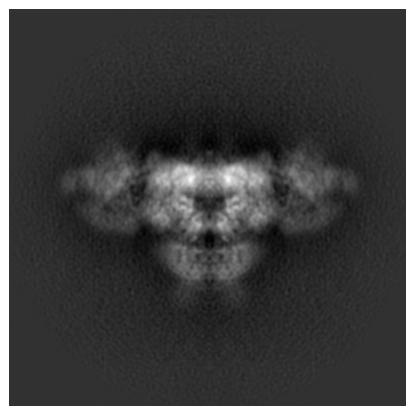
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8388. These allow visual inspection of the internal detail of the map and identification of artifacts.

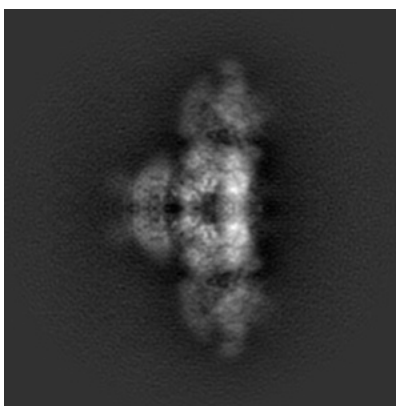
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

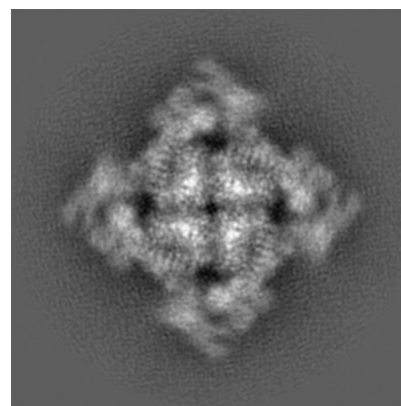
#### 6.1.1 Primary map



X

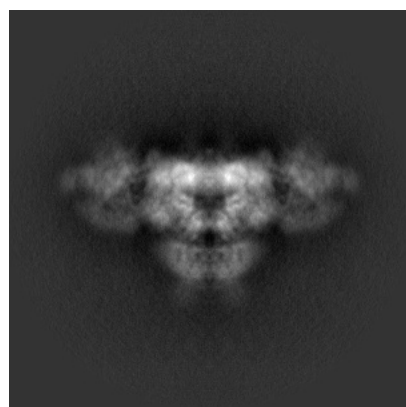


Y

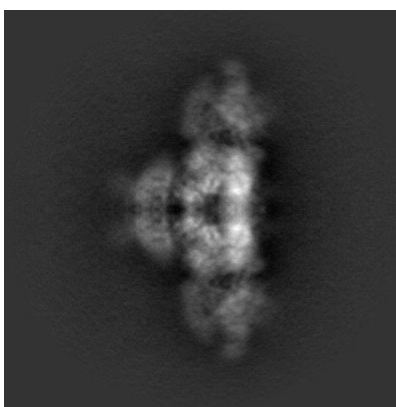


Z

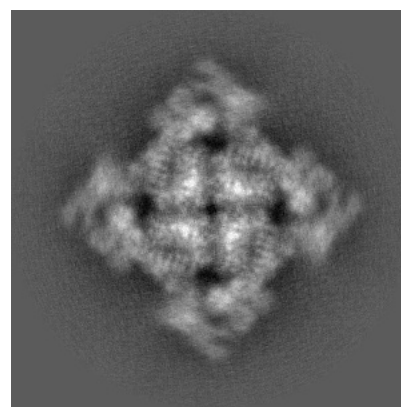
#### 6.1.2 Raw map



X



Y

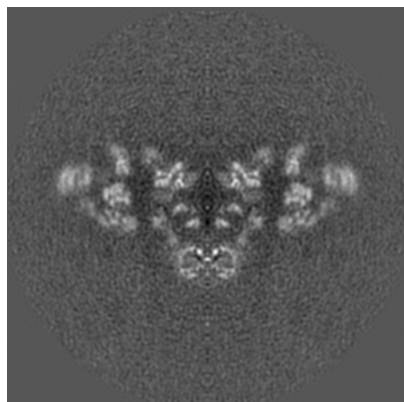


Z

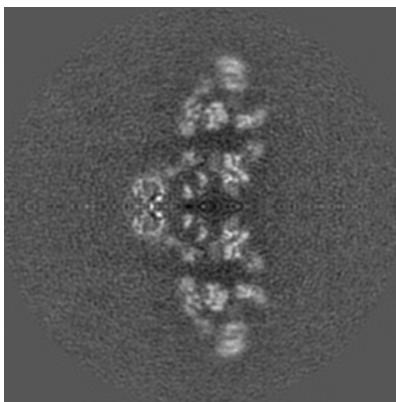
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

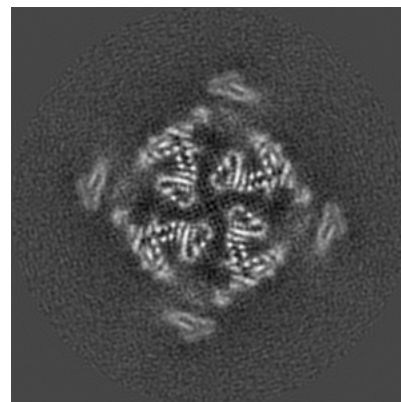
### 6.2.1 Primary map



X Index: 200

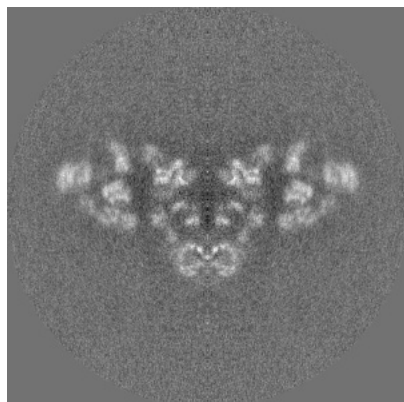


Y Index: 200

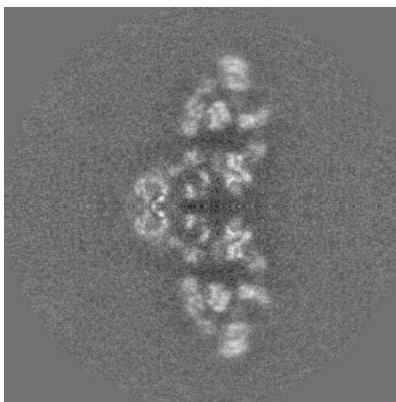


Z Index: 200

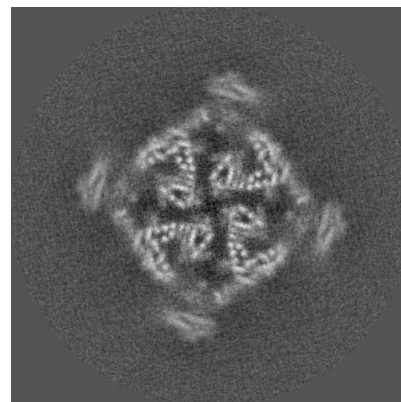
### 6.2.2 Raw map



X Index: 200



Y Index: 200

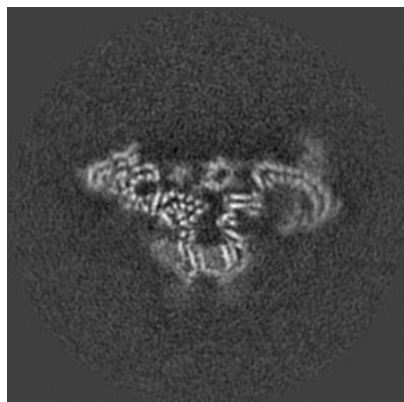


Z Index: 200

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

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

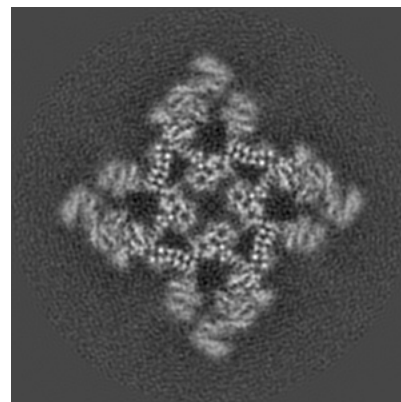
### 6.3.1 Primary map



X Index: 225

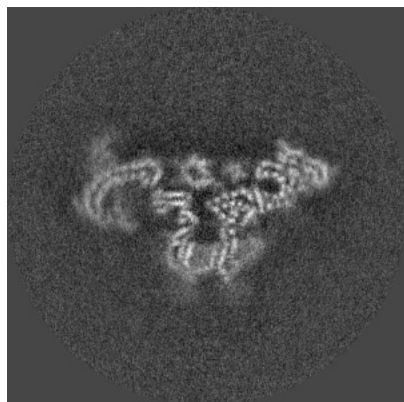


Y Index: 225

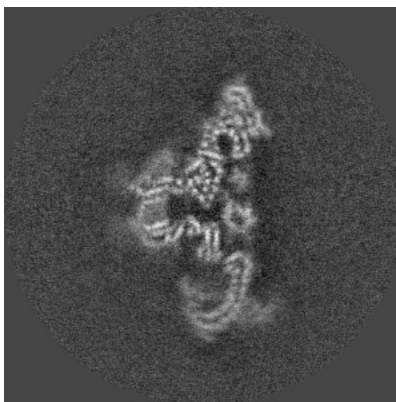


Z Index: 226

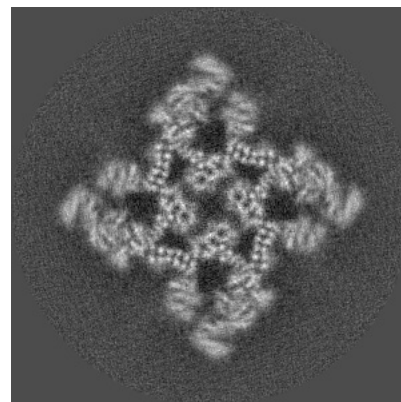
### 6.3.2 Raw map



X Index: 175



Y Index: 225

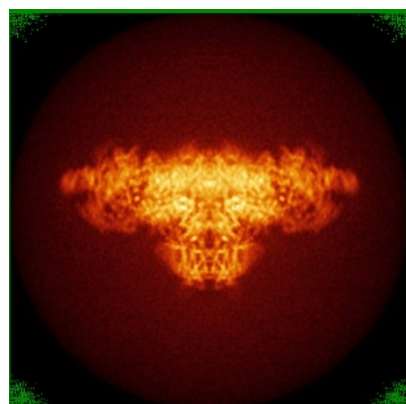


Z Index: 229

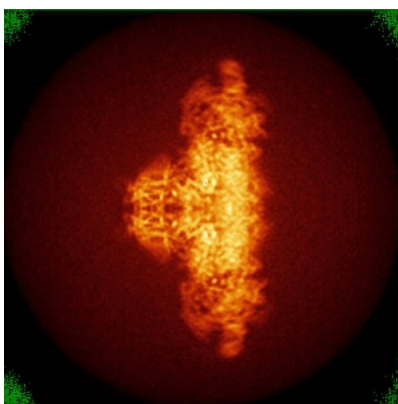
The images above show the largest variance slices of the map in three orthogonal directions.

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

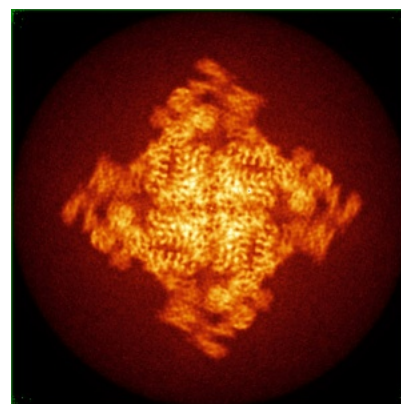
### 6.4.1 Primary map



X

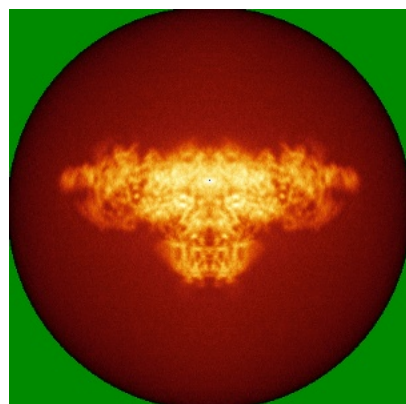


Y

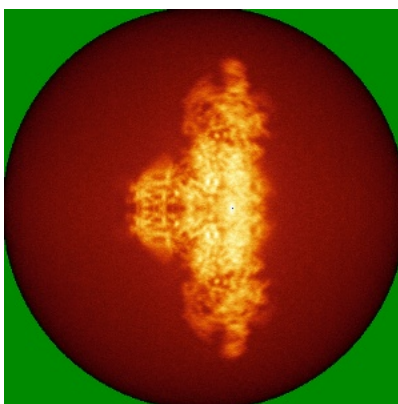


Z

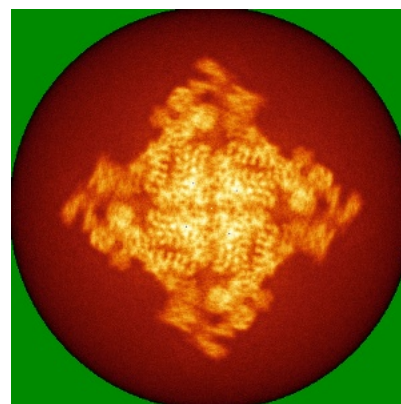
### 6.4.2 Raw map



X



Y

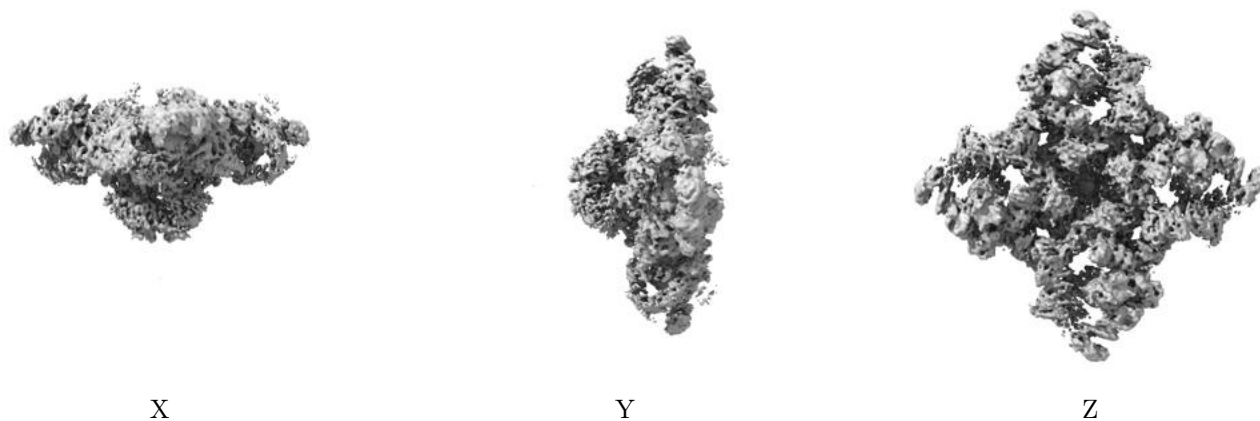


Z

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

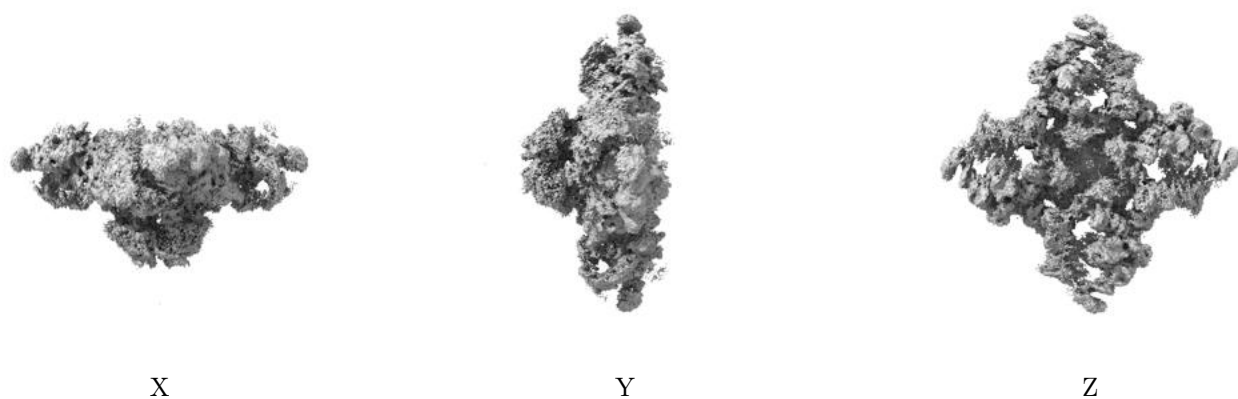
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

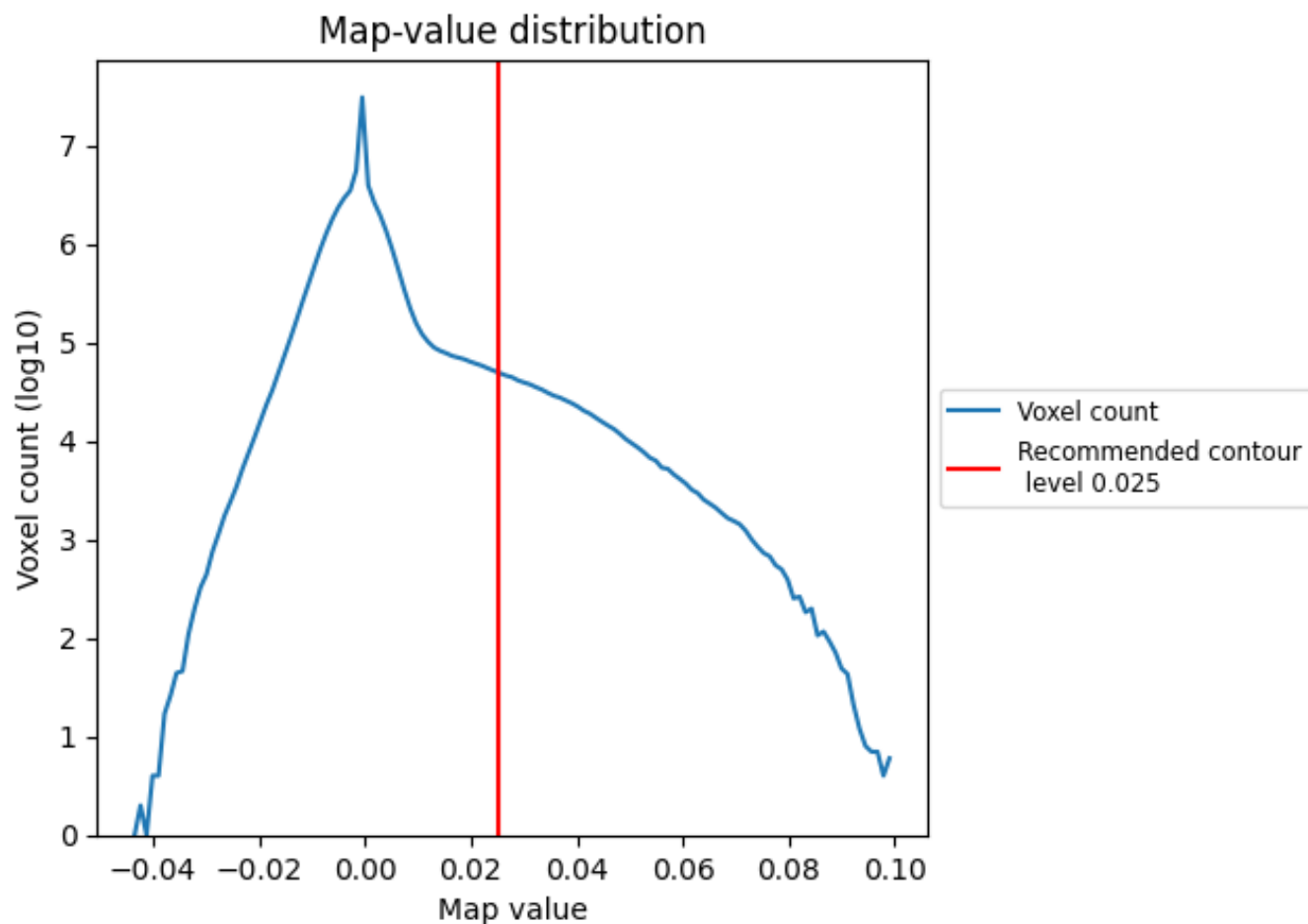
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

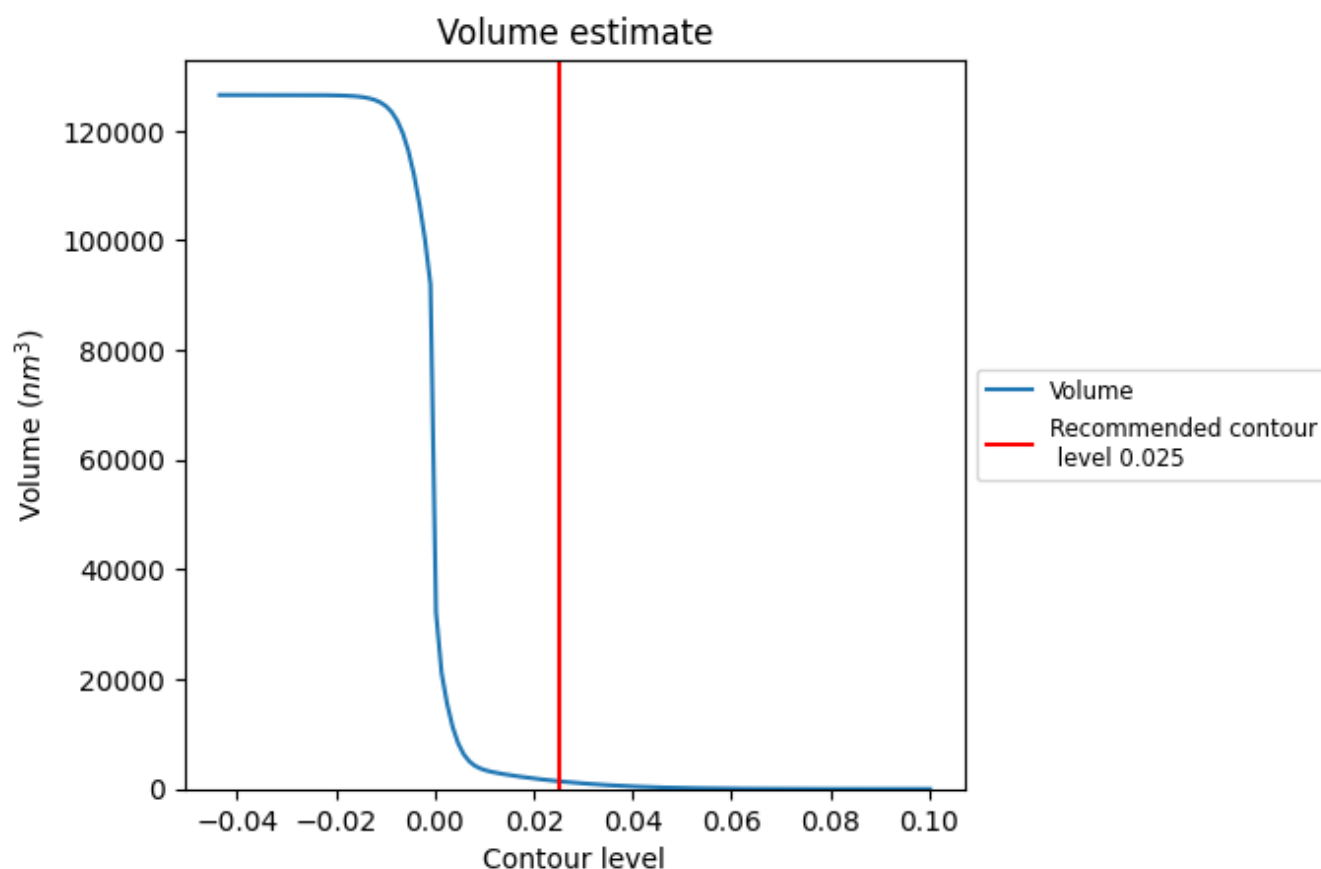
This section contains the results of statistical analysis of the map.

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



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

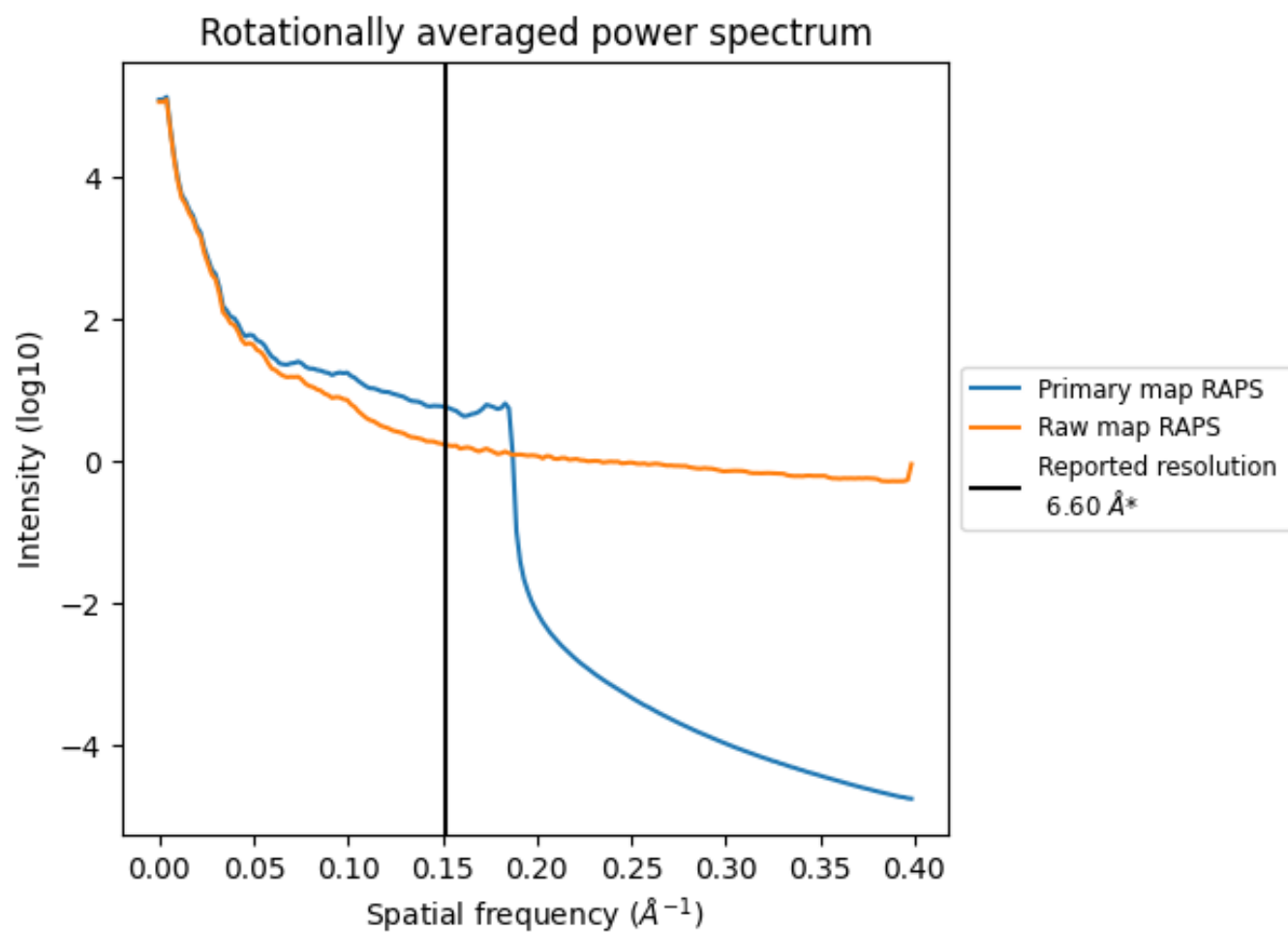
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1411 nm<sup>3</sup>; this corresponds to an approximate mass of 1274 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 ⓘ

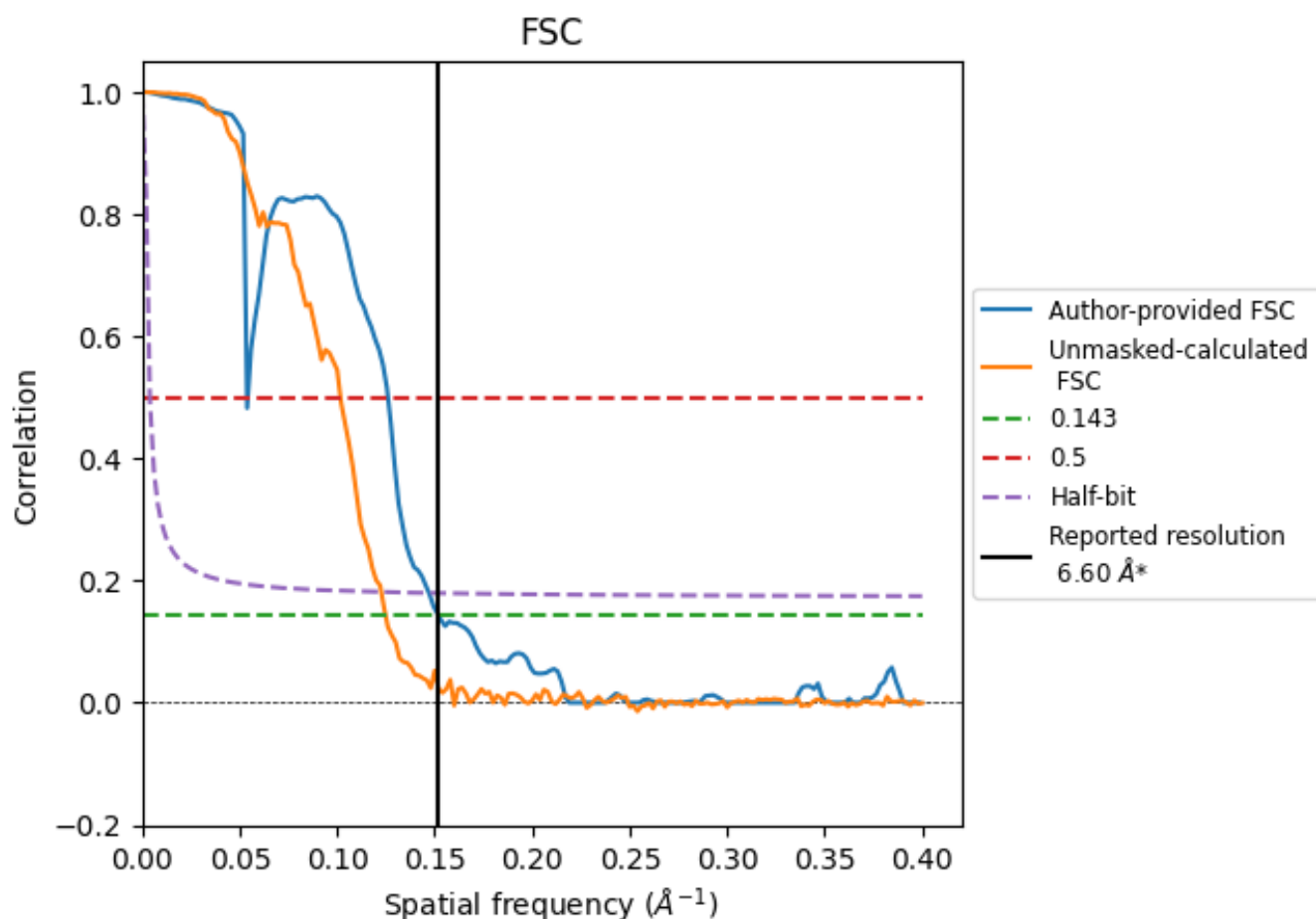


\*Reported resolution corresponds to spatial frequency of 0.152 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.152 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

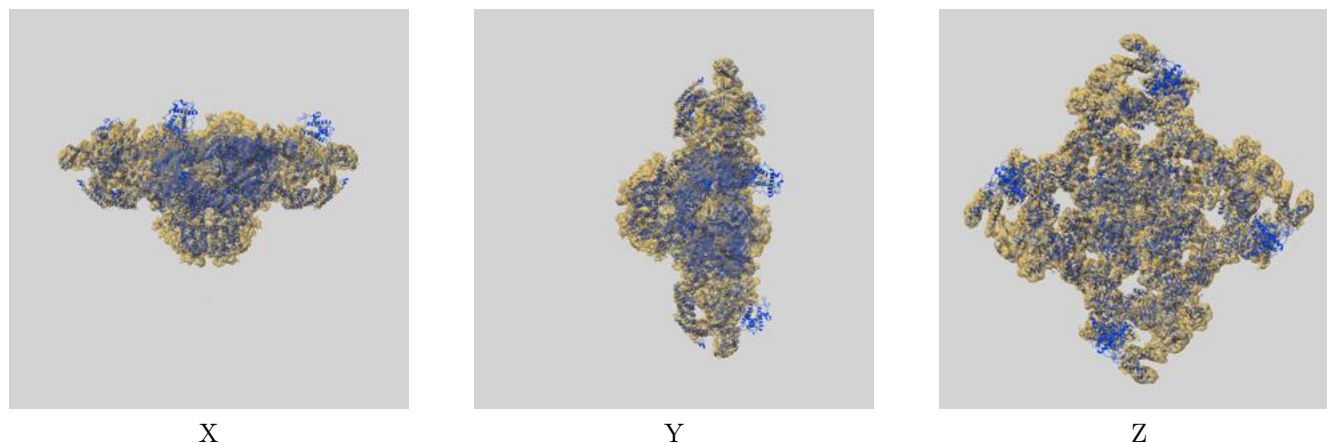
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 6.60                               | -     | -        |
| Author-provided FSC curve | 6.58                               | 18.62 | 6.80     |
| Unmasked-calculated*      | 8.01                               | 9.83  | 8.16     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.01 differs from the reported value 6.6 by more than 10 %

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

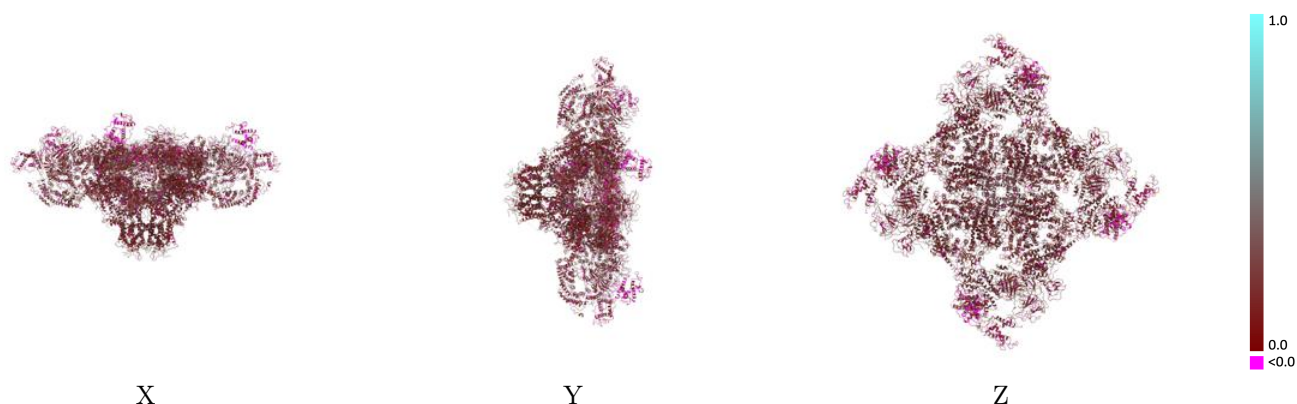
This section contains information regarding the fit between EMDB map EMD-8388 and PDB model 5TAX. Per-residue inclusion information can be found in section 3 on page 6.

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



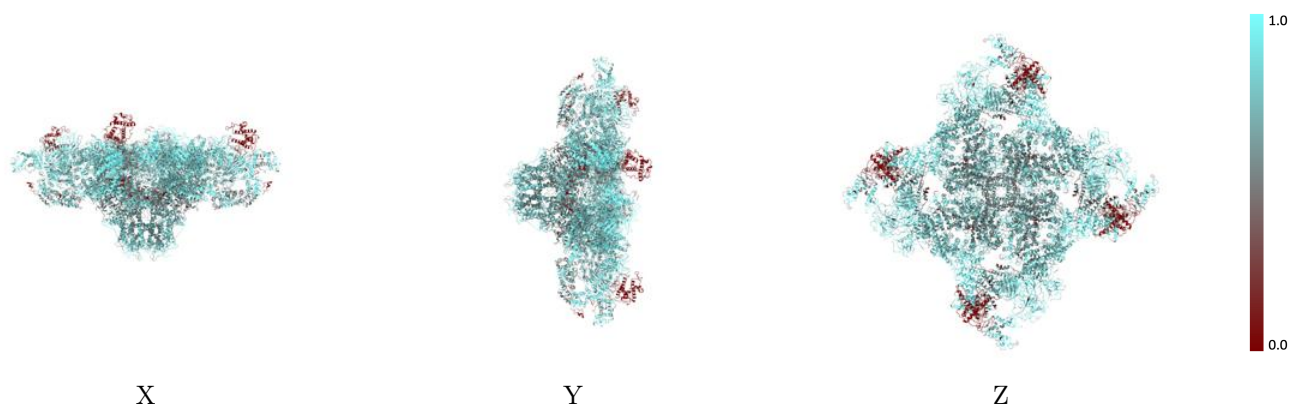
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



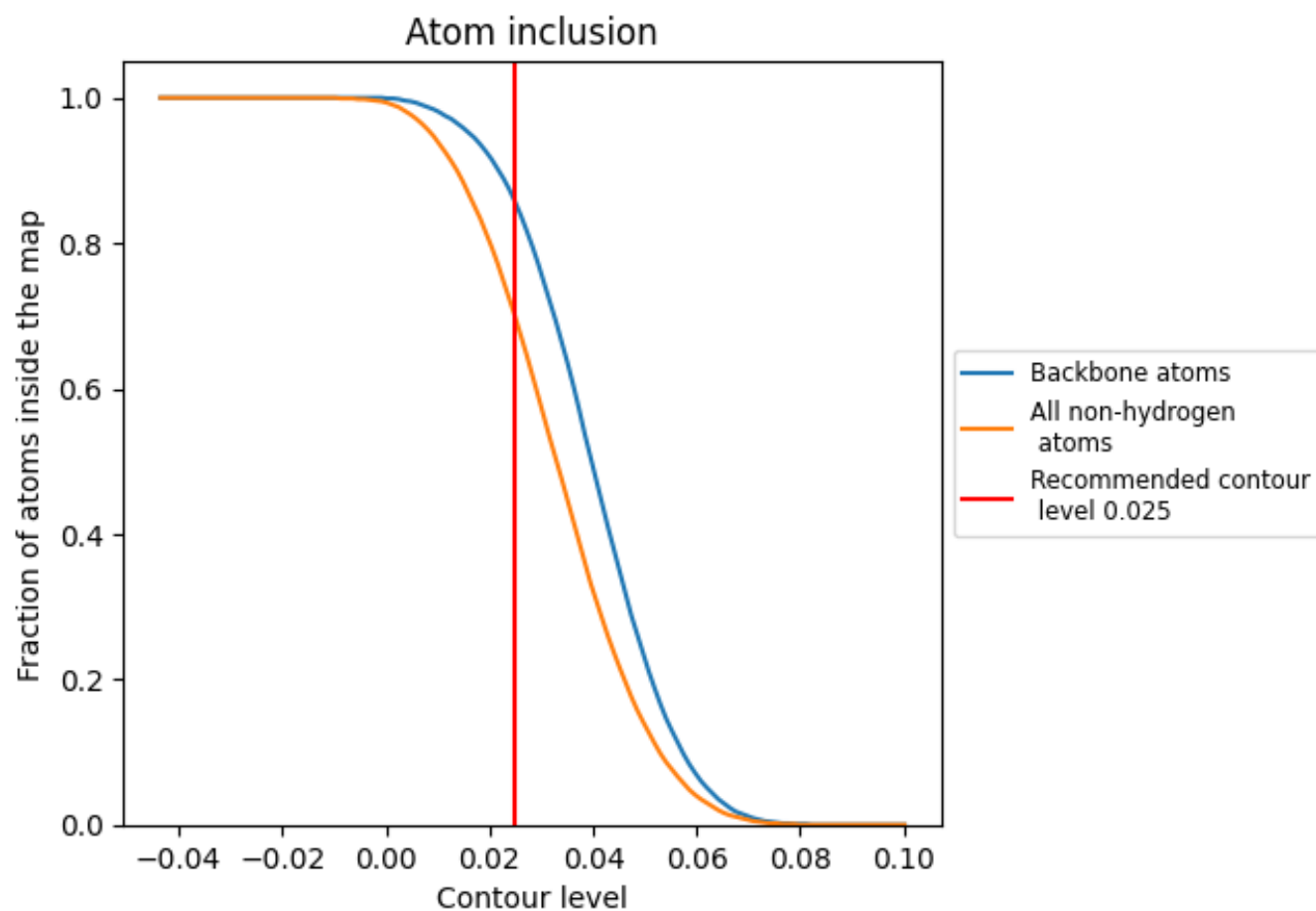
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.6980 | <div></div> 0.1910 |
| A     | <div></div> 0.8060 | <div></div> 0.1870 |
| B     | <div></div> 0.6950 | <div></div> 0.1910 |
| E     | <div></div> 0.6960 | <div></div> 0.1910 |
| F     | <div></div> 0.8060 | <div></div> 0.1910 |
| G     | <div></div> 0.6930 | <div></div> 0.1910 |
| H     | <div></div> 0.8080 | <div></div> 0.1900 |
| I     | <div></div> 0.6960 | <div></div> 0.1910 |
| J     | <div></div> 0.8080 | <div></div> 0.1870 |

1.0

0.0

<0.0