



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:56 PM UTC

PDB ID : 9C5X / pdb\_00009c5x  
EMDB ID : EMD-45234  
Title : Molecular basis for HerA-Duf supramolecular complex in anti-phage defense - Assembly 3  
Authors : Rish, A.D.; Fu, T.M.; Fosuah, E.  
Deposited on : 2024-06-06  
Resolution : 3.01 Å(reported)  
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

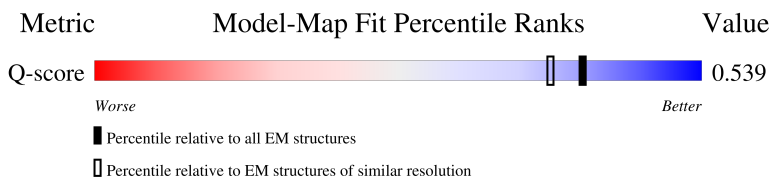
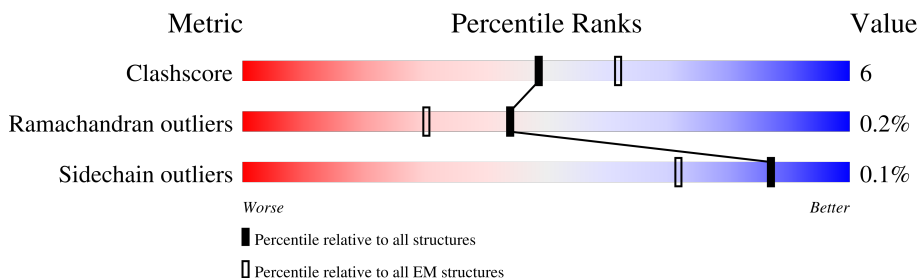
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.01 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.



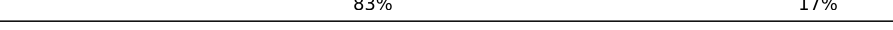
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 13882 ( 2.51 - 3.51 )                                    |

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     | 436    |  |
| 1   | B     | 436    |  |
| 1   | C     | 436    |  |
| 1   | D     | 436    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | E     | 436    |    |
| 1   | F     | 436    |    |
| 1   | G     | 436    |    |
| 1   | H     | 436    |    |
| 1   | I     | 436    |    |
| 1   | J     | 436    |    |
| 1   | K     | 436    |    |
| 1   | L     | 436    |    |
| 2   | M     | 585    |    |
| 2   | N     | 585    |    |
| 2   | O     | 585    |    |
| 2   | P     | 585    |   |
| 2   | Q     | 585    |  |
| 2   | R     | 585    |  |

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 45990 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 DUF4297 domain-containing protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | A     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1423  | 915 | 234 | 269 | 5 |         |       |
| 1   | B     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1423  | 915 | 234 | 269 | 5 |         |       |
| 1   | C     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1423  | 915 | 234 | 269 | 5 |         |       |
| 1   | D     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1423  | 915 | 234 | 269 | 5 |         |       |
| 1   | E     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1423  | 915 | 234 | 269 | 5 |         |       |
| 1   | F     | 170      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1423  | 915 | 234 | 269 | 5 |         |       |
| 1   | G     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 970 | 250 | 281 | 5 |         |       |
| 1   | H     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 970 | 250 | 281 | 5 |         |       |
| 1   | I     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 970 | 250 | 281 | 5 |         |       |
| 1   | J     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 970 | 250 | 281 | 5 |         |       |
| 1   | K     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 970 | 250 | 281 | 5 |         |       |
| 1   | L     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1506  | 970 | 250 | 281 | 5 |         |       |

- Molecule 2 is a protein called ATP-binding protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | M     | 585      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4736  | 3025 | 790 | 909 | 12 |         |       |
| 2   | N     | 585      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4736  | 3025 | 790 | 909 | 12 |         |       |
| 2   | O     | 585      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4736  | 3025 | 790 | 909 | 12 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | P     | 585      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4736  | 3025 | 790 | 909 | 12 |         |       |
| 2   | Q     | 585      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4736  | 3025 | 790 | 909 | 12 |         |       |
| 2   | R     | 585      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4736  | 3025 | 790 | 909 | 12 |         |       |

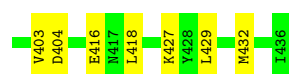




- Molecule 1: DUF4297 domain-containing protein

Chain C: 32% 7% 61%

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     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| TYR | LEU | LYS | GLY | ASN | LYS | LYS | THR | ALA | MET | SER | ARG | GLU | VAL | LEU | GLN | THR | LEU | VAL | LEU | THR | ARG | LYS | LYS | VAL | R267 | K268 | Q270 | L271 | V272 | P273 | S274 | R280 | S281 | R282 | D295 | D296 | Y305 | L306 | D307 | S311 | K312 | F322 | K325 | R337 | I378 | N381 | D396 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     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    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| GLU | ILE | GLY | LEU | SER | TYR | GLU | GLU | THR | ASN | GLU | THR | THR | LYS | GLY | ASN | GLN | LEU | GLY | GLU | GLY | GLU | VAL | THR | LYS | ASP  | VAL  | ASP  | PHE  | PRO  | PRO  | ASP  | LEU  | GLN  | TYR  | TYR  | GLY  | ALA  | GLU  | THR  | SER  | ILE  | GLY  | LEU  | THR  | GLY  | GLU  | GLY  | THR | GLY | GLY | THR | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY |



- Molecule 1: DUF4297 domain-containing protein

Chain D: 35% 7% 61%

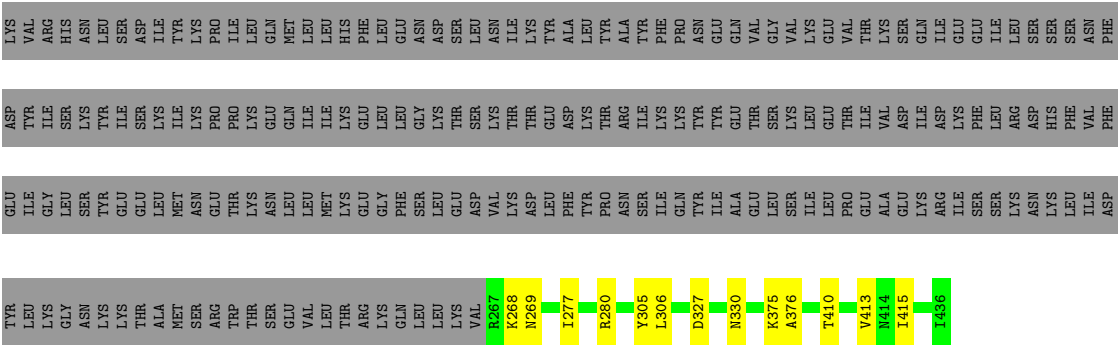
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     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| TYR | LEU | LYS | GLY | ASN | LYS | THR | THR | ALA | MET | SER | ARG | TRP | SER | SER | GLU | VAL | LEU | VAL | LEU | THR | ARG | LYS | GLN | LEU | R267 | V272 | P273 | I285 | N293 | F294 | D295 | D296 | E297 | Y305 | L306 | Y309 | I323 | R337 | E373 | F374 | K375 | V403 | I420 | L426 | I430 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     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| THR | LEU | LYS | GLY | ASN | LYS | THR | THR | ALA | MET | SER | ARG | TRP | SER | SER | GLU | VAL | LEU | VAL | LEU | THR | ARG | LYS | GLN | LEU | R267 | V272 | P273 | I285 | N293 | F294 | D295 | D296 | E297 | Y305 | L306 | Y309 | I323 | R337 | E373 | F374 | K375 | V403 | I420 | L426 | I430 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 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|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| GLY | ILE | GLY | LEU | SER | ASN | GLU | THR | THR | GLU | GLY | THR | THR | GLY | GLY | ASP | VAL | LEU | VAL | LEU | THR | ARG | LYS | GLN | LEU | R267 | V272 | P273 | I285 | N293 | F294 | D295 | D296 | E297 | Y305 | L306 | Y309 | I323 | R337 | E373 | F374 | K375 | V403 | I420 | L426 | I430 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |  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    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
| ASP | TYR | ILE | SER | LYS | THR | ILE | PRO | PRO | GLN | ILE | ILE | GLY | GLY | GLY | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR  | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |



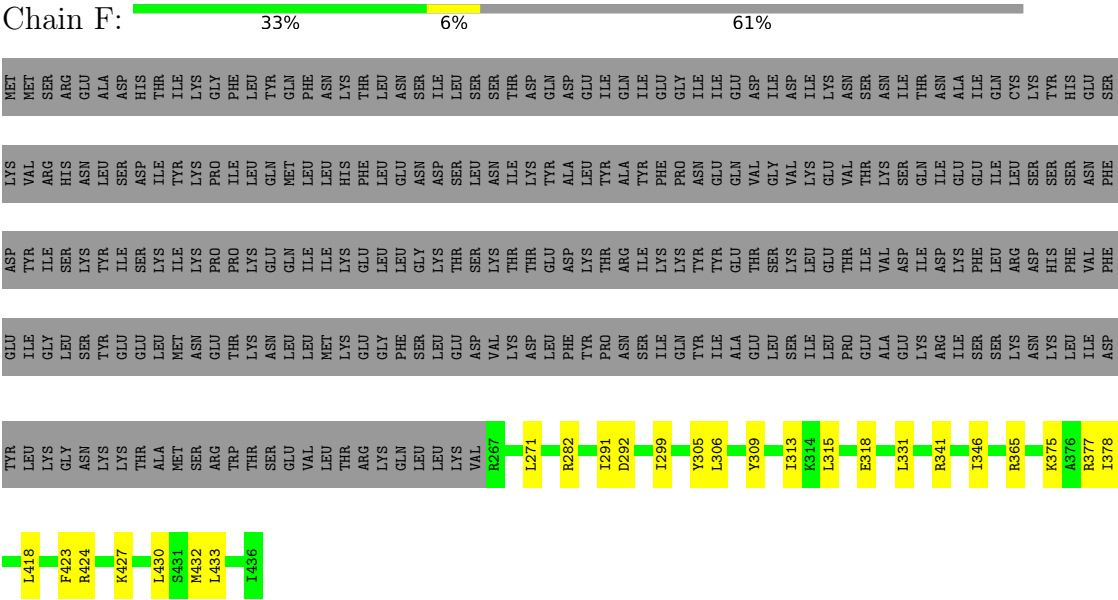
- Molecule 1: DUF4297 domain-containing protein

Chain E: 36% 7% 61%

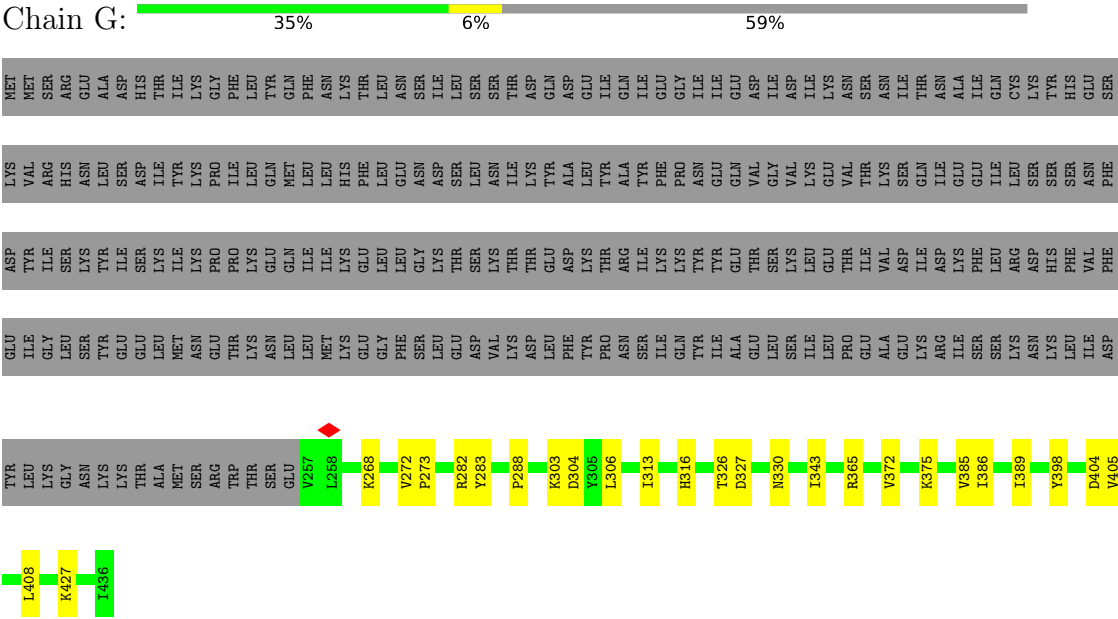
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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----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



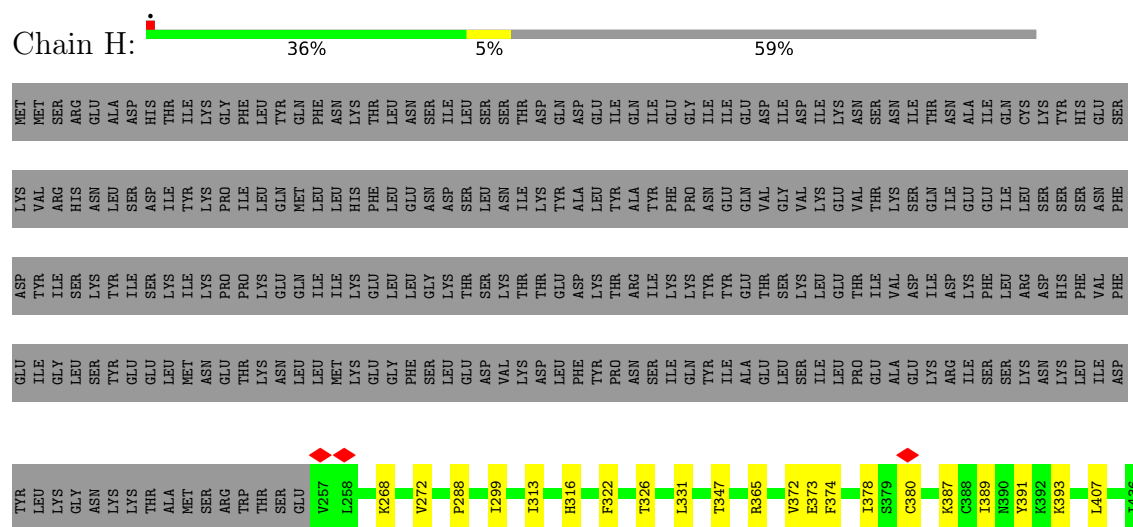
● Molecule 1: DUF4297 domain-containing protein



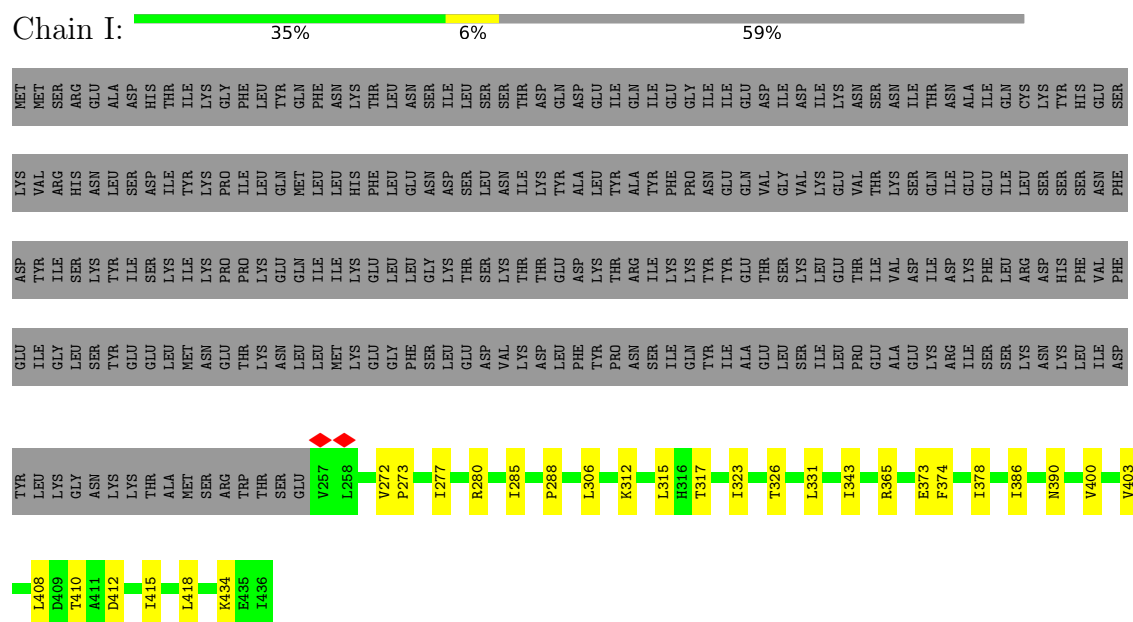
● Molecule 1: DUF4297 domain-containing protein



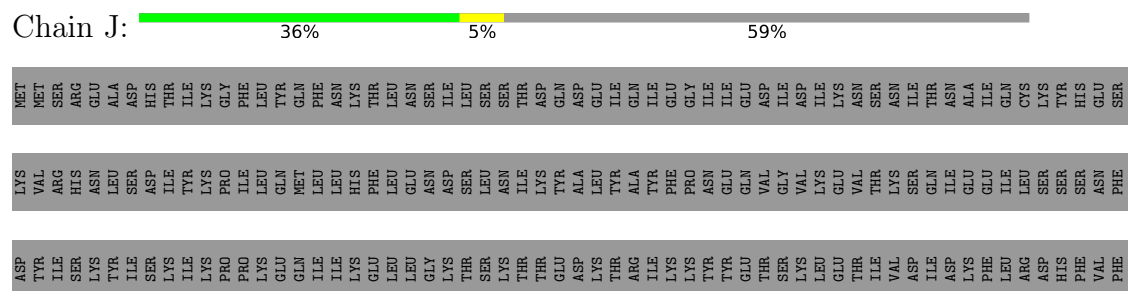
- Molecule 1: DUF4297 domain-containing protein



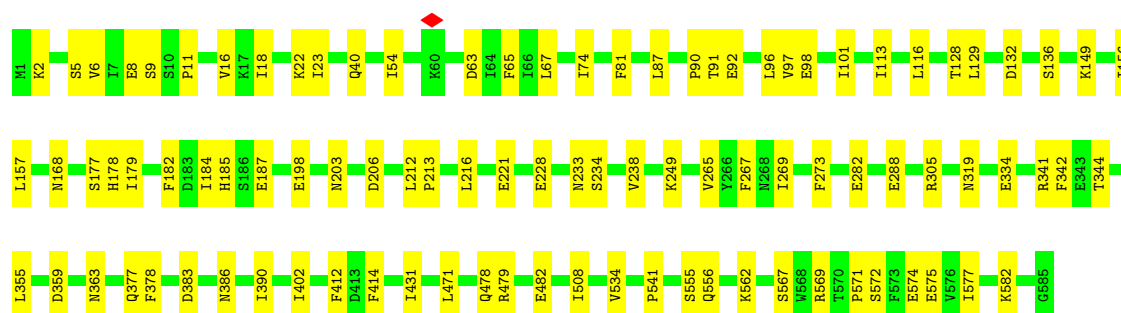
- Molecule 1: DUF4297 domain-containing protein



- Molecule 1: DUF4297 domain-containing protein

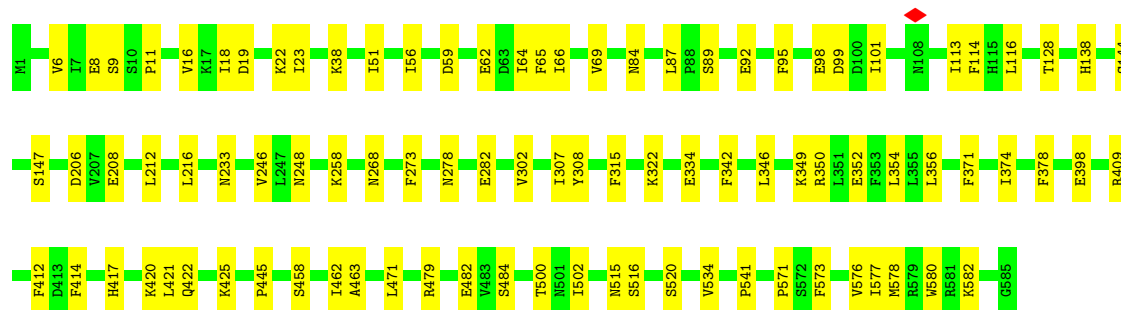






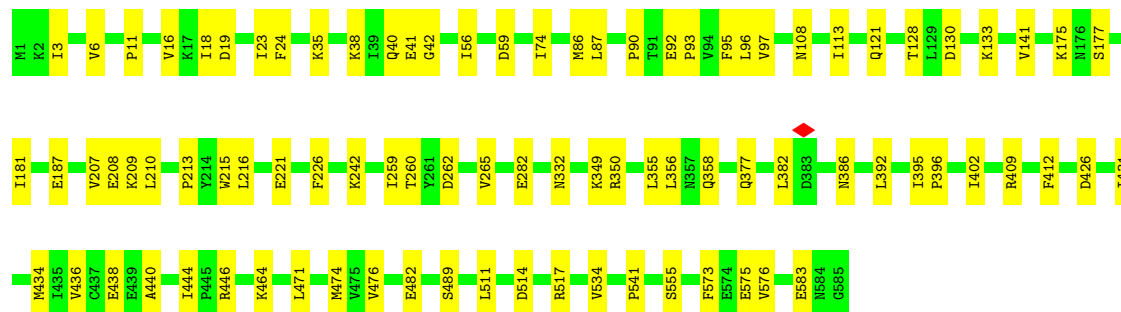
- Molecule 2: ATP-binding protein

Chain N: 84% 16%



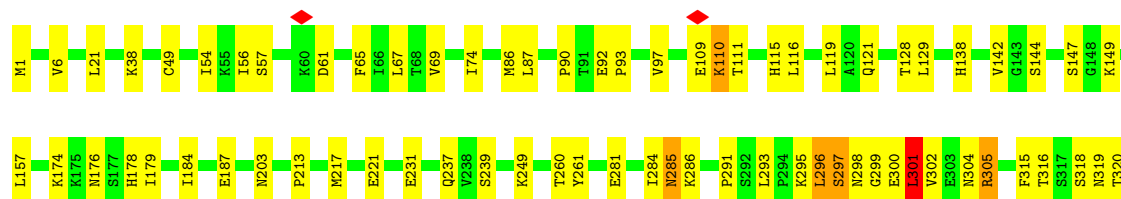
- Molecule 2: ATP-binding protein

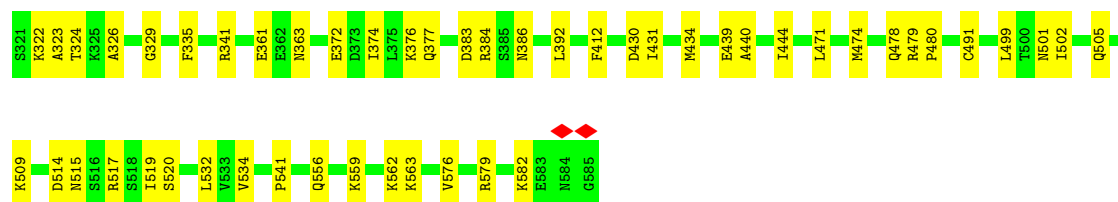
Chain O: 85% 15%



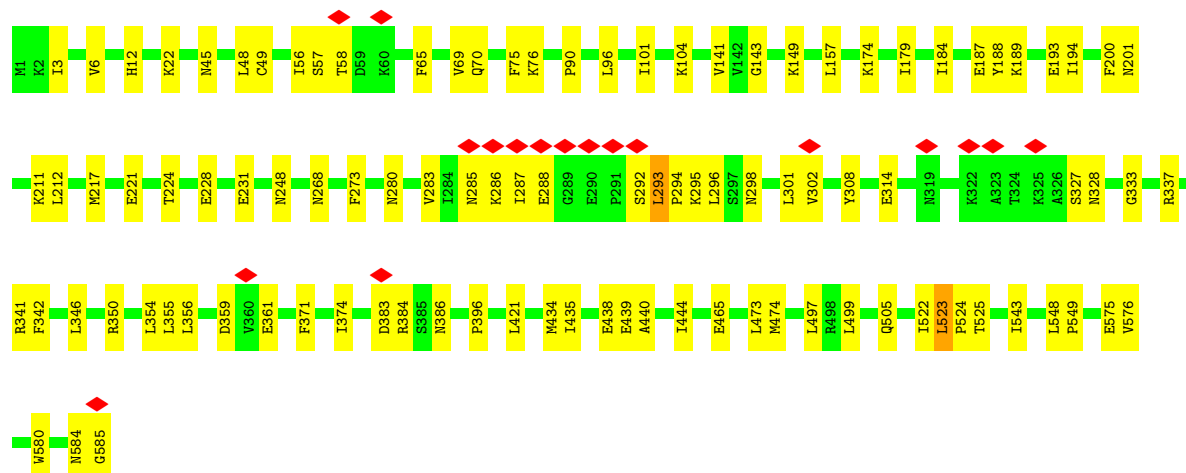
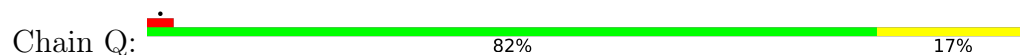
- Molecule 2: ATP-binding protein

Chain P: 79% 20%

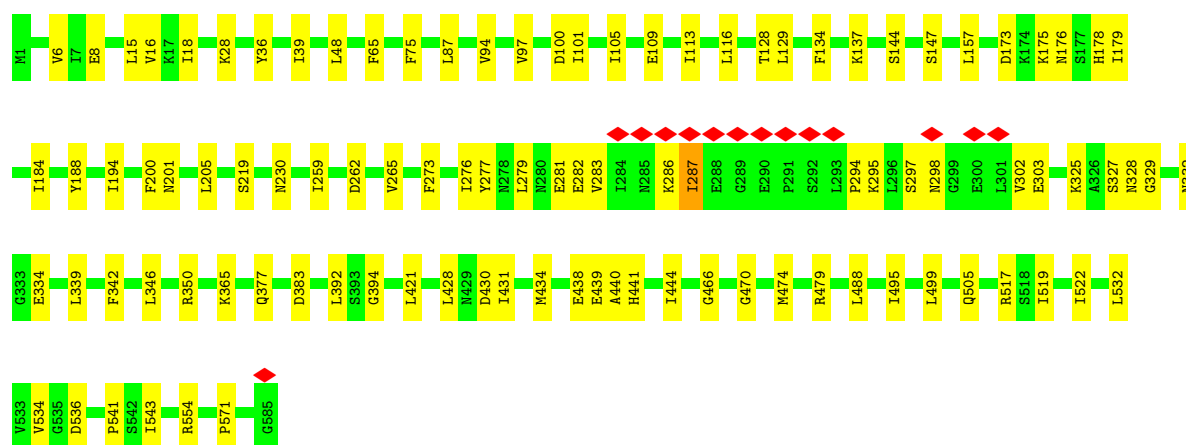
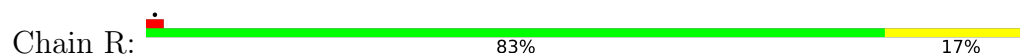




• Molecule 2: ATP-binding protein



• Molecule 2: ATP-binding protein



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, Not provided             |           |
| Number of particles used             | 530769                          | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | NONE                            | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                              | Depositor |
| Minimum defocus (nm)                 | 500                             | Depositor |
| Maximum defocus (nm)                 | 2500                            | Depositor |
| Magnification                        | Not provided                    |           |
| Image detector                       | GATAN K3 (6k x 4k)              | Depositor |
| Maximum map value                    | 2.684                           | Depositor |
| Minimum map value                    | -1.477                          | Depositor |
| Average map value                    | 0.002                           | Depositor |
| Map value standard deviation         | 0.068                           | Depositor |
| Recommended contour level            | 0.14                            | Depositor |
| Map size ( $\text{\AA}$ )            | 366.24002, 366.24002, 366.24002 | wwPDB     |
| Map dimensions                       | 336, 336, 336                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.09, 1.09, 1.09                | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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     | 0.09         | 0/1450  | 0.26        | 0/1954  |
| 1   | B     | 0.09         | 0/1450  | 0.31        | 0/1954  |
| 1   | C     | 0.08         | 0/1450  | 0.27        | 0/1954  |
| 1   | D     | 0.08         | 0/1450  | 0.24        | 0/1954  |
| 1   | E     | 0.07         | 0/1450  | 0.23        | 0/1954  |
| 1   | F     | 0.07         | 0/1450  | 0.24        | 0/1954  |
| 1   | G     | 0.10         | 0/1533  | 0.33        | 0/2065  |
| 1   | H     | 0.08         | 0/1533  | 0.26        | 0/2065  |
| 1   | I     | 0.08         | 0/1533  | 0.25        | 0/2065  |
| 1   | J     | 0.08         | 0/1533  | 0.24        | 0/2065  |
| 1   | K     | 0.09         | 0/1533  | 0.24        | 0/2065  |
| 1   | L     | 0.08         | 0/1533  | 0.24        | 0/2065  |
| 2   | M     | 0.09         | 0/4832  | 0.25        | 0/6519  |
| 2   | N     | 0.08         | 0/4832  | 0.25        | 0/6519  |
| 2   | O     | 0.07         | 0/4832  | 0.21        | 0/6519  |
| 2   | P     | 0.14         | 0/4832  | 0.30        | 0/6519  |
| 2   | Q     | 0.09         | 0/4832  | 0.27        | 0/6519  |
| 2   | R     | 0.08         | 0/4832  | 0.24        | 0/6519  |
| All | All   | 0.09         | 0/46890 | 0.26        | 0/63228 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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     | 1423  | 0        | 1423     | 20      | 0            |
| 1   | B     | 1423  | 0        | 1423     | 12      | 0            |
| 1   | C     | 1423  | 0        | 1423     | 17      | 0            |
| 1   | D     | 1423  | 0        | 1423     | 10      | 0            |
| 1   | E     | 1423  | 0        | 1423     | 9       | 0            |
| 1   | F     | 1423  | 0        | 1423     | 15      | 0            |
| 1   | G     | 1506  | 0        | 1528     | 18      | 0            |
| 1   | H     | 1506  | 0        | 1528     | 13      | 0            |
| 1   | I     | 1506  | 0        | 1528     | 16      | 0            |
| 1   | J     | 1506  | 0        | 1528     | 12      | 0            |
| 1   | K     | 1506  | 0        | 1528     | 12      | 0            |
| 1   | L     | 1506  | 0        | 1528     | 18      | 0            |
| 2   | M     | 4736  | 0        | 4725     | 63      | 0            |
| 2   | N     | 4736  | 0        | 4725     | 60      | 0            |
| 2   | O     | 4736  | 0        | 4725     | 60      | 0            |
| 2   | P     | 4736  | 0        | 4725     | 80      | 0            |
| 2   | Q     | 4736  | 0        | 4725     | 69      | 0            |
| 2   | R     | 4736  | 0        | 4725     | 66      | 0            |
| All | All   | 45990 | 0        | 46056    | 534     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (534) 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:P:293:LEU:HB2  | 2:P:301:LEU:HD23 | 1.65                     | 0.79              |
| 2:P:6:VAL:HG12   | 2:P:92:GLU:H     | 1.54                     | 0.72              |
| 2:O:260:THR:OG1  | 2:R:230:ASN:ND2  | 2.22                     | 0.72              |
| 1:E:306:LEU:HD23 | 1:E:375:LYS:HB3  | 1.71                     | 0.71              |
| 2:M:273:PHE:HB2  | 2:M:342:PHE:HE2  | 1.57                     | 0.69              |
| 1:C:267:ARG:NH2  | 1:C:416:GLU:OE1  | 2.25                     | 0.69              |
| 1:B:380:CYS:SG   | 1:B:381:ASN:N    | 2.64                     | 0.69              |
| 2:Q:273:PHE:HB2  | 2:Q:342:PHE:HE2  | 1.56                     | 0.68              |
| 2:M:571:PRO:HB3  | 2:R:431:ILE:HD13 | 1.74                     | 0.68              |
| 2:R:439:GLU:OE1  | 2:R:441:HIS:NE2  | 2.27                     | 0.68              |
| 1:E:306:LEU:HD21 | 1:E:376:ALA:HB2  | 1.76                     | 0.68              |
| 2:R:176:ASN:OD1  | 2:R:178:HIS:NE2  | 2.25                     | 0.68              |
| 1:H:365:ARG:HG2  | 1:H:372:VAL:HG12 | 1.76                     | 0.67              |
| 2:P:49:CYS:HB3   | 2:P:69:VAL:HG22  | 1.76                     | 0.67              |
| 2:R:434:MET:HE2  | 2:R:474:MET:HB2  | 1.77                     | 0.66              |
| 1:L:264:LEU:HD12 | 1:L:429:LEU:HD11 | 1.76                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:306:LEU:HD23 | 1:G:375:LYS:HE3  | 1.78                     | 0.66              |
| 1:E:327:ASP:OD1  | 1:E:330:ASN:ND2  | 2.29                     | 0.65              |
| 1:I:306:LEU:HD12 | 1:I:343:ILE:HD11 | 1.77                     | 0.65              |
| 2:P:237:GLN:O    | 2:P:239:SER:N    | 2.29                     | 0.65              |
| 2:O:74:ILE:HD12  | 2:O:86:MET:HG3   | 1.78                     | 0.65              |
| 2:M:8:GLU:HA     | 2:P:57:SER:HB2   | 1.78                     | 0.64              |
| 2:N:502:ILE:HG13 | 2:P:517:ARG:HE   | 1.62                     | 0.64              |
| 2:O:431:ILE:HD13 | 2:R:571:PRO:HG2  | 1.79                     | 0.64              |
| 1:H:288:PRO:HG2  | 1:H:326:THR:HG23 | 1.80                     | 0.64              |
| 2:M:534:VAL:HG22 | 2:M:541:PRO:HB3  | 1.79                     | 0.64              |
| 1:K:313:ILE:HD12 | 1:K:367:ILE:HA   | 1.81                     | 0.63              |
| 1:J:267:ARG:NH2  | 1:J:270:GLN:OE1  | 2.32                     | 0.62              |
| 2:O:534:VAL:HG22 | 2:O:541:PRO:HB3  | 1.80                     | 0.62              |
| 1:A:345:ILE:HG22 | 1:A:376:ALA:HB3  | 1.82                     | 0.62              |
| 2:O:207:VAL:HG11 | 2:O:392:LEU:HD23 | 1.81                     | 0.62              |
| 2:P:184:ILE:HG22 | 2:P:392:LEU:HB2  | 1.81                     | 0.62              |
| 2:P:203:ASN:ND2  | 2:P:377:GLN:O    | 2.31                     | 0.62              |
| 2:P:187:GLU:OE2  | 2:P:556:GLN:NE2  | 2.34                     | 0.61              |
| 2:Q:45:ASN:ND2   | 2:Q:76:LYS:O     | 2.34                     | 0.61              |
| 2:M:319:ASN:HD22 | 2:R:286:LYS:HZ3  | 1.48                     | 0.61              |
| 1:I:400:VAL:HG12 | 1:I:418:LEU:HB2  | 1.83                     | 0.61              |
| 2:Q:6:VAL:HG13   | 2:Q:90:PRO:HA    | 1.83                     | 0.61              |
| 1:J:362:GLU:OE2  | 1:J:392:LYS:NZ   | 2.30                     | 0.60              |
| 1:H:316:HIS:O    | 1:H:365:ARG:NH2  | 2.34                     | 0.60              |
| 2:P:297:SER:HA   | 2:P:316:THR:HG22 | 1.84                     | 0.60              |
| 2:P:322:LYS:HD3  | 2:P:323:ALA:N    | 2.17                     | 0.60              |
| 1:A:420:ILE:HD13 | 1:A:426:LEU:HB2  | 1.84                     | 0.60              |
| 1:I:312:LYS:HD3  | 1:I:315:LEU:HD12 | 1.84                     | 0.60              |
| 2:M:177:SER:O    | 2:M:386:ASN:ND2  | 2.34                     | 0.59              |
| 2:Q:383:ASP:O    | 2:Q:384:ARG:HG3  | 2.02                     | 0.59              |
| 1:F:305:TYR:HD2  | 1:F:306:LEU:HD12 | 1.67                     | 0.59              |
| 2:M:273:PHE:HB2  | 2:M:342:PHE:CE2  | 2.37                     | 0.59              |
| 1:D:306:LEU:HD23 | 1:D:375:LYS:HB3  | 1.85                     | 0.59              |
| 1:L:277:ILE:HD12 | 1:L:280:ARG:HH11 | 1.67                     | 0.59              |
| 2:R:287:ILE:HD11 | 2:R:295:LYS:HB2  | 1.85                     | 0.59              |
| 1:H:268:LYS:O    | 1:H:272:VAL:HG23 | 2.02                     | 0.59              |
| 2:Q:174:LYS:NZ   | 2:Q:386:ASN:OD1  | 2.34                     | 0.59              |
| 1:L:331:LEU:HD21 | 1:L:379:SER:HA   | 1.85                     | 0.59              |
| 2:O:350:ARG:NH2  | 2:Q:465:GLU:OE2  | 2.36                     | 0.59              |
| 2:Q:292:SER:O    | 2:Q:293:LEU:HB2  | 2.03                     | 0.58              |
| 1:K:268:LYS:O    | 1:K:272:VAL:HG13 | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:305:TYR:HD1  | 1:D:306:LEU:HD12 | 1.68                     | 0.58              |
| 2:N:571:PRO:HG3  | 2:P:431:ILE:HD13 | 1.85                     | 0.58              |
| 2:Q:184:ILE:HD11 | 2:Q:439:GLU:HB2  | 1.86                     | 0.58              |
| 2:M:11:PRO:HA    | 2:M:87:LEU:HD21  | 1.85                     | 0.58              |
| 2:R:279:LEU:HD11 | 2:R:334:GLU:H    | 1.67                     | 0.58              |
| 1:E:305:TYR:HD1  | 1:E:306:LEU:HD12 | 1.69                     | 0.58              |
| 2:Q:522:ILE:HG12 | 2:Q:543:ILE:HD11 | 1.86                     | 0.58              |
| 2:R:8:GLU:HB2    | 2:R:15:LEU:HB2   | 1.85                     | 0.57              |
| 2:M:233:ASN:HD21 | 2:M:334:GLU:HB3  | 1.69                     | 0.57              |
| 2:Q:48:LEU:HB2   | 2:Q:75:PHE:HE1   | 1.68                     | 0.57              |
| 1:A:364:LYS:H    | 1:A:373:GLU:HG2  | 1.69                     | 0.57              |
| 2:O:242:LYS:NZ   | 2:R:230:ASN:O    | 2.30                     | 0.57              |
| 2:P:297:SER:HA   | 2:P:316:THR:CG2  | 2.35                     | 0.57              |
| 2:O:6:VAL:HG12   | 2:O:16:VAL:HG12  | 1.86                     | 0.57              |
| 2:P:297:SER:O    | 2:P:298:ASN:C    | 2.47                     | 0.57              |
| 2:Q:143:GLY:HA2  | 2:Q:497:LEU:HB2  | 1.85                     | 0.57              |
| 2:R:157:LEU:HD22 | 2:R:179:ILE:HD13 | 1.86                     | 0.57              |
| 1:F:306:LEU:HD23 | 1:F:375:LYS:HB3  | 1.87                     | 0.57              |
| 2:R:188:TYR:HE2  | 2:R:438:GLU:HG3  | 1.70                     | 0.57              |
| 1:A:306:LEU:HD23 | 1:A:375:LYS:HB3  | 1.87                     | 0.57              |
| 2:Q:371:PHE:HA   | 2:Q:374:ILE:HD12 | 1.87                     | 0.57              |
| 2:Q:211:LYS:HD3  | 2:Q:355:LEU:HD11 | 1.87                     | 0.57              |
| 2:P:176:ASN:OD1  | 2:P:178:HIS:NE2  | 2.35                     | 0.56              |
| 2:P:285:ASN:HD22 | 2:P:301:LEU:HD21 | 1.70                     | 0.56              |
| 2:O:6:VAL:HG23   | 2:O:90:PRO:HA    | 1.87                     | 0.56              |
| 1:F:318:GLU:OE2  | 2:Q:22:LYS:NZ    | 2.38                     | 0.56              |
| 1:H:313:ILE:O    | 1:H:365:ARG:NH1  | 2.38                     | 0.56              |
| 1:K:309:TYR:OH   | 1:K:430:LEU:O    | 2.21                     | 0.56              |
| 1:L:313:ILE:HD12 | 1:L:367:ILE:HA   | 1.86                     | 0.56              |
| 2:N:258:LYS:HE3  | 2:Q:584:ASN:HB2  | 1.88                     | 0.56              |
| 2:P:284:ILE:HG13 | 2:P:286:LYS:HG2  | 1.87                     | 0.56              |
| 2:P:440:ALA:HB1  | 2:P:444:ILE:HD11 | 1.87                     | 0.56              |
| 1:L:427:LYS:HA   | 1:L:432:MET:HE3  | 1.88                     | 0.56              |
| 2:M:157:LEU:HD22 | 2:M:179:ILE:HD13 | 1.88                     | 0.56              |
| 2:N:233:ASN:HD21 | 2:N:334:GLU:HB3  | 1.71                     | 0.56              |
| 2:Q:293:LEU:H    | 2:Q:295:LYS:HZ2  | 1.53                     | 0.56              |
| 2:M:249:LYS:HG3  | 2:M:267:PHE:HB3  | 1.88                     | 0.56              |
| 2:P:38:LYS:HG3   | 2:P:97:VAL:HB    | 1.87                     | 0.56              |
| 1:C:280:ARG:NE   | 1:C:396:ASP:OD2  | 2.39                     | 0.56              |
| 2:R:201:ASN:ND2  | 2:R:383:ASP:O    | 2.38                     | 0.56              |
| 2:M:2:LYS:HE3    | 2:M:96:LEU:HD12  | 1.87                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:M:187:GLU:HG2  | 2:M:555:SER:HB2  | 1.87                     | 0.55              |
| 2:M:282:GLU:OE2  | 2:M:305:ARG:NH2  | 2.38                     | 0.55              |
| 2:N:233:ASN:ND2  | 2:N:334:GLU:O    | 2.40                     | 0.55              |
| 2:P:231:GLU:OE2  | 2:P:341:ARG:NH2  | 2.39                     | 0.55              |
| 2:Q:248:ASN:ND2  | 2:Q:268:ASN:O    | 2.39                     | 0.55              |
| 1:L:313:ILE:HD13 | 1:L:370:ASN:HA   | 1.87                     | 0.55              |
| 1:A:305:TYR:HD2  | 1:A:306:LEU:HD12 | 1.72                     | 0.55              |
| 1:C:295:ASP:O    | 1:C:337:ARG:NH1  | 2.39                     | 0.55              |
| 2:N:354:LEU:HD23 | 2:N:356:LEU:HD12 | 1.87                     | 0.55              |
| 2:P:174:LYS:NZ   | 2:P:386:ASN:OD1  | 2.39                     | 0.55              |
| 2:N:346:LEU:HD23 | 2:N:356:LEU:HD23 | 1.88                     | 0.55              |
| 1:D:295:ASP:O    | 1:D:337:ARG:NH1  | 2.40                     | 0.55              |
| 2:N:534:VAL:HG22 | 2:N:541:PRO:HB3  | 1.88                     | 0.55              |
| 2:O:177:SER:O    | 2:O:386:ASN:ND2  | 2.39                     | 0.55              |
| 2:P:157:LEU:HD22 | 2:P:179:ILE:HD13 | 1.88                     | 0.55              |
| 1:B:299:ILE:HD13 | 1:B:337:ARG:HH11 | 1.70                     | 0.54              |
| 2:O:514:ASP:HA   | 2:O:517:ARG:HG3  | 1.88                     | 0.54              |
| 2:M:574:GLU:HA   | 2:M:577:ILE:HG12 | 1.88                     | 0.54              |
| 2:O:216:LEU:O    | 2:O:409:ARG:NH2  | 2.41                     | 0.54              |
| 1:D:285:ILE:HG22 | 1:D:403:VAL:HG21 | 1.90                     | 0.54              |
| 1:D:420:ILE:HD13 | 1:D:426:LEU:HB2  | 1.89                     | 0.54              |
| 2:N:6:VAL:HG12   | 2:N:16:VAL:HG22  | 1.88                     | 0.54              |
| 1:C:267:ARG:HH21 | 1:C:271:LEU:HD21 | 1.72                     | 0.54              |
| 2:N:11:PRO:O     | 2:N:84:ASN:ND2   | 2.40                     | 0.54              |
| 1:K:277:ILE:HD12 | 1:K:280:ARG:HD2  | 1.90                     | 0.54              |
| 2:N:212:LEU:HD21 | 2:N:378:PHE:CE1  | 2.42                     | 0.54              |
| 2:M:149:LYS:HZ3  | 2:M:478:GLN:HB3  | 1.73                     | 0.54              |
| 1:I:410:THR:HB   | 1:I:415:ILE:HD11 | 1.90                     | 0.54              |
| 2:O:108:ASN:HB2  | 2:O:113:ILE:HD11 | 1.90                     | 0.54              |
| 2:Q:350:ARG:HD2  | 2:Q:396:PRO:HG3  | 1.89                     | 0.54              |
| 1:K:396:ASP:OD1  | 1:K:414:ASN:ND2  | 2.38                     | 0.53              |
| 2:N:573:PHE:HA   | 2:N:576:VAL:HG22 | 1.91                     | 0.53              |
| 2:O:11:PRO:HD3   | 2:O:87:LEU:HD21  | 1.90                     | 0.53              |
| 1:G:405:VAL:HG23 | 1:G:408:LEU:HD12 | 1.90                     | 0.53              |
| 2:P:372:GLU:OE2  | 2:P:376:LYS:NZ   | 2.42                     | 0.53              |
| 1:L:272:VAL:O    | 1:L:276:ASN:ND2  | 2.39                     | 0.53              |
| 2:M:116:LEU:HD11 | 2:M:156:ILE:HG12 | 1.89                     | 0.53              |
| 1:F:331:LEU:HD11 | 1:F:378:ILE:HG22 | 1.89                     | 0.53              |
| 2:Q:285:ASN:HD21 | 2:Q:327:SER:HB3  | 1.73                     | 0.53              |
| 1:H:299:ILE:HD11 | 1:I:412:ASP:CG   | 2.34                     | 0.53              |
| 2:P:119:LEU:HD13 | 2:P:121:GLN:HE21 | 1.74                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:R:277:TYR:HA   | 2:R:339:LEU:HD21 | 1.90                     | 0.53              |
| 2:O:6:VAL:HG22   | 2:O:92:GLU:H     | 1.73                     | 0.53              |
| 2:M:5:SER:HB2    | 2:M:91:THR:HA    | 1.90                     | 0.52              |
| 2:N:500:THR:HB   | 2:P:515:ASN:HA   | 1.91                     | 0.52              |
| 2:P:579:ARG:HA   | 2:P:582:LYS:HG2  | 1.90                     | 0.52              |
| 2:R:282:GLU:HA   | 2:R:328:ASN:HA   | 1.91                     | 0.52              |
| 1:J:312:LYS:HD3  | 1:J:315:LEU:HD12 | 1.91                     | 0.52              |
| 1:G:327:ASP:OD1  | 1:G:330:ASN:ND2  | 2.43                     | 0.52              |
| 1:I:390:ASN:HD21 | 1:I:408:LEU:HA   | 1.75                     | 0.52              |
| 2:M:18:ILE:HD11  | 2:M:67:LEU:HD13  | 1.90                     | 0.52              |
| 2:M:182:PHE:HE1  | 2:M:390:ILE:HD12 | 1.74                     | 0.52              |
| 2:O:464:LYS:O    | 2:R:479:ARG:NH2  | 2.41                     | 0.52              |
| 2:Q:440:ALA:HB1  | 2:Q:444:ILE:HD11 | 1.90                     | 0.52              |
| 2:N:479:ARG:NH1  | 2:N:482:GLU:OE2  | 2.43                     | 0.52              |
| 2:Q:286:LYS:HE3  | 2:Q:288:GLU:HA   | 1.92                     | 0.52              |
| 2:R:499:LEU:O    | 2:R:505:GLN:NE2  | 2.38                     | 0.52              |
| 2:R:116:LEU:HD22 | 2:R:129:LEU:HD11 | 1.92                     | 0.52              |
| 1:G:288:PRO:HG2  | 1:G:326:THR:HG23 | 1.91                     | 0.52              |
| 2:N:206:ASP:O    | 2:N:208:GLU:N    | 2.42                     | 0.52              |
| 2:R:109:GLU:HB2  | 2:R:113:ILE:HB   | 1.92                     | 0.52              |
| 2:R:325:LYS:HE2  | 2:R:327:SER:HB3  | 1.91                     | 0.52              |
| 2:R:144:SER:O    | 2:R:147:SER:OG   | 2.28                     | 0.51              |
| 1:C:274:SER:O    | 1:C:282:ARG:NH1  | 2.43                     | 0.51              |
| 1:J:309:TYR:OH   | 1:J:430:LEU:O    | 2.21                     | 0.51              |
| 2:Q:359:ASP:O    | 2:Q:361:GLU:N    | 2.44                     | 0.51              |
| 2:P:285:ASN:ND2  | 2:P:301:LEU:HD21 | 2.25                     | 0.51              |
| 2:M:288:GLU:HG2  | 2:N:322:LYS:HE3  | 1.93                     | 0.51              |
| 2:R:350:ARG:NH2  | 2:R:394:GLY:O    | 2.43                     | 0.51              |
| 2:N:59:ASP:HB3   | 2:N:62:GLU:HB2   | 1.93                     | 0.51              |
| 1:B:325:LYS:HE3  | 1:B:403:VAL:HG13 | 1.93                     | 0.51              |
| 1:C:305:TYR:HD2  | 1:C:306:LEU:HD12 | 1.76                     | 0.51              |
| 1:F:309:TYR:OH   | 1:F:430:LEU:O    | 2.26                     | 0.51              |
| 2:Q:212:LEU:O    | 2:Q:354:LEU:HA   | 2.11                     | 0.51              |
| 2:Q:231:GLU:OE2  | 2:Q:341:ARG:NH2  | 2.37                     | 0.51              |
| 1:A:357:LYS:NZ   | 1:A:358:GLU:OE2  | 2.43                     | 0.51              |
| 2:R:294:PRO:HG3  | 2:R:303:GLU:HA   | 1.93                     | 0.51              |
| 2:M:74:ILE:HG22  | 2:M:81:PHE:HB2   | 1.93                     | 0.51              |
| 2:P:430:ASP:OD1  | 2:P:431:ILE:HD12 | 2.11                     | 0.51              |
| 1:J:287:ASP:HB2  | 1:J:403:VAL:HG23 | 1.93                     | 0.50              |
| 2:M:6:VAL:HG12   | 2:M:16:VAL:HG22  | 1.93                     | 0.50              |
| 2:P:74:ILE:HG12  | 2:P:86:MET:HG2   | 1.92                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:331:LEU:HD13 | 1:H:380:CYS:H    | 1.76                     | 0.50              |
| 1:L:306:LEU:HD23 | 1:L:375:LYS:HD2  | 1.93                     | 0.50              |
| 2:N:38:LYS:HE3   | 2:N:95:PHE:HB2   | 1.92                     | 0.50              |
| 2:P:110:LYS:HG3  | 2:P:111:THR:HG23 | 1.94                     | 0.50              |
| 1:G:385:VAL:HG12 | 1:G:385:VAL:O    | 2.11                     | 0.50              |
| 2:O:41:GLU:OE2   | 2:R:28:LYS:NZ    | 2.31                     | 0.50              |
| 2:Q:296:LEU:HD13 | 2:Q:308:TYR:HE1  | 1.75                     | 0.50              |
| 2:N:19:ASP:HB2   | 2:N:23:ILE:HD12  | 1.93                     | 0.50              |
| 1:F:315:LEU:HD21 | 2:N:89:SER:HB2   | 1.93                     | 0.50              |
| 2:N:64:ILE:HG22  | 2:N:66:ILE:HG12  | 1.94                     | 0.50              |
| 2:O:259:ILE:HD12 | 2:O:265:VAL:HG21 | 1.93                     | 0.50              |
| 2:Q:143:GLY:HA3  | 2:Q:149:LYS:HG2  | 1.92                     | 0.50              |
| 1:G:316:HIS:O    | 1:G:365:ARG:NH2  | 2.45                     | 0.50              |
| 1:K:313:ILE:HD13 | 1:K:370:ASN:HA   | 1.94                     | 0.50              |
| 2:O:434:MET:HE2  | 2:O:474:MET:HB2  | 1.94                     | 0.50              |
| 2:R:281:GLU:O    | 2:R:332:ASN:ND2  | 2.44                     | 0.50              |
| 2:P:534:VAL:HG22 | 2:P:541:PRO:HB3  | 1.94                     | 0.49              |
| 1:A:331:LEU:HD21 | 1:A:379:SER:HA   | 1.94                     | 0.49              |
| 2:M:221:GLU:HB3  | 2:M:402:ILE:HG23 | 1.94                     | 0.49              |
| 2:M:249:LYS:HG2  | 2:M:265:VAL:HG23 | 1.93                     | 0.49              |
| 2:P:149:LYS:NZ   | 2:P:439:GLU:OE2  | 2.44                     | 0.49              |
| 1:J:271:LEU:HD11 | 1:J:418:LEU:HD11 | 1.93                     | 0.49              |
| 2:Q:522:ILE:HD12 | 2:Q:525:THR:HB   | 1.95                     | 0.49              |
| 1:B:331:LEU:HD11 | 1:B:378:ILE:HG22 | 1.94                     | 0.49              |
| 1:C:325:LYS:HA   | 1:C:381:ASN:HB2  | 1.94                     | 0.49              |
| 1:K:399:ILE:HD13 | 1:K:415:ILE:HG23 | 1.94                     | 0.49              |
| 1:K:424:ARG:HH21 | 1:K:436:ILE:HD11 | 1.77                     | 0.49              |
| 2:Q:285:ASN:OD1  | 2:Q:327:SER:N    | 2.44                     | 0.49              |
| 1:G:386:ILE:HG13 | 1:G:389:ILE:HD13 | 1.95                     | 0.49              |
| 2:P:296:LEU:HD11 | 2:P:300:GLU:HB3  | 1.94                     | 0.49              |
| 2:P:6:VAL:HG13   | 2:P:90:PRO:HA    | 1.94                     | 0.49              |
| 2:P:320:THR:HG22 | 2:P:320:THR:O    | 2.13                     | 0.49              |
| 2:Q:49:CYS:HB3   | 2:Q:69:VAL:HG22  | 1.95                     | 0.49              |
| 2:M:206:ASP:OD1  | 2:M:206:ASP:N    | 2.46                     | 0.49              |
| 2:P:116:LEU:HD22 | 2:P:129:LEU:HD11 | 1.95                     | 0.49              |
| 2:P:322:LYS:HD3  | 2:P:324:THR:H    | 1.78                     | 0.49              |
| 1:C:404:ASP:OD1  | 1:C:404:ASP:N    | 2.45                     | 0.49              |
| 1:G:268:LYS:O    | 1:G:272:VAL:HG13 | 2.12                     | 0.49              |
| 1:I:272:VAL:N    | 1:I:273:PRO:HD2  | 2.27                     | 0.49              |
| 2:M:479:ARG:NH1  | 2:M:482:GLU:OE2  | 2.46                     | 0.49              |
| 2:N:116:LEU:O    | 2:N:116:LEU:HD23 | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:258:LYS:NZ   | 2:Q:585:GLY:OXT  | 2.44                     | 0.48              |
| 2:O:426:ASP:OD1  | 2:R:554:ARG:NH2  | 2.39                     | 0.48              |
| 1:A:335:HIS:O    | 1:A:339:VAL:HG23 | 2.13                     | 0.48              |
| 2:M:575:GLU:HB3  | 2:R:421:LEU:HD21 | 1.95                     | 0.48              |
| 2:M:383:ASP:N    | 2:M:383:ASP:OD1  | 2.47                     | 0.48              |
| 2:O:226:PHE:HZ   | 2:O:356:LEU:HD11 | 1.78                     | 0.48              |
| 2:Q:273:PHE:HB2  | 2:Q:342:PHE:CE2  | 2.45                     | 0.48              |
| 2:R:178:HIS:NE2  | 2:R:431:ILE:HG23 | 2.29                     | 0.48              |
| 2:M:344:THR:OG1  | 2:R:262:ASP:OD2  | 2.27                     | 0.48              |
| 2:O:349:LYS:NZ   | 2:O:583:GLU:O    | 2.47                     | 0.48              |
| 2:Q:188:TYR:HE2  | 2:Q:438:GLU:HG3  | 1.79                     | 0.48              |
| 1:A:271:LEU:HD22 | 1:A:398:TYR:HE2  | 1.77                     | 0.48              |
| 2:P:21:LEU:HA    | 2:P:65:PHE:HE2   | 1.79                     | 0.48              |
| 2:R:440:ALA:HB1  | 2:R:444:ILE:HD11 | 1.95                     | 0.48              |
| 1:F:291:ILE:HG21 | 1:F:423:PHE:CE2  | 2.49                     | 0.47              |
| 1:K:267:ARG:NH1  | 1:K:417:ASN:O    | 2.44                     | 0.47              |
| 2:N:8:GLU:HG3    | 2:Q:57:SER:HB2   | 1.96                     | 0.47              |
| 2:O:446:ARG:N    | 2:O:482:GLU:O    | 2.46                     | 0.47              |
| 2:O:489:SER:HA   | 2:O:511:LEU:HD11 | 1.96                     | 0.47              |
| 1:A:388:CYS:O    | 1:A:390:ASN:N    | 2.43                     | 0.47              |
| 2:M:213:PRO:HG2  | 2:M:216:LEU:HG   | 1.96                     | 0.47              |
| 1:J:420:ILE:HD13 | 1:J:426:LEU:HB2  | 1.95                     | 0.47              |
| 1:F:424:ARG:HH21 | 1:F:433:LEU:HD21 | 1.80                     | 0.47              |
| 2:M:132:ASP:O    | 2:M:136:SER:OG   | 2.30                     | 0.47              |
| 2:Q:217:MET:HB3  | 2:Q:221:GLU:HB2  | 1.96                     | 0.47              |
| 1:C:312:LYS:NZ   | 2:O:42:GLY:O     | 2.48                     | 0.47              |
| 2:M:54:ILE:HG12  | 2:M:67:LEU:HG    | 1.96                     | 0.47              |
| 2:N:216:LEU:O    | 2:N:409:ARG:NH2  | 2.47                     | 0.47              |
| 2:N:371:PHE:HA   | 2:N:374:ILE:HD12 | 1.96                     | 0.47              |
| 1:G:404:ASP:OD1  | 1:G:404:ASP:N    | 2.47                     | 0.47              |
| 2:M:113:ILE:HG23 | 2:M:128:THR:HB   | 1.96                     | 0.47              |
| 2:N:349:LYS:HB2  | 2:N:352:GLU:HG3  | 1.96                     | 0.47              |
| 2:N:412:PHE:HA   | 2:N:471:LEU:HD11 | 1.97                     | 0.47              |
| 1:J:345:ILE:HG22 | 1:J:376:ALA:HB3  | 1.97                     | 0.47              |
| 2:M:22:LYS:HG3   | 2:M:23:ILE:HD12  | 1.96                     | 0.47              |
| 2:O:412:PHE:HA   | 2:O:471:LEU:HD11 | 1.96                     | 0.47              |
| 2:P:514:ASP:N    | 2:P:514:ASP:OD1  | 2.47                     | 0.47              |
| 2:R:184:ILE:HG22 | 2:R:392:LEU:HB2  | 1.97                     | 0.47              |
| 2:N:420:LYS:C    | 2:N:422:GLN:H    | 2.22                     | 0.47              |
| 2:Q:141:VAL:HG12 | 2:Q:141:VAL:O    | 2.14                     | 0.46              |
| 2:R:273:PHE:HB2  | 2:R:342:PHE:HE2  | 1.80                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:273:PHE:HB2  | 2:N:342:PHE:CE2  | 2.50                     | 0.46              |
| 2:P:138:HIS:HB2  | 2:P:491:CYS:HA   | 1.97                     | 0.46              |
| 2:P:237:GLN:HG2  | 2:P:335:PHE:HE1  | 1.80                     | 0.46              |
| 2:R:194:ILE:HD11 | 2:R:200:PHE:HB3  | 1.97                     | 0.46              |
| 2:R:219:SER:N    | 2:R:262:ASP:OD1  | 2.47                     | 0.46              |
| 1:B:309:TYR:OH   | 1:B:430:LEU:O    | 2.30                     | 0.46              |
| 2:Q:189:LYS:NZ   | 2:Q:193:GLU:OE1  | 2.48                     | 0.46              |
| 2:Q:434:MET:HE2  | 2:Q:474:MET:HB2  | 1.96                     | 0.46              |
| 1:K:277:ILE:HD12 | 1:K:280:ARG:HH11 | 1.81                     | 0.46              |
| 2:N:11:PRO:HA    | 2:N:87:LEU:HD21  | 1.97                     | 0.46              |
| 2:N:578:MET:O    | 2:N:582:LYS:HB2  | 2.15                     | 0.46              |
| 1:G:304:ASP:OD2  | 1:G:427:LYS:NZ   | 2.45                     | 0.46              |
| 2:M:359:ASP:OD1  | 2:M:359:ASP:N    | 2.46                     | 0.46              |
| 2:N:98:GLU:HG2   | 2:N:101:ILE:HG22 | 1.97                     | 0.46              |
| 2:Q:12:HIS:O     | 2:Q:70:GLN:NE2   | 2.48                     | 0.46              |
| 2:R:48:LEU:HB2   | 2:R:75:PHE:HE2   | 1.80                     | 0.46              |
| 1:L:327:ASP:OD2  | 1:L:329:ASN:ND2  | 2.39                     | 0.46              |
| 2:O:187:GLU:HG2  | 2:O:555:SER:HB2  | 1.96                     | 0.46              |
| 2:M:98:GLU:HG3   | 2:M:101:ILE:HG12 | 1.98                     | 0.46              |
| 2:N:22:LYS:HB3   | 2:N:22:LYS:HE3   | 1.71                     | 0.46              |
| 2:Q:157:LEU:HD22 | 2:Q:179:ILE:HD13 | 1.96                     | 0.46              |
| 2:R:466:GLY:O    | 2:R:470:GLY:N    | 2.49                     | 0.46              |
| 1:L:420:ILE:HD13 | 1:L:426:LEU:HB2  | 1.98                     | 0.46              |
| 2:N:138:HIS:NE2  | 2:N:463:ALA:HA   | 2.31                     | 0.46              |
| 2:Q:149:LYS:HB2  | 2:Q:149:LYS:HE3  | 1.68                     | 0.46              |
| 2:R:298:ASN:HB3  | 2:R:302:VAL:HG11 | 1.97                     | 0.46              |
| 1:I:288:PRO:HG2  | 1:I:326:THR:HG23 | 1.97                     | 0.46              |
| 2:P:478:GLN:HG3  | 2:P:479:ARG:HD3  | 1.98                     | 0.46              |
| 2:Q:287:ILE:HD12 | 2:Q:294:PRO:HB3  | 1.96                     | 0.46              |
| 2:N:9:SER:HB2    | 2:Q:56:ILE:HG21  | 1.98                     | 0.46              |
| 2:O:438:GLU:HA   | 2:O:476:VAL:HB   | 1.96                     | 0.46              |
| 2:P:281:GLU:O    | 2:P:329:GLY:N    | 2.47                     | 0.46              |
| 1:A:333:GLU:OE2  | 1:A:336:LYS:NZ   | 2.50                     | 0.45              |
| 1:D:309:TYR:OH   | 1:D:430:LEU:O    | 2.28                     | 0.45              |
| 2:M:97:VAL:HG23  | 2:M:101:ILE:HD11 | 1.97                     | 0.45              |
| 2:M:355:LEU:HG   | 2:M:363:ASN:HB3  | 1.98                     | 0.45              |
| 1:H:322:PHE:HB2  | 1:H:378:ILE:HG23 | 1.97                     | 0.45              |
| 1:K:288:PRO:HG2  | 1:K:326:THR:HG23 | 1.99                     | 0.45              |
| 2:M:6:VAL:HG23   | 2:M:90:PRO:HA    | 1.99                     | 0.45              |
| 2:O:208:GLU:HG3  | 2:O:209:LYS:HG2  | 1.97                     | 0.45              |
| 1:C:272:VAL:CG1  | 1:C:273:PRO:HD3  | 2.46                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:272:VAL:N    | 1:G:273:PRO:HD2  | 2.31                     | 0.45              |
| 2:P:237:GLN:HG2  | 2:P:335:PHE:CE1  | 2.51                     | 0.45              |
| 2:P:499:LEU:O    | 2:P:505:GLN:NE2  | 2.49                     | 0.45              |
| 1:G:405:VAL:O    | 1:G:405:VAL:HG13 | 2.17                     | 0.45              |
| 1:E:277:ILE:HD12 | 1:E:280:ARG:HD3  | 1.98                     | 0.45              |
| 2:M:9:SER:HB2    | 2:P:56:ILE:HB    | 1.98                     | 0.45              |
| 2:O:282:GLU:O    | 2:O:332:ASN:ND2  | 2.48                     | 0.45              |
| 1:A:325:LYS:HE3  | 1:A:403:VAL:HG13 | 1.98                     | 0.45              |
| 1:C:322:PHE:HB2  | 1:C:378:ILE:HG12 | 1.98                     | 0.45              |
| 1:D:373:GLU:HG3  | 1:D:374:PHE:CD2  | 2.52                     | 0.45              |
| 1:F:282:ARG:HH22 | 1:F:309:TYR:HB3  | 1.80                     | 0.45              |
| 2:Q:101:ILE:O    | 2:Q:104:LYS:HG2  | 2.16                     | 0.45              |
| 1:A:382:SER:O    | 1:A:386:ILE:HG12 | 2.16                     | 0.45              |
| 1:G:372:VAL:HG13 | 1:G:375:LYS:HG3  | 1.99                     | 0.45              |
| 2:P:144:SER:O    | 2:P:147:SER:OG   | 2.34                     | 0.45              |
| 2:P:296:LEU:HD12 | 2:P:299:GLY:H    | 1.81                     | 0.45              |
| 2:R:113:ILE:HG13 | 2:R:128:THR:HB   | 1.98                     | 0.45              |
| 1:I:434:LYS:HA   | 1:I:434:LYS:HD3  | 1.71                     | 0.45              |
| 1:L:282:ARG:HG3  | 1:L:396:ASP:HB2  | 1.98                     | 0.45              |
| 2:R:430:ASP:OD1  | 2:R:430:ASP:N    | 2.45                     | 0.45              |
| 2:N:18:ILE:HB    | 2:N:65:PHE:HB2   | 1.99                     | 0.45              |
| 2:N:56:ILE:HG23  | 2:N:65:PHE:HD1   | 1.82                     | 0.45              |
| 2:N:350:ARG:NH1  | 2:N:398:GLU:OE2  | 2.38                     | 0.45              |
| 2:R:75:PHE:HZ    | 2:R:105:ILE:HD11 | 1.82                     | 0.45              |
| 2:R:281:GLU:O    | 2:R:329:GLY:N    | 2.41                     | 0.45              |
| 1:I:331:LEU:HD11 | 1:I:378:ILE:HG22 | 1.99                     | 0.44              |
| 2:O:19:ASP:HB2   | 2:O:23:ILE:HD12  | 1.98                     | 0.44              |
| 2:O:35:LYS:HD3   | 2:O:121:GLN:HG2  | 1.98                     | 0.44              |
| 2:P:1:MET:HA     | 2:P:93:PRO:HB3   | 1.99                     | 0.44              |
| 2:R:276:ILE:HG22 | 2:R:339:LEU:HD11 | 1.99                     | 0.44              |
| 1:E:410:THR:HG21 | 1:E:415:ILE:HD11 | 2.00                     | 0.44              |
| 2:O:573:PHE:HA   | 2:O:576:VAL:HG22 | 1.99                     | 0.44              |
| 2:Q:548:LEU:HD12 | 2:Q:549:PRO:HD2  | 1.99                     | 0.44              |
| 1:D:285:ILE:HD13 | 1:D:323:ILE:HB   | 1.99                     | 0.44              |
| 1:F:346:ILE:HD11 | 1:F:377:ARG:HG2  | 1.99                     | 0.44              |
| 2:O:130:ASP:HB3  | 2:O:133:LYS:HB2  | 1.98                     | 0.44              |
| 2:O:40:GLN:O     | 2:O:92:GLU:HG2   | 2.17                     | 0.44              |
| 2:O:93:PRO:HB2   | 2:O:95:PHE:CE2   | 2.52                     | 0.44              |
| 2:O:260:THR:HG23 | 2:O:262:ASP:H    | 1.83                     | 0.44              |
| 2:M:567:SER:OG   | 2:R:173:ASP:OD2  | 2.35                     | 0.44              |
| 2:P:178:HIS:NE2  | 2:P:431:ILE:HG23 | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:3:ILE:HD11   | 2:Q:96:LEU:HD22  | 1.98                     | 0.44              |
| 2:Q:149:LYS:NZ   | 2:Q:439:GLU:OE2  | 2.45                     | 0.44              |
| 2:Q:283:VAL:HA   | 2:Q:328:ASN:HA   | 2.00                     | 0.44              |
| 1:I:317:THR:O    | 1:I:365:ARG:NH2  | 2.51                     | 0.44              |
| 2:R:519:ILE:HG23 | 2:R:532:LEU:HD21 | 1.99                     | 0.44              |
| 2:M:571:PRO:O    | 2:M:572:SER:C    | 2.61                     | 0.44              |
| 2:M:582:LYS:HD2  | 2:M:582:LYS:HA   | 1.80                     | 0.44              |
| 2:P:383:ASP:O    | 2:P:384:ARG:HG3  | 2.17                     | 0.44              |
| 2:P:434:MET:HE2  | 2:P:474:MET:HB2  | 1.99                     | 0.44              |
| 1:B:272:VAL:HG12 | 1:B:273:PRO:HD3  | 2.00                     | 0.44              |
| 2:P:109:GLU:O    | 2:P:110:LYS:HG2  | 2.18                     | 0.43              |
| 2:Q:58:THR:HG22  | 2:Q:58:THR:O     | 2.18                     | 0.43              |
| 2:R:18:ILE:HB    | 2:R:65:PHE:HB2   | 2.00                     | 0.43              |
| 2:R:100:ASP:OD1  | 2:R:101:ILE:N    | 2.50                     | 0.43              |
| 2:M:212:LEU:HD13 | 2:M:378:PHE:HZ   | 1.83                     | 0.43              |
| 2:P:61:ASP:OD1   | 2:P:61:ASP:N     | 2.50                     | 0.43              |
| 2:P:412:PHE:HA   | 2:P:471:LEU:HD11 | 1.99                     | 0.43              |
| 1:I:285:ILE:HD13 | 1:I:323:ILE:HB   | 2.00                     | 0.43              |
| 2:M:562:LYS:HB2  | 2:M:562:LYS:HE3  | 1.68                     | 0.43              |
| 2:N:144:SER:O    | 2:N:147:SER:OG   | 2.25                     | 0.43              |
| 2:N:422:GLN:HA   | 2:N:425:LYS:HZ3  | 1.83                     | 0.43              |
| 2:O:350:ARG:NE   | 2:O:396:PRO:HG3  | 2.34                     | 0.43              |
| 2:Q:342:PHE:CE2  | 2:Q:346:LEU:HD11 | 2.53                     | 0.43              |
| 2:R:438:GLU:OE2  | 2:R:439:GLU:HG2  | 2.17                     | 0.43              |
| 1:F:292:ASP:N    | 1:F:292:ASP:OD1  | 2.50                     | 0.43              |
| 1:G:313:ILE:HG23 | 1:G:365:ARG:NH1  | 2.33                     | 0.43              |
| 2:Q:523:LEU:H    | 2:Q:524:PRO:HD2  | 1.83                     | 0.43              |
| 2:R:283:VAL:HG11 | 2:R:297:SER:OG   | 2.18                     | 0.43              |
| 2:P:304:ASN:O    | 2:P:305:ARG:HB3  | 2.19                     | 0.43              |
| 1:B:316:HIS:O    | 1:B:365:ARG:NH2  | 2.52                     | 0.43              |
| 2:M:184:ILE:HG13 | 2:M:185:HIS:N    | 2.32                     | 0.43              |
| 2:O:221:GLU:HB3  | 2:O:402:ILE:HG23 | 1.99                     | 0.43              |
| 2:Q:56:ILE:HG13  | 2:Q:65:PHE:HD1   | 1.83                     | 0.43              |
| 1:G:282:ARG:HG2  | 1:G:398:TYR:HE1  | 1.83                     | 0.43              |
| 1:I:285:ILE:HG22 | 1:I:403:VAL:HG21 | 2.01                     | 0.43              |
| 2:Q:224:THR:HA   | 2:Q:228:GLU:HB2  | 2.01                     | 0.43              |
| 2:R:205:LEU:HD22 | 2:R:377:GLN:HE21 | 1.82                     | 0.43              |
| 2:P:115:HIS:HA   | 2:P:128:THR:HG22 | 1.99                     | 0.43              |
| 2:P:260:THR:OG1  | 2:P:261:TYR:N    | 2.52                     | 0.43              |
| 2:P:519:ILE:HG23 | 2:P:532:LEU:HD21 | 2.00                     | 0.43              |
| 1:B:397:LEU:HD23 | 1:B:399:ILE:HD11 | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:299:ILE:HG21 | 1:F:341:ARG:HG3  | 2.00                     | 0.43              |
| 1:L:295:ASP:OD1  | 1:L:334:TYR:OH   | 2.28                     | 0.43              |
| 1:F:313:ILE:O    | 1:F:365:ARG:NH1  | 2.51                     | 0.43              |
| 2:O:207:VAL:HA   | 2:O:210:LEU:HB3  | 2.01                     | 0.43              |
| 2:P:249:LYS:NZ   | 2:P:261:TYR:O    | 2.51                     | 0.43              |
| 2:P:322:LYS:HD3  | 2:P:323:ALA:H    | 1.82                     | 0.43              |
| 2:P:383:ASP:OD1  | 2:P:383:ASP:N    | 2.46                     | 0.43              |
| 2:R:36:TYR:HB2   | 2:R:97:VAL:HG11  | 2.01                     | 0.43              |
| 1:B:322:PHE:HB2  | 1:B:378:ILE:HG13 | 2.00                     | 0.42              |
| 1:H:331:LEU:HD21 | 1:H:347:THR:HB   | 2.00                     | 0.42              |
| 2:N:113:ILE:HG13 | 2:N:128:THR:HB   | 2.01                     | 0.42              |
| 2:O:213:PRO:HB2  | 2:O:215:TRP:CD1  | 2.54                     | 0.42              |
| 1:H:331:LEU:HB2  | 1:H:380:CYS:HB2  | 2.00                     | 0.42              |
| 1:H:387:LYS:HE3  | 1:H:407:LEU:HD12 | 2.02                     | 0.42              |
| 2:M:182:PHE:CE1  | 2:M:390:ILE:HD12 | 2.54                     | 0.42              |
| 2:N:114:PHE:HE2  | 2:N:116:LEU:HD12 | 1.84                     | 0.42              |
| 2:O:59:ASP:N     | 2:O:59:ASP:OD1   | 2.50                     | 0.42              |
| 2:P:559:LYS:HB2  | 2:P:562:LYS:HG2  | 2.01                     | 0.42              |
| 2:N:248:ASN:ND2  | 2:N:268:ASN:O    | 2.53                     | 0.42              |
| 2:P:142:VAL:HB   | 2:P:480:PRO:HG3  | 2.00                     | 0.42              |
| 2:Q:295:LYS:HE3  | 2:Q:301:LEU:HB2  | 2.00                     | 0.42              |
| 2:R:259:ILE:HD12 | 2:R:265:VAL:HG21 | 2.00                     | 0.42              |
| 1:I:386:ILE:HG23 | 1:I:408:LEU:HB3  | 2.00                     | 0.42              |
| 2:M:178:HIS:CE1  | 2:M:431:ILE:HG23 | 2.54                     | 0.42              |
| 2:O:175:LYS:HA   | 2:O:175:LYS:HD3  | 1.78                     | 0.42              |
| 2:O:431:ILE:O    | 2:O:431:ILE:HG13 | 2.19                     | 0.42              |
| 2:Q:201:ASN:ND2  | 2:Q:384:ARG:O    | 2.53                     | 0.42              |
| 2:R:365:LYS:HD3  | 2:R:365:LYS:HA   | 1.70                     | 0.42              |
| 1:A:399:ILE:HG23 | 1:A:417:ASN:HA   | 2.01                     | 0.42              |
| 1:I:373:GLU:HG3  | 1:I:374:PHE:CD1  | 2.55                     | 0.42              |
| 2:M:63:ASP:HB3   | 2:M:65:PHE:HE1   | 1.83                     | 0.42              |
| 2:N:445:PRO:O    | 2:N:484:SER:OG   | 2.34                     | 0.42              |
| 2:R:488:LEU:HD23 | 2:R:488:LEU:HA   | 1.94                     | 0.42              |
| 1:C:268:LYS:C    | 1:C:270:GLN:H    | 2.28                     | 0.42              |
| 1:G:303:LYS:HG3  | 1:G:343:ILE:HD11 | 2.01                     | 0.42              |
| 2:N:56:ILE:HD11  | 2:P:87:LEU:HD23  | 2.01                     | 0.42              |
| 2:O:575:GLU:HB3  | 2:Q:421:LEU:HD21 | 2.02                     | 0.42              |
| 2:P:54:ILE:HG23  | 2:P:67:LEU:HD23  | 2.01                     | 0.42              |
| 1:B:405:VAL:HB   | 1:B:408:LEU:HD12 | 2.01                     | 0.42              |
| 1:E:410:THR:HA   | 1:E:413:VAL:HG22 | 2.01                     | 0.42              |
| 2:N:246:VAL:HG12 | 2:Q:337:ARG:HH22 | 1.84                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:427:LYS:HA   | 1:B:432:MET:HE3  | 2.01                     | 0.42              |
| 1:C:427:LYS:HG2  | 1:C:432:MET:HE2  | 2.02                     | 0.42              |
| 1:F:427:LYS:HG2  | 1:F:432:MET:HE2  | 2.01                     | 0.42              |
| 1:G:283:TYR:CE2  | 1:G:389:ILE:HG23 | 2.54                     | 0.42              |
| 1:G:313:ILE:HG23 | 1:G:365:ARG:HH11 | 1.85                     | 0.42              |
| 2:N:414:PHE:CE1  | 2:Q:576:VAL:HG21 | 2.55                     | 0.42              |
| 2:O:56:ILE:HD12  | 2:Q:90:PRO:HD3   | 2.00                     | 0.42              |
| 2:R:39:ILE:HG13  | 2:R:94:VAL:HG22  | 2.01                     | 0.42              |
| 2:M:414:PHE:CE2  | 2:P:576:VAL:HG21 | 2.54                     | 0.42              |
| 2:N:577:ILE:HA   | 2:N:580:TRP:HB2  | 2.02                     | 0.42              |
| 2:O:377:GLN:HA   | 2:O:382:LEU:HD11 | 2.01                     | 0.42              |
| 2:P:361:GLU:HG3  | 2:P:363:ASN:H    | 1.84                     | 0.42              |
| 1:J:350:ILE:HG22 | 1:J:350:ILE:O    | 2.20                     | 0.42              |
| 1:L:309:TYR:OH   | 1:L:430:LEU:O    | 2.27                     | 0.42              |
| 1:L:410:THR:HB   | 1:L:415:ILE:HD11 | 2.02                     | 0.42              |
| 2:M:40:GLN:HB3   | 2:M:92:GLU:OE2   | 2.20                     | 0.42              |
| 2:M:168:ASN:HB2  | 2:M:198:GLU:HB3  | 2.02                     | 0.42              |
| 2:Q:499:LEU:O    | 2:Q:505:GLN:NE2  | 2.36                     | 0.42              |
| 1:H:373:GLU:HB3  | 1:H:374:PHE:H    | 1.66                     | 0.41              |
| 2:M:234:SER:O    | 2:M:238:VAL:HG23 | 2.19                     | 0.41              |
| 2:O:213:PRO:HB3  | 2:O:355:LEU:HD12 | 2.00                     | 0.41              |
| 2:P:285:ASN:ND2  | 2:P:291:PRO:O    | 2.52                     | 0.41              |
| 2:P:509:LYS:HE2  | 2:P:520:SER:HB2  | 2.02                     | 0.41              |
| 2:R:137:LYS:NZ   | 2:R:536:ASP:OD2  | 2.52                     | 0.41              |
| 2:R:342:PHE:O    | 2:R:346:LEU:HG   | 2.20                     | 0.41              |
| 2:R:522:ILE:HG21 | 2:R:543:ILE:HD11 | 2.01                     | 0.41              |
| 2:N:6:VAL:HG22   | 2:N:92:GLU:H     | 1.86                     | 0.41              |
| 2:O:18:ILE:HG21  | 2:O:24:PHE:HB2   | 2.02                     | 0.41              |
| 2:O:355:LEU:O    | 2:O:358:GLN:NE2  | 2.50                     | 0.41              |
| 1:E:268:LYS:O    | 1:E:269:ASN:HB2  | 2.20                     | 0.41              |
| 1:I:277:ILE:HD12 | 1:I:280:ARG:HD2  | 2.03                     | 0.41              |
| 2:O:96:LEU:HB3   | 2:O:97:VAL:H     | 1.78                     | 0.41              |
| 2:O:209:LYS:HB3  | 2:O:209:LYS:HE3  | 1.73                     | 0.41              |
| 2:R:6:VAL:HG22   | 2:R:16:VAL:HG22  | 2.02                     | 0.41              |
| 1:A:284:PHE:HB3  | 1:A:286:ILE:HG13 | 2.03                     | 0.41              |
| 1:A:386:ILE:O    | 1:A:390:ASN:ND2  | 2.54                     | 0.41              |
| 1:F:271:LEU:HD11 | 1:F:418:LEU:HD11 | 2.01                     | 0.41              |
| 1:K:386:ILE:HD12 | 1:K:408:LEU:HD11 | 2.02                     | 0.41              |
| 2:N:302:VAL:HG13 | 2:N:307:ILE:HD11 | 2.02                     | 0.41              |
| 2:O:3:ILE:HD13   | 2:O:3:ILE:HA     | 1.92                     | 0.41              |
| 2:Q:174:LYS:HB3  | 2:Q:384:ARG:NH2  | 2.35                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:Q:435:ILE:HB   | 2:Q:473:LEU:HD23 | 2.01                     | 0.41              |
| 1:A:274:SER:HB2  | 1:A:280:ARG:HH21 | 1.86                     | 0.41              |
| 1:C:307:ASP:O    | 1:C:311:SER:OG   | 2.38                     | 0.41              |
| 1:J:285:ILE:HD13 | 1:J:323:ILE:HB   | 2.03                     | 0.41              |
| 2:M:203:ASN:ND2  | 2:M:377:GLN:O    | 2.52                     | 0.41              |
| 2:N:421:LEU:HD11 | 2:Q:575:GLU:HB3  | 2.03                     | 0.41              |
| 2:O:141:VAL:HB   | 2:O:476:VAL:HG22 | 2.01                     | 0.41              |
| 2:O:181:ILE:HG23 | 2:O:436:VAL:HB   | 2.02                     | 0.41              |
| 1:L:352:ASP:N    | 1:L:352:ASP:OD1  | 2.53                     | 0.41              |
| 2:R:87:LEU:HD23  | 2:R:87:LEU:HA    | 1.86                     | 0.41              |
| 2:R:273:PHE:HB2  | 2:R:342:PHE:CE2  | 2.55                     | 0.41              |
| 2:M:149:LYS:HE3  | 2:M:149:LYS:HB2  | 1.86                     | 0.41              |
| 2:M:556:GLN:HG2  | 2:R:428:LEU:HD11 | 2.03                     | 0.41              |
| 2:N:51:ILE:HA    | 2:N:69:VAL:HG12  | 2.03                     | 0.41              |
| 2:N:99:ASP:OD1   | 2:N:99:ASP:N     | 2.43                     | 0.41              |
| 2:N:417:HIS:NE2  | 2:Q:580:TRP:HE3  | 2.19                     | 0.41              |
| 2:O:207:VAL:HG13 | 2:O:395:ILE:HD11 | 2.02                     | 0.41              |
| 2:P:174:LYS:HB3  | 2:P:384:ARG:NH2  | 2.35                     | 0.41              |
| 2:R:134:PHE:HZ   | 2:R:495:ILE:HD11 | 1.85                     | 0.41              |
| 1:L:386:ILE:HG23 | 1:L:408:LEU:HD12 | 2.03                     | 0.41              |
| 2:M:269:ILE:HG13 | 2:M:342:PHE:HZ   | 1.86                     | 0.41              |
| 2:P:213:PRO:HG2  | 2:P:374:ILE:HD13 | 2.03                     | 0.41              |
| 2:R:517:ARG:HA   | 2:R:517:ARG:HD2  | 1.87                     | 0.41              |
| 1:A:286:ILE:HG13 | 1:A:286:ILE:H    | 1.73                     | 0.41              |
| 1:B:399:ILE:HG12 | 1:B:405:VAL:HG11 | 2.01                     | 0.41              |
| 2:M:569:ARG:O    | 2:M:571:PRO:HD3  | 2.21                     | 0.41              |
| 2:N:278:ASN:HD22 | 2:N:308:TYR:HA   | 1.86                     | 0.41              |
| 2:N:515:ASN:OD1  | 2:N:516:SER:N    | 2.54                     | 0.41              |
| 2:P:149:LYS:HE2  | 2:P:149:LYS:HB3  | 1.85                     | 0.41              |
| 2:P:301:LEU:O    | 2:P:302:VAL:C    | 2.63                     | 0.41              |
| 2:P:563:LYS:HA   | 2:P:563:LYS:HD2  | 1.84                     | 0.41              |
| 2:Q:346:LEU:HD23 | 2:Q:356:LEU:HD12 | 2.03                     | 0.41              |
| 1:A:332:SER:O    | 1:A:336:LYS:HG3  | 2.21                     | 0.41              |
| 1:C:418:LEU:HD12 | 1:C:429:LEU:HD13 | 2.03                     | 0.41              |
| 2:O:38:LYS:HG2   | 2:O:96:LEU:O     | 2.20                     | 0.41              |
| 2:O:113:ILE:HG23 | 2:O:128:THR:HB   | 2.02                     | 0.41              |
| 2:P:296:LEU:HB3  | 2:P:315:PHE:HD1  | 1.85                     | 0.41              |
| 2:Q:522:ILE:HG23 | 2:Q:522:ILE:O    | 2.21                     | 0.41              |
| 1:A:378:ILE:HD12 | 1:A:378:ILE:H    | 1.86                     | 0.40              |
| 1:D:272:VAL:N    | 1:D:273:PRO:HD2  | 2.36                     | 0.40              |
| 1:E:327:ASP:OD1  | 1:E:327:ASP:N    | 2.52                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:N:516:SER:O    | 2:N:520:SER:OG   | 2.34                     | 0.40              |
| 2:P:56:ILE:HD13  | 2:P:56:ILE:HA    | 1.94                     | 0.40              |
| 2:P:217:MET:HB3  | 2:P:221:GLU:HB2  | 2.03                     | 0.40              |
| 1:J:270:GLN:HG2  | 1:L:424:ARG:HH22 | 1.85                     | 0.40              |
| 1:L:285:ILE:HG22 | 1:L:403:VAL:HG11 | 2.02                     | 0.40              |
| 2:N:282:GLU:HA   | 2:N:315:PHE:CE2  | 2.56                     | 0.40              |
| 2:O:113:ILE:HD13 | 2:O:113:ILE:HA   | 1.95                     | 0.40              |
| 2:O:440:ALA:HB1  | 2:O:444:ILE:HD11 | 2.04                     | 0.40              |
| 2:Q:298:ASN:HB2  | 2:Q:314:GLU:O    | 2.22                     | 0.40              |
| 2:P:501:ASN:OD1  | 2:P:502:ILE:N    | 2.54                     | 0.40              |
| 2:Q:194:ILE:HD11 | 2:Q:200:PHE:HB3  | 2.02                     | 0.40              |
| 2:Q:296:LEU:HD21 | 2:Q:302:VAL:HB   | 2.03                     | 0.40              |
| 2:R:175:LYS:HA   | 2:R:175:LYS:HD3  | 1.81                     | 0.40              |
| 1:C:296:ASP:HA   | 1:C:337:ARG:HH22 | 1.86                     | 0.40              |
| 1:D:293:ASN:ND2  | 1:D:297:GLU:OE2  | 2.51                     | 0.40              |
| 2:M:228:GLU:HG3  | 2:M:341:ARG:NH1  | 2.36                     | 0.40              |
| 2:M:412:PHE:HD1  | 2:M:471:LEU:HD22 | 1.86                     | 0.40              |
| 2:M:508:ILE:HD13 | 2:M:508:ILE:HA   | 1.89                     | 0.40              |
| 2:N:458:SER:O    | 2:N:462:ILE:HG13 | 2.21                     | 0.40              |
| 2:P:318:SER:O    | 2:P:320:THR:N    | 2.54                     | 0.40              |
| 1:C:325:LYS:HD2  | 1:C:403:VAL:HG23 | 2.03                     | 0.40              |
| 1:H:389:ILE:C    | 1:H:391:TYR:H    | 2.28                     | 0.40              |
| 1:J:410:THR:HB   | 1:J:415:ILE:HD11 | 2.04                     | 0.40              |
| 2:M:129:LEU:HD23 | 2:M:129:LEU:HA   | 1.90                     | 0.40              |
| 2:Q:280:ASN:O    | 2:Q:333:GLY:N    | 2.37                     | 0.40              |
| 2:R:534:VAL:HG22 | 2:R:541:PRO:HB3  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 168/436 (38%)   | 160 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 1   | B     | 168/436 (38%)   | 157 (94%)  | 10 (6%)  | 1 (1%)   | 21          | 54  |
| 1   | C     | 168/436 (38%)   | 160 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 1   | D     | 168/436 (38%)   | 165 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 1   | E     | 168/436 (38%)   | 162 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 1   | F     | 168/436 (38%)   | 164 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 1   | G     | 178/436 (41%)   | 165 (93%)  | 13 (7%)  | 0        | 100         | 100 |
| 1   | H     | 178/436 (41%)   | 165 (93%)  | 12 (7%)  | 1 (1%)   | 21          | 54  |
| 1   | I     | 178/436 (41%)   | 172 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 1   | J     | 178/436 (41%)   | 171 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 1   | K     | 178/436 (41%)   | 171 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 1   | L     | 178/436 (41%)   | 173 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 2   | M     | 583/585 (100%)  | 562 (96%)  | 21 (4%)  | 0        | 100         | 100 |
| 2   | N     | 583/585 (100%)  | 567 (97%)  | 16 (3%)  | 0        | 100         | 100 |
| 2   | O     | 583/585 (100%)  | 565 (97%)  | 18 (3%)  | 0        | 100         | 100 |
| 2   | P     | 583/585 (100%)  | 538 (92%)  | 38 (6%)  | 7 (1%)   | 10          | 38  |
| 2   | Q     | 583/585 (100%)  | 548 (94%)  | 32 (6%)  | 3 (0%)   | 24          | 59  |
| 2   | R     | 583/585 (100%)  | 553 (95%)  | 29 (5%)  | 1 (0%)   | 43          | 75  |
| All | All   | 5574/8742 (64%) | 5318 (95%) | 243 (4%) | 13 (0%)  | 44          | 75  |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 305 | ARG  |
| 2   | Q     | 293 | LEU  |
| 1   | B     | 412 | ASP  |
| 2   | Q     | 187 | GLU  |
| 2   | P     | 297 | SER  |
| 2   | P     | 319 | ASN  |
| 2   | Q     | 523 | LEU  |
| 2   | P     | 285 | ASN  |
| 2   | P     | 301 | LEU  |
| 2   | R     | 287 | ILE  |
| 1   | H     | 393 | LYS  |
| 2   | P     | 110 | LYS  |
| 2   | P     | 326 | ALA  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | B     | 159/416 (38%)   | 159 (100%)  | 0        | 100         | 100 |
| 1   | C     | 142/416 (34%)   | 142 (100%)  | 0        | 100         | 100 |
| 1   | D     | 164/416 (39%)   | 164 (100%)  | 0        | 100         | 100 |
| 1   | E     | 164/416 (39%)   | 164 (100%)  | 0        | 100         | 100 |
| 1   | F     | 164/416 (39%)   | 164 (100%)  | 0        | 100         | 100 |
| 1   | G     | 174/416 (42%)   | 174 (100%)  | 0        | 100         | 100 |
| 1   | H     | 174/416 (42%)   | 174 (100%)  | 0        | 100         | 100 |
| 1   | I     | 174/416 (42%)   | 174 (100%)  | 0        | 100         | 100 |
| 1   | J     | 174/416 (42%)   | 174 (100%)  | 0        | 100         | 100 |
| 1   | K     | 174/416 (42%)   | 174 (100%)  | 0        | 100         | 100 |
| 1   | L     | 174/416 (42%)   | 174 (100%)  | 0        | 100         | 100 |
| 2   | M     | 542/542 (100%)  | 542 (100%)  | 0        | 100         | 100 |
| 2   | N     | 542/542 (100%)  | 542 (100%)  | 0        | 100         | 100 |
| 2   | O     | 542/542 (100%)  | 542 (100%)  | 0        | 100         | 100 |
| 2   | P     | 542/542 (100%)  | 539 (99%)   | 3 (1%)   | 78          | 87  |
| 2   | Q     | 542/542 (100%)  | 542 (100%)  | 0        | 100         | 100 |
| 2   | R     | 542/542 (100%)  | 542 (100%)  | 0        | 100         | 100 |
| All | All   | 5089/7828 (65%) | 5086 (100%) | 3 (0%)   | 87          | 92  |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | P     | 295 | LYS  |
| 2   | P     | 296 | LEU  |
| 2   | P     | 301 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 344 | GLN  |
| 1   | D     | 278 | ASN  |
| 1   | E     | 330 | ASN  |
| 1   | F     | 278 | ASN  |
| 1   | H     | 293 | ASN  |
| 1   | H     | 390 | ASN  |
| 1   | I     | 269 | ASN  |
| 1   | I     | 293 | ASN  |
| 1   | I     | 335 | HIS  |
| 1   | I     | 414 | ASN  |
| 1   | J     | 370 | ASN  |
| 1   | J     | 381 | ASN  |
| 1   | K     | 330 | ASN  |
| 1   | L     | 370 | ASN  |
| 2   | M     | 170 | ASN  |
| 2   | M     | 270 | ASN  |
| 2   | M     | 442 | ASN  |
| 2   | M     | 501 | ASN  |
| 2   | M     | 505 | GLN  |
| 2   | N     | 12  | HIS  |
| 2   | N     | 52  | GLN  |
| 2   | N     | 185 | HIS  |
| 2   | N     | 203 | ASN  |
| 2   | N     | 233 | ASN  |
| 2   | N     | 253 | ASN  |
| 2   | N     | 492 | ASN  |
| 2   | O     | 197 | ASN  |
| 2   | O     | 270 | ASN  |
| 2   | O     | 386 | ASN  |
| 2   | O     | 422 | GLN  |
| 2   | O     | 423 | HIS  |
| 2   | O     | 510 | ASN  |
| 2   | P     | 70  | GLN  |
| 2   | P     | 121 | GLN  |
| 2   | P     | 122 | ASN  |
| 2   | P     | 328 | ASN  |
| 2   | P     | 358 | GLN  |
| 2   | P     | 515 | ASN  |
| 2   | P     | 556 | GLN  |
| 2   | Q     | 118 | ASN  |
| 2   | Q     | 122 | ASN  |
| 2   | Q     | 170 | ASN  |
| 2   | Q     | 203 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | R     | 115 | HIS  |
| 2   | R     | 203 | ASN  |
| 2   | R     | 230 | ASN  |
| 2   | R     | 237 | GLN  |
| 2   | R     | 442 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

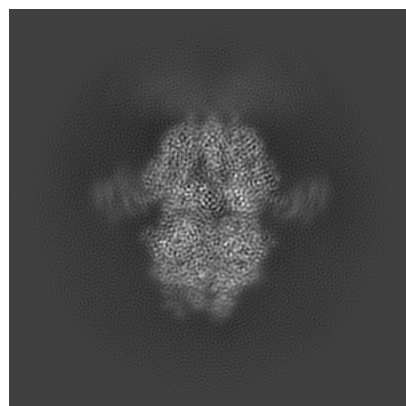
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45234. These allow visual inspection of the internal detail of the map and identification of artifacts.

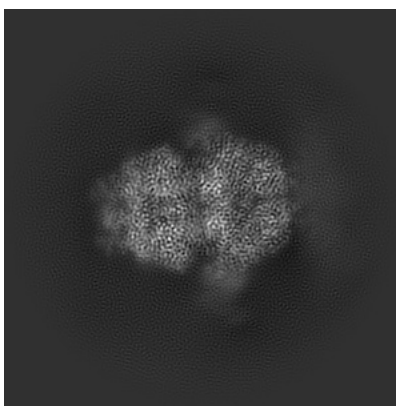
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

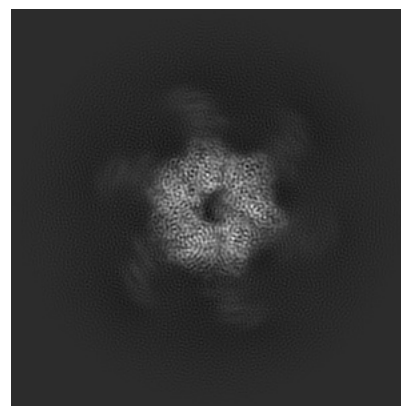
#### 6.1.1 Primary map



X

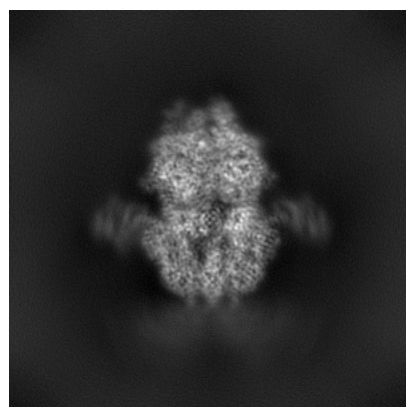


Y

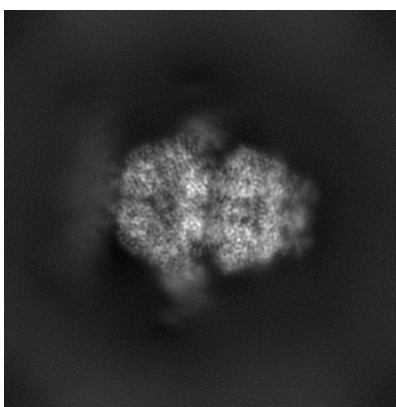


Z

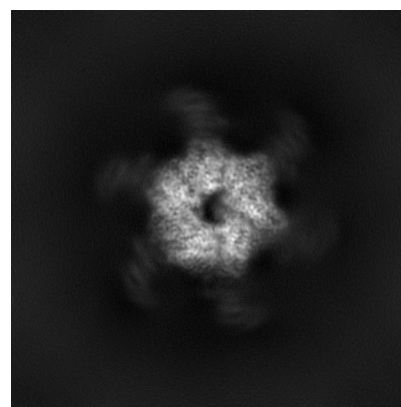
#### 6.1.2 Raw map



X



Y

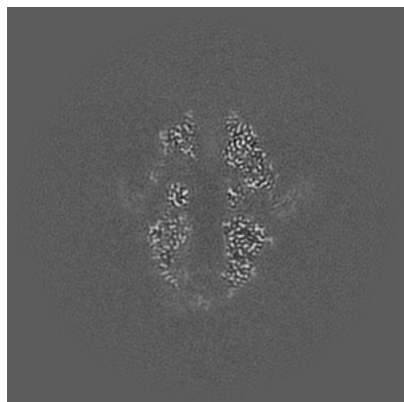


Z

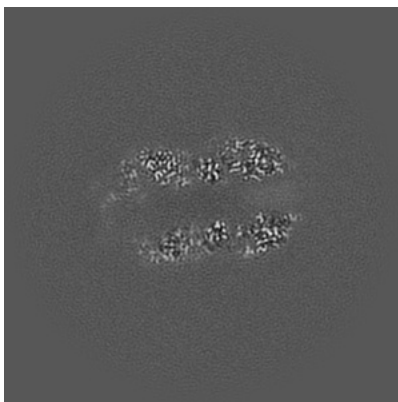
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

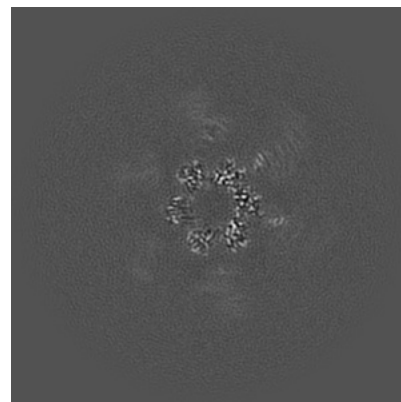
### 6.2.1 Primary map



X Index: 168

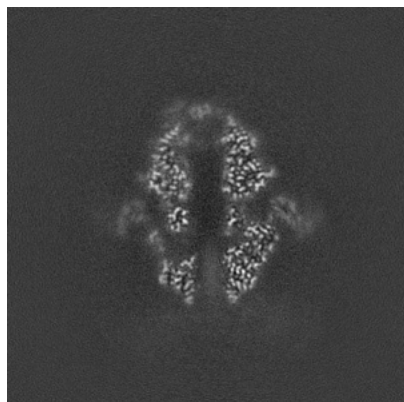


Y Index: 168

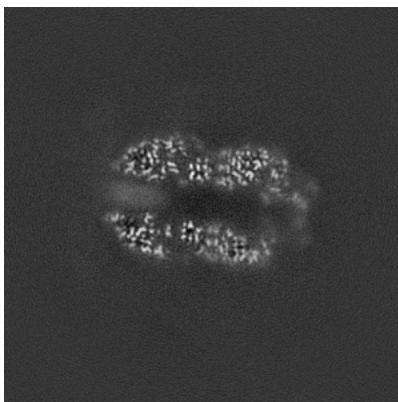


Z Index: 168

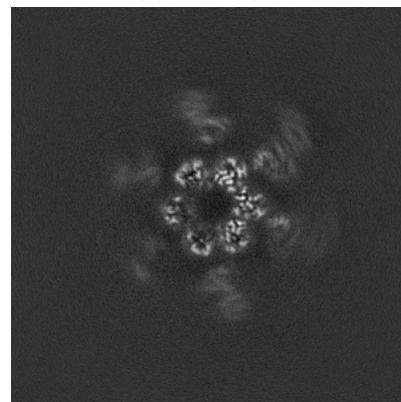
### 6.2.2 Raw map



X Index: 168



Y Index: 168

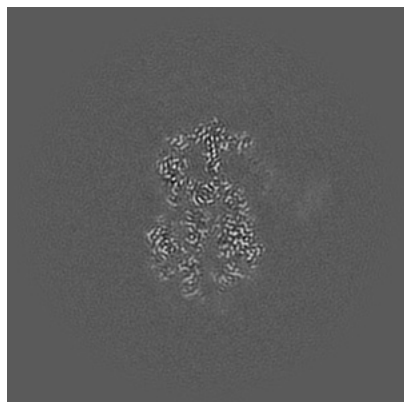


Z Index: 168

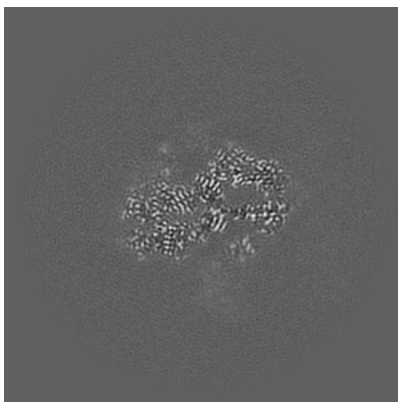
The images above show central slices of the map in three orthogonal directions.

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

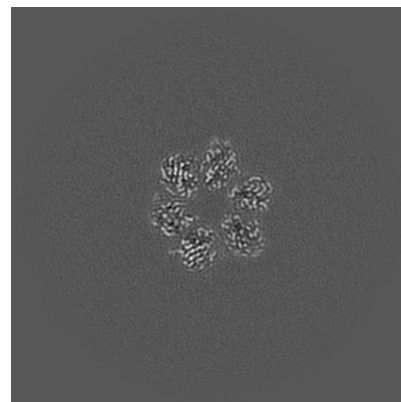
### 6.3.1 Primary map



X Index: 147

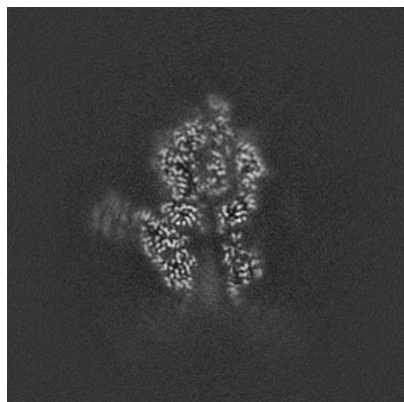


Y Index: 194

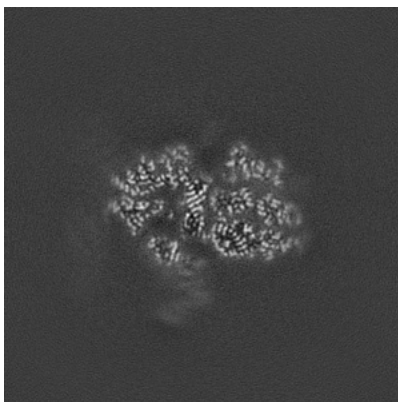


Z Index: 139

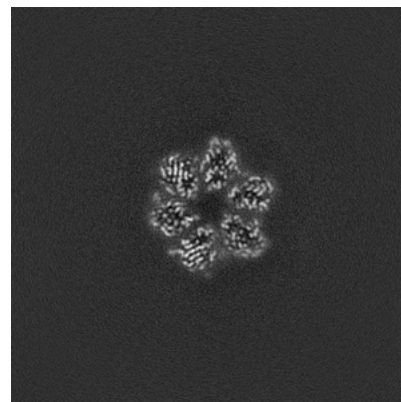
### 6.3.2 Raw map



X Index: 186



Y Index: 189

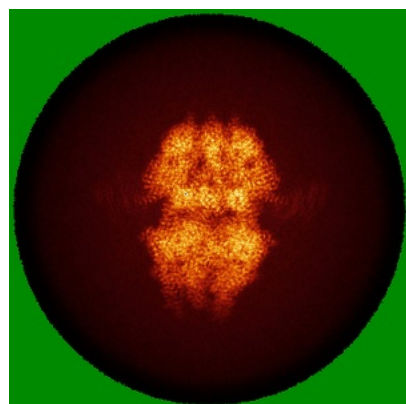


Z Index: 196

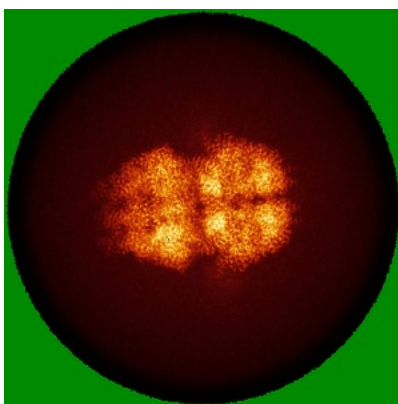
The images above show the largest variance slices of the map in three orthogonal directions.

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

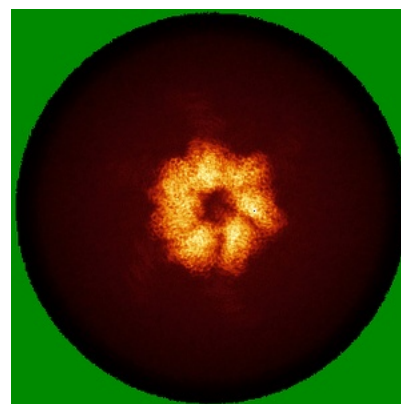
### 6.4.1 Primary map



X

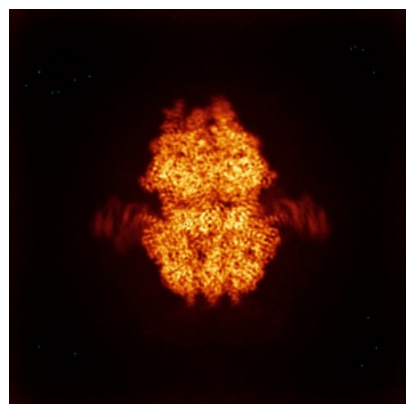


Y

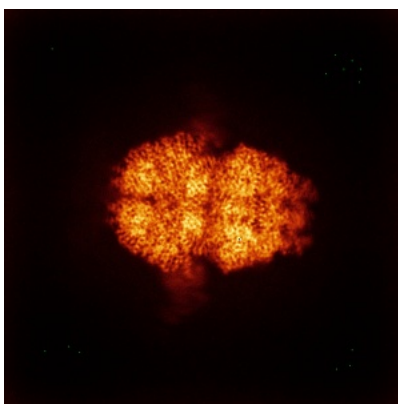


Z

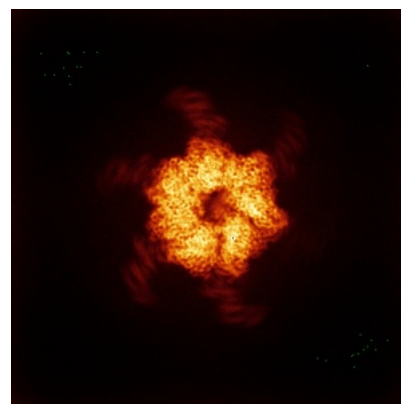
### 6.4.2 Raw map



X



Y

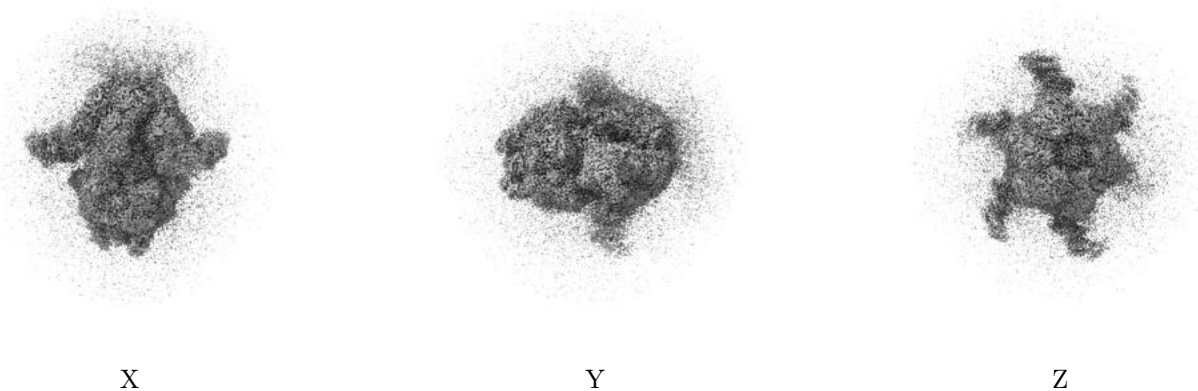


Z

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

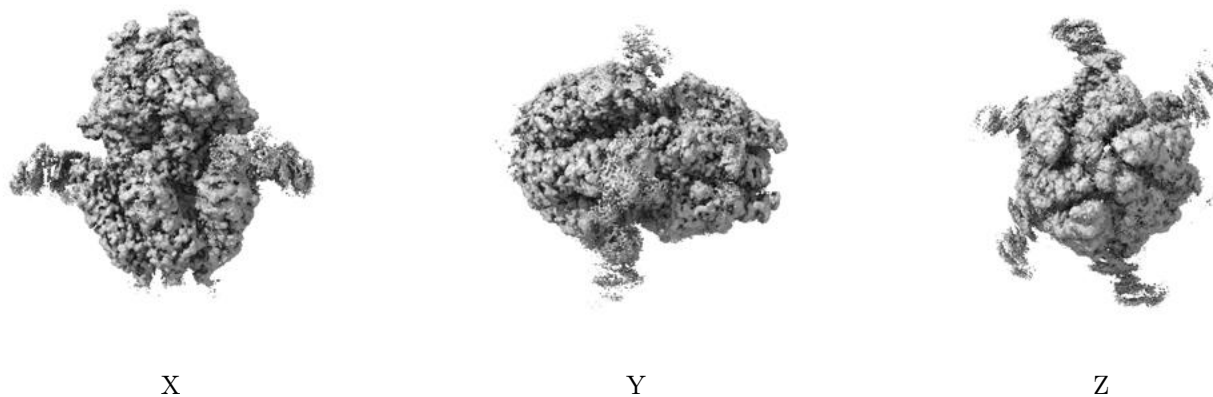
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

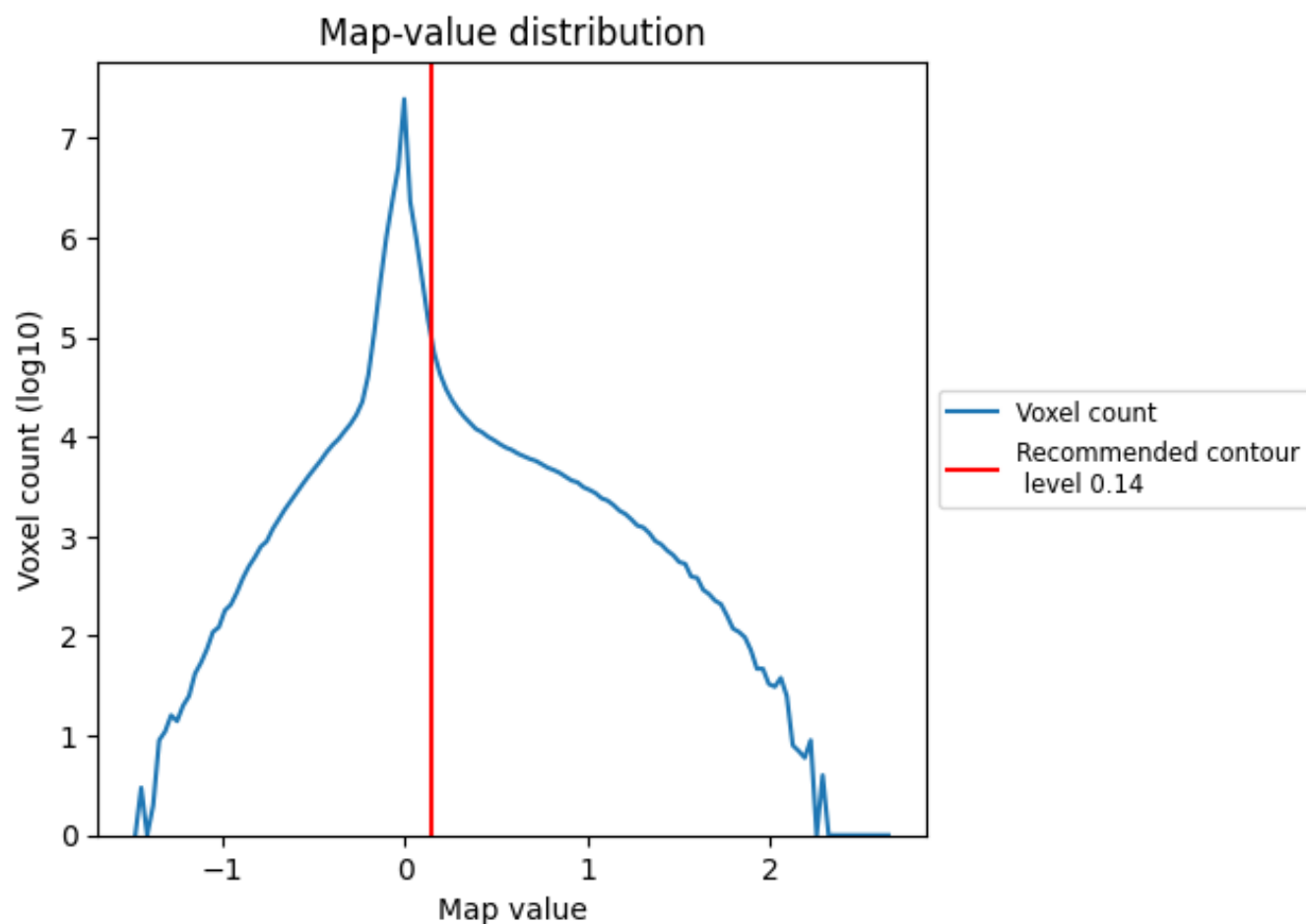
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

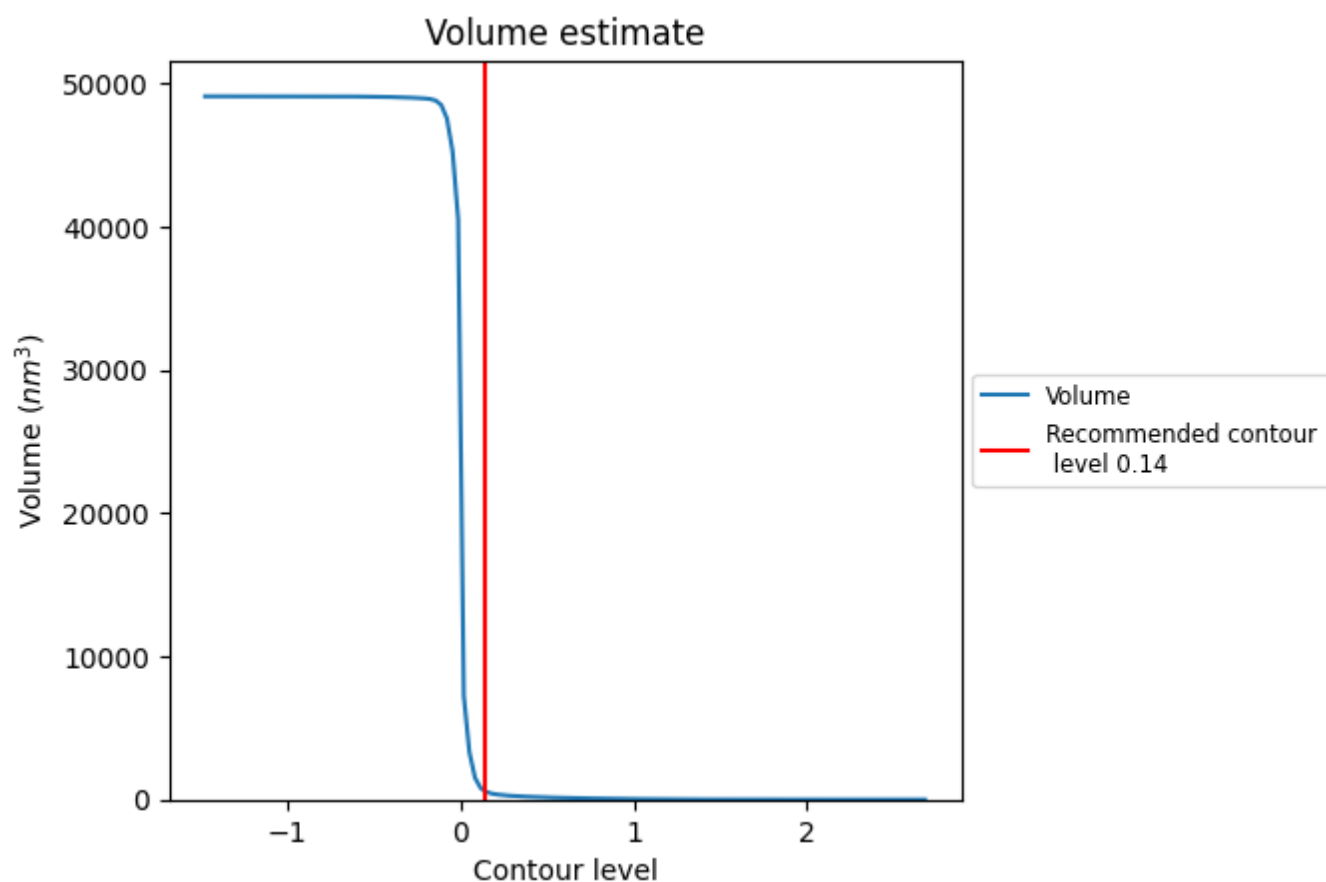
This section contains the results of statistical analysis of the map.

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



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

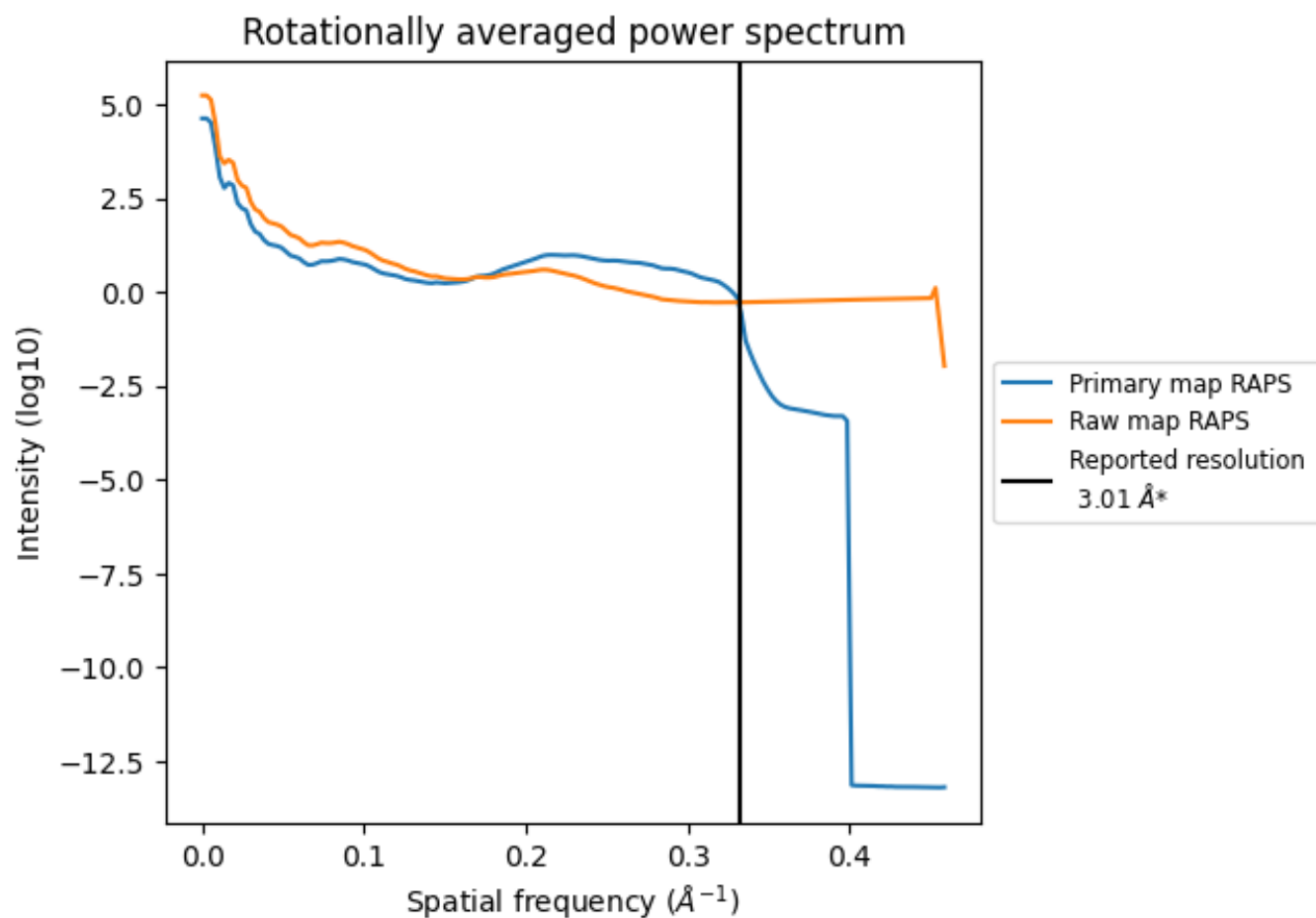
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 599 nm<sup>3</sup>; this corresponds to an approximate mass of 541 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 ⓘ

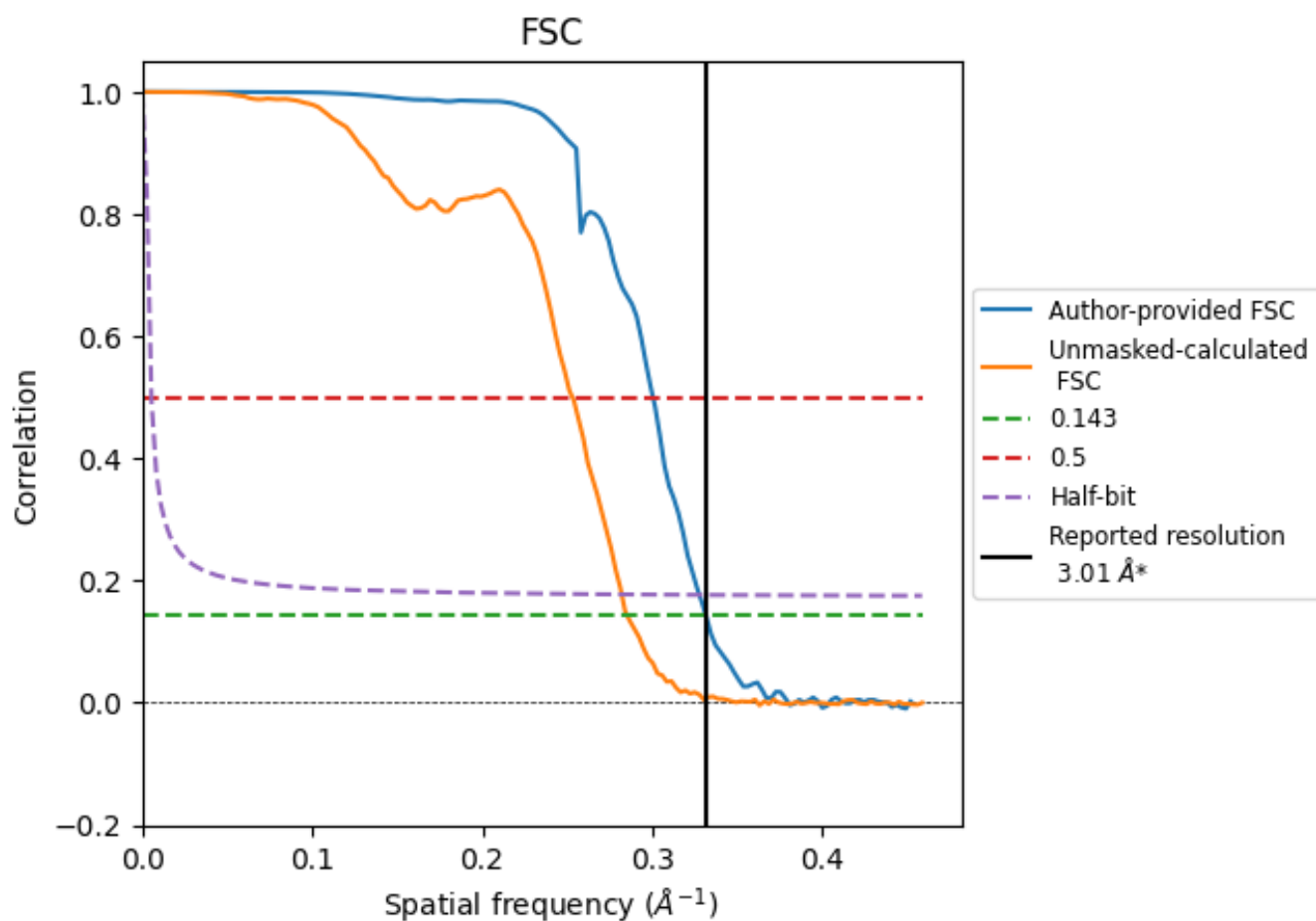


\*Reported resolution corresponds to spatial frequency of 0.332  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.332  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.01                               | -    | -        |
| Author-provided FSC curve | 3.02                               | 3.33 | 3.05     |
| Unmasked-calculated*      | 3.51                               | 3.95 | 3.55     |

\*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 3.51 differs from the reported value 3.01 by more than 10 %

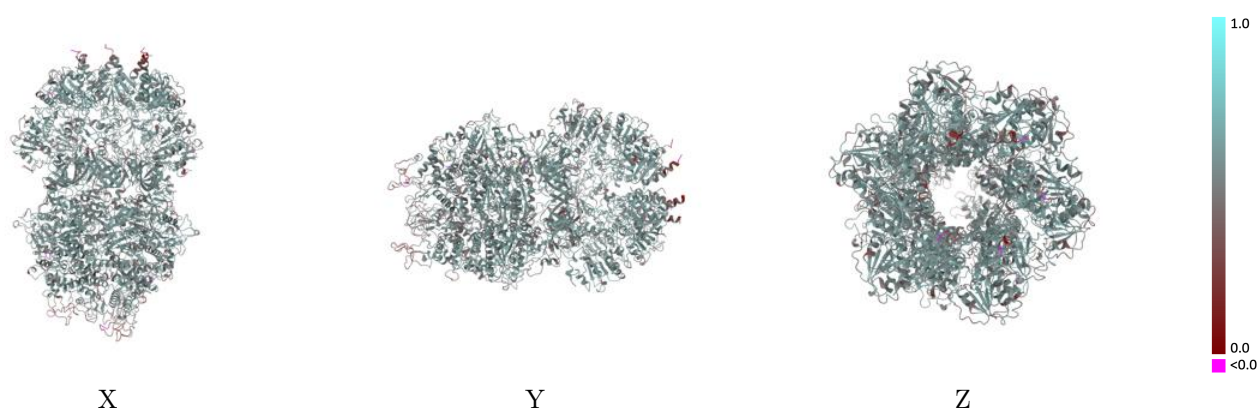
## 9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-45234 and PDB model 9C5X. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay ⓘ

This section was not generated.

### 9.2 Q-score mapped to coordinate model ⓘ

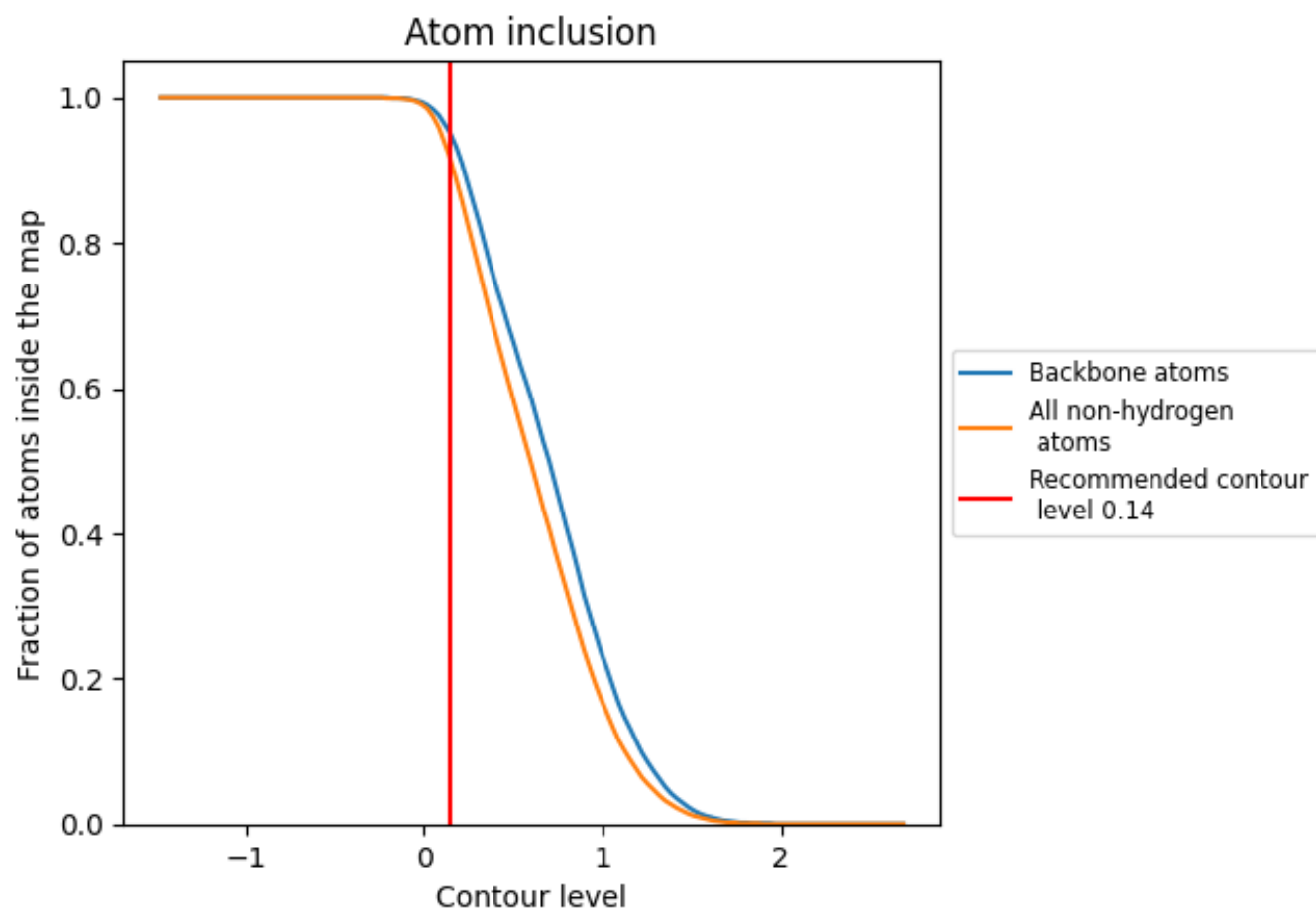


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

### 9.3 Atom inclusion mapped to coordinate model ⓘ

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.14) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9210   |  0.5390   |
| A     |  0.9140   |  0.5350   |
| B     |  0.9250   |  0.5380   |
| C     |  0.9270   |  0.5410   |
| D     |  0.9510   |  0.5570   |
| E     |  0.9330   |  0.5500   |
| F     |  0.9230   |  0.5430   |
| G     |  0.9160   |  0.5420   |
| H     |  0.9150   |  0.5410   |
| I     |  0.9230   |  0.5530   |
| J     |  0.9160   |  0.5450   |
| K     |  0.9330   |  0.5590   |
| L     |  0.9340   |  0.5570   |
| M     |  0.9230   |  0.5390   |
| N     |  0.9320  |  0.5420  |
| O     |  0.9230 |  0.5420 |
| P     |  0.9090 |  0.5260 |
| Q     |  0.9060 |  0.5240 |
| R     |  0.9170 |  0.5350 |

