



## Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 05:18 AM UTC

PDB ID : 8K49 / pdb\_00008k49  
EMDB ID : EMD-36880  
Title : Structure of partial Banna virus  
Authors : Li, Z.; Cao, S.  
Deposited on : 2023-07-17  
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

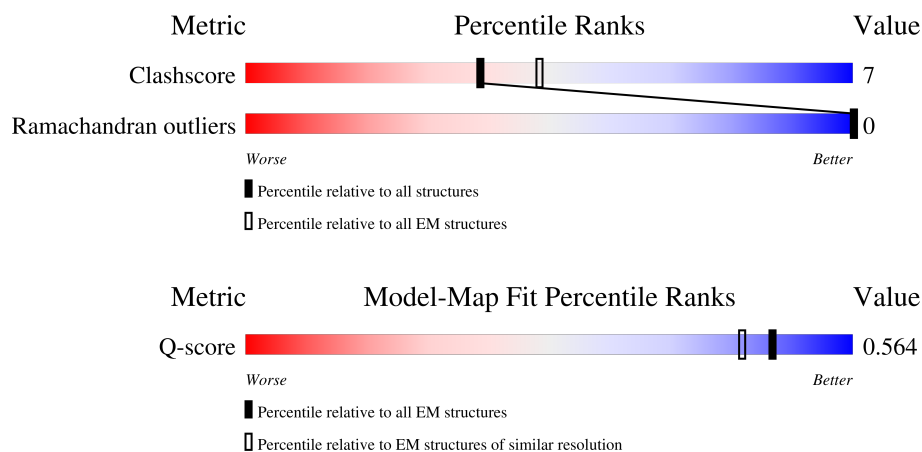
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



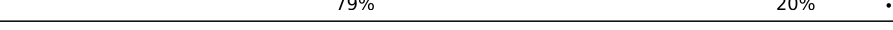
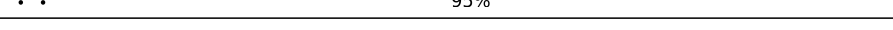
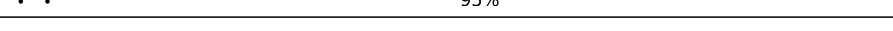
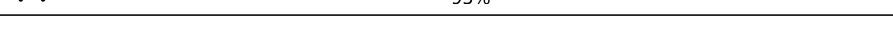
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Q-score               | -                           | 25397                       | 13054 ( 2.40 - 3.40 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 955    |                  |
| 1   | B     | 955    |                  |
| 2   | C     | 302    |                  |
| 2   | D     | 302    |                  |
| 2   | E     | 302    |                  |

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| Mol | Chain | Length | Quality of chain                                                                               |
|-----|-------|--------|------------------------------------------------------------------------------------------------|
| 2   | F     | 302    |  91% 8% .    |
| 2   | G     | 302    |  83% 16% .   |
| 2   | H     | 302    |  89% 10% .   |
| 2   | I     | 302    |  88% 11% .   |
| 2   | J     | 302    |  88% 11% .   |
| 2   | K     | 302    |  87% 12% .   |
| 2   | L     | 302    |  86% 12% .   |
| 2   | M     | 302    |  86% 12% .   |
| 2   | N     | 302    |  84% 15% .   |
| 2   | O     | 302    |  85% 13% .   |
| 3   | P     | 249    |  82% 18% .   |
| 3   | Q     | 249    |  80% 19% .  |
| 4   | R     | 628    |  75% 21% . |
| 4   | S     | 628    |  79% 20% . |
| 4   | T     | 628    |  77% 22% . |
| 5   | r     | 283    |  95% . .   |
| 5   | s     | 283    |  95% . .   |
| 5   | t     | 283    |  95% . .   |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 61697 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 VP2.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 751      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 6045  | 3848 | 1025 | 1145 | 27 |         |       |
| 1   | B     | 902      | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 7210  | 4578 | 1221 | 1384 | 27 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 97      | LYS      | ARG    | conflict | UNP Q9INH3 |
| B     | 97      | LYS      | ARG    | conflict | UNP Q9INH3 |

- Molecule 2 is a protein called VP8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | C     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2288  | 1449 | 397 | 435 | 7 |         |       |
| 2   | D     | 298      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2277  | 1443 | 393 | 434 | 7 |         |       |
| 2   | E     | 298      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2277  | 1443 | 393 | 434 | 7 |         |       |
| 2   | F     | 298      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2277  | 1443 | 393 | 434 | 7 |         |       |
| 2   | G     | 298      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2277  | 1443 | 393 | 434 | 7 |         |       |
| 2   | H     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2288  | 1449 | 397 | 435 | 7 |         |       |
| 2   | I     | 298      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2277  | 1443 | 393 | 434 | 7 |         |       |
| 2   | J     | 299      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2288  | 1449 | 397 | 435 | 7 |         |       |
| 2   | K     | 298      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2277  | 1443 | 393 | 434 | 7 |         |       |
| 2   | L     | 297      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2270  | 1438 | 392 | 433 | 7 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | M     | 298      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2277  | 1443 | 393 | 434 | 7 |         |       |
| 2   | N     | 298      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2277  | 1443 | 393 | 434 | 7 |         |       |
| 2   | O     | 298      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2277  | 1443 | 393 | 434 | 7 |         |       |

There are 39 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| C     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| C     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| C     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| D     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| D     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| D     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| E     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| E     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| E     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| F     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| F     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| F     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| G     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| G     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| G     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| H     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| H     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| H     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| I     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| I     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| I     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| J     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| J     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| J     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| K     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| K     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| K     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| L     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| L     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| L     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| M     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| M     | 185     | LEU      | MET    | conflict | UNP W0G587 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| M     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| N     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| N     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| N     | 266     | SER      | ALA    | conflict | UNP W0G587 |
| O     | 136     | ARG      | GLN    | conflict | UNP W0G587 |
| O     | 185     | LEU      | MET    | conflict | UNP W0G587 |
| O     | 266     | SER      | ALA    | conflict | UNP W0G587 |

- Molecule 3 is a protein called VP10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | P     | 249      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2014  | 1276 | 353 | 377 | 8 |         |       |
| 3   | Q     | 246      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1986  | 1258 | 347 | 373 | 8 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| P     | 79      | VAL      | ILE    | conflict | UNP A0A2H4QDD3 |
| Q     | 79      | VAL      | ILE    | conflict | UNP A0A2H4QDD3 |

- Molecule 4 is a protein called VP4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | R     | 601      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4706  | 2969 | 814 | 907 | 16 |         |       |
| 4   | S     | 622      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4858  | 3060 | 841 | 941 | 16 |         |       |
| 4   | T     | 627      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4900  | 3088 | 848 | 948 | 16 |         |       |

There are 81 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| R     | 15      | ASN      | SER    | conflict | UNP B4Y048 |
| R     | 61      | LEU      | ILE    | conflict | UNP B4Y048 |
| R     | 62      | ASN      | ILE    | conflict | UNP B4Y048 |
| R     | 65      | ALA      | THR    | conflict | UNP B4Y048 |
| R     | 80      | ASN      | LYS    | conflict | UNP B4Y048 |
| R     | 94      | ILE      | VAL    | conflict | UNP B4Y048 |
| R     | 130     | VAL      | ILE    | conflict | UNP B4Y048 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| R     | 154     | VAL      | ILE    | conflict | UNP B4Y048 |
| R     | 235     | ALA      | SER    | conflict | UNP B4Y048 |
| R     | 271     | VAL      | THR    | conflict | UNP B4Y048 |
| R     | 278     | ILE      | VAL    | conflict | UNP B4Y048 |
| R     | 307     | LEU      | MET    | conflict | UNP B4Y048 |
| R     | 322     | ASN      | THR    | conflict | UNP B4Y048 |
| R     | 369     | ALA      | VAL    | conflict | UNP B4Y048 |
| R     | 436     | ASP      | GLU    | conflict | UNP B4Y048 |
| R     | 439     | GLN      | LYS    | conflict | UNP B4Y048 |
| R     | 444     | THR      | ALA    | conflict | UNP B4Y048 |
| R     | 470     | LYS      | ARG    | conflict | UNP B4Y048 |
| R     | 500     | THR      | ALA    | conflict | UNP B4Y048 |
| R     | 524     | VAL      | ILE    | conflict | UNP B4Y048 |
| R     | 537     | ASN      | ASP    | conflict | UNP B4Y048 |
| R     | 539     | SER      | ASP    | conflict | UNP B4Y048 |
| R     | 543     | SER      | LEU    | conflict | UNP B4Y048 |
| R     | 545     | ASN      | LYS    | conflict | UNP B4Y048 |
| R     | 547     | ARG      | LYS    | conflict | UNP B4Y048 |
| R     | 575     | ALA      | THR    | conflict | UNP B4Y048 |
| R     | 628     | PRO      | SER    | conflict | UNP B4Y048 |
| S     | 15      | ASN      | SER    | conflict | UNP B4Y048 |
| S     | 61      | LEU      | ILE    | conflict | UNP B4Y048 |
| S     | 62      | ASN      | ILE    | conflict | UNP B4Y048 |
| S     | 65      | ALA      | THR    | conflict | UNP B4Y048 |
| S     | 80      | ASN      | LYS    | conflict | UNP B4Y048 |
| S     | 94      | ILE      | VAL    | conflict | UNP B4Y048 |
| S     | 130     | VAL      | ILE    | conflict | UNP B4Y048 |
| S     | 154     | VAL      | ILE    | conflict | UNP B4Y048 |
| S     | 235     | ALA      | SER    | conflict | UNP B4Y048 |
| S     | 271     | VAL      | THR    | conflict | UNP B4Y048 |
| S     | 278     | ILE      | VAL    | conflict | UNP B4Y048 |
| S     | 307     | LEU      | MET    | conflict | UNP B4Y048 |
| S     | 322     | ASN      | THR    | conflict | UNP B4Y048 |
| S     | 369     | ALA      | VAL    | conflict | UNP B4Y048 |
| S     | 436     | ASP      | GLU    | conflict | UNP B4Y048 |
| S     | 439     | GLN      | LYS    | conflict | UNP B4Y048 |
| S     | 444     | THR      | ALA    | conflict | UNP B4Y048 |
| S     | 470     | LYS      | ARG    | conflict | UNP B4Y048 |
| S     | 500     | THR      | ALA    | conflict | UNP B4Y048 |
| S     | 524     | VAL      | ILE    | conflict | UNP B4Y048 |
| S     | 537     | ASN      | ASP    | conflict | UNP B4Y048 |
| S     | 539     | SER      | ASP    | conflict | UNP B4Y048 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| S     | 543     | SER      | LEU    | conflict | UNP B4Y048 |
| S     | 545     | ASN      | LYS    | conflict | UNP B4Y048 |
| S     | 547     | ARG      | LYS    | conflict | UNP B4Y048 |
| S     | 575     | ALA      | THR    | conflict | UNP B4Y048 |
| S     | 628     | PRO      | SER    | conflict | UNP B4Y048 |
| T     | 15      | ASN      | SER    | conflict | UNP B4Y048 |
| T     | 61      | LEU      | ILE    | conflict | UNP B4Y048 |
| T     | 62      | ASN      | ILE    | conflict | UNP B4Y048 |
| T     | 65      | ALA      | THR    | conflict | UNP B4Y048 |
| T     | 80      | ASN      | LYS    | conflict | UNP B4Y048 |
| T     | 94      | ILE      | VAL    | conflict | UNP B4Y048 |
| T     | 130     | VAL      | ILE    | conflict | UNP B4Y048 |
| T     | 154     | VAL      | ILE    | conflict | UNP B4Y048 |
| T     | 235     | ALA      | SER    | conflict | UNP B4Y048 |
| T     | 271     | VAL      | THR    | conflict | UNP B4Y048 |
| T     | 278     | ILE      | VAL    | conflict | UNP B4Y048 |
| T     | 307     | LEU      | MET    | conflict | UNP B4Y048 |
| T     | 322     | ASN      | THR    | conflict | UNP B4Y048 |
| T     | 369     | ALA      | VAL    | conflict | UNP B4Y048 |
| T     | 436     | ASP      | GLU    | conflict | UNP B4Y048 |
| T     | 439     | GLN      | LYS    | conflict | UNP B4Y048 |
| T     | 444     | THR      | ALA    | conflict | UNP B4Y048 |
| T     | 470     | LYS      | ARG    | conflict | UNP B4Y048 |
| T     | 500     | THR      | ALA    | conflict | UNP B4Y048 |
| T     | 524     | VAL      | ILE    | conflict | UNP B4Y048 |
| T     | 537     | ASN      | ASP    | conflict | UNP B4Y048 |
| T     | 539     | SER      | ASP    | conflict | UNP B4Y048 |
| T     | 543     | SER      | LEU    | conflict | UNP B4Y048 |
| T     | 545     | ASN      | LYS    | conflict | UNP B4Y048 |
| T     | 547     | ARG      | LYS    | conflict | UNP B4Y048 |
| T     | 575     | ALA      | THR    | conflict | UNP B4Y048 |
| T     | 628     | PRO      | SER    | conflict | UNP B4Y048 |

- Molecule 5 is a protein called VP9.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 5   | r     | 15       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 117   | 73 | 20 | 24 |         |       |
| 5   | s     | 15       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 117   | 73 | 20 | 24 |         |       |
| 5   | t     | 15       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 117   | 73 | 20 | 24 |         |       |

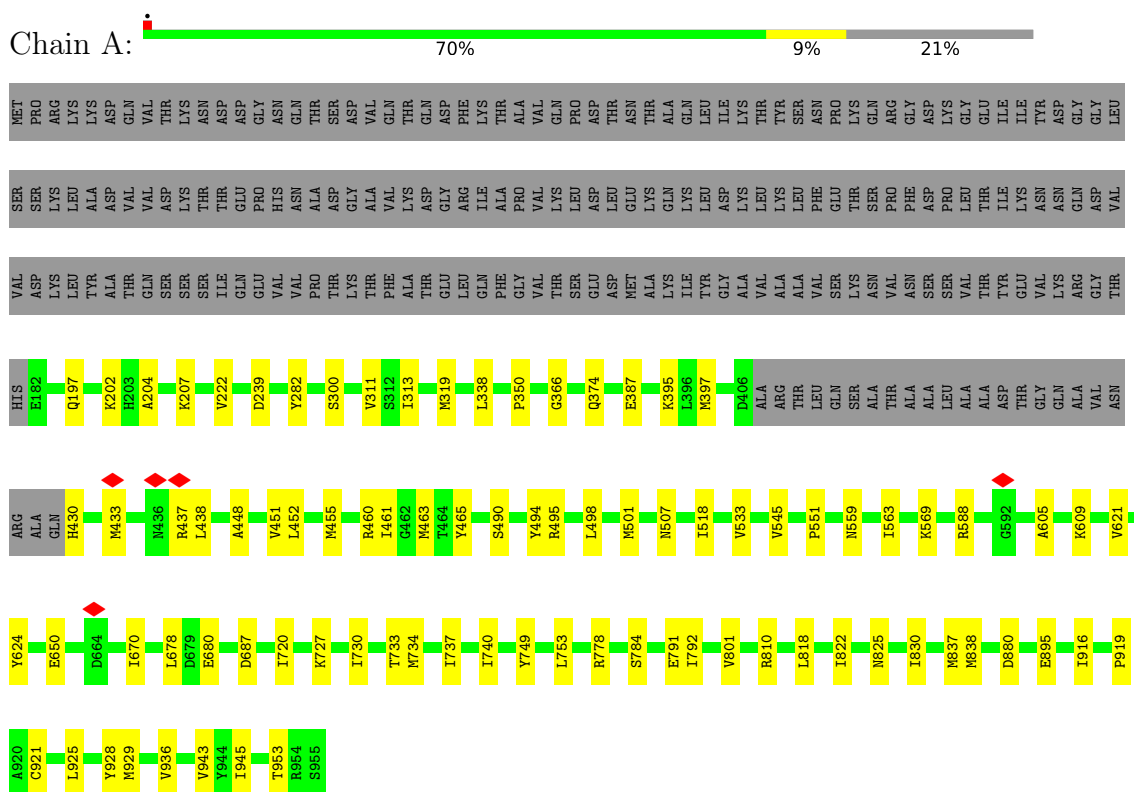
There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| r     | 150     | TYR      | HIS    | conflict | UNP Q9YWN5 |
| r     | 156     | LEU      | GLN    | conflict | UNP Q9YWN5 |
| r     | 184     | THR      | ALA    | conflict | UNP Q9YWN5 |
| r     | 191     | ASN      | ASP    | conflict | UNP Q9YWN5 |
| s     | 150     | TYR      | HIS    | conflict | UNP Q9YWN5 |
| s     | 156     | LEU      | GLN    | conflict | UNP Q9YWN5 |
| s     | 184     | THR      | ALA    | conflict | UNP Q9YWN5 |
| s     | 191     | ASN      | ASP    | conflict | UNP Q9YWN5 |
| t     | 150     | TYR      | HIS    | conflict | UNP Q9YWN5 |
| t     | 156     | LEU      | GLN    | conflict | UNP Q9YWN5 |
| t     | 184     | THR      | ALA    | conflict | UNP Q9YWN5 |
| t     | 191     | ASN      | ASP    | conflict | UNP Q9YWN5 |

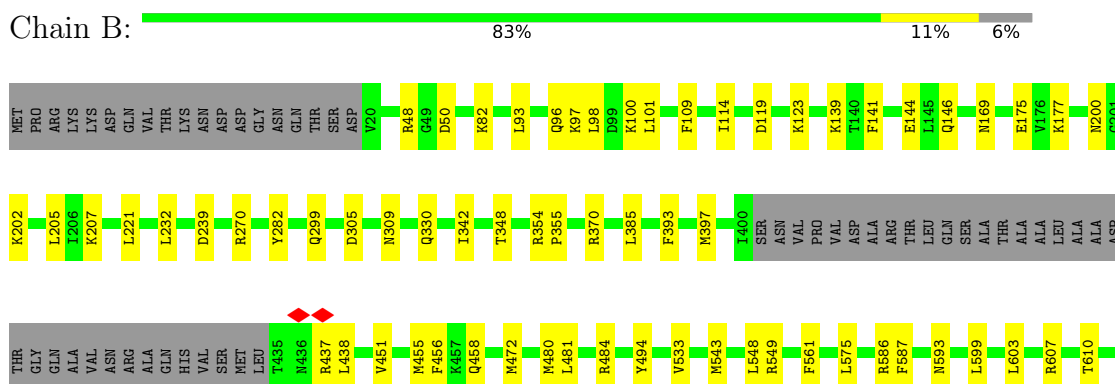
### 3 Residue-property plots

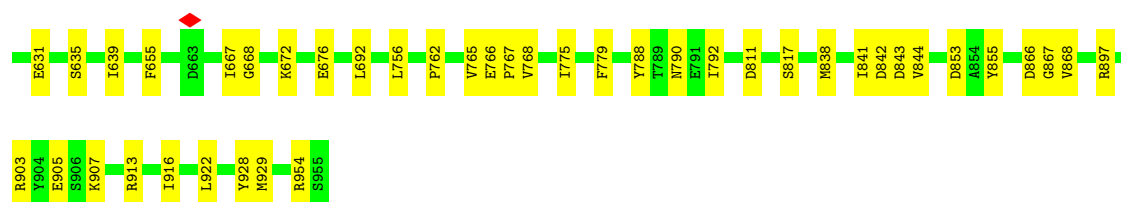
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: VP2



#### • Molecule 1: VP2





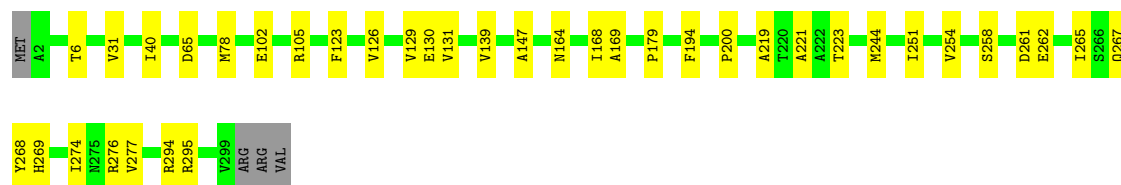
• Molecule 2: VP8

Chain C: 87% 12%



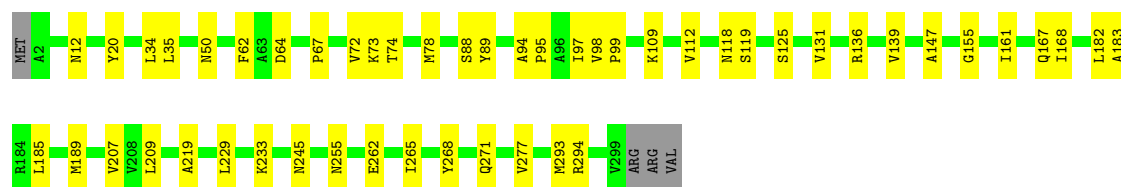
• Molecule 2: VP8

Chain D: 86% 13%



• Molecule 2: VP8

Chain E: 82% 17%



• Molecule 2: VP8

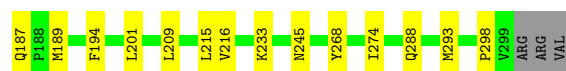
Chain F: 91% 8%



• Molecule 2: VP8

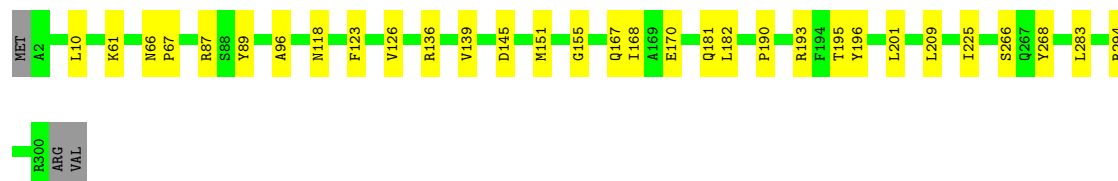
Chain G: 83% 16%





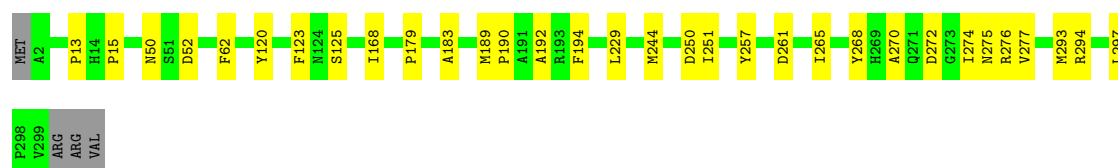
- Molecule 2: VP8

Chain H: 89% 10%



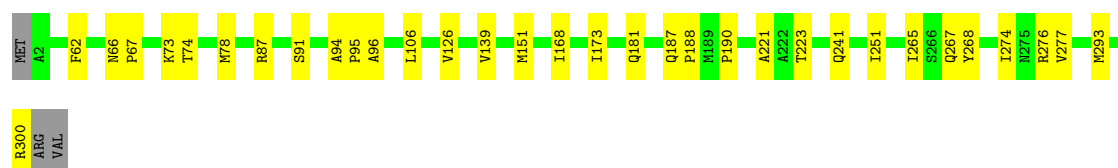
- Molecule 2: VP8

Chain I: 88% 11%



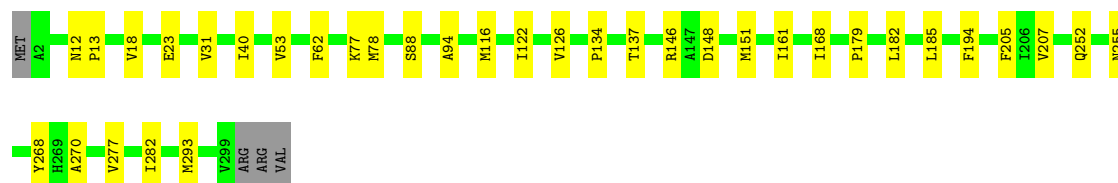
- Molecule 2: VP8

Chain J: 88% 11%



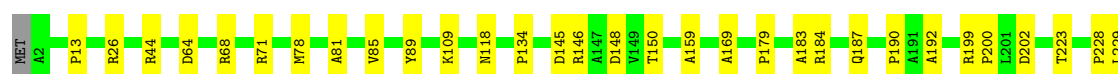
- Molecule 2: VP8

Chain K: 87% 12%



- Molecule 2: VP8

Chain L: 86% 12%





• Molecule 2: VP8

Chain M: 86% 12%



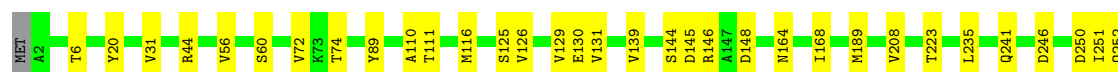
• Molecule 2: VP8

Chain N: 84% 15%



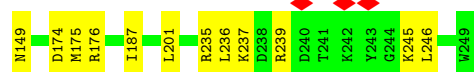
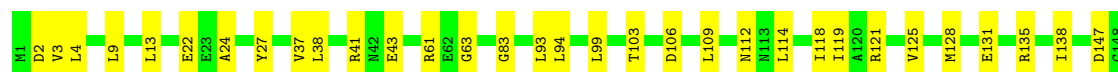
• Molecule 2: VP8

Chain O: 85% 13%



• Molecule 3: VP10

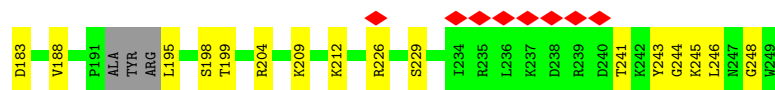
Chain P: 82% 18%



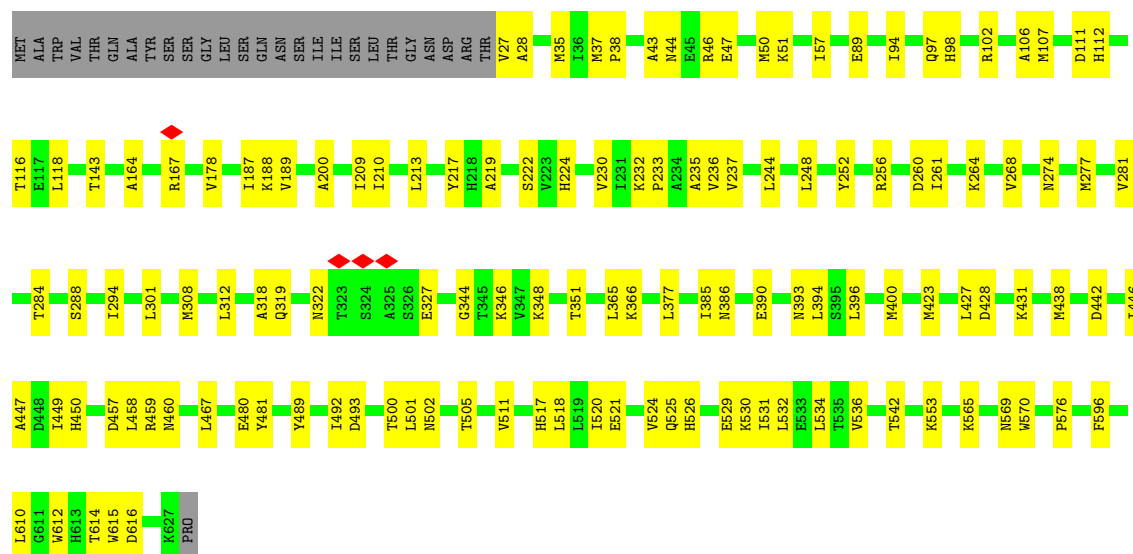
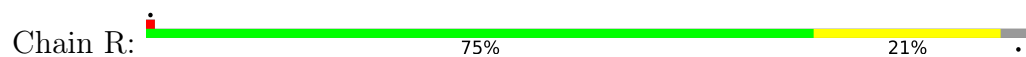
• Molecule 3: VP10

Chain Q: 80% 19%

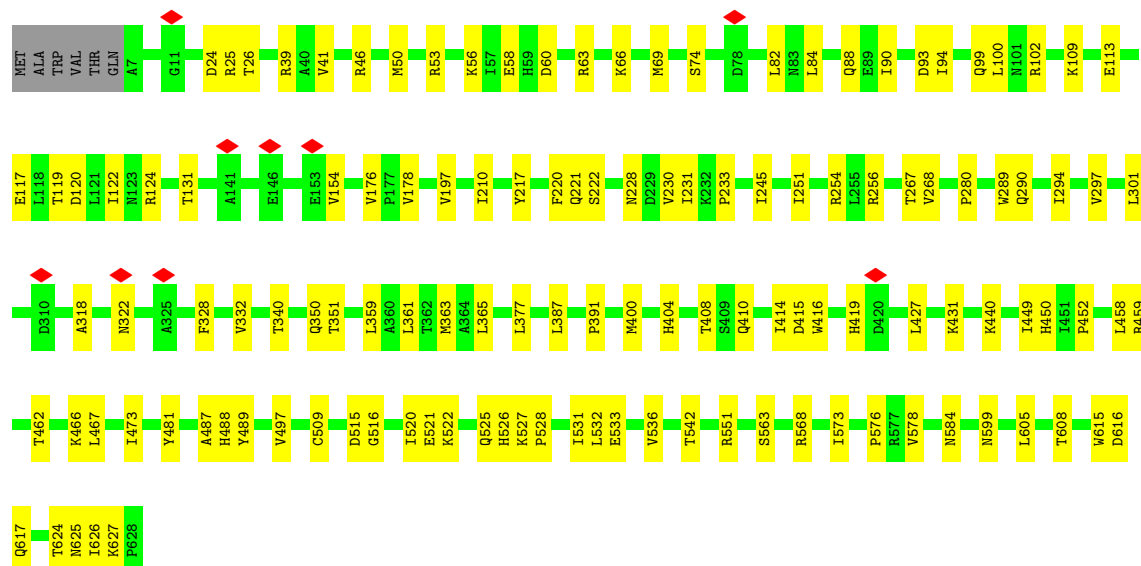
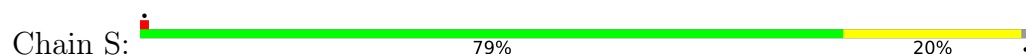




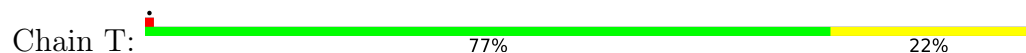
• Molecule 4: VP4

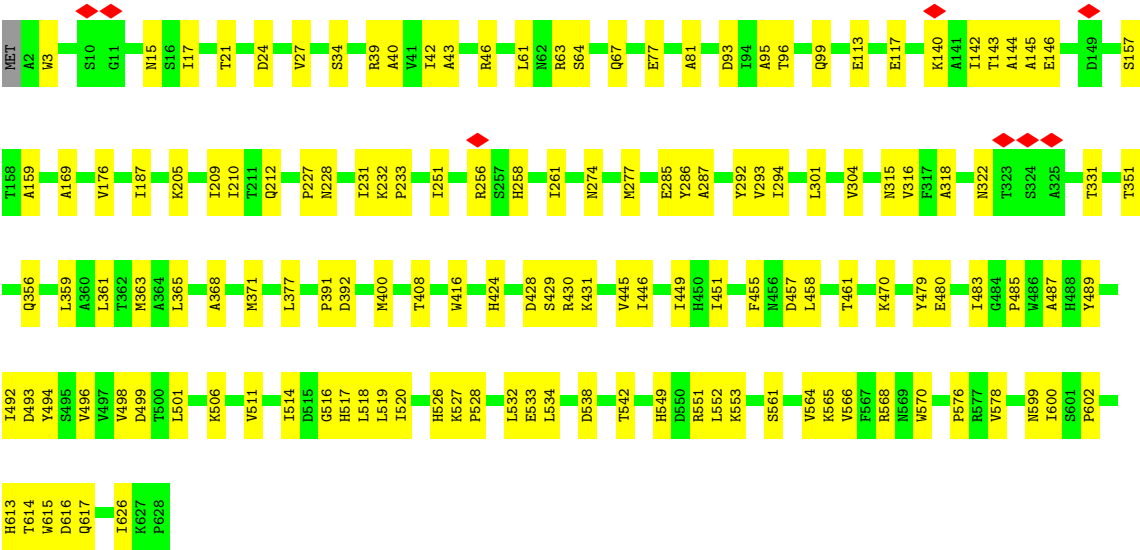


• Molecule 4: VP4

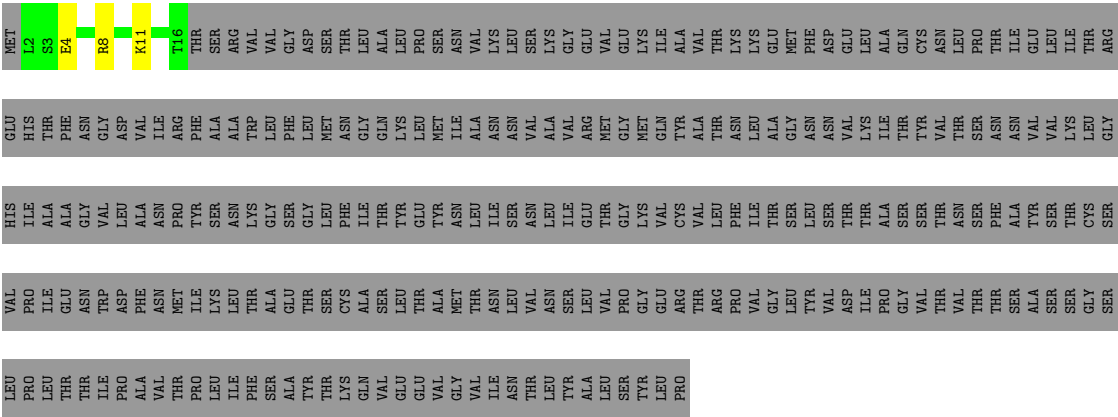


• Molecule 4: VP4

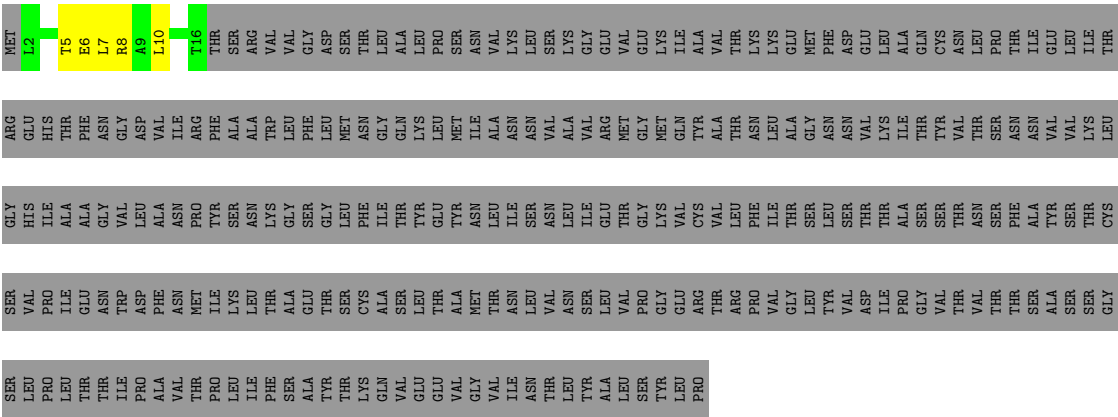




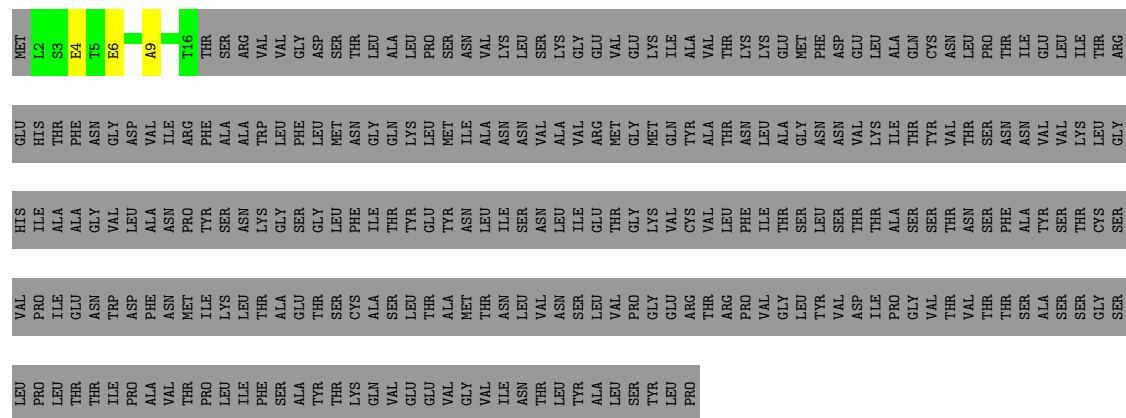
• Molecule 5: VP9



• Molecule 5: VP9



Chain t:  95%



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 136575                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | JEOL CRYO ARM 300                       | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 40                                      | 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                    | 1.753                                   | Depositor |
| Minimum map value                    | -0.003                                  | Depositor |
| Average map value                    | 0.016                                   | Depositor |
| Map value standard deviation         | 0.092                                   | Depositor |
| Recommended contour level            | 0.1                                     | Depositor |
| Map size (Å)                         | 437.0, 437.0, 437.0                     | wwPDB     |
| Map dimensions                       | 460, 460, 460                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.95, 0.95, 0.95                        | 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     | 0.15         | 0/6179  | 0.25        | 0/8387  |
| 1   | B     | 0.17         | 0/7361  | 0.29        | 0/9987  |
| 2   | C     | 0.16         | 0/2333  | 0.27        | 0/3179  |
| 2   | D     | 0.14         | 0/2322  | 0.26        | 0/3165  |
| 2   | E     | 0.15         | 0/2322  | 0.25        | 0/3165  |
| 2   | F     | 0.16         | 0/2322  | 0.27        | 0/3165  |
| 2   | G     | 0.16         | 0/2322  | 0.28        | 0/3165  |
| 2   | H     | 0.14         | 0/2333  | 0.25        | 0/3179  |
| 2   | I     | 0.15         | 0/2322  | 0.29        | 0/3165  |
| 2   | J     | 0.16         | 0/2333  | 0.27        | 0/3179  |
| 2   | K     | 0.15         | 0/2322  | 0.25        | 0/3165  |
| 2   | L     | 0.15         | 0/2315  | 0.27        | 0/3155  |
| 2   | M     | 0.15         | 0/2322  | 0.27        | 0/3165  |
| 2   | N     | 0.15         | 0/2322  | 0.27        | 0/3165  |
| 2   | O     | 0.15         | 0/2322  | 0.25        | 0/3165  |
| 3   | P     | 0.15         | 0/2050  | 0.24        | 0/2772  |
| 3   | Q     | 0.14         | 0/2020  | 0.26        | 0/2730  |
| 4   | R     | 0.14         | 0/4799  | 0.29        | 0/6515  |
| 4   | S     | 0.14         | 0/4953  | 0.29        | 0/6725  |
| 4   | T     | 0.15         | 0/4997  | 0.28        | 0/6787  |
| 5   | r     | 0.10         | 0/116   | 0.13        | 0/154   |
| 5   | s     | 0.12         | 0/116   | 0.23        | 0/154   |
| 5   | t     | 0.11         | 0/116   | 0.26        | 0/154   |
| All | All   | 0.15         | 0/62919 | 0.27        | 0/85542 |

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 ⓘ

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     | 6045  | 0        | 5960     | 67      | 0            |
| 1   | B     | 7210  | 0        | 7136     | 86      | 0            |
| 2   | C     | 2288  | 0        | 2283     | 34      | 0            |
| 2   | D     | 2277  | 0        | 2270     | 26      | 0            |
| 2   | E     | 2277  | 0        | 2270     | 35      | 0            |
| 2   | F     | 2277  | 0        | 2270     | 21      | 0            |
| 2   | G     | 2277  | 0        | 2270     | 36      | 0            |
| 2   | H     | 2288  | 0        | 2283     | 30      | 0            |
| 2   | I     | 2277  | 0        | 2270     | 29      | 0            |
| 2   | J     | 2288  | 0        | 2283     | 27      | 0            |
| 2   | K     | 2277  | 0        | 2270     | 33      | 0            |
| 2   | L     | 2270  | 0        | 2261     | 28      | 0            |
| 2   | M     | 2277  | 0        | 2270     | 33      | 0            |
| 2   | N     | 2277  | 0        | 2270     | 35      | 0            |
| 2   | O     | 2277  | 0        | 2270     | 32      | 0            |
| 3   | P     | 2014  | 0        | 2036     | 31      | 0            |
| 3   | Q     | 1986  | 0        | 2008     | 37      | 0            |
| 4   | R     | 4706  | 0        | 4649     | 108     | 0            |
| 4   | S     | 4858  | 0        | 4796     | 99      | 0            |
| 4   | T     | 4900  | 0        | 4835     | 125     | 0            |
| 5   | r     | 117   | 0        | 130      | 3       | 0            |
| 5   | s     | 117   | 0        | 130      | 9       | 0            |
| 5   | t     | 117   | 0        | 130      | 3       | 0            |
| All | All   | 61697 | 0        | 61350    | 900     | 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 7.

All (900) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 4:S:74:SER:HB3   | 5:s:5:THR:HG22  | 1.35                     | 1.07              |
| 4:T:210:ILE:CG2  | 4:T:212:GLN:HG2 | 1.85                     | 1.05              |
| 4:S:74:SER:HB3   | 5:s:5:THR:CG2   | 1.86                     | 1.04              |
| 2:I:168:ILE:HG12 | 2:I:268:TYR:CD2 | 1.93                     | 1.03              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:T:258:HIS:CE1  | 4:T:356:GLN:HE22 | 1.79                     | 1.00              |
| 2:H:182:LEU:HB3  | 2:H:196:TYR:CE2  | 1.97                     | 0.99              |
| 4:T:517:HIS:CD2  | 4:T:519:LEU:HD23 | 1.97                     | 0.99              |
| 4:T:81:ALA:HB1   | 4:T:527:LYS:CE   | 1.93                     | 0.98              |
| 4:T:99:GLN:HE22  | 4:T:187:ILE:HD13 | 1.27                     | 0.98              |
| 2:E:119:SER:HB2  | 2:E:229:LEU:HD23 | 1.43                     | 0.98              |
| 4:R:438:MET:HE2  | 4:R:447:ALA:HA   | 1.42                     | 0.98              |
| 2:M:268:TYR:CD1  | 2:M:277:VAL:HG21 | 1.99                     | 0.97              |
| 4:S:233:PRO:CG   | 4:S:404:HIS:HD2  | 1.76                     | 0.97              |
| 4:T:81:ALA:HB1   | 4:T:527:LYS:HE3  | 1.44                     | 0.96              |
| 3:P:235:ARG:O    | 3:P:239:ARG:HG3  | 1.64                     | 0.96              |
| 2:O:268:TYR:CD1  | 2:O:277:VAL:HG11 | 2.00                     | 0.96              |
| 4:T:210:ILE:HG23 | 4:T:212:GLN:HG2  | 1.47                     | 0.96              |
| 2:K:18:VAL:HG21  | 3:Q:127:LYS:HG2  | 1.45                     | 0.95              |
| 2:C:183:ALA:HB3  | 2:C:189:MET:CE   | 1.95                     | 0.95              |
| 2:D:168:ILE:HD13 | 2:D:269:HIS:CD2  | 2.01                     | 0.95              |
| 1:B:438:LEU:HD13 | 1:B:655:PHE:HD1  | 1.32                     | 0.95              |
| 2:I:168:ILE:HG12 | 2:I:268:TYR:HD2  | 1.29                     | 0.95              |
| 4:T:258:HIS:HE1  | 4:T:356:GLN:HE22 | 1.07                     | 0.92              |
| 1:B:438:LEU:HD13 | 1:B:655:PHE:CD1  | 2.06                     | 0.90              |
| 1:B:370:ARG:HG3  | 1:B:370:ARG:HH11 | 1.38                     | 0.89              |
| 1:B:169:ASN:HD21 | 1:B:668:GLY:HA3  | 1.39                     | 0.88              |
| 2:C:183:ALA:HB3  | 2:C:189:MET:HE1  | 1.55                     | 0.87              |
| 4:R:438:MET:CE   | 4:R:447:ALA:HA   | 2.05                     | 0.86              |
| 2:H:182:LEU:HB3  | 2:H:196:TYR:HE2  | 1.41                     | 0.85              |
| 4:S:233:PRO:HG2  | 4:S:404:HIS:CD2  | 2.13                     | 0.83              |
| 3:P:112:ASN:OD1  | 3:P:147:ASP:HB3  | 1.78                     | 0.83              |
| 2:H:193:ARG:HB2  | 2:H:196:TYR:HE1  | 1.42                     | 0.82              |
| 4:T:21:THR:HG22  | 4:T:27:VAL:HB    | 1.61                     | 0.82              |
| 4:T:517:HIS:HD2  | 4:T:519:LEU:HD23 | 1.40                     | 0.82              |
| 4:R:256:ARG:CZ   | 4:R:459:ARG:HH21 | 1.92                     | 0.81              |
| 4:S:233:PRO:HG2  | 4:S:404:HIS:HD2  | 1.43                     | 0.81              |
| 4:R:50:MET:SD    | 4:S:50:MET:HE1   | 2.21                     | 0.81              |
| 4:S:233:PRO:CG   | 4:S:404:HIS:CD2  | 2.62                     | 0.81              |
| 4:T:258:HIS:HE1  | 4:T:356:GLN:NE2  | 1.79                     | 0.80              |
| 2:M:268:TYR:HD1  | 2:M:277:VAL:HG21 | 1.45                     | 0.80              |
| 2:M:168:ILE:HD12 | 2:M:268:TYR:HE2  | 1.46                     | 0.80              |
| 4:T:15:ASN:HD22  | 4:T:371:MET:HG2  | 1.45                     | 0.80              |
| 2:D:251:ILE:O    | 2:D:254:VAL:HG12 | 1.82                     | 0.80              |
| 2:H:168:ILE:HG21 | 2:H:268:TYR:CD2  | 2.17                     | 0.79              |
| 2:K:182:LEU:HD12 | 2:K:207:VAL:HG22 | 1.65                     | 0.79              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:T:368:ALA:HA   | 4:T:371:MET:HE3  | 1.65                     | 0.79              |
| 2:C:168:ILE:HG23 | 2:C:268:TYR:CE2  | 2.18                     | 0.78              |
| 2:J:168:ILE:HD12 | 2:J:268:TYR:CE2  | 2.19                     | 0.78              |
| 2:M:272:ASP:OD2  | 2:M:275:ASN:HB3  | 1.83                     | 0.78              |
| 2:J:168:ILE:HD12 | 2:J:268:TYR:HE2  | 1.46                     | 0.78              |
| 4:T:81:ALA:CB    | 4:T:527:LYS:HE3  | 2.13                     | 0.78              |
| 2:N:199:ARG:NH2  | 2:N:201:LEU:HD23 | 1.98                     | 0.78              |
| 2:C:168:ILE:HD13 | 2:C:269:HIS:CD2  | 2.19                     | 0.77              |
| 2:K:168:ILE:HG21 | 2:K:268:TYR:CD2  | 2.20                     | 0.77              |
| 4:R:44:ASN:HB3   | 4:R:47:GLU:HB2   | 1.65                     | 0.76              |
| 3:Q:241:THR:HG23 | 3:Q:243:TYR:H    | 1.51                     | 0.76              |
| 2:N:136:ARG:HE   | 2:N:155:GLY:HA2  | 1.50                     | 0.76              |
| 4:S:322:ASN:OD1  | 4:S:322:ASN:O    | 2.04                     | 0.76              |
| 1:B:438:LEU:CD1  | 1:B:655:PHE:CD1  | 2.68                     | 0.76              |
| 1:A:720:ILE:HD11 | 1:A:753:LEU:HD12 | 1.68                     | 0.76              |
| 2:E:268:TYR:CD1  | 2:E:277:VAL:HG21 | 2.21                     | 0.76              |
| 4:R:553:LYS:HD2  | 4:R:596:PHE:HB3  | 1.67                     | 0.76              |
| 4:S:536:VAL:HG12 | 4:S:542:THR:HB   | 1.68                     | 0.75              |
| 2:J:274:ILE:O    | 2:J:277:VAL:HG12 | 1.86                     | 0.75              |
| 2:L:223:THR:HG21 | 2:L:265:ILE:HD11 | 1.66                     | 0.75              |
| 4:T:457:ASP:OD2  | 4:T:458:LEU:N    | 2.20                     | 0.74              |
| 2:L:81:ALA:O     | 2:L:85:VAL:HG23  | 1.88                     | 0.74              |
| 2:I:168:ILE:CG1  | 2:I:268:TYR:CD2  | 2.70                     | 0.74              |
| 2:J:168:ILE:HG21 | 2:J:268:TYR:CD2  | 2.22                     | 0.74              |
| 4:R:189:VAL:HG22 | 4:R:209:ILE:HD11 | 1.70                     | 0.74              |
| 4:T:256:ARG:NH2  | 4:T:485:PRO:O    | 2.20                     | 0.74              |
| 4:T:534:LEU:HD12 | 4:T:542:THR:HG21 | 1.68                     | 0.74              |
| 1:B:437:ARG:HD2  | 1:B:472:MET:HE3  | 1.68                     | 0.74              |
| 4:R:50:MET:CE    | 4:T:46:ARG:NH2   | 2.51                     | 0.74              |
| 1:B:169:ASN:ND2  | 1:B:668:GLY:HA3  | 2.02                     | 0.73              |
| 4:S:361:LEU:HD13 | 4:S:400:MET:SD   | 2.28                     | 0.73              |
| 3:P:63:GLY:HA2   | 4:T:286:TYR:OH   | 1.89                     | 0.73              |
| 4:R:438:MET:HE1  | 4:R:450:HIS:HB2  | 1.70                     | 0.73              |
| 4:S:74:SER:HB3   | 5:s:5:THR:HG23   | 1.69                     | 0.73              |
| 4:T:210:ILE:HG21 | 4:T:212:GLN:HG2  | 1.70                     | 0.73              |
| 4:R:294:ILE:HG23 | 4:R:351:THR:HG21 | 1.71                     | 0.72              |
| 2:C:183:ALA:HB3  | 2:C:189:MET:HE2  | 1.72                     | 0.72              |
| 2:H:181:GLN:NE2  | 2:H:190:PRO:O    | 2.22                     | 0.72              |
| 2:C:168:ILE:HG21 | 2:C:268:TYR:CD2  | 2.24                     | 0.71              |
| 2:F:262:GLU:OE1  | 2:G:175:LYS:NZ   | 2.23                     | 0.71              |
| 4:T:143:THR:HB   | 4:T:146:GLU:HG2  | 1.73                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:168:ILE:HG21 | 2:G:268:TYR:CD2  | 2.26                     | 0.71              |
| 3:Q:244:GLY:O    | 3:Q:245:LYS:HG3  | 1.90                     | 0.71              |
| 1:B:868:VAL:HG21 | 1:B:905:GLU:HG2  | 1.73                     | 0.70              |
| 4:T:64:SER:OG    | 4:T:67:GLN:HB2   | 1.91                     | 0.70              |
| 4:R:236:VAL:HG13 | 4:R:237:VAL:HG13 | 1.74                     | 0.70              |
| 1:B:458:GLN:HG3  | 1:B:639:ILE:O    | 1.92                     | 0.70              |
| 2:N:183:ALA:HB3  | 2:N:189:MET:HE2  | 1.74                     | 0.70              |
| 2:O:251:ILE:HG22 | 2:O:252:GLN:N    | 2.08                     | 0.69              |
| 4:R:51:LYS:HE2   | 4:R:386:ASN:CG   | 2.17                     | 0.69              |
| 2:N:199:ARG:HH22 | 2:N:201:LEU:HD23 | 1.57                     | 0.69              |
| 4:R:189:VAL:CG2  | 4:R:209:ILE:HD11 | 2.23                     | 0.68              |
| 4:R:457:ASP:HB3  | 4:R:460:ASN:HB2  | 1.75                     | 0.68              |
| 1:B:561:PHE:HB3  | 1:B:610:THR:HG23 | 1.74                     | 0.68              |
| 2:I:15:PRO:HA    | 2:I:276:ARG:HH21 | 1.57                     | 0.68              |
| 4:R:517:HIS:ND1  | 4:R:615:TRP:CZ3  | 2.62                     | 0.68              |
| 2:H:182:LEU:HB3  | 2:H:196:TYR:CD2  | 2.28                     | 0.68              |
| 2:C:151:MET:HE3  | 2:C:161:ILE:HD12 | 1.74                     | 0.68              |
| 4:S:63:ARG:NH2   | 4:S:176:VAL:O    | 2.26                     | 0.67              |
| 4:S:74:SER:HB2   | 5:s:8:ARG:HH21   | 1.60                     | 0.67              |
| 2:J:66:ASN:OD1   | 2:J:67:PRO:HD2   | 1.94                     | 0.67              |
| 4:R:187:ILE:CG2  | 4:R:209:ILE:HG12 | 2.25                     | 0.67              |
| 4:R:423:MET:HE3  | 4:R:427:LEU:HD11 | 1.74                     | 0.67              |
| 2:H:167:GLN:HG2  | 2:H:201:LEU:HD12 | 1.76                     | 0.67              |
| 2:K:168:ILE:HG21 | 2:K:268:TYR:CE2  | 2.30                     | 0.67              |
| 2:K:179:PRO:HG3  | 2:K:194:PHE:CE2  | 2.30                     | 0.67              |
| 4:S:294:ILE:HG23 | 4:S:351:THR:HG21 | 1.76                     | 0.67              |
| 1:A:749:TYR:CE2  | 1:A:753:LEU:HD11 | 2.30                     | 0.67              |
| 4:T:142:ILE:HD12 | 4:T:146:GLU:HB2  | 1.76                     | 0.67              |
| 2:H:193:ARG:HB2  | 2:H:196:TYR:CE1  | 2.28                     | 0.66              |
| 4:R:189:VAL:HG22 | 4:R:209:ILE:CD1  | 2.25                     | 0.66              |
| 4:S:233:PRO:HG3  | 4:S:404:HIS:HD2  | 1.57                     | 0.66              |
| 2:M:168:ILE:HD12 | 2:M:268:TYR:CE2  | 2.29                     | 0.66              |
| 4:S:489:TYR:HA   | 4:S:536:VAL:HG23 | 1.76                     | 0.66              |
| 4:R:256:ARG:CZ   | 4:R:459:ARG:NH2  | 2.58                     | 0.66              |
| 2:C:271:GLN:OE1  | 2:C:271:GLN:N    | 2.25                     | 0.66              |
| 2:I:13:PRO:HG2   | 2:I:270:ALA:HB2  | 1.78                     | 0.66              |
| 2:L:64:ASP:OD1   | 2:L:109:LYS:CE   | 2.43                     | 0.66              |
| 2:L:78:MET:HE1   | 2:L:109:LYS:HD3  | 1.76                     | 0.66              |
| 4:S:69:MET:HE3   | 4:T:470:LYS:HD3  | 1.78                     | 0.66              |
| 1:A:801:VAL:HG12 | 1:A:822:ILE:CD1  | 2.26                     | 0.66              |
| 2:F:168:ILE:HG21 | 2:F:268:TYR:CD2  | 2.30                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:T:205:LYS:HE2  | 4:T:446:ILE:HG12 | 1.77                     | 0.65              |
| 3:Q:86:ILE:HB    | 3:Q:89:ILE:HD11  | 1.77                     | 0.65              |
| 4:S:221:GLN:NE2  | 4:S:350:GLN:OE1  | 2.29                     | 0.65              |
| 2:K:116:MET:HE2  | 2:K:282:ILE:HG12 | 1.79                     | 0.64              |
| 2:C:168:ILE:CG2  | 2:C:268:TYR:CE2  | 2.81                     | 0.64              |
| 2:J:168:ILE:HG23 | 2:J:268:TYR:CE2  | 2.33                     | 0.64              |
| 2:D:274:ILE:O    | 2:D:277:VAL:HG12 | 1.97                     | 0.64              |
| 2:D:267:GLN:HE21 | 2:D:276:ARG:HD3  | 1.63                     | 0.63              |
| 2:E:161:ILE:HD11 | 2:E:209:LEU:HD22 | 1.80                     | 0.63              |
| 4:T:46:ARG:HG3   | 4:T:46:ARG:HH11  | 1.64                     | 0.63              |
| 2:O:168:ILE:HG12 | 2:O:268:TYR:CD2  | 2.33                     | 0.63              |
| 2:J:139:VAL:HG22 | 2:J:151:MET:HG2  | 1.80                     | 0.63              |
| 4:R:46:ARG:HH12  | 4:R:50:MET:HB2   | 1.61                     | 0.63              |
| 2:C:168:ILE:HG12 | 2:C:268:TYR:CD2  | 2.34                     | 0.63              |
| 4:S:391:PRO:HD2  | 4:S:400:MET:HE1  | 1.81                     | 0.63              |
| 2:M:168:ILE:HG21 | 2:M:268:TYR:CD2  | 2.34                     | 0.63              |
| 2:I:229:LEU:HD11 | 2:K:40:ILE:CD1   | 2.29                     | 0.62              |
| 2:E:119:SER:HB2  | 2:E:229:LEU:CD2  | 2.26                     | 0.62              |
| 3:P:118:ILE:H    | 3:P:118:ILE:HD12 | 1.64                     | 0.62              |
| 1:B:299:GLN:HG3  | 1:B:929:MET:HE1  | 1.80                     | 0.62              |
| 2:E:118:ASN:HB3  | 2:E:229:LEU:HG   | 1.81                     | 0.62              |
| 2:K:168:ILE:CG2  | 2:K:268:TYR:CE2  | 2.82                     | 0.62              |
| 2:L:78:MET:HE1   | 2:L:109:LYS:CD   | 2.29                     | 0.62              |
| 4:R:501:LEU:HD13 | 5:t:9:ALA:HB3    | 1.81                     | 0.62              |
| 1:A:605:ALA:O    | 1:A:609:LYS:HG2  | 2.00                     | 0.62              |
| 1:B:370:ARG:HG3  | 1:B:370:ARG:NH1  | 2.08                     | 0.62              |
| 2:L:184:ARG:HD3  | 2:L:202:ASP:HB3  | 1.82                     | 0.62              |
| 1:B:587:PHE:O    | 1:B:593:ASN:ND2  | 2.32                     | 0.62              |
| 4:T:96:THR:HG22  | 4:T:209:ILE:HG22 | 1.82                     | 0.62              |
| 3:P:41:ARG:NH1   | 3:P:201:LEU:O    | 2.31                     | 0.61              |
| 4:S:74:SER:CB    | 5:s:5:THR:HG22   | 2.21                     | 0.61              |
| 1:A:730:ILE:HD12 | 1:A:734:MET:HE2  | 1.82                     | 0.61              |
| 2:F:22:ASP:OD1   | 2:F:22:ASP:N     | 2.33                     | 0.61              |
| 4:R:489:TYR:HA   | 4:R:536:VAL:HG23 | 1.82                     | 0.61              |
| 2:C:168:ILE:HG12 | 2:C:268:TYR:HD2  | 1.66                     | 0.61              |
| 2:O:223:THR:HG21 | 2:O:265:ILE:CD1  | 2.31                     | 0.61              |
| 4:R:480:GLU:HB3  | 4:R:553:LYS:NZ   | 2.16                     | 0.61              |
| 4:R:500:THR:HG21 | 4:R:505:THR:HG21 | 1.83                     | 0.61              |
| 1:A:810:ARG:HB2  | 1:A:895:GLU:HB2  | 1.83                     | 0.61              |
| 2:G:78:MET:HE3   | 2:G:106:LEU:HB3  | 1.81                     | 0.61              |
| 2:I:168:ILE:HG13 | 2:I:268:TYR:CE2  | 2.35                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:136:ARG:HD2  | 2:H:155:GLY:HA3  | 1.81                     | 0.60              |
| 2:J:78:MET:HE3   | 2:J:106:LEU:HB3  | 1.83                     | 0.60              |
| 2:J:181:GLN:NE2  | 2:J:190:PRO:O    | 2.33                     | 0.60              |
| 2:D:102:GLU:OE2  | 2:D:105:ARG:NH2  | 2.32                     | 0.60              |
| 4:T:251:ILE:HG12 | 4:T:408:THR:HG21 | 1.83                     | 0.60              |
| 2:K:182:LEU:HD12 | 2:K:207:VAL:CG2  | 2.30                     | 0.60              |
| 2:C:168:ILE:CG2  | 2:C:268:TYR:CD2  | 2.84                     | 0.59              |
| 2:C:184:ARG:HD3  | 2:C:202:ASP:HB3  | 1.84                     | 0.59              |
| 2:J:168:ILE:CG2  | 2:J:268:TYR:CD2  | 2.85                     | 0.59              |
| 1:B:897:ARG:HH12 | 1:B:903:ARG:HD3  | 1.67                     | 0.59              |
| 2:I:229:LEU:HD11 | 2:K:40:ILE:HD13  | 1.84                     | 0.59              |
| 4:T:99:GLN:NE2   | 4:T:187:ILE:HD13 | 2.07                     | 0.59              |
| 1:B:494:TYR:OH   | 1:B:533:VAL:O    | 2.20                     | 0.59              |
| 2:L:145:ASP:OD1  | 2:L:146:ARG:N    | 2.34                     | 0.59              |
| 2:L:146:ARG:NH1  | 2:L:148:ASP:OD1  | 2.34                     | 0.59              |
| 2:L:85:VAL:HG12  | 2:L:89:TYR:CE1   | 2.36                     | 0.59              |
| 1:B:385:LEU:HD12 | 1:B:635:SER:OG   | 2.03                     | 0.59              |
| 1:A:791:GLU:HG2  | 1:A:818:LEU:HD12 | 1.84                     | 0.59              |
| 4:R:438:MET:HE2  | 4:R:447:ALA:CA   | 2.27                     | 0.59              |
| 2:L:223:THR:HG21 | 2:L:265:ILE:CD1  | 2.33                     | 0.59              |
| 4:T:493:ASP:OD1  | 4:T:533:GLU:HG2  | 2.02                     | 0.59              |
| 1:A:460:ARG:NH1  | 1:A:490:SER:CB   | 2.65                     | 0.58              |
| 4:T:517:HIS:CD2  | 4:T:519:LEU:CD2  | 2.82                     | 0.58              |
| 1:B:232:LEU:HD23 | 1:B:775:ILE:CG2  | 2.33                     | 0.58              |
| 2:G:115:ASP:OD1  | 2:G:115:ASP:N    | 2.37                     | 0.58              |
| 2:H:168:ILE:HG21 | 2:H:268:TYR:CE2  | 2.38                     | 0.58              |
| 3:Q:57:ASP:OD1   | 3:Q:204:ARG:HG2  | 2.02                     | 0.58              |
| 2:I:274:ILE:O    | 2:I:277:VAL:HG12 | 2.03                     | 0.58              |
| 4:S:60:ASP:HB2   | 4:T:61:LEU:HD21  | 1.85                     | 0.58              |
| 2:O:145:ASP:OD1  | 2:O:146:ARG:N    | 2.36                     | 0.58              |
| 3:P:93:LEU:HD21  | 3:P:109:LEU:HD13 | 1.86                     | 0.58              |
| 4:R:51:LYS:HE2   | 4:R:386:ASN:OD1  | 2.03                     | 0.58              |
| 4:S:497:VAL:HG22 | 4:S:528:PRO:HA   | 1.85                     | 0.58              |
| 2:G:26:ARG:HD2   | 2:G:116:MET:HG3  | 1.85                     | 0.58              |
| 2:N:168:ILE:HG21 | 2:N:268:TYR:CD2  | 2.38                     | 0.58              |
| 3:Q:244:GLY:O    | 3:Q:245:LYS:CG   | 2.50                     | 0.58              |
| 4:T:117:GLU:HB3  | 4:T:227:PRO:HG3  | 1.85                     | 0.58              |
| 1:A:801:VAL:HG12 | 1:A:822:ILE:HD11 | 1.85                     | 0.57              |
| 4:R:525:GLN:HB3  | 4:R:526:HIS:ND1  | 2.18                     | 0.57              |
| 4:R:390:GLU:HG2  | 4:R:400:MET:HE1  | 1.86                     | 0.57              |
| 4:T:565:LYS:NZ   | 5:t:4:GLU:OE1    | 2.37                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:Q:226:ARG:O    | 3:Q:229:SER:OG   | 2.20                     | 0.57              |
| 4:T:322:ASN:OD1  | 4:T:322:ASN:O    | 2.23                     | 0.57              |
| 4:T:496:VAL:HG22 | 4:T:566:VAL:HG22 | 1.85                     | 0.57              |
| 2:L:229:LEU:O    | 2:N:44:ARG:NH1   | 2.38                     | 0.57              |
| 1:B:330:GLN:HB3  | 1:B:767:PRO:HB3  | 1.86                     | 0.57              |
| 1:B:239:ASP:OD1  | 1:B:239:ASP:N    | 2.36                     | 0.57              |
| 1:B:561:PHE:HB3  | 1:B:610:THR:CG2  | 2.34                     | 0.57              |
| 2:H:145:ASP:OD1  | 2:H:145:ASP:N    | 2.34                     | 0.57              |
| 2:O:251:ILE:CG2  | 2:O:252:GLN:N    | 2.68                     | 0.57              |
| 4:T:455:PHE:O    | 4:T:461:THR:OG1  | 2.22                     | 0.57              |
| 2:H:168:ILE:CG2  | 2:H:268:TYR:CE2  | 2.88                     | 0.56              |
| 2:J:187:GLN:HG3  | 2:J:188:PRO:HD2  | 1.88                     | 0.56              |
| 3:P:118:ILE:HG23 | 3:P:121:ARG:HH12 | 1.70                     | 0.56              |
| 3:P:174:ASP:OD2  | 3:P:176:ARG:NH1  | 2.38                     | 0.56              |
| 4:R:505:THR:OG1  | 4:R:525:GLN:OE1  | 2.20                     | 0.56              |
| 2:G:131:VAL:HG11 | 2:G:139:VAL:HG11 | 1.87                     | 0.56              |
| 2:I:168:ILE:CG1  | 2:I:268:TYR:CE2  | 2.88                     | 0.56              |
| 4:R:614:THR:OG1  | 4:R:616:ASP:OD1  | 2.23                     | 0.56              |
| 1:B:667:ILE:HD12 | 1:B:672:LYS:CD   | 2.35                     | 0.56              |
| 4:R:517:HIS:ND1  | 4:R:615:TRP:CH2  | 2.74                     | 0.56              |
| 2:E:136:ARG:HH12 | 2:E:155:GLY:HA2  | 1.69                     | 0.56              |
| 4:R:442:ASP:HB2  | 4:R:446:ILE:HD12 | 1.87                     | 0.56              |
| 1:A:239:ASP:OD1  | 1:A:239:ASP:N    | 2.33                     | 0.56              |
| 4:R:57:ILE:HD11  | 4:S:58:GLU:HG3   | 1.88                     | 0.56              |
| 4:R:230:VAL:HG12 | 4:R:248:LEU:HD23 | 1.88                     | 0.56              |
| 4:R:500:THR:HG22 | 4:R:502:ASN:H    | 1.71                     | 0.56              |
| 4:S:533:GLU:N    | 4:S:533:GLU:OE1  | 2.39                     | 0.56              |
| 1:B:842:ASP:OD1  | 1:B:843:ASP:N    | 2.38                     | 0.56              |
| 2:D:258:SER:OG   | 2:D:262:GLU:OE2  | 2.24                     | 0.56              |
| 2:G:245:ASN:ND2  | 2:H:170:GLU:OE1  | 2.39                     | 0.56              |
| 2:O:223:THR:HG21 | 2:O:265:ILE:HD11 | 1.88                     | 0.56              |
| 4:T:538:ASP:O    | 4:T:578:VAL:HG12 | 2.06                     | 0.56              |
| 2:N:20:TYR:O     | 2:N:89:TYR:OH    | 2.22                     | 0.55              |
| 2:N:146:ARG:NH1  | 2:N:148:ASP:OD1  | 2.39                     | 0.55              |
| 2:N:169:ALA:HB3  | 2:N:200:PRO:HG2  | 1.88                     | 0.55              |
| 4:S:122:ILE:HG23 | 4:S:245:ILE:HD12 | 1.89                     | 0.55              |
| 2:J:241:GLN:HB2  | 2:K:122:ILE:HD13 | 1.88                     | 0.55              |
| 2:K:12:ASN:O     | 2:K:255:ASN:ND2  | 2.39                     | 0.55              |
| 4:R:565:LYS:NZ   | 5:r:4:GLU:OE1    | 2.37                     | 0.55              |
| 4:S:459:ARG:HA   | 4:S:568:ARG:HH12 | 1.72                     | 0.55              |
| 1:B:438:LEU:CD1  | 1:B:655:PHE:CE1  | 2.89                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:132:LEU:HB2  | 2:G:162:THR:HB   | 1.89                     | 0.55              |
| 1:A:737:ILE:O    | 1:A:740:ILE:HG22 | 2.06                     | 0.55              |
| 2:K:268:TYR:CD1  | 2:K:277:VAL:HG21 | 2.42                     | 0.55              |
| 4:T:315:ASN:HD22 | 4:T:331:THR:HG21 | 1.71                     | 0.55              |
| 2:F:168:ILE:HG23 | 2:F:268:TYR:CE2  | 2.42                     | 0.55              |
| 2:G:62:PHE:CZ    | 2:G:293:MET:SD   | 3.00                     | 0.55              |
| 2:G:134:PRO:HG2  | 2:G:159:ALA:HB1  | 1.89                     | 0.55              |
| 2:N:26:ARG:HD2   | 2:N:116:MET:HG2  | 1.88                     | 0.55              |
| 2:M:134:PRO:O    | 2:M:137:THR:OG1  | 2.24                     | 0.55              |
| 3:P:2:ASP:OD1    | 3:P:3:VAL:N      | 2.39                     | 0.55              |
| 4:S:93:ASP:OD1   | 4:S:93:ASP:N     | 2.37                     | 0.55              |
| 1:B:667:ILE:HD12 | 1:B:672:LYS:HD2  | 1.88                     | 0.55              |
| 1:B:838:MET:SD   | 1:B:844:VAL:HG21 | 2.47                     | 0.55              |
| 4:T:501:LEU:HD21 | 5:s:6:GLU:HG2    | 1.88                     | 0.55              |
| 4:T:205:LYS:CE   | 4:T:446:ILE:HG23 | 2.37                     | 0.54              |
| 4:T:498:VAL:HG22 | 4:T:564:VAL:HG22 | 1.88                     | 0.54              |
| 4:S:473:ILE:HD11 | 4:S:599:ASN:HD22 | 1.71                     | 0.54              |
| 4:S:509:CYS:HB2  | 4:S:520:ILE:HG12 | 1.90                     | 0.54              |
| 4:T:365:LEU:HD22 | 4:T:377:LEU:HD23 | 1.89                     | 0.54              |
| 1:A:730:ILE:HD12 | 1:A:734:MET:CE   | 2.38                     | 0.54              |
| 1:A:784:SER:HB3  | 1:A:919:PRO:HA   | 1.88                     | 0.54              |
| 2:I:250:ASP:OD1  | 2:I:250:ASP:O    | 2.26                     | 0.54              |
| 1:B:561:PHE:CB   | 1:B:610:THR:HG23 | 2.37                     | 0.54              |
| 1:B:393:PHE:O    | 1:B:397:MET:HG2  | 2.07                     | 0.54              |
| 2:E:50:ASN:OD1   | 2:F:68:ARG:NH2   | 2.41                     | 0.54              |
| 4:R:502:ASN:O    | 5:r:11:LYS:NZ    | 2.41                     | 0.54              |
| 4:S:41:VAL:HG21  | 4:S:387:LEU:HD13 | 1.90                     | 0.54              |
| 1:A:928:TYR:CE1  | 1:A:929:MET:HE2  | 2.43                     | 0.54              |
| 1:B:766:GLU:HG2  | 1:B:768:VAL:HG12 | 1.90                     | 0.54              |
| 2:C:136:ARG:CZ   | 2:C:155:GLY:HA2  | 2.38                     | 0.53              |
| 2:N:136:ARG:NH2  | 2:N:154:THR:O    | 2.41                     | 0.53              |
| 4:R:98:HIS:CE1   | 4:R:102:ARG:HD2  | 2.43                     | 0.53              |
| 4:R:274:ASN:N    | 4:R:274:ASN:OD1  | 2.41                     | 0.53              |
| 4:T:316:VAL:O    | 4:T:331:THR:HG23 | 2.08                     | 0.53              |
| 4:R:209:ILE:HD12 | 4:R:210:ILE:O    | 2.09                     | 0.53              |
| 1:B:811:ASP:OD2  | 1:B:913:ARG:NH2  | 2.42                     | 0.53              |
| 2:E:125:SER:HB2  | 2:E:265:ILE:HG13 | 1.90                     | 0.53              |
| 4:R:89:GLU:OE2   | 4:R:89:GLU:N     | 2.33                     | 0.53              |
| 4:R:489:TYR:CE1  | 4:R:576:PRO:HB2  | 2.42                     | 0.53              |
| 1:B:599:LEU:O    | 1:B:603:LEU:HG   | 2.08                     | 0.53              |
| 2:C:201:LEU:HD21 | 2:G:201:LEU:HD13 | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:D:251:ILE:O    | 2:D:254:VAL:CG1  | 2.56                     | 0.53              |
| 2:L:26:ARG:HG2   | 2:L:282:ILE:HD11 | 1.91                     | 0.53              |
| 2:O:116:MET:HE2  | 2:O:282:ILE:HG12 | 1.90                     | 0.53              |
| 1:B:928:TYR:CE2  | 1:B:929:MET:HE2  | 2.44                     | 0.53              |
| 2:I:125:SER:HB2  | 2:I:265:ILE:HG13 | 1.89                     | 0.53              |
| 4:S:616:ASP:N    | 4:S:616:ASP:OD2  | 2.33                     | 0.53              |
| 1:A:680:GLU:HG3  | 1:A:733:THR:HG21 | 1.90                     | 0.53              |
| 2:E:12:ASN:O     | 2:E:255:ASN:ND2  | 2.41                     | 0.53              |
| 4:T:24:ASP:OD1   | 4:T:24:ASP:N     | 2.42                     | 0.53              |
| 4:T:205:LYS:HE2  | 4:T:446:ILE:CG1  | 2.39                     | 0.53              |
| 1:A:498:LEU:HA   | 1:A:501:MET:HE2  | 1.90                     | 0.53              |
| 1:B:109:PHE:CB   | 1:B:123:LYS:HG2  | 2.38                     | 0.53              |
| 4:R:520:ILE:HD11 | 4:R:531:ILE:HG22 | 1.90                     | 0.53              |
| 4:S:230:VAL:O    | 4:S:233:PRO:HD2  | 2.08                     | 0.53              |
| 2:E:118:ASN:CB   | 2:E:229:LEU:HG   | 2.38                     | 0.53              |
| 2:D:223:THR:HG21 | 2:D:265:ILE:HD11 | 1.91                     | 0.53              |
| 2:G:56:VAL:O     | 2:G:60:SER:OG    | 2.24                     | 0.53              |
| 4:S:74:SER:CB    | 5:s:5:THR:CG2    | 2.75                     | 0.53              |
| 2:D:130:GLU:HG3  | 2:D:164:ASN:HB3  | 1.91                     | 0.52              |
| 2:H:123:PHE:HE2  | 2:H:225:ILE:HB   | 1.74                     | 0.52              |
| 2:O:251:ILE:HG22 | 2:O:252:GLN:H    | 1.75                     | 0.52              |
| 2:L:68:ARG:HD2   | 2:L:71:ARG:HD2   | 1.90                     | 0.52              |
| 2:D:31:VAL:HG12  | 2:D:78:MET:HE1   | 1.91                     | 0.52              |
| 2:H:195:THR:C    | 2:H:196:TYR:HD1  | 2.17                     | 0.52              |
| 2:I:62:PHE:CZ    | 2:I:293:MET:SD   | 3.02                     | 0.52              |
| 3:Q:130:CYS:SG   | 3:Q:134:LYS:HE3  | 2.50                     | 0.52              |
| 4:R:143:THR:HG21 | 4:R:394:LEU:HD12 | 1.91                     | 0.52              |
| 4:R:457:ASP:OD1  | 4:R:458:LEU:N    | 2.42                     | 0.52              |
| 4:T:600:ILE:HG13 | 4:T:602:PRO:HD3  | 1.91                     | 0.52              |
| 2:E:168:ILE:HG21 | 2:E:268:TYR:CD2  | 2.44                     | 0.52              |
| 2:F:145:ASP:OD1  | 2:F:146:ARG:N    | 2.43                     | 0.52              |
| 2:H:66:ASN:OD1   | 2:H:67:PRO:HD2   | 2.10                     | 0.52              |
| 2:I:244:MET:SD   | 2:J:173:ILE:HD11 | 2.50                     | 0.52              |
| 1:B:144:GLU:OE2  | 1:B:146:GLN:HG2  | 2.09                     | 0.52              |
| 2:E:183:ALA:HB3  | 2:E:189:MET:HE2  | 1.91                     | 0.52              |
| 4:T:487:ALA:C    | 4:T:578:VAL:HG22 | 2.34                     | 0.52              |
| 2:M:46:SER:HB3   | 2:M:54:PRO:HG2   | 1.92                     | 0.52              |
| 4:R:351:THR:HG22 | 4:R:385:ILE:CG2  | 2.40                     | 0.52              |
| 2:N:126:VAL:O    | 2:N:126:VAL:HG13 | 2.10                     | 0.52              |
| 4:T:391:PRO:HD2  | 4:T:400:MET:HE1  | 1.92                     | 0.52              |
| 4:R:46:ARG:NH1   | 4:R:50:MET:HB2   | 2.25                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:T:487:ALA:O    | 4:T:578:VAL:HG22 | 2.10                     | 0.52              |
| 2:F:100:GLN:HG2  | 3:P:131:GLU:OE1  | 2.10                     | 0.52              |
| 2:G:274:ILE:H    | 2:G:274:ILE:HD12 | 1.74                     | 0.52              |
| 2:M:31:VAL:HG22  | 2:M:110:ALA:HB3  | 1.91                     | 0.52              |
| 2:O:251:ILE:CG2  | 2:O:252:GLN:H    | 2.23                     | 0.52              |
| 1:A:397:MET:HG2  | 1:A:448:ALA:HB1  | 1.92                     | 0.52              |
| 1:B:175:GLU:OE1  | 1:B:177:LYS:NZ   | 2.43                     | 0.52              |
| 2:M:168:ILE:HG23 | 2:M:268:TYR:CE2  | 2.45                     | 0.51              |
| 2:O:130:GLU:HG3  | 2:O:164:ASN:HB3  | 1.91                     | 0.51              |
| 4:T:43:ALA:HA    | 4:T:277:MET:HE1  | 1.92                     | 0.51              |
| 2:I:294:ARG:NH1  | 2:I:297:LEU:O    | 2.43                     | 0.51              |
| 2:K:126:VAL:O    | 2:K:126:VAL:HG13 | 2.10                     | 0.51              |
| 4:T:205:LYS:HE2  | 4:T:446:ILE:HG23 | 1.93                     | 0.51              |
| 2:M:145:ASP:OD1  | 2:M:145:ASP:N    | 2.38                     | 0.51              |
| 4:R:232:LYS:HB2  | 4:R:233:PRO:HD3  | 1.92                     | 0.51              |
| 4:S:82:LEU:HD23  | 4:S:84:LEU:HD21  | 1.92                     | 0.51              |
| 4:T:518:LEU:HD23 | 4:T:520:ILE:HD11 | 1.93                     | 0.51              |
| 4:T:294:ILE:HG23 | 4:T:351:THR:HG21 | 1.93                     | 0.51              |
| 2:G:51:SER:OG    | 2:G:53:VAL:HG23  | 2.10                     | 0.51              |
| 2:L:199:ARG:NH2  | 2:L:202:ASP:OD1  | 2.36                     | 0.51              |
| 2:O:235:LEU:HD12 | 2:O:288:GLN:HE21 | 1.76                     | 0.51              |
| 4:T:205:LYS:HE2  | 4:T:446:ILE:CG2  | 2.41                     | 0.51              |
| 2:G:64:ASP:OD1   | 2:G:109:LYS:NZ   | 2.40                     | 0.51              |
| 2:N:4:ARG:HH11   | 2:N:130:GLU:HG3  | 1.74                     | 0.51              |
| 4:T:143:THR:HG22 | 4:T:145:ALA:H    | 1.76                     | 0.51              |
| 2:N:199:ARG:HG3  | 2:N:202:ASP:HB2  | 1.93                     | 0.51              |
| 4:R:284:THR:O    | 4:R:288:SER:OG   | 2.27                     | 0.51              |
| 2:G:61:LYS:O     | 2:G:109:LYS:NZ   | 2.43                     | 0.51              |
| 2:I:179:PRO:HD3  | 2:I:194:PHE:CZ   | 2.45                     | 0.51              |
| 1:A:452:LEU:HA   | 1:A:455:MET:HG2  | 1.93                     | 0.51              |
| 1:A:460:ARG:HH11 | 1:A:490:SER:HB3  | 1.76                     | 0.51              |
| 2:O:6:THR:OG1    | 2:O:129:VAL:O    | 2.26                     | 0.51              |
| 4:S:527:LYS:HG3  | 4:S:528:PRO:HD2  | 1.93                     | 0.51              |
| 1:A:463:MET:SD   | 1:A:465:TYR:CE1  | 3.04                     | 0.51              |
| 1:B:575:LEU:HD23 | 1:B:607:ARG:HD2  | 1.93                     | 0.51              |
| 2:H:126:VAL:HG13 | 2:H:126:VAL:O    | 2.11                     | 0.51              |
| 2:O:20:TYR:O     | 2:O:89:TYR:OH    | 2.27                     | 0.51              |
| 3:P:24:ALA:O     | 3:P:83:GLY:HA3   | 2.10                     | 0.51              |
| 4:T:514:ILE:HG13 | 4:T:549:HIS:NE2  | 2.26                     | 0.51              |
| 1:A:460:ARG:NH1  | 1:A:490:SER:HB2  | 2.25                     | 0.50              |
| 2:K:268:TYR:CE1  | 2:K:277:VAL:HG21 | 2.46                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:L:44:ARG:NH1   | 2:M:229:LEU:O    | 2.43                     | 0.50              |
| 4:S:608:THR:O    | 4:S:608:THR:HG22 | 2.11                     | 0.50              |
| 2:C:168:ILE:HD13 | 2:C:269:HIS:CG   | 2.46                     | 0.50              |
| 4:S:440:LYS:NZ   | 4:S:440:LYS:HB3  | 2.26                     | 0.50              |
| 1:A:801:VAL:HG12 | 1:A:822:ILE:HD13 | 1.92                     | 0.50              |
| 2:E:95:PRO:HB2   | 2:E:97:ILE:HG23  | 1.93                     | 0.50              |
| 2:N:168:ILE:HG23 | 2:N:268:TYR:CE2  | 2.46                     | 0.50              |
| 2:N:228:PRO:HG2  | 2:N:285:LEU:HD22 | 1.92                     | 0.50              |
| 4:R:467:LEU:HD21 | 4:R:481:TYR:HD1  | 1.76                     | 0.50              |
| 4:R:517:HIS:CE1  | 4:R:615:TRP:CZ3  | 3.00                     | 0.50              |
| 4:S:290:GLN:N    | 4:S:290:GLN:OE1  | 2.45                     | 0.50              |
| 2:C:126:VAL:O    | 2:C:126:VAL:HG13 | 2.10                     | 0.50              |
| 2:K:252:GLN:H    | 2:K:252:GLN:CD   | 2.18                     | 0.50              |
| 2:L:134:PRO:HG2  | 2:L:159:ALA:HB1  | 1.92                     | 0.50              |
| 2:O:189:MET:HE3  | 2:O:208:VAL:HG23 | 1.92                     | 0.50              |
| 4:R:264:LYS:HG2  | 4:R:427:LEU:HD13 | 1.92                     | 0.50              |
| 1:A:338:LEU:HD13 | 1:A:945:ILE:HD13 | 1.93                     | 0.50              |
| 1:A:953:THR:HG22 | 1:B:141:PHE:HB2  | 1.93                     | 0.50              |
| 2:E:34:LEU:HD22  | 2:E:112:VAL:HG11 | 1.94                     | 0.50              |
| 2:M:233:LYS:HE3  | 2:M:261:ASP:OD1  | 2.12                     | 0.50              |
| 4:R:346:LYS:HZ1  | 4:R:348:LYS:HE2  | 1.77                     | 0.50              |
| 4:S:88:GLN:HG2   | 4:S:573:ILE:HB   | 1.92                     | 0.50              |
| 4:S:626:ILE:HD12 | 4:S:627:LYS:H    | 1.77                     | 0.50              |
| 2:C:11:ASP:C     | 2:C:11:ASP:OD1   | 2.55                     | 0.50              |
| 4:R:521:GLU:HB2  | 4:R:610:LEU:HD11 | 1.93                     | 0.50              |
| 1:A:387:GLU:N    | 1:A:387:GLU:OE1  | 2.44                     | 0.50              |
| 3:Q:25:ILE:HG21  | 3:Q:89:ILE:HD13  | 1.94                     | 0.50              |
| 2:D:179:PRO:HG3  | 2:D:194:PHE:CE2  | 2.47                     | 0.50              |
| 2:E:136:ARG:NH1  | 2:E:155:GLY:HA2  | 2.27                     | 0.50              |
| 2:F:126:VAL:O    | 2:F:126:VAL:HG13 | 2.11                     | 0.50              |
| 2:L:183:ALA:HB2  | 2:L:190:PRO:HD3  | 1.92                     | 0.50              |
| 2:N:246:ASP:OD2  | 2:N:290:TYR:OH   | 2.30                     | 0.50              |
| 2:J:168:ILE:CG2  | 2:J:268:TYR:CE2  | 2.95                     | 0.49              |
| 2:K:23:GLU:OE2   | 3:Q:209:LYS:NZ   | 2.45                     | 0.49              |
| 4:R:319:GLN:O    | 4:R:322:ASN:ND2  | 2.45                     | 0.49              |
| 4:T:96:THR:CG2   | 4:T:209:ILE:HG22 | 2.41                     | 0.49              |
| 2:D:126:VAL:O    | 2:D:126:VAL:HG13 | 2.12                     | 0.49              |
| 2:M:272:ASP:CG   | 2:M:275:ASN:HB3  | 2.37                     | 0.49              |
| 3:Q:204:ARG:HG3  | 3:Q:204:ARG:HH11 | 1.77                     | 0.49              |
| 1:B:305:ASP:C    | 1:B:305:ASP:OD1  | 2.55                     | 0.49              |
| 2:L:187:GLN:OE1  | 2:L:187:GLN:N    | 2.44                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:O:168:ILE:HG12 | 2:O:268:TYR:HD2  | 1.75                     | 0.49              |
| 3:Q:244:GLY:C    | 3:Q:245:LYS:HG3  | 2.37                     | 0.49              |
| 4:R:281:VAL:HG23 | 4:R:344:GLY:HA2  | 1.94                     | 0.49              |
| 1:B:543:MET:HE1  | 1:B:625:ARG:HG2  | 1.94                     | 0.49              |
| 2:I:50:ASN:OD1   | 2:M:68:ARG:NH1   | 2.45                     | 0.49              |
| 4:T:95:ALA:O     | 4:T:99:GLN:HG2   | 2.12                     | 0.49              |
| 4:T:520:ILE:HD12 | 4:T:520:ILE:H    | 1.77                     | 0.49              |
| 4:T:527:LYS:HD2  | 4:T:528:PRO:HD2  | 1.95                     | 0.49              |
| 1:A:880:ASP:OD1  | 1:A:880:ASP:N    | 2.43                     | 0.49              |
| 1:B:200:ASN:OD1  | 1:B:200:ASN:N    | 2.39                     | 0.49              |
| 4:T:511:VAL:CG1  | 4:T:552:LEU:HD23 | 2.42                     | 0.49              |
| 2:L:179:PRO:HB2  | 2:L:192:ALA:HB1  | 1.92                     | 0.49              |
| 2:M:4:ARG:HG3    | 2:M:4:ARG:HH11   | 1.76                     | 0.49              |
| 2:J:87:ARG:NH1   | 3:P:38:LEU:O     | 2.46                     | 0.49              |
| 3:Q:95:ARG:HG3   | 3:Q:95:ARG:HH11  | 1.78                     | 0.49              |
| 4:S:466:LYS:NZ   | 4:S:563:SER:HB2  | 2.28                     | 0.49              |
| 4:S:520:ILE:HD12 | 4:S:522:LYS:NZ   | 2.28                     | 0.49              |
| 4:T:17:ILE:HD12  | 4:T:368:ALA:HB2  | 1.95                     | 0.49              |
| 2:C:136:ARG:NH2  | 2:C:155:GLY:HA2  | 2.28                     | 0.49              |
| 2:L:64:ASP:OD1   | 2:L:109:LYS:HE3  | 2.11                     | 0.49              |
| 4:S:268:VAL:HG21 | 4:S:427:LEU:HD22 | 1.94                     | 0.49              |
| 1:B:232:LEU:HD23 | 1:B:775:ILE:HG21 | 1.94                     | 0.49              |
| 3:P:114:LEU:HD13 | 3:P:119:ILE:HD11 | 1.94                     | 0.49              |
| 4:R:27:VAL:HG12  | 4:R:28:ALA:N     | 2.28                     | 0.49              |
| 4:S:531:ILE:HG22 | 4:S:532:LEU:HB2  | 1.95                     | 0.49              |
| 1:B:205:LEU:C    | 1:B:205:LEU:HD12 | 2.38                     | 0.48              |
| 1:B:866:ASP:OD1  | 1:B:867:GLY:N    | 2.45                     | 0.48              |
| 2:G:151:MET:HB2  | 2:G:151:MET:HE3  | 1.80                     | 0.48              |
| 2:N:102:GLU:OE2  | 2:N:105:ARG:NH1  | 2.46                     | 0.48              |
| 4:R:112:HIS:O    | 4:R:116:THR:HG23 | 2.13                     | 0.48              |
| 2:C:175:LYS:NZ   | 2:E:262:GLU:OE1  | 2.46                     | 0.48              |
| 3:Q:195:LEU:HD11 | 3:Q:212:LYS:HD2  | 1.96                     | 0.48              |
| 4:S:46:ARG:HH12  | 4:S:50:MET:HB2   | 1.78                     | 0.48              |
| 4:S:131:THR:HG21 | 4:S:154:VAL:HG21 | 1.94                     | 0.48              |
| 4:T:143:THR:HG22 | 4:T:144:ALA:N    | 2.27                     | 0.48              |
| 4:T:551:ARG:C    | 4:T:552:LEU:HD12 | 2.38                     | 0.48              |
| 2:G:126:VAL:HG13 | 2:G:126:VAL:O    | 2.13                     | 0.48              |
| 2:N:268:TYR:CD2  | 2:N:268:TYR:O    | 2.66                     | 0.48              |
| 4:S:254:ARG:HG2  | 4:S:254:ARG:HH11 | 1.79                     | 0.48              |
| 4:S:178:VAL:HG22 | 4:S:222:SER:HB3  | 1.94                     | 0.48              |
| 4:T:538:ASP:O    | 4:T:578:VAL:CG1  | 2.62                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:P:118:ILE:HG23 | 3:P:121:ARG:NH1  | 2.29                     | 0.48              |
| 4:R:37:MET:SD    | 4:R:38:PRO:HD2   | 2.53                     | 0.48              |
| 2:E:182:LEU:HD12 | 2:E:207:VAL:HG22 | 1.96                     | 0.48              |
| 2:M:168:ILE:CG2  | 2:M:268:TYR:CE2  | 2.97                     | 0.48              |
| 2:O:146:ARG:NH1  | 2:O:148:ASP:OD1  | 2.46                     | 0.48              |
| 3:P:13:LEU:HB3   | 3:P:246:LEU:HD21 | 1.96                     | 0.48              |
| 4:S:415:ASP:C    | 4:S:415:ASP:OD2  | 2.56                     | 0.48              |
| 4:T:210:ILE:CG2  | 4:T:212:GLN:CG   | 2.77                     | 0.48              |
| 2:C:170:GLU:OE2  | 2:E:245:ASN:ND2  | 2.47                     | 0.48              |
| 2:F:70:LEU:C     | 2:F:70:LEU:HD12  | 2.38                     | 0.48              |
| 2:G:62:PHE:CE2   | 2:G:293:MET:SD   | 3.07                     | 0.48              |
| 4:R:50:MET:HE3   | 4:T:46:ARG:HH22  | 1.79                     | 0.48              |
| 1:B:48:ARG:HG3   | 1:B:50:ASP:H     | 1.78                     | 0.48              |
| 2:K:146:ARG:NH1  | 2:K:148:ASP:OD1  | 2.45                     | 0.48              |
| 2:K:182:LEU:HD21 | 2:K:205:PHE:HB3  | 1.96                     | 0.48              |
| 1:B:437:ARG:HD2  | 1:B:472:MET:CE   | 2.40                     | 0.48              |
| 1:B:672:LYS:O    | 1:B:676:GLU:HG3  | 2.13                     | 0.48              |
| 2:M:130:GLU:HG3  | 2:M:164:ASN:HB3  | 1.95                     | 0.48              |
| 4:R:98:HIS:NE2   | 4:R:102:ARG:HD2  | 2.28                     | 0.48              |
| 4:S:119:THR:HG22 | 4:S:551:ARG:HH11 | 1.79                     | 0.48              |
| 4:S:120:ASP:O    | 4:S:124:ARG:HG2  | 2.14                     | 0.48              |
| 4:S:466:LYS:HZ3  | 4:S:563:SER:HB2  | 1.79                     | 0.48              |
| 1:A:319:MET:HE1  | 1:A:778:ARG:HD3  | 1.94                     | 0.47              |
| 1:B:114:ILE:HG23 | 1:B:119:ASP:HB2  | 1.96                     | 0.47              |
| 1:B:817:SER:HB3  | 2:G:105:ARG:HG3  | 1.94                     | 0.47              |
| 2:J:62:PHE:CZ    | 2:J:293:MET:SD   | 3.07                     | 0.47              |
| 3:Q:33:PRO:HA    | 3:Q:61:ARG:HD2   | 1.96                     | 0.47              |
| 4:R:106:ALA:HB1  | 4:R:178:VAL:CG1  | 2.43                     | 0.47              |
| 4:R:501:LEU:HD11 | 5:t:6:GLU:HA     | 1.96                     | 0.47              |
| 2:H:182:LEU:CB   | 2:H:196:TYR:CE2  | 2.85                     | 0.47              |
| 3:P:4:LEU:HD22   | 3:P:187:ILE:HD12 | 1.97                     | 0.47              |
| 4:S:359:LEU:O    | 4:S:363:MET:HG3  | 2.13                     | 0.47              |
| 4:T:277:MET:SD   | 4:T:292:TYR:CE2  | 3.06                     | 0.47              |
| 2:C:235:LEU:HD13 | 2:C:292:GLN:NE2  | 2.29                     | 0.47              |
| 2:K:88:SER:HA    | 2:K:94:ALA:HB3   | 1.96                     | 0.47              |
| 4:R:493:ASP:HB3  | 4:R:530:LYS:HZ1  | 1.78                     | 0.47              |
| 1:A:397:MET:HE2  | 1:A:397:MET:HB3  | 1.76                     | 0.47              |
| 1:B:232:LEU:HD23 | 1:B:775:ILE:HG23 | 1.94                     | 0.47              |
| 2:L:293:MET:HE2  | 2:L:293:MET:HB3  | 1.76                     | 0.47              |
| 4:S:467:LEU:HD11 | 4:S:481:TYR:HB2  | 1.96                     | 0.47              |
| 4:T:356:GLN:HG3  | 4:T:416:TRP:CZ2  | 2.49                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:792:ILE:HG22 | 1:A:916:ILE:HG22 | 1.97                     | 0.47              |
| 1:B:548:LEU:HD23 | 1:B:548:LEU:HA   | 1.78                     | 0.47              |
| 2:C:20:TYR:O     | 2:C:89:TYR:OH    | 2.26                     | 0.47              |
| 2:K:168:ILE:HG23 | 2:K:268:TYR:CE2  | 2.49                     | 0.47              |
| 4:R:526:HIS:HB3  | 5:r:8:ARG:HE     | 1.79                     | 0.47              |
| 1:A:837:MET:HE1  | 1:B:354:ARG:HD3  | 1.97                     | 0.47              |
| 2:L:223:THR:CG2  | 2:L:265:ILE:HD11 | 2.42                     | 0.47              |
| 3:P:125:VAL:HA   | 3:P:128:MET:HG3  | 1.95                     | 0.47              |
| 4:S:113:GLU:O    | 4:S:117:GLU:HG3  | 2.15                     | 0.47              |
| 1:A:437:ARG:HA   | 1:A:437:ARG:HD3  | 1.79                     | 0.47              |
| 2:N:168:ILE:HD12 | 2:N:268:TYR:HE2  | 1.79                     | 0.47              |
| 2:O:72:VAL:CG1   | 2:O:74:THR:HG23  | 2.45                     | 0.47              |
| 4:S:449:ILE:HG22 | 4:S:450:HIS:CD2  | 2.50                     | 0.47              |
| 1:A:507:ASN:OD1  | 1:A:588:ARG:NH1  | 2.48                     | 0.47              |
| 2:C:131:VAL:HG11 | 2:C:139:VAL:HG11 | 1.96                     | 0.47              |
| 2:C:145:ASP:OD1  | 2:C:146:ARG:N    | 2.48                     | 0.47              |
| 2:C:149:VAL:HG13 | 2:C:149:VAL:O    | 2.15                     | 0.47              |
| 3:P:175:MET:HG2  | 3:P:245:LYS:HB2  | 1.97                     | 0.47              |
| 4:R:46:ARG:NE    | 4:S:387:LEU:HD21 | 2.30                     | 0.47              |
| 4:R:256:ARG:NH2  | 4:R:459:ARG:HH21 | 2.12                     | 0.47              |
| 3:Q:151:ASN:O    | 3:Q:155:ILE:HG13 | 2.15                     | 0.47              |
| 4:T:285:GLU:CG   | 4:T:287:ALA:O    | 2.63                     | 0.47              |
| 1:A:928:TYR:HE1  | 1:A:929:MET:HE2  | 1.80                     | 0.47              |
| 2:E:64:ASP:CG    | 2:E:109:LYS:HZ1  | 2.21                     | 0.47              |
| 2:G:168:ILE:HG23 | 2:G:268:TYR:CE2  | 2.50                     | 0.47              |
| 2:G:233:LYS:HE2  | 2:G:233:LYS:HB3  | 1.56                     | 0.47              |
| 2:H:89:TYR:HB2   | 2:H:283:LEU:HD13 | 1.97                     | 0.47              |
| 2:O:131:VAL:HG11 | 2:O:139:VAL:HG11 | 1.97                     | 0.47              |
| 3:P:22:GLU:OE2   | 3:P:27:TYR:OH    | 2.25                     | 0.47              |
| 4:R:164:ALA:HA   | 4:R:167:ARG:HH21 | 1.80                     | 0.47              |
| 1:B:139:LYS:HB2  | 1:B:139:LYS:HE2  | 1.73                     | 0.46              |
| 2:H:139:VAL:HG22 | 2:H:151:MET:HG2  | 1.97                     | 0.46              |
| 1:A:374:GLN:OE1  | 1:B:146:GLN:NE2  | 2.48                     | 0.46              |
| 2:E:20:TYR:O     | 2:E:89:TYR:OH    | 2.23                     | 0.46              |
| 2:K:62:PHE:HZ    | 2:K:293:MET:HE2  | 1.79                     | 0.46              |
| 4:T:480:GLU:HB3  | 4:T:553:LYS:HE2  | 1.96                     | 0.46              |
| 1:B:790:ASN:OD1  | 1:B:790:ASN:N    | 2.48                     | 0.46              |
| 2:K:179:PRO:HD3  | 2:K:194:PHE:CZ   | 2.50                     | 0.46              |
| 4:S:100:LEU:HD22 | 4:S:267:THR:HG22 | 1.96                     | 0.46              |
| 1:A:207:LYS:NZ   | 1:A:921:CYS:SG   | 2.89                     | 0.46              |
| 1:A:451:VAL:HG13 | 1:A:621:VAL:HG22 | 1.96                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:370:ARG:NH1  | 1:B:370:ARG:CG   | 2.75                     | 0.46              |
| 2:M:180:PHE:HE2  | 2:M:182:LEU:HD12 | 1.81                     | 0.46              |
| 3:Q:65:ARG:HH12  | 3:Q:248:GLY:HA3  | 1.81                     | 0.46              |
| 4:T:228:ASN:O    | 4:T:231:ILE:HG22 | 2.15                     | 0.46              |
| 1:B:342:ILE:HG23 | 1:B:355:PRO:HG2  | 1.98                     | 0.46              |
| 2:D:223:THR:HG21 | 2:D:265:ILE:CD1  | 2.45                     | 0.46              |
| 2:F:168:ILE:CG2  | 2:F:268:TYR:CE2  | 2.97                     | 0.46              |
| 2:O:223:THR:CG2  | 2:O:265:ILE:HD11 | 2.46                     | 0.46              |
| 1:A:311:VAL:HG22 | 1:A:936:VAL:HG22 | 1.96                     | 0.46              |
| 2:K:31:VAL:HG12  | 2:K:78:MET:HE1   | 1.98                     | 0.46              |
| 2:N:35:LEU:HD12  | 2:N:78:MET:HE1   | 1.96                     | 0.46              |
| 3:Q:92:MET:HE3   | 3:Q:92:MET:HB3   | 1.81                     | 0.46              |
| 1:B:907:LYS:HB2  | 1:B:907:LYS:HE3  | 1.65                     | 0.46              |
| 2:J:94:ALA:HB2   | 2:J:251:ILE:HD13 | 1.98                     | 0.46              |
| 2:O:125:SER:HB2  | 2:O:265:ILE:HG13 | 1.98                     | 0.46              |
| 4:T:599:ASN:N    | 4:T:599:ASN:OD1  | 2.48                     | 0.46              |
| 2:C:72:VAL:O     | 2:C:72:VAL:HG12  | 2.16                     | 0.46              |
| 2:G:184:ARG:HB2  | 2:G:187:GLN:HG3  | 1.96                     | 0.46              |
| 2:L:169:ALA:HB3  | 2:L:200:PRO:HG2  | 1.98                     | 0.46              |
| 2:O:31:VAL:HG22  | 2:O:110:ALA:HB3  | 1.98                     | 0.46              |
| 3:P:22:GLU:HG3   | 3:P:94:LEU:HB3   | 1.97                     | 0.46              |
| 4:R:94:ILE:HB    | 4:R:97:GLN:HG3   | 1.98                     | 0.46              |
| 4:R:322:ASN:OD1  | 4:R:327:GLU:O    | 2.33                     | 0.46              |
| 4:S:66:LYS:HE3   | 4:S:66:LYS:HB3   | 1.58                     | 0.46              |
| 4:S:256:ARG:HB3  | 4:S:459:ARG:HH12 | 1.81                     | 0.46              |
| 1:A:222:VAL:HG21 | 2:K:53:VAL:HG13  | 1.97                     | 0.46              |
| 1:A:830:ILE:HD13 | 1:A:838:MET:HE1  | 1.98                     | 0.46              |
| 2:E:62:PHE:CE2   | 2:E:293:MET:SD   | 3.08                     | 0.46              |
| 2:E:185:LEU:HD23 | 2:E:185:LEU:HA   | 1.81                     | 0.46              |
| 2:N:132:LEU:HB2  | 2:N:162:THR:HB   | 1.97                     | 0.46              |
| 4:T:489:TYR:CE1  | 4:T:576:PRO:HB2  | 2.51                     | 0.46              |
| 2:N:184:ARG:NE   | 2:N:202:ASP:OD1  | 2.49                     | 0.46              |
| 2:O:223:THR:HG21 | 2:O:265:ILE:HD12 | 1.97                     | 0.46              |
| 3:Q:92:MET:HB2   | 3:Q:246:LEU:HD13 | 1.98                     | 0.46              |
| 4:R:268:VAL:HG12 | 4:R:431:LYS:HB2  | 1.97                     | 0.46              |
| 4:S:431:LYS:NZ   | 4:S:452:PRO:O    | 2.40                     | 0.46              |
| 2:D:126:VAL:HG23 | 2:D:221:ALA:HB2  | 1.97                     | 0.45              |
| 2:H:10:LEU:HD23  | 2:H:266:SER:HA   | 1.97                     | 0.45              |
| 2:J:67:PRO:HB3   | 2:J:73:LYS:HD3   | 1.96                     | 0.45              |
| 4:R:213:LEU:HD11 | 4:R:217:TYR:CE1  | 2.51                     | 0.45              |
| 4:S:617:GLN:HB3  | 4:S:626:ILE:HD11 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:s:7:LEU:HD12   | 5:s:10:LEU:HD11  | 1.97                     | 0.45              |
| 1:B:692:LEU:HD23 | 1:B:756:LEU:HD12 | 1.98                     | 0.45              |
| 2:I:179:PRO:HB2  | 2:I:192:ALA:HB1  | 1.97                     | 0.45              |
| 3:Q:111:THR:OG1  | 3:Q:147:ASP:OD1  | 2.32                     | 0.45              |
| 4:R:187:ILE:HG21 | 4:R:209:ILE:HG12 | 1.97                     | 0.45              |
| 4:S:525:GLN:HG3  | 4:S:526:HIS:ND1  | 2.32                     | 0.45              |
| 2:G:168:ILE:CG2  | 2:G:268:TYR:CE2  | 2.99                     | 0.45              |
| 2:J:91:SER:HB3   | 2:J:251:ILE:HD12 | 1.97                     | 0.45              |
| 3:P:135:ARG:HA   | 3:P:138:ILE:HD12 | 1.99                     | 0.45              |
| 2:D:169:ALA:HB3  | 2:D:200:PRO:HG2  | 1.99                     | 0.45              |
| 2:N:116:MET:SD   | 2:N:228:PRO:HG3  | 2.56                     | 0.45              |
| 3:P:106:ASP:OD1  | 3:P:106:ASP:O    | 2.34                     | 0.45              |
| 4:R:377:LEU:HD12 | 4:R:377:LEU:HA   | 1.82                     | 0.45              |
| 4:S:56:LYS:NZ    | 4:T:169:ALA:O    | 2.50                     | 0.45              |
| 4:T:285:GLU:HG3  | 4:T:287:ALA:O    | 2.17                     | 0.45              |
| 1:B:456:PHE:HB3  | 1:B:458:GLN:NE2  | 2.31                     | 0.45              |
| 2:D:168:ILE:CD1  | 2:D:269:HIS:CD2  | 2.88                     | 0.45              |
| 2:E:168:ILE:HG23 | 2:E:268:TYR:CE2  | 2.52                     | 0.45              |
| 2:F:64:ASP:OD1   | 2:F:109:LYS:NZ   | 2.44                     | 0.45              |
| 1:B:631:GLU:H    | 1:B:631:GLU:CD   | 2.25                     | 0.45              |
| 2:D:65:ASP:OD1   | 2:D:65:ASP:O     | 2.34                     | 0.45              |
| 2:N:272:ASP:OD1  | 2:N:272:ASP:N    | 2.49                     | 0.45              |
| 4:S:220:PHE:CE1  | 4:S:297:VAL:HG21 | 2.52                     | 0.45              |
| 2:D:123:PHE:HB3  | 2:D:261:ASP:OD1  | 2.16                     | 0.45              |
| 2:F:252:GLN:OE1  | 2:F:252:GLN:N    | 2.30                     | 0.45              |
| 2:K:168:ILE:HD12 | 2:K:268:TYR:HE2  | 1.81                     | 0.45              |
| 3:Q:70:LEU:HD23  | 3:Q:70:LEU:HA    | 1.80                     | 0.45              |
| 4:T:301:LEU:HD23 | 4:T:318:ALA:HA   | 1.98                     | 0.45              |
| 2:D:244:MET:HE3  | 2:D:244:MET:HB2  | 1.80                     | 0.45              |
| 2:D:294:ARG:HA   | 2:D:294:ARG:HD3  | 1.72                     | 0.45              |
| 2:F:41:ASP:OD1   | 2:F:41:ASP:N     | 2.50                     | 0.45              |
| 2:H:151:MET:HE2  | 2:H:209:LEU:HD13 | 1.97                     | 0.45              |
| 2:J:96:ALA:O     | 3:P:61:ARG:NH1   | 2.47                     | 0.45              |
| 2:N:145:ASP:OD1  | 2:N:146:ARG:N    | 2.49                     | 0.45              |
| 4:R:50:MET:CE    | 4:T:46:ARG:HH22  | 2.27                     | 0.45              |
| 4:R:492:ILE:HD12 | 4:R:570:TRP:CZ2  | 2.51                     | 0.45              |
| 4:T:232:LYS:HB2  | 4:T:233:PRO:HD3  | 1.97                     | 0.45              |
| 4:T:492:ILE:HD11 | 4:T:568:ARG:HG2  | 1.98                     | 0.45              |
| 1:B:348:THR:OG1  | 1:B:549:ARG:NH2  | 2.44                     | 0.45              |
| 2:L:150:THR:O    | 2:L:150:THR:HG23 | 2.16                     | 0.45              |
| 4:T:261:ILE:HD11 | 4:T:424:HIS:CD2  | 2.52                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:495:ARG:HG3  | 1:A:518:ILE:HG13 | 1.99                     | 0.44              |
| 1:A:569:LYS:NZ   | 1:A:569:LYS:HB2  | 2.32                     | 0.44              |
| 1:B:792:ILE:HG22 | 1:B:916:ILE:HG22 | 1.99                     | 0.44              |
| 2:C:179:PRO:HG3  | 2:C:194:PHE:CE2  | 2.52                     | 0.44              |
| 4:R:301:LEU:HD23 | 4:R:318:ALA:HA   | 1.97                     | 0.44              |
| 4:T:81:ALA:HB1   | 4:T:527:LYS:CD   | 2.44                     | 0.44              |
| 4:T:293:VAL:HG22 | 4:T:304:VAL:HG22 | 1.99                     | 0.44              |
| 4:T:361:LEU:HD13 | 4:T:400:MET:HE2  | 1.99                     | 0.44              |
| 2:K:185:LEU:HD23 | 2:K:185:LEU:HA   | 1.87                     | 0.44              |
| 2:L:85:VAL:CG1   | 2:L:89:TYR:CE1   | 3.00                     | 0.44              |
| 3:Q:246:LEU:HD12 | 3:Q:246:LEU:HA   | 1.89                     | 0.44              |
| 4:T:520:ILE:HD12 | 4:T:520:ILE:N    | 2.31                     | 0.44              |
| 1:A:678:LEU:HD23 | 1:A:678:LEU:HA   | 1.87                     | 0.44              |
| 2:E:167:GLN:N    | 2:E:167:GLN:OE1  | 2.50                     | 0.44              |
| 2:J:95:PRO:HB3   | 3:P:37:VAL:HG11  | 1.98                     | 0.44              |
| 3:Q:24:ALA:O     | 3:Q:83:GLY:HA3   | 2.17                     | 0.44              |
| 4:R:178:VAL:HG22 | 4:R:222:SER:HB3  | 1.99                     | 0.44              |
| 4:T:27:VAL:O     | 4:T:27:VAL:HG13  | 2.18                     | 0.44              |
| 1:B:109:PHE:HB2  | 1:B:123:LYS:HG2  | 1.99                     | 0.44              |
| 2:M:201:LEU:HD23 | 2:M:201:LEU:HA   | 1.87                     | 0.44              |
| 2:N:39:LEU:HD23  | 2:N:39:LEU:HA    | 1.84                     | 0.44              |
| 2:O:250:ASP:OD1  | 2:O:250:ASP:N    | 2.51                     | 0.44              |
| 2:O:258:SER:OG   | 2:O:262:GLU:OE2  | 2.35                     | 0.44              |
| 4:R:50:MET:HE3   | 4:T:46:ARG:NH2   | 2.28                     | 0.44              |
| 1:A:822:ILE:HG22 | 3:Q:182:GLN:HG3  | 1.99                     | 0.44              |
| 2:D:6:THR:HG23   | 2:D:129:VAL:O    | 2.18                     | 0.44              |
| 4:R:524:VAL:HG11 | 4:R:529:GLU:HG3  | 2.00                     | 0.44              |
| 2:E:64:ASP:OD1   | 2:E:109:LYS:NZ   | 2.41                     | 0.44              |
| 2:K:134:PRO:O    | 2:K:137:THR:OG1  | 2.33                     | 0.44              |
| 2:K:268:TYR:CD1  | 2:K:277:VAL:CG2  | 3.00                     | 0.44              |
| 2:O:56:VAL:O     | 2:O:60:SER:OG    | 2.30                     | 0.44              |
| 3:P:112:ASN:HB2  | 4:S:26:THR:HG21  | 1.99                     | 0.44              |
| 4:R:308:MET:HE2  | 4:R:308:MET:HB3  | 1.73                     | 0.44              |
| 4:R:312:LEU:HD22 | 4:R:366:LYS:HB2  | 2.00                     | 0.44              |
| 4:T:81:ALA:HB1   | 4:T:527:LYS:HE2  | 1.93                     | 0.44              |
| 1:A:687:ASP:HB3  | 1:A:730:ILE:HD13 | 2.00                     | 0.44              |
| 4:S:515:ASP:OD2  | 4:S:515:ASP:N    | 2.46                     | 0.44              |
| 2:D:131:VAL:HG11 | 2:D:139:VAL:HG11 | 2.00                     | 0.44              |
| 2:G:168:ILE:CG2  | 2:G:268:TYR:CD2  | 3.00                     | 0.44              |
| 2:L:13:PRO:HB2   | 2:L:276:ARG:HH12 | 1.82                     | 0.44              |
| 3:P:236:LEU:HD12 | 3:P:239:ARG:HD2  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:Q:198:SER:OG   | 3:Q:199:THR:N    | 2.51                     | 0.44              |
| 4:S:99:GLN:O     | 4:S:217:TYR:OH   | 2.33                     | 0.44              |
| 4:T:205:LYS:HE3  | 4:T:446:ILE:HG23 | 1.99                     | 0.44              |
| 1:A:461:ILE:HD12 | 1:A:461:ILE:HA   | 1.81                     | 0.44              |
| 2:E:67:PRO:HB3   | 2:E:73:LYS:HE3   | 1.99                     | 0.44              |
| 2:G:178:VAL:HG22 | 2:G:215:LEU:HD13 | 1.98                     | 0.44              |
| 2:H:168:ILE:HG23 | 2:H:268:TYR:CE2  | 2.53                     | 0.44              |
| 2:I:272:ASP:OD1  | 2:I:275:ASN:HB2  | 2.17                     | 0.44              |
| 2:J:267:GLN:OE1  | 2:J:276:ARG:NH1  | 2.50                     | 0.44              |
| 4:S:328:PHE:CE2  | 4:S:340:THR:HG21 | 2.53                     | 0.44              |
| 4:T:63:ARG:NH1   | 4:T:176:VAL:HG23 | 2.33                     | 0.44              |
| 4:T:274:ASN:OD1  | 4:T:274:ASN:N    | 2.50                     | 0.44              |
| 2:K:151:MET:HE2  | 2:K:161:ILE:HD12 | 1.99                     | 0.43              |
| 4:T:457:ASP:O    | 4:T:461:THR:OG1  | 2.35                     | 0.43              |
| 2:G:62:PHE:HZ    | 2:G:293:MET:SD   | 2.41                     | 0.43              |
| 2:G:150:THR:HG23 | 2:G:216:VAL:HG22 | 1.99                     | 0.43              |
| 2:N:59:TYR:CD1   | 2:N:67:PRO:HG3   | 2.54                     | 0.43              |
| 4:R:188:LYS:O    | 4:R:209:ILE:HG13 | 2.17                     | 0.43              |
| 4:R:520:ILE:CD1  | 4:R:531:ILE:HG22 | 2.48                     | 0.43              |
| 1:A:202:LYS:HD2  | 1:A:282:TYR:CE2  | 2.53                     | 0.43              |
| 1:B:853:ASP:O    | 1:B:853:ASP:CG   | 2.61                     | 0.43              |
| 2:F:152:LEU:HD22 | 2:F:154:THR:HG23 | 2.00                     | 0.43              |
| 2:L:263:PHE:O    | 2:L:267:GLN:HG2  | 2.18                     | 0.43              |
| 4:T:430:ARG:HA   | 4:T:430:ARG:HD2  | 1.83                     | 0.43              |
| 2:M:18:VAL:HG21  | 4:T:3:TRP:HH2    | 1.82                     | 0.43              |
| 2:M:39:LEU:HD12  | 2:M:39:LEU:HA    | 1.91                     | 0.43              |
| 2:O:44:ARG:CZ    | 2:O:44:ARG:HB3   | 2.49                     | 0.43              |
| 4:R:118:LEU:HD22 | 4:R:252:TYR:CD2  | 2.54                     | 0.43              |
| 4:R:187:ILE:HG22 | 4:R:209:ILE:HG12 | 2.00                     | 0.43              |
| 1:B:305:ASP:OD2  | 1:B:309:ASN:HB2  | 2.19                     | 0.43              |
| 2:I:251:ILE:HD12 | 2:I:251:ILE:HA   | 1.83                     | 0.43              |
| 3:P:99:LEU:O     | 3:P:103:THR:HG22 | 2.19                     | 0.43              |
| 4:S:516:GLY:H    | 4:S:615:TRP:CD1  | 2.36                     | 0.43              |
| 4:T:157:SER:C    | 4:T:159:ALA:H    | 2.26                     | 0.43              |
| 2:M:68:ARG:HE    | 2:M:68:ARG:HB3   | 1.67                     | 0.43              |
| 3:P:149:ASN:ND2  | 4:S:24:ASP:OD2   | 2.41                     | 0.43              |
| 4:R:111:ASP:OD1  | 4:R:224:HIS:ND1  | 2.49                     | 0.43              |
| 4:S:365:LEU:HD22 | 4:S:377:LEU:HD23 | 2.00                     | 0.43              |
| 1:A:460:ARG:HH11 | 1:A:490:SER:CB   | 2.29                     | 0.43              |
| 1:A:463:MET:HE1  | 1:A:650:GLU:CB   | 2.48                     | 0.43              |
| 2:E:147:ALA:HB3  | 2:E:219:ALA:HB3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:R:235:ALA:HB2  | 4:R:244:LEU:HD13 | 2.01                     | 0.43              |
| 4:R:260:ASP:OD2  | 4:R:459:ARG:HD2  | 2.18                     | 0.43              |
| 4:S:332:VAL:HG21 | 4:S:419:HIS:NE2  | 2.33                     | 0.43              |
| 4:S:414:ILE:HD11 | 4:S:416:TRP:CZ2  | 2.54                     | 0.43              |
| 4:T:492:ILE:HD13 | 4:T:570:TRP:CE2  | 2.53                     | 0.43              |
| 1:A:197:GLN:HG3  | 1:A:204:ALA:HB2  | 2.01                     | 0.43              |
| 1:A:430:HIS:HA   | 1:A:433:MET:HE3  | 2.01                     | 0.43              |
| 2:H:87:ARG:NH1   | 3:Q:38:LEU:O     | 2.51                     | 0.43              |
| 2:I:52:ASP:OD1   | 2:I:52:ASP:N     | 2.51                     | 0.43              |
| 2:I:183:ALA:HB2  | 2:I:190:PRO:HD3  | 2.01                     | 0.43              |
| 4:S:74:SER:H     | 5:s:5:THR:CG2    | 2.31                     | 0.43              |
| 4:S:90:ILE:HD12  | 4:S:462:THR:OG1  | 2.18                     | 0.43              |
| 4:S:410:GLN:NE2  | 4:S:584:ASN:H    | 2.16                     | 0.43              |
| 1:B:100:LYS:HB2  | 1:B:100:LYS:HE2  | 1.78                     | 0.43              |
| 1:B:270:ARG:HG3  | 1:B:270:ARG:HH11 | 1.84                     | 0.43              |
| 2:C:134:PRO:HG2  | 2:C:159:ALA:HB1  | 2.01                     | 0.43              |
| 2:D:168:ILE:HG21 | 2:D:268:TYR:CD2  | 2.53                     | 0.43              |
| 4:T:43:ALA:CA    | 4:T:277:MET:HE1  | 2.48                     | 0.43              |
| 2:D:147:ALA:HB3  | 2:D:219:ALA:HB3  | 2.00                     | 0.43              |
| 2:F:168:ILE:CG2  | 2:F:268:TYR:CD2  | 3.01                     | 0.43              |
| 4:R:365:LEU:HD22 | 4:R:377:LEU:HD12 | 2.01                     | 0.43              |
| 4:R:536:VAL:HG12 | 4:R:542:THR:HB   | 2.01                     | 0.43              |
| 4:S:69:MET:HE2   | 4:S:102:ARG:HH12 | 1.84                     | 0.43              |
| 4:T:519:LEU:HD13 | 4:T:519:LEU:HA   | 1.90                     | 0.43              |
| 1:A:319:MET:HE3  | 1:A:319:MET:HA   | 2.01                     | 0.42              |
| 2:M:44:ARG:HA    | 2:M:44:ARG:HD2   | 1.90                     | 0.42              |
| 4:R:393:ASN:HB3  | 4:R:396:LEU:HB2  | 2.01                     | 0.42              |
| 4:T:93:ASP:OD1   | 4:T:93:ASP:N     | 2.51                     | 0.42              |
| 4:T:140:LYS:HD3  | 4:T:140:LYS:HA   | 1.86                     | 0.42              |
| 4:T:479:TYR:HH   | 4:T:561:SER:HG   | 1.66                     | 0.42              |
| 4:T:506:LYS:HB2  | 4:T:506:LYS:HE2  | 1.86                     | 0.42              |
| 1:A:727:LYS:H    | 1:A:727:LYS:HG2  | 1.70                     | 0.42              |
| 2:N:182:LEU:HD12 | 2:N:207:VAL:HG22 | 2.01                     | 0.42              |
| 4:T:392:ASP:OD1  | 4:T:392:ASP:N    | 2.52                     | 0.42              |
| 1:A:366:GLY:HA2  | 1:A:943:VAL:HG23 | 2.01                     | 0.42              |
| 2:E:35:LEU:HD12  | 2:E:78:MET:HE1   | 1.99                     | 0.42              |
| 2:F:233:LYS:HE3  | 2:F:233:LYS:HB3  | 1.84                     | 0.42              |
| 4:T:431:LYS:HG3  | 4:T:451:ILE:HD11 | 2.01                     | 0.42              |
| 1:A:953:THR:HG23 | 1:B:139:LYS:O    | 2.20                     | 0.42              |
| 2:F:252:GLN:H    | 2:F:252:GLN:CD   | 2.21                     | 0.42              |
| 3:P:9:LEU:HD12   | 3:P:9:LEU:HA     | 1.87                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:228:ASN:O    | 4:S:231:ILE:HG22 | 2.18                     | 0.42              |
| 4:T:77:GLU:OE1   | 4:T:77:GLU:HA    | 2.19                     | 0.42              |
| 4:T:445:VAL:O    | 4:T:449:ILE:HG13 | 2.20                     | 0.42              |
| 1:A:837:MET:HG2  | 1:B:954:ARG:HB2  | 2.01                     | 0.42              |
| 1:B:93:LEU:HD23  | 1:B:93:LEU:HA    | 1.87                     | 0.42              |
| 1:B:437:ARG:O    | 1:B:437:ARG:HG2  | 2.18                     | 0.42              |
| 1:B:762:PRO:O    | 1:B:765:VAL:HG23 | 2.20                     | 0.42              |
| 2:C:6:THR:HG23   | 2:C:129:VAL:O    | 2.19                     | 0.42              |
| 2:C:89:TYR:HB2   | 2:C:283:LEU:HD13 | 2.01                     | 0.42              |
| 2:M:152:LEU:HD13 | 2:M:214:PRO:HG3  | 2.01                     | 0.42              |
| 3:Q:99:LEU:HD12  | 3:Q:99:LEU:HA    | 1.91                     | 0.42              |
| 4:T:511:VAL:O    | 4:T:517:HIS:HA   | 2.19                     | 0.42              |
| 2:E:131:VAL:HG11 | 2:E:139:VAL:HG11 | 2.02                     | 0.42              |
| 2:H:182:LEU:CB   | 2:H:196:TYR:HE2  | 2.22                     | 0.42              |
| 2:I:189:MET:HA   | 2:I:190:PRO:HD3  | 1.95                     | 0.42              |
| 2:L:118:ASN:OD1  | 2:L:228:PRO:HA   | 2.20                     | 0.42              |
| 2:N:88:SER:HA    | 2:N:94:ALA:HB3   | 2.02                     | 0.42              |
| 4:R:261:ILE:HD13 | 4:R:261:ILE:HA   | 1.85                     | 0.42              |
| 4:S:25:ARG:HG3   | 4:S:25:ARG:HH11  | 1.84                     | 0.42              |
| 4:S:197:VAL:HG12 | 4:S:197:VAL:O    | 2.20                     | 0.42              |
| 4:T:42:ILE:HG22  | 4:T:277:MET:HE2  | 2.02                     | 0.42              |
| 2:D:274:ILE:O    | 2:D:277:VAL:CG1  | 2.68                     | 0.42              |
| 2:G:151:MET:HE3  | 2:G:209:LEU:HD13 | 2.00                     | 0.42              |
| 2:G:179:PRO:HG3  | 2:G:194:PHE:CZ   | 2.54                     | 0.42              |
| 2:G:183:ALA:HB3  | 2:G:189:MET:SD   | 2.60                     | 0.42              |
| 2:I:294:ARG:HD3  | 2:I:294:ARG:HA   | 1.88                     | 0.42              |
| 2:J:300:ARG:CD   | 3:Q:46:ASN:HD21  | 2.32                     | 0.42              |
| 2:M:137:THR:HG22 | 2:M:153:ASN:HA   | 2.02                     | 0.42              |
| 4:R:107:MET:HE2  | 4:R:458:LEU:HD13 | 2.00                     | 0.42              |
| 4:R:502:ASN:HB2  | 4:R:505:THR:HG23 | 2.01                     | 0.42              |
| 4:S:109:LYS:O    | 4:S:113:GLU:HG2  | 2.20                     | 0.42              |
| 4:S:624:THR:HG23 | 4:S:625:ASN:N    | 2.35                     | 0.42              |
| 4:T:616:ASP:OD1  | 4:T:617:GLN:N    | 2.53                     | 0.42              |
| 1:A:374:GLN:NE2  | 1:A:551:PRO:HD3  | 2.34                     | 0.42              |
| 1:A:463:MET:SD   | 1:A:465:TYR:HE1  | 2.41                     | 0.42              |
| 1:A:825:ASN:ND2  | 3:Q:183:ASP:HA   | 2.34                     | 0.42              |
| 2:I:120:TYR:CD1  | 2:I:120:TYR:C    | 2.98                     | 0.42              |
| 3:P:237:LYS:HB2  | 3:P:237:LYS:HE3  | 1.82                     | 0.42              |
| 3:Q:93:LEU:HG    | 3:Q:246:LEU:HD11 | 2.02                     | 0.42              |
| 2:C:184:ARG:CD   | 2:C:202:ASP:HB3  | 2.48                     | 0.42              |
| 2:F:151:MET:HE3  | 2:F:161:ILE:HD12 | 2.02                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:96:ALA:O     | 3:Q:59:VAL:HG11  | 2.20                     | 0.42              |
| 2:M:294:ARG:HA   | 2:M:294:ARG:HD3  | 1.70                     | 0.42              |
| 3:Q:152:ASP:OD1  | 3:Q:152:ASP:N    | 2.52                     | 0.42              |
| 4:R:35:MET:HE3   | 4:T:40:ALA:HB2   | 2.01                     | 0.42              |
| 4:S:131:THR:CG2  | 4:S:154:VAL:HG21 | 2.50                     | 0.42              |
| 4:T:210:ILE:HG23 | 4:T:212:GLN:H    | 1.84                     | 0.42              |
| 4:T:483:ILE:HG23 | 4:T:494:TYR:CZ   | 2.54                     | 0.42              |
| 2:H:294:ARG:HH12 | 3:Q:42:ASN:HD21  | 1.68                     | 0.42              |
| 2:J:223:THR:HG21 | 2:J:265:ILE:HD11 | 2.01                     | 0.42              |
| 2:K:13:PRO:HG2   | 2:K:270:ALA:HB2  | 2.01                     | 0.42              |
| 2:O:246:ASP:OD1  | 2:O:246:ASP:N    | 2.53                     | 0.42              |
| 4:R:534:LEU:HD23 | 4:R:534:LEU:HA   | 1.90                     | 0.42              |
| 4:S:94:ILE:HD13  | 4:S:449:ILE:HD12 | 2.02                     | 0.42              |
| 1:A:559:ASN:ND2  | 1:A:563:ILE:O    | 2.50                     | 0.41              |
| 2:G:298:PRO:HG2  | 2:H:118:ASN:O    | 2.20                     | 0.41              |
| 2:H:136:ARG:H    | 2:H:136:ARG:HG2  | 1.70                     | 0.41              |
| 2:M:53:VAL:N     | 2:M:54:PRO:HD2   | 2.35                     | 0.41              |
| 2:O:126:VAL:HG12 | 2:O:144:SER:O    | 2.20                     | 0.41              |
| 4:S:280:PRO:HG3  | 4:S:289:TRP:CE2  | 2.55                     | 0.41              |
| 1:A:749:TYR:O    | 1:A:753:LEU:HG   | 2.19                     | 0.41              |
| 1:B:779:PHE:O    | 1:B:788:TYR:OH   | 2.37                     | 0.41              |
| 2:M:182:LEU:HD21 | 2:M:205:PHE:HB3  | 2.02                     | 0.41              |
| 4:R:428:ASP:OD1  | 4:R:428:ASP:N    | 2.53                     | 0.41              |
| 4:S:39:ARG:HD3   | 4:T:39:ARG:NH2   | 2.34                     | 0.41              |
| 4:S:459:ARG:HB2  | 4:S:488:HIS:NE2  | 2.35                     | 0.41              |
| 1:B:480:MET:HA   | 1:B:484:ARG:HG2  | 2.02                     | 0.41              |
| 2:D:40:ILE:HD13  | 2:D:295:ARG:HH21 | 1.84                     | 0.41              |
| 2:E:98:VAL:HA    | 2:E:99:PRO:HD3   | 1.92                     | 0.41              |
| 2:M:11:ASP:OD2   | 2:N:194:PHE:HD2  | 2.02                     | 0.41              |
| 3:Q:188:VAL:HG23 | 3:Q:212:LYS:HA   | 2.02                     | 0.41              |
| 4:R:489:TYR:CZ   | 4:R:576:PRO:HB2  | 2.55                     | 0.41              |
| 4:S:458:LEU:HD12 | 4:S:458:LEU:HA   | 1.84                     | 0.41              |
| 2:F:205:PHE:C    | 2:F:206:ILE:HD13 | 2.45                     | 0.41              |
| 2:I:272:ASP:O    | 2:I:276:ARG:HG3  | 2.19                     | 0.41              |
| 2:M:83:THR:O     | 2:M:87:ARG:HG3   | 2.20                     | 0.41              |
| 4:R:219:ALA:HB1  | 4:R:274:ASN:HB3  | 2.02                     | 0.41              |
| 4:T:614:THR:HG22 | 4:T:615:TRP:H    | 1.85                     | 0.41              |
| 1:B:766:GLU:CG   | 1:B:768:VAL:HG12 | 2.49                     | 0.41              |
| 2:I:62:PHE:CE2   | 2:I:293:MET:SD   | 3.13                     | 0.41              |
| 2:I:123:PHE:HD1  | 2:I:261:ASP:OD1  | 2.03                     | 0.41              |
| 2:J:126:VAL:HA   | 2:J:221:ALA:HB3  | 2.01                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:S:50:MET:O     | 4:S:53:ARG:N     | 2.52                     | 0.41              |
| 4:T:359:LEU:O    | 4:T:363:MET:HG3  | 2.20                     | 0.41              |
| 4:T:511:VAL:HG21 | 4:T:532:LEU:HD22 | 2.02                     | 0.41              |
| 1:B:202:LYS:HE3  | 1:B:282:TYR:CE1  | 2.55                     | 0.41              |
| 2:E:72:VAL:HG12  | 2:E:74:THR:HG23  | 2.02                     | 0.41              |
| 2:J:62:PHE:CE2   | 2:J:293:MET:SD   | 3.14                     | 0.41              |
| 4:R:511:VAL:HG21 | 4:R:532:LEU:HD22 | 2.02                     | 0.41              |
| 4:S:449:ILE:HG22 | 4:S:450:HIS:HD2  | 1.85                     | 0.41              |
| 4:S:605:LEU:HD13 | 4:S:624:THR:OG1  | 2.21                     | 0.41              |
| 4:T:46:ARG:HG3   | 4:T:46:ARG:NH1   | 2.30                     | 0.41              |
| 4:T:113:GLU:OE1  | 4:T:113:GLU:C    | 2.64                     | 0.41              |
| 4:T:516:GLY:HA3  | 4:T:613:HIS:O    | 2.20                     | 0.41              |
| 1:A:204:ALA:HB3  | 1:A:925:LEU:HD22 | 2.03                     | 0.41              |
| 1:A:494:TYR:OH   | 1:A:533:VAL:O    | 2.33                     | 0.41              |
| 2:K:77:LYS:HE2   | 2:K:77:LYS:HB3   | 1.80                     | 0.41              |
| 4:R:43:ALA:HB2   | 4:R:277:MET:HE1  | 2.03                     | 0.41              |
| 4:R:449:ILE:C    | 4:R:449:ILE:HD12 | 2.45                     | 0.41              |
| 4:S:489:TYR:CE1  | 4:S:576:PRO:HB2  | 2.55                     | 0.41              |
| 1:B:82:LYS:HE3   | 1:B:82:LYS:HB3   | 1.74                     | 0.41              |
| 1:B:98:LEU:HD22  | 1:B:101:LEU:HB3  | 2.02                     | 0.41              |
| 1:B:481:LEU:HD23 | 1:B:481:LEU:HA   | 1.90                     | 0.41              |
| 2:C:40:ILE:HD11  | 2:C:292:GLN:HA   | 2.03                     | 0.41              |
| 2:N:271:GLN:HG2  | 2:N:272:ASP:OD1  | 2.21                     | 0.41              |
| 2:O:241:GLN:H    | 2:O:241:GLN:HG2  | 1.72                     | 0.41              |
| 4:R:27:VAL:CG1   | 4:R:28:ALA:N     | 2.84                     | 0.41              |
| 1:B:96:GLN:O     | 1:B:97:LYS:NZ    | 2.48                     | 0.41              |
| 1:B:586:ARG:HG3  | 1:B:586:ARG:NH1  | 2.36                     | 0.41              |
| 2:J:74:THR:HG21  | 3:P:43:GLU:HB2   | 2.03                     | 0.41              |
| 2:K:179:PRO:HG3  | 2:K:194:PHE:CD2  | 2.55                     | 0.41              |
| 2:M:181:GLN:HB2  | 2:M:208:VAL:HG22 | 2.03                     | 0.41              |
| 2:N:268:TYR:O    | 2:N:268:TYR:HD2  | 2.04                     | 0.41              |
| 3:Q:65:ARG:HD2   | 3:Q:87:PRO:O     | 2.21                     | 0.41              |
| 4:R:200:ALA:HB1  | 4:S:624:THR:HG21 | 2.03                     | 0.41              |
| 4:R:493:ASP:HB2  | 4:R:569:ASN:OD1  | 2.21                     | 0.41              |
| 4:T:534:LEU:CD1  | 4:T:542:THR:HG21 | 2.46                     | 0.41              |
| 4:T:626:ILE:HD12 | 4:T:626:ILE:HA   | 1.89                     | 0.41              |
| 1:B:756:LEU:HD12 | 1:B:756:LEU:HA   | 1.97                     | 0.41              |
| 2:M:65:ASP:N     | 2:M:65:ASP:OD1   | 2.52                     | 0.41              |
| 4:S:487:ALA:C    | 4:S:578:VAL:HG12 | 2.46                     | 0.41              |
| 1:A:438:LEU:HD22 | 1:A:438:LEU:H    | 1.86                     | 0.40              |
| 1:A:624:TYR:CZ   | 1:A:670:ILE:HD11 | 2.56                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:207:LYS:HG3  | 1:B:922:LEU:HD23 | 2.03                     | 0.40              |
| 2:G:126:VAL:HG11 | 2:G:147:ALA:HB2  | 2.02                     | 0.40              |
| 2:G:160:ASN:C    | 2:G:161:ILE:HD13 | 2.46                     | 0.40              |
| 2:N:168:ILE:CG2  | 2:N:268:TYR:CD2  | 3.04                     | 0.40              |
| 2:N:183:ALA:HB2  | 2:N:190:PRO:HD3  | 2.02                     | 0.40              |
| 2:O:168:ILE:HG13 | 2:O:268:TYR:CE2  | 2.55                     | 0.40              |
| 4:S:521:GLU:OE1  | 4:S:521:GLU:C    | 2.64                     | 0.40              |
| 1:B:593:ASN:OD1  | 1:B:593:ASN:N    | 2.54                     | 0.40              |
| 2:I:244:MET:HE1  | 2:I:257:TYR:O    | 2.21                     | 0.40              |
| 2:O:111:THR:O    | 2:O:111:THR:HG23 | 2.21                     | 0.40              |
| 4:T:428:ASP:OD1  | 4:T:429:SER:N    | 2.54                     | 0.40              |
| 1:A:350:PRO:HA   | 1:A:545:VAL:HG11 | 2.02                     | 0.40              |
| 2:E:233:LYS:HB3  | 2:E:233:LYS:HE2  | 1.72                     | 0.40              |
| 2:E:271:GLN:OE1  | 2:E:271:GLN:HA   | 2.21                     | 0.40              |
| 2:F:26:ARG:HG2   | 2:F:116:MET:HE3  | 2.03                     | 0.40              |
| 2:G:33:GLU:OE2   | 2:G:288:GLN:NE2  | 2.54                     | 0.40              |
| 3:Q:174:ASP:OD1  | 3:Q:175:MET:N    | 2.54                     | 0.40              |
| 4:R:492:ILE:HD12 | 4:R:570:TRP:CE2  | 2.57                     | 0.40              |
| 4:S:210:ILE:HA   | 4:S:210:ILE:HD12 | 1.84                     | 0.40              |
| 4:T:27:VAL:HG22  | 4:T:34:SER:HB2   | 2.04                     | 0.40              |
| 1:A:300:SER:HA   | 1:A:313:ILE:O    | 2.21                     | 0.40              |
| 1:A:395:LYS:HE2  | 1:A:395:LYS:HB3  | 1.73                     | 0.40              |
| 2:C:172:VAL:HG23 | 2:C:200:PRO:HG3  | 2.04                     | 0.40              |
| 2:F:244:MET:SD   | 2:G:173:ILE:HD11 | 2.62                     | 0.40              |
| 4:S:251:ILE:HG12 | 4:S:408:THR:HG21 | 2.02                     | 0.40              |
| 4:S:301:LEU:HD23 | 4:S:318:ALA:HA   | 2.04                     | 0.40              |
| 1:B:221:LEU:HD22 | 1:B:855:TYR:CZ   | 2.56                     | 0.40              |
| 1:B:451:VAL:HG12 | 1:B:455:MET:HE2  | 2.03                     | 0.40              |
| 1:B:841:ILE:HD12 | 1:B:841:ILE:HA   | 1.95                     | 0.40              |
| 2:E:88:SER:HA    | 2:E:94:ALA:HB3   | 2.04                     | 0.40              |
| 2:E:294:ARG:HA   | 2:E:294:ARG:HD3  | 1.93                     | 0.40              |
| 2:H:61:LYS:HD2   | 2:H:61:LYS:HA    | 1.71                     | 0.40              |
| 3:Q:20:PRO:HA    | 3:Q:97:SER:HA    | 2.04                     | 0.40              |
| 4:R:518:LEU:HB2  | 4:R:612:TRP:HE3  | 1.86                     | 0.40              |
| 4:T:499:ASP:CG   | 4:T:526:HIS:HD1  | 2.30                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | A     | 747/955 (78%)   | 737 (99%)  | 10 (1%)  | 0        | 100         | 100 |
| 1   | B     | 898/955 (94%)   | 880 (98%)  | 18 (2%)  | 0        | 100         | 100 |
| 2   | C     | 297/302 (98%)   | 293 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 2   | D     | 296/302 (98%)   | 287 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 2   | E     | 296/302 (98%)   | 290 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 2   | F     | 296/302 (98%)   | 290 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 2   | G     | 296/302 (98%)   | 290 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 2   | H     | 297/302 (98%)   | 292 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | I     | 296/302 (98%)   | 286 (97%)  | 10 (3%)  | 0        | 100         | 100 |
| 2   | J     | 297/302 (98%)   | 292 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | K     | 296/302 (98%)   | 293 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 2   | L     | 295/302 (98%)   | 286 (97%)  | 9 (3%)   | 0        | 100         | 100 |
| 2   | M     | 296/302 (98%)   | 291 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | N     | 296/302 (98%)   | 289 (98%)  | 7 (2%)   | 0        | 100         | 100 |
| 2   | O     | 296/302 (98%)   | 291 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 3   | P     | 247/249 (99%)   | 245 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 3   | Q     | 242/249 (97%)   | 233 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 4   | R     | 599/628 (95%)   | 593 (99%)  | 6 (1%)   | 0        | 100         | 100 |
| 4   | S     | 620/628 (99%)   | 610 (98%)  | 10 (2%)  | 0        | 100         | 100 |
| 4   | T     | 625/628 (100%)  | 609 (97%)  | 16 (3%)  | 0        | 100         | 100 |
| 5   | r     | 13/283 (5%)     | 13 (100%)  | 0        | 0        | 100         | 100 |
| 5   | s     | 13/283 (5%)     | 13 (100%)  | 0        | 0        | 100         | 100 |
| 5   | t     | 13/283 (5%)     | 13 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 7867/9067 (87%) | 7716 (98%) | 151 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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.

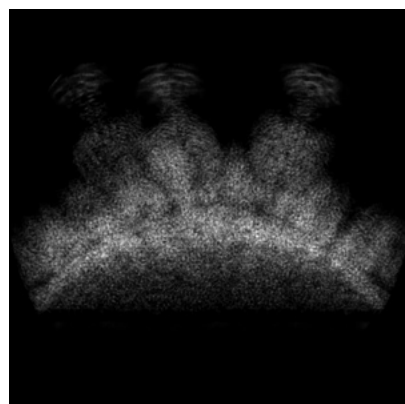
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36880. These allow visual inspection of the internal detail of the map and identification of artifacts.

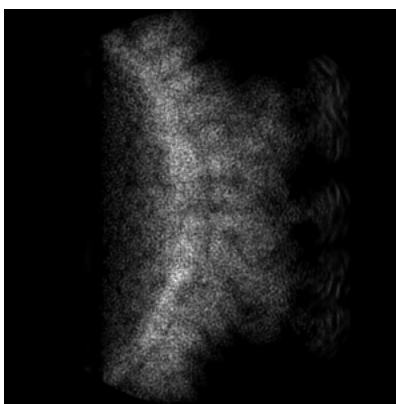
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

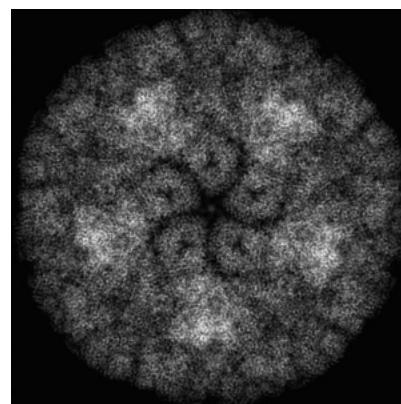
#### 6.1.1 Primary map



X

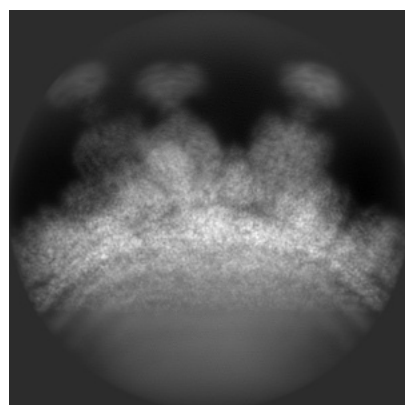


Y

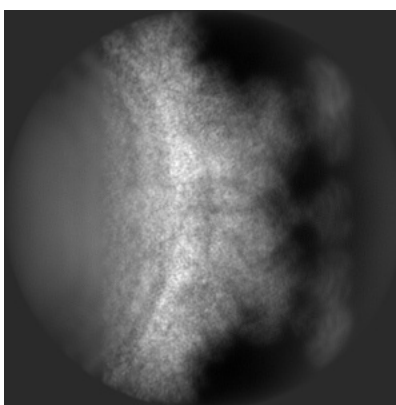


Z

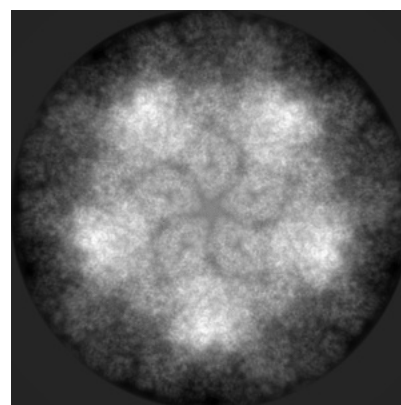
#### 6.1.2 Raw map



X



Y



Z

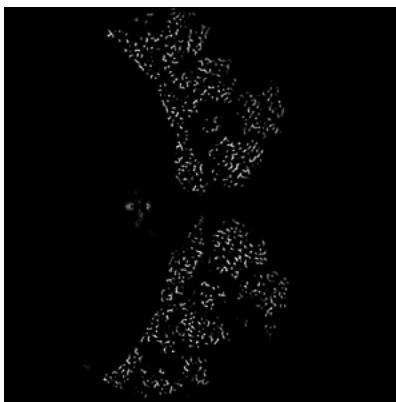
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 230

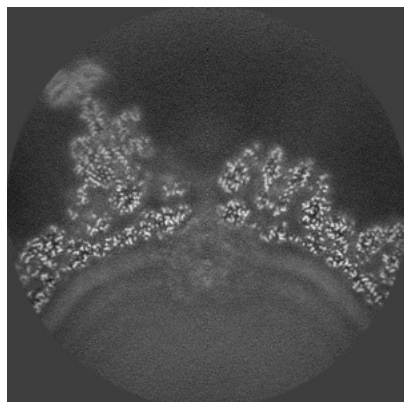


Y Index: 230

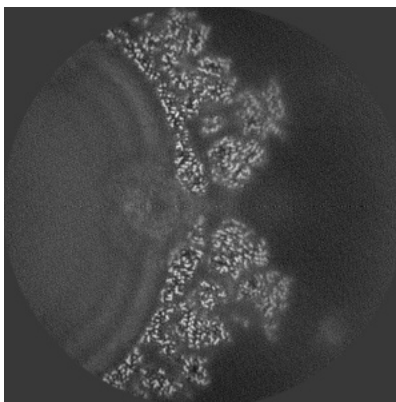


Z Index: 230

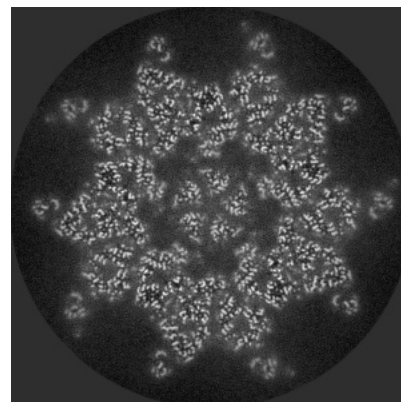
### 6.2.2 Raw map



X Index: 230



Y Index: 230



Z Index: 230

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

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

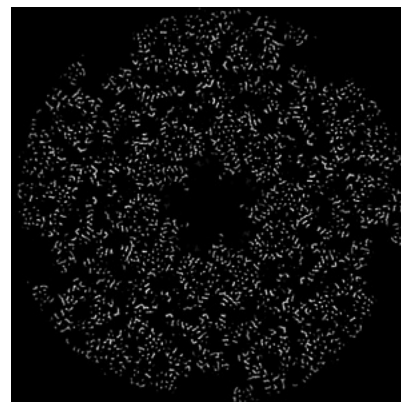
### 6.3.1 Primary map



X Index: 307

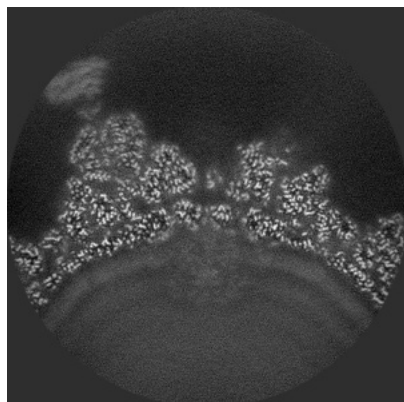


Y Index: 177

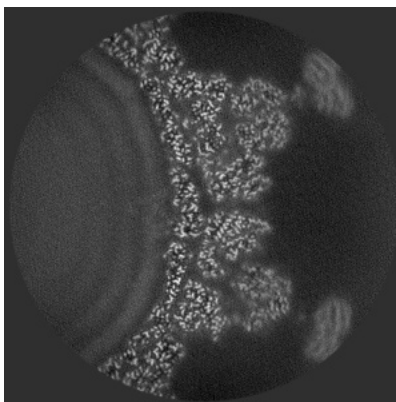


Z Index: 198

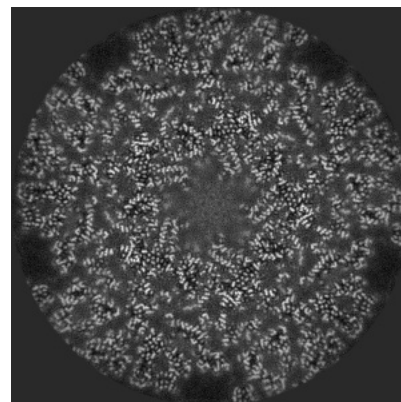
### 6.3.2 Raw map



X Index: 213



Y Index: 172

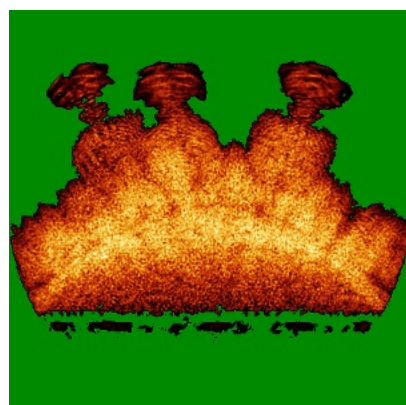


Z Index: 198

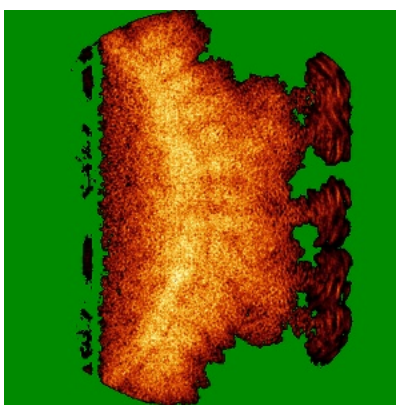
The images above show the largest variance slices of the map in three orthogonal directions.

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

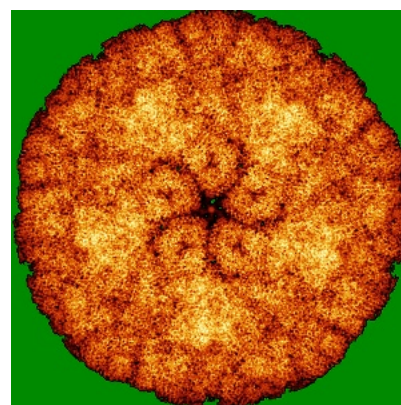
### 6.4.1 Primary map



X

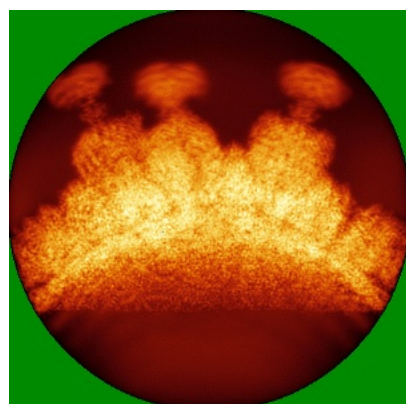


Y

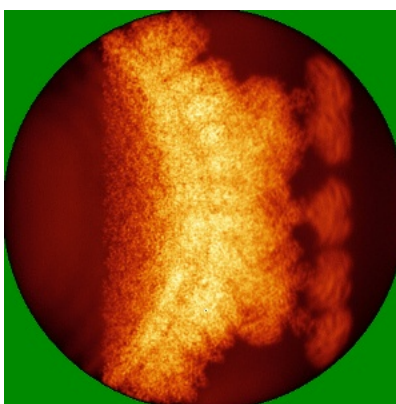


Z

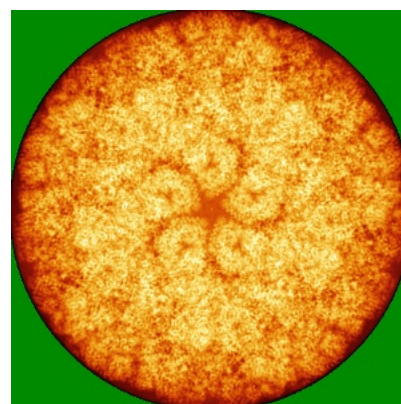
### 6.4.2 Raw map



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](#)

This section was not generated.

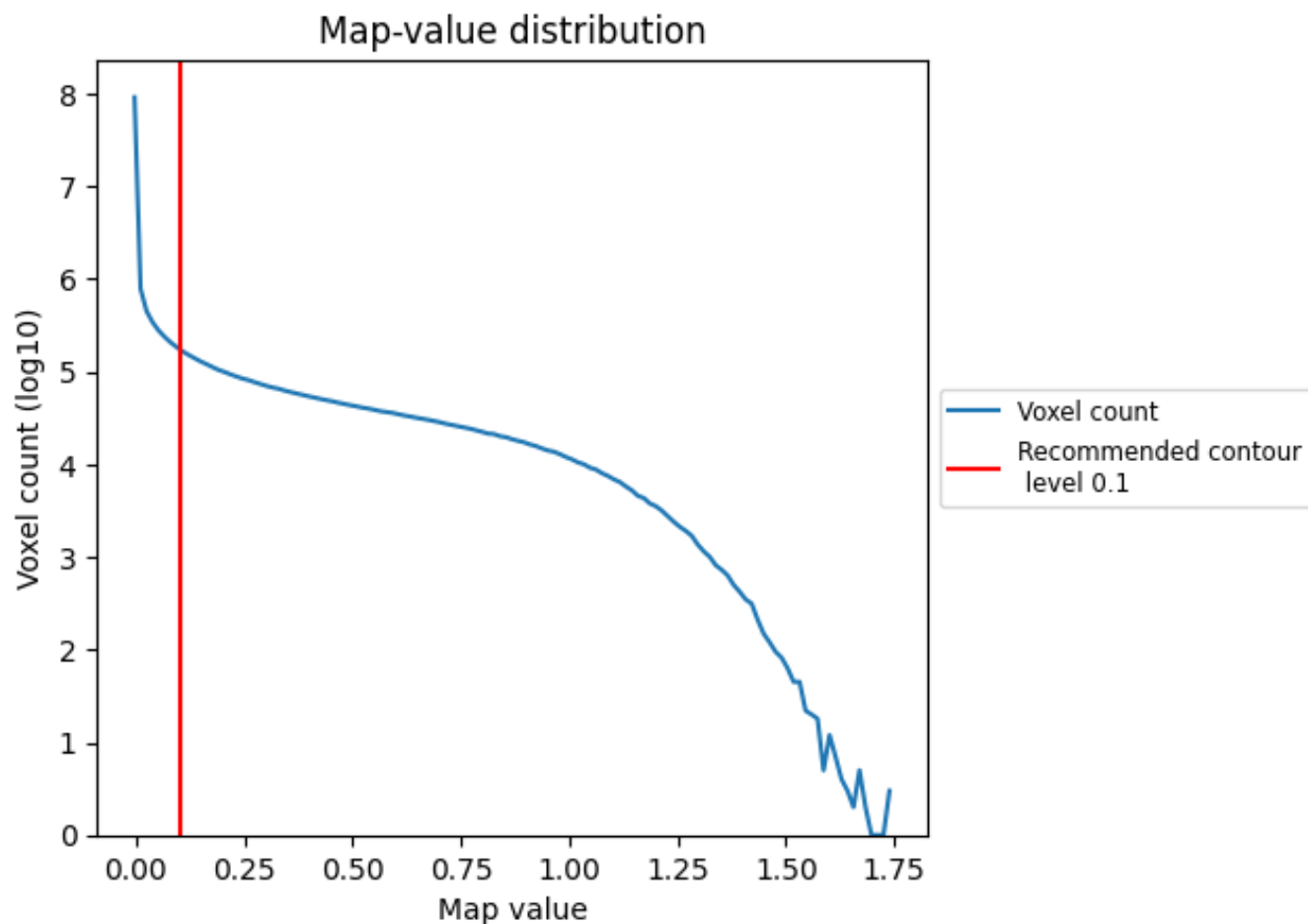
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

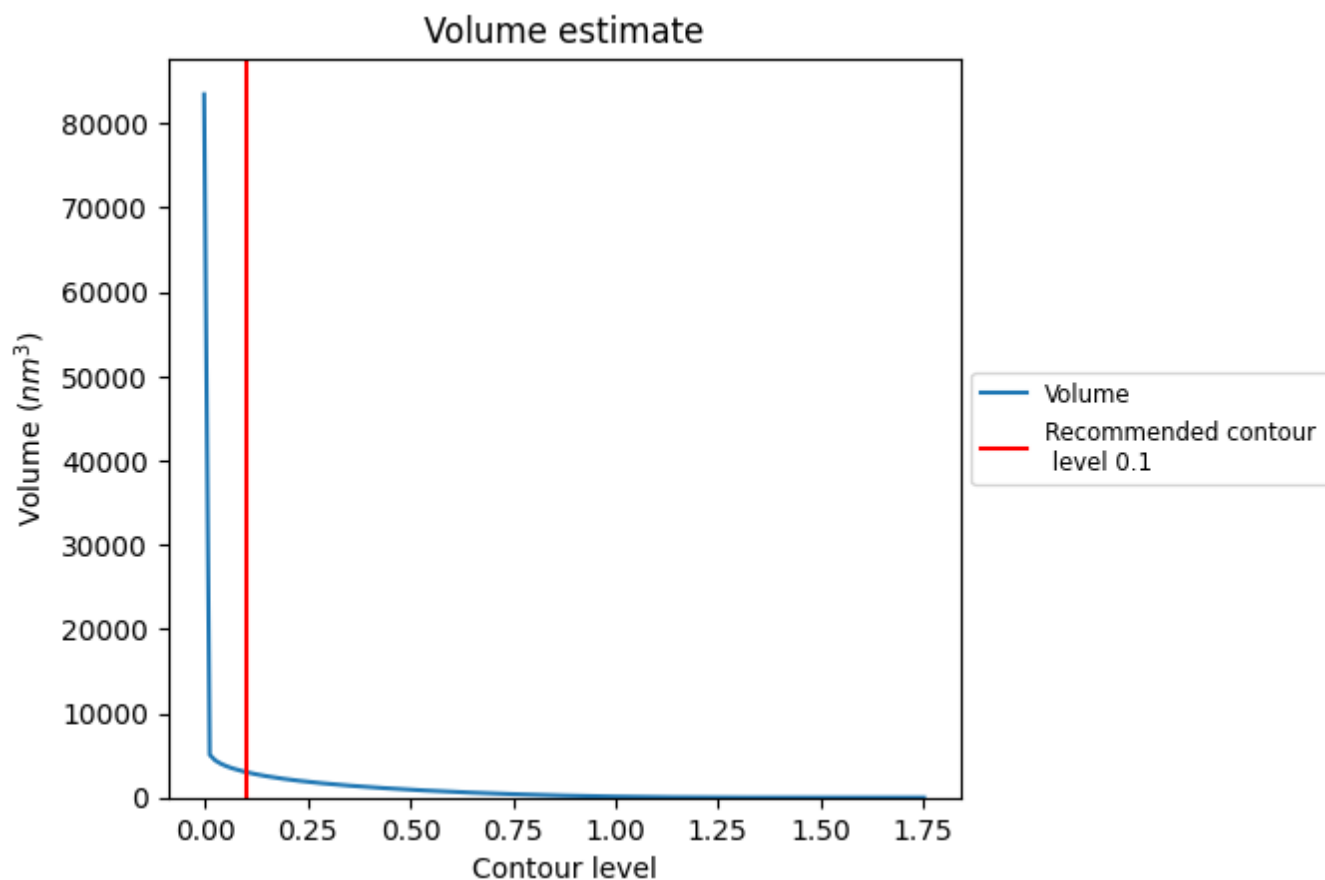
This section contains the results of statistical analysis of the map.

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



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

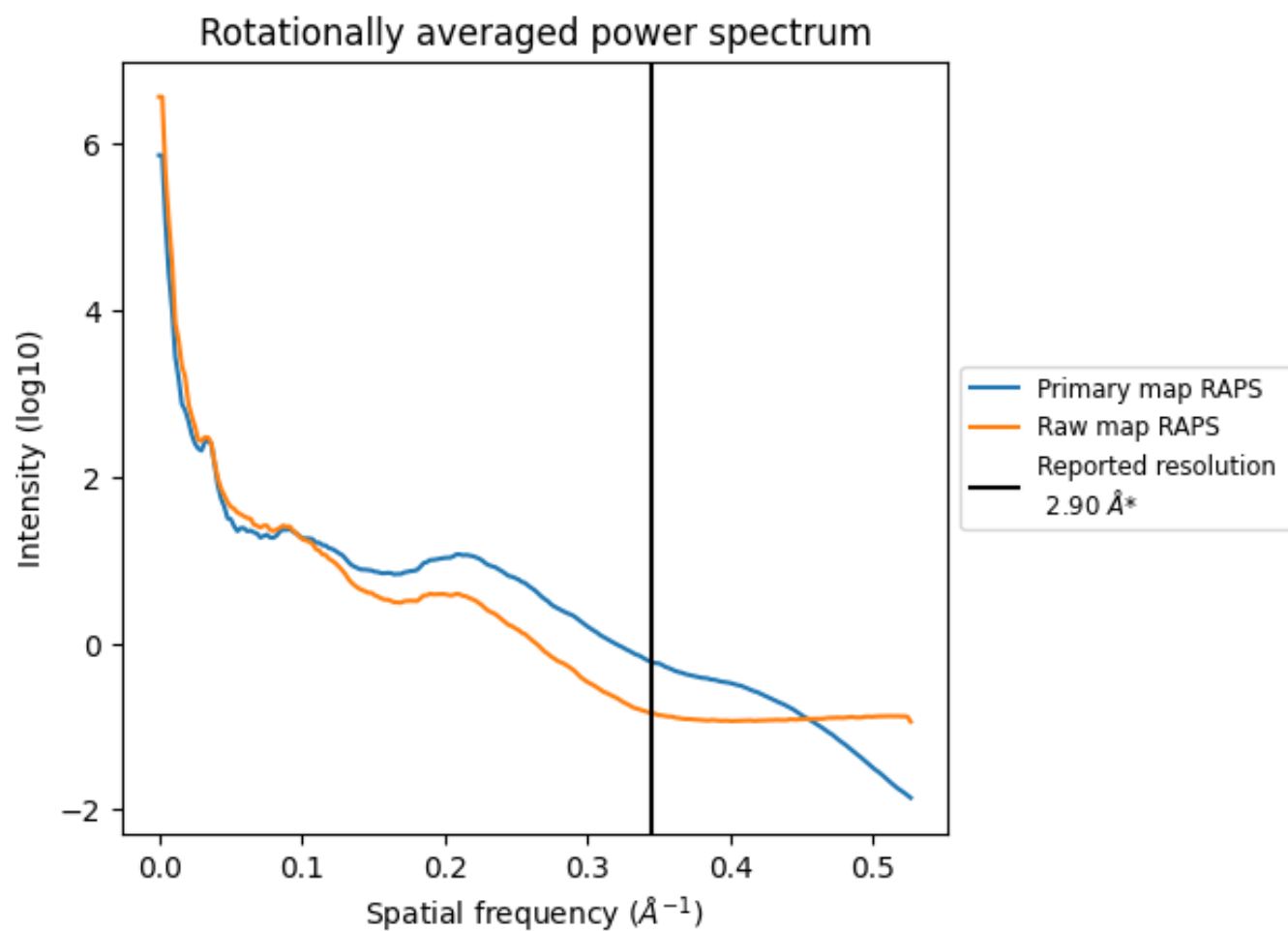
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3013  $\text{nm}^3$ ; this corresponds to an approximate mass of 2722 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 ⓘ

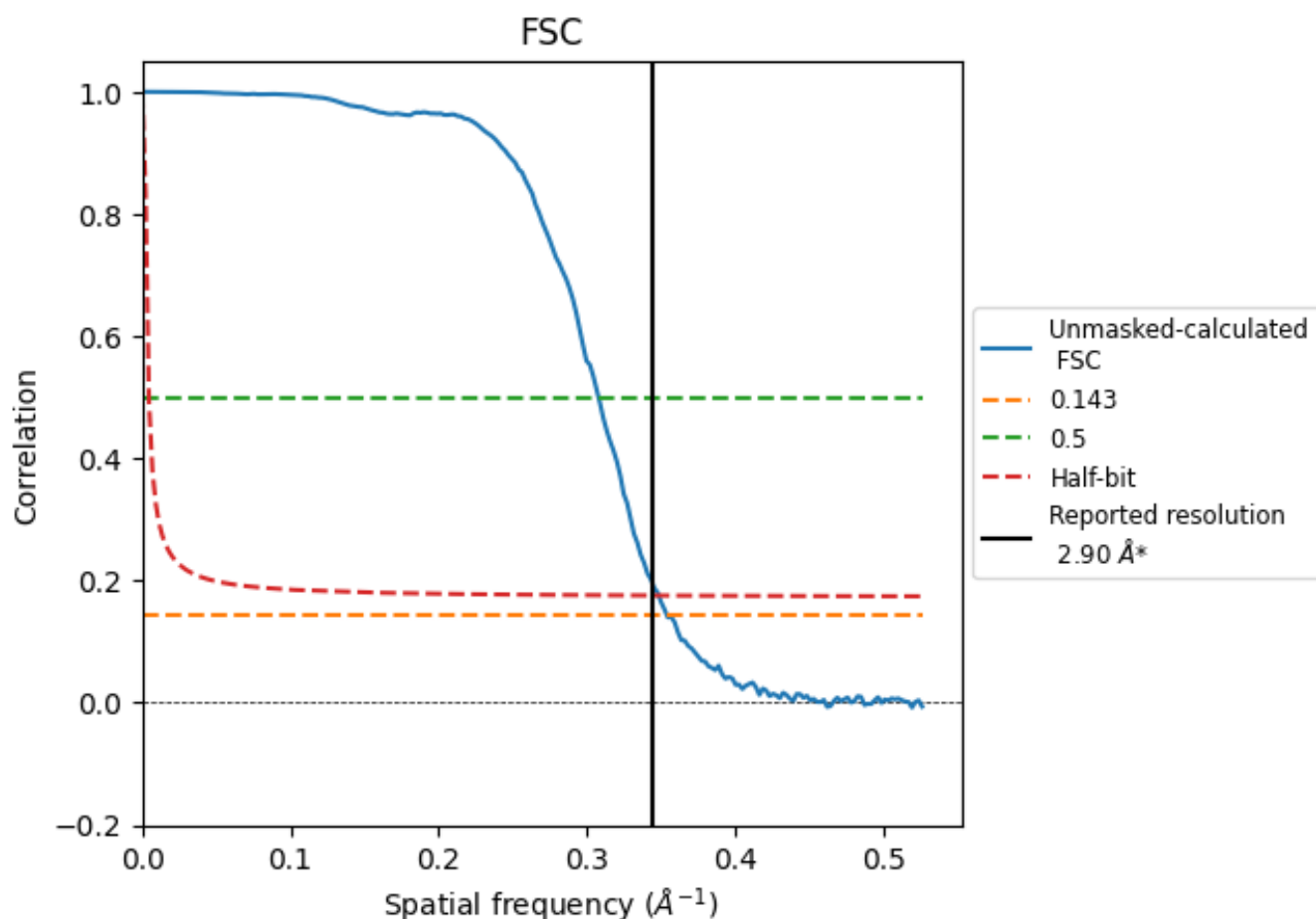


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.345  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.90                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 2.82                               | 3.25 | 2.87     |

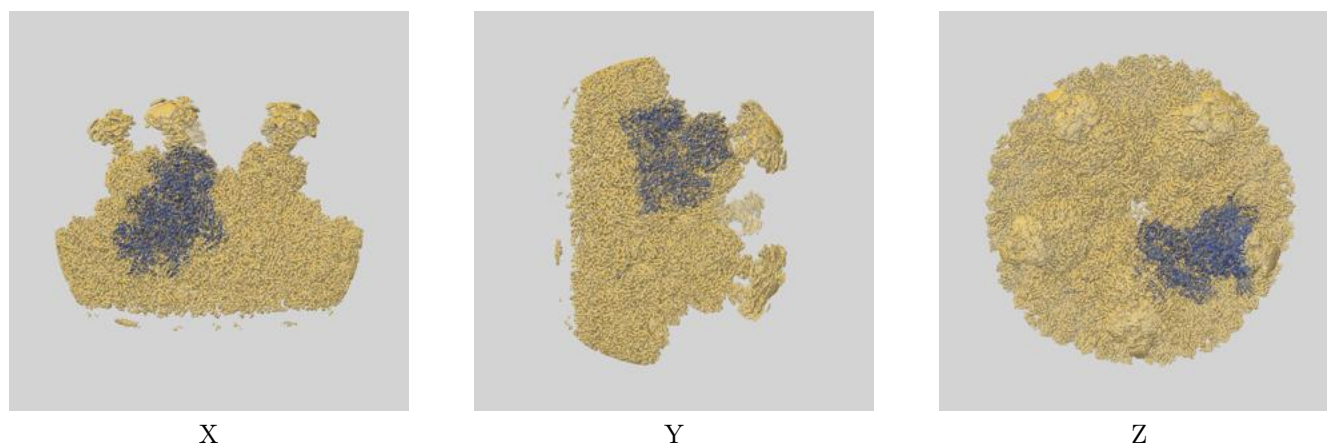
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

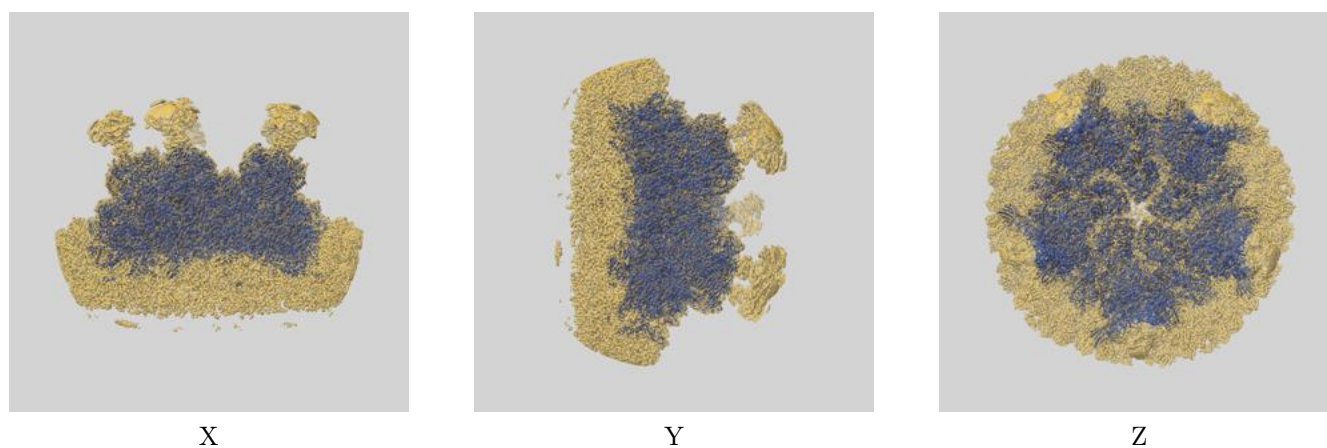
This section contains information regarding the fit between EMDB map EMD-36880 and PDB model 8K49. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlays

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

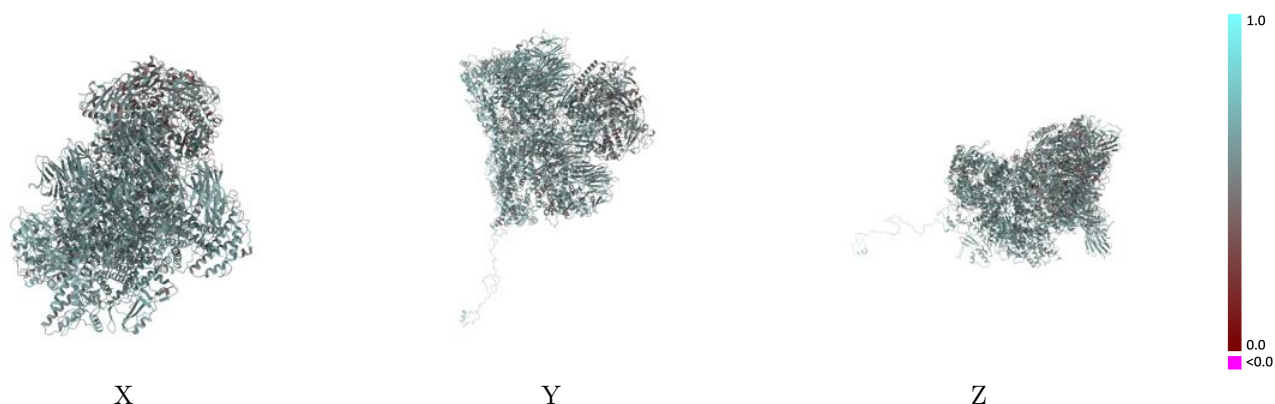


#### 9.1.2 Map-model assembly overlay [i](#)



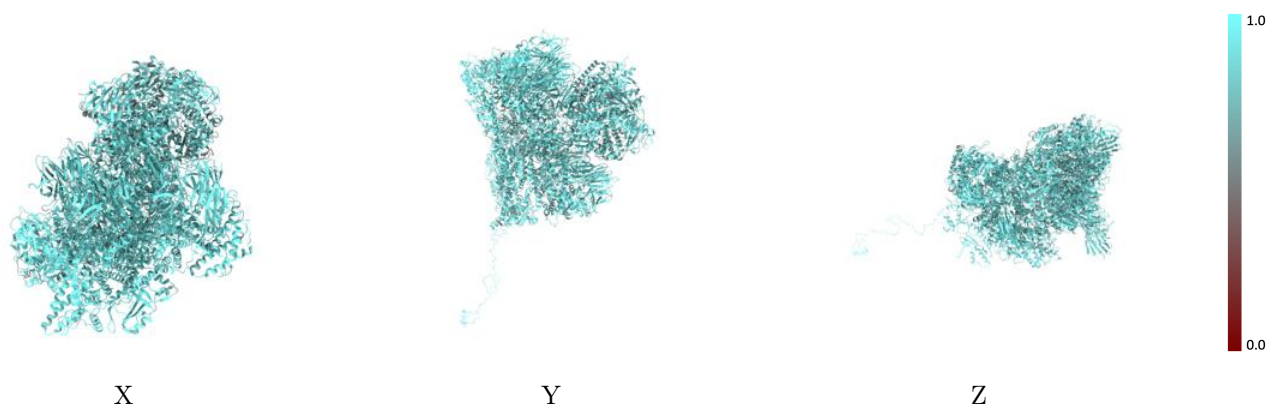
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



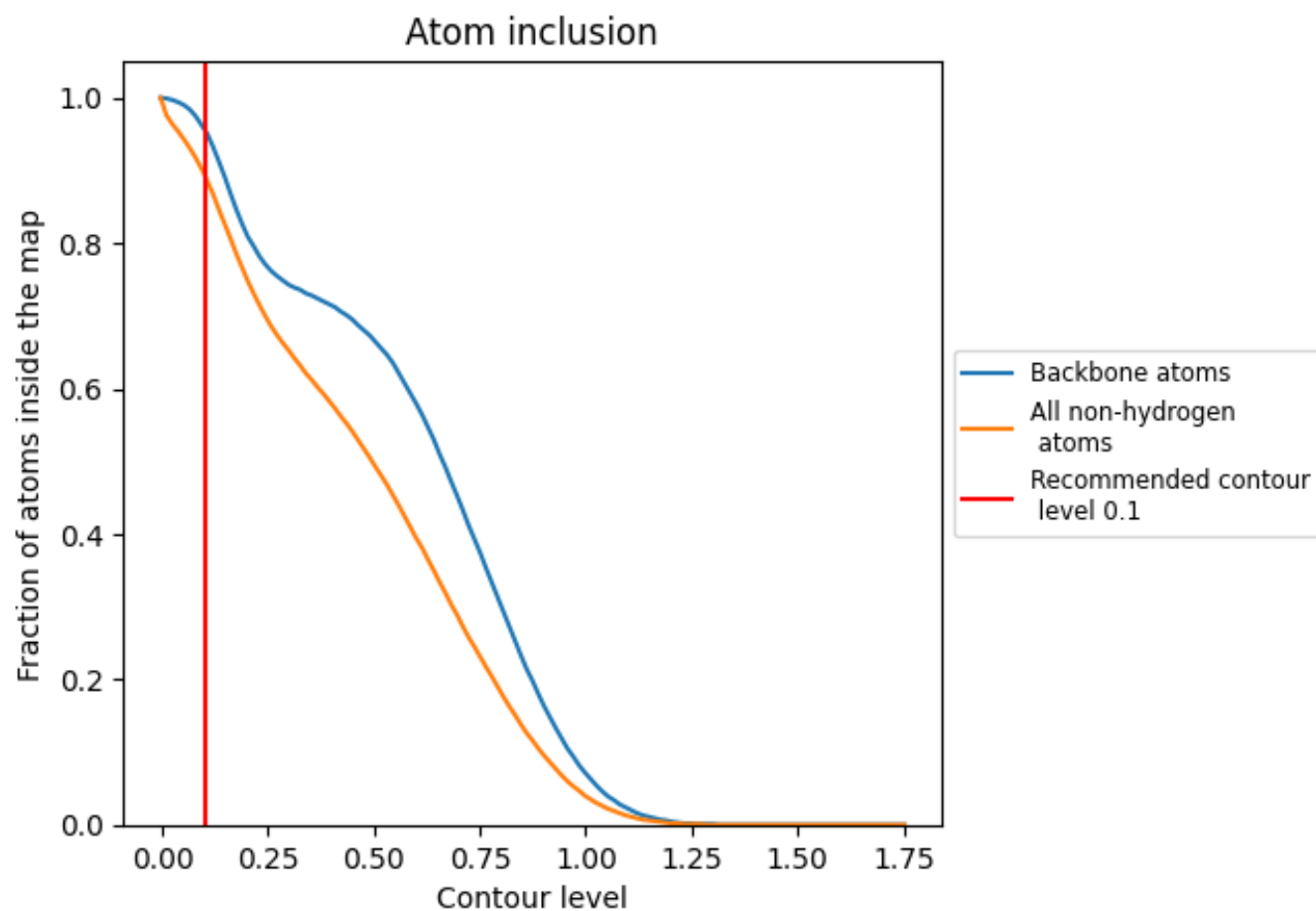
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8950   |  0.5640   |
| A     |  0.9120   |  0.5830   |
| B     |  0.9150   |  0.5850   |
| C     |  0.9190   |  0.5770   |
| D     |  0.9020   |  0.5690   |
| E     |  0.9080   |  0.5730   |
| F     |  0.9260   |  0.5880   |
| G     |  0.9180   |  0.5770   |
| H     |  0.9060   |  0.5740   |
| I     |  0.9070   |  0.5710   |
| J     |  0.9140   |  0.5770   |
| K     |  0.9280   |  0.5930   |
| L     |  0.8870   |  0.5490   |
| M     |  0.9100   |  0.5650   |
| N     |  0.9020  |  0.5590  |
| O     |  0.9130 |  0.5830 |
| P     |  0.9180 |  0.5840 |
| Q     |  0.8710 |  0.5610 |
| R     |  0.8550 |  0.5330 |
| S     |  0.8330 |  0.5160 |
| T     |  0.8530 |  0.5280 |
| r     |  0.8000 |  0.4670 |
| s     |  0.7390 |  0.4320 |
| t     |  0.8000 |  0.4920 |

