



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:59 AM UTC

PDB ID : 5TAW / pdb\_00005taw  
EMDB ID : EMD-8387  
Title : Structure of rabbit RyR1 (ryanodine dataset, all particles)  
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;  
Frank, J.  
Deposited on : 2016-09-10  
Resolution : 4.40 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:

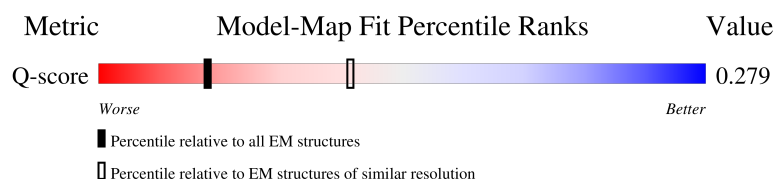
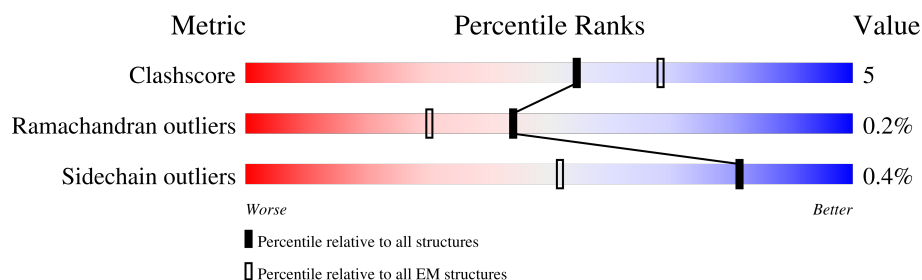
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

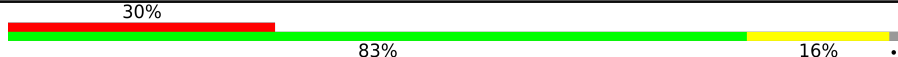
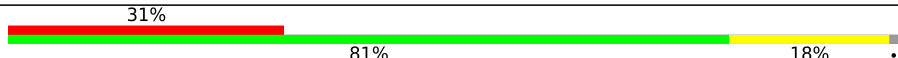
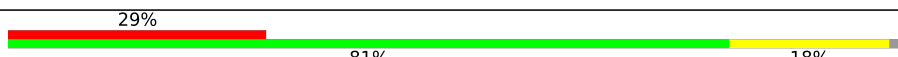
The reported resolution of this entry is 4.40 Å.

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                       | 3132 ( 3.91 - 4.90 )                                     |

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   | <div><div>43%</div><div><div></div><div>83%</div><div>11%</div><div>5%</div></div></div> |
| 2   | E     | 4416   | <div><div>43%</div><div><div></div><div>84%</div><div>11%</div><div>5%</div></div></div> |
| 2   | G     | 4416   | <div><div>43%</div><div><div></div><div>84%</div><div>11%</div><div>5%</div></div></div> |
| 2   | I     | 4416   | <div><div>43%</div><div><div></div><div>84%</div><div>11%</div><div>5%</div></div></div> |

## 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   | G     | 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   | 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   | G     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | I     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 3   | E     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

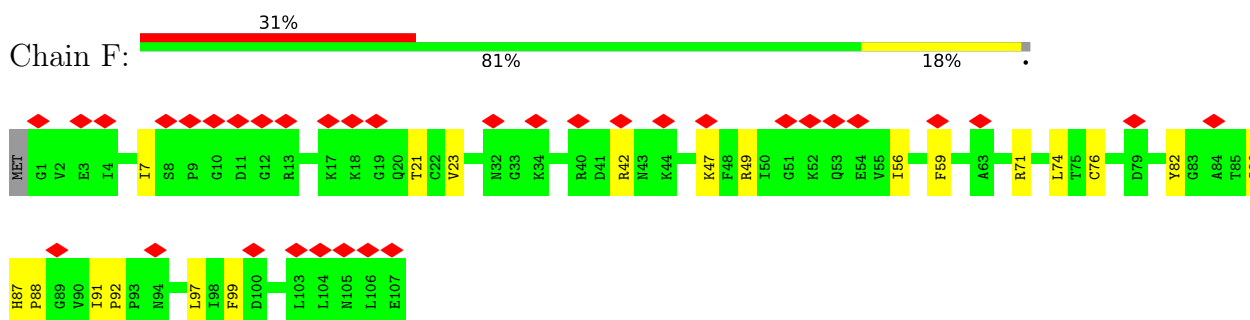
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

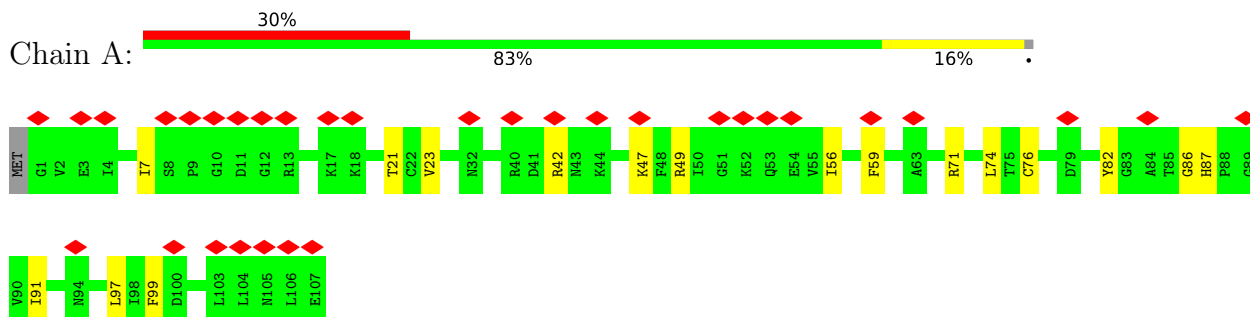
### 3 Residue-property plots [i](#)

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.

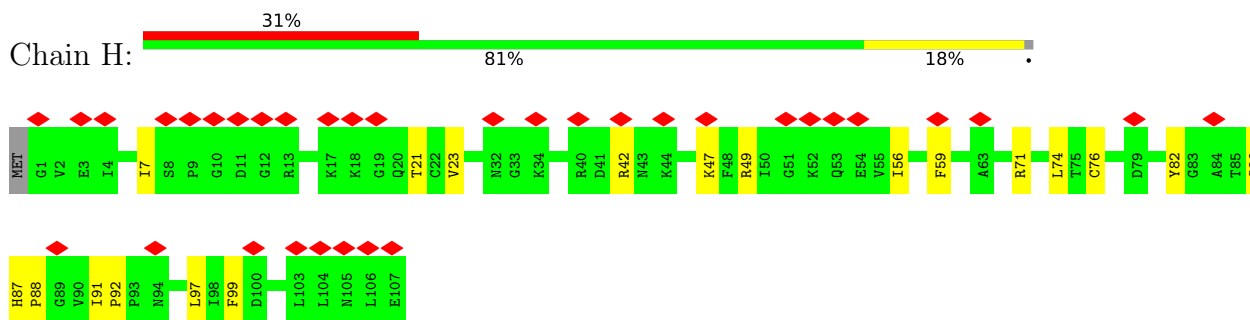
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



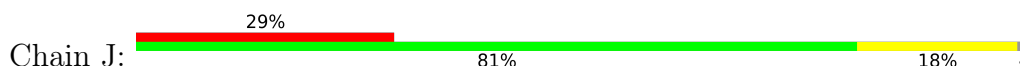
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

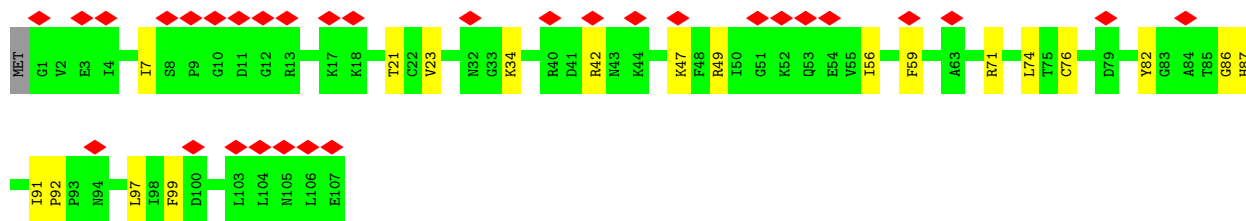


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

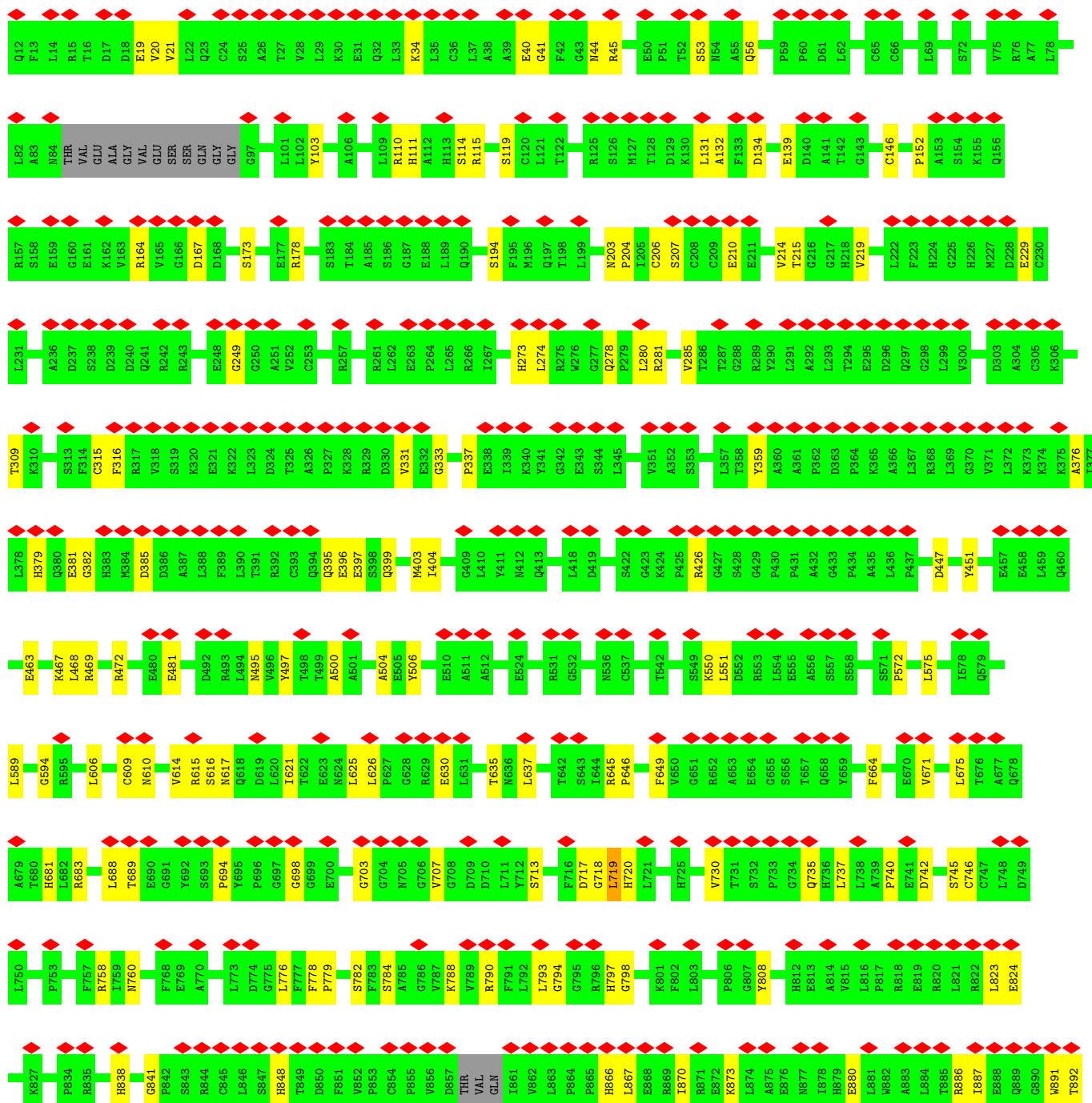
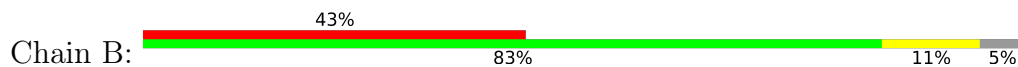


- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

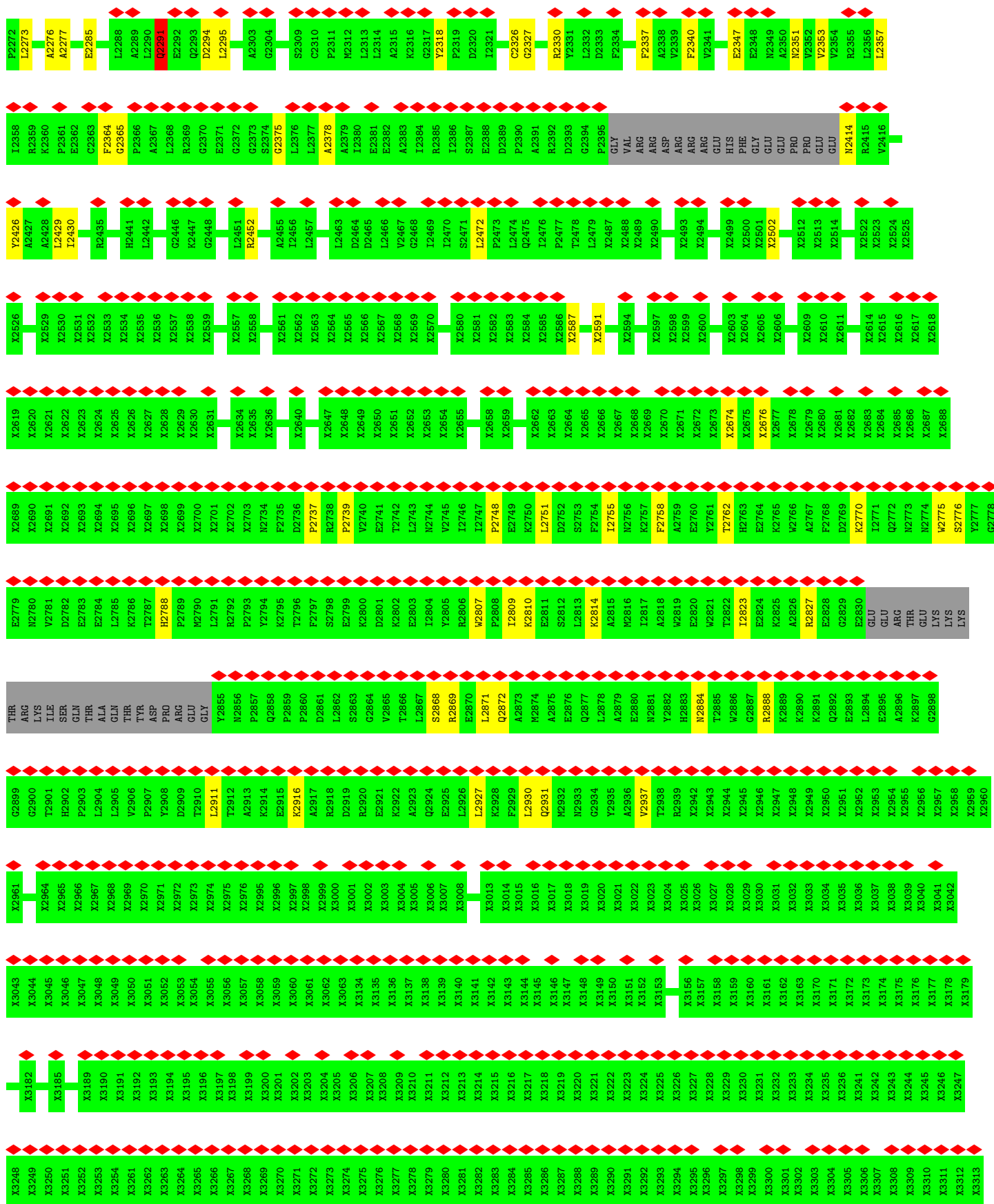




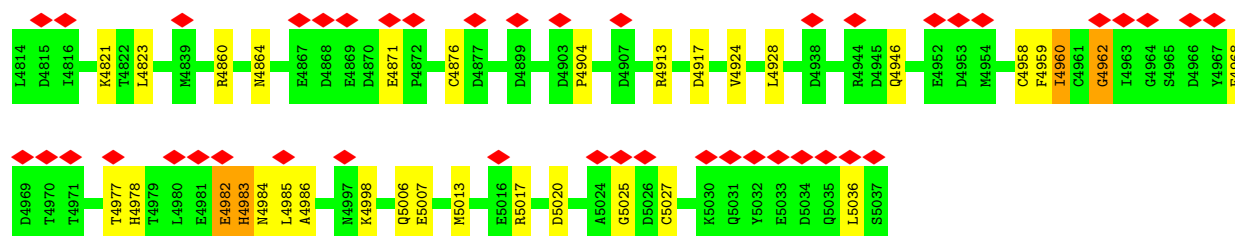
• Molecule 2: Ryanodine receptor 1



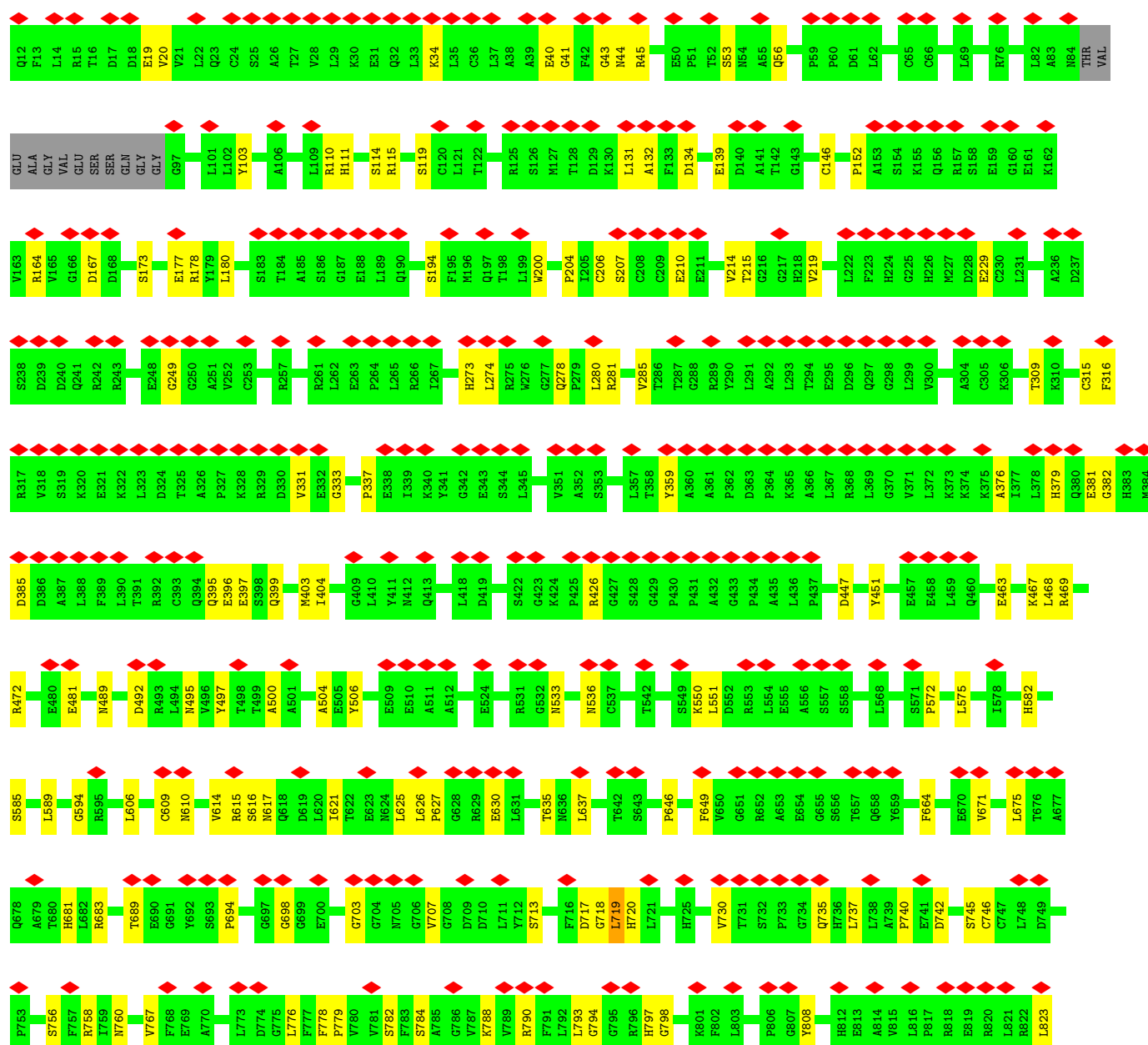
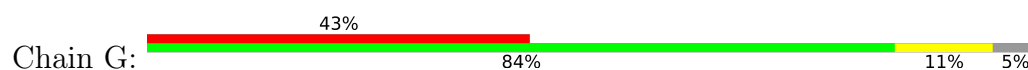




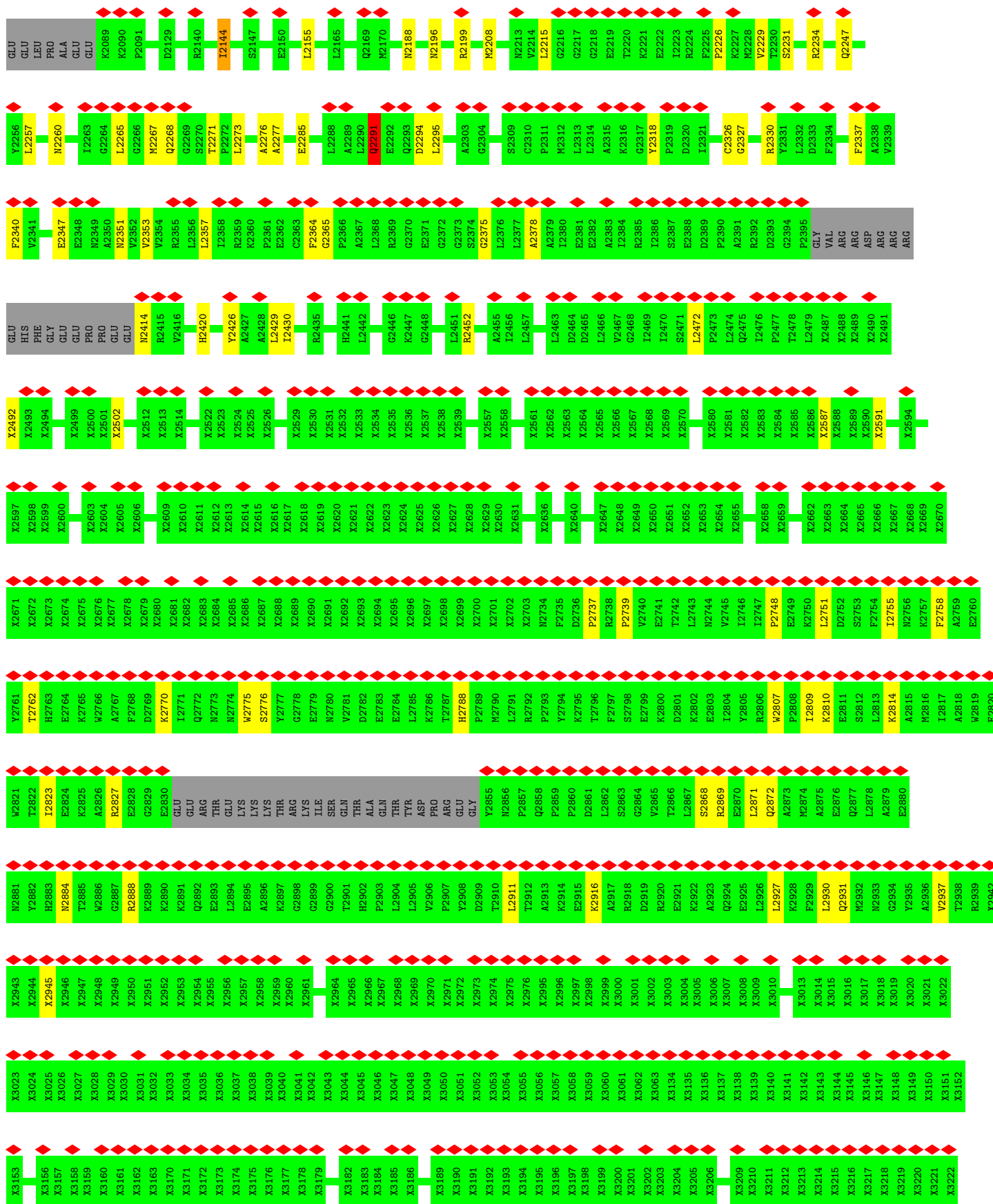
|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |    |
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| S4713 | S4714 | D4717 | K4718 | D4726 | K4727 | H4728 | D4729 | D4730 | L4731 | E4735 | R4736 | A4738 | L4741 | G4742 | M4743 | L4744 | L4745 | A4746 | S4747 | L4748 | E4749 | L4750 | T4751 | H4752 | H4753 | N4754 | E4755 | R4756 | K4757 | P4758 | D4759 | P4760 | P4761 | P4762 | G4763 | L4764 | L4765 | T4766 | H4767 | G4699 | Q4700 | H4701 | D4702 | R4703 | L4704 | L4705 | L4706 | N4707 | N4805 | N4806 | F4807 | F4808 | F4809 | L4813 |       |       |       |       |       |       |       |       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |    |
| GLY   | ALA   | GLY   | GLY   | GLY   | ASP   | GLY   | ASP   | GLY   | GLY   | N4626 | N4627 | V4628 | E4634 | S4635 | T4636 | G4637 | Y4638 | P4641 | W4644 | C4645 | L4646 | S4647 | L4648 | R4673 | E4674 | R4679 | K4680 | L4681 | E4682 | F4683 | Y4687 | I4688 | T4689 | P4760 | P4761 | P4762 | G4693 | D4694 | ASP   | D4695 | D4696 | V4697 | K4698 | C4699 | Q4700 | H4701 | D4702 | R4703 | L4704 | L4705 | L4706 | N4707 | N4805 | N4806 | F4807 | F4808 | F4809 | L4813 |       |       |       |       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |    |
| E4232 | L4233 | S4236 | E4239 | Q4250 | L4251 | S4252 | E4253 | X4320 | X4321 | X4340 | X4345 | X4346 | X4347 | D4070 | Y4071 | G4073 | S4074 | E4075 | A4076 | F4077 | Q4078 | D4079 | Y4080 | T4081 | G4082 | D4083 | P4084 | R4085 | G4086 | L4087 | I4088 | K4091 | D4092 | F4093 | Q4094 | K4095 | A4096 | M4097 | D4098 | S4099 | Q4100 | K4101 | Q4102 | F4103 | T4104 | G4105 | P4106 | E4107 | F4110 | A4117 | D4118 | N4119 | E4121 | M4122 | I4123 | F4124 | F4125 | E4126 | E4127 | F4128 | N4129 | N4130 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |    |
| R4131 | F4132 | Q4133 | E4134 | R4137 | D4138 | L4139 | N4142 | E4152 | P4155 | H4156 | D4157 | P4158 | R4159 | L4160 | R4161 | L4164 | E4165 | I4170 | F4174 | R4180 | M4184 | Q4185 | A4186 | S4187 | R4188 | R4189 | L4190 | E4191 | Y4194 | E4199 | E4206 | E4212 | R4215 | F4219 | M4223 | E4224 | G4225 | G4226 | E4227 | A4228 | E4229 | K4230 | M4231 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |    |
| F4062 | D4063 | M4064 | F4065 | L4066 | D4070 | Y4071 | G4073 | S4074 | E4075 | A4076 | F4077 | Q4078 | D4079 | Y4080 | T4081 | G4082 | D4083 | P4084 | R4085 | G4086 | L4087 | I4088 | K4091 | D4092 | F4093 | Q4094 | K4095 | A4096 | M4097 | D4098 | S4099 | Q4100 | K4101 | Q4102 | F4103 | T4104 | G4105 | P4106 | E4107 | F4110 | A4117 | D4118 | N4119 | E4121 | M4122 | I4123 | F4124 | F4125 | E4126 | E4127 | F4128 | N4129 | N4130 |       |       |       |       |       |       |       |       |       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |    |
| M3836 | L3842 | D3843 | Q3850 | A3853 | E3854 | G3855 | L3856 | G3857 | M3858 | V3859 | N3860 | E3861 | D3862 | G3863 | T3864 | V3865 | R3866 | N3867 | R3868 | Q3869 | G3871 | E3872 | L3770 | R3773 | G3774 | A3775 | V3779 | L3780 | Q3781 | K3782 | L3783 | S3784 | N3897 | D3898 | F3899 | G3908 | N3909 | T3910 | T3911 | T3912 | N3913 | N3914 | I3915 | R3925 | D3932 | Y3937 | S3938 | G3939 | K3940 | D3941 | V3942 | I3943 | E3944 | E3945 | Q3946 |       |       |       |       |       |       |       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |    |
| N3950 | N3955 | K3959 | N3963 | G3971 | P3972 | C3973 | N3976 | Q3977 | Q3978 | S3979 | L3980 | A3981 | H3982 | S3983 | R3984 | L3985 | V3986 | L3993 | H3994 | A3997 | M4000 | M4001 | K4002 | L4003 | A4004 | Q4005 | D4006 | L4017 | D4018 | L4019 | D4022 | L4030 | L4031 | E4032 | G4033 | M4034 | V4035 | M4037 | G4038 | E4050 | M4057 | L4058 | L4059 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |    |
| F4062 | D4063 | M4064 | F4065 | L4066 | D4070 | Y4071 | G4073 | S4074 | E4075 | A4076 | F4077 | Q4078 | D4079 | Y4080 | T4081 | G4082 | D4083 | P4084 | R4085 | G4086 | L4087 | I4088 | K4091 | D4092 | F4093 | Q4094 | K4095 | A4096 | M4097 | D4098 | S4099 | Q4100 | K4101 | Q4102 | F4103 | T4104 | G4105 | P4106 | E4107 | F4110 | A4117 | D4118 | N4119 | E4121 | M4122 | I4123 | F4124 | F4125 | E4126 | E4127 | F4128 | N4129 | N4130 |       |       |       |       |       |       |       |       |       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |    |
| R4131 | F4132 | Q4133 | E4134 | R4137 | D4138 | L4139 | N4142 | E4152 | P4155 | H4156 | D4157 | P4158 | R4159 | L4160 | R4161 | L4164 | E4165 | I4170 | F4174 | R4180 | M4184 | Q4185 | A4186 | S4187 | R4188 | R4189 | L4190 | E4191 | Y4194 | E4199 | E4206 | E4212 | R4215 | F4219 | M4223 | E4224 | G4225 | G4226 | E4227 | A4228 | E4229 | K4230 | M4231 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | </ |



• Molecule 2: Ryanodine receptor 1







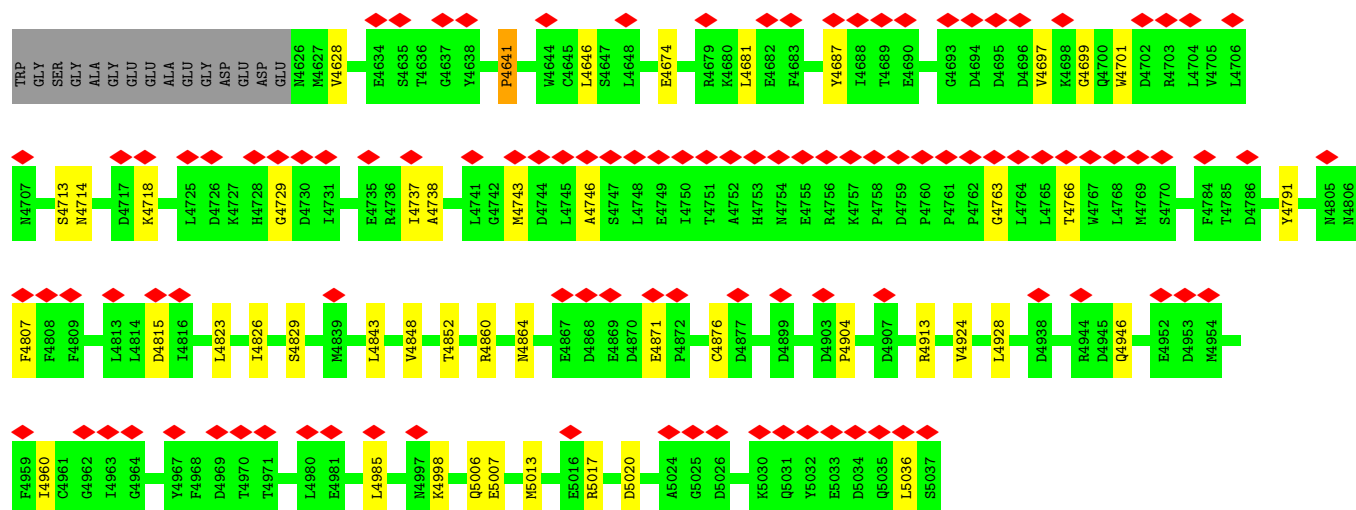




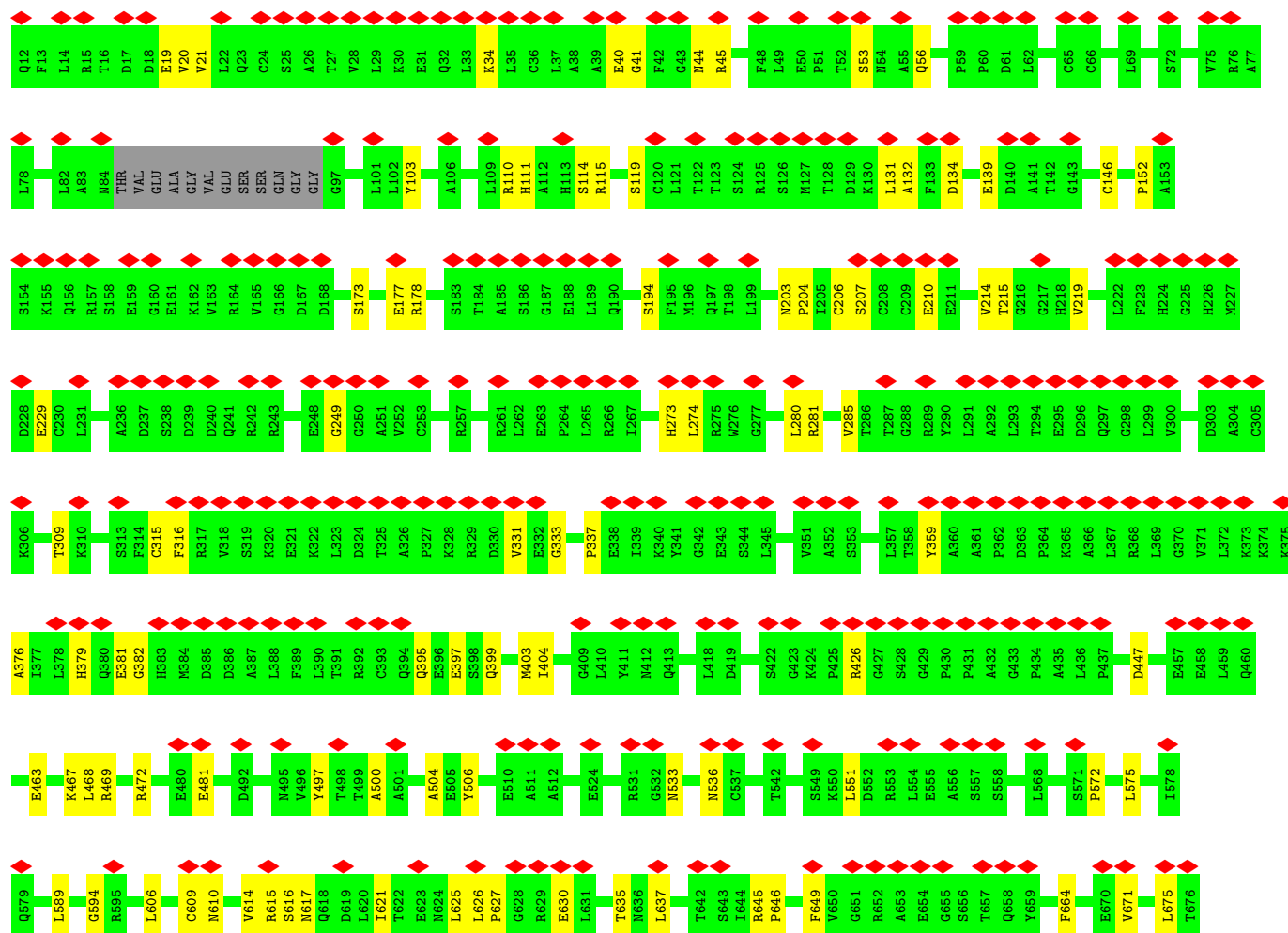
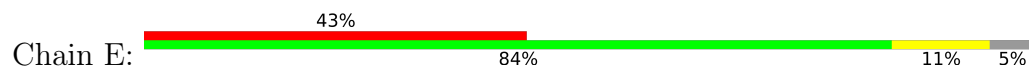


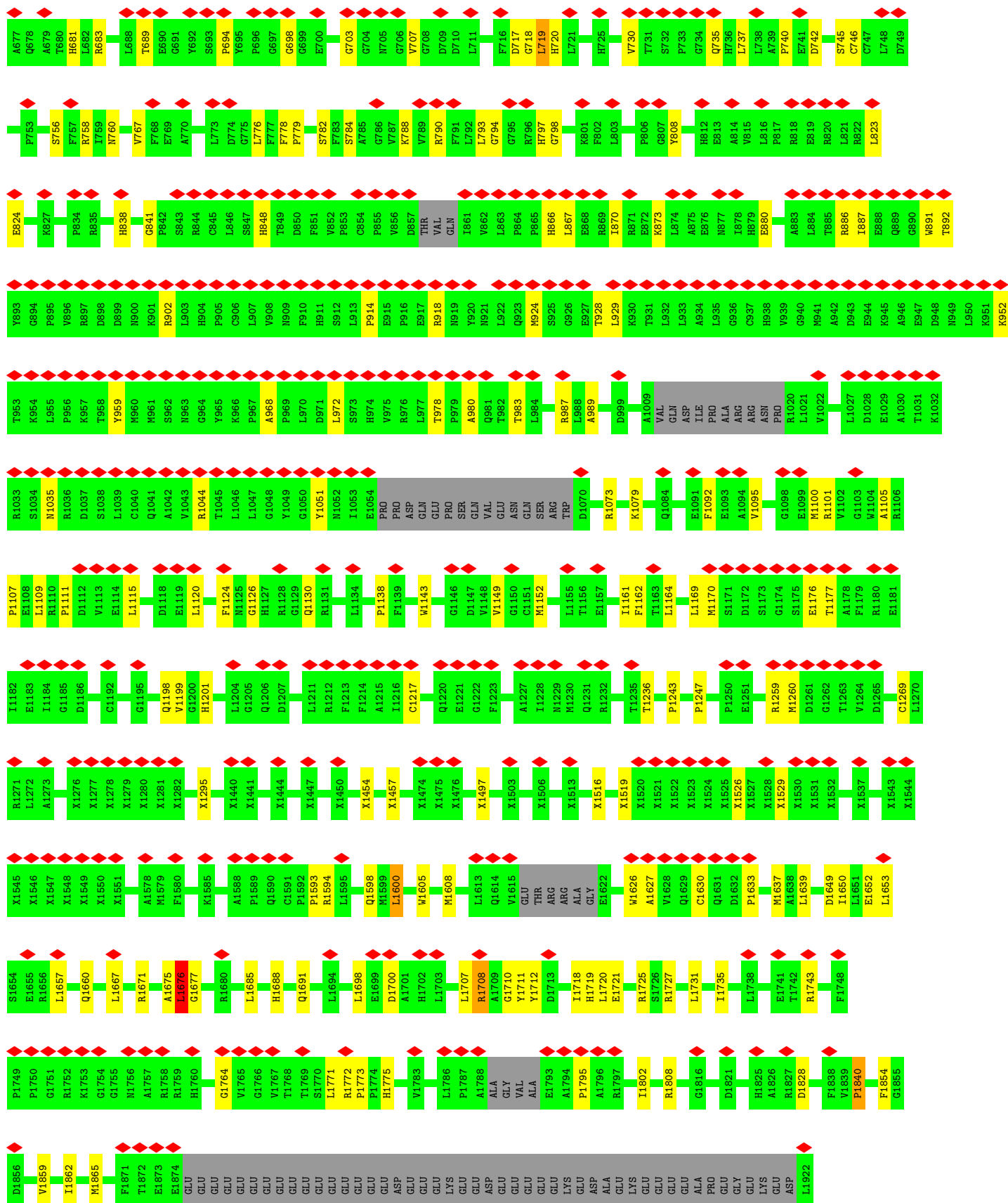


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| X3190 | X3191 | X3192 | X3193 | X3194 | X3195 | X3196 | X3197 | X3200 | X3201 | X3202 | X3203 | X3204 | X3207 | X3208 | X3209 | X3210 | X3211 | X3212 | X3213 | X3214 | X3215 | X3216 | X3217 | X3218 | X3219 | X3220 | X3221 | X3222 | X3223 | X3224 | X3225 | X3226 | X3227 | X3228 | X3229 | X3230 | X3231 | X3232 | X3233 | X3234 | X3235 | X3236 | X3241 | X3242 | X3243 | X3244 | X3245 | X3246 | X3247 | X3248 | X3249 | X3250 | X3251 | X3252 | X3253 | X3254 | X3261 |       |       |
| X3262 | X3263 | X3264 | X3265 | X3266 | X3267 | X3268 | X3269 | X3270 | X3271 | X3272 | X3273 | X3274 | X3275 | X3276 | X3277 | X3278 | X3279 | X3280 | X3281 | X3282 | X3283 | X3284 | X3285 | X3286 | X3287 | X3288 | X3289 | X3290 | X3291 | X3292 | X3293 | X3294 | X3295 | X3296 | X3297 | X3298 | X3299 | X3300 | X3301 | X3302 | X3303 | X3304 | X3305 | X3306 | X3307 | X3308 | X3309 | X3310 | X3311 | X3312 | X3313 | X3314 | X3315 | X3316 | X3317 | X3318 | X3319 | X3320 | X3321 |
| X3322 | X3323 | X3324 | X3325 | X3326 | X3327 | X3328 | X3329 | X3330 | X3331 | X3332 | X3333 | X3334 | X3335 | X3336 | X3337 | X3338 | X3339 | X3340 | X3341 | X3342 | X3343 | X3344 | X3345 | X3346 | X3347 | X3348 | X3349 | X3350 | X3351 | X3352 | X3353 | X3354 | X3355 | X3356 | X3357 | X3358 | X3359 | X3360 | X3361 | X3362 | X3363 | X3364 | X3365 | X3366 | X3367 | X3368 | X3369 | X3370 | X3371 | X3372 | X3373 | X3374 | X3375 | X3376 | X3377 | X3378 | X3379 | X3380 | X3381 |
| X3382 | X3383 | X3384 | X3385 | X3386 | X3387 | X3388 | X3389 | X3390 | X3391 | X3392 | X3393 | X3394 | X3395 | X3396 | X3397 | X3398 | X3399 | X3400 | X3401 | X3402 | X3403 | X3404 | X3405 | X3406 | X3407 | X3408 | X3409 | X3410 | X3411 | X3412 | X3413 | X3414 | X3417 | X3418 | X3419 | X3420 | X3421 | X3422 | X3423 | X3426 | X3427 | X3428 | X3429 | X3430 | X3431 | X3432 | X3433 | X3434 | X3435 | X3436 | X3437 | X3438 | X3439 | X3440 | X3441 | X3442 | X3443 |       |       |
| X3446 | X3450 | X3451 | X3452 | X3453 | X3454 | X3455 | X3456 | X3457 | X3458 | X3459 | X3463 | X3464 | X3465 | X3466 | X3467 | X3468 | X3511 | X3512 | X3513 | X3514 | X3515 | X3516 | X3517 | X3518 | X3519 | X3520 | X3521 | X3522 | X3523 | X3524 | X3525 | X3526 | X3527 | X3528 | X3529 | X3530 | X3531 | X3532 | X3533 | X3534 | X3535 | X3536 | X3537 | X3538 | X3539 | X3540 | X3541 | X3542 | X3543 | X3544 | X3545 | X3546 | X3547 | X3548 | X3549 | X3550 |       |       |       |
| X3551 | X3552 | X3553 | X3554 | X3555 | X3556 | X3557 | X3558 | X3559 | X3560 | X3561 | X3562 | X3563 | X3564 | X3565 | X3566 | X3567 | X3568 | X3569 | X3570 | X3571 | X3572 | X3573 | X3574 | X3577 | X3578 | X3579 | X3580 | X3581 | X3582 | X3583 | X3584 | X3585 | X3586 | X3587 | X3588 | X3589 | X3590 | X3591 | X3592 | X3595 | X3596 | X3597 | X3598 | X3599 | X3600 | X3601 | X3604 | X3605 | X3606 | X3607 | X3608 | X3609 | X3610 | X3611 | X3612 | X3613 |       |       |       |
| N3643 | L3644 | S3656 | GLU   | X3657 | X3658 | X3659 | X3660 | X3661 | X3662 | X3663 | X3664 | X3665 | X3666 | H3667 | S3668 | F3669 | I3674 | D3675 | D3676 | A3680 | G3681 | E3682 | Q3683 | E3684 | E3685 | E3686 | E3687 | E3688 | E3689 | V3690 | E3691 | E3692 | K3693 | K3694 | R3707 | E3712 | K3713 | S3714 | K3715 | D3716 | L3717 | E3718 | Y3722 | M3723 | I3728 | C3733 | H3734 | L3735 | E3736 | E3737 | G3738 |       |       |       |       |       |       |       |       |
| G3739 | E3740 | N3741 | GLY   | ALA   | GLU   | GLU   | E3747 | E3748 | V3749 | E3750 | V3751 | S3752 | F3753 | E3754 | E3755 | K3756 | Q3761 | R3762 | Q3766 | R3769 | L3770 | R3773 | G3774 | A3775 | M3778 | V3779 | L3780 | Q3781 | M3782 | L3783 | S3784 | L3804 | L3805 | N3809 | L3817 | K3821 | D3822 | E3825 | V3826 | G3827 | F3828 | F3829 | Q3830 | Q3833 | M3836 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| L3842 | D3843 | Q3850 | A3853 | E3854 | G3855 | L3856 | G3857 | G3858 | V3859 | N3860 | E3861 | D3862 | G3863 | T3864 | V3865 | I3866 | N3867 | R3868 | Q3869 | G3871 | E3872 | K3873 | V3874 | D3878 | R3886 | N3897 | D3898 | F3899 | G3908 | N3909 | T3910 | T3911 | T3912 | L3913 | N3914 | L3915 | R3925 | D3932 | Y3937 | S3938 | G3939 | K3940 | D3941 | V3942 | L3943 | E3944 | E3945 | Q3946 |       |       |       |       |       |       |       |       |       |       |       |
| N3950 | M3955 | K3959 | N3963 | G3971 | F3972 | C3973 | N3976 | Q3977 | Q3978 | S3979 | L3980 | A3981 | H3982 | S3983 | R3984 | L3985 | W3986 | L3993 | H3994 | M4000 | M4001 | K4002 | L4003 | A4004 | Q4005 | D4006 | L4017 | D4018 | L4019 | D4022 | L4030 | L4031 | E4032 | G4033 | M4034 | V4035 | V4036 | M4037 | C4038 | E4050 | M4057 | L4058 | L4059 | F4062 | D4063 | M4064 |       |       |       |       |       |       |       |       |       |       |       |       |       |
| F4065 | L4066 | D4070 | I4071 | V4072 | G4073 | E4075 | A4076 | Q4077 | D4079 | V4080 | V4081 | T4082 | D4083 | P4084 | R4085 | G4086 | L4087 | T4088 | K4091 | D4092 | F4093 | Q4094 | K4095 | A4096 | M4097 | D4098 | S4099 | Q4100 | K4101 | Q4102 | F4103 | T4104 | G4105 | P4106 | E4107 | F4110 | A4117 | D4118 | E4119 | N4120 | E4121 | M4122 | T4123 | N4124 | F4125 | E4126 | E4127 | F4128 | A4129 | N4130 | R4131 | F4132 | Q4133 |       |       |       |       |       |       |
| E4134 | R4137 | D4138 | I4139 | N4142 | E4152 | P4155 | H4156 | D4157 | P4158 | R4159 | L4160 | R4161 | L4164 | E4165 | I4170 | F4174 | R4180 | M4184 | G4185 | A4186 | S4187 | R4188 | R4189 | I4190 | E4191 | Y4194 | E4199 | E4206 | E4212 | R4215 | F4219 | N4223 | E4224 | G4225 | G4226 | E4227 | A4228 | E4229 | K4230 | M4231 | E4232 | L4233 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |
| S4236 | E4239 | I4242 | Q4246 | Q4250 | I4251 | S4252 | E4253 | E4254 | E4259 | X4321 | X4331 | X4340 | X4345 | F4540 | W4541 | O4542 | E4543 | L4544 | E4545 | F4551 | L4569 | V4582 | S4583 | D4584 | S4585 | P4586 | P4587 | GLY   | GLU   | ASP   | ASP   | MET   | GLU   | GLY   | SER   | ALA   | ALA   | GLY   | ASP   | LEU   | ALA   | GLY   | ALA   | SER   | GLY   | GLY   | GLY   | SER   | GLY   |       |       |       |       |       |       |       |       |       |       |



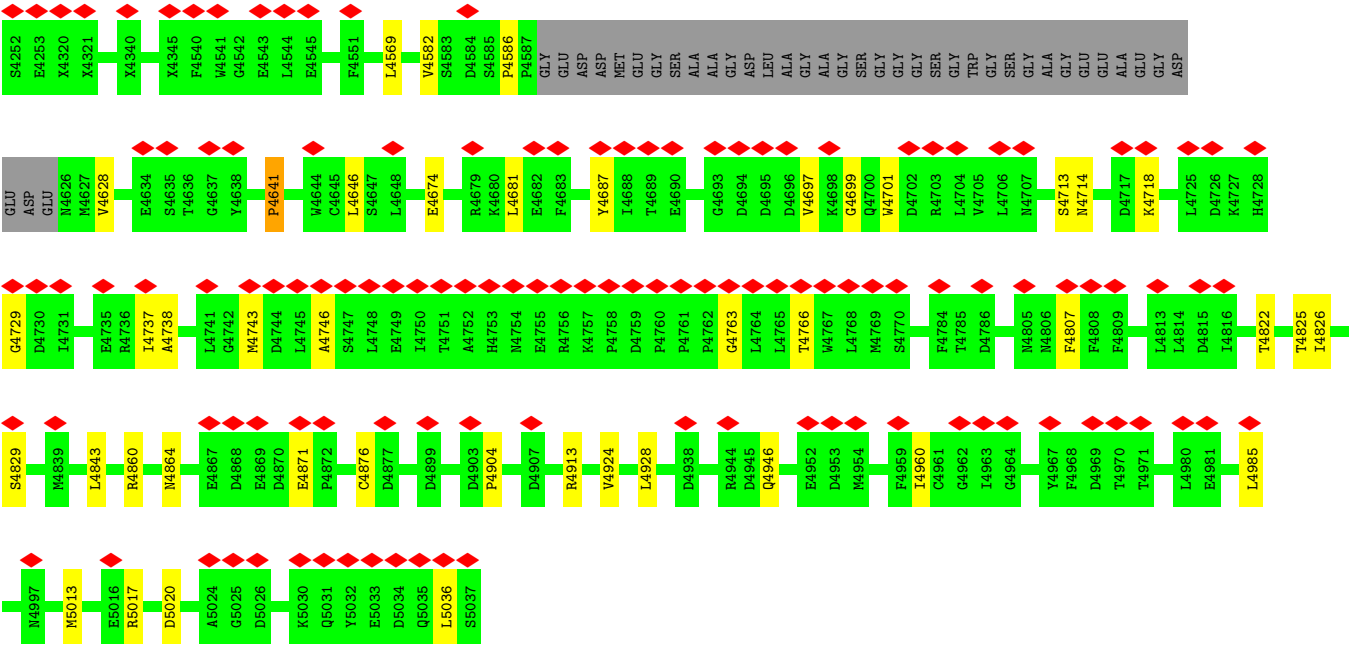
• Molecule 2: Ryanodine receptor 1





|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|
| X2967 | X2968 | X2969 | X2970 | X2971 | X2972 | X2973 | X2974 | X2975 | X2976 | X2977 | X2978 | X2979 | X3000 | X3001 | X3002 | X3003 | X3004 | X3005 | X3006 | X3007 | X3008 | X3012 | X3013 | X3014 | X3015 | X3016 | X3017 | X3018 | X3019 | X3020 | X3021 | X3022 | X3023 | X3024 | X3025 | X3026 | X3027 | X3028 | X3029 | X3030 | X3031 | X3032 | X3033 | X3034 | X3035 | X3036 | X3037 | X3038 | X3039 | X3040 | X3041 | X3042 | X3043 | X3044 | X3045 | X3046 |       |       |       |       |     |     |     |
| L2904 | L2905 | V2906 | P2907 | V2908 | D2909 | T2910 | L2911 | T2912 | A2913 | K2914 | E2915 | Y2916 | A2917 | R2918 | D2919 | R2920 | E2921 | K2922 | A2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | P2929 | L2930 | Q2931 | M2932 | N2933 | G2934 | Y2935 | A2936 | Y2937 | T2938 | R2939 | X2940 | X2941 | X2942 | X2943 | X2944 | X2945 | X2946 | X2947 | X2948 | X2949 | X2950 | X2951 | X2952 | X2953 | X2954 | X2955 | X2956 | X2957 | X2958 | X2959 | X2960 | X2961 | X2964 | X2965 | X2966 |     |     |     |
| GLN   | THR   | ALA   | GLN   | THR   | T2787 | H2788 | P2789 | M2790 | L2791 | K2792 | P2793 | Y2794 | K2795 | T2796 | F2797 | S2798 | E2799 | D2800 | K2801 | K2802 | E2803 | L2804 | Y2805 | E2806 | W2807 | P2808 | L2809 | K2810 | E2811 | S2812 | L2813 | K2814 | A2815 | L2816 | L2817 | A2818 | W2819 | E2820 | W2821 | T2822 | L2823 | E2824 | K2825 | A2826 | E2827 | E2828 | G2829 | E2830 | GLU   | GLU   | ARG   | THR   | GLU   | LVS   | LVS   | THR   | G2898 | G2899 | G2900 | ARG   | LVS | ILE | SER |
| R2140 | L2144 | S2147 | E2150 | L2155 | Q2169 | M2170 | N2188 | N2196 | R2199 | M2208 | N2213 | W2214 | L2215 | Q2216 | Q2217 | Q2218 | E2219 | T2220 | K2221 | E2222 | I2223 | R2224 | F2225 | P2226 | Q2227 | M2228 | V2229 | T2230 | S2231 | R2234 | Q2247 | Y2256 | L2257 | N2260 | I2263 | L2264 | L2265 | Q2266 | M2267 | Q2268 | Q2269 | S2270 | T2271 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |
| P2272 | L2273 | A2276 | A2277 | E2285 | L2286 | A2287 | L2288 | A2289 | L2290 | Q2291 | E2292 | Q2293 | D2294 | L2295 | A2303 | G2304 | S2309 | C2310 | P2311 | M2312 | L2313 | L2314 | A2315 | K2316 | G2317 | Y2318 | P2319 | D2320 | I2321 | C2326 | Q2327 | R2330 | Y2331 | L2332 | F2337 | A2338 | V2339 | F2340 | V2341 | E2347 | E2348 | N2349 | A2350 | N2351 | V2352 | L2353 | V2354 | R2355 | L2356 | L2357 | I2358 |       |       |       |       |       |       |       |       |       |     |     |     |
| R2359 | K2360 | P2361 | E2362 | C2363 | F2364 | Q2365 | P2366 | A2367 | L2368 | R2369 | G2370 | E2371 | Q2372 | G2373 | S2374 | G2375 | L2376 | L2377 | A2378 | L2379 | I2380 | E2381 | E2382 | A2383 | L2384 | R2385 | L2386 | S2387 | E2388 | D2389 | P2390 | A2391 | R2392 | D2393 | G2394 | P2395 | GLY   | VAL   | ARG   | ASP   | ARG   | ARG   | ARG   | GLU   | HIS   | PHE   | GLY   | GLU   | GLU   | PRO   | PRO   | GLU   | N2414 | R2415 | V2416 | Y2426 |       |       |       |       |     |     |     |
| K2427 | A2428 | L2429 | R2435 | H2441 | L2442 | G2446 | K2447 | G2448 | L2451 | A2455 | L2456 | L2457 | L2463 | D2464 | D2465 | L2466 | V2467 | Q2468 | L2469 | L2470 | S2471 | L2472 | P2473 | L2474 | Q2475 | L2476 | P2477 | T2478 | L2479 | K2487 | X2488 | X2489 | X2490 | X2493 | X2494 | X2500 | Y2512 | X2513 | Y2514 | X2522 | X2523 | X2524 | X2525 | X2526 | X2529 | X2530 | X2531 | X2532 |       |       |       |       |       |       |       |       |       |       |       |       |     |     |     |
| X2533 | X2534 | X2535 | X2536 | X2537 | X2538 | X2539 | X2557 | X2558 | X2561 | X2562 | X2563 | X2564 | X2565 | X2566 | X2567 | X2568 | X2569 | X2570 | X2571 | X2580 | X2581 | X2582 | X2583 | X2584 | X2585 | X2586 | X2587 | X2591 | X2594 | X2597 | X2598 | X2602 | X2603 | X2604 | X2605 | X2606 | X2607 | X2608 | X2609 | X2610 | X2611 | X2614 | X2615 | X2616 | X2617 | X2618 | X2619 | X2620 | X2621 | X2622 | X2623 |       |       |       |       |       |       |       |       |       |     |     |     |
| X2624 | X2625 | X2626 | X2627 | X2628 | X2629 | X2630 | X2631 | X2634 | X2635 | X2636 | X2640 | X2647 | X2648 | X2649 | X2650 | X2651 | X2652 | X2653 | X2654 | X2655 | X2656 | X2657 | X2658 | X2659 | X2662 | X2663 | X2664 | X2665 | X2666 | X2667 | X2668 | X2669 | X2670 | X2671 | X2672 | X2673 | X2674 | X2675 | X2676 | X2677 | X2678 | X2679 | X2680 | X2681 | X2682 | X2683 | X2684 | X2685 | X2686 | X2687 | X2688 | X2689 | X2690 | X2691 | X2692 | X2693 |       |       |       |       |     |     |     |
| X2694 | X2695 | X2696 | X2697 | X2698 | X2699 | X2700 | X2701 | X2702 | X2703 | N2734 | F2735 | D2736 | R2737 | R2738 | P2739 | V2740 | E2741 | T2742 | L2743 | N2744 | X2745 | L2746 | L2747 | P2748 | E2749 | K2750 | L2751 | D2752 | S2753 | F2754 | L2755 | N2756 | K2757 | F2758 | A2759 | E2760 | Y2761 | T2762 | H2763 | E2764 | K2765 | W2766 | A2767 | D2768 | D2769 | K2770 | I2771 | Q2772 | N2773 | M2774 | W2775 | S2776 | Y2777 | G2778 | E2779 | V2781 | D2782 | E2783 |       |       |     |     |     |
| E2784 | L2785 | K2786 | T2787 | H2788 | P2789 | M2790 | L2791 | K2792 | P2793 | Y2794 | K2795 | T2796 | F2797 | S2798 | E2799 | D2800 | K2801 | K2802 | E2803 | L2804 | Y2805 | E2806 | W2807 | P2808 | L2809 | K2810 | E2811 | S2812 | L2813 | K2814 | A2815 | L2816 | L2817 | A2818 | W2819 | E2820 | W2821 | T2822 | L2823 | E2824 | K2825 | A2826 | E2827 | E2828 | G2829 | E2830 | GLU   | GLU   | ARG   | THR   | GLU   | LVS   | LVS   | THR   | G2898 | G2899 | G2900 | ARG   | LVS   | ILE   | SER |     |     |
| GLN   | THR   | ALA   | GLN   | THR   | TYR   | ASP   | PRO   | ARG   | GLU   | GLY   | Y2855 | N2856 | P2857 | Q2858 | P2859 | P2860 | D2861 | L2862 | S2863 | G2864 | T2865 | L2866 | L2867 | S2868 | R2869 | E2870 | L2871 | Q2872 | A2873 | N2874 | A2875 | E2876 | Q2877 | L2878 | A2879 | E2880 | N2881 | X2882 | H2883 | N2884 | T2885 | W2886 | G2887 | R2888 | K2889 | K2890 | X2891 | Q2892 | E2893 | L2894 | E2895 | A2896 | Q2897 | G2898 | G2899 | G2900 | T2901 | H2902 | P2903 |       |     |     |     |
| L2904 | L2905 | V2906 | P2907 | V2908 | D2909 | T2910 | L2911 | T2912 | A2913 | K2914 | E2915 | Y2916 | A2917 | R2918 | D2919 | R2920 | E2921 | K2922 | A2923 | Q2924 | E2925 | L2926 | L2927 | K2928 | P2929 | L2930 | Q2931 | M2932 | N2933 | G2934 | Y2935 | A2936 | Y2937 | T2938 | R2939 | X2940 | X2941 | X2942 | X2943 | X2944 | X2945 | X2946 | X2947 | X2948 | X2949 | X2950 | X2951 | X2952 | X2953 | X2954 | X2955 | X2956 | X2957 | X2958 | X2959 | X2960 | X2961 | X2964 | X2965 | X2966 |     |     |     |





## 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                    | 0.110                                   | Depositor |
| Minimum map value                    | -0.053                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.04                                    | Depositor |
| Map size (Å)                         | 502.0, 502.0, 502.0                     | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 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: CA, ZN

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

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 1   | A     | 0.20         | 0/834    | 0.47        | 0/1123          |
| 1   | F     | 0.20         | 0/834    | 0.47        | 0/1123          |
| 1   | H     | 0.20         | 0/834    | 0.47        | 0/1123          |
| 1   | J     | 0.20         | 0/834    | 0.47        | 0/1123          |
| 2   | B     | 0.21         | 0/25428  | 0.51        | 2/34534 (0.0%)  |
| 2   | E     | 0.21         | 0/25428  | 0.51        | 2/34534 (0.0%)  |
| 2   | G     | 0.21         | 0/25428  | 0.51        | 2/34534 (0.0%)  |
| 2   | I     | 0.21         | 0/25428  | 0.51        | 2/34534 (0.0%)  |
| All | All   | 0.21         | 0/105048 | 0.51        | 8/142628 (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                   | 14                  |
| 2   | E     | 0                   | 14                  |
| 2   | G     | 0                   | 14                  |
| 2   | I     | 0                   | 14                  |
| All | All   | 0                   | 56                  |

There are no bond length outliers.

All (8) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|------|-------------|----------|
| 2   | I     | 2291 | GLN  | CA-C-N | 5.61 | 132.25      | 121.54   |
| 2   | I     | 2291 | GLN  | C-N-CA | 5.61 | 132.25      | 121.54   |
| 2   | B     | 2291 | GLN  | CA-C-N | 5.60 | 132.23      | 121.54   |
| 2   | B     | 2291 | GLN  | C-N-CA | 5.60 | 132.23      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|------|-------------|----------|
| 2   | E     | 2291 | GLN  | CA-C-N | 5.59 | 132.22      | 121.54   |
| 2   | E     | 2291 | GLN  | C-N-CA | 5.59 | 132.22      | 121.54   |
| 2   | G     | 2291 | GLN  | CA-C-N | 5.58 | 132.20      | 121.54   |
| 2   | G     | 2291 | GLN  | C-N-CA | 5.58 | 132.20      | 121.54   |

There are no chirality outliers.

All (56) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | B     | 139  | GLU  | Peptide |
| 2   | B     | 1676 | LEU  | Peptide |
| 2   | B     | 1720 | LEU  | Peptide |
| 2   | B     | 1795 | PRO  | Peptide |
| 2   | B     | 1828 | ASP  | Peptide |
| 2   | B     | 1840 | PRO  | 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     | 4807 | PHE  | Peptide |
| 2   | B     | 694  | PRO  | Peptide |
| 2   | B     | 808  | TYR  | Peptide |
| 2   | E     | 139  | GLU  | Peptide |
| 2   | E     | 1676 | LEU  | Peptide |
| 2   | E     | 1720 | LEU  | Peptide |
| 2   | E     | 1795 | PRO  | Peptide |
| 2   | E     | 1828 | ASP  | Peptide |
| 2   | E     | 1840 | PRO  | 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     | 4807 | PHE  | Peptide |
| 2   | E     | 694  | PRO  | Peptide |
| 2   | E     | 808  | TYR  | Peptide |
| 2   | G     | 139  | GLU  | Peptide |
| 2   | G     | 1676 | LEU  | Peptide |
| 2   | G     | 1720 | LEU  | Peptide |
| 2   | G     | 1795 | PRO  | Peptide |
| 2   | G     | 1828 | ASP  | Peptide |

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| Mol | Chain | Res  | Type | Group   |
|-----|-------|------|------|---------|
| 2   | G     | 1840 | PRO  | 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     | 4807 | PHE  | Peptide |
| 2   | G     | 694  | PRO  | Peptide |
| 2   | G     | 808  | TYR  | Peptide |
| 2   | I     | 139  | GLU  | Peptide |
| 2   | I     | 1676 | LEU  | Peptide |
| 2   | I     | 1720 | LEU  | Peptide |
| 2   | I     | 1795 | PRO  | Peptide |
| 2   | I     | 1828 | ASP  | Peptide |
| 2   | I     | 1840 | PRO  | 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     | 4807 | PHE  | Peptide |
| 2   | I     | 694  | 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      | 10      | 0            |
| 1   | F     | 818   | 0        | 824      | 12      | 0            |
| 1   | H     | 818   | 0        | 824      | 12      | 0            |
| 1   | J     | 818   | 0        | 824      | 12      | 0            |
| 2   | B     | 29499 | 0        | 24749    | 295     | 0            |
| 2   | E     | 29499 | 0        | 24749    | 266     | 0            |
| 2   | G     | 29499 | 0        | 24750    | 276     | 0            |
| 2   | I     | 29499 | 0        | 24749    | 272     | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | E     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 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            |
| 4   | G     | 1      | 0        | 0        | 0       | 0            |
| 4   | I     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 121276 | 0        | 102293   | 1137    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1137) 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:B:4968:PHE:CE2 | 2:B:4978:HIS:CE1 | 2.28                     | 1.20              |
| 2:B:4230:LYS:HD2 | 2:B:4959:PHE:HE2 | 0.99                     | 1.10              |
| 2:B:4230:LYS:HD2 | 2:B:4959:PHE:CE2 | 1.92                     | 1.04              |
| 2:B:4983:HIS:CE1 | 2:B:5027:CYS:SG  | 2.57                     | 0.98              |
| 2:B:4230:LYS:CD  | 2:B:4959:PHE:HE2 | 1.87                     | 0.87              |
| 2:B:4983:HIS:HE1 | 2:B:5027:CYS:SG  | 1.98                     | 0.85              |
| 2:I:2318:TYR:HH  | 2:I:2414:ASN:N   | 1.86                     | 0.74              |
| 2:B:4968:PHE:HE2 | 2:B:4978:HIS:CE1 | 1.98                     | 0.72              |
| 2:E:2318:TYR:HH  | 2:E:2414:ASN:N   | 1.86                     | 0.72              |
| 2:G:2318:TYR:HH  | 2:G:2414:ASN:N   | 1.87                     | 0.71              |
| 2:B:2318:TYR:HH  | 2:B:2414:ASN:N   | 1.86                     | 0.71              |
| 2:G:1260:MET:HB2 | 2:G:1269:CYS:H   | 1.57                     | 0.69              |
| 2:I:1260:MET:HB2 | 2:I:1269:CYS:H   | 1.57                     | 0.69              |
| 2:B:1260:MET:HB2 | 2:B:1269:CYS:H   | 1.57                     | 0.68              |
| 2:E:1260:MET:HB2 | 2:E:1269:CYS:H   | 1.57                     | 0.68              |
| 2:B:4968:PHE:HE2 | 2:B:4978:HIS:NE2 | 1.93                     | 0.67              |
| 2:E:111:HIS:HD2  | 2:E:114:SER:H    | 1.43                     | 0.67              |
| 2:E:379:HIS:HD2  | 2:E:382:GLY:H    | 1.43                     | 0.66              |
| 2:B:379:HIS:HD2  | 2:B:382:GLY:H    | 1.43                     | 0.66              |
| 2:G:111:HIS:HD2  | 2:G:114:SER:H    | 1.43                     | 0.66              |
| 2:B:111:HIS:HD2  | 2:B:114:SER:H    | 1.43                     | 0.66              |
| 2:G:379:HIS:HD2  | 2:G:382:GLY:H    | 1.43                     | 0.65              |
| 2:I:111:HIS:HD2  | 2:I:114:SER:H    | 1.43                     | 0.65              |
| 2:B:4968:PHE:CE2 | 2:B:4978:HIS:NE2 | 2.64                     | 0.64              |
| 2:E:1685:LEU:HA  | 2:E:1688:HIS:HD2 | 1.63                     | 0.64              |
| 2:B:1152:MET:HE1 | 2:B:1217:CYS:HB3 | 1.80                     | 0.64              |
| 2:I:1152:MET:HE1 | 2:I:1217:CYS:HB3 | 1.80                     | 0.64              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:I:379:HIS:HD2  | 2:I:382:GLY:H     | 1.43                     | 0.64              |
| 2:G:1152:MET:HE1 | 2:G:1217:CYS:HB3  | 1.80                     | 0.63              |
| 2:E:1152:MET:HE1 | 2:E:1217:CYS:HB3  | 1.80                     | 0.63              |
| 2:B:1685:LEU:HA  | 2:B:1688:HIS:HD2  | 1.63                     | 0.63              |
| 2:G:1685:LEU:HA  | 2:G:1688:HIS:HD2  | 1.63                     | 0.62              |
| 2:I:1685:LEU:HA  | 2:I:1688:HIS:HD2  | 1.63                     | 0.62              |
| 2:B:1170:MET:HE1 | 2:B:1176:GLU:HG3  | 1.82                     | 0.62              |
| 2:I:1079:LYS:NZ  | 2:I:1107:PRO:O    | 2.33                     | 0.62              |
| 2:B:1079:LYS:NZ  | 2:B:1107:PRO:O    | 2.33                     | 0.62              |
| 2:G:1170:MET:HE1 | 2:G:1176:GLU:HG3  | 1.82                     | 0.62              |
| 2:G:4860:ARG:HD2 | 2:I:4582:VAL:HG11 | 1.81                     | 0.62              |
| 2:B:1637:MET:SD  | 2:B:1708:ARG:NH1  | 2.74                     | 0.61              |
| 2:G:3937:TYR:O   | 2:G:4002:LYS:NZ   | 2.34                     | 0.61              |
| 2:E:1637:MET:SD  | 2:E:1708:ARG:NH1  | 2.74                     | 0.61              |
| 2:G:1079:LYS:NZ  | 2:G:1107:PRO:O    | 2.33                     | 0.61              |
| 2:B:683:ARG:NH1  | 2:B:707:VAL:O     | 2.34                     | 0.61              |
| 2:E:1079:LYS:NZ  | 2:E:1107:PRO:O    | 2.33                     | 0.61              |
| 2:B:3937:TYR:O   | 2:B:4002:LYS:NZ   | 2.34                     | 0.60              |
| 2:I:1170:MET:HE1 | 2:I:1176:GLU:HG3  | 1.82                     | 0.60              |
| 2:E:614:VAL:HG22 | 2:E:616:SER:H     | 1.66                     | 0.60              |
| 2:B:110:ARG:HH21 | 2:B:115:ARG:HB3   | 1.67                     | 0.60              |
| 2:I:1637:MET:SD  | 2:I:1708:ARG:NH1  | 2.74                     | 0.60              |
| 2:G:1637:MET:SD  | 2:G:1708:ARG:NH1  | 2.74                     | 0.60              |
| 2:G:1721:GLU:OE2 | 2:G:1725:ARG:NH2  | 2.34                     | 0.60              |
| 2:I:3937:TYR:O   | 2:I:4002:LYS:NZ   | 2.34                     | 0.60              |
| 2:E:110:ARG:HH21 | 2:E:115:ARG:HB3   | 1.67                     | 0.60              |
| 2:B:614:VAL:HG22 | 2:B:616:SER:H     | 1.66                     | 0.60              |
| 2:G:683:ARG:NH1  | 2:G:707:VAL:O     | 2.34                     | 0.60              |
| 2:E:1170:MET:HE1 | 2:E:1176:GLU:HG3  | 1.82                     | 0.60              |
| 2:E:2022:PRO:O   | 2:E:2028:ARG:NH2  | 2.35                     | 0.60              |
| 2:E:3937:TYR:O   | 2:E:4002:LYS:NZ   | 2.34                     | 0.60              |
| 2:I:132:ALA:HA   | 2:I:194:SER:HB2   | 1.83                     | 0.60              |
| 2:G:614:VAL:HG22 | 2:G:616:SER:H     | 1.66                     | 0.60              |
| 2:G:132:ALA:HA   | 2:G:194:SER:HB2   | 1.83                     | 0.60              |
| 2:E:1721:GLU:OE2 | 2:E:1725:ARG:NH2  | 2.34                     | 0.60              |
| 2:B:1721:GLU:OE2 | 2:B:1725:ARG:NH2  | 2.34                     | 0.60              |
| 2:I:173:SER:HB3  | 2:I:178:ARG:H     | 1.67                     | 0.60              |
| 2:I:1721:GLU:OE2 | 2:I:1725:ARG:NH2  | 2.34                     | 0.59              |
| 2:I:683:ARG:NH1  | 2:I:707:VAL:O     | 2.34                     | 0.59              |
| 2:I:2022:PRO:O   | 2:I:2028:ARG:NH2  | 2.35                     | 0.59              |
| 2:G:173:SER:HB3  | 2:G:178:ARG:H     | 1.67                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:173:SER:HB3   | 2:B:178:ARG:H     | 1.67                     | 0.59              |
| 2:I:110:ARG:HH21  | 2:I:115:ARG:HB3   | 1.67                     | 0.59              |
| 2:B:4582:VAL:HG11 | 2:I:4860:ARG:HD2  | 1.83                     | 0.59              |
| 2:G:110:ARG:HH21  | 2:G:115:ARG:HB3   | 1.67                     | 0.59              |
| 2:B:132:ALA:HA    | 2:B:194:SER:HB2   | 1.83                     | 0.59              |
| 2:E:132:ALA:HA    | 2:E:194:SER:HB2   | 1.83                     | 0.59              |
| 2:E:1667:LEU:HD23 | 2:E:1671:ARG:HH12 | 1.68                     | 0.59              |
| 2:G:1667:LEU:HD23 | 2:G:1671:ARG:HH12 | 1.68                     | 0.59              |
| 2:I:315:CYS:SG    | 2:I:316:PHE:N     | 2.76                     | 0.59              |
| 2:I:614:VAL:HG22  | 2:I:616:SER:H     | 1.66                     | 0.59              |
| 2:G:315:CYS:SG    | 2:G:316:PHE:N     | 2.76                     | 0.58              |
| 2:E:683:ARG:NH1   | 2:E:707:VAL:O     | 2.34                     | 0.58              |
| 2:I:40:GLU:HB3    | 2:I:44:ASN:HB3    | 1.85                     | 0.58              |
| 2:E:4674:GLU:HG3  | 2:E:4714:ASN:HB3  | 1.85                     | 0.58              |
| 2:B:40:GLU:HB3    | 2:B:44:ASN:HB3    | 1.85                     | 0.58              |
| 2:E:315:CYS:SG    | 2:E:316:PHE:N     | 2.76                     | 0.58              |
| 2:G:2022:PRO:O    | 2:G:2028:ARG:NH2  | 2.35                     | 0.58              |
| 2:E:173:SER:HB3   | 2:E:178:ARG:H     | 1.67                     | 0.58              |
| 2:B:315:CYS:SG    | 2:B:316:PHE:N     | 2.76                     | 0.58              |
| 2:G:4104:THR:HG22 | 2:G:4106:PRO:HD2  | 1.86                     | 0.58              |
| 2:I:4104:THR:HG22 | 2:I:4106:PRO:HD2  | 1.86                     | 0.58              |
| 2:I:4674:GLU:HG3  | 2:I:4714:ASN:HB3  | 1.85                     | 0.58              |
| 2:B:1667:LEU:HD23 | 2:B:1671:ARG:HH12 | 1.68                     | 0.58              |
| 2:B:4860:ARG:HD2  | 2:E:4582:VAL:HG11 | 1.84                     | 0.58              |
| 2:E:4223:ASN:OD1  | 2:E:4946:GLN:NE2  | 2.37                     | 0.58              |
| 1:J:42:ARG:HG2    | 2:I:1691:GLN:HG2  | 1.86                     | 0.57              |
| 2:B:2022:PRO:O    | 2:B:2028:ARG:NH2  | 2.35                     | 0.57              |
| 2:I:4223:ASN:OD1  | 2:I:4946:GLN:NE2  | 2.37                     | 0.57              |
| 2:B:229:GLU:HA    | 2:B:249:GLY:HA2   | 1.87                     | 0.57              |
| 2:B:4674:GLU:HG3  | 2:B:4714:ASN:HB3  | 1.85                     | 0.57              |
| 2:B:497:TYR:HB3   | 2:B:500:ALA:HB2   | 1.87                     | 0.57              |
| 2:B:4104:THR:HG22 | 2:B:4106:PRO:HD2  | 1.86                     | 0.57              |
| 2:G:497:TYR:HB3   | 2:G:500:ALA:HB2   | 1.87                     | 0.57              |
| 2:G:4674:GLU:HG3  | 2:G:4714:ASN:HB3  | 1.85                     | 0.57              |
| 2:E:497:TYR:HB3   | 2:E:500:ALA:HB2   | 1.87                     | 0.57              |
| 2:B:4223:ASN:OD1  | 2:B:4946:GLN:NE2  | 2.37                     | 0.57              |
| 2:E:229:GLU:HA    | 2:E:249:GLY:HA2   | 1.87                     | 0.57              |
| 2:G:3762:ARG:O    | 2:G:3766:GLN:NE2  | 2.38                     | 0.57              |
| 2:G:4223:ASN:OD1  | 2:G:4946:GLN:NE2  | 2.37                     | 0.57              |
| 2:I:3762:ARG:O    | 2:I:3766:GLN:NE2  | 2.38                     | 0.57              |
| 2:E:40:GLU:HB3    | 2:E:44:ASN:HB3    | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:497:TYR:HB3   | 2:I:500:ALA:HB2   | 1.87                     | 0.57              |
| 2:I:989:ALA:O     | 2:I:1035:ASN:ND2  | 2.38                     | 0.57              |
| 2:E:683:ARG:HB2   | 2:E:782:SER:HB3   | 1.87                     | 0.57              |
| 2:E:4104:THR:HG22 | 2:E:4106:PRO:HD2  | 1.86                     | 0.57              |
| 2:I:1667:LEU:HD23 | 2:I:1671:ARG:HH12 | 1.68                     | 0.57              |
| 2:E:2748:PRO:HD2  | 2:E:2751:LEU:HD12 | 1.87                     | 0.57              |
| 2:B:683:ARG:HB2   | 2:B:782:SER:HB3   | 1.87                     | 0.57              |
| 2:E:609:CYS:SG    | 2:E:610:ASN:N     | 2.78                     | 0.57              |
| 2:B:2326:CYS:SG   | 2:B:2327:GLY:N    | 2.78                     | 0.56              |
| 2:B:2748:PRO:HD2  | 2:B:2751:LEU:HD12 | 1.87                     | 0.56              |
| 2:B:3762:ARG:O    | 2:B:3766:GLN:NE2  | 2.38                     | 0.56              |
| 2:I:2748:PRO:HD2  | 2:I:2751:LEU:HD12 | 1.87                     | 0.56              |
| 2:B:609:CYS:SG    | 2:B:610:ASN:N     | 2.78                     | 0.56              |
| 2:B:2827:ARG:HH21 | 2:B:2931:GLN:HG3  | 1.70                     | 0.56              |
| 2:G:683:ARG:HB2   | 2:G:782:SER:HB3   | 1.87                     | 0.56              |
| 2:G:2748:PRO:HD2  | 2:G:2751:LEU:HD12 | 1.87                     | 0.56              |
| 2:I:2291:GLN:HB2  | 2:I:2295:LEU:HG   | 1.88                     | 0.56              |
| 2:I:2326:CYS:SG   | 2:I:2327:GLY:N    | 2.78                     | 0.56              |
| 2:B:1259:ARG:HH12 | 2:B:1593:PRO:HA   | 1.70                     | 0.56              |
| 2:B:2291:GLN:HB2  | 2:B:2295:LEU:HG   | 1.88                     | 0.56              |
| 2:G:229:GLU:HA    | 2:G:249:GLY:HA2   | 1.87                     | 0.56              |
| 2:I:229:GLU:HA    | 2:I:249:GLY:HA2   | 1.87                     | 0.56              |
| 2:E:2827:ARG:HH21 | 2:E:2931:GLN:HG3  | 1.70                     | 0.56              |
| 2:B:1764:GLY:HA3  | 2:B:1859:VAL:HG11 | 1.87                     | 0.56              |
| 2:G:40:GLU:HB3    | 2:G:44:ASN:HB3    | 1.85                     | 0.56              |
| 2:E:788:LYS:HG2   | 2:E:1630:CYS:H    | 1.71                     | 0.56              |
| 2:E:1259:ARG:HH12 | 2:E:1593:PRO:HA   | 1.70                     | 0.56              |
| 2:G:609:CYS:SG    | 2:G:610:ASN:N     | 2.78                     | 0.56              |
| 2:G:2291:GLN:HB2  | 2:G:2295:LEU:HG   | 1.88                     | 0.56              |
| 2:I:646:PRO:HD2   | 2:I:779:PRO:HB2   | 1.87                     | 0.56              |
| 2:I:4860:ARG:HG3  | 2:I:4876:CYS:HB3  | 1.88                     | 0.56              |
| 2:B:4860:ARG:HG3  | 2:B:4876:CYS:HB3  | 1.88                     | 0.56              |
| 2:G:972:LEU:O     | 2:G:1044:ARG:NH2  | 2.39                     | 0.56              |
| 2:G:989:ALA:O     | 2:G:1035:ASN:ND2  | 2.38                     | 0.56              |
| 2:G:2326:CYS:SG   | 2:G:2327:GLY:N    | 2.78                     | 0.56              |
| 2:I:1519:UNK:HA   | 2:I:1526:UNK:HA   | 1.88                     | 0.56              |
| 2:E:1109:LEU:HA   | 2:E:1120:LEU:HD21 | 1.87                     | 0.56              |
| 2:E:2326:CYS:SG   | 2:E:2327:GLY:N    | 2.78                     | 0.56              |
| 2:B:646:PRO:HD2   | 2:B:779:PRO:HB2   | 1.87                     | 0.56              |
| 2:E:1519:UNK:HA   | 2:E:1526:UNK:HA   | 1.88                     | 0.56              |
| 2:G:1109:LEU:HA   | 2:G:1120:LEU:HD21 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1519:UNK:HA   | 2:G:1526:UNK:HA   | 1.88                     | 0.56              |
| 2:I:683:ARG:HB2   | 2:I:782:SER:HB3   | 1.87                     | 0.56              |
| 2:I:1764:GLY:HA3  | 2:I:1859:VAL:HG11 | 1.87                     | 0.56              |
| 2:B:1519:UNK:HA   | 2:B:1526:UNK:HA   | 1.88                     | 0.56              |
| 2:I:609:CYS:SG    | 2:I:610:ASN:N     | 2.78                     | 0.56              |
| 2:B:745:SER:HB2   | 2:B:758:ARG:HB3   | 1.89                     | 0.55              |
| 2:B:1691:GLN:HE22 | 2:B:1802:ILE:HG12 | 1.71                     | 0.55              |
| 2:B:4982:GLU:OE1  | 2:B:4982:GLU:HA   | 2.06                     | 0.55              |
| 2:G:4860:ARG:HG3  | 2:G:4876:CYS:HB3  | 1.88                     | 0.55              |
| 2:I:1691:GLN:HE22 | 2:I:1802:ILE:HG12 | 1.71                     | 0.55              |
| 2:E:646:PRO:HD2   | 2:E:779:PRO:HB2   | 1.87                     | 0.55              |
| 2:E:1691:GLN:HE22 | 2:E:1802:ILE:HG12 | 1.71                     | 0.55              |
| 2:E:3762:ARG:O    | 2:E:3766:GLN:NE2  | 2.38                     | 0.55              |
| 2:B:626:LEU:HD23  | 2:B:630:GLU:H     | 1.71                     | 0.55              |
| 2:B:788:LYS:HG2   | 2:B:1630:CYS:H    | 1.71                     | 0.55              |
| 2:G:1259:ARG:HH12 | 2:G:1593:PRO:HA   | 1.70                     | 0.55              |
| 2:I:745:SER:HB2   | 2:I:758:ARG:HB3   | 1.88                     | 0.55              |
| 2:E:972:LEU:O     | 2:E:1044:ARG:NH2  | 2.39                     | 0.55              |
| 2:E:2291:GLN:HB2  | 2:E:2295:LEU:HG   | 1.88                     | 0.55              |
| 2:G:745:SER:HB2   | 2:G:758:ARG:HB3   | 1.88                     | 0.55              |
| 2:I:2770:LYS:HB3  | 2:I:2775:TRP:HB2  | 1.88                     | 0.55              |
| 2:B:1109:LEU:HA   | 2:B:1120:LEU:HD21 | 1.87                     | 0.55              |
| 2:G:2770:LYS:HB3  | 2:G:2775:TRP:HB2  | 1.89                     | 0.55              |
| 2:E:2347:GLU:O    | 2:E:2351:ASN:N    | 2.40                     | 0.55              |
| 2:G:626:LEU:HD23  | 2:G:630:GLU:H     | 1.71                     | 0.55              |
| 2:G:2827:ARG:HH21 | 2:G:2931:GLN:HG3  | 1.70                     | 0.55              |
| 2:I:1259:ARG:HH12 | 2:I:1593:PRO:HA   | 1.70                     | 0.55              |
| 2:E:626:LEU:HD23  | 2:E:630:GLU:H     | 1.71                     | 0.55              |
| 2:G:788:LYS:HG2   | 2:G:1630:CYS:H    | 1.71                     | 0.55              |
| 2:E:4860:ARG:HG3  | 2:E:4876:CYS:HB3  | 1.88                     | 0.55              |
| 2:G:2347:GLU:O    | 2:G:2351:ASN:N    | 2.40                     | 0.55              |
| 2:E:1764:GLY:HA3  | 2:E:1859:VAL:HG11 | 1.87                     | 0.55              |
| 2:B:972:LEU:O     | 2:B:1044:ARG:NH2  | 2.39                     | 0.55              |
| 2:B:2737:PRO:O    | 2:B:2888:ARG:NH2  | 2.40                     | 0.55              |
| 2:I:103:TYR:HB3   | 2:I:152:PRO:HD3   | 1.89                     | 0.55              |
| 2:E:745:SER:HB2   | 2:E:758:ARG:HB3   | 1.88                     | 0.55              |
| 2:G:646:PRO:HD2   | 2:G:779:PRO:HB2   | 1.87                     | 0.55              |
| 2:G:1764:GLY:HA3  | 2:G:1859:VAL:HG11 | 1.87                     | 0.55              |
| 2:I:1109:LEU:HA   | 2:I:1120:LEU:HD21 | 1.87                     | 0.55              |
| 2:E:1671:ARG:NH2  | 2:E:1710:GLY:O    | 2.40                     | 0.55              |
| 2:B:1671:ARG:NH2  | 2:B:1710:GLY:O    | 2.40                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1691:GLN:HE22 | 2:G:1802:ILE:HG12 | 1.71                     | 0.54              |
| 2:I:626:LEU:HD23  | 2:I:630:GLU:H     | 1.71                     | 0.54              |
| 2:B:103:TYR:HB3   | 2:B:152:PRO:HD3   | 1.89                     | 0.54              |
| 1:H:42:ARG:HG2    | 2:G:1691:GLN:HG2  | 1.90                     | 0.54              |
| 2:B:2770:LYS:HB3  | 2:B:2775:TRP:HB2  | 1.88                     | 0.54              |
| 2:B:3981:ALA:HA   | 2:B:3986:TRP:HE1  | 1.72                     | 0.54              |
| 2:I:1671:ARG:NH2  | 2:I:1710:GLY:O    | 2.40                     | 0.54              |
| 2:I:2827:ARG:HH21 | 2:I:2931:GLN:HG3  | 1.70                     | 0.54              |
| 2:E:989:ALA:O     | 2:E:1035:ASN:ND2  | 2.38                     | 0.54              |
| 2:E:730:VAL:O     | 2:E:735:GLN:NE2   | 2.41                     | 0.54              |
| 2:G:103:TYR:HB3   | 2:G:152:PRO:HD3   | 1.89                     | 0.54              |
| 2:G:1671:ARG:NH2  | 2:G:1710:GLY:O    | 2.40                     | 0.54              |
| 2:G:2737:PRO:O    | 2:G:2888:ARG:NH2  | 2.40                     | 0.54              |
| 2:I:972:LEU:O     | 2:I:1044:ARG:NH2  | 2.39                     | 0.54              |
| 1:H:23:VAL:HG22   | 1:H:47:LYS:HG2    | 1.90                     | 0.54              |
| 2:I:637:LEU:HD23  | 2:I:1637:MET:HB3  | 1.90                     | 0.54              |
| 2:I:2737:PRO:O    | 2:I:2888:ARG:NH2  | 2.40                     | 0.54              |
| 2:B:989:ALA:O     | 2:B:1035:ASN:ND2  | 2.38                     | 0.54              |
| 2:G:730:VAL:O     | 2:G:735:GLN:NE2   | 2.41                     | 0.54              |
| 2:E:2737:PRO:O    | 2:E:2888:ARG:NH2  | 2.40                     | 0.54              |
| 1:F:23:VAL:HG22   | 1:F:47:LYS:HG2    | 1.90                     | 0.54              |
| 2:I:730:VAL:O     | 2:I:735:GLN:NE2   | 2.41                     | 0.54              |
| 2:I:2347:GLU:O    | 2:I:2351:ASN:N    | 2.40                     | 0.54              |
| 2:E:3981:ALA:HA   | 2:E:3986:TRP:HE1  | 1.72                     | 0.54              |
| 2:B:359:TYR:HA    | 2:B:376:ALA:HA    | 1.90                     | 0.54              |
| 1:F:42:ARG:HG2    | 2:E:1691:GLN:HG2  | 1.89                     | 0.54              |
| 2:G:637:LEU:HD23  | 2:G:1637:MET:HB3  | 1.90                     | 0.54              |
| 2:E:2770:LYS:HB3  | 2:E:2775:TRP:HB2  | 1.89                     | 0.54              |
| 2:E:359:TYR:HA    | 2:E:376:ALA:HA    | 1.90                     | 0.53              |
| 2:E:1164:LEU:HB3  | 2:E:1169:LEU:HD21 | 1.90                     | 0.53              |
| 2:E:4924:VAL:HA   | 2:E:4928:LEU:HB2  | 1.90                     | 0.53              |
| 2:G:41:GLY:O      | 2:G:45:ARG:NH1    | 2.42                     | 0.53              |
| 2:G:395:GLN:HG3   | 2:G:397:GLU:H     | 1.74                     | 0.53              |
| 2:I:359:TYR:HA    | 2:I:376:ALA:HA    | 1.90                     | 0.53              |
| 2:I:788:LYS:HG2   | 2:I:1630:CYS:H    | 1.71                     | 0.53              |
| 2:B:4924:VAL:HA   | 2:B:4928:LEU:HB2  | 1.90                     | 0.53              |
| 2:G:1731:LEU:HA   | 2:G:1772:ARG:HH12 | 1.73                     | 0.53              |
| 2:I:1731:LEU:HA   | 2:I:1772:ARG:HH12 | 1.73                     | 0.53              |
| 2:I:3910:THR:HG23 | 2:I:3911:THR:HG23 | 1.91                     | 0.53              |
| 2:I:3981:ALA:HA   | 2:I:3986:TRP:HE1  | 1.72                     | 0.53              |
| 1:J:23:VAL:HG22   | 1:J:47:LYS:HG2    | 1.90                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1164:LEU:HB3  | 2:B:1169:LEU:HD21 | 1.90                     | 0.53              |
| 2:B:2347:GLU:O    | 2:B:2351:ASN:N    | 2.40                     | 0.53              |
| 2:B:3910:THR:HG23 | 2:B:3911:THR:HG23 | 1.91                     | 0.53              |
| 2:G:359:TYR:HA    | 2:G:376:ALA:HA    | 1.90                     | 0.53              |
| 2:G:4001:MET:HE3  | 2:G:4057:MET:HE3  | 1.91                     | 0.53              |
| 2:I:19:GLU:HB2    | 2:I:206:CYS:HB3   | 1.91                     | 0.53              |
| 2:E:103:TYR:HB3   | 2:E:152:PRO:HD3   | 1.89                     | 0.53              |
| 1:A:23:VAL:HG22   | 1:A:47:LYS:HG2    | 1.90                     | 0.53              |
| 2:B:730:VAL:O     | 2:B:735:GLN:NE2   | 2.41                     | 0.53              |
| 2:I:41:GLY:O      | 2:I:45:ARG:NH1    | 2.42                     | 0.53              |
| 2:I:4001:MET:HE3  | 2:I:4057:MET:HE3  | 1.91                     | 0.53              |
| 2:B:1243:PRO:HB2  | 2:B:1600:LEU:HD22 | 1.91                     | 0.53              |
| 2:G:2755:ILE:HD13 | 2:G:2810:LYS:HG2  | 1.91                     | 0.53              |
| 2:E:41:GLY:O      | 2:E:45:ARG:NH1    | 2.42                     | 0.53              |
| 2:G:3910:THR:HG23 | 2:G:3911:THR:HG23 | 1.91                     | 0.53              |
| 2:I:4924:VAL:HA   | 2:I:4928:LEU:HB2  | 1.90                     | 0.53              |
| 2:E:19:GLU:HB2    | 2:E:206:CYS:HB3   | 1.91                     | 0.53              |
| 2:E:4001:MET:HE3  | 2:E:4057:MET:HE3  | 1.91                     | 0.53              |
| 2:B:395:GLN:HG3   | 2:B:397:GLU:H     | 1.74                     | 0.53              |
| 2:B:637:LEU:HD23  | 2:B:1637:MET:HB3  | 1.90                     | 0.53              |
| 2:B:867:LEU:HB3   | 2:B:929:LEU:HD13  | 1.91                     | 0.53              |
| 2:B:2755:ILE:HD13 | 2:B:2810:LYS:HG2  | 1.91                     | 0.53              |
| 2:G:3981:ALA:HA   | 2:G:3986:TRP:HE1  | 1.72                     | 0.53              |
| 2:G:4924:VAL:HA   | 2:G:4928:LEU:HB2  | 1.90                     | 0.53              |
| 2:E:395:GLN:HG3   | 2:E:397:GLU:H     | 1.74                     | 0.53              |
| 2:E:637:LEU:HD23  | 2:E:1637:MET:HB3  | 1.90                     | 0.53              |
| 2:E:867:LEU:HB3   | 2:E:929:LEU:HD13  | 1.91                     | 0.53              |
| 2:E:1650:ILE:HG13 | 2:E:1707:LEU:HD21 | 1.91                     | 0.53              |
| 2:B:19:GLU:HB2    | 2:B:206:CYS:HB3   | 1.91                     | 0.52              |
| 2:B:1650:ILE:HG13 | 2:B:1707:LEU:HD21 | 1.91                     | 0.52              |
| 2:G:1164:LEU:HB3  | 2:G:1169:LEU:HD21 | 1.90                     | 0.52              |
| 2:I:823:LEU:HD23  | 2:I:1626:TRP:HB3  | 1.91                     | 0.52              |
| 2:E:2755:ILE:HD13 | 2:E:2810:LYS:HG2  | 1.91                     | 0.52              |
| 2:E:3910:THR:HG23 | 2:E:3911:THR:HG23 | 1.91                     | 0.52              |
| 2:G:867:LEU:HB3   | 2:G:929:LEU:HD13  | 1.91                     | 0.52              |
| 2:I:1100:MET:HE2  | 2:I:1198:GLN:HB3  | 1.90                     | 0.52              |
| 2:I:1164:LEU:HB3  | 2:I:1169:LEU:HD21 | 1.90                     | 0.52              |
| 2:E:718:GLY:HA3   | 2:E:737:LEU:HA    | 1.92                     | 0.52              |
| 2:E:823:LEU:HD23  | 2:E:1626:TRP:HB3  | 1.92                     | 0.52              |
| 2:B:838:HIS:HA    | 2:B:1201:HIS:HB3  | 1.92                     | 0.52              |
| 2:E:886:ARG:HB3   | 2:E:891:TRP:HB2   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:1100:MET:HE2  | 2:B:1198:GLN:HB3  | 1.90                     | 0.52              |
| 2:B:4959:PHE:C    | 2:B:4959:PHE:CD2  | 2.86                     | 0.52              |
| 2:I:887:ILE:HG21  | 2:I:959:TYR:HA    | 1.92                     | 0.52              |
| 2:I:1243:PRO:HB2  | 2:I:1600:LEU:HD22 | 1.91                     | 0.52              |
| 2:E:1731:LEU:HA   | 2:E:1772:ARG:HH12 | 1.73                     | 0.52              |
| 2:E:2911:LEU:HB2  | 2:E:2916:LYS:HE3  | 1.91                     | 0.52              |
| 1:A:42:ARG:HG2    | 2:B:1691:GLN:HG2  | 1.91                     | 0.52              |
| 2:B:776:LEU:HG    | 2:B:848:HIS:HA    | 1.92                     | 0.52              |
| 2:B:886:ARG:HB3   | 2:B:891:TRP:HB2   | 1.91                     | 0.52              |
| 2:B:887:ILE:HG21  | 2:B:959:TYR:HA    | 1.92                     | 0.52              |
| 2:G:19:GLU:HB2    | 2:G:206:CYS:HB3   | 1.91                     | 0.52              |
| 2:G:718:GLY:HA3   | 2:G:737:LEU:HA    | 1.91                     | 0.52              |
| 2:G:776:LEU:HG    | 2:G:848:HIS:HA    | 1.92                     | 0.52              |
| 2:G:823:LEU:HD23  | 2:G:1626:TRP:HB3  | 1.92                     | 0.52              |
| 2:G:1100:MET:HE2  | 2:G:1198:GLN:HB3  | 1.90                     | 0.52              |
| 2:G:4582:VAL:HG11 | 2:E:4860:ARG:HD2  | 1.89                     | 0.52              |
| 2:E:838:HIS:HA    | 2:E:1201:HIS:HB3  | 1.92                     | 0.52              |
| 2:E:1100:MET:HE2  | 2:E:1198:GLN:HB3  | 1.90                     | 0.52              |
| 2:B:823:LEU:HD23  | 2:B:1626:TRP:HB3  | 1.92                     | 0.52              |
| 2:I:2755:ILE:HD13 | 2:I:2810:LYS:HG2  | 1.91                     | 0.52              |
| 2:B:4001:MET:HE3  | 2:B:4057:MET:HE3  | 1.91                     | 0.52              |
| 2:G:2452:ARG:HH12 | 2:E:177:GLU:HG3   | 1.73                     | 0.52              |
| 2:I:1650:ILE:HG13 | 2:I:1707:LEU:HD21 | 1.91                     | 0.52              |
| 2:B:41:GLY:O      | 2:B:45:ARG:NH1    | 2.41                     | 0.52              |
| 2:G:887:ILE:HG21  | 2:G:959:TYR:HA    | 1.92                     | 0.52              |
| 2:B:1731:LEU:HA   | 2:B:1772:ARG:HH12 | 1.73                     | 0.52              |
| 2:I:281:ARG:NH2   | 2:I:309:THR:OG1   | 2.43                     | 0.52              |
| 2:I:1152:MET:HB2  | 2:I:1161:ILE:HB   | 1.92                     | 0.52              |
| 2:E:1243:PRO:HB2  | 2:E:1600:LEU:HD22 | 1.91                     | 0.52              |
| 2:B:2364:PHE:HD1  | 2:B:2429:LEU:HD21 | 1.75                     | 0.52              |
| 2:G:2911:LEU:HB2  | 2:G:2916:LYS:HE3  | 1.91                     | 0.52              |
| 2:I:776:LEU:HG    | 2:I:848:HIS:HA    | 1.92                     | 0.52              |
| 2:I:838:HIS:HA    | 2:I:1201:HIS:HB3  | 1.92                     | 0.52              |
| 2:E:1152:MET:HB2  | 2:E:1161:ILE:HB   | 1.92                     | 0.52              |
| 2:E:3751:VAL:O    | 2:E:3756:LYS:NZ   | 2.43                     | 0.52              |
| 2:E:4681:LEU:HD21 | 2:E:4687:TYR:HD2  | 1.75                     | 0.52              |
| 2:B:1152:MET:HB2  | 2:B:1161:ILE:HB   | 1.92                     | 0.51              |
| 2:G:838:HIS:HA    | 2:G:1201:HIS:HB3  | 1.92                     | 0.51              |
| 2:G:1152:MET:HB2  | 2:G:1161:ILE:HB   | 1.92                     | 0.51              |
| 2:I:2364:PHE:HD1  | 2:I:2429:LEU:HD21 | 1.75                     | 0.51              |
| 2:E:776:LEU:HG    | 2:E:848:HIS:HA    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:887:ILE:HG21  | 2:E:959:TYR:HA    | 1.92                     | 0.51              |
| 2:B:3751:VAL:O    | 2:B:3756:LYS:NZ   | 2.44                     | 0.51              |
| 2:B:4126:GLU:O    | 2:B:4130:ASN:ND2  | 2.44                     | 0.51              |
| 2:G:1243:PRO:HB2  | 2:G:1600:LEU:HD22 | 1.91                     | 0.51              |
| 2:G:1650:ILE:HG13 | 2:G:1707:LEU:HD21 | 1.91                     | 0.51              |
| 2:I:469:ARG:HH21  | 2:I:3712:GLU:HB3  | 1.76                     | 0.51              |
| 2:I:886:ARG:HB3   | 2:I:891:TRP:HB2   | 1.91                     | 0.51              |
| 2:B:281:ARG:NH2   | 2:B:309:THR:OG1   | 2.43                     | 0.51              |
| 2:I:4126:GLU:O    | 2:I:4130:ASN:ND2  | 2.44                     | 0.51              |
| 2:E:281:ARG:NH2   | 2:E:309:THR:OG1   | 2.43                     | 0.51              |
| 2:G:56:GLN:O      | 2:G:309:THR:OG1   | 2.26                     | 0.51              |
| 2:G:469:ARG:HH21  | 2:G:3712:GLU:HB3  | 1.76                     | 0.51              |
| 2:I:867:LEU:HB3   | 2:I:929:LEU:HD13  | 1.91                     | 0.51              |
| 2:I:2911:LEU:HB2  | 2:I:2916:LYS:HE3  | 1.91                     | 0.51              |
| 2:E:2364:PHE:HD1  | 2:E:2429:LEU:HD21 | 1.75                     | 0.51              |
| 2:B:718:GLY:HA3   | 2:B:737:LEU:HA    | 1.91                     | 0.51              |
| 2:G:1743:ARG:O    | 2:G:1964:ARG:NH2  | 2.44                     | 0.51              |
| 2:I:395:GLN:HG3   | 2:I:397:GLU:H     | 1.74                     | 0.51              |
| 2:I:2042:CYS:SG   | 2:I:2043:GLY:N    | 2.81                     | 0.51              |
| 2:B:219:VAL:HG13  | 2:B:285:VAL:HG21  | 1.93                     | 0.51              |
| 2:B:1516:UNK:N    | 2:B:1529:UNK:O    | 2.44                     | 0.51              |
| 2:B:1743:ARG:O    | 2:B:1964:ARG:NH2  | 2.44                     | 0.51              |
| 2:B:2042:CYS:SG   | 2:B:2043:GLY:N    | 2.81                     | 0.51              |
| 2:B:2911:LEU:HB2  | 2:B:2916:LYS:HE3  | 1.91                     | 0.51              |
| 2:G:1516:UNK:N    | 2:G:1529:UNK:O    | 2.44                     | 0.51              |
| 2:I:3751:VAL:O    | 2:I:3756:LYS:NZ   | 2.43                     | 0.51              |
| 2:E:2365:GLY:HA3  | 2:E:2426:TYR:HE1  | 1.76                     | 0.51              |
| 2:I:718:GLY:HA3   | 2:I:737:LEU:HA    | 1.91                     | 0.51              |
| 2:I:2318:TYR:OH   | 2:I:2414:ASN:N    | 2.44                     | 0.51              |
| 2:G:2364:PHE:HD1  | 2:G:2429:LEU:HD21 | 1.75                     | 0.51              |
| 2:I:4081:VAL:HB   | 2:I:4088:ILE:HD12 | 1.93                     | 0.51              |
| 2:E:219:VAL:HG13  | 2:E:285:VAL:HG21  | 1.93                     | 0.51              |
| 2:E:1516:UNK:N    | 2:E:1529:UNK:O    | 2.44                     | 0.51              |
| 2:E:3980:LEU:HD22 | 2:E:3985:LEU:HD22 | 1.93                     | 0.51              |
| 2:E:4126:GLU:O    | 2:E:4130:ASN:ND2  | 2.44                     | 0.51              |
| 2:G:4681:LEU:HD21 | 2:G:4687:TYR:HD2  | 1.75                     | 0.51              |
| 2:B:469:ARG:HH21  | 2:B:3712:GLU:HB3  | 1.76                     | 0.51              |
| 2:G:3751:VAL:O    | 2:G:3756:LYS:NZ   | 2.43                     | 0.51              |
| 2:G:4126:GLU:O    | 2:G:4130:ASN:ND2  | 2.44                     | 0.51              |
| 2:E:4230:LYS:HE3  | 2:E:4231:MET:HE2  | 1.94                     | 0.51              |
| 2:E:4904:PRO:HB3  | 2:E:4913:ARG:HD3  | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2365:GLY:HA3  | 2:B:2426:TYR:HE1  | 1.76                     | 0.50              |
| 2:B:2739:PRO:HB3  | 2:B:2884:ASN:HB3  | 1.93                     | 0.50              |
| 2:G:331:VAL:HG12  | 2:G:333:GLY:H     | 1.76                     | 0.50              |
| 2:G:886:ARG:HB3   | 2:G:891:TRP:HB2   | 1.91                     | 0.50              |
| 2:I:717:ASP:OD1   | 2:I:720:HIS:ND1   | 2.45                     | 0.50              |
| 2:B:45:ARG:NH2    | 2:B:447:ASP:OD1   | 2.45                     | 0.50              |
| 2:B:606:LEU:HG    | 2:B:617:ASN:HD22  | 1.77                     | 0.50              |
| 2:B:671:VAL:HG22  | 2:B:740:PRO:HG3   | 1.94                     | 0.50              |
| 2:B:717:ASP:OD1   | 2:B:720:HIS:ND1   | 2.45                     | 0.50              |
| 2:G:281:ARG:NH2   | 2:G:309:THR:OG1   | 2.43                     | 0.50              |
| 2:G:606:LEU:HG    | 2:G:617:ASN:HD22  | 1.77                     | 0.50              |
| 2:G:794:GLY:H     | 2:G:798:GLY:HA3   | 1.76                     | 0.50              |
| 2:G:3980:LEU:HD22 | 2:G:3985:LEU:HD22 | 1.93                     | 0.50              |
| 2:I:794:GLY:H     | 2:I:798:GLY:HA3   | 1.76                     | 0.50              |
| 2:I:4904:PRO:HB3  | 2:I:4913:ARG:HD3  | 1.93                     | 0.50              |
| 2:E:56:GLN:O      | 2:E:309:THR:OG1   | 2.26                     | 0.50              |
| 2:G:2265:LEU:HD22 | 2:G:2330:ARG:HB3  | 1.94                     | 0.50              |
| 2:I:1516:UNK:N    | 2:I:1529:UNK:O    | 2.44                     | 0.50              |
| 2:E:331:VAL:HG12  | 2:E:333:GLY:H     | 1.76                     | 0.50              |
| 1:A:21:THR:HA     | 1:A:49:ARG:HA     | 1.94                     | 0.50              |
| 2:B:4681:LEU:HD21 | 2:B:4687:TYR:HD2  | 1.75                     | 0.50              |
| 2:G:219:VAL:HG13  | 2:G:285:VAL:HG21  | 1.93                     | 0.50              |
| 2:E:2739:PRO:HB3  | 2:E:2884:ASN:HB3  | 1.93                     | 0.50              |
| 1:J:21:THR:HA     | 1:J:49:ARG:HA     | 1.94                     | 0.50              |
| 2:G:4230:LYS:HE3  | 2:G:4231:MET:HE2  | 1.94                     | 0.50              |
| 2:E:606:LEU:HG    | 2:E:617:ASN:HD22  | 1.77                     | 0.50              |
| 2:E:717:ASP:OD1   | 2:E:720:HIS:ND1   | 2.44                     | 0.50              |
| 2:E:4729:GLY:HA2  | 2:E:4737:ILE:HG13 | 1.93                     | 0.50              |
| 1:F:21:THR:HA     | 1:F:49:ARG:HA     | 1.94                     | 0.50              |
| 2:B:4230:LYS:HE3  | 2:B:4231:MET:HE2  | 1.93                     | 0.50              |
| 2:B:4983:HIS:ND1  | 2:B:4983:HIS:N    | 2.59                     | 0.50              |
| 2:G:45:ARG:NH2    | 2:G:447:ASP:OD1   | 2.44                     | 0.50              |
| 2:I:2365:GLY:HA3  | 2:I:2426:TYR:HE1  | 1.76                     | 0.50              |
| 2:I:4681:LEU:HD21 | 2:I:4687:TYR:HD2  | 1.75                     | 0.50              |
| 2:E:3830:GLN:HA   | 2:E:3833:GLN:HG2  | 1.94                     | 0.50              |
| 2:B:952:LYS:HB3   | 2:B:968:ALA:HB1   | 1.94                     | 0.50              |
| 2:E:2265:LEU:HD22 | 2:E:2330:ARG:HB3  | 1.94                     | 0.50              |
| 2:B:794:GLY:H     | 2:B:798:GLY:HA3   | 1.76                     | 0.50              |
| 2:B:3830:GLN:HA   | 2:B:3833:GLN:HG2  | 1.94                     | 0.50              |
| 2:B:4081:VAL:HB   | 2:B:4088:ILE:HD12 | 1.93                     | 0.50              |
| 2:B:4904:PRO:HB3  | 2:B:4913:ARG:HD3  | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:717:ASP:OD1   | 2:G:720:HIS:ND1   | 2.45                     | 0.50              |
| 2:I:426:ARG:HB2   | 2:I:506:TYR:HA    | 1.94                     | 0.50              |
| 2:E:469:ARG:HH21  | 2:E:3712:GLU:HB3  | 1.76                     | 0.50              |
| 2:E:952:LYS:HB3   | 2:E:968:ALA:HB1   | 1.94                     | 0.50              |
| 2:E:4081:VAL:HB   | 2:E:4088:ILE:HD12 | 1.93                     | 0.50              |
| 2:G:4904:PRO:HB3  | 2:G:4913:ARG:HD3  | 1.93                     | 0.50              |
| 2:I:2739:PRO:HB3  | 2:I:2884:ASN:HB3  | 1.93                     | 0.50              |
| 2:I:3830:GLN:HA   | 2:I:3833:GLN:HG2  | 1.94                     | 0.50              |
| 2:I:3980:LEU:HD22 | 2:I:3985:LEU:HD22 | 1.93                     | 0.50              |
| 2:E:794:GLY:H     | 2:E:798:GLY:HA3   | 1.76                     | 0.50              |
| 2:B:2265:LEU:HD22 | 2:B:2330:ARG:HB3  | 1.94                     | 0.49              |
| 2:G:952:LYS:HB3   | 2:G:968:ALA:HB1   | 1.94                     | 0.49              |
| 2:G:4998:LYS:NZ   | 2:G:5007:GLU:OE1  | 2.45                     | 0.49              |
| 2:I:219:VAL:HG13  | 2:I:285:VAL:HG21  | 1.93                     | 0.49              |
| 2:I:331:VAL:HG12  | 2:I:333:GLY:H     | 1.76                     | 0.49              |
| 2:I:635:THR:HB    | 2:I:1639:LEU:HD23 | 1.94                     | 0.49              |
| 2:E:426:ARG:HB2   | 2:E:506:TYR:HA    | 1.94                     | 0.49              |
| 1:H:21:THR:HA     | 1:H:49:ARG:HA     | 1.94                     | 0.49              |
| 2:B:4738:ALA:HA   | 2:B:4743:MET:HE3  | 1.94                     | 0.49              |
| 2:G:1111:PRO:HD3  | 2:G:1605:TRP:HE1  | 1.77                     | 0.49              |
| 2:G:2739:PRO:HB3  | 2:G:2884:ASN:HB3  | 1.93                     | 0.49              |
| 2:I:45:ARG:NH2    | 2:I:447:ASP:OD1   | 2.44                     | 0.49              |
| 2:E:2257:LEU:HD11 | 2:E:2276:ALA:HB2  | 1.94                     | 0.49              |
| 2:B:331:VAL:HG12  | 2:B:333:GLY:H     | 1.76                     | 0.49              |
| 2:B:1111:PRO:HD3  | 2:B:1605:TRP:HE1  | 1.77                     | 0.49              |
| 2:B:4968:PHE:CD2  | 2:B:4978:HIS:CE1  | 2.94                     | 0.49              |
| 2:G:2758:PHE:HD2  | 2:G:2809:ILE:HG12 | 1.77                     | 0.49              |
| 2:G:3830:GLN:HA   | 2:G:3833:GLN:HG2  | 1.94                     | 0.49              |
| 2:B:635:THR:HB    | 2:B:1639:LEU:HD23 | 1.94                     | 0.49              |
| 2:B:3980:LEU:HD22 | 2:B:3985:LEU:HD22 | 1.93                     | 0.49              |
| 2:G:2318:TYR:OH   | 2:G:2414:ASN:N    | 2.44                     | 0.49              |
| 2:G:4081:VAL:HB   | 2:G:4088:ILE:HD12 | 1.93                     | 0.49              |
| 2:I:671:VAL:HG22  | 2:I:740:PRO:HG3   | 1.94                     | 0.49              |
| 2:I:3850:GLN:HA   | 2:I:3853:ALA:HB3  | 1.95                     | 0.49              |
| 2:I:4738:ALA:HA   | 2:I:4743:MET:HE3  | 1.94                     | 0.49              |
| 2:E:45:ARG:NH2    | 2:E:447:ASP:OD1   | 2.45                     | 0.49              |
| 2:E:2291:GLN:HB3  | 2:E:2294:ASP:H    | 1.77                     | 0.49              |
| 2:B:615:ARG:NH2   | 2:B:1677:GLY:O    | 2.43                     | 0.49              |
| 2:G:399:GLN:HG2   | 2:G:403:MET:HE3   | 1.95                     | 0.49              |
| 2:G:2365:GLY:HA3  | 2:G:2426:TYR:HE1  | 1.76                     | 0.49              |
| 2:E:111:HIS:CD2   | 2:E:114:SER:H     | 2.29                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1960:ALA:O    | 2:G:1964:ARG:NE   | 2.46                     | 0.49              |
| 2:I:2265:LEU:HD22 | 2:I:2330:ARG:HB3  | 1.94                     | 0.49              |
| 2:I:4230:LYS:HE3  | 2:I:4231:MET:HE2  | 1.93                     | 0.49              |
| 2:G:635:THR:HB    | 2:G:1639:LEU:HD23 | 1.94                     | 0.49              |
| 2:G:2257:LEU:HD11 | 2:G:2276:ALA:HB2  | 1.94                     | 0.49              |
| 2:G:3850:GLN:HA   | 2:G:3853:ALA:HB3  | 1.95                     | 0.49              |
| 2:G:4729:GLY:HA2  | 2:G:4737:ILE:HG13 | 1.93                     | 0.49              |
| 2:I:399:GLN:HG2   | 2:I:403:MET:HE3   | 1.95                     | 0.49              |
| 2:I:606:LEU:HG    | 2:I:617:ASN:HD22  | 1.77                     | 0.49              |
| 2:I:1111:PRO:HD3  | 2:I:1605:TRP:HE1  | 1.77                     | 0.49              |
| 2:B:2758:PHE:HD2  | 2:B:2809:ILE:HG12 | 1.77                     | 0.49              |
| 2:G:671:VAL:HG22  | 2:G:740:PRO:HG3   | 1.93                     | 0.49              |
| 2:G:2291:GLN:HB3  | 2:G:2294:ASP:H    | 1.78                     | 0.49              |
| 2:B:4984:ASN:C    | 2:B:4986:ALA:H    | 2.21                     | 0.49              |
| 2:E:2042:CYS:SG   | 2:E:2043:GLY:N    | 2.81                     | 0.49              |
| 2:G:4152:GLU:OE1  | 2:G:4194:TYR:OH   | 2.31                     | 0.49              |
| 2:I:56:GLN:O      | 2:I:309:THR:OG1   | 2.26                     | 0.49              |
| 2:I:2291:GLN:HB3  | 2:I:2294:ASP:H    | 1.78                     | 0.49              |
| 2:I:4152:GLU:OE1  | 2:I:4194:TYR:OH   | 2.31                     | 0.48              |
| 2:E:671:VAL:HG22  | 2:E:740:PRO:HG3   | 1.93                     | 0.48              |
| 2:E:3850:GLN:HA   | 2:E:3853:ALA:HB3  | 1.95                     | 0.48              |
| 2:B:4729:GLY:HA2  | 2:B:4737:ILE:HG13 | 1.94                     | 0.48              |
| 2:B:4962:GLY:H    | 2:B:5025:GLY:N    | 2.12                     | 0.48              |
| 2:I:4998:LYS:NZ   | 2:I:5007:GLU:OE1  | 2.45                     | 0.48              |
| 2:E:399:GLN:HG2   | 2:E:403:MET:HE3   | 1.95                     | 0.48              |
| 2:E:2758:PHE:HD2  | 2:E:2809:ILE:HG12 | 1.77                     | 0.48              |
| 2:B:426:ARG:HB2   | 2:B:506:TYR:HA    | 1.94                     | 0.48              |
| 2:G:1700:ASP:OD2  | 2:G:1708:ARG:NH2  | 2.47                     | 0.48              |
| 2:G:3946:GLN:OE1  | 2:G:3950:ASN:ND2  | 2.47                     | 0.48              |
| 2:G:4687:TYR:OH   | 2:G:4699:GLY:O    | 2.30                     | 0.48              |
| 2:I:952:LYS:HB3   | 2:I:968:ALA:HB1   | 1.94                     | 0.48              |
| 2:I:1743:ARG:O    | 2:I:1964:ARG:NH2  | 2.44                     | 0.48              |
| 2:E:1700:ASP:OD2  | 2:E:1708:ARG:NH2  | 2.47                     | 0.48              |
| 2:E:1743:ARG:O    | 2:E:1964:ARG:NH2  | 2.44                     | 0.48              |
| 2:E:4152:GLU:OE1  | 2:E:4194:TYR:OH   | 2.31                     | 0.48              |
| 2:B:1126:GLY:HA3  | 2:B:1143:TRP:CE2  | 2.49                     | 0.48              |
| 2:G:426:ARG:HB2   | 2:G:506:TYR:HA    | 1.94                     | 0.48              |
| 2:G:2337:PHE:HA   | 2:G:2340:PHE:HB2  | 1.95                     | 0.48              |
| 2:G:3781:GLN:HA   | 2:G:3784:SER:HB3  | 1.95                     | 0.48              |
| 2:G:4738:ALA:HA   | 2:G:4743:MET:HE3  | 1.94                     | 0.48              |
| 2:E:34:LYS:H      | 2:E:53:SER:HG     | 1.60                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:635:THR:HB    | 2:E:1639:LEU:HD23 | 1.94                     | 0.48              |
| 2:E:1111:PRO:HD3  | 2:E:1605:TRP:HE1  | 1.77                     | 0.48              |
| 2:B:3946:GLN:OE1  | 2:B:3950:ASN:ND2  | 2.47                     | 0.48              |
| 2:E:2337:PHE:HA   | 2:E:2340:PHE:HB2  | 1.95                     | 0.48              |
| 2:E:3946:GLN:OE1  | 2:E:3950:ASN:ND2  | 2.47                     | 0.48              |
| 2:B:2291:GLN:HB3  | 2:B:2294:ASP:H    | 1.77                     | 0.48              |
| 2:G:1126:GLY:HA3  | 2:G:1143:TRP:CE2  | 2.49                     | 0.48              |
| 2:I:2257:LEU:HD11 | 2:I:2276:ALA:HB2  | 1.94                     | 0.48              |
| 2:E:1457:UNK:N    | 2:E:1497:UNK:O    | 2.47                     | 0.48              |
| 2:E:4697:VAL:O    | 2:E:4701:TRP:N    | 2.47                     | 0.48              |
| 2:B:4152:GLU:OE1  | 2:B:4194:TYR:OH   | 2.31                     | 0.48              |
| 2:B:4586:PRO:HB3  | 2:B:4628:VAL:HG21 | 1.96                     | 0.48              |
| 2:I:615:ARG:NH2   | 2:I:1677:GLY:O    | 2.44                     | 0.48              |
| 2:I:1126:GLY:HA3  | 2:I:1143:TRP:CE2  | 2.49                     | 0.48              |
| 2:I:1936:LYS:HZ3  | 2:I:2105:TRP:CG   | 2.31                     | 0.48              |
| 2:I:4586:PRO:HB3  | 2:I:4628:VAL:HG21 | 1.96                     | 0.48              |
| 2:I:4729:GLY:HA2  | 2:I:4737:ILE:HG13 | 1.94                     | 0.48              |
| 2:E:4738:ALA:HA   | 2:E:4743:MET:HE3  | 1.94                     | 0.48              |
| 2:B:664:PHE:HB2   | 2:B:746:CYS:HB2   | 1.96                     | 0.48              |
| 2:B:1457:UNK:N    | 2:B:1497:UNK:O    | 2.46                     | 0.48              |
| 2:B:2257:LEU:HD11 | 2:B:2276:ALA:HB2  | 1.94                     | 0.48              |
| 2:B:2337:PHE:HA   | 2:B:2340:PHE:HB2  | 1.95                     | 0.48              |
| 2:B:3850:GLN:HA   | 2:B:3853:ALA:HB3  | 1.95                     | 0.48              |
| 2:E:3781:GLN:HA   | 2:E:3784:SER:HB3  | 1.95                     | 0.48              |
| 2:B:399:GLN:HG2   | 2:B:403:MET:HE3   | 1.95                     | 0.48              |
| 2:B:1960:ALA:O    | 2:B:1964:ARG:NE   | 2.46                     | 0.48              |
| 2:I:280:LEU:HD21  | 2:I:316:PHE:HE2   | 1.79                     | 0.48              |
| 2:E:4687:TYR:OH   | 2:E:4699:GLY:O    | 2.30                     | 0.48              |
| 2:B:280:LEU:HD21  | 2:B:316:PHE:HE2   | 1.79                     | 0.48              |
| 2:B:2375:GLY:HA3  | 2:B:2378:ALA:HB3  | 1.96                     | 0.48              |
| 2:G:177:GLU:HG3   | 2:I:2452:ARG:HH12 | 1.79                     | 0.48              |
| 2:I:3781:GLN:HA   | 2:I:3784:SER:HB3  | 1.95                     | 0.48              |
| 2:E:280:LEU:HD21  | 2:E:316:PHE:HE2   | 1.79                     | 0.48              |
| 2:E:1126:GLY:HA3  | 2:E:1143:TRP:CE2  | 2.49                     | 0.48              |
| 2:E:2375:GLY:HA3  | 2:E:2378:ALA:HB3  | 1.96                     | 0.48              |
| 2:B:1700:ASP:OD2  | 2:B:1708:ARG:NH2  | 2.47                     | 0.47              |
| 2:I:1457:UNK:N    | 2:I:1497:UNK:O    | 2.46                     | 0.47              |
| 2:I:3946:GLN:OE1  | 2:I:3950:ASN:ND2  | 2.47                     | 0.47              |
| 2:E:1960:ALA:O    | 2:E:1964:ARG:NE   | 2.46                     | 0.47              |
| 2:E:2318:TYR:OH   | 2:E:2414:ASN:N    | 2.44                     | 0.47              |
| 2:I:34:LYS:H      | 2:I:53:SER:HG     | 1.60                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:1700:ASP:OD2  | 2:I:1708:ARG:NH2  | 2.47                     | 0.47              |
| 2:I:2758:PHE:HD2  | 2:I:2809:ILE:HG12 | 1.77                     | 0.47              |
| 2:G:1457:UNK:N    | 2:G:1497:UNK:O    | 2.47                     | 0.47              |
| 2:G:4586:PRO:HB3  | 2:G:4628:VAL:HG21 | 1.96                     | 0.47              |
| 2:B:3733:CYS:HA   | 2:B:3766:GLN:HG2  | 1.97                     | 0.47              |
| 2:G:111:HIS:CD2   | 2:G:114:SER:H     | 2.29                     | 0.47              |
| 2:E:615:ARG:NH2   | 2:E:1677:GLY:O    | 2.44                     | 0.47              |
| 2:E:2751:LEU:HD11 | 2:E:2823:ILE:HG21 | 1.96                     | 0.47              |
| 1:J:34:LYS:HD3    | 2:I:629:ARG:HD2   | 1.95                     | 0.47              |
| 2:B:1973:GLN:O    | 2:B:1977:TYR:N    | 2.45                     | 0.47              |
| 2:B:2318:TYR:OH   | 2:B:2414:ASN:N    | 2.44                     | 0.47              |
| 2:G:2751:LEU:HD11 | 2:G:2823:ILE:HG21 | 1.96                     | 0.47              |
| 2:G:3817:LEU:HD13 | 2:G:3899:PHE:HD1  | 1.80                     | 0.47              |
| 2:G:4697:VAL:O    | 2:G:4701:TRP:N    | 2.47                     | 0.47              |
| 2:E:2277:ALA:HB1  | 2:E:2337:PHE:HD2  | 1.80                     | 0.47              |
| 2:E:2868:SER:O    | 2:E:2872:GLN:N    | 2.48                     | 0.47              |
| 2:B:2277:ALA:HB1  | 2:B:2337:PHE:HD2  | 1.80                     | 0.47              |
| 2:G:280:LEU:HD21  | 2:G:316:PHE:HE2   | 1.79                     | 0.47              |
| 2:G:2042:CYS:SG   | 2:G:2043:GLY:N    | 2.81                     | 0.47              |
| 2:G:3733:CYS:HA   | 2:G:3766:GLN:HG2  | 1.97                     | 0.47              |
| 2:I:111:HIS:CD2   | 2:I:114:SER:H     | 2.29                     | 0.47              |
| 2:I:664:PHE:HB2   | 2:I:746:CYS:HB2   | 1.96                     | 0.47              |
| 2:I:2375:GLY:HA3  | 2:I:2378:ALA:HB3  | 1.96                     | 0.47              |
| 2:E:664:PHE:HB2   | 2:E:746:CYS:HB2   | 1.96                     | 0.47              |
| 2:B:56:GLN:O      | 2:B:309:THR:OG1   | 2.26                     | 0.47              |
| 2:B:621:ILE:O     | 2:B:625:LEU:N     | 2.46                     | 0.47              |
| 2:B:2452:ARG:HH12 | 2:I:177:GLU:HG3   | 1.79                     | 0.47              |
| 2:G:664:PHE:HB2   | 2:G:746:CYS:HB2   | 1.96                     | 0.47              |
| 2:I:2337:PHE:HA   | 2:I:2340:PHE:HB2  | 1.95                     | 0.47              |
| 2:I:3733:CYS:HA   | 2:I:3766:GLN:HG2  | 1.97                     | 0.47              |
| 2:I:4697:VAL:O    | 2:I:4701:TRP:N    | 2.47                     | 0.47              |
| 2:E:2758:PHE:O    | 2:E:2762:THR:N    | 2.47                     | 0.47              |
| 2:B:20:VAL:HG12   | 2:B:204:PRO:HA    | 1.97                     | 0.47              |
| 2:I:924:MET:O     | 2:I:928:THR:OG1   | 2.30                     | 0.47              |
| 2:I:1960:ALA:O    | 2:I:1964:ARG:NE   | 2.46                     | 0.47              |
| 2:E:20:VAL:HG12   | 2:E:204:PRO:HA    | 1.97                     | 0.47              |
| 2:E:4586:PRO:HB3  | 2:E:4628:VAL:HG21 | 1.96                     | 0.47              |
| 2:G:2353:VAL:O    | 2:G:2357:LEU:N    | 2.48                     | 0.47              |
| 2:I:1649:ASP:HB3  | 2:I:1652:GLU:HG2  | 1.97                     | 0.47              |
| 2:I:2751:LEU:HD11 | 2:I:2823:ILE:HG21 | 1.96                     | 0.47              |
| 2:I:3817:LEU:HD13 | 2:I:3899:PHE:HD1  | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:2868:SER:O    | 2:B:2872:GLN:N    | 2.48                     | 0.47              |
| 2:B:3781:GLN:HA   | 2:B:3784:SER:HB3  | 1.95                     | 0.47              |
| 2:B:4232:GLU:OE2  | 2:B:5017:ARG:NH1  | 2.48                     | 0.47              |
| 2:B:4864:ASN:ND2  | 2:B:4871:GLU:OE1  | 2.46                     | 0.47              |
| 2:G:2868:SER:O    | 2:G:2872:GLN:N    | 2.48                     | 0.47              |
| 2:G:4227:GLU:HG3  | 2:G:4228:ALA:H    | 1.79                     | 0.47              |
| 2:G:4864:ASN:ND2  | 2:G:4871:GLU:OE1  | 2.46                     | 0.47              |
| 2:I:20:VAL:HG12   | 2:I:204:PRO:HA    | 1.97                     | 0.47              |
| 2:I:34:LYS:N      | 2:I:53:SER:OG     | 2.44                     | 0.47              |
| 2:B:3817:LEU:HD13 | 2:B:3899:PHE:HD1  | 1.80                     | 0.46              |
| 2:G:1649:ASP:HB3  | 2:G:1652:GLU:HG2  | 1.97                     | 0.46              |
| 2:G:2277:ALA:HB1  | 2:G:2337:PHE:HD2  | 1.80                     | 0.46              |
| 2:E:2196:ASN:OD1  | 2:E:2199:ARG:NH1  | 2.40                     | 0.46              |
| 2:E:2927:LEU:HD23 | 2:E:2930:LEU:HD12 | 1.98                     | 0.46              |
| 2:E:3817:LEU:HD13 | 2:E:3899:PHE:HD1  | 1.80                     | 0.46              |
| 2:I:2810:LYS:O    | 2:I:2814:LYS:N    | 2.39                     | 0.46              |
| 2:E:4227:GLU:HG3  | 2:E:4228:ALA:H    | 1.79                     | 0.46              |
| 2:G:20:VAL:HG12   | 2:G:204:PRO:HA    | 1.97                     | 0.46              |
| 2:G:615:ARG:NH2   | 2:G:1677:GLY:O    | 2.44                     | 0.46              |
| 2:I:2155:LEU:HD13 | 2:I:2188:ASN:HD21 | 1.80                     | 0.46              |
| 2:I:2277:ALA:HB1  | 2:I:2337:PHE:HD2  | 1.80                     | 0.46              |
| 2:E:1973:GLN:O    | 2:E:1977:TYR:N    | 2.46                     | 0.46              |
| 2:E:3770:LEU:HD21 | 2:E:3775:ALA:HB3  | 1.97                     | 0.46              |
| 2:B:978:THR:HB    | 2:B:980:ALA:H     | 1.80                     | 0.46              |
| 2:B:2751:LEU:HD11 | 2:B:2823:ILE:HG21 | 1.96                     | 0.46              |
| 2:B:2758:PHE:O    | 2:B:2762:THR:N    | 2.47                     | 0.46              |
| 2:G:463:GLU:OE2   | 2:G:467:LYS:NZ    | 2.49                     | 0.46              |
| 2:E:866:HIS:O     | 2:E:1051:TYR:OH   | 2.31                     | 0.46              |
| 2:E:924:MET:O     | 2:E:928:THR:OG1   | 2.30                     | 0.46              |
| 2:G:1973:GLN:O    | 2:G:1977:TYR:N    | 2.45                     | 0.46              |
| 2:I:2024:PRO:HB2  | 2:I:2027:ILE:HG12 | 1.98                     | 0.46              |
| 2:I:2247:GLN:NE2  | 2:I:2285:GLU:OE2  | 2.49                     | 0.46              |
| 2:E:3733:CYS:HA   | 2:E:3766:GLN:HG2  | 1.96                     | 0.46              |
| 2:B:551:LEU:HD21  | 2:B:589:LEU:HD13  | 1.98                     | 0.46              |
| 2:B:1649:ASP:HB3  | 2:B:1652:GLU:HG2  | 1.97                     | 0.46              |
| 2:B:1808:ARG:HD2  | 2:B:1854:PHE:HA   | 1.97                     | 0.46              |
| 2:B:2353:VAL:O    | 2:B:2357:LEU:N    | 2.48                     | 0.46              |
| 2:B:2927:LEU:HD23 | 2:B:2930:LEU:HD12 | 1.98                     | 0.46              |
| 2:G:4232:GLU:OE2  | 2:G:5017:ARG:NH1  | 2.48                     | 0.46              |
| 2:I:2003:GLN:O    | 2:I:2007:ASN:ND2  | 2.49                     | 0.46              |
| 2:I:4864:ASN:ND2  | 2:I:4871:GLU:OE1  | 2.46                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:214:VAL:HG12  | 2:E:274:LEU:HD12  | 1.98                     | 0.46              |
| 2:E:683:ARG:HG2   | 2:E:717:ASP:HB3   | 1.98                     | 0.46              |
| 2:B:4184:MET:HE2  | 2:B:4188:ARG:HA   | 1.98                     | 0.46              |
| 2:B:4227:GLU:HG3  | 2:B:4228:ALA:H    | 1.79                     | 0.46              |
| 2:G:2758:PHE:O    | 2:G:2762:THR:N    | 2.47                     | 0.46              |
| 2:I:1808:ARG:HD2  | 2:I:1854:PHE:HA   | 1.97                     | 0.46              |
| 2:I:1973:GLN:O    | 2:I:1977:TYR:N    | 2.46                     | 0.46              |
| 2:I:4232:GLU:OE2  | 2:I:5017:ARG:NH1  | 2.48                     | 0.46              |
| 1:F:87:HIS:H      | 1:F:91:ILE:HB     | 1.81                     | 0.46              |
| 2:B:2024:PRO:HB2  | 2:B:2027:ILE:HG12 | 1.98                     | 0.46              |
| 2:B:2247:GLN:NE2  | 2:B:2285:GLU:OE2  | 2.49                     | 0.46              |
| 2:G:2247:GLN:NE2  | 2:G:2285:GLU:OE2  | 2.49                     | 0.46              |
| 2:I:551:LEU:HD21  | 2:I:589:LEU:HD13  | 1.98                     | 0.46              |
| 2:I:2927:LEU:HD23 | 2:I:2930:LEU:HD12 | 1.98                     | 0.46              |
| 2:I:4687:TYR:OH   | 2:I:4699:GLY:O    | 2.30                     | 0.46              |
| 2:E:2353:VAL:O    | 2:E:2357:LEU:N    | 2.48                     | 0.46              |
| 1:H:87:HIS:H      | 1:H:91:ILE:HB     | 1.81                     | 0.46              |
| 2:B:3940:LYS:O    | 2:B:4002:LYS:NZ   | 2.49                     | 0.46              |
| 2:G:880:GLU:OE1   | 2:G:968:ALA:N     | 2.44                     | 0.46              |
| 2:G:2003:GLN:O    | 2:G:2007:ASN:ND2  | 2.49                     | 0.46              |
| 2:G:2375:GLY:HA3  | 2:G:2378:ALA:HB3  | 1.96                     | 0.46              |
| 2:E:2247:GLN:NE2  | 2:E:2285:GLU:OE2  | 2.49                     | 0.46              |
| 2:E:4184:MET:HE2  | 2:E:4188:ARG:HA   | 1.98                     | 0.46              |
| 2:B:111:HIS:CD2   | 2:B:114:SER:H     | 2.29                     | 0.46              |
| 2:B:4155:PRO:HD2  | 2:B:5036:LEU:HD23 | 1.98                     | 0.46              |
| 2:G:551:LEU:HD21  | 2:G:589:LEU:HD13  | 1.98                     | 0.46              |
| 2:G:1808:ARG:HD2  | 2:G:1854:PHE:HA   | 1.97                     | 0.46              |
| 2:G:2155:LEU:HD13 | 2:G:2188:ASN:HD21 | 1.81                     | 0.46              |
| 2:G:4017:LEU:HB3  | 2:G:4139:ILE:HG13 | 1.98                     | 0.46              |
| 2:I:2868:SER:O    | 2:I:2872:GLN:N    | 2.48                     | 0.46              |
| 2:I:4227:GLU:HG3  | 2:I:4228:ALA:H    | 1.79                     | 0.46              |
| 2:E:551:LEU:HD21  | 2:E:589:LEU:HD13  | 1.98                     | 0.46              |
| 2:B:4713:SER:HA   | 2:B:4718:LYS:HE2  | 1.99                     | 0.45              |
| 2:G:978:THR:HB    | 2:G:980:ALA:H     | 1.80                     | 0.45              |
| 2:G:3770:LEU:HD21 | 2:G:3775:ALA:HB3  | 1.97                     | 0.45              |
| 2:I:4017:LEU:HB3  | 2:I:4139:ILE:HG13 | 1.98                     | 0.45              |
| 2:E:2024:PRO:HB2  | 2:E:2027:ILE:HG12 | 1.98                     | 0.45              |
| 2:E:4232:GLU:OE2  | 2:E:5017:ARG:NH1  | 2.48                     | 0.45              |
| 2:I:3770:LEU:HD21 | 2:I:3775:ALA:HB3  | 1.97                     | 0.45              |
| 2:I:4184:MET:HE2  | 2:I:4188:ARG:HA   | 1.98                     | 0.45              |
| 2:E:1649:ASP:HB3  | 2:E:1652:GLU:HG2  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:4155:PRO:HD2  | 2:E:5036:LEU:HD23 | 1.98                     | 0.45              |
| 2:B:214:VAL:HG12  | 2:B:274:LEU:HD12  | 1.98                     | 0.45              |
| 2:B:683:ARG:HG2   | 2:B:717:ASP:HB3   | 1.98                     | 0.45              |
| 2:B:3955:MET:HG3  | 2:B:4019:LEU:HD22 | 1.98                     | 0.45              |
| 2:B:4687:TYR:OH   | 2:B:4699:GLY:O    | 2.30                     | 0.45              |
| 2:G:34:LYS:N      | 2:G:53:SER:OG     | 2.44                     | 0.45              |
| 2:G:2024:PRO:HB2  | 2:G:2027:ILE:HG12 | 1.98                     | 0.45              |
| 2:G:2927:LEU:HD23 | 2:G:2930:LEU:HD12 | 1.98                     | 0.45              |
| 2:G:4713:SER:HA   | 2:G:4718:LYS:HE2  | 1.98                     | 0.45              |
| 2:I:978:THR:HB    | 2:I:980:ALA:H     | 1.80                     | 0.45              |
| 2:E:4713:SER:HA   | 2:E:4718:LYS:HE2  | 1.98                     | 0.45              |
| 2:B:463:GLU:OE2   | 2:B:467:LYS:NZ    | 2.49                     | 0.45              |
| 2:B:1865:MET:SD   | 2:B:1865:MET:N    | 2.90                     | 0.45              |
| 2:G:4031:LEU:HB3  | 2:G:4034:ASN:HB2  | 1.98                     | 0.45              |
| 2:E:892:THR:N     | 2:E:902:ARG:O     | 2.49                     | 0.45              |
| 2:E:2155:LEU:HD13 | 2:E:2188:ASN:HD21 | 1.81                     | 0.45              |
| 2:E:4763:GLY:O    | 2:E:4766:THR:OG1  | 2.28                     | 0.45              |
| 1:F:7:ILE:HB      | 1:F:71:ARG:HB3    | 1.99                     | 0.45              |
| 2:G:214:VAL:HG12  | 2:G:274:LEU:HD12  | 1.98                     | 0.45              |
| 2:G:3361:UNK:O    | 2:G:3365:UNK:N    | 2.50                     | 0.45              |
| 2:G:4184:MET:HE2  | 2:G:4188:ARG:HA   | 1.98                     | 0.45              |
| 2:E:1865:MET:SD   | 2:E:1865:MET:N    | 2.90                     | 0.45              |
| 2:E:2003:GLN:O    | 2:E:2007:ASN:ND2  | 2.49                     | 0.45              |
| 2:E:3955:MET:HG3  | 2:E:4019:LEU:HD22 | 1.99                     | 0.45              |
| 1:A:87:HIS:H      | 1:A:91:ILE:HB     | 1.81                     | 0.45              |
| 1:H:7:ILE:HB      | 1:H:71:ARG:HB3    | 1.99                     | 0.45              |
| 2:B:606:LEU:O     | 2:B:617:ASN:ND2   | 2.50                     | 0.45              |
| 2:B:2003:GLN:O    | 2:B:2007:ASN:ND2  | 2.49                     | 0.45              |
| 2:I:4031:LEU:HB3  | 2:I:4034:ASN:HB2  | 1.98                     | 0.45              |
| 2:E:978:THR:HB    | 2:E:980:ALA:H     | 1.80                     | 0.45              |
| 2:E:1808:ARG:HD2  | 2:E:1854:PHE:HA   | 1.97                     | 0.45              |
| 1:J:76:CYS:HB2    | 1:J:97:LEU:HB2    | 1.98                     | 0.45              |
| 1:J:87:HIS:H      | 1:J:91:ILE:HB     | 1.81                     | 0.45              |
| 2:B:359:TYR:OH    | 2:B:385:ASP:OD2   | 2.32                     | 0.45              |
| 2:B:3770:LEU:HD21 | 2:B:3775:ALA:HB3  | 1.97                     | 0.45              |
| 2:I:582:HIS:O     | 2:I:585:SER:OG    | 2.29                     | 0.45              |
| 2:I:790:ARG:HG2   | 2:I:1627:ALA:HA   | 1.99                     | 0.45              |
| 2:E:621:ILE:O     | 2:E:625:LEU:N     | 2.46                     | 0.45              |
| 2:E:3365:UNK:O    | 2:E:3369:UNK:N    | 2.50                     | 0.45              |
| 2:B:1095:VAL:HB   | 2:B:1199:VAL:HG23 | 1.99                     | 0.45              |
| 2:B:3365:UNK:O    | 2:B:3369:UNK:N    | 2.50                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:4697:VAL:O    | 2:B:4701:TRP:N    | 2.47                     | 0.45              |
| 2:B:4960:ILE:H    | 2:B:4960:ILE:HG12 | 1.51                     | 0.45              |
| 2:B:4968:PHE:CZ   | 2:B:4978:HIS:CE1  | 2.96                     | 0.45              |
| 2:G:606:LEU:O     | 2:G:617:ASN:ND2   | 2.50                     | 0.45              |
| 2:G:2776:SER:O    | 2:G:2788:HIS:N    | 2.50                     | 0.45              |
| 2:G:4155:PRO:HD2  | 2:G:5036:LEU:HD23 | 1.98                     | 0.45              |
| 2:I:606:LEU:O     | 2:I:617:ASN:ND2   | 2.50                     | 0.45              |
| 2:I:2353:VAL:O    | 2:I:2357:LEU:N    | 2.48                     | 0.45              |
| 2:I:3365:UNK:O    | 2:I:3369:UNK:N    | 2.50                     | 0.45              |
| 2:I:4155:PRO:HD2  | 2:I:5036:LEU:HD23 | 1.98                     | 0.45              |
| 2:E:880:GLU:OE1   | 2:E:968:ALA:N     | 2.44                     | 0.45              |
| 2:B:404:ILE:HG21  | 2:B:481:GLU:HG3   | 1.99                     | 0.45              |
| 2:B:2155:LEU:HD13 | 2:B:2188:ASN:HD21 | 1.81                     | 0.45              |
| 2:G:134:ASP:OD1   | 2:G:134:ASP:N     | 2.50                     | 0.45              |
| 2:G:3365:UNK:O    | 2:G:3369:UNK:N    | 2.50                     | 0.45              |
| 2:I:1865:MET:SD   | 2:I:1865:MET:N    | 2.90                     | 0.45              |
| 2:I:2869:ARG:HA   | 2:I:2872:GLN:HB3  | 1.98                     | 0.45              |
| 2:E:2869:ARG:HA   | 2:E:2872:GLN:HB3  | 1.98                     | 0.45              |
| 1:F:76:CYS:HB2    | 1:F:97:LEU:HB2    | 1.98                     | 0.45              |
| 2:B:1247:PRO:HA   | 2:B:1598:GLN:HA   | 1.99                     | 0.45              |
| 2:G:683:ARG:HG2   | 2:G:717:ASP:HB3   | 1.98                     | 0.45              |
| 2:I:404:ILE:HG21  | 2:I:481:GLU:HG3   | 1.99                     | 0.45              |
| 2:I:1095:VAL:HB   | 2:I:1199:VAL:HG23 | 1.99                     | 0.45              |
| 2:E:1092:PHE:N    | 2:E:1149:VAL:O    | 2.41                     | 0.45              |
| 2:E:4864:ASN:ND2  | 2:E:4871:GLU:OE1  | 2.46                     | 0.45              |
| 1:H:76:CYS:HB2    | 1:H:97:LEU:HB2    | 1.98                     | 0.44              |
| 2:B:396:GLU:OE2   | 2:B:451:TYR:OH    | 2.28                     | 0.44              |
| 2:G:34:LYS:H      | 2:G:53:SER:HG     | 1.63                     | 0.44              |
| 2:I:4233:LEU:HA   | 2:I:4236:SER:HB3  | 1.99                     | 0.44              |
| 2:I:4713:SER:HA   | 2:I:4718:LYS:HE2  | 1.98                     | 0.44              |
| 2:E:2776:SER:O    | 2:E:2788:HIS:N    | 2.50                     | 0.44              |
| 2:E:4075:GLU:HA   | 2:E:4078:GLN:HB2  | 2.00                     | 0.44              |
| 2:G:43:GLY:N      | 2:G:447:ASP:OD2   | 2.45                     | 0.44              |
| 2:G:621:ILE:O     | 2:G:625:LEU:N     | 2.46                     | 0.44              |
| 2:G:1865:MET:SD   | 2:G:1865:MET:N    | 2.90                     | 0.44              |
| 2:G:2430:ILE:HG21 | 2:G:2502:UNK:HA   | 1.99                     | 0.44              |
| 2:G:3955:MET:HG3  | 2:G:4019:LEU:HD22 | 1.98                     | 0.44              |
| 2:G:4233:LEU:HA   | 2:G:4236:SER:HB3  | 2.00                     | 0.44              |
| 2:I:533:ASN:ND2   | 2:I:536:ASN:OD1   | 2.40                     | 0.44              |
| 1:H:74:LEU:HB2    | 1:H:99:PHE:HB2    | 2.00                     | 0.44              |
| 2:B:2231:SER:HA   | 2:B:2234:ARG:HG2  | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:4017:LEU:HB3  | 2:B:4139:ILE:HG13 | 1.98                     | 0.44              |
| 2:G:396:GLU:OE2   | 2:G:451:TYR:OH    | 2.28                     | 0.44              |
| 2:G:790:ARG:HG2   | 2:G:1627:ALA:HA   | 1.99                     | 0.44              |
| 2:G:3658:LYS:HA   | 2:G:3661:TRP:CE2  | 2.53                     | 0.44              |
| 2:I:134:ASP:OD1   | 2:I:134:ASP:N     | 2.50                     | 0.44              |
| 2:I:683:ARG:HG2   | 2:I:717:ASP:HB3   | 1.98                     | 0.44              |
| 2:I:3955:MET:HG3  | 2:I:4019:LEU:HD22 | 1.99                     | 0.44              |
| 2:E:533:ASN:ND2   | 2:E:536:ASN:OD1   | 2.40                     | 0.44              |
| 2:E:4017:LEU:HB3  | 2:E:4139:ILE:HG13 | 1.98                     | 0.44              |
| 2:B:1727:ARG:HH21 | 2:B:1775:HIS:CE1  | 2.36                     | 0.44              |
| 2:B:2776:SER:O    | 2:B:2788:HIS:N    | 2.50                     | 0.44              |
| 2:B:3973:CYS:SG   | 2:B:3976:ASN:ND2  | 2.91                     | 0.44              |
| 2:G:3973:CYS:SG   | 2:G:3976:ASN:ND2  | 2.91                     | 0.44              |
| 2:I:1727:ARG:HH21 | 2:I:1775:HIS:CE1  | 2.36                     | 0.44              |
| 2:E:3361:UNK:O    | 2:E:3365:UNK:N    | 2.50                     | 0.44              |
| 1:A:56:ILE:HG13   | 1:A:59:PHE:H      | 1.83                     | 0.44              |
| 2:B:892:THR:N     | 2:B:902:ARG:O     | 2.49                     | 0.44              |
| 2:B:983:THR:O     | 2:B:987:ARG:N     | 2.49                     | 0.44              |
| 2:B:3658:LYS:HA   | 2:B:3661:TRP:CE2  | 2.53                     | 0.44              |
| 2:B:4075:GLU:HA   | 2:B:4078:GLN:HB2  | 2.00                     | 0.44              |
| 2:B:4968:PHE:CE2  | 2:B:4978:HIS:HE1  | 2.21                     | 0.44              |
| 2:G:404:ILE:HG21  | 2:G:481:GLU:HG3   | 1.99                     | 0.44              |
| 2:G:1095:VAL:HB   | 2:G:1199:VAL:HG23 | 1.99                     | 0.44              |
| 2:I:164:ARG:N     | 2:I:167:ASP:OD2   | 2.46                     | 0.44              |
| 2:I:214:VAL:HG12  | 2:I:274:LEU:HD12  | 1.98                     | 0.44              |
| 2:I:3658:LYS:HA   | 2:I:3661:TRP:CE2  | 2.53                     | 0.44              |
| 2:E:606:LEU:O     | 2:E:617:ASN:ND2   | 2.50                     | 0.44              |
| 2:E:1095:VAL:HB   | 2:E:1199:VAL:HG23 | 1.99                     | 0.44              |
| 2:E:1247:PRO:HA   | 2:E:1598:GLN:HA   | 1.99                     | 0.44              |
| 2:E:3973:CYS:SG   | 2:E:3976:ASN:ND2  | 2.91                     | 0.44              |
| 2:B:34:LYS:H      | 2:B:53:SER:HG     | 1.64                     | 0.44              |
| 2:G:1105:ALA:HB1  | 2:G:1109:LEU:HD21 | 2.00                     | 0.44              |
| 2:G:1653:LEU:HB3  | 2:G:1660:GLN:HB2  | 2.00                     | 0.44              |
| 2:G:1727:ARG:HH21 | 2:G:1775:HIS:CE1  | 2.36                     | 0.44              |
| 2:I:2231:SER:HA   | 2:I:2234:ARG:HG2  | 2.00                     | 0.44              |
| 2:I:2776:SER:O    | 2:I:2788:HIS:N    | 2.50                     | 0.44              |
| 2:I:3973:CYS:SG   | 2:I:3976:ASN:ND2  | 2.91                     | 0.44              |
| 2:E:1105:ALA:HB1  | 2:E:1109:LEU:HD21 | 2.00                     | 0.44              |
| 2:E:3940:LYS:O    | 2:E:4002:LYS:NZ   | 2.49                     | 0.44              |
| 1:A:7:ILE:HB      | 1:A:71:ARG:HB3    | 1.99                     | 0.44              |
| 2:G:2869:ARG:HA   | 2:G:2872:GLN:HB3  | 1.98                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:I:3361:UNK:O    | 2:I:3365:UNK:N    | 2.50                     | 0.44              |
| 2:E:119:SER:HA    | 2:E:146:CYS:HA    | 1.99                     | 0.44              |
| 2:E:914:PRO:O     | 2:E:918:ARG:N     | 2.51                     | 0.44              |
| 1:F:92:PRO:HD3    | 2:E:627:PRO:HB2   | 1.99                     | 0.44              |
| 1:A:76:CYS:HB2    | 1:A:97:LEU:HB2    | 1.98                     | 0.44              |
| 2:B:2869:ARG:HA   | 2:B:2872:GLN:HB3  | 1.98                     | 0.44              |
| 2:B:4031:LEU:HB3  | 2:B:4034:ASN:HB2  | 1.98                     | 0.44              |
| 2:G:892:THR:N     | 2:G:902:ARG:O     | 2.49                     | 0.44              |
| 2:G:1247:PRO:HA   | 2:G:1598:GLN:HA   | 1.99                     | 0.44              |
| 2:G:1972:ASN:HD21 | 2:G:2024:PRO:HB3  | 1.83                     | 0.44              |
| 2:I:793:LEU:HB2   | 2:I:797:HIS:H     | 1.83                     | 0.44              |
| 2:E:404:ILE:HG21  | 2:E:481:GLU:HG3   | 1.99                     | 0.44              |
| 2:E:1727:ARG:HH21 | 2:E:1775:HIS:CE1  | 2.36                     | 0.44              |
| 2:E:3658:LYS:HA   | 2:E:3661:TRP:CE2  | 2.53                     | 0.44              |
| 2:E:4826:ILE:O    | 2:E:4829:SER:OG   | 2.31                     | 0.44              |
| 1:F:56:ILE:HG13   | 1:F:59:PHE:H      | 1.83                     | 0.44              |
| 1:F:74:LEU:HB2    | 1:F:99:PHE:HB2    | 2.00                     | 0.44              |
| 1:J:7:ILE:HB      | 1:J:71:ARG:HB3    | 1.99                     | 0.44              |
| 2:B:3361:UNK:O    | 2:B:3365:UNK:N    | 2.50                     | 0.44              |
| 2:G:793:LEU:HB2   | 2:G:797:HIS:H     | 1.83                     | 0.44              |
| 2:G:2196:ASN:OD1  | 2:G:2199:ARG:NH1  | 2.40                     | 0.44              |
| 2:G:4075:GLU:HA   | 2:G:4078:GLN:HB2  | 1.99                     | 0.44              |
| 2:I:4075:GLU:HA   | 2:I:4078:GLN:HB2  | 1.99                     | 0.44              |
| 2:I:4743:MET:HB3  | 2:I:4746:ALA:HB3  | 2.00                     | 0.44              |
| 2:I:4763:GLY:O    | 2:I:4766:THR:OG1  | 2.28                     | 0.44              |
| 2:I:4826:ILE:O    | 2:I:4829:SER:OG   | 2.31                     | 0.44              |
| 2:E:790:ARG:HG2   | 2:E:1627:ALA:HA   | 1.99                     | 0.44              |
| 1:J:74:LEU:HB2    | 1:J:99:PHE:HB2    | 2.00                     | 0.43              |
| 2:B:3674:ILE:HD11 | 2:B:3728:ILE:HG22 | 1.99                     | 0.43              |
| 2:B:4743:MET:HB3  | 2:B:4746:ALA:HB3  | 2.00                     | 0.43              |
| 2:G:1727:ARG:NH2  | 2:G:1773:PRO:O    | 2.50                     | 0.43              |
| 2:I:396:GLU:OE2   | 2:I:451:TYR:OH    | 2.28                     | 0.43              |
| 2:I:572:PRO:HA    | 2:I:575:LEU:HD13  | 2.00                     | 0.43              |
| 2:I:681:HIS:HB3   | 2:I:784:SER:HB3   | 2.00                     | 0.43              |
| 2:E:463:GLU:OE2   | 2:E:467:LYS:NZ    | 2.49                     | 0.43              |
| 2:E:681:HIS:HB3   | 2:E:784:SER:HB3   | 2.00                     | 0.43              |
| 2:E:4031:LEU:HB3  | 2:E:4034:ASN:HB2  | 1.98                     | 0.43              |
| 2:B:572:PRO:HA    | 2:B:575:LEU:HD13  | 2.00                     | 0.43              |
| 2:B:841:GLY:HA2   | 2:B:1073:ARG:HD2  | 2.00                     | 0.43              |
| 2:I:3674:ILE:HD11 | 2:I:3728:ILE:HG22 | 1.99                     | 0.43              |
| 2:E:1236:THR:OG1  | 2:E:1608:MET:SD   | 2.76                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:1972:ASN:HD21 | 2:E:2024:PRO:HB3  | 1.83                     | 0.43              |
| 2:E:3676:ASP:N    | 2:E:3676:ASP:OD1  | 2.50                     | 0.43              |
| 2:B:866:HIS:O     | 2:B:1051:TYR:OH   | 2.31                     | 0.43              |
| 2:B:1859:VAL:HA   | 2:B:1862:ILE:HG12 | 2.00                     | 0.43              |
| 2:B:1972:ASN:HD21 | 2:B:2024:PRO:HB3  | 1.83                     | 0.43              |
| 2:B:4233:LEU:HA   | 2:B:4236:SER:HB3  | 1.99                     | 0.43              |
| 2:G:533:ASN:ND2   | 2:G:536:ASN:OD1   | 2.40                     | 0.43              |
| 2:I:1653:LEU:HB3  | 2:I:1660:GLN:HB2  | 2.00                     | 0.43              |
| 2:E:1859:VAL:HA   | 2:E:1862:ILE:HG12 | 2.01                     | 0.43              |
| 2:B:790:ARG:HG2   | 2:B:1627:ALA:HA   | 1.99                     | 0.43              |
| 2:B:793:LEU:HB2   | 2:B:797:HIS:H     | 1.83                     | 0.43              |
| 2:B:1130:GLN:HG2  | 2:B:1138:PRO:HA   | 2.01                     | 0.43              |
| 2:G:681:HIS:HB3   | 2:G:784:SER:HB3   | 2.00                     | 0.43              |
| 2:G:1130:GLN:HG2  | 2:G:1138:PRO:HA   | 2.01                     | 0.43              |
| 2:I:463:GLU:OE2   | 2:I:467:LYS:NZ    | 2.49                     | 0.43              |
| 2:I:4569:LEU:HD11 | 2:I:4646:LEU:HD22 | 2.00                     | 0.43              |
| 2:E:4743:MET:HB3  | 2:E:4746:ALA:HB3  | 2.00                     | 0.43              |
| 1:A:7:ILE:HD13    | 1:A:71:ARG:HG2    | 2.01                     | 0.43              |
| 1:A:82:TYR:O      | 1:A:86:GLY:N      | 2.52                     | 0.43              |
| 1:H:82:TYR:O      | 1:H:86:GLY:N      | 2.52                     | 0.43              |
| 2:G:119:SER:HA    | 2:G:146:CYS:HA    | 1.99                     | 0.43              |
| 2:G:1236:THR:OG1  | 2:G:1608:MET:SD   | 2.76                     | 0.43              |
| 2:G:1859:VAL:HA   | 2:G:1862:ILE:HG12 | 2.01                     | 0.43              |
| 2:I:1698:LEU:N    | 2:I:1712:TYR:OH   | 2.52                     | 0.43              |
| 2:I:3779:VAL:HG23 | 2:I:3780:LEU:HD12 | 2.01                     | 0.43              |
| 2:E:2231:SER:HA   | 2:E:2234:ARG:HG2  | 2.00                     | 0.43              |
| 2:B:1105:ALA:HB1  | 2:B:1109:LEU:HD21 | 2.00                     | 0.43              |
| 2:B:3779:VAL:HG23 | 2:B:3780:LEU:HD12 | 2.01                     | 0.43              |
| 2:G:841:GLY:HA2   | 2:G:1073:ARG:HD2  | 2.00                     | 0.43              |
| 2:G:3674:ILE:HD11 | 2:G:3728:ILE:HG22 | 1.99                     | 0.43              |
| 2:G:3779:VAL:HG23 | 2:G:3780:LEU:HD12 | 2.01                     | 0.43              |
| 2:G:3805:LEU:HA   | 2:G:3809:ASN:HD22 | 1.84                     | 0.43              |
| 2:I:1972:ASN:HD21 | 2:I:2024:PRO:HB3  | 1.83                     | 0.43              |
| 2:E:206:CYS:SG    | 2:E:207:SER:N     | 2.92                     | 0.43              |
| 2:E:793:LEU:HB2   | 2:E:797:HIS:H     | 1.83                     | 0.43              |
| 2:E:4233:LEU:HA   | 2:E:4236:SER:HB3  | 2.00                     | 0.43              |
| 2:B:914:PRO:O     | 2:B:918:ARG:N     | 2.51                     | 0.43              |
| 2:B:4978:HIS:CE1  | 2:B:4982:GLU:HG3  | 2.53                     | 0.43              |
| 2:G:3940:LYS:O    | 2:G:4002:LYS:NZ   | 2.49                     | 0.43              |
| 2:I:1247:PRO:HA   | 2:I:1598:GLN:HA   | 1.99                     | 0.43              |
| 2:I:1859:VAL:HA   | 2:I:1862:ILE:HG12 | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:841:GLY:HA2   | 2:E:1073:ARG:HD2  | 2.00                     | 0.43              |
| 2:E:1295:UNK:N    | 2:E:1454:UNK:O    | 2.52                     | 0.43              |
| 2:E:1653:LEU:HB3  | 2:E:1660:GLN:HB2  | 2.00                     | 0.43              |
| 2:G:500:ALA:HB1   | 2:G:504:ALA:HB2   | 2.01                     | 0.43              |
| 2:G:2231:SER:HA   | 2:G:2234:ARG:HG2  | 2.00                     | 0.43              |
| 2:G:4083:ASP:HB3  | 2:G:4086:GLY:H    | 1.84                     | 0.43              |
| 2:G:4743:MET:HB3  | 2:G:4746:ALA:HB3  | 2.00                     | 0.43              |
| 2:I:119:SER:HA    | 2:I:146:CYS:HA    | 1.99                     | 0.43              |
| 2:I:841:GLY:HA2   | 2:I:1073:ARG:HD2  | 2.00                     | 0.43              |
| 2:I:907:LEU:O     | 2:I:963:ASN:ND2   | 2.42                     | 0.43              |
| 2:E:4083:ASP:HB3  | 2:E:4086:GLY:H    | 1.84                     | 0.43              |
| 2:E:4569:LEU:HD11 | 2:E:4646:LEU:HD22 | 2.00                     | 0.43              |
| 1:A:74:LEU:HB2    | 1:A:99:PHE:HB2    | 1.99                     | 0.43              |
| 1:J:82:TYR:O      | 1:J:86:GLY:N      | 2.52                     | 0.43              |
| 2:B:681:HIS:HB3   | 2:B:784:SER:HB3   | 2.00                     | 0.43              |
| 2:G:1698:LEU:N    | 2:G:1712:TYR:OH   | 2.52                     | 0.43              |
| 2:G:3804:ILE:O    | 2:G:3809:ASN:ND2  | 2.52                     | 0.43              |
| 2:I:3676:ASP:OD1  | 2:I:3676:ASP:N    | 2.51                     | 0.43              |
| 2:I:3804:ILE:O    | 2:I:3809:ASN:ND2  | 2.52                     | 0.43              |
| 2:I:4083:ASP:HB3  | 2:I:4086:GLY:H    | 1.84                     | 0.43              |
| 2:E:572:PRO:HA    | 2:E:575:LEU:HD13  | 2.00                     | 0.43              |
| 2:E:645:ARG:N     | 2:E:824:GLU:O     | 2.43                     | 0.43              |
| 1:H:7:ILE:HD13    | 1:H:71:ARG:HG2    | 2.01                     | 0.43              |
| 1:H:56:ILE:HG13   | 1:H:59:PHE:H      | 1.83                     | 0.43              |
| 1:J:56:ILE:HG13   | 1:J:59:PHE:H      | 1.83                     | 0.43              |
| 2:B:1727:ARG:NH2  | 2:B:1773:PRO:O    | 2.50                     | 0.43              |
| 2:B:2587:UNK:O    | 2:B:2591:UNK:N    | 2.52                     | 0.43              |
| 2:B:3804:ILE:O    | 2:B:3809:ASN:ND2  | 2.52                     | 0.43              |
| 2:B:3805:LEU:HA   | 2:B:3809:ASN:HD22 | 1.84                     | 0.43              |
| 2:I:206:CYS:SG    | 2:I:207:SER:N     | 2.92                     | 0.43              |
| 2:I:500:ALA:HB1   | 2:I:504:ALA:HB2   | 2.01                     | 0.43              |
| 2:E:1698:LEU:N    | 2:E:1712:TYR:OH   | 2.52                     | 0.43              |
| 2:E:3779:VAL:HG23 | 2:E:3780:LEU:HD12 | 2.01                     | 0.43              |
| 1:F:82:TYR:O      | 1:F:86:GLY:N      | 2.52                     | 0.42              |
| 2:B:206:CYS:SG    | 2:B:207:SER:N     | 2.92                     | 0.42              |
| 2:B:719:LEU:HD22  | 2:B:735:GLN:HG2   | 2.01                     | 0.42              |
| 2:B:1295:UNK:N    | 2:B:1454:UNK:O    | 2.52                     | 0.42              |
| 2:B:1698:LEU:N    | 2:B:1712:TYR:OH   | 2.52                     | 0.42              |
| 2:B:2810:LYS:O    | 2:B:2814:LYS:N    | 2.39                     | 0.42              |
| 2:I:1236:THR:OG1  | 2:I:1608:MET:SD   | 2.76                     | 0.42              |
| 2:I:1295:UNK:N    | 2:I:1454:UNK:O    | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:E:134:ASP:N     | 2:E:134:ASP:OD1   | 2.50                     | 0.42              |
| 2:E:2742:THR:OG1  | 2:E:2811:GLU:OE1  | 2.31                     | 0.42              |
| 2:E:3674:ILE:HD11 | 2:E:3728:ILE:HG22 | 1.99                     | 0.42              |
| 2:E:3850:GLN:HB3  | 2:E:3873:LYS:HD3  | 2.00                     | 0.42              |
| 2:B:119:SER:HA    | 2:B:146:CYS:HA    | 2.00                     | 0.42              |
| 2:B:134:ASP:OD1   | 2:B:134:ASP:N     | 2.50                     | 0.42              |
| 2:G:572:PRO:HA    | 2:G:575:LEU:HD13  | 2.00                     | 0.42              |
| 2:G:2810:LYS:O    | 2:G:2814:LYS:N    | 2.39                     | 0.42              |
| 2:I:1105:ALA:HB1  | 2:I:1109:LEU:HD21 | 2.00                     | 0.42              |
| 2:I:1931:LEU:HB3  | 2:I:1935:VAL:HB   | 2.01                     | 0.42              |
| 2:E:3805:LEU:HA   | 2:E:3809:ASN:HD22 | 1.84                     | 0.42              |
| 1:J:7:ILE:HD13    | 1:J:71:ARG:HG2    | 2.01                     | 0.42              |
| 2:B:500:ALA:HB1   | 2:B:504:ALA:HB2   | 2.01                     | 0.42              |
| 2:B:742:ASP:HA    | 2:B:760:ASN:HD21  | 1.84                     | 0.42              |
| 2:B:870:ILE:HD12  | 2:B:873:LYS:HB2   | 2.01                     | 0.42              |
| 2:B:2002:PRO:HA   | 2:B:2005:GLN:HB3  | 2.02                     | 0.42              |
| 2:B:3734:HIS:O    | 2:B:3738:GLY:N    | 2.43                     | 0.42              |
| 2:B:4083:ASP:HB3  | 2:B:4086:GLY:H    | 1.84                     | 0.42              |
| 2:G:870:ILE:HD12  | 2:G:873:LYS:HB2   | 2.02                     | 0.42              |
| 2:I:675:LEU:HD11  | 2:I:1633:PRO:HB3  | 2.02                     | 0.42              |
| 2:I:742:ASP:HA    | 2:I:760:ASN:HD21  | 1.84                     | 0.42              |
| 2:I:2271:THR:HG22 | 2:I:2273:LEU:H    | 1.85                     | 0.42              |
| 2:I:2871:LEU:HD22 | 2:I:2927:LEU:HD22 | 2.02                     | 0.42              |
| 2:E:594:GLY:H     | 2:E:1594:ARG:HD3  | 1.85                     | 0.42              |
| 2:E:719:LEU:HD22  | 2:E:735:GLN:HG2   | 2.01                     | 0.42              |
| 2:B:880:GLU:OE1   | 2:B:968:ALA:N     | 2.44                     | 0.42              |
| 2:B:1653:LEU:HB3  | 2:B:1660:GLN:HB2  | 2.00                     | 0.42              |
| 2:B:2871:LEU:HD22 | 2:B:2927:LEU:HD22 | 2.02                     | 0.42              |
| 2:B:3676:ASP:N    | 2:B:3676:ASP:OD1  | 2.50                     | 0.42              |
| 2:B:4569:LEU:HD11 | 2:B:4646:LEU:HD22 | 2.00                     | 0.42              |
| 2:G:210:GLU:HG3   | 2:G:337:PRO:HG3   | 2.02                     | 0.42              |
| 2:I:594:GLY:H     | 2:I:1594:ARG:HD3  | 1.85                     | 0.42              |
| 2:I:621:ILE:O     | 2:I:625:LEU:N     | 2.46                     | 0.42              |
| 2:I:870:ILE:HD12  | 2:I:873:LYS:HB2   | 2.01                     | 0.42              |
| 2:I:1130:GLN:HG2  | 2:I:1138:PRO:HA   | 2.01                     | 0.42              |
| 2:I:1718:ILE:HG13 | 2:I:1719:HIS:CD2  | 2.55                     | 0.42              |
| 2:E:2871:LEU:HD22 | 2:E:2927:LEU:HD22 | 2.01                     | 0.42              |
| 2:B:594:GLY:H     | 2:B:1594:ARG:HD3  | 1.85                     | 0.42              |
| 2:B:1675:ALA:HB1  | 2:B:1676:LEU:HD13 | 2.02                     | 0.42              |
| 2:B:2271:THR:HG22 | 2:B:2273:LEU:H    | 1.84                     | 0.42              |
| 2:B:2823:ILE:HG12 | 2:B:2937:VAL:HG22 | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:1295:UNK:N    | 2:G:1454:UNK:O    | 2.52                     | 0.42              |
| 2:G:2871:LEU:HD22 | 2:G:2927:LEU:HD22 | 2.02                     | 0.42              |
| 2:G:3676:ASP:OD1  | 2:G:3676:ASP:N    | 2.51                     | 0.42              |
| 2:G:4960:ILE:HD11 | 2:G:4985:LEU:HD23 | 2.02                     | 0.42              |
| 2:E:649:PHE:HB3   | 2:E:776:LEU:HD13  | 2.02                     | 0.42              |
| 2:E:2215:LEU:HD23 | 2:E:2260:ASN:HB3  | 2.01                     | 0.42              |
| 2:E:3804:ILE:O    | 2:E:3809:ASN:ND2  | 2.52                     | 0.42              |
| 2:B:675:LEU:HD11  | 2:B:1633:PRO:HB3  | 2.02                     | 0.42              |
| 2:B:1236:THR:OG1  | 2:B:1608:MET:SD   | 2.76                     | 0.42              |
| 2:G:215:THR:HG22  | 2:G:273:HIS:HA    | 2.02                     | 0.42              |
| 2:G:594:GLY:H     | 2:G:1594:ARG:HD3  | 1.85                     | 0.42              |
| 2:G:742:ASP:HA    | 2:G:760:ASN:HD21  | 1.84                     | 0.42              |
| 2:G:3850:GLN:HB3  | 2:G:3873:LYS:HD3  | 2.00                     | 0.42              |
| 2:I:2479:LEU:O    | 2:I:2487:UNK:N    | 2.53                     | 0.42              |
| 2:I:4960:ILE:HD11 | 2:I:4985:LEU:HD23 | 2.02                     | 0.42              |
| 2:E:870:ILE:HD12  | 2:E:873:LYS:HB2   | 2.02                     | 0.42              |
| 2:E:1130:GLN:HG2  | 2:E:1138:PRO:HA   | 2.00                     | 0.42              |
| 2:E:1727:ARG:NH2  | 2:E:1773:PRO:O    | 2.50                     | 0.42              |
| 2:B:1718:ILE:HG13 | 2:B:1719:HIS:CD2  | 2.55                     | 0.42              |
| 2:G:206:CYS:SG    | 2:G:207:SER:N     | 2.92                     | 0.42              |
| 2:G:1718:ILE:HG13 | 2:G:1719:HIS:CD2  | 2.55                     | 0.42              |
| 2:G:2012:PHE:CG   | 2:G:2022:PRO:HD3  | 2.55                     | 0.42              |
| 2:I:2012:PHE:CG   | 2:I:2022:PRO:HD3  | 2.55                     | 0.42              |
| 2:I:2587:UNK:O    | 2:I:2591:UNK:N    | 2.53                     | 0.42              |
| 2:E:210:GLU:HG3   | 2:E:337:PRO:HG3   | 2.02                     | 0.42              |
| 2:E:2587:UNK:O    | 2:E:2591:UNK:N    | 2.53                     | 0.42              |
| 2:E:3663:LEU:H    | 2:E:3663:LEU:HG   | 1.72                     | 0.42              |
| 2:B:649:PHE:HB3   | 2:B:776:LEU:HD13  | 2.02                     | 0.42              |
| 2:B:2215:LEU:HD23 | 2:B:2260:ASN:HB3  | 2.01                     | 0.42              |
| 2:B:4998:LYS:NZ   | 2:B:5007:GLU:OE1  | 2.45                     | 0.42              |
| 2:G:3829:PHE:HD1  | 2:G:3915:ILE:HD11 | 1.85                     | 0.42              |
| 2:I:379:HIS:CD2   | 2:I:381:GLU:H     | 2.38                     | 0.42              |
| 2:I:2823:ILE:HG12 | 2:I:2937:VAL:HG22 | 2.02                     | 0.42              |
| 2:I:3850:GLN:HB3  | 2:I:3873:LYS:HD3  | 2.00                     | 0.42              |
| 2:I:4791:TYR:OH   | 2:I:4815:ASP:OD1  | 2.32                     | 0.42              |
| 2:E:500:ALA:HB1   | 2:E:504:ALA:HB2   | 2.01                     | 0.42              |
| 2:E:2823:ILE:HG12 | 2:E:2937:VAL:HG22 | 2.02                     | 0.42              |
| 1:J:92:PRO:HD3    | 2:I:627:PRO:HB2   | 2.02                     | 0.42              |
| 2:G:582:HIS:O     | 2:G:585:SER:OG    | 2.29                     | 0.42              |
| 2:G:2271:THR:HG22 | 2:G:2273:LEU:H    | 1.85                     | 0.42              |
| 2:I:2002:PRO:HA   | 2:I:2005:GLN:HB3  | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:379:HIS:CD2   | 2:G:381:GLU:H     | 2.38                     | 0.42              |
| 2:G:675:LEU:HD11  | 2:G:1633:PRO:HB3  | 2.02                     | 0.42              |
| 2:G:689:THR:H     | 2:G:778:PHE:HE2   | 1.68                     | 0.42              |
| 2:B:215:THR:HG22  | 2:B:273:HIS:HA    | 2.02                     | 0.41              |
| 2:B:3850:GLN:HB3  | 2:B:3873:LYS:HD3  | 2.00                     | 0.41              |
| 2:B:5013:MET:HE1  | 2:B:5020:ASP:HB3  | 2.02                     | 0.41              |
| 2:G:1124:PHE:HB2  | 2:G:1162:PHE:CE2  | 2.55                     | 0.41              |
| 2:I:689:THR:H     | 2:I:778:PHE:HE2   | 1.68                     | 0.41              |
| 2:I:719:LEU:HD22  | 2:I:735:GLN:HG2   | 2.01                     | 0.41              |
| 2:E:34:LYS:N      | 2:E:53:SER:OG     | 2.44                     | 0.41              |
| 2:E:468:LEU:HB3   | 2:E:472:ARG:HH12  | 1.85                     | 0.41              |
| 2:E:2002:PRO:HA   | 2:E:2005:GLN:HB3  | 2.01                     | 0.41              |
| 2:E:3829:PHE:HD1  | 2:E:3915:ILE:HD11 | 1.85                     | 0.41              |
| 1:F:7:ILE:HD13    | 1:F:71:ARG:HG2    | 2.01                     | 0.41              |
| 2:B:698:GLY:HA2   | 2:B:703:GLY:HA2   | 2.02                     | 0.41              |
| 2:B:2267:MET:HE3  | 2:B:2268:GLN:HG2  | 2.02                     | 0.41              |
| 2:B:3552:UNK:O    | 2:B:3556:UNK:N    | 2.54                     | 0.41              |
| 2:G:1931:LEU:HB3  | 2:G:1935:VAL:HB   | 2.01                     | 0.41              |
| 2:I:210:GLU:HG3   | 2:I:337:PRO:HG3   | 2.02                     | 0.41              |
| 2:I:1675:ALA:HB1  | 2:I:1676:LEU:HD13 | 2.02                     | 0.41              |
| 2:I:3805:LEU:HA   | 2:I:3809:ASN:HD22 | 1.84                     | 0.41              |
| 2:E:675:LEU:HD11  | 2:E:1633:PRO:HB3  | 2.02                     | 0.41              |
| 2:B:164:ARG:N     | 2:B:167:ASP:OD2   | 2.46                     | 0.41              |
| 2:B:1931:LEU:HB3  | 2:B:1935:VAL:HB   | 2.01                     | 0.41              |
| 2:B:4984:ASN:C    | 2:B:4986:ALA:N    | 2.77                     | 0.41              |
| 2:G:983:THR:O     | 2:G:987:ARG:N     | 2.49                     | 0.41              |
| 2:G:1161:ILE:HA   | 2:G:1177:THR:HB   | 2.02                     | 0.41              |
| 2:G:2002:PRO:HA   | 2:G:2005:GLN:HB3  | 2.02                     | 0.41              |
| 2:G:2420:HIS:HB2  | 2:G:2492:UNK:C    | 2.50                     | 0.41              |
| 2:G:2587:UNK:O    | 2:G:2591:UNK:N    | 2.52                     | 0.41              |
| 2:G:4569:LEU:HD11 | 2:G:4646:LEU:HD22 | 2.00                     | 0.41              |
| 2:I:215:THR:HG22  | 2:I:273:HIS:HA    | 2.02                     | 0.41              |
| 2:I:892:THR:N     | 2:I:902:ARG:O     | 2.49                     | 0.41              |
| 2:I:1727:ARG:NH2  | 2:I:1773:PRO:O    | 2.50                     | 0.41              |
| 2:I:2196:ASN:OD1  | 2:I:2199:ARG:NH1  | 2.40                     | 0.41              |
| 2:I:3552:UNK:O    | 2:I:3556:UNK:N    | 2.54                     | 0.41              |
| 2:E:983:THR:O     | 2:E:987:ARG:N     | 2.49                     | 0.41              |
| 2:E:1931:LEU:HB3  | 2:E:1935:VAL:HB   | 2.01                     | 0.41              |
| 2:B:34:LYS:N      | 2:B:53:SER:OG     | 2.44                     | 0.41              |
| 2:B:1708:ARG:HG2  | 2:B:1711:TYR:CE2  | 2.55                     | 0.41              |
| 2:B:4763:GLY:O    | 2:B:4766:THR:OG1  | 2.28                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:359:TYR:OH    | 2:G:385:ASP:OD2   | 2.32                     | 0.41              |
| 2:G:468:LEU:HB3   | 2:G:472:ARG:HH12  | 1.85                     | 0.41              |
| 2:I:278:GLN:N     | 2:I:315:CYS:SG    | 2.94                     | 0.41              |
| 2:I:321:GLU:HB3   | 2:I:322:LYS:H     | 1.75                     | 0.41              |
| 2:E:215:THR:HG22  | 2:E:273:HIS:HA    | 2.02                     | 0.41              |
| 2:E:742:ASP:HA    | 2:E:760:ASN:HD21  | 1.84                     | 0.41              |
| 2:E:4960:ILE:HD11 | 2:E:4985:LEU:HD23 | 2.02                     | 0.41              |
| 2:B:4823:LEU:HD23 | 2:I:4843:LEU:HD12 | 2.02                     | 0.41              |
| 2:B:4982:GLU:HB3  | 2:B:4983:HIS:H    | 1.63                     | 0.41              |
| 2:G:1708:ARG:HG2  | 2:G:1711:TYR:CE2  | 2.55                     | 0.41              |
| 2:G:3959:LYS:O    | 2:G:3963:ASN:ND2  | 2.53                     | 0.41              |
| 2:G:5013:MET:HE1  | 2:G:5020:ASP:HB3  | 2.02                     | 0.41              |
| 2:I:495:ASN:HD21  | 2:I:550:LYS:HG3   | 1.86                     | 0.41              |
| 2:E:1708:ARG:HG2  | 2:E:1711:TYR:CE2  | 2.55                     | 0.41              |
| 2:E:3552:UNK:O    | 2:E:3556:UNK:N    | 2.54                     | 0.41              |
| 2:E:3959:LYS:O    | 2:E:3963:ASN:ND2  | 2.53                     | 0.41              |
| 2:B:379:HIS:CD2   | 2:B:381:GLU:H     | 2.38                     | 0.41              |
| 2:B:1092:PHE:N    | 2:B:1149:VAL:O    | 2.41                     | 0.41              |
| 2:B:2012:PHE:CG   | 2:B:2022:PRO:HD3  | 2.55                     | 0.41              |
| 2:G:649:PHE:HB3   | 2:G:776:LEU:HD13  | 2.02                     | 0.41              |
| 2:G:1078:GLU:HB3  | 2:G:1081:TYR:HD2  | 1.86                     | 0.41              |
| 2:G:1675:ALA:HB1  | 2:G:1676:LEU:HD13 | 2.02                     | 0.41              |
| 2:G:2823:ILE:HG12 | 2:G:2937:VAL:HG22 | 2.02                     | 0.41              |
| 2:G:4843:LEU:HD12 | 2:I:4823:LEU:HD23 | 2.03                     | 0.41              |
| 2:E:698:GLY:HA2   | 2:E:703:GLY:HA2   | 2.02                     | 0.41              |
| 2:E:5013:MET:HE1  | 2:E:5020:ASP:HB3  | 2.02                     | 0.41              |
| 2:B:468:LEU:HB3   | 2:B:472:ARG:HH12  | 1.85                     | 0.41              |
| 2:G:698:GLY:HA2   | 2:G:703:GLY:HA2   | 2.02                     | 0.41              |
| 2:G:924:MET:O     | 2:G:928:THR:OG1   | 2.30                     | 0.41              |
| 2:G:3722:TYR:CZ   | 2:G:3782:MET:HE3  | 2.56                     | 0.41              |
| 2:G:4848:VAL:O    | 2:G:4852:THR:OG1  | 2.29                     | 0.41              |
| 2:I:698:GLY:HA2   | 2:I:703:GLY:HA2   | 2.02                     | 0.41              |
| 2:I:983:THR:O     | 2:I:987:ARG:N     | 2.49                     | 0.41              |
| 2:I:1101:ARG:HH21 | 2:I:1115:LEU:HB3  | 1.86                     | 0.41              |
| 2:I:1708:ARG:HG2  | 2:I:1711:TYR:CE2  | 2.55                     | 0.41              |
| 2:I:2215:LEU:HD23 | 2:I:2260:ASN:HB3  | 2.01                     | 0.41              |
| 2:I:3722:TYR:CZ   | 2:I:3782:MET:HE3  | 2.56                     | 0.41              |
| 2:I:5013:MET:HE1  | 2:I:5020:ASP:HB3  | 2.02                     | 0.41              |
| 2:G:495:ASN:HD21  | 2:G:550:LYS:HG3   | 1.86                     | 0.41              |
| 2:G:1101:ARG:HH21 | 2:G:1115:LEU:HB3  | 1.86                     | 0.41              |
| 2:G:2215:LEU:HD23 | 2:G:2260:ASN:HB3  | 2.01                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:4822:THR:O    | 2:G:4825:THR:OG1  | 2.39                     | 0.41              |
| 2:G:4823:LEU:HD23 | 2:E:4843:LEU:HD12 | 2.03                     | 0.41              |
| 2:I:1124:PHE:HB2  | 2:I:1162:PHE:CE2  | 2.55                     | 0.41              |
| 2:I:2267:MET:HE3  | 2:I:2268:GLN:HG2  | 2.02                     | 0.41              |
| 2:I:3829:PHE:HD1  | 2:I:3915:ILE:HD11 | 1.85                     | 0.41              |
| 2:E:756:SER:HB3   | 2:E:767:VAL:HG22  | 2.03                     | 0.41              |
| 2:E:1124:PHE:HB2  | 2:E:1162:PHE:CE2  | 2.55                     | 0.41              |
| 2:E:1161:ILE:HA   | 2:E:1177:THR:HB   | 2.02                     | 0.41              |
| 2:E:1718:ILE:HG13 | 2:E:1719:HIS:CD2  | 2.55                     | 0.41              |
| 2:E:2285:GLU:HG3  | 2:E:2286:LEU:HG   | 2.03                     | 0.41              |
| 2:B:210:GLU:HG3   | 2:B:337:PRO:HG3   | 2.02                     | 0.41              |
| 2:B:278:GLN:N     | 2:B:315:CYS:SG    | 2.94                     | 0.41              |
| 2:B:2196:ASN:OD1  | 2:B:2199:ARG:NH1  | 2.40                     | 0.41              |
| 2:B:3722:TYR:CZ   | 2:B:3782:MET:HE3  | 2.56                     | 0.41              |
| 2:B:3829:PHE:HD1  | 2:B:3915:ILE:HD11 | 1.85                     | 0.41              |
| 2:G:180:LEU:O     | 2:G:200:TRP:NE1   | 2.41                     | 0.41              |
| 2:G:719:LEU:HD22  | 2:G:735:GLN:HG2   | 2.01                     | 0.41              |
| 2:G:756:SER:HB3   | 2:G:767:VAL:HG22  | 2.03                     | 0.41              |
| 2:G:2267:MET:HE3  | 2:G:2268:GLN:HG2  | 2.02                     | 0.41              |
| 2:G:2869:ARG:NH1  | 2:G:2945:UNK:O    | 2.53                     | 0.41              |
| 2:G:3552:UNK:O    | 2:G:3556:UNK:N    | 2.54                     | 0.41              |
| 2:I:649:PHE:HB3   | 2:I:776:LEU:HD13  | 2.02                     | 0.41              |
| 2:I:756:SER:HB3   | 2:I:767:VAL:HG22  | 2.03                     | 0.41              |
| 2:I:1161:ILE:HA   | 2:I:1177:THR:HB   | 2.02                     | 0.41              |
| 2:E:379:HIS:CD2   | 2:E:381:GLU:H     | 2.38                     | 0.41              |
| 2:E:1735:ILE:HG23 | 2:E:1771:LEU:HD23 | 2.03                     | 0.41              |
| 2:E:2012:PHE:CG   | 2:E:2022:PRO:HD3  | 2.55                     | 0.41              |
| 2:E:2226:PRO:HA   | 2:E:2229:VAL:HG12 | 2.03                     | 0.41              |
| 2:E:2271:THR:HG22 | 2:E:2273:LEU:H    | 1.84                     | 0.41              |
| 2:B:1101:ARG:HH21 | 2:B:1115:LEU:HB3  | 1.86                     | 0.41              |
| 2:B:1161:ILE:HA   | 2:B:1177:THR:HB   | 2.02                     | 0.41              |
| 2:B:2430:ILE:HG21 | 2:B:2502:UNK:HA   | 2.02                     | 0.41              |
| 2:B:2927:LEU:HA   | 2:B:2930:LEU:HD12 | 2.03                     | 0.41              |
| 2:G:2144:ILE:H    | 2:G:2144:ILE:HG13 | 1.81                     | 0.41              |
| 2:G:2226:PRO:HA   | 2:G:2229:VAL:HG12 | 2.03                     | 0.41              |
| 2:I:468:LEU:HB3   | 2:I:472:ARG:HH12  | 1.85                     | 0.41              |
| 2:I:2758:PHE:O    | 2:I:2762:THR:N    | 2.47                     | 0.41              |
| 2:E:21:VAL:HG22   | 2:E:203:ASN:HB2   | 2.03                     | 0.41              |
| 2:E:1675:ALA:HB1  | 2:E:1676:LEU:HD13 | 2.02                     | 0.41              |
| 2:E:4822:THR:O    | 2:E:4825:THR:OG1  | 2.39                     | 0.41              |
| 2:B:645:ARG:N     | 2:B:824:GLU:O     | 2.43                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:B:707:VAL:HG23  | 2:B:713:SER:HB2   | 2.03                     | 0.40              |
| 2:B:4982:GLU:CD   | 2:B:5027:CYS:SG   | 3.04                     | 0.40              |
| 2:E:2208:MET:HE2  | 2:E:2208:MET:HB3  | 1.90                     | 0.40              |
| 1:H:92:PRO:HD3    | 2:G:627:PRO:HB2   | 2.02                     | 0.40              |
| 2:B:495:ASN:HD21  | 2:B:550:LYS:HG3   | 1.86                     | 0.40              |
| 2:B:1679:ASN:ND2  | 2:B:1798:LEU:O    | 2.54                     | 0.40              |
| 2:B:1735:ILE:HG23 | 2:B:1771:LEU:HD23 | 2.03                     | 0.40              |
| 2:B:2144:ILE:H    | 2:B:2144:ILE:HG13 | 1.81                     | 0.40              |
| 2:G:707:VAL:HG23  | 2:G:713:SER:HB2   | 2.03                     | 0.40              |
| 2:G:1679:ASN:ND2  | 2:G:1798:LEU:O    | 2.54                     | 0.40              |
| 2:G:4191:GLU:OE1  | 2:G:5006:GLN:NE2  | 2.54                     | 0.40              |
| 2:I:1078:GLU:HB3  | 2:I:1081:TYR:HD2  | 1.86                     | 0.40              |
| 2:I:3959:LYS:O    | 2:I:3963:ASN:ND2  | 2.53                     | 0.40              |
| 2:I:4242:ILE:O    | 2:I:4246:GLN:N    | 2.54                     | 0.40              |
| 2:I:4928:LEU:HD13 | 2:I:4928:LEU:HA   | 1.92                     | 0.40              |
| 2:E:1101:ARG:HH21 | 2:E:1115:LEU:HB3  | 1.86                     | 0.40              |
| 2:E:2267:MET:HE3  | 2:E:2268:GLN:HG2  | 2.02                     | 0.40              |
| 1:F:87:HIS:HA     | 1:F:88:PRO:HD3    | 1.90                     | 0.40              |
| 2:B:21:VAL:HG22   | 2:B:203:ASN:HB2   | 2.03                     | 0.40              |
| 2:B:2291:GLN:HE21 | 2:B:2294:ASP:H    | 1.70                     | 0.40              |
| 2:B:3959:LYS:O    | 2:B:3963:ASN:ND2  | 2.53                     | 0.40              |
| 2:B:4913:ARG:O    | 2:B:4917:ASP:N    | 2.48                     | 0.40              |
| 2:G:164:ARG:N     | 2:G:167:ASP:OD2   | 2.46                     | 0.40              |
| 2:G:278:GLN:N     | 2:G:315:CYS:SG    | 2.94                     | 0.40              |
| 2:I:4191:GLU:OE1  | 2:I:5006:GLN:NE2  | 2.54                     | 0.40              |
| 1:H:87:HIS:HA     | 1:H:88:PRO:HD3    | 1.90                     | 0.40              |
| 2:B:1078:GLU:HB3  | 2:B:1081:TYR:HD2  | 1.86                     | 0.40              |
| 2:B:2674:UNK:O    | 2:B:2676:UNK:N    | 2.55                     | 0.40              |
| 2:G:489:ASN:HA    | 2:G:492:ASP:HB2   | 2.03                     | 0.40              |
| 2:E:689:THR:H     | 2:E:778:PHE:HE2   | 1.68                     | 0.40              |
| 2:E:2144:ILE:H    | 2:E:2144:ILE:HG13 | 1.80                     | 0.40              |
| 2:E:3722:TYR:CZ   | 2:E:3782:MET:HE3  | 2.56                     | 0.40              |
| 2:B:689:THR:H     | 2:B:778:PHE:HE2   | 1.68                     | 0.40              |
| 2:B:870:ILE:HD12  | 2:B:870:ILE:HA    | 1.98                     | 0.40              |
| 2:B:2226:PRO:HA   | 2:B:2229:VAL:HG12 | 2.03                     | 0.40              |
| 2:B:4191:GLU:OE1  | 2:B:5006:GLN:NE2  | 2.54                     | 0.40              |
| 2:B:4673:ARG:HH22 | 2:B:4698:LYS:HB2  | 1.87                     | 0.40              |
| 2:B:4821:LYS:HE2  | 2:B:4821:LYS:HB3  | 1.95                     | 0.40              |
| 2:G:2208:MET:HB3  | 2:G:2208:MET:HE2  | 1.90                     | 0.40              |
| 2:G:3662:ILE:H    | 2:G:3662:ILE:HG13 | 1.78                     | 0.40              |
| 2:I:395:GLN:NE2   | 2:I:397:GLU:OE1   | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:1679:ASN:ND2 | 2:I:1798:LEU:O   | 2.54                     | 0.40              |
| 2:I:4848:VAL:O   | 2:I:4852:THR:OG1 | 2.28                     | 0.40              |
| 2:E:2810:LYS:O   | 2:E:2814:LYS:N   | 2.39                     | 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%)     | 94 (90%)    | 11 (10%)   | 0        | 100         | 100 |
| 1   | F     | 105/108 (97%)     | 94 (90%)    | 11 (10%)   | 0        | 100         | 100 |
| 1   | H     | 105/108 (97%)     | 94 (90%)    | 11 (10%)   | 0        | 100         | 100 |
| 1   | J     | 105/108 (97%)     | 94 (90%)    | 11 (10%)   | 0        | 100         | 100 |
| 2   | B     | 3235/4416 (73%)   | 2894 (90%)  | 333 (10%)  | 8 (0%)   | 43          | 77  |
| 2   | E     | 3235/4416 (73%)   | 2898 (90%)  | 332 (10%)  | 5 (0%)   | 43          | 77  |
| 2   | G     | 3235/4416 (73%)   | 2896 (90%)  | 334 (10%)  | 5 (0%)   | 43          | 77  |
| 2   | I     | 3235/4416 (73%)   | 2898 (90%)  | 332 (10%)  | 5 (0%)   | 43          | 77  |
| All | All   | 13360/18096 (74%) | 11962 (90%) | 1375 (10%) | 23 (0%)  | 44          | 77  |

All (23) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 4962 | GLY  |
| 2   | B     | 1708 | ARG  |
| 2   | G     | 1708 | ARG  |
| 2   | I     | 1708 | ARG  |
| 2   | E     | 1708 | ARG  |
| 2   | B     | 1932 | PRO  |
| 2   | B     | 4982 | GLU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 4985 | LEU  |
| 2   | G     | 1932 | PRO  |
| 2   | I     | 1932 | PRO  |
| 2   | E     | 1932 | PRO  |
| 2   | B     | 1840 | PRO  |
| 2   | B     | 4641 | PRO  |
| 2   | G     | 1840 | PRO  |
| 2   | G     | 4641 | PRO  |
| 2   | I     | 1840 | PRO  |
| 2   | I     | 4641 | PRO  |
| 2   | E     | 1840 | PRO  |
| 2   | E     | 4641 | PRO  |
| 2   | B     | 2291 | GLN  |
| 2   | G     | 2291 | GLN  |
| 2   | I     | 2291 | GLN  |
| 2   | E     | 2291 | GLN  |

### 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%)   | 2479 (99%)   | 14 (1%)  | 78          | 80  |
| 2   | E     | 2493/3022 (82%)   | 2484 (100%)  | 9 (0%)   | 84          | 82  |
| 2   | G     | 2493/3022 (82%)   | 2484 (100%)  | 9 (0%)   | 84          | 82  |
| 2   | I     | 2493/3022 (82%)   | 2485 (100%)  | 8 (0%)   | 86          | 84  |
| All | All   | 10324/12444 (83%) | 10284 (100%) | 40 (0%)  | 81          | 82  |

All (40) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 131  | LEU  |
| 2   | B     | 688  | LEU  |
| 2   | B     | 719  | LEU  |
| 2   | B     | 1600 | LEU  |
| 2   | B     | 1657 | LEU  |
| 2   | B     | 1676 | LEU  |
| 2   | B     | 2144 | ILE  |
| 2   | B     | 3663 | LEU  |
| 2   | B     | 3805 | LEU  |
| 2   | B     | 4081 | VAL  |
| 2   | B     | 4958 | CYS  |
| 2   | B     | 4960 | ILE  |
| 2   | B     | 4977 | THR  |
| 2   | B     | 4983 | HIS  |
| 2   | G     | 131  | LEU  |
| 2   | G     | 719  | LEU  |
| 2   | G     | 1600 | LEU  |
| 2   | G     | 1657 | LEU  |
| 2   | G     | 1676 | LEU  |
| 2   | G     | 2144 | ILE  |
| 2   | G     | 3663 | LEU  |
| 2   | G     | 3805 | LEU  |
| 2   | G     | 4081 | VAL  |
| 2   | I     | 131  | LEU  |
| 2   | I     | 719  | LEU  |
| 2   | I     | 1600 | LEU  |
| 2   | I     | 1657 | LEU  |
| 2   | I     | 1676 | LEU  |
| 2   | I     | 2144 | ILE  |
| 2   | I     | 3663 | LEU  |
| 2   | I     | 3805 | LEU  |
| 2   | E     | 131  | LEU  |
| 2   | E     | 719  | LEU  |
| 2   | E     | 1600 | LEU  |
| 2   | E     | 1657 | LEU  |
| 2   | E     | 1676 | LEU  |
| 2   | E     | 2144 | ILE  |
| 2   | E     | 3663 | LEU  |
| 2   | E     | 3805 | LEU  |
| 2   | E     | 4081 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (242) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | F     | 87   | HIS  |
| 1   | A     | 87   | HIS  |
| 1   | H     | 87   | HIS  |
| 1   | J     | 87   | HIS  |
| 2   | B     | 57   | ASN  |
| 2   | B     | 105  | HIS  |
| 2   | B     | 113  | HIS  |
| 2   | B     | 190  | GLN  |
| 2   | B     | 273  | HIS  |
| 2   | B     | 379  | HIS  |
| 2   | B     | 395  | GLN  |
| 2   | B     | 413  | GLN  |
| 2   | B     | 479  | GLN  |
| 2   | B     | 489  | ASN  |
| 2   | B     | 520  | ASN  |
| 2   | B     | 582  | HIS  |
| 2   | B     | 593  | HIS  |
| 2   | B     | 725  | HIS  |
| 2   | B     | 765  | GLN  |
| 2   | B     | 797  | HIS  |
| 2   | B     | 838  | HIS  |
| 2   | B     | 1041 | GLN  |
| 2   | B     | 1220 | GLN  |
| 2   | B     | 1598 | GLN  |
| 2   | B     | 1679 | ASN  |
| 2   | B     | 1688 | HIS  |
| 2   | B     | 1691 | GLN  |
| 2   | B     | 1693 | GLN  |
| 2   | B     | 1719 | HIS  |
| 2   | B     | 1775 | HIS  |
| 2   | B     | 1861 | GLN  |
| 2   | B     | 1949 | GLN  |
| 2   | B     | 1953 | HIS  |
| 2   | B     | 1973 | GLN  |
| 2   | B     | 2007 | ASN  |
| 2   | B     | 2100 | HIS  |
| 2   | B     | 2127 | GLN  |
| 2   | B     | 2260 | ASN  |
| 2   | B     | 2291 | GLN  |
| 2   | B     | 2324 | ASN  |
| 2   | B     | 2772 | GLN  |
| 2   | B     | 2773 | ASN  |
| 2   | B     | 3704 | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | B     | 3809 | ASN  |
| 2   | B     | 3814 | GLN  |
| 2   | B     | 3830 | GLN  |
| 2   | B     | 3896 | ASN  |
| 2   | B     | 3946 | GLN  |
| 2   | B     | 3950 | ASN  |
| 2   | B     | 3960 | GLN  |
| 2   | B     | 3976 | ASN  |
| 2   | B     | 3994 | HIS  |
| 2   | B     | 4054 | ASN  |
| 2   | B     | 4120 | ASN  |
| 2   | B     | 4246 | GLN  |
| 2   | B     | 4553 | ASN  |
| 2   | B     | 4574 | ASN  |
| 2   | B     | 4806 | ASN  |
| 2   | B     | 4946 | GLN  |
| 2   | B     | 4949 | GLN  |
| 2   | B     | 4978 | HIS  |
| 2   | B     | 4983 | HIS  |
| 2   | B     | 4987 | ASN  |
| 2   | B     | 5006 | GLN  |
| 2   | G     | 57   | ASN  |
| 2   | G     | 98   | HIS  |
| 2   | G     | 105  | HIS  |
| 2   | G     | 113  | HIS  |
| 2   | G     | 190  | GLN  |
| 2   | G     | 273  | HIS  |
| 2   | G     | 379  | HIS  |
| 2   | G     | 395  | GLN  |
| 2   | G     | 413  | GLN  |
| 2   | G     | 479  | GLN  |
| 2   | G     | 489  | ASN  |
| 2   | G     | 520  | ASN  |
| 2   | G     | 582  | HIS  |
| 2   | G     | 593  | HIS  |
| 2   | G     | 725  | HIS  |
| 2   | G     | 765  | GLN  |
| 2   | G     | 797  | HIS  |
| 2   | G     | 838  | HIS  |
| 2   | G     | 1220 | GLN  |
| 2   | G     | 1274 | HIS  |
| 2   | G     | 1598 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | G     | 1679 | ASN  |
| 2   | G     | 1688 | HIS  |
| 2   | G     | 1691 | GLN  |
| 2   | G     | 1693 | GLN  |
| 2   | G     | 1719 | HIS  |
| 2   | G     | 1775 | HIS  |
| 2   | G     | 1861 | GLN  |
| 2   | G     | 1949 | GLN  |
| 2   | G     | 1953 | HIS  |
| 2   | G     | 1973 | GLN  |
| 2   | G     | 2007 | ASN  |
| 2   | G     | 2100 | HIS  |
| 2   | G     | 2127 | GLN  |
| 2   | G     | 2260 | ASN  |
| 2   | G     | 2291 | GLN  |
| 2   | G     | 2324 | ASN  |
| 2   | G     | 2772 | GLN  |
| 2   | G     | 2773 | ASN  |
| 2   | G     | 3704 | HIS  |
| 2   | G     | 3809 | ASN  |
| 2   | G     | 3814 | GLN  |
| 2   | G     | 3830 | GLN  |
| 2   | G     | 3896 | ASN  |
| 2   | G     | 3946 | GLN  |
| 2   | G     | 3950 | ASN  |
| 2   | G     | 3960 | GLN  |
| 2   | G     | 3976 | ASN  |
| 2   | G     | 3994 | HIS  |
| 2   | G     | 4034 | ASN  |
| 2   | G     | 4054 | ASN  |
| 2   | G     | 4120 | ASN  |
| 2   | G     | 4246 | GLN  |
| 2   | G     | 4553 | ASN  |
| 2   | G     | 4574 | ASN  |
| 2   | G     | 4806 | ASN  |
| 2   | G     | 4833 | ASN  |
| 2   | G     | 4949 | GLN  |
| 2   | G     | 4983 | HIS  |
| 2   | G     | 5006 | GLN  |
| 2   | I     | 57   | ASN  |
| 2   | I     | 105  | HIS  |
| 2   | I     | 113  | HIS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 190  | GLN  |
| 2   | I     | 273  | HIS  |
| 2   | I     | 379  | HIS  |
| 2   | I     | 395  | GLN  |
| 2   | I     | 413  | GLN  |
| 2   | I     | 479  | GLN  |
| 2   | I     | 489  | ASN  |
| 2   | I     | 520  | ASN  |
| 2   | I     | 582  | HIS  |
| 2   | I     | 593  | HIS  |
| 2   | I     | 725  | HIS  |
| 2   | I     | 765  | GLN  |
| 2   | I     | 797  | HIS  |
| 2   | I     | 838  | HIS  |
| 2   | I     | 1220 | GLN  |
| 2   | I     | 1598 | GLN  |
| 2   | I     | 1611 | HIS  |
| 2   | I     | 1679 | ASN  |
| 2   | I     | 1688 | HIS  |
| 2   | I     | 1691 | GLN  |
| 2   | I     | 1693 | GLN  |
| 2   | I     | 1719 | HIS  |
| 2   | I     | 1775 | HIS  |
| 2   | I     | 1861 | GLN  |
| 2   | I     | 1949 | GLN  |
| 2   | I     | 1953 | HIS  |
| 2   | I     | 1973 | GLN  |
| 2   | I     | 2007 | ASN  |
| 2   | I     | 2100 | HIS  |
| 2   | I     | 2127 | GLN  |
| 2   | I     | 2260 | ASN  |
| 2   | I     | 2291 | GLN  |
| 2   | I     | 2324 | ASN  |
| 2   | I     | 2772 | GLN  |
| 2   | I     | 2773 | ASN  |
| 2   | I     | 3704 | HIS  |
| 2   | I     | 3809 | ASN  |
| 2   | I     | 3814 | GLN  |
| 2   | I     | 3830 | GLN  |
| 2   | I     | 3896 | ASN  |
| 2   | I     | 3946 | GLN  |
| 2   | I     | 3950 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | I     | 3960 | GLN  |
| 2   | I     | 3976 | ASN  |
| 2   | I     | 3994 | HIS  |
| 2   | I     | 4034 | ASN  |
| 2   | I     | 4054 | ASN  |
| 2   | I     | 4120 | ASN  |
| 2   | I     | 4246 | GLN  |
| 2   | I     | 4553 | ASN  |
| 2   | I     | 4574 | ASN  |
| 2   | I     | 4806 | ASN  |
| 2   | I     | 4946 | GLN  |
| 2   | I     | 4947 | GLN  |
| 2   | I     | 4949 | GLN  |
| 2   | I     | 4983 | HIS  |
| 2   | I     | 5006 | GLN  |
| 2   | E     | 57   | ASN  |
| 2   | E     | 105  | HIS  |
| 2   | E     | 113  | HIS  |
| 2   | E     | 190  | GLN  |
| 2   | E     | 273  | HIS  |
| 2   | E     | 379  | HIS  |
| 2   | E     | 395  | GLN  |
| 2   | E     | 413  | GLN  |
| 2   | E     | 479  | GLN  |
| 2   | E     | 489  | ASN  |
| 2   | E     | 520  | ASN  |
| 2   | E     | 582  | HIS  |
| 2   | E     | 593  | HIS  |
| 2   | E     | 725  | HIS  |
| 2   | E     | 797  | HIS  |
| 2   | E     | 838  | HIS  |
| 2   | E     | 1041 | GLN  |
| 2   | E     | 1220 | GLN  |
| 2   | E     | 1598 | GLN  |
| 2   | E     | 1679 | ASN  |
| 2   | E     | 1688 | HIS  |
| 2   | E     | 1691 | GLN  |
| 2   | E     | 1693 | GLN  |
| 2   | E     | 1719 | HIS  |
| 2   | E     | 1775 | HIS  |
| 2   | E     | 1861 | GLN  |
| 2   | E     | 1949 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | E     | 1953 | HIS  |
| 2   | E     | 1973 | GLN  |
| 2   | E     | 2007 | ASN  |
| 2   | E     | 2100 | HIS  |
| 2   | E     | 2127 | GLN  |
| 2   | E     | 2260 | ASN  |
| 2   | E     | 2291 | GLN  |
| 2   | E     | 2324 | ASN  |
| 2   | E     | 2772 | GLN  |
| 2   | E     | 2773 | ASN  |
| 2   | E     | 3704 | HIS  |
| 2   | E     | 3809 | ASN  |
| 2   | E     | 3814 | GLN  |
| 2   | E     | 3830 | GLN  |
| 2   | E     | 3896 | ASN  |
| 2   | E     | 3946 | GLN  |
| 2   | E     | 3950 | ASN  |
| 2   | E     | 3960 | GLN  |
| 2   | E     | 3976 | ASN  |
| 2   | E     | 3994 | HIS  |
| 2   | E     | 4054 | ASN  |
| 2   | E     | 4120 | ASN  |
| 2   | E     | 4246 | GLN  |
| 2   | E     | 4553 | ASN  |
| 2   | E     | 4574 | ASN  |
| 2   | E     | 4806 | ASN  |
| 2   | E     | 4833 | ASN  |
| 2   | E     | 4946 | GLN  |
| 2   | E     | 4949 | GLN  |
| 2   | E     | 4983 | HIS  |
| 2   | E     | 5006 | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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   | G     | 14               |
| 2   | B     | 14               |
| 2   | I     | 14               |
| 2   | E     | 14               |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | G     | 4345:UNK  | C      | 4540:PHE  | N      | 73.65        |
| 1     | B     | 4345:UNK  | C      | 4540:PHE  | N      | 73.61        |
| 1     | I     | 4345:UNK  | C      | 4540:PHE  | N      | 73.61        |
| 1     | E     | 4345:UNK  | C      | 4540:PHE  | N      | 73.59        |
| 1     | G     | 3613:UNK  | C      | 3639:THR  | N      | 45.21        |
| 1     | B     | 3613:UNK  | C      | 3639:THR  | N      | 45.16        |
| 1     | E     | 3613:UNK  | C      | 3639:THR  | N      | 45.11        |
| 1     | I     | 3613:UNK  | C      | 3639:THR  | N      | 45.10        |
| 1     | G     | 4253:GLU  | C      | 4320:UNK  | N      | 28.96        |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | I     | 4253:GLU  | C      | 4320:UNK  | N      | 28.94        |
| 1     | B     | 4253:GLU  | C      | 4320:UNK  | N      | 28.93        |
| 1     | E     | 4253:GLU  | C      | 4320:UNK  | N      | 28.92        |
| 1     | B     | 3163:UNK  | C      | 3170:UNK  | N      | 16.13        |
| 1     | G     | 3163:UNK  | C      | 3170:UNK  | N      | 16.13        |
| 1     | I     | 3163:UNK  | C      | 3170:UNK  | N      | 16.13        |
| 1     | E     | 3163:UNK  | C      | 3170:UNK  | N      | 16.13        |
| 1     | I     | 3063:UNK  | C      | 3134:UNK  | N      | 14.80        |
| 1     | E     | 3063:UNK  | C      | 3134:UNK  | N      | 14.80        |
| 1     | B     | 3063:UNK  | C      | 3134:UNK  | N      | 14.79        |
| 1     | G     | 3063:UNK  | C      | 3134:UNK  | N      | 14.79        |
| 1     | G     | 3468:UNK  | C      | 3511:UNK  | N      | 14.32        |
| 1     | B     | 3468:UNK  | C      | 3511:UNK  | N      | 14.31        |
| 1     | E     | 3468:UNK  | C      | 3511:UNK  | N      | 14.31        |
| 1     | I     | 3468:UNK  | C      | 3511:UNK  | N      | 14.30        |
| 1     | I     | 2703:UNK  | C      | 2734:ASN  | N      | 13.53        |
| 1     | E     | 2703:UNK  | C      | 2734:ASN  | N      | 13.51        |
| 1     | B     | 2703:UNK  | C      | 2734:ASN  | N      | 13.49        |
| 1     | G     | 2703:UNK  | C      | 2734:ASN  | N      | 13.47        |
| 1     | I     | 3236:UNK  | C      | 3241:UNK  | N      | 12.90        |
| 1     | E     | 3236:UNK  | C      | 3241:UNK  | N      | 12.90        |
| 1     | B     | 3236:UNK  | C      | 3241:UNK  | N      | 12.89        |
| 1     | G     | 3236:UNK  | C      | 3241:UNK  | N      | 12.89        |
| 1     | B     | 2976:UNK  | C      | 2995:UNK  | N      | 12.39        |
| 1     | I     | 2976:UNK  | C      | 2995:UNK  | N      | 12.39        |
| 1     | E     | 2976:UNK  | C      | 2995:UNK  | N      | 12.39        |
| 1     | G     | 2976:UNK  | C      | 2995:UNK  | N      | 12.38        |
| 1     | E     | 1564:UNK  | C      | 1573:MET  | N      | 12.31        |
| 1     | I     | 1564:UNK  | C      | 1573:MET  | N      | 12.30        |
| 1     | B     | 1564:UNK  | C      | 1573:MET  | N      | 12.29        |
| 1     | G     | 1564:UNK  | C      | 1573:MET  | N      | 12.23        |
| 1     | B     | 3254:UNK  | C      | 3261:UNK  | N      | 8.56         |
| 1     | G     | 3254:UNK  | C      | 3261:UNK  | N      | 8.56         |
| 1     | I     | 3254:UNK  | C      | 3261:UNK  | N      | 8.56         |
| 1     | E     | 3254:UNK  | C      | 3261:UNK  | N      | 8.56         |
| 1     | B     | 1297:UNK  | C      | 1430:UNK  | N      | 5.76         |
| 1     | G     | 1297:UNK  | C      | 1430:UNK  | N      | 5.76         |
| 1     | I     | 1297:UNK  | C      | 1430:UNK  | N      | 5.75         |
| 1     | E     | 1297:UNK  | C      | 1430:UNK  | N      | 5.75         |
| 1     | G     | 2479:LEU  | C      | 2487:UNK  | N      | 3.50         |
| 1     | B     | 2479:LEU  | C      | 2487:UNK  | N      | 3.44         |
| 1     | E     | 2479:LEU  | C      | 2487:UNK  | N      | 3.38         |

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| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | I     | 2479:LEU  | C      | 2487:UNK  | N      | 3.34         |
| 1     | I     | 2939:ARG  | C      | 2942:UNK  | N      | 3.22         |
| 1     | E     | 2939:ARG  | C      | 2942:UNK  | N      | 3.21         |
| 1     | B     | 2939:ARG  | C      | 2942:UNK  | N      | 3.20         |
| 1     | G     | 2939:ARG  | C      | 2942:UNK  | N      | 3.20         |

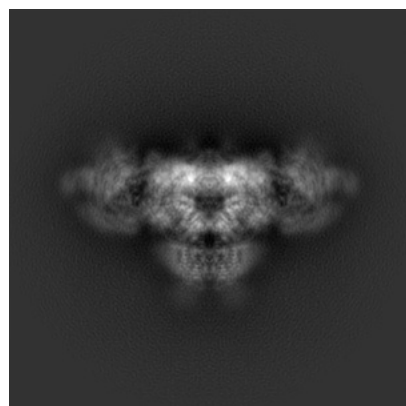
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8387. These allow visual inspection of the internal detail of the map and identification of artifacts.

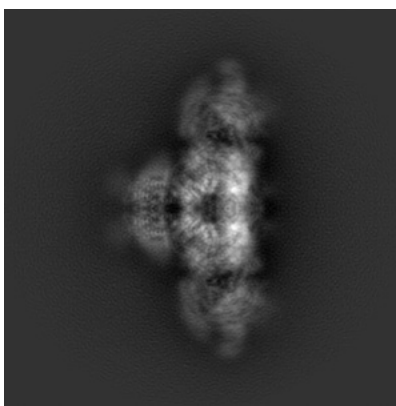
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

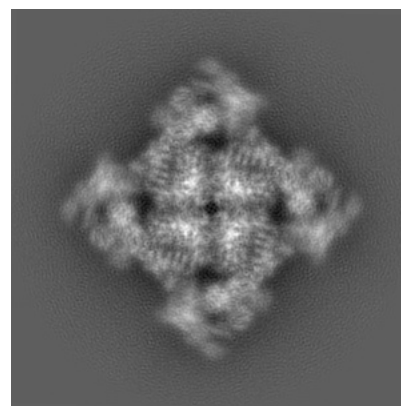
#### 6.1.1 Primary map



X

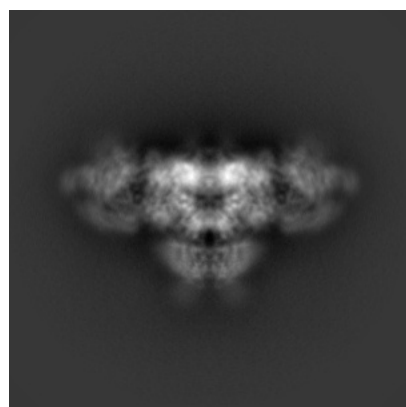


Y

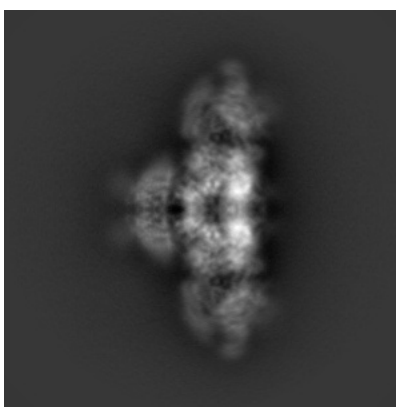


Z

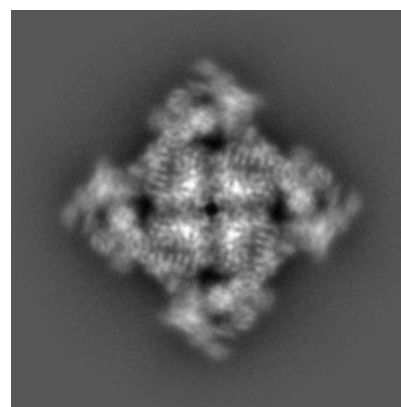
#### 6.1.2 Raw map



X



Y

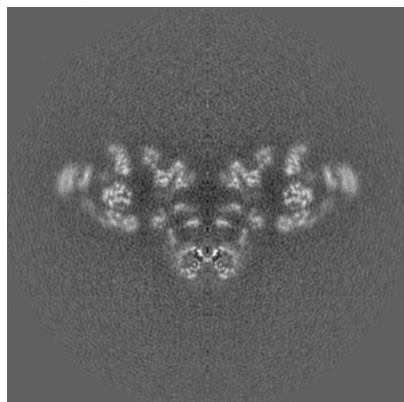


Z

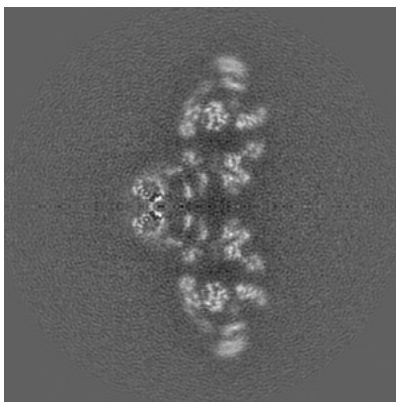
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

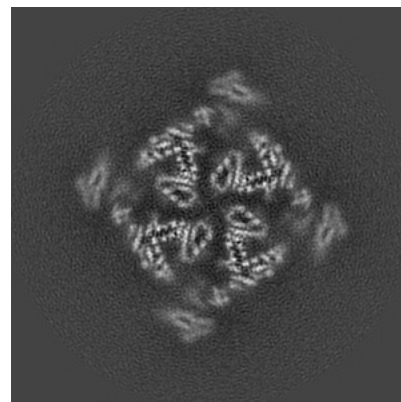
### 6.2.1 Primary map



X Index: 200

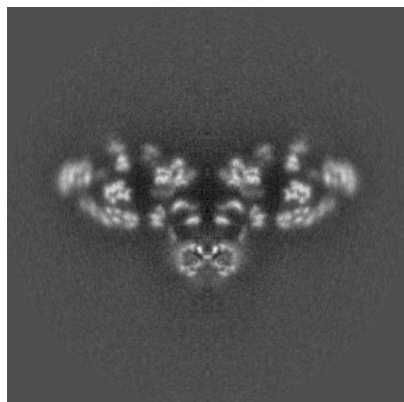


Y Index: 200

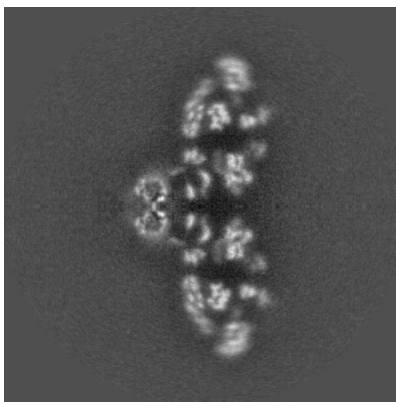


Z Index: 200

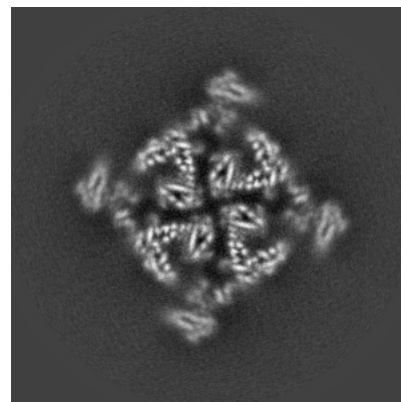
### 6.2.2 Raw map



X Index: 200



Y Index: 200

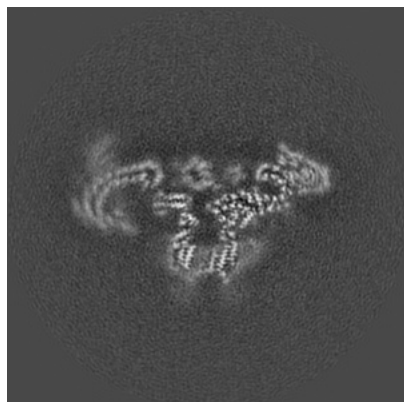


Z Index: 200

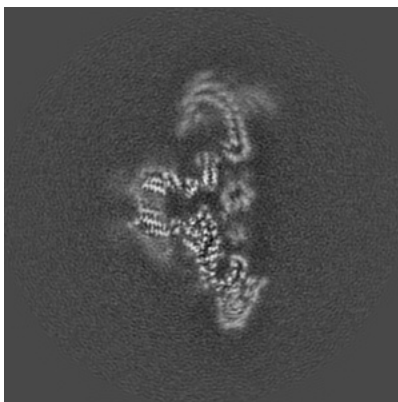
The images above show central slices of the map in three orthogonal directions.

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

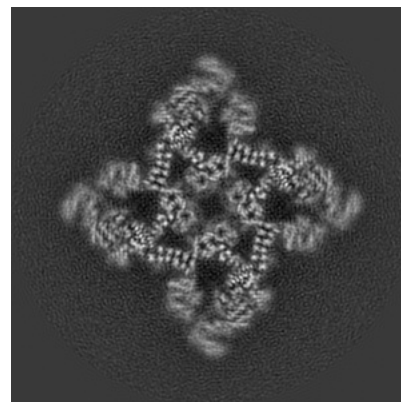
### 6.3.1 Primary map



X Index: 175

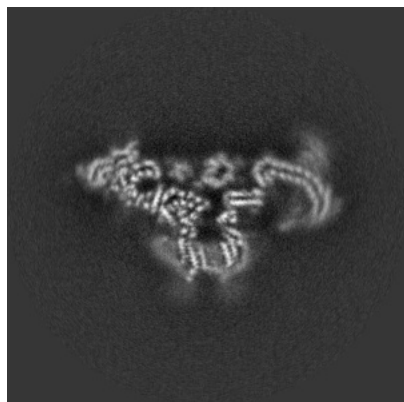


Y Index: 175

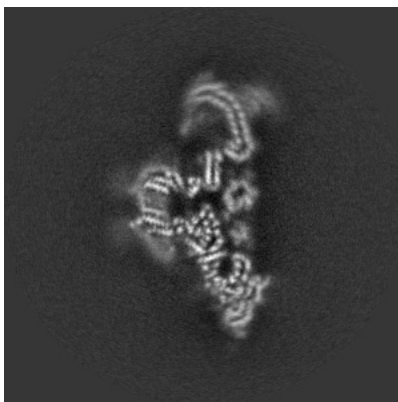


Z Index: 227

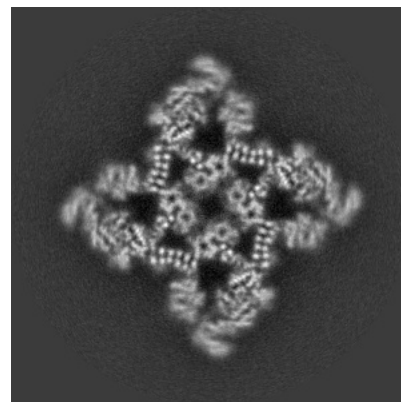
### 6.3.2 Raw map



X Index: 225



Y Index: 175

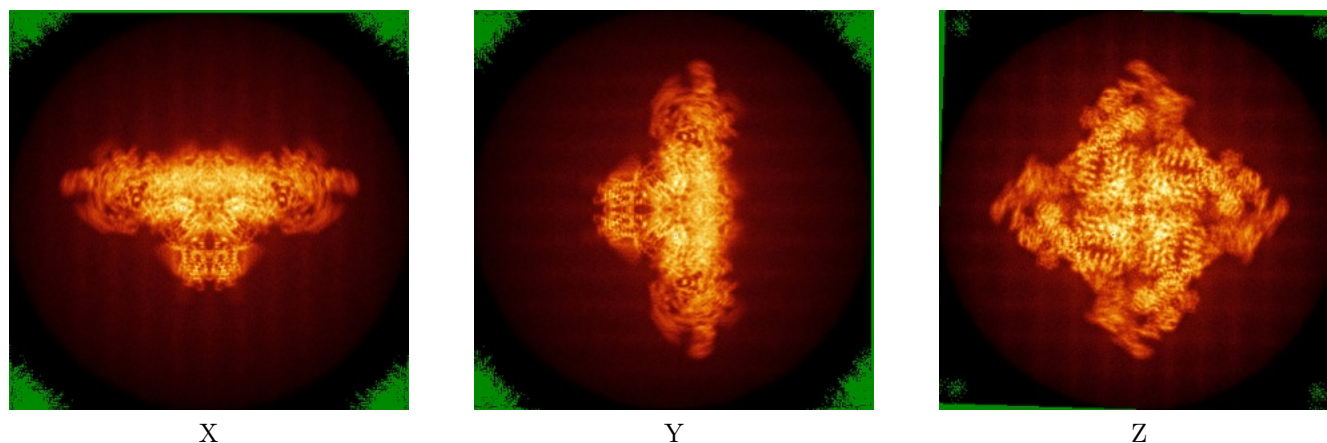


Z Index: 229

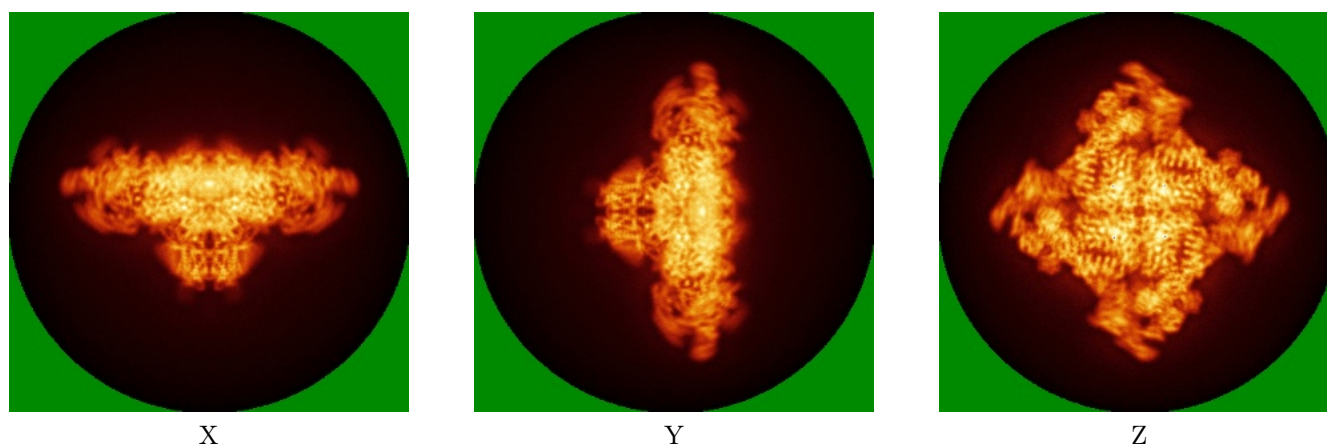
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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

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

This section was not generated.

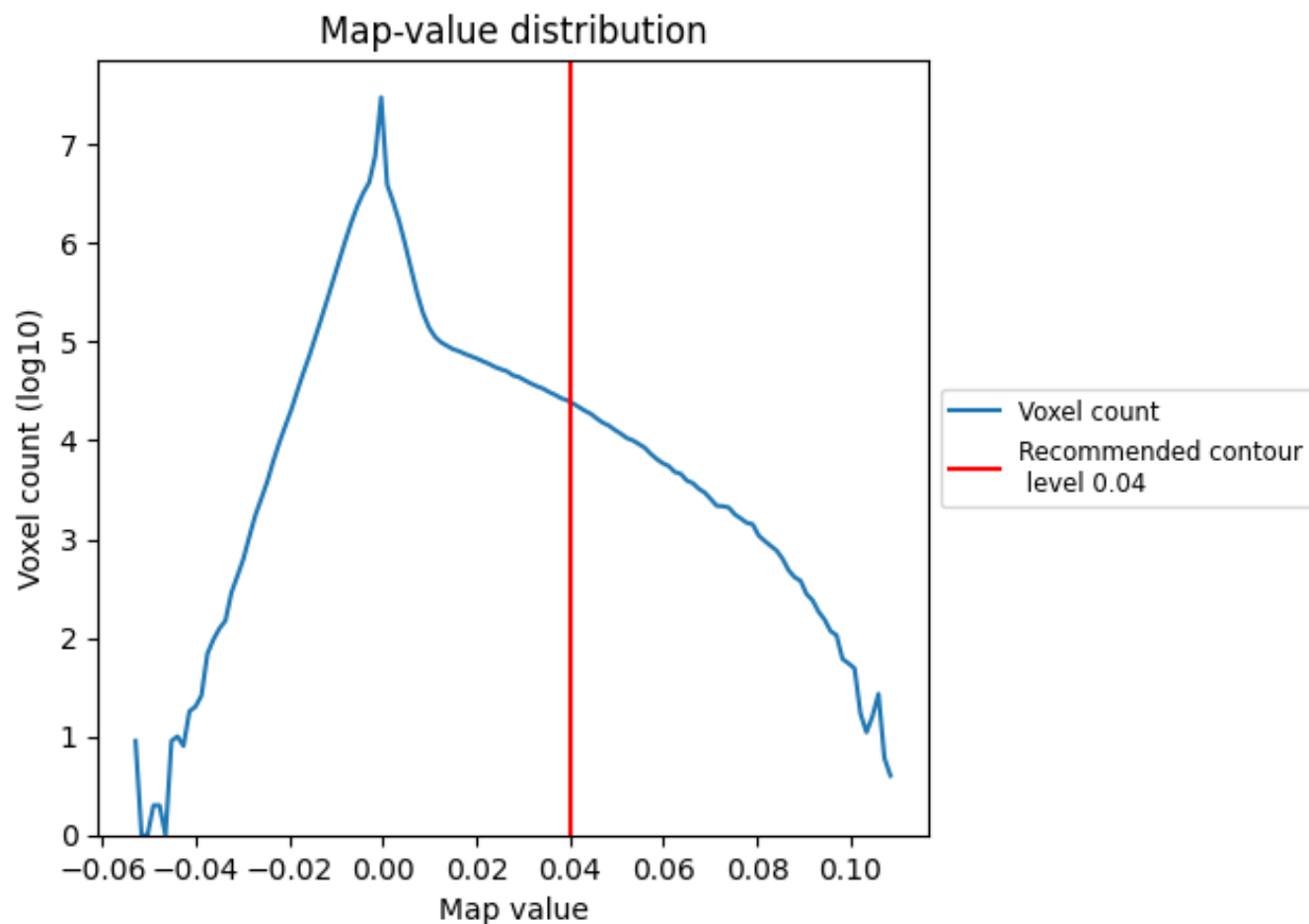
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

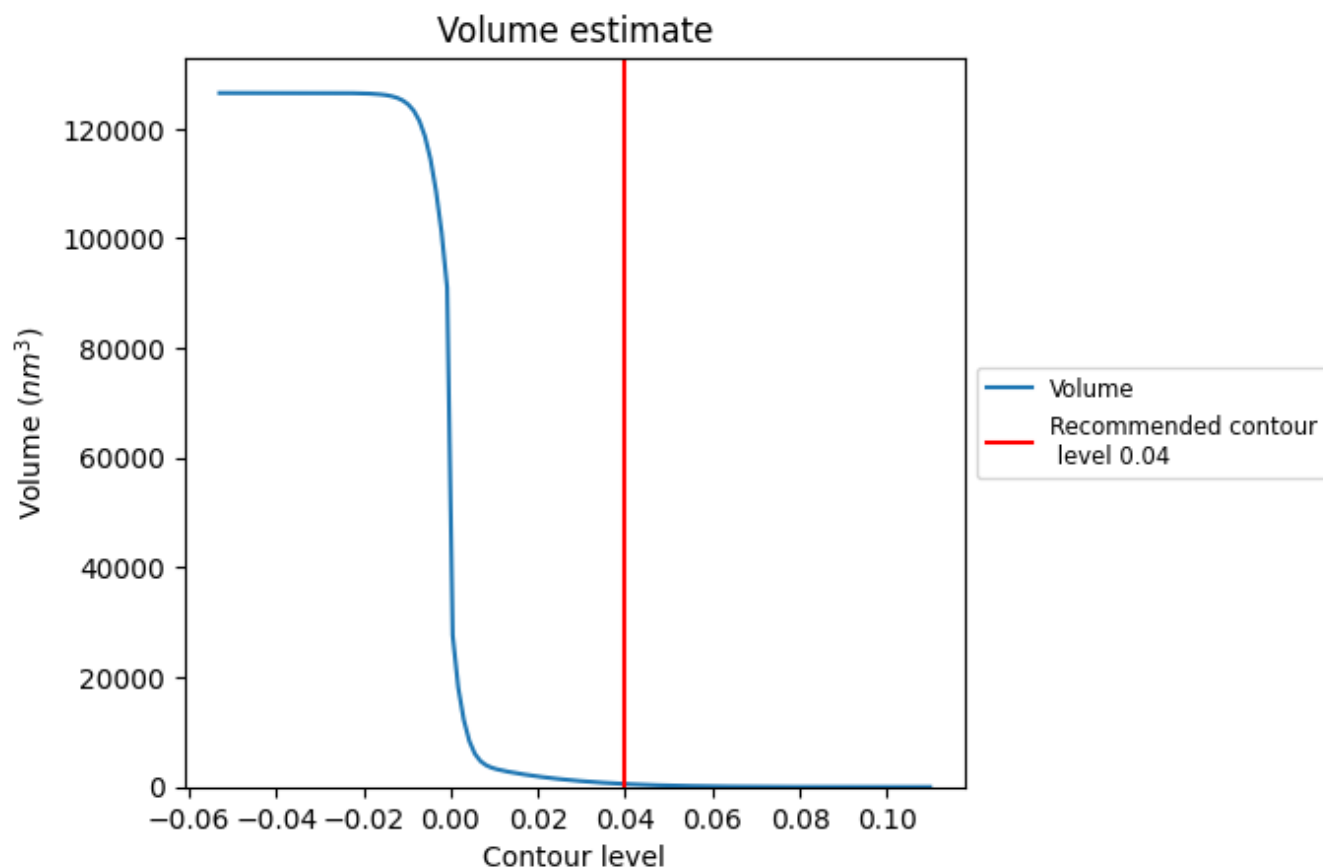
This section contains the results of statistical analysis of the map.

### 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.

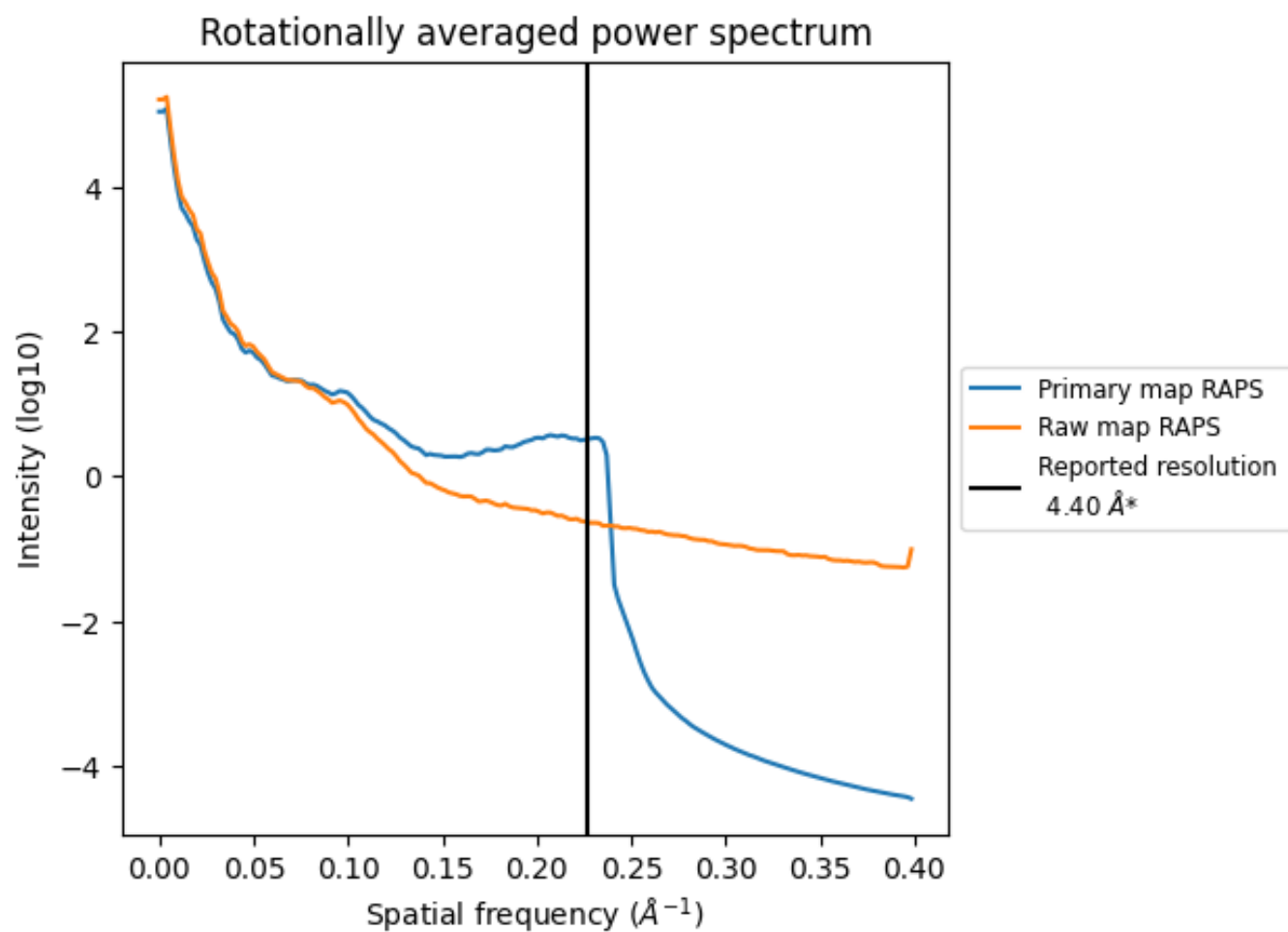
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 547  $\text{nm}^3$ ; this corresponds to an approximate mass of 494 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 ⓘ

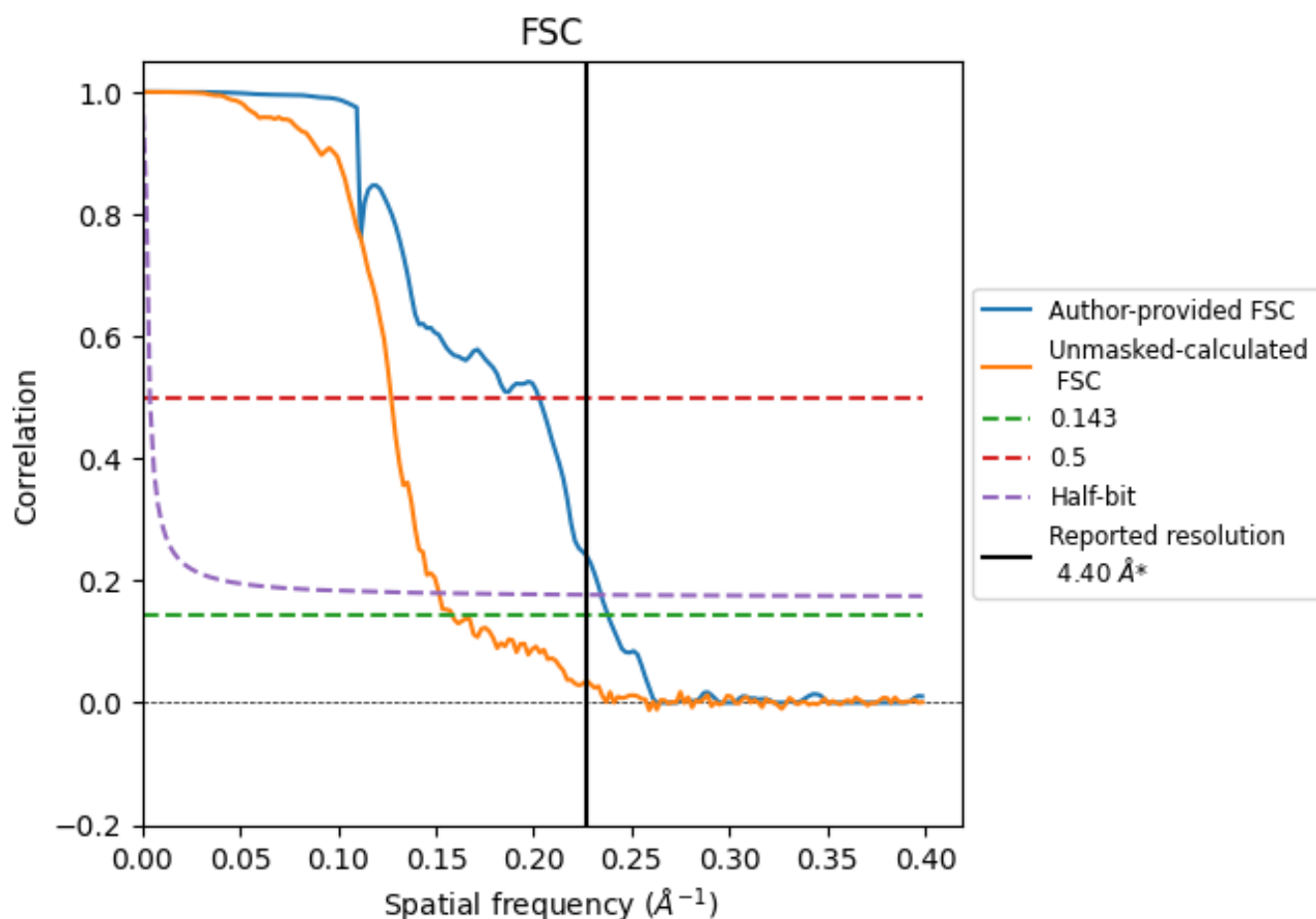


\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

## 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 0.227  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.40                               | -    | -        |
| Author-provided FSC curve | 4.20                               | 4.94 | 4.27     |
| Unmasked-calculated*      | 6.31                               | 7.87 | 6.60     |

\*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 6.31 differs from the reported value 4.4 by more than 10 %

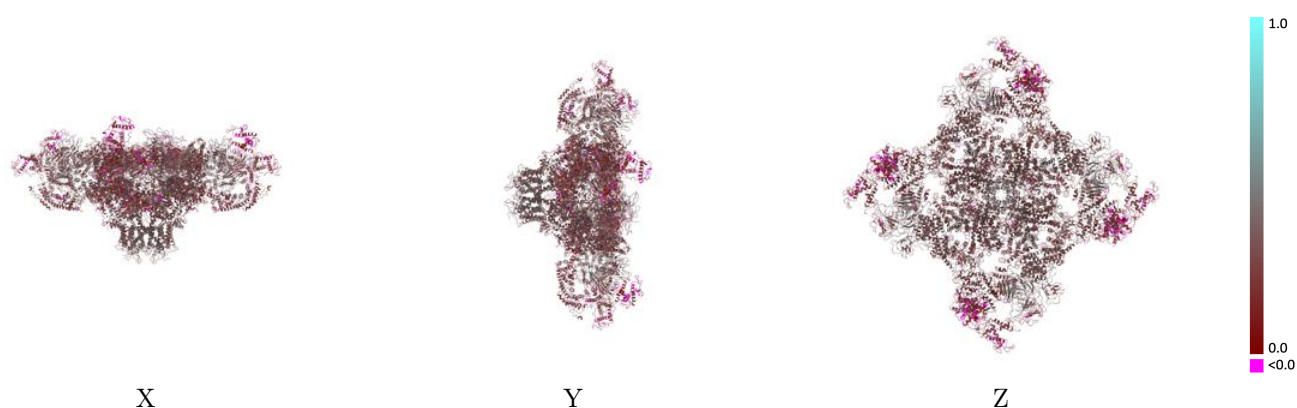
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8387 and PDB model 5TAW. Per-residue inclusion information can be found in section 3 on page 6.

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

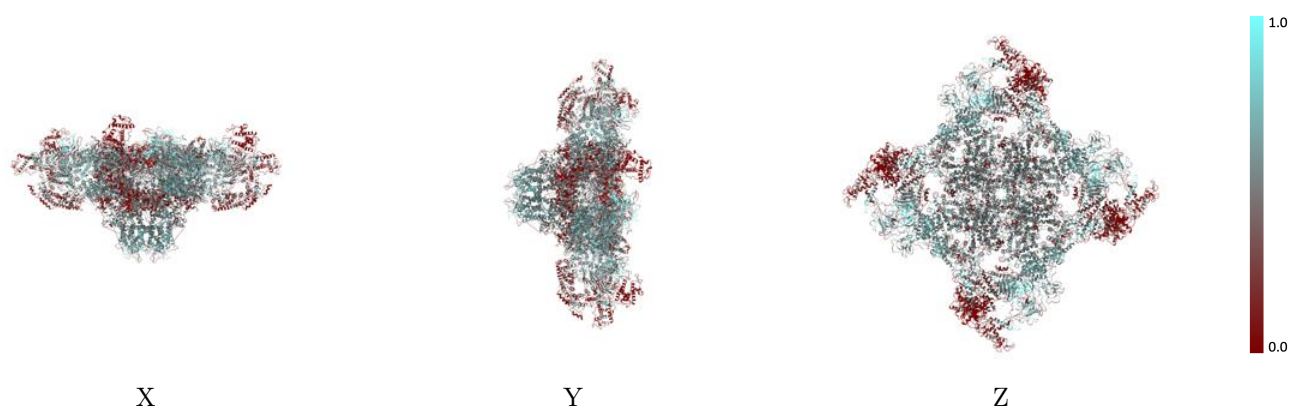
This section was not generated.

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



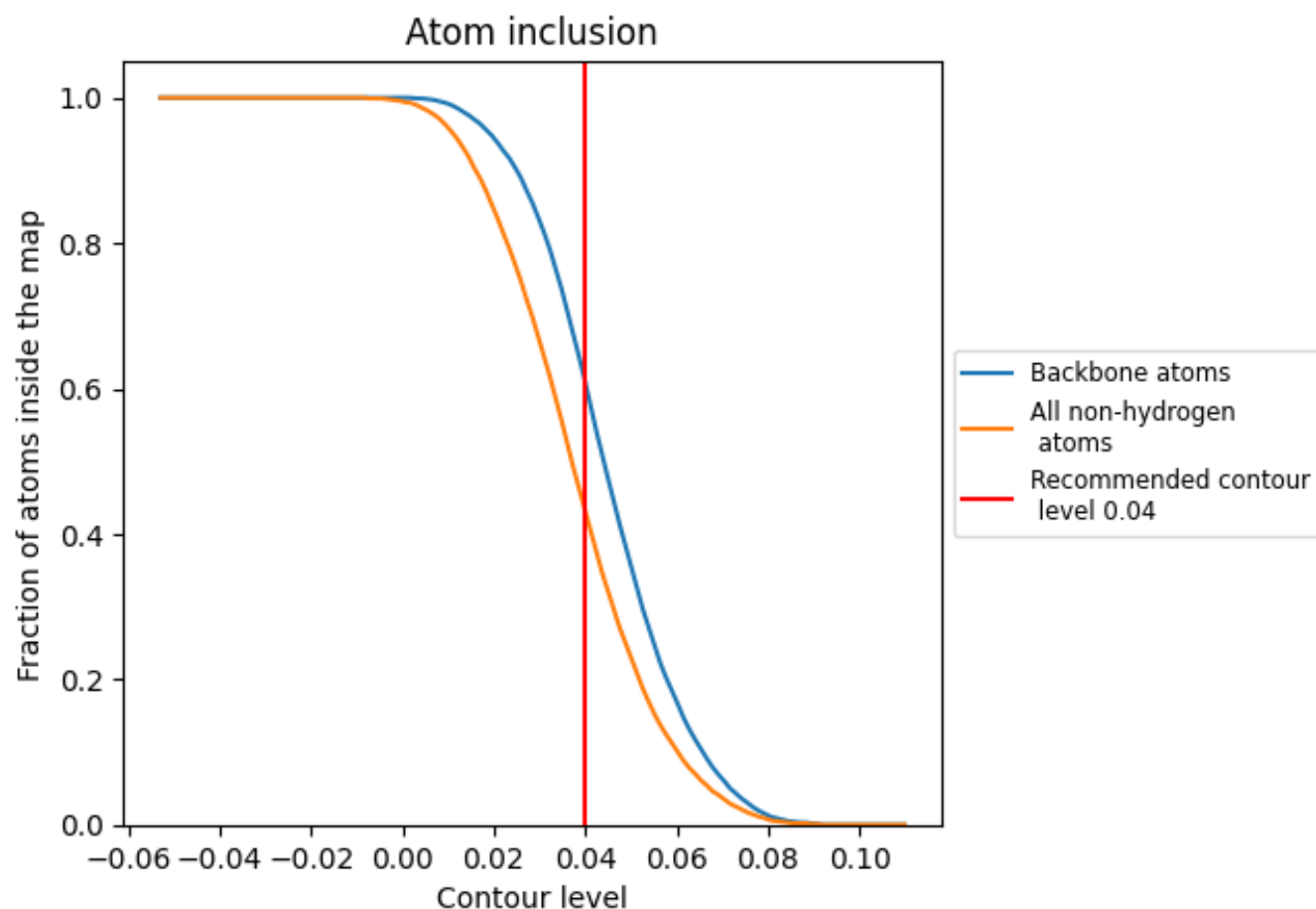
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 43% 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 (0.04) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion     | Q-score            |
|-------|--------------------|--------------------|
| All   | <div></div> 0.4320 | <div></div> 0.2790 |
| A     | <div></div> 0.4970 | <div></div> 0.3250 |
| B     | <div></div> 0.4300 | <div></div> 0.2780 |
| E     | <div></div> 0.4300 | <div></div> 0.2780 |
| F     | <div></div> 0.4940 | <div></div> 0.3290 |
| G     | <div></div> 0.4310 | <div></div> 0.2780 |
| H     | <div></div> 0.4950 | <div></div> 0.3280 |
| I     | <div></div> 0.4300 | <div></div> 0.2780 |
| J     | <div></div> 0.4990 | <div></div> 0.3270 |

1.0

0.0

<0.0