



## Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 06:58 PM UTC

PDB ID : 8U7I / pdb\_00008u7i  
EMDB ID : EMD-41983  
Title : Structure of the phage immune evasion protein Gad1 bound to the Gabija GajAB complex  
Authors : Antine, S.P.; Johnson, A.G.; Mooney, S.E.; Mayer, M.L.; Kranzusch, P.J.  
Deposited on : 2023-09-15  
Resolution : 2.57 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

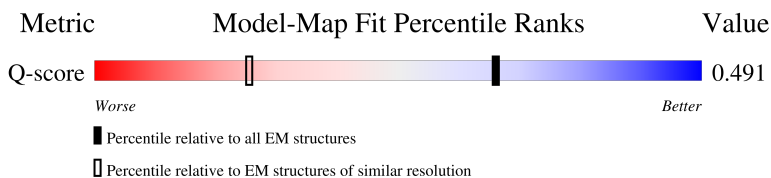
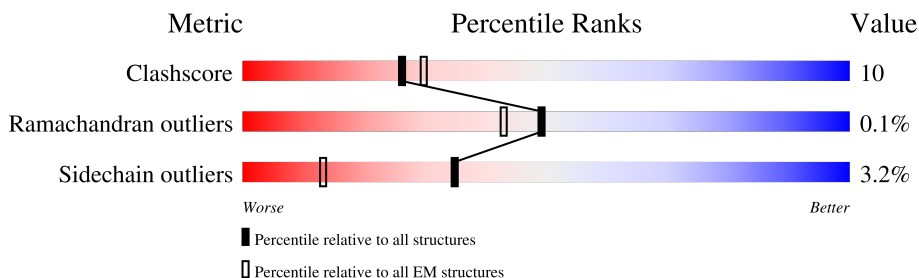
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.57 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 7615 ( 2.07 - 3.07 )                                     |

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     | 675    |                  |
| 1   | B     | 675    |                  |
| 1   | C     | 675    |                  |
| 1   | D     | 675    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | E     | 494    |                  |
| 2   | F     | 494    |                  |
| 2   | G     | 494    |                  |
| 2   | H     | 494    |                  |
| 3   | I     | 295    |                  |
| 3   | J     | 295    |                  |
| 3   | K     | 295    |                  |
| 3   | L     | 295    |                  |
| 3   | M     | 295    |                  |
| 3   | N     | 295    |                  |
| 3   | O     | 295    |                  |
| 3   | P     | 295    |                  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38864 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 Endonuclease GajA.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 626      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5111  | 3268 | 849 | 977 | 17 |         |       |
| 1   | B     | 626      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5111  | 3268 | 849 | 977 | 17 |         |       |
| 1   | C     | 626      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5111  | 3268 | 849 | 977 | 17 |         |       |
| 1   | D     | 626      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 5111  | 3268 | 849 | 977 | 17 |         |       |

There are 392 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -96     | MET      | -      | expression tag | UNP J8H9C1 |
| A     | -95     | GLY      | -      | expression tag | UNP J8H9C1 |
| A     | -94     | SER      | -      | expression tag | UNP J8H9C1 |
| A     | -93     | SER      | -      | expression tag | UNP J8H9C1 |
| A     | -92     | HIS      | -      | expression tag | UNP J8H9C1 |
| A     | -91     | HIS      | -      | expression tag | UNP J8H9C1 |
| A     | -90     | HIS      | -      | expression tag | UNP J8H9C1 |
| A     | -89     | HIS      | -      | expression tag | UNP J8H9C1 |
| A     | -88     | HIS      | -      | expression tag | UNP J8H9C1 |
| A     | -87     | HIS      | -      | expression tag | UNP J8H9C1 |
| A     | -86     | GLY      | -      | expression tag | UNP J8H9C1 |
| A     | -85     | SER      | -      | expression tag | UNP J8H9C1 |
| A     | -84     | GLY      | -      | expression tag | UNP J8H9C1 |
| A     | -83     | VAL      | -      | expression tag | UNP J8H9C1 |
| A     | -82     | LYS      | -      | expression tag | UNP J8H9C1 |
| A     | -81     | THR      | -      | expression tag | UNP J8H9C1 |
| A     | -80     | GLU      | -      | expression tag | UNP J8H9C1 |
| A     | -79     | ASN      | -      | expression tag | UNP J8H9C1 |
| A     | -78     | ASN      | -      | expression tag | UNP J8H9C1 |
| A     | -77     | ASP      | -      | expression tag | UNP J8H9C1 |
| A     | -76     | HIS      | -      | expression tag | UNP J8H9C1 |
| A     | -75     | ILE      | -      | expression tag | UNP J8H9C1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -74     | ASN      | -      | expression tag | UNP J8H9C1 |
| A     | -73     | LEU      | -      | expression tag | UNP J8H9C1 |
| A     | -72     | LYS      | -      | expression tag | UNP J8H9C1 |
| A     | -71     | VAL      | -      | expression tag | UNP J8H9C1 |
| A     | -70     | ALA      | -      | expression tag | UNP J8H9C1 |
| A     | -69     | GLY      | -      | expression tag | UNP J8H9C1 |
| A     | -68     | GLN      | -      | expression tag | UNP J8H9C1 |
| A     | -67     | ASP      | -      | expression tag | UNP J8H9C1 |
| A     | -66     | GLY      | -      | expression tag | UNP J8H9C1 |
| A     | -65     | SER      | -      | expression tag | UNP J8H9C1 |
| A     | -64     | VAL      | -      | expression tag | UNP J8H9C1 |
| A     | -63     | VAL      | -      | expression tag | UNP J8H9C1 |
| A     | -62     | GLN      | -      | expression tag | UNP J8H9C1 |
| A     | -61     | PHE      | -      | expression tag | UNP J8H9C1 |
| A     | -60     | LYS      | -      | expression tag | UNP J8H9C1 |
| A     | -59     | ILE      | -      | expression tag | UNP J8H9C1 |
| A     | -58     | LYS      | -      | expression tag | UNP J8H9C1 |
| A     | -57     | ARG      | -      | expression tag | UNP J8H9C1 |
| A     | -56     | HIS      | -      | expression tag | UNP J8H9C1 |
| A     | -55     | THR      | -      | expression tag | UNP J8H9C1 |
| A     | -54     | PRO      | -      | expression tag | UNP J8H9C1 |
| A     | -53     | LEU      | -      | expression tag | UNP J8H9C1 |
| A     | -52     | SER      | -      | expression tag | UNP J8H9C1 |
| A     | -51     | LYS      | -      | expression tag | UNP J8H9C1 |
| A     | -50     | LEU      | -      | expression tag | UNP J8H9C1 |
| A     | -49     | MET      | -      | expression tag | UNP J8H9C1 |
| A     | -48     | LYS      | -      | expression tag | UNP J8H9C1 |
| A     | -47     | ALA      | -      | expression tag | UNP J8H9C1 |
| A     | -46     | TYR      | -      | expression tag | UNP J8H9C1 |
| A     | -45     | CYS      | -      | expression tag | UNP J8H9C1 |
| A     | -44     | GLU      | -      | expression tag | UNP J8H9C1 |
| A     | -43     | ARG      | -      | expression tag | UNP J8H9C1 |
| A     | -42     | GLN      | -      | expression tag | UNP J8H9C1 |
| A     | -41     | GLY      | -      | expression tag | UNP J8H9C1 |
| A     | -40     | LEU      | -      | expression tag | UNP J8H9C1 |
| A     | -39     | SER      | -      | expression tag | UNP J8H9C1 |
| A     | -38     | MET      | -      | expression tag | UNP J8H9C1 |
| A     | -37     | ARG      | -      | expression tag | UNP J8H9C1 |
| A     | -36     | GLN      | -      | expression tag | UNP J8H9C1 |
| A     | -35     | ILE      | -      | expression tag | UNP J8H9C1 |
| A     | -34     | ARG      | -      | expression tag | UNP J8H9C1 |
| A     | -33     | PHE      | -      | expression tag | UNP J8H9C1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -32     | ARG      | -      | expression tag | UNP J8H9C1 |
| A     | -31     | PHE      | -      | expression tag | UNP J8H9C1 |
| A     | -30     | ASP      | -      | expression tag | UNP J8H9C1 |
| A     | -29     | GLY      | -      | expression tag | UNP J8H9C1 |
| A     | -28     | GLN      | -      | expression tag | UNP J8H9C1 |
| A     | -27     | PRO      | -      | expression tag | UNP J8H9C1 |
| A     | -26     | ILE      | -      | expression tag | UNP J8H9C1 |
| A     | -25     | ASN      | -      | expression tag | UNP J8H9C1 |
| A     | -24     | GLU      | -      | expression tag | UNP J8H9C1 |
| A     | -23     | THR      | -      | expression tag | UNP J8H9C1 |
| A     | -22     | ASP      | -      | expression tag | UNP J8H9C1 |
| A     | -21     | THR      | -      | expression tag | UNP J8H9C1 |
| A     | -20     | PRO      | -      | expression tag | UNP J8H9C1 |
| A     | -19     | ALA      | -      | expression tag | UNP J8H9C1 |
| A     | -18     | GLN      | -      | expression tag | UNP J8H9C1 |
| A     | -17     | LEU      | -      | expression tag | UNP J8H9C1 |
| A     | -16     | GLU      | -      | expression tag | UNP J8H9C1 |
| A     | -15     | MET      | -      | expression tag | UNP J8H9C1 |
| A     | -14     | GLU      | -      | expression tag | UNP J8H9C1 |
| A     | -13     | ASP      | -      | expression tag | UNP J8H9C1 |
| A     | -12     | GLU      | -      | expression tag | UNP J8H9C1 |
| A     | -11     | ASP      | -      | expression tag | UNP J8H9C1 |
| A     | -10     | THR      | -      | expression tag | UNP J8H9C1 |
| A     | -9      | ILE      | -      | expression tag | UNP J8H9C1 |
| A     | -8      | ASP      | -      | expression tag | UNP J8H9C1 |
| A     | -7      | VAL      | -      | expression tag | UNP J8H9C1 |
| A     | -6      | PHE      | -      | expression tag | UNP J8H9C1 |
| A     | -5      | GLN      | -      | expression tag | UNP J8H9C1 |
| A     | -4      | GLN      | -      | expression tag | UNP J8H9C1 |
| A     | -3      | GLN      | -      | expression tag | UNP J8H9C1 |
| A     | -2      | THR      | -      | expression tag | UNP J8H9C1 |
| A     | -1      | GLY      | -      | expression tag | UNP J8H9C1 |
| A     | 0       | GLY      | -      | expression tag | UNP J8H9C1 |
| A     | 1       | SER      | -      | expression tag | UNP J8H9C1 |
| B     | -96     | MET      | -      | expression tag | UNP J8H9C1 |
| B     | -95     | GLY      | -      | expression tag | UNP J8H9C1 |
| B     | -94     | SER      | -      | expression tag | UNP J8H9C1 |
| B     | -93     | SER      | -      | expression tag | UNP J8H9C1 |
| B     | -92     | HIS      | -      | expression tag | UNP J8H9C1 |
| B     | -91     | HIS      | -      | expression tag | UNP J8H9C1 |
| B     | -90     | HIS      | -      | expression tag | UNP J8H9C1 |
| B     | -89     | HIS      | -      | expression tag | UNP J8H9C1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -88     | HIS      | -      | expression tag | UNP J8H9C1 |
| B     | -87     | HIS      | -      | expression tag | UNP J8H9C1 |
| B     | -86     | GLY      | -      | expression tag | UNP J8H9C1 |
| B     | -85     | SER      | -      | expression tag | UNP J8H9C1 |
| B     | -84     | GLY      | -      | expression tag | UNP J8H9C1 |
| B     | -83     | VAL      | -      | expression tag | UNP J8H9C1 |
| B     | -82     | LYS      | -      | expression tag | UNP J8H9C1 |
| B     | -81     | THR      | -      | expression tag | UNP J8H9C1 |
| B     | -80     | GLU      | -      | expression tag | UNP J8H9C1 |
| B     | -79     | ASN      | -      | expression tag | UNP J8H9C1 |
| B     | -78     | ASN      | -      | expression tag | UNP J8H9C1 |
| B     | -77     | ASP      | -      | expression tag | UNP J8H9C1 |
| B     | -76     | HIS      | -      | expression tag | UNP J8H9C1 |
| B     | -75     | ILE      | -      | expression tag | UNP J8H9C1 |
| B     | -74     | ASN      | -      | expression tag | UNP J8H9C1 |
| B     | -73     | LEU      | -      | expression tag | UNP J8H9C1 |
| B     | -72     | LYS      | -      | expression tag | UNP J8H9C1 |
| B     | -71     | VAL      | -      | expression tag | UNP J8H9C1 |
| B     | -70     | ALA      | -      | expression tag | UNP J8H9C1 |
| B     | -69     | GLY      | -      | expression tag | UNP J8H9C1 |
| B     | -68     | GLN      | -      | expression tag | UNP J8H9C1 |
| B     | -67     | ASP      | -      | expression tag | UNP J8H9C1 |
| B     | -66     | GLY      | -      | expression tag | UNP J8H9C1 |
| B     | -65     | SER      | -      | expression tag | UNP J8H9C1 |
| B     | -64     | VAL      | -      | expression tag | UNP J8H9C1 |
| B     | -63     | VAL      | -      | expression tag | UNP J8H9C1 |
| B     | -62     | GLN      | -      | expression tag | UNP J8H9C1 |
| B     | -61     | PHE      | -      | expression tag | UNP J8H9C1 |
| B     | -60     | LYS      | -      | expression tag | UNP J8H9C1 |
| B     | -59     | ILE      | -      | expression tag | UNP J8H9C1 |
| B     | -58     | LYS      | -      | expression tag | UNP J8H9C1 |
| B     | -57     | ARG      | -      | expression tag | UNP J8H9C1 |
| B     | -56     | HIS      | -      | expression tag | UNP J8H9C1 |
| B     | -55     | THR      | -      | expression tag | UNP J8H9C1 |
| B     | -54     | PRO      | -      | expression tag | UNP J8H9C1 |
| B     | -53     | LEU      | -      | expression tag | UNP J8H9C1 |
| B     | -52     | SER      | -      | expression tag | UNP J8H9C1 |
| B     | -51     | LYS      | -      | expression tag | UNP J8H9C1 |
| B     | -50     | LEU      | -      | expression tag | UNP J8H9C1 |
| B     | -49     | MET      | -      | expression tag | UNP J8H9C1 |
| B     | -48     | LYS      | -      | expression tag | UNP J8H9C1 |
| B     | -47     | ALA      | -      | expression tag | UNP J8H9C1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -46     | TYR      | -      | expression tag | UNP J8H9C1 |
| B     | -45     | CYS      | -      | expression tag | UNP J8H9C1 |
| B     | -44     | GLU      | -      | expression tag | UNP J8H9C1 |
| B     | -43     | ARG      | -      | expression tag | UNP J8H9C1 |
| B     | -42     | GLN      | -      | expression tag | UNP J8H9C1 |
| B     | -41     | GLY      | -      | expression tag | UNP J8H9C1 |
| B     | -40     | LEU      | -      | expression tag | UNP J8H9C1 |
| B     | -39     | SER      | -      | expression tag | UNP J8H9C1 |
| B     | -38     | MET      | -      | expression tag | UNP J8H9C1 |
| B     | -37     | ARG      | -      | expression tag | UNP J8H9C1 |
| B     | -36     | GLN      | -      | expression tag | UNP J8H9C1 |
| B     | -35     | ILE      | -      | expression tag | UNP J8H9C1 |
| B     | -34     | ARG      | -      | expression tag | UNP J8H9C1 |
| B     | -33     | PHE      | -      | expression tag | UNP J8H9C1 |
| B     | -32     | ARG      | -      | expression tag | UNP J8H9C1 |
| B     | -31     | PHE      | -      | expression tag | UNP J8H9C1 |
| B     | -30     | ASP      | -      | expression tag | UNP J8H9C1 |
| B     | -29     | GLY      | -      | expression tag | UNP J8H9C1 |
| B     | -28     | GLN      | -      | expression tag | UNP J8H9C1 |
| B     | -27     | PRO      | -      | expression tag | UNP J8H9C1 |
| B     | -26     | ILE      | -      | expression tag | UNP J8H9C1 |
| B     | -25     | ASN      | -      | expression tag | UNP J8H9C1 |
| B     | -24     | GLU      | -      | expression tag | UNP J8H9C1 |
| B     | -23     | THR      | -      | expression tag | UNP J8H9C1 |
| B     | -22     | ASP      | -      | expression tag | UNP J8H9C1 |
| B     | -21     | THR      | -      | expression tag | UNP J8H9C1 |
| B     | -20     | PRO      | -      | expression tag | UNP J8H9C1 |
| B     | -19     | ALA      | -      | expression tag | UNP J8H9C1 |
| B     | -18     | GLN      | -      | expression tag | UNP J8H9C1 |
| B     | -17     | LEU      | -      | expression tag | UNP J8H9C1 |
| B     | -16     | GLU      | -      | expression tag | UNP J8H9C1 |
| B     | -15     | MET      | -      | expression tag | UNP J8H9C1 |
| B     | -14     | GLU      | -      | expression tag | UNP J8H9C1 |
| B     | -13     | ASP      | -      | expression tag | UNP J8H9C1 |
| B     | -12     | GLU      | -      | expression tag | UNP J8H9C1 |
| B     | -11     | ASP      | -      | expression tag | UNP J8H9C1 |
| B     | -10     | THR      | -      | expression tag | UNP J8H9C1 |
| B     | -9      | ILE      | -      | expression tag | UNP J8H9C1 |
| B     | -8      | ASP      | -      | expression tag | UNP J8H9C1 |
| B     | -7      | VAL      | -      | expression tag | UNP J8H9C1 |
| B     | -6      | PHE      | -      | expression tag | UNP J8H9C1 |
| B     | -5      | GLN      | -      | expression tag | UNP J8H9C1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | -4      | GLN      | -      | expression tag | UNP J8H9C1 |
| B     | -3      | GLN      | -      | expression tag | UNP J8H9C1 |
| B     | -2      | THR      | -      | expression tag | UNP J8H9C1 |
| B     | -1      | GLY      | -      | expression tag | UNP J8H9C1 |
| B     | 0       | GLY      | -      | expression tag | UNP J8H9C1 |
| B     | 1       | SER      | -      | expression tag | UNP J8H9C1 |
| C     | -96     | MET      | -      | expression tag | UNP J8H9C1 |
| C     | -95     | GLY      | -      | expression tag | UNP J8H9C1 |
| C     | -94     | SER      | -      | expression tag | UNP J8H9C1 |
| C     | -93     | SER      | -      | expression tag | UNP J8H9C1 |
| C     | -92     | HIS      | -      | expression tag | UNP J8H9C1 |
| C     | -91     | HIS      | -      | expression tag | UNP J8H9C1 |
| C     | -90     | HIS      | -      | expression tag | UNP J8H9C1 |
| C     | -89     | HIS      | -      | expression tag | UNP J8H9C1 |
| C     | -88     | HIS      | -      | expression tag | UNP J8H9C1 |
| C     | -87     | HIS      | -      | expression tag | UNP J8H9C1 |
| C     | -86     | GLY      | -      | expression tag | UNP J8H9C1 |
| C     | -85     | SER      | -      | expression tag | UNP J8H9C1 |
| C     | -84     | GLY      | -      | expression tag | UNP J8H9C1 |
| C     | -83     | VAL      | -      | expression tag | UNP J8H9C1 |
| C     | -82     | LYS      | -      | expression tag | UNP J8H9C1 |
| C     | -81     | THR      | -      | expression tag | UNP J8H9C1 |
| C     | -80     | GLU      | -      | expression tag | UNP J8H9C1 |
| C     | -79     | ASN      | -      | expression tag | UNP J8H9C1 |
| C     | -78     | ASN      | -      | expression tag | UNP J8H9C1 |
| C     | -77     | ASP      | -      | expression tag | UNP J8H9C1 |
| C     | -76     | HIS      | -      | expression tag | UNP J8H9C1 |
| C     | -75     | ILE      | -      | expression tag | UNP J8H9C1 |
| C     | -74     | ASN      | -      | expression tag | UNP J8H9C1 |
| C     | -73     | LEU      | -      | expression tag | UNP J8H9C1 |
| C     | -72     | LYS      | -      | expression tag | UNP J8H9C1 |
| C     | -71     | VAL      | -      | expression tag | UNP J8H9C1 |
| C     | -70     | ALA      | -      | expression tag | UNP J8H9C1 |
| C     | -69     | GLY      | -      | expression tag | UNP J8H9C1 |
| C     | -68     | GLN      | -      | expression tag | UNP J8H9C1 |
| C     | -67     | ASP      | -      | expression tag | UNP J8H9C1 |
| C     | -66     | GLY      | -      | expression tag | UNP J8H9C1 |
| C     | -65     | SER      | -      | expression tag | UNP J8H9C1 |
| C     | -64     | VAL      | -      | expression tag | UNP J8H9C1 |
| C     | -63     | VAL      | -      | expression tag | UNP J8H9C1 |
| C     | -62     | GLN      | -      | expression tag | UNP J8H9C1 |
| C     | -61     | PHE      | -      | expression tag | UNP J8H9C1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -60     | LYS      | -      | expression tag | UNP J8H9C1 |
| C     | -59     | ILE      | -      | expression tag | UNP J8H9C1 |
| C     | -58     | LYS      | -      | expression tag | UNP J8H9C1 |
| C     | -57     | ARG      | -      | expression tag | UNP J8H9C1 |
| C     | -56     | HIS      | -      | expression tag | UNP J8H9C1 |
| C     | -55     | THR      | -      | expression tag | UNP J8H9C1 |
| C     | -54     | PRO      | -      | expression tag | UNP J8H9C1 |
| C     | -53     | LEU      | -      | expression tag | UNP J8H9C1 |
| C     | -52     | SER      | -      | expression tag | UNP J8H9C1 |
| C     | -51     | LYS      | -      | expression tag | UNP J8H9C1 |
| C     | -50     | LEU      | -      | expression tag | UNP J8H9C1 |
| C     | -49     | MET      | -      | expression tag | UNP J8H9C1 |
| C     | -48     | LYS      | -      | expression tag | UNP J8H9C1 |
| C     | -47     | ALA      | -      | expression tag | UNP J8H9C1 |
| C     | -46     | TYR      | -      | expression tag | UNP J8H9C1 |
| C     | -45     | CYS      | -      | expression tag | UNP J8H9C1 |
| C     | -44     | GLU      | -      | expression tag | UNP J8H9C1 |
| C     | -43     | ARG      | -      | expression tag | UNP J8H9C1 |
| C     | -42     | GLN      | -      | expression tag | UNP J8H9C1 |
| C     | -41     | GLY      | -      | expression tag | UNP J8H9C1 |
| C     | -40     | LEU      | -      | expression tag | UNP J8H9C1 |
| C     | -39     | SER      | -      | expression tag | UNP J8H9C1 |
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| C     | -35     | ILE      | -      | expression tag | UNP J8H9C1 |
| C     | -34     | ARG      | -      | expression tag | UNP J8H9C1 |
| C     | -33     | PHE      | -      | expression tag | UNP J8H9C1 |
| C     | -32     | ARG      | -      | expression tag | UNP J8H9C1 |
| C     | -31     | PHE      | -      | expression tag | UNP J8H9C1 |
| C     | -30     | ASP      | -      | expression tag | UNP J8H9C1 |
| C     | -29     | GLY      | -      | expression tag | UNP J8H9C1 |
| C     | -28     | GLN      | -      | expression tag | UNP J8H9C1 |
| C     | -27     | PRO      | -      | expression tag | UNP J8H9C1 |
| C     | -26     | ILE      | -      | expression tag | UNP J8H9C1 |
| C     | -25     | ASN      | -      | expression tag | UNP J8H9C1 |
| C     | -24     | GLU      | -      | expression tag | UNP J8H9C1 |
| C     | -23     | THR      | -      | expression tag | UNP J8H9C1 |
| C     | -22     | ASP      | -      | expression tag | UNP J8H9C1 |
| C     | -21     | THR      | -      | expression tag | UNP J8H9C1 |
| C     | -20     | PRO      | -      | expression tag | UNP J8H9C1 |
| C     | -19     | ALA      | -      | expression tag | UNP J8H9C1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -18     | GLN      | -      | expression tag | UNP J8H9C1 |
| C     | -17     | LEU      | -      | expression tag | UNP J8H9C1 |
| C     | -16     | GLU      | -      | expression tag | UNP J8H9C1 |
| C     | -15     | MET      | -      | expression tag | UNP J8H9C1 |
| C     | -14     | GLU      | -      | expression tag | UNP J8H9C1 |
| C     | -13     | ASP      | -      | expression tag | UNP J8H9C1 |
| C     | -12     | GLU      | -      | expression tag | UNP J8H9C1 |
| C     | -11     | ASP      | -      | expression tag | UNP J8H9C1 |
| C     | -10     | THR      | -      | expression tag | UNP J8H9C1 |
| C     | -9      | ILE      | -      | expression tag | UNP J8H9C1 |
| C     | -8      | ASP      | -      | expression tag | UNP J8H9C1 |
| C     | -7      | VAL      | -      | expression tag | UNP J8H9C1 |
| C     | -6      | PHE      | -      | expression tag | UNP J8H9C1 |
| C     | -5      | GLN      | -      | expression tag | UNP J8H9C1 |
| C     | -4      | GLN      | -      | expression tag | UNP J8H9C1 |
| C     | -3      | GLN      | -      | expression tag | UNP J8H9C1 |
| C     | -2      | THR      | -      | expression tag | UNP J8H9C1 |
| C     | -1      | GLY      | -      | expression tag | UNP J8H9C1 |
| C     | 0       | GLY      | -      | expression tag | UNP J8H9C1 |
| C     | 1       | SER      | -      | expression tag | UNP J8H9C1 |
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| D     | -95     | GLY      | -      | expression tag | UNP J8H9C1 |
| D     | -94     | SER      | -      | expression tag | UNP J8H9C1 |
| D     | -93     | SER      | -      | expression tag | UNP J8H9C1 |
| D     | -92     | HIS      | -      | expression tag | UNP J8H9C1 |
| D     | -91     | HIS      | -      | expression tag | UNP J8H9C1 |
| D     | -90     | HIS      | -      | expression tag | UNP J8H9C1 |
| D     | -89     | HIS      | -      | expression tag | UNP J8H9C1 |
| D     | -88     | HIS      | -      | expression tag | UNP J8H9C1 |
| D     | -87     | HIS      | -      | expression tag | UNP J8H9C1 |
| D     | -86     | GLY      | -      | expression tag | UNP J8H9C1 |
| D     | -85     | SER      | -      | expression tag | UNP J8H9C1 |
| D     | -84     | GLY      | -      | expression tag | UNP J8H9C1 |
| D     | -83     | VAL      | -      | expression tag | UNP J8H9C1 |
| D     | -82     | LYS      | -      | expression tag | UNP J8H9C1 |
| D     | -81     | THR      | -      | expression tag | UNP J8H9C1 |
| D     | -80     | GLU      | -      | expression tag | UNP J8H9C1 |
| D     | -79     | ASN      | -      | expression tag | UNP J8H9C1 |
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| D     | -77     | ASP      | -      | expression tag | UNP J8H9C1 |
| D     | -76     | HIS      | -      | expression tag | UNP J8H9C1 |
| D     | -75     | ILE      | -      | expression tag | UNP J8H9C1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -74     | ASN      | -      | expression tag | UNP J8H9C1 |
| D     | -73     | LEU      | -      | expression tag | UNP J8H9C1 |
| D     | -72     | LYS      | -      | expression tag | UNP J8H9C1 |
| D     | -71     | VAL      | -      | expression tag | UNP J8H9C1 |
| D     | -70     | ALA      | -      | expression tag | UNP J8H9C1 |
| D     | -69     | GLY      | -      | expression tag | UNP J8H9C1 |
| D     | -68     | GLN      | -      | expression tag | UNP J8H9C1 |
| D     | -67     | ASP      | -      | expression tag | UNP J8H9C1 |
| D     | -66     | GLY      | -      | expression tag | UNP J8H9C1 |
| D     | -65     | SER      | -      | expression tag | UNP J8H9C1 |
| D     | -64     | VAL      | -      | expression tag | UNP J8H9C1 |
| D     | -63     | VAL      | -      | expression tag | UNP J8H9C1 |
| D     | -62     | GLN      | -      | expression tag | UNP J8H9C1 |
| D     | -61     | PHE      | -      | expression tag | UNP J8H9C1 |
| D     | -60     | LYS      | -      | expression tag | UNP J8H9C1 |
| D     | -59     | ILE      | -      | expression tag | UNP J8H9C1 |
| D     | -58     | LYS      | -      | expression tag | UNP J8H9C1 |
| D     | -57     | ARG      | -      | expression tag | UNP J8H9C1 |
| D     | -56     | HIS      | -      | expression tag | UNP J8H9C1 |
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| D     | -53     | LEU      | -      | expression tag | UNP J8H9C1 |
| D     | -52     | SER      | -      | expression tag | UNP J8H9C1 |
| D     | -51     | LYS      | -      | expression tag | UNP J8H9C1 |
| D     | -50     | LEU      | -      | expression tag | UNP J8H9C1 |
| D     | -49     | MET      | -      | expression tag | UNP J8H9C1 |
| D     | -48     | LYS      | -      | expression tag | UNP J8H9C1 |
| D     | -47     | ALA      | -      | expression tag | UNP J8H9C1 |
| D     | -46     | TYR      | -      | expression tag | UNP J8H9C1 |
| D     | -45     | CYS      | -      | expression tag | UNP J8H9C1 |
| D     | -44     | GLU      | -      | expression tag | UNP J8H9C1 |
| D     | -43     | ARG      | -      | expression tag | UNP J8H9C1 |
| D     | -42     | GLN      | -      | expression tag | UNP J8H9C1 |
| D     | -41     | GLY      | -      | expression tag | UNP J8H9C1 |
| D     | -40     | LEU      | -      | expression tag | UNP J8H9C1 |
| D     | -39     | SER      | -      | expression tag | UNP J8H9C1 |
| D     | -38     | MET      | -      | expression tag | UNP J8H9C1 |
| D     | -37     | ARG      | -      | expression tag | UNP J8H9C1 |
| D     | -36     | GLN      | -      | expression tag | UNP J8H9C1 |
| D     | -35     | ILE      | -      | expression tag | UNP J8H9C1 |
| D     | -34     | ARG      | -      | expression tag | UNP J8H9C1 |
| D     | -33     | PHE      | -      | expression tag | UNP J8H9C1 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| D     | -32     | ARG      | -      | expression tag | UNP J8H9C1 |
| D     | -31     | PHE      | -      | expression tag | UNP J8H9C1 |
| D     | -30     | ASP      | -      | expression tag | UNP J8H9C1 |
| D     | -29     | GLY      | -      | expression tag | UNP J8H9C1 |
| D     | -28     | GLN      | -      | expression tag | UNP J8H9C1 |
| D     | -27     | PRO      | -      | expression tag | UNP J8H9C1 |
| D     | -26     | ILE      | -      | expression tag | UNP J8H9C1 |
| D     | -25     | ASN      | -      | expression tag | UNP J8H9C1 |
| D     | -24     | GLU      | -      | expression tag | UNP J8H9C1 |
| D     | -23     | THR      | -      | expression tag | UNP J8H9C1 |
| D     | -22     | ASP      | -      | expression tag | UNP J8H9C1 |
| D     | -21     | THR      | -      | expression tag | UNP J8H9C1 |
| D     | -20     | PRO      | -      | expression tag | UNP J8H9C1 |
| D     | -19     | ALA      | -      | expression tag | UNP J8H9C1 |
| D     | -18     | GLN      | -      | expression tag | UNP J8H9C1 |
| D     | -17     | LEU      | -      | expression tag | UNP J8H9C1 |
| D     | -16     | GLU      | -      | expression tag | UNP J8H9C1 |
| D     | -15     | MET      | -      | expression tag | UNP J8H9C1 |
| D     | -14     | GLU      | -      | expression tag | UNP J8H9C1 |
| D     | -13     | ASP      | -      | expression tag | UNP J8H9C1 |
| D     | -12     | GLU      | -      | expression tag | UNP J8H9C1 |
| D     | -11     | ASP      | -      | expression tag | UNP J8H9C1 |
| D     | -10     | THR      | -      | expression tag | UNP J8H9C1 |
| D     | -9      | ILE      | -      | expression tag | UNP J8H9C1 |
| D     | -8      | ASP      | -      | expression tag | UNP J8H9C1 |
| D     | -7      | VAL      | -      | expression tag | UNP J8H9C1 |
| D     | -6      | PHE      | -      | expression tag | UNP J8H9C1 |
| D     | -5      | GLN      | -      | expression tag | UNP J8H9C1 |
| D     | -4      | GLN      | -      | expression tag | UNP J8H9C1 |
| D     | -3      | GLN      | -      | expression tag | UNP J8H9C1 |
| D     | -2      | THR      | -      | expression tag | UNP J8H9C1 |
| D     | -1      | GLY      | -      | expression tag | UNP J8H9C1 |
| D     | 0       | GLY      | -      | expression tag | UNP J8H9C1 |
| D     | 1       | SER      | -      | expression tag | UNP J8H9C1 |

- Molecule 2 is a protein called Gabija protein GajB.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | E     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2326  | 1502 | 381 | 441 | 2 |         |       |
| 2   | F     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2326  | 1502 | 381 | 441 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | G     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2326  | 1502 | 381 | 441 | 2 |         |       |
| 2   | H     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2326  | 1502 | 381 | 441 | 2 |         |       |

- Molecule 3 is a protein called Gabija Anti-Defense 1.

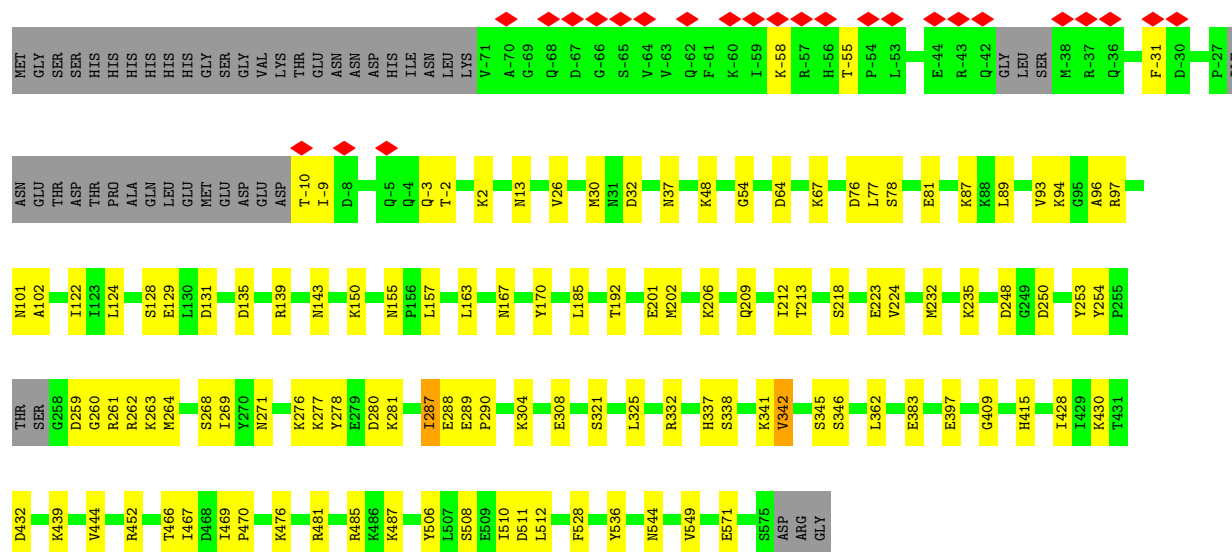
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | I     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1346  | 867 | 231 | 240 | 8 |         |       |
| 3   | J     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1346  | 867 | 231 | 240 | 8 |         |       |
| 3   | K     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1346  | 867 | 231 | 240 | 8 |         |       |
| 3   | L     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1346  | 867 | 231 | 240 | 8 |         |       |
| 3   | M     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 933   | 602 | 152 | 172 | 7 |         |       |
| 3   | N     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 933   | 602 | 152 | 172 | 7 |         |       |
| 3   | O     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 933   | 602 | 152 | 172 | 7 |         |       |
| 3   | P     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 933   | 602 | 152 | 172 | 7 |         |       |





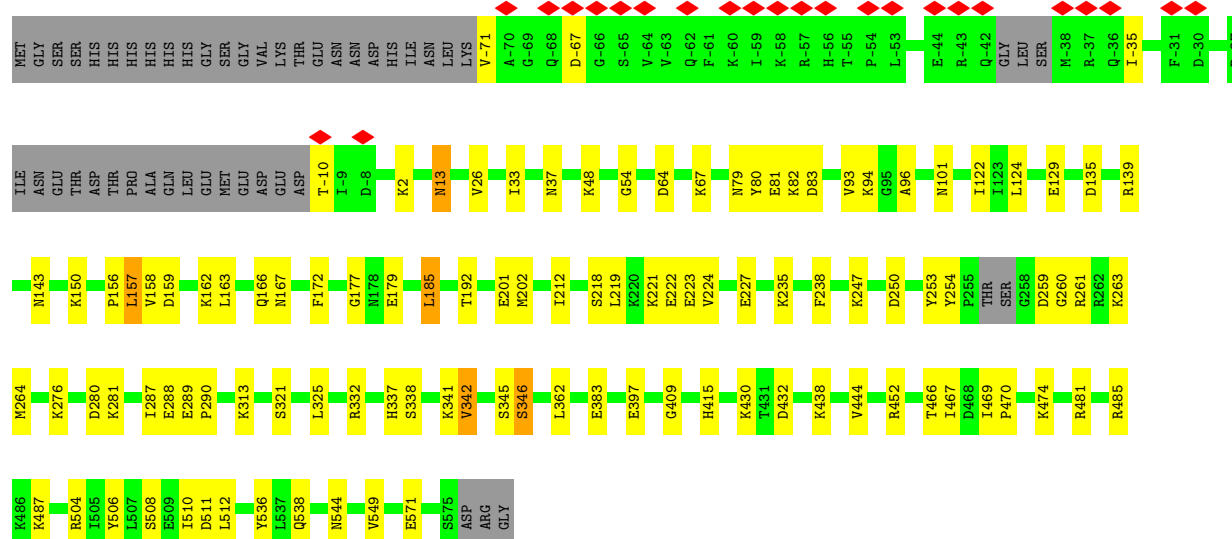
• Molecule 1: Endonuclease GajA

Chain C: 75% 17% 7%



• Molecule 1: Endonuclease GajA

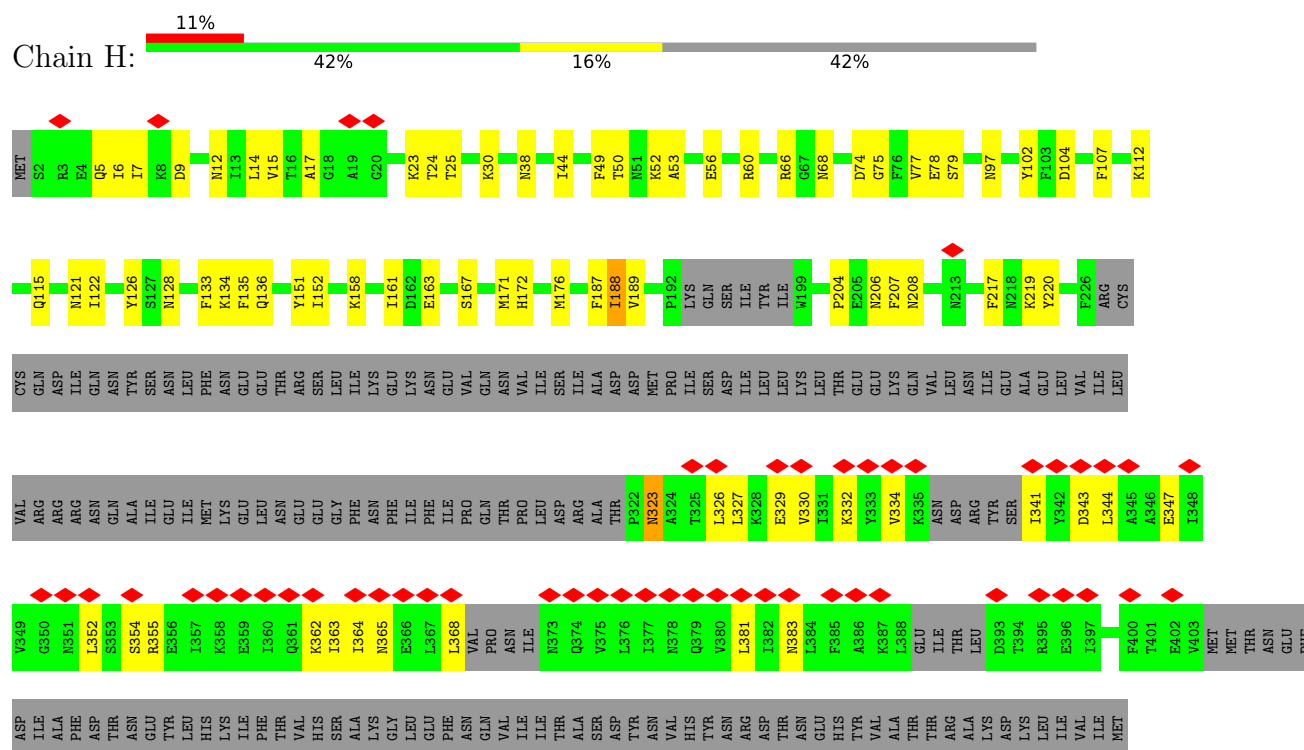
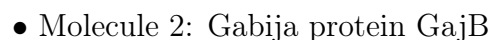
Chain D: 77% 15% 7%



• Molecule 2: Gabija protein GajB

Chain E: 9% 40% 17% 42%





ASP  
ASN  
LYS  
LYS  
TYR  
SER  
ASP  
TYR  
ILE  
THR  
LEU  
MET  
LYS  
GLU  
LEU  
LYS  
LYS  
ILE  
ASN  
SER  
ILE

### • Molecule 3: Gabija Anti-Defense 1

Chain I:  34% 20% 45%

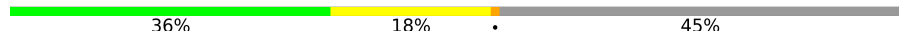
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GLY  
ILE  
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THR  
SER  
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ASN  
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VAL  
ASP  
SER  
ASN  
ILE  
GLY  
GLY  
LYS  
TYR  
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LEU  
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ARG  
ALA  
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GLY  
PHE  
GLN  
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SER  
GLY  
LEU  
TYR  
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LYS  
ALA  
SER  
GLY  
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TYR  
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VAL  
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LYS  
THR  
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THR  
GLY  
PHE  
MET

MET  
ASN  
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GLY  
ASN  
HIS  
ASP  
GLY  
LEU  
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K133  
Q134  
S135  
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F137  
F138  
M139  
L140  
N141  
L144  
L145  
D146  
R147  
I148  
Q149  
T150  
H151  
P152  
M153  
L154  
L155  
K158  
L162  
S163  
S167  
Y168  
K169  
M173  
H174  
D189  
L189  
L194  
K198  
Y203  
E207  
Y208  
L209  
V210  
D211

L212  
N213  
A214  
M215  
Y216  
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K241  
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Y243  
Q244  
I248  
K255  
D256  
V257  
E258  
D259  
L268  
D269  
D270  
L271  
M272  
L279  
V280  
E281  
C282  
C285  
R288  
G289  
V290  
I291  
L292  
N293  
GLU  
ASN

### • Molecule 3: Gabija Anti-Defense 1

Chain J:  36% 18% 45%

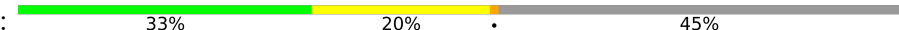
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GLY  
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LYS  
THR  
SER  
GLY  
ASN  
CYS  
PHE  
LEU  
VAL  
ASP  
SER  
ASN  
ILE  
GLY  
GLY  
LYS  
TYR  
ARG  
PHE  
HIS  
SER  
GLN  
LEU  
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ARG  
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THR  
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PRO  
GLN  
SER  
VAL  
ILE  
GLY  
LYS  
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PRO  
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K132  
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Q134  
S135  
H136  
F137  
F138  
M139  
L140  
N141  
L144  
L145  
D146  
R147  
I148  
Q149  
T150  
C160  
Y161  
L162  
S163  
Q164  
E165  
E166  
S167  
Y168  
H174  
I175  
I179  
A184  
R185  
I186  
D189  
V199  
L200  
E201  
L202  
V203  
R204  
F205  
H206

M215  
Y216  
K217  
R219  
K222  
R226  
Q228  
T229  
K230  
E232  
K241  
Y249  
F252  
S253  
V257  
L260  
L268  
P278  
E281  
C282  
K283  
C284  
C285  
V286  
G287  
R288  
L292  
N293  
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ASN

### • Molecule 3: Gabija Anti-Defense 1

Chain K:  33% 20% 45%

MET  
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K132  
K133  
H136  
N137  
F138  
M141  
Y142  
D146  
R147  
I148  
Q149  
M153  
K158  
P159  
C160  
Y161  
L162  
S163  
Q164  
E165  
E166  
S167  
Y168  
I179  
F183  
A184  
R185  
I186  
T187  
S188  
D189  
V196  
V197  
K198  
V199  
L200  
H206  
E207  
V210

D211  
L212  
N213  
A214  
M215  
Y216  
K217  
R219  
K222  
K225  
R226  
F227  
Q228  
T229  
K230  
R231  
E232  
K241  
V249  
S253  
G254  
K255  
D256  
D259  
D270  
L271  
M272  
L275  
N276  
E277  
P278  
L279  
C282  
K283  
C284  
C285  
R288  
L292  
N293  
GLU  
ASN

### • Molecule 3: Gabija Anti-Defense 1

- Molecule 3: Gabija Anti-Defense 1

- Molecule 3: Gabija Anti-Defense 1

- Molecule 3: Gabija Anti-Defense 1



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided |           |
| Number of particles used             | 351193              | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | NONE                | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 41.1                | Depositor |
| Minimum defocus (nm)                 | 800                 | Depositor |
| Maximum defocus (nm)                 | 1900                | Depositor |
| Magnification                        | Not provided        |           |
| Image detector                       | GATAN K3 (6k x 4k)  | Depositor |
| Maximum map value                    | 0.269               | Depositor |
| Minimum map value                    | -0.095              | Depositor |
| Average map value                    | 0.000               | Depositor |
| Map value standard deviation         | 0.009               | Depositor |
| Recommended contour level            | 0.028               | Depositor |
| Map size ( $\text{\AA}$ )            | 311.5, 311.5, 311.5 | wwPDB     |
| Map dimensions                       | 350, 350, 350       | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0    | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.89, 0.89, 0.89    | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | A     | 0.19         | 0/5196  | 0.26        | 0/6968         |
| 1   | B     | 0.19         | 0/5196  | 0.26        | 0/6968         |
| 1   | C     | 0.19         | 0/5196  | 0.26        | 0/6968         |
| 1   | D     | 0.19         | 0/5196  | 0.28        | 0/6968         |
| 2   | E     | 0.13         | 0/2365  | 0.33        | 0/3179         |
| 2   | F     | 0.15         | 0/2365  | 0.36        | 1/3179 (0.0%)  |
| 2   | G     | 0.11         | 0/2365  | 0.28        | 0/3179         |
| 2   | H     | 0.12         | 0/2365  | 0.31        | 0/3179         |
| 3   | I     | 0.14         | 0/1374  | 0.38        | 0/1849         |
| 3   | J     | 0.14         | 0/1374  | 0.30        | 0/1849         |
| 3   | K     | 0.15         | 0/1374  | 0.39        | 0/1849         |
| 3   | L     | 0.16         | 0/1374  | 0.39        | 0/1849         |
| 3   | M     | 0.17         | 0/951   | 0.49        | 0/1280         |
| 3   | N     | 0.22         | 0/951   | 0.51        | 0/1280         |
| 3   | O     | 0.21         | 0/951   | 0.57        | 0/1280         |
| 3   | P     | 0.19         | 0/951   | 0.46        | 0/1280         |
| All | All   | 0.17         | 0/39544 | 0.32        | 1/53104 (0.0%) |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2   | F     | 129 | PRO  | CA-N-CD | -6.48 | 102.93      | 112.00   |

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     | 5111  | 0        | 5155     | 80      | 0            |
| 1   | B     | 5111  | 0        | 5155     | 72      | 0            |
| 1   | C     | 5111  | 0        | 5155     | 76      | 0            |
| 1   | D     | 5111  | 0        | 5155     | 78      | 0            |
| 2   | E     | 2326  | 0        | 2331     | 62      | 0            |
| 2   | F     | 2326  | 0        | 2331     | 60      | 0            |
| 2   | G     | 2326  | 0        | 2331     | 60      | 0            |
| 2   | H     | 2326  | 0        | 2331     | 60      | 0            |
| 3   | I     | 1346  | 0        | 1388     | 49      | 0            |
| 3   | J     | 1346  | 0        | 1388     | 39      | 0            |
| 3   | K     | 1346  | 0        | 1388     | 49      | 0            |
| 3   | L     | 1346  | 0        | 1388     | 54      | 0            |
| 3   | M     | 933   | 0        | 946      | 25      | 0            |
| 3   | N     | 933   | 0        | 946      | 38      | 0            |
| 3   | O     | 933   | 0        | 946      | 27      | 0            |
| 3   | P     | 933   | 0        | 946      | 34      | 0            |
| All | All   | 38864 | 0        | 39280    | 787     | 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 10.

All (787) 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) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:182:LYS:HD3  | 3:O:204:LYS:HB3  | 1.53                     | 0.88              |
| 3:L:263:ASN:HA   | 3:L:266:LYS:HE3  | 1.57                     | 0.85              |
| 3:O:198:LYS:HB2  | 3:O:235:ILE:HD11 | 1.63                     | 0.80              |
| 3:M:185:ARG:HH22 | 3:N:177:ALA:HA   | 1.45                     | 0.80              |
| 2:E:112:LYS:HA   | 2:E:115:GLN:HE22 | 1.46                     | 0.79              |
| 1:A:13:ASN:HB3   | 1:A:342:VAL:HG21 | 1.65                     | 0.79              |
| 2:E:129:PRO:HB3  | 2:E:200:ARG:HG2  | 1.66                     | 0.78              |
| 1:B:162:LYS:O    | 1:B:162:LYS:NZ   | 2.18                     | 0.74              |
| 2:F:28:VAL:HG21  | 2:F:60:ARG:HD3   | 1.70                     | 0.73              |
| 1:D:397:GLU:OE1  | 1:D:397:GLU:N    | 2.19                     | 0.72              |
| 3:K:164:GLN:NE2  | 3:K:249:VAL:O    | 2.22                     | 0.72              |
| 3:J:229:THR:HG23 | 3:J:230:LYS:HG3  | 1.71                     | 0.72              |
| 3:N:182:LYS:HB2  | 3:N:204:LYS:HD3  | 1.71                     | 0.71              |
| 2:G:5:GLN:N      | 2:G:5:GLN:OE1    | 2.22                     | 0.71              |
| 2:E:5:GLN:N      | 2:E:5:GLN:OE1    | 2.23                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:383:GLU:HG3  | 1:B:512:LEU:HD22 | 1.73                     | 0.70              |
| 3:M:232:GLU:N    | 3:M:232:GLU:OE1  | 2.24                     | 0.70              |
| 3:O:203:TYR:CD1  | 3:O:205:PRO:HD2  | 2.26                     | 0.70              |
| 2:E:115:GLN:OE1  | 2:E:115:GLN:N    | 2.24                     | 0.70              |
| 3:K:200:LEU:HA   | 3:K:279:LEU:HD13 | 1.74                     | 0.70              |
| 1:A:383:GLU:HG3  | 1:A:512:LEU:HD22 | 1.75                     | 0.69              |
| 1:D:511:ASP:OD2  | 1:D:538:GLN:NE2  | 2.25                     | 0.69              |
| 1:D:383:GLU:HG3  | 1:D:512:LEU:HD22 | 1.74                     | 0.69              |
| 1:A:511:ASP:OD2  | 1:A:538:GLN:NE2  | 2.25                     | 0.69              |
| 1:C:13:ASN:HB3   | 1:C:342:VAL:HG21 | 1.74                     | 0.69              |
| 2:H:161:ILE:HB   | 2:H:188:ILE:HG22 | 1.75                     | 0.69              |
| 3:L:211:ASP:HB3  | 3:L:214:ALA:HB2  | 1.75                     | 0.68              |
| 2:E:51:ASN:OD1   | 2:E:55:LYS:NZ    | 2.26                     | 0.68              |
| 2:F:5:GLN:OE1    | 2:F:5:GLN:N      | 2.25                     | 0.68              |
| 2:H:14:LEU:HD23  | 2:H:188:ILE:HD11 | 1.74                     | 0.68              |
| 1:B:-4:GLN:NE2   | 1:B:103:ASP:OD2  | 2.22                     | 0.68              |
| 1:C:383:GLU:HG3  | 1:C:512:LEU:HD22 | 1.76                     | 0.68              |
| 1:C:170:TYR:OH   | 1:C:276:LYS:O    | 2.10                     | 0.68              |
| 1:D:2:LYS:NZ     | 1:D:83:ASP:OD2   | 2.27                     | 0.68              |
| 2:E:97:ASN:ND2   | 2:F:97:ASN:O     | 2.26                     | 0.68              |
| 3:M:185:ARG:HE   | 3:M:199:VAL:HG11 | 1.60                     | 0.67              |
| 2:G:121:ASN:HB3  | 2:H:122:ILE:HG12 | 1.77                     | 0.67              |
| 1:B:511:ASP:OD2  | 1:B:538:GLN:NE2  | 2.27                     | 0.67              |
| 1:B:65:THR:HG23  | 1:B:113:TYR:HB3  | 1.76                     | 0.67              |
| 1:D:13:ASN:OD1   | 1:D:13:ASN:N     | 2.27                     | 0.67              |
| 2:H:126:TYR:HD2  | 2:H:133:PHE:HB2  | 1.60                     | 0.67              |
| 3:O:166:GLU:OE2  | 3:O:166:GLU:N    | 2.25                     | 0.67              |
| 3:L:266:LYS:HD2  | 3:L:267:PHE:N    | 2.09                     | 0.67              |
| 2:E:393:ASP:HB3  | 2:E:396:GLU:HB2  | 1.75                     | 0.66              |
| 2:F:120:GLN:HE21 | 2:F:122:ILE:HG22 | 1.61                     | 0.66              |
| 1:D:223:GLU:OE2  | 3:I:241:LYS:NZ   | 2.29                     | 0.66              |
| 1:C:13:ASN:OD1   | 1:C:37:ASN:ND2   | 2.29                     | 0.66              |
| 3:I:285:CYS:HB3  | 3:I:288:ARG:HE   | 1.59                     | 0.66              |
| 3:I:270:ASP:OD1  | 3:I:271:LEU:N    | 2.29                     | 0.65              |
| 2:G:120:GLN:HG3  | 2:G:122:ILE:H    | 1.62                     | 0.65              |
| 3:N:174:HIS:CE1  | 3:N:268:LEU:HD21 | 2.32                     | 0.65              |
| 1:A:527:ILE:HD12 | 1:A:551:ASN:HB2  | 1.79                     | 0.65              |
| 3:P:200:LEU:HD11 | 3:P:233:VAL:HG12 | 1.79                     | 0.65              |
| 2:F:74:ASP:OD2   | 2:F:75:GLY:N     | 2.30                     | 0.64              |
| 1:C:287:ILE:HG22 | 1:C:290:PRO:HG3  | 1.80                     | 0.64              |
| 2:F:51:ASN:HB3   | 2:F:346:ALA:HA   | 1.79                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:GLN:OE1  | 3:I:226:ARG:NH2  | 2.30                     | 0.64              |
| 2:G:329:GLU:HG3  | 2:G:347:GLU:HG3  | 1.80                     | 0.64              |
| 3:I:272:MET:HE2  | 3:I:272:MET:HA   | 1.78                     | 0.64              |
| 1:B:287:ILE:HG22 | 1:B:290:PRO:HG3  | 1.79                     | 0.64              |
| 3:M:166:GLU:OE2  | 3:M:166:GLU:N    | 2.24                     | 0.64              |
| 2:H:323:ASN:OD1  | 2:H:323:ASN:N    | 2.28                     | 0.63              |
| 3:M:196:VAL:HG22 | 3:M:235:ILE:HD11 | 1.80                     | 0.63              |
| 2:F:102:TYR:O    | 2:F:106:GLN:NE2  | 2.32                     | 0.63              |
| 1:A:172:PHE:HD2  | 1:A:238:PHE:HE1  | 1.45                     | 0.63              |
| 1:C:250:ASP:OD2  | 1:C:254:TYR:OH   | 2.16                     | 0.63              |
| 1:D:235:LYS:HD3  | 3:J:218:ARG:HH21 | 1.63                     | 0.63              |
| 3:L:153:MET:HA   | 3:L:153:MET:HE3  | 1.80                     | 0.63              |
| 2:H:332:LYS:NZ   | 2:H:343:ASP:OD2  | 2.32                     | 0.62              |
| 2:H:74:ASP:OD2   | 2:H:75:GLY:N     | 2.33                     | 0.62              |
| 3:I:203:TYR:OH   | 3:I:281:GLU:O    | 2.15                     | 0.62              |
| 2:E:14:LEU:HB2   | 2:E:219:LYS:HA   | 1.81                     | 0.62              |
| 3:L:147:ARG:HH11 | 3:L:148:ILE:HG12 | 1.64                     | 0.62              |
| 1:D:287:ILE:HG22 | 1:D:290:PRO:HG3  | 1.80                     | 0.62              |
| 1:A:287:ILE:HG22 | 1:A:290:PRO:HG3  | 1.81                     | 0.62              |
| 2:H:75:GLY:O     | 2:H:79:SER:OG    | 2.18                     | 0.62              |
| 3:L:270:ASP:OD2  | 3:L:271:LEU:N    | 2.32                     | 0.62              |
| 1:A:340:GLU:OE2  | 1:A:340:GLU:N    | 2.26                     | 0.62              |
| 1:A:432:ASP:HB2  | 1:A:511:ASP:HA   | 1.82                     | 0.61              |
| 3:N:203:TYR:HD2  | 3:N:205:PRO:HD2  | 1.65                     | 0.61              |
| 2:F:5:GLN:HA     | 2:F:8:LYS:HZ3    | 1.65                     | 0.61              |
| 3:J:285:CYS:HB3  | 3:J:288:ARG:HG2  | 1.81                     | 0.61              |
| 2:H:112:LYS:HA   | 2:H:115:GLN:HG3  | 1.82                     | 0.61              |
| 3:J:206:HIS:HB3  | 3:J:228:GLN:HG3  | 1.82                     | 0.61              |
| 2:F:329:GLU:HG3  | 2:F:347:GLU:HG3  | 1.82                     | 0.61              |
| 1:B:487:LYS:HE3  | 1:B:510:ILE:HD11 | 1.82                     | 0.61              |
| 1:D:13:ASN:HD21  | 1:D:33:ILE:HG22  | 1.66                     | 0.61              |
| 2:E:17:ALA:O     | 2:E:23:LYS:NZ    | 2.34                     | 0.61              |
| 3:I:212:LEU:HD23 | 3:I:222:LYS:HZ1  | 1.65                     | 0.61              |
| 3:N:182:LYS:HD3  | 3:N:204:LYS:HG2  | 1.81                     | 0.61              |
| 1:A:163:LEU:O    | 1:A:167:ASN:ND2  | 2.33                     | 0.61              |
| 1:D:64:ASP:HB3   | 1:D:67:LYS:HE2   | 1.83                     | 0.61              |
| 2:F:83:ARG:NH2   | 2:F:98:PHE:O     | 2.34                     | 0.61              |
| 1:B:212:ILE:HD11 | 1:C:269:ILE:HG13 | 1.83                     | 0.60              |
| 1:C:155:ASN:ND2  | 1:C:157:LEU:O    | 2.34                     | 0.60              |
| 1:D:177:GLY:O    | 3:J:226:ARG:NH1  | 2.34                     | 0.60              |
| 3:M:178:ASN:HD21 | 3:N:205:PRO:HA   | 1.65                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:206:ASN:OD1  | 2:G:207:PHE:N    | 2.35                     | 0.60              |
| 1:B:432:ASP:HB2  | 1:B:511:ASP:HA   | 1.84                     | 0.60              |
| 3:K:272:MET:HE3  | 3:K:272:MET:O    | 2.01                     | 0.60              |
| 3:L:272:MET:HE2  | 3:L:272:MET:HA   | 1.84                     | 0.60              |
| 1:D:156:PRO:HG2  | 1:D:157:LEU:HD22 | 1.84                     | 0.60              |
| 3:O:272:MET:O    | 3:O:276:ASN:ND2  | 2.35                     | 0.60              |
| 1:C:223:GLU:OE2  | 3:K:241:LYS:NZ   | 2.25                     | 0.59              |
| 1:A:414:ASN:OD1  | 1:A:455:ASN:ND2  | 2.34                     | 0.59              |
| 2:G:78:GLU:OE2   | 2:G:134:LYS:NZ   | 2.34                     | 0.59              |
| 3:L:180:ASN:HD21 | 3:L:183:PHE:HB2  | 1.68                     | 0.59              |
| 3:P:198:LYS:HB2  | 3:P:235:ILE:HD11 | 1.83                     | 0.59              |
| 3:M:185:ARG:NH1  | 3:N:176:LYS:O    | 2.35                     | 0.59              |
| 2:F:5:GLN:HA     | 2:F:8:LYS:NZ     | 2.17                     | 0.59              |
| 3:K:185:ARG:HH21 | 3:K:187:THR:HG22 | 1.68                     | 0.59              |
| 2:G:4:GLU:OE1    | 2:G:8:LYS:NZ     | 2.30                     | 0.59              |
| 3:L:279:LEU:HD22 | 3:L:290:VAL:HG23 | 1.83                     | 0.59              |
| 2:E:38:ASN:OD1   | 2:E:66:ARG:NH2   | 2.36                     | 0.59              |
| 1:B:527:ILE:HD12 | 1:B:551:ASN:HB2  | 1.83                     | 0.58              |
| 1:C:64:ASP:HB3   | 1:C:67:LYS:HE2   | 1.84                     | 0.58              |
| 3:O:232:GLU:OE1  | 3:O:232:GLU:N    | 2.34                     | 0.58              |
| 2:F:38:ASN:OD1   | 2:F:66:ARG:NH2   | 2.36                     | 0.58              |
| 3:I:144:LEU:HD12 | 3:I:145:LEU:HD12 | 1.86                     | 0.58              |
| 1:A:-3:GLN:NE2   | 1:A:78:SER:O     | 2.37                     | 0.58              |
| 3:K:213:ASN:HD22 | 3:K:219:ARG:HG3  | 1.69                     | 0.58              |
| 1:D:260:GLY:HA2  | 1:D:263:LYS:HG3  | 1.85                     | 0.58              |
| 3:K:163:SER:HB3  | 3:K:166:GLU:HB3  | 1.84                     | 0.58              |
| 2:H:14:LEU:HD12  | 2:H:219:LYS:HB3  | 1.85                     | 0.58              |
| 2:H:38:ASN:OD1   | 2:H:66:ARG:NH2   | 2.36                     | 0.58              |
| 3:M:203:TYR:CD2  | 3:M:205:PRO:HD2  | 2.38                     | 0.58              |
| 1:C:-3:GLN:NE2   | 1:C:81:GLU:OE2   | 2.36                     | 0.58              |
| 2:E:164:TYR:OH   | 2:E:172:HIS:ND1  | 2.33                     | 0.58              |
| 3:I:146:ASP:O    | 3:I:149:GLN:NE2  | 2.35                     | 0.58              |
| 3:J:136:HIS:O    | 3:J:136:HIS:ND1  | 2.36                     | 0.58              |
| 1:A:269:ILE:HG13 | 1:D:212:ILE:HD11 | 1.85                     | 0.58              |
| 2:E:78:GLU:OE2   | 2:E:134:LYS:NZ   | 2.37                     | 0.58              |
| 2:F:382:ILE:HD12 | 2:F:383:ASN:N    | 2.18                     | 0.58              |
| 1:D:444:VAL:HA   | 1:D:466:THR:HA   | 1.86                     | 0.58              |
| 1:A:337:HIS:NE2  | 1:A:345:SER:OG   | 2.32                     | 0.57              |
| 2:G:93:ASP:N     | 2:G:93:ASP:OD1   | 2.36                     | 0.57              |
| 2:G:97:ASN:O     | 2:H:97:ASN:ND2   | 2.36                     | 0.57              |
| 2:F:104:ASP:OD2  | 2:F:355:ARG:NH2  | 2.37                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:38:ASN:OD1   | 2:G:66:ARG:NH2   | 2.37                     | 0.57              |
| 3:I:209:ILE:HG12 | 3:I:223:LEU:HD12 | 1.85                     | 0.57              |
| 1:A:255:PRO:O    | 1:A:262:ARG:NH1  | 2.37                     | 0.57              |
| 1:A:536:TYR:O    | 1:A:544:ASN:ND2  | 2.37                     | 0.57              |
| 2:E:161:ILE:HB   | 2:E:188:ILE:HG22 | 1.87                     | 0.57              |
| 2:H:78:GLU:OE2   | 2:H:134:LYS:NZ   | 2.38                     | 0.57              |
| 3:L:168:TYR:HB2  | 3:L:249:VAL:HG11 | 1.85                     | 0.57              |
| 1:C:163:LEU:O    | 1:C:167:ASN:ND2  | 2.36                     | 0.57              |
| 1:C:536:TYR:O    | 1:C:544:ASN:ND2  | 2.38                     | 0.57              |
| 2:F:101:GLU:OE2  | 2:F:105:ASN:ND2  | 2.31                     | 0.57              |
| 1:B:192:THR:OG1  | 3:K:217:LYS:NZ   | 2.38                     | 0.57              |
| 3:J:222:LYS:O    | 3:J:222:LYS:NZ   | 2.31                     | 0.56              |
| 1:B:-35:ILE:HD11 | 1:B:-7:VAL:HB    | 1.88                     | 0.56              |
| 1:D:81:GLU:OE2   | 1:D:82:LYS:NZ    | 2.38                     | 0.56              |
| 3:J:168:TYR:HB2  | 3:J:249:VAL:HG11 | 1.87                     | 0.56              |
| 3:L:189:ASP:OD1  | 3:L:189:ASP:N    | 2.38                     | 0.56              |
| 1:A:202:MET:HE1  | 1:D:185:LEU:HD23 | 1.87                     | 0.56              |
| 1:D:280:ASP:OD1  | 1:D:280:ASP:N    | 2.38                     | 0.56              |
| 2:G:131:LYS:HB3  | 2:G:136:GLN:HE22 | 1.71                     | 0.56              |
| 3:J:288:ARG:HH22 | 3:N:280:VAL:HB   | 1.71                     | 0.56              |
| 2:G:181:GLN:N    | 2:G:181:GLN:OE1  | 2.39                     | 0.56              |
| 1:C:487:LYS:HE2  | 1:C:510:ILE:HD11 | 1.88                     | 0.56              |
| 2:E:218:ASN:HB3  | 2:E:220:TYR:HE1  | 1.71                     | 0.56              |
| 3:I:134:GLN:HB2  | 3:I:136:HIS:HD2  | 1.70                     | 0.56              |
| 3:L:260:LEU:O    | 3:L:264:ILE:HG12 | 2.06                     | 0.56              |
| 3:N:196:VAL:HG22 | 3:N:235:ILE:HD11 | 1.87                     | 0.56              |
| 3:O:185:ARG:HH22 | 3:P:177:ALA:HA   | 1.71                     | 0.56              |
| 1:D:487:LYS:HE2  | 1:D:510:ILE:HD11 | 1.88                     | 0.55              |
| 2:G:323:ASN:OD1  | 2:G:323:ASN:N    | 2.29                     | 0.55              |
| 3:L:241:LYS:HG2  | 3:L:242:ALA:H    | 1.71                     | 0.55              |
| 2:H:327:LEU:HD23 | 2:H:327:LEU:H    | 1.70                     | 0.55              |
| 3:J:281:GLU:HB3  | 3:J:287:GLY:HA2  | 1.88                     | 0.55              |
| 3:K:255:LYS:N    | 3:K:259:ASP:OD2  | 2.38                     | 0.55              |
| 3:L:285:CYS:HB3  | 3:L:288:ARG:HB3  | 1.89                     | 0.55              |
| 1:B:64:ASP:HB3   | 1:B:67:LYS:HE2   | 1.88                     | 0.55              |
| 3:L:174:HIS:CD2  | 3:L:268:LEU:HD13 | 2.41                     | 0.55              |
| 1:A:192:THR:OG1  | 3:I:217:LYS:NZ   | 2.39                     | 0.55              |
| 2:G:343:ASP:OD1  | 2:G:343:ASP:N    | 2.38                     | 0.55              |
| 3:I:189:ASP:OD2  | 3:I:189:ASP:N    | 2.40                     | 0.55              |
| 3:K:168:TYR:HB2  | 3:K:249:VAL:HG11 | 1.89                     | 0.55              |
| 1:B:542:LEU:HD13 | 1:D:409:GLY:HA3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:97:ASN:ND2   | 2:H:97:ASN:O     | 2.40                     | 0.55              |
| 3:L:201:GLU:HB3  | 3:L:230:LYS:HG2  | 1.88                     | 0.55              |
| 3:N:280:VAL:HG12 | 3:N:282:CYS:H    | 1.71                     | 0.55              |
| 3:P:170:ILE:HD12 | 3:P:264:ILE:HD11 | 1.88                     | 0.55              |
| 2:E:15:VAL:HB    | 2:E:189:VAL:HG22 | 1.88                     | 0.55              |
| 2:F:206:ASN:OD1  | 2:F:207:PHE:N    | 2.40                     | 0.55              |
| 3:M:182:LYS:HA   | 3:M:204:LYS:HG3  | 1.89                     | 0.55              |
| 1:A:280:ASP:N    | 1:A:280:ASP:OD1  | 2.40                     | 0.54              |
| 1:D:221:LYS:HE2  | 1:D:221:LYS:N    | 2.23                     | 0.54              |
| 3:P:256:ASP:OD2  | 3:P:257:VAL:N    | 2.39                     | 0.54              |
| 1:B:247:LYS:HG2  | 1:B:254:TYR:HE2  | 1.72                     | 0.54              |
| 1:C:467:ILE:HD11 | 1:C:485:ARG:HG2  | 1.89                     | 0.54              |
| 3:M:171:ILE:HG22 | 3:M:268:LEU:HD21 | 1.90                     | 0.54              |
| 2:F:179:LYS:HD3  | 2:F:186:LEU:HD12 | 1.88                     | 0.54              |
| 2:H:17:ALA:HB3   | 2:H:23:LYS:HB3   | 1.89                     | 0.54              |
| 3:I:216:TYR:HB2  | 3:I:219:ARG:HD3  | 1.89                     | 0.54              |
| 3:L:255:LYS:N    | 3:L:259:ASP:OD2  | 2.40                     | 0.54              |
| 2:E:329:GLU:H    | 2:E:329:GLU:CD   | 2.14                     | 0.54              |
| 1:B:504:ARG:HD3  | 1:B:571:GLU:HG2  | 1.90                     | 0.54              |
| 3:K:199:VAL:HG22 | 3:K:232:GLU:HG2  | 1.90                     | 0.54              |
| 1:B:162:LYS:NZ   | 1:B:166:GLN:OE1  | 2.39                     | 0.54              |
| 1:C:397:GLU:HG3  | 1:D:221:LYS:HE3  | 1.89                     | 0.54              |
| 1:B:170:TYR:OH   | 1:B:276:LYS:O    | 2.26                     | 0.53              |
| 2:F:52:LYS:HB3   | 2:F:346:ALA:HB1  | 1.89                     | 0.53              |
| 2:F:93:ASP:OD1   | 2:F:93:ASP:N     | 2.41                     | 0.53              |
| 3:I:169:LYS:NZ   | 3:I:173:ASN:OD1  | 2.35                     | 0.53              |
| 1:B:264:MET:HE2  | 1:B:264:MET:HA   | 1.89                     | 0.53              |
| 2:G:15:VAL:HB    | 2:G:189:VAL:HG22 | 1.90                     | 0.53              |
| 3:J:163:SER:O    | 3:J:167:SER:OG   | 2.27                     | 0.53              |
| 1:D:467:ILE:HD11 | 1:D:485:ARG:HG2  | 1.89                     | 0.53              |
| 2:F:50:THR:HG22  | 2:F:53:ALA:H     | 1.74                     | 0.53              |
| 3:I:140:LEU:HD21 | 3:I:257:VAL:HG22 | 1.91                     | 0.53              |
| 1:D:163:LEU:O    | 1:D:167:ASN:ND2  | 2.35                     | 0.53              |
| 2:H:6:ILE:HG13   | 2:H:220:TYR:HD2  | 1.74                     | 0.53              |
| 3:P:283:LYS:HE3  | 3:P:284:CYS:HB3  | 1.91                     | 0.53              |
| 1:D:504:ARG:HD3  | 1:D:571:GLU:HG2  | 1.91                     | 0.53              |
| 3:K:211:ASP:HB3  | 3:K:214:ALA:HB2  | 1.91                     | 0.53              |
| 3:L:275:ILE:HD12 | 3:L:275:ILE:H    | 1.73                     | 0.53              |
| 1:D:94:LYS:HG3   | 2:H:151:TYR:CZ   | 2.44                     | 0.53              |
| 3:J:147:ARG:HD3  | 3:J:147:ARG:C    | 2.32                     | 0.53              |
| 3:J:140:LEU:HD22 | 3:J:257:VAL:HG22 | 1.91                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:163:SER:OG   | 3:O:164:GLN:N    | 2.39                     | 0.53              |
| 1:B:295:HIS:HB3  | 1:B:298:MET:HE3  | 1.91                     | 0.53              |
| 1:B:536:TYR:O    | 1:B:544:ASN:ND2  | 2.41                     | 0.53              |
| 1:A:223:GLU:OE2  | 3:J:241:LYS:NZ   | 2.42                     | 0.53              |
| 1:D:536:TYR:O    | 1:D:544:ASN:ND2  | 2.42                     | 0.53              |
| 3:L:271:LEU:O    | 3:L:275:ILE:HD12 | 2.08                     | 0.53              |
| 2:E:74:ASP:OD2   | 2:E:75:GLY:N     | 2.42                     | 0.53              |
| 1:B:13:ASN:HB3   | 1:B:342:VAL:HG21 | 1.91                     | 0.52              |
| 1:C:94:LYS:HG3   | 2:G:151:TYR:CZ   | 2.44                     | 0.52              |
| 2:H:104:ASP:OD1  | 2:H:355:ARG:NH2  | 2.43                     | 0.52              |
| 3:K:136:HIS:O    | 3:K:136:HIS:ND1  | 2.42                     | 0.52              |
| 1:D:341:LYS:HA   | 1:D:341:LYS:HE2  | 1.91                     | 0.52              |
| 2:E:376:LEU:HA   | 2:E:379:GLN:HE21 | 1.74                     | 0.52              |
| 2:F:180:ASP:OD1  | 2:F:181:GLN:N    | 2.42                     | 0.52              |
| 3:K:147:ARG:HD3  | 3:K:147:ARG:C    | 2.35                     | 0.52              |
| 1:B:150:LYS:HB2  | 1:B:281:LYS:HD3  | 1.91                     | 0.52              |
| 2:E:206:ASN:OD1  | 2:E:207:PHE:N    | 2.42                     | 0.52              |
| 2:F:343:ASP:N    | 2:F:343:ASP:OD1  | 2.43                     | 0.52              |
| 3:I:208:TYR:CE1  | 3:I:226:ARG:HB2  | 2.45                     | 0.52              |
| 3:N:204:LYS:HG3  | 3:N:205:PRO:HD3  | 1.90                     | 0.52              |
| 1:A:185:LEU:HD21 | 3:I:215:MET:HG3  | 1.90                     | 0.52              |
| 2:H:23:LYS:NZ    | 2:H:163:GLU:OE2  | 2.42                     | 0.52              |
| 2:H:341:ILE:HD12 | 2:H:344:LEU:HD21 | 1.92                     | 0.52              |
| 3:K:226:ARG:HH11 | 3:K:226:ARG:HB3  | 1.74                     | 0.52              |
| 2:E:355:ARG:HD2  | 2:F:118:LYS:HG2  | 1.90                     | 0.52              |
| 2:E:98:PHE:HB2   | 2:E:122:ILE:HA   | 1.92                     | 0.52              |
| 1:D:192:THR:OG1  | 3:J:217:LYS:NZ   | 2.42                     | 0.52              |
| 3:I:255:LYS:N    | 3:I:259:ASP:OD2  | 2.42                     | 0.52              |
| 3:M:166:GLU:HA   | 3:M:169:LYS:HB2  | 1.92                     | 0.52              |
| 1:A:94:LYS:HG3   | 2:E:151:TYR:CZ   | 2.45                     | 0.52              |
| 1:A:504:ARG:HD3  | 1:A:571:GLU:HG2  | 1.91                     | 0.52              |
| 1:B:94:LYS:HG3   | 2:F:151:TYR:CZ   | 2.45                     | 0.52              |
| 2:H:206:ASN:OD1  | 2:H:207:PHE:N    | 2.43                     | 0.52              |
| 1:D:506:TYR:OH   | 1:D:571:GLU:OE1  | 2.28                     | 0.51              |
| 3:I:153:MET:HE3  | 3:I:153:MET:O    | 2.10                     | 0.51              |
| 3:K:285:CYS:SG   | 3:K:288:ARG:HD2  | 2.51                     | 0.51              |
| 3:I:207:GLU:HG3  | 3:I:227:PHE:CE1  | 2.44                     | 0.51              |
| 1:C:506:TYR:OH   | 1:C:571:GLU:OE1  | 2.27                     | 0.51              |
| 2:F:3:ARG:O      | 2:F:7:ILE:HD13   | 2.10                     | 0.51              |
| 3:M:196:VAL:HG13 | 3:M:236:TYR:HB3  | 1.92                     | 0.51              |
| 1:B:467:ILE:HD11 | 1:B:485:ARG:HG2  | 1.92                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:260:GLY:HA2  | 1:C:263:LYS:HG3  | 1.92                     | 0.51              |
| 1:D:332:ARG:NH1  | 1:D:346:SER:OG   | 2.41                     | 0.51              |
| 1:D:337:HIS:NE2  | 1:D:345:SER:OG   | 2.36                     | 0.51              |
| 2:G:14:LEU:HB3   | 2:G:219:LYS:HA   | 1.92                     | 0.51              |
| 3:I:242:ALA:HA   | 3:I:248:ILE:HD11 | 1.92                     | 0.51              |
| 3:L:147:ARG:HD3  | 3:L:147:ARG:C    | 2.36                     | 0.51              |
| 2:F:382:ILE:HD12 | 2:F:383:ASN:H    | 1.73                     | 0.51              |
| 2:E:109:SER:O    | 2:E:113:GLY:N    | 2.34                     | 0.51              |
| 2:H:121:ASN:C    | 2:H:122:ILE:HD12 | 2.35                     | 0.51              |
| 3:L:262:SER:HA   | 3:L:265:LYS:HG2  | 1.92                     | 0.51              |
| 3:P:284:CYS:SG   | 3:P:285:CYS:N    | 2.83                     | 0.51              |
| 2:E:116:VAL:C    | 2:E:120:GLN:HE21 | 2.18                     | 0.51              |
| 3:O:181:PRO:HG2  | 3:P:179:ILE:O    | 2.11                     | 0.51              |
| 1:A:506:TYR:OH   | 1:A:571:GLU:OE1  | 2.28                     | 0.51              |
| 1:D:162:LYS:HD3  | 1:D:162:LYS:C    | 2.36                     | 0.51              |
| 2:G:326:LEU:HD12 | 2:G:327:LEU:HD22 | 1.92                     | 0.51              |
| 1:D:13:ASN:HB2   | 1:D:342:VAL:HG21 | 1.92                     | 0.51              |
| 3:K:206:HIS:HB3  | 3:K:228:GLN:HG3  | 1.93                     | 0.51              |
| 2:E:50:THR:HG22  | 2:E:52:LYS:H     | 1.76                     | 0.51              |
| 3:P:174:HIS:ND1  | 3:P:268:LEU:HD13 | 2.26                     | 0.51              |
| 1:D:185:LEU:HD11 | 3:J:215:MET:HG3  | 1.93                     | 0.50              |
| 2:H:24:THR:HG22  | 2:H:60:ARG:HH21  | 1.75                     | 0.50              |
| 3:L:134:GLN:HG2  | 3:L:257:VAL:HG11 | 1.91                     | 0.50              |
| 1:A:487:LYS:HE2  | 1:A:510:ILE:HD11 | 1.93                     | 0.50              |
| 1:C:192:THR:OG1  | 3:L:217:LYS:NZ   | 2.40                     | 0.50              |
| 3:J:189:ASP:OD2  | 3:J:189:ASP:N    | 2.38                     | 0.50              |
| 3:M:174:HIS:CG   | 3:M:268:LEU:HD13 | 2.46                     | 0.50              |
| 3:N:164:GLN:O    | 3:N:167:SER:OG   | 2.28                     | 0.50              |
| 1:D:101:ASN:ND2  | 1:D:129:GLU:OE2  | 2.45                     | 0.50              |
| 1:D:166:GLN:N    | 1:D:166:GLN:OE1  | 2.44                     | 0.50              |
| 3:P:252:PHE:HB3  | 3:P:260:LEU:HD11 | 1.93                     | 0.50              |
| 2:G:169:LYS:HA   | 2:G:206:ASN:HD22 | 1.77                     | 0.50              |
| 2:H:53:ALA:HA    | 2:H:56:GLU:HG2   | 1.93                     | 0.50              |
| 3:K:226:ARG:HB3  | 3:K:226:ARG:NH1  | 2.25                     | 0.50              |
| 1:D:250:ASP:OD2  | 1:D:254:TYR:OH   | 2.25                     | 0.50              |
| 3:I:279:LEU:HB3  | 3:I:290:VAL:HG21 | 1.94                     | 0.50              |
| 3:L:141:ASN:HB2  | 3:L:161:TYR:CE2  | 2.46                     | 0.50              |
| 3:I:209:ILE:HD11 | 3:I:223:LEU:HB3  | 1.93                     | 0.50              |
| 2:E:78:GLU:HA    | 2:E:82:ILE:HB    | 1.93                     | 0.50              |
| 2:E:80:GLU:OE2   | 2:E:156:TYR:OH   | 2.25                     | 0.50              |
| 2:F:150:GLN:O    | 2:F:154:SER:OG   | 2.26                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:362:LEU:HD21 | 1:A:415:HIS:CD2  | 2.47                     | 0.49              |
| 1:B:229:LYS:HG3  | 1:C:253:TYR:HE1  | 1.77                     | 0.49              |
| 3:L:216:TYR:HB2  | 3:L:219:ARG:HD3  | 1.94                     | 0.49              |
| 3:L:262:SER:O    | 3:L:266:LYS:HG3  | 2.12                     | 0.49              |
| 1:A:250:ASP:OD2  | 1:A:254:TYR:OH   | 2.28                     | 0.49              |
| 1:A:332:ARG:HD2  | 1:A:346:SER:OG   | 2.12                     | 0.49              |
| 1:B:-71:VAL:HA   | 1:B:-9:ILE:H     | 1.76                     | 0.49              |
| 1:C:201:GLU:HA   | 1:C:201:GLU:OE1  | 2.13                     | 0.49              |
| 2:E:133:PHE:HA   | 2:E:136:GLN:HE21 | 1.77                     | 0.49              |
| 3:O:209:ILE:O    | 3:P:261:LYS:NZ   | 2.45                     | 0.49              |
| 2:E:343:ASP:OD1  | 2:E:343:ASP:N    | 2.43                     | 0.49              |
| 1:A:150:LYS:HB2  | 1:A:281:LYS:HD3  | 1.94                     | 0.49              |
| 1:A:246:LYS:NZ   | 1:A:250:ASP:O    | 2.34                     | 0.49              |
| 2:F:377:ILE:O    | 2:F:381:LEU:HD13 | 2.11                     | 0.49              |
| 2:H:5:GLN:OE1    | 2:H:5:GLN:HA     | 2.13                     | 0.49              |
| 3:K:142:TYR:CE1  | 3:K:160:CYS:HB3  | 2.48                     | 0.49              |
| 1:A:172:PHE:HB3  | 3:I:215:MET:HE1  | 1.94                     | 0.49              |
| 1:C:264:MET:HA   | 1:C:264:MET:HE2  | 1.95                     | 0.49              |
| 2:H:329:GLU:O    | 2:H:332:LYS:HG3  | 2.12                     | 0.49              |
| 2:H:330:VAL:HG21 | 2:H:364:ILE:HD12 | 1.93                     | 0.49              |
| 1:C:341:LYS:HE2  | 1:C:341:LYS:HA   | 1.94                     | 0.49              |
| 1:D:261:ARG:HG2  | 1:D:261:ARG:HH11 | 1.77                     | 0.49              |
| 3:K:212:LEU:HB2  | 3:K:222:LYS:NZ   | 2.28                     | 0.49              |
| 1:B:280:ASP:OD1  | 1:B:280:ASP:N    | 2.44                     | 0.49              |
| 3:I:211:ASP:HB2  | 3:I:214:ALA:HB2  | 1.94                     | 0.49              |
| 3:K:183:PHE:HA   | 3:K:279:LEU:HD21 | 1.95                     | 0.49              |
| 2:G:329:GLU:O    | 2:G:332:LYS:HG3  | 2.13                     | 0.49              |
| 1:C:-31:PHE:HB2  | 1:C:-9:ILE:HG22  | 1.95                     | 0.49              |
| 1:D:159:ASP:HB3  | 1:D:162:LYS:HB3  | 1.95                     | 0.49              |
| 1:D:150:LYS:HB2  | 1:D:281:LYS:HD3  | 1.95                     | 0.48              |
| 1:D:264:MET:HE2  | 1:D:264:MET:HA   | 1.95                     | 0.48              |
| 2:F:126:TYR:HD2  | 2:F:131:LYS:HG3  | 1.78                     | 0.48              |
| 2:F:129:PRO:HD3  | 2:F:200:ARG:NH1  | 2.28                     | 0.48              |
| 3:L:216:TYR:CB   | 3:L:219:ARG:HD3  | 2.43                     | 0.48              |
| 1:B:13:ASN:OD1   | 1:B:13:ASN:N     | 2.45                     | 0.48              |
| 1:D:332:ARG:HD2  | 1:D:346:SER:OG   | 2.13                     | 0.48              |
| 3:I:147:ARG:C    | 3:I:147:ARG:HD2  | 2.38                     | 0.48              |
| 2:E:14:LEU:HG    | 2:E:217:PHE:HD2  | 1.79                     | 0.48              |
| 2:H:158:LYS:HE3  | 2:H:187:PHE:HB2  | 1.95                     | 0.48              |
| 3:L:256:ASP:O    | 3:L:260:LEU:N    | 2.34                     | 0.48              |
| 1:C:332:ARG:HD2  | 1:C:346:SER:OG   | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:G:150:GLN:O    | 2:G:154:SER:OG   | 2.31                     | 0.48              |
| 2:G:159:ILE:HB   | 2:G:186:LEU:HD23 | 1.95                     | 0.48              |
| 2:H:343:ASP:OD1  | 2:H:343:ASP:N    | 2.36                     | 0.48              |
| 3:O:185:ARG:NH1  | 3:P:176:LYS:O    | 2.36                     | 0.48              |
| 2:G:98:PHE:HB2   | 2:G:122:ILE:HA   | 1.95                     | 0.48              |
| 2:H:362:LYS:HA   | 2:H:365:ASN:HD21 | 1.78                     | 0.48              |
| 3:I:146:ASP:O    | 3:I:158:LYS:NZ   | 2.46                     | 0.48              |
| 3:L:212:LEU:HD21 | 3:L:224:GLU:HB2  | 1.96                     | 0.48              |
| 1:C:26:VAL:HG11  | 1:C:325:LEU:HD21 | 1.95                     | 0.48              |
| 3:J:161:TYR:HA   | 3:J:253:SER:HA   | 1.95                     | 0.48              |
| 3:J:175:ILE:HG22 | 3:J:186:ILE:HD11 | 1.96                     | 0.48              |
| 1:A:64:ASP:HB3   | 1:A:67:LYS:HE2   | 1.95                     | 0.48              |
| 1:B:93:VAL:HG13  | 1:B:96:ALA:HB3   | 1.96                     | 0.48              |
| 2:F:325:THR:HA   | 2:F:328:LYS:HD2  | 1.95                     | 0.48              |
| 2:H:135:PHE:CZ   | 2:H:171:MET:HG2  | 2.49                     | 0.48              |
| 3:I:216:TYR:HB2  | 3:I:219:ARG:CD   | 2.44                     | 0.48              |
| 3:K:284:CYS:SG   | 3:K:285:CYS:N    | 2.87                     | 0.48              |
| 3:M:203:TYR:HD2  | 3:M:205:PRO:HD2  | 1.79                     | 0.48              |
| 2:G:106:GLN:HG3  | 2:G:125:THR:HG23 | 1.95                     | 0.48              |
| 3:L:201:GLU:HA   | 3:L:230:LYS:HA   | 1.95                     | 0.48              |
| 1:B:33:ILE:HD11  | 1:D:259:ASP:HB2  | 1.96                     | 0.48              |
| 1:B:469:ILE:O    | 1:B:469:ILE:HD12 | 2.14                     | 0.48              |
| 1:D:26:VAL:HG11  | 1:D:325:LEU:HD21 | 1.96                     | 0.48              |
| 3:I:163:SER:O    | 3:I:167:SER:OG   | 2.32                     | 0.48              |
| 3:K:141:ASN:HD22 | 3:K:161:TYR:HE2  | 1.60                     | 0.48              |
| 1:B:474:LYS:O    | 1:D:474:LYS:NZ   | 2.47                     | 0.47              |
| 3:O:264:ILE:HG21 | 3:P:209:ILE:HG12 | 1.96                     | 0.47              |
| 1:B:225:SER:OG   | 1:C:248:ASP:OD1  | 2.33                     | 0.47              |
| 1:B:506:TYR:OH   | 1:B:571:GLU:OE1  | 2.30                     | 0.47              |
| 3:N:174:HIS:CG   | 3:N:268:LEU:HD11 | 2.49                     | 0.47              |
| 1:A:209:GLN:HA   | 1:A:212:ILE:HG22 | 1.96                     | 0.47              |
| 2:E:4:GLU:OE1    | 2:E:8:LYS:NZ     | 2.36                     | 0.47              |
| 3:N:284:CYS:SG   | 3:N:285:CYS:N    | 2.87                     | 0.47              |
| 1:A:469:ILE:HD12 | 1:A:469:ILE:O    | 2.14                     | 0.47              |
| 1:C:280:ASP:OD1  | 1:C:280:ASP:N    | 2.46                     | 0.47              |
| 3:J:142:TYR:CE1  | 3:J:160:CYS:HB3  | 2.50                     | 0.47              |
| 3:K:272:MET:HE2  | 3:K:276:ASN:HD22 | 1.79                     | 0.47              |
| 3:O:235:ILE:N    | 3:O:235:ILE:HD12 | 2.29                     | 0.47              |
| 1:B:167:ASN:O    | 1:B:171:ILE:HG13 | 2.15                     | 0.47              |
| 1:C:209:GLN:HA   | 1:C:212:ILE:HG22 | 1.96                     | 0.47              |
| 2:E:53:ALA:HA    | 2:E:56:GLU:HG2   | 1.97                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:73:ASN:OD1   | 2:F:73:ASN:N     | 2.39                     | 0.47              |
| 3:O:167:SER:O    | 3:O:171:ILE:HG13 | 2.15                     | 0.47              |
| 1:A:93:VAL:HG13  | 1:A:96:ALA:HB3   | 1.96                     | 0.47              |
| 1:C:362:LEU:HD21 | 1:C:415:HIS:CD2  | 2.50                     | 0.47              |
| 1:D:93:VAL:HG13  | 1:D:96:ALA:HB3   | 1.96                     | 0.47              |
| 1:D:432:ASP:HA   | 1:D:508:SER:HB2  | 1.95                     | 0.47              |
| 3:N:252:PHE:HB3  | 3:N:260:LEU:HD11 | 1.97                     | 0.47              |
| 3:P:166:GLU:O    | 3:P:170:ILE:HG12 | 2.14                     | 0.47              |
| 1:A:444:VAL:HA   | 1:A:466:THR:HA   | 1.97                     | 0.47              |
| 1:B:524:MET:HG2  | 1:B:533:PRO:HB2  | 1.97                     | 0.47              |
| 2:E:98:PHE:CD2   | 2:E:123:LEU:HB2  | 2.50                     | 0.47              |
| 2:F:36:LYS:HB2   | 2:F:36:LYS:HE2   | 1.72                     | 0.47              |
| 2:H:172:HIS:ND1  | 2:H:176:MET:HE3  | 2.30                     | 0.47              |
| 3:J:179:ILE:HD12 | 3:J:186:ILE:HG13 | 1.96                     | 0.47              |
| 3:J:216:TYR:HB2  | 3:J:219:ARG:HG2  | 1.97                     | 0.47              |
| 3:K:162:LEU:HD12 | 3:K:162:LEU:HA   | 1.75                     | 0.47              |
| 3:L:241:LYS:NZ   | 3:L:241:LYS:HB2  | 2.30                     | 0.47              |
| 1:A:54:GLY:HA2   | 1:A:122:ILE:HD12 | 1.97                     | 0.47              |
| 1:B:26:VAL:HG11  | 1:B:325:LEU:HD21 | 1.97                     | 0.47              |
| 1:B:159:ASP:HB3  | 1:B:162:LYS:HB3  | 1.95                     | 0.47              |
| 2:G:112:LYS:HA   | 2:G:115:GLN:HG3  | 1.95                     | 0.47              |
| 3:K:212:LEU:HB2  | 3:K:222:LYS:HZ3  | 1.80                     | 0.47              |
| 3:O:265:LYS:HB2  | 3:O:265:LYS:HE2  | 1.57                     | 0.47              |
| 1:D:54:GLY:HA2   | 1:D:122:ILE:HD12 | 1.97                     | 0.47              |
| 1:D:469:ILE:HD12 | 1:D:469:ILE:O    | 2.15                     | 0.47              |
| 2:E:178:LEU:HD23 | 2:E:182:LEU:HD12 | 1.96                     | 0.47              |
| 2:F:78:GLU:OE2   | 2:F:134:LYS:NZ   | 2.48                     | 0.47              |
| 3:L:184:ALA:HA   | 3:L:199:VAL:HG23 | 1.97                     | 0.47              |
| 3:M:185:ARG:HH12 | 3:N:176:LYS:C    | 2.22                     | 0.47              |
| 1:C:-3:GLN:HA    | 1:C:78:SER:HB2   | 1.97                     | 0.47              |
| 1:C:150:LYS:HB2  | 1:C:281:LYS:HD3  | 1.97                     | 0.47              |
| 1:C:332:ARG:NH1  | 1:C:346:SER:OG   | 2.41                     | 0.47              |
| 3:I:174:HIS:CG   | 3:I:268:LEU:HD13 | 2.50                     | 0.47              |
| 3:I:282:CYS:HB3  | 3:M:285:CYS:HB3  | 1.49                     | 0.47              |
| 1:A:332:ARG:NH1  | 1:A:346:SER:OG   | 2.40                     | 0.46              |
| 2:G:204:PRO:O    | 2:G:208:ASN:ND2  | 2.39                     | 0.46              |
| 2:G:362:LYS:HA   | 2:G:365:ASN:ND2  | 2.30                     | 0.46              |
| 3:J:163:SER:HB3  | 3:J:166:GLU:HB3  | 1.96                     | 0.46              |
| 3:M:264:ILE:HD11 | 3:N:209:ILE:CG2  | 2.45                     | 0.46              |
| 3:N:209:ILE:HD12 | 3:N:210:VAL:N    | 2.30                     | 0.46              |
| 3:O:200:LEU:HD11 | 3:O:233:VAL:HG12 | 1.97                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:304:LYS:HG3  | 1:B:308:GLU:HG3  | 1.98                     | 0.46              |
| 1:C:48:LYS:HB3   | 1:C:48:LYS:HE2   | 1.78                     | 0.46              |
| 1:C:432:ASP:HA   | 1:C:508:SER:HB2  | 1.97                     | 0.46              |
| 2:F:164:TYR:OH   | 2:F:172:HIS:ND1  | 2.37                     | 0.46              |
| 2:F:378:ASN:O    | 2:F:382:ILE:HG13 | 2.14                     | 0.46              |
| 2:G:78:GLU:HA    | 2:G:82:ILE:HB    | 1.97                     | 0.46              |
| 3:K:189:ASP:OD2  | 3:K:189:ASP:N    | 2.42                     | 0.46              |
| 1:A:527:ILE:HD11 | 1:A:548:LEU:HD12 | 1.98                     | 0.46              |
| 1:B:185:LEU:HD13 | 1:C:202:MET:HE1  | 1.97                     | 0.46              |
| 1:C:444:VAL:HA   | 1:C:466:THR:HA   | 1.97                     | 0.46              |
| 2:E:14:LEU:HD11  | 2:E:217:PHE:HB3  | 1.98                     | 0.46              |
| 2:G:172:HIS:CE1  | 2:G:176:MET:HE3  | 2.50                     | 0.46              |
| 1:A:397:GLU:OE1  | 1:A:397:GLU:N    | 2.45                     | 0.46              |
| 1:B:185:LEU:HD23 | 3:K:214:ALA:HB3  | 1.97                     | 0.46              |
| 1:B:202:MET:HE2  | 1:B:202:MET:HB3  | 1.69                     | 0.46              |
| 2:E:135:PHE:CE2  | 2:E:171:MET:HG2  | 2.51                     | 0.46              |
| 2:E:150:GLN:O    | 2:E:154:SER:OG   | 2.27                     | 0.46              |
| 2:G:36:LYS:HE2   | 2:G:36:LYS:HB2   | 1.66                     | 0.46              |
| 3:K:146:ASP:O    | 3:K:149:GLN:NE2  | 2.48                     | 0.46              |
| 3:K:216:TYR:HB2  | 3:K:219:ARG:CD   | 2.46                     | 0.46              |
| 3:P:272:MET:O    | 3:P:275:ILE:HG13 | 2.16                     | 0.46              |
| 1:B:49:GLU:OE1   | 1:B:52:LYS:NZ    | 2.42                     | 0.46              |
| 2:F:57:ILE:O     | 2:F:61:LEU:HD22  | 2.16                     | 0.46              |
| 3:L:257:VAL:HG12 | 3:L:261:LYS:NZ   | 2.31                     | 0.46              |
| 1:D:172:PHE:HD2  | 1:D:238:PHE:HE1  | 1.64                     | 0.46              |
| 1:D:201:GLU:HA   | 1:D:201:GLU:OE1  | 2.16                     | 0.46              |
| 2:E:377:ILE:O    | 2:E:381:LEU:HD13 | 2.15                     | 0.46              |
| 3:L:183:PHE:CZ   | 3:L:278:PRO:HB3  | 2.51                     | 0.46              |
| 1:A:5:ASN:ND2    | 1:A:18:ASN:OD1   | 2.49                     | 0.46              |
| 1:B:172:PHE:HD2  | 1:B:238:PHE:HE1  | 1.62                     | 0.46              |
| 2:E:6:ILE:HG22   | 2:E:220:TYR:CD2  | 2.51                     | 0.46              |
| 2:E:159:ILE:HB   | 2:E:186:LEU:HD23 | 1.97                     | 0.46              |
| 2:G:121:ASN:O    | 2:G:121:ASN:ND2  | 2.49                     | 0.46              |
| 3:L:146:ASP:HB2  | 3:L:158:LYS:NZ   | 2.31                     | 0.46              |
| 3:O:185:ARG:HH12 | 3:P:176:LYS:C    | 2.21                     | 0.46              |
| 3:O:256:ASP:OD2  | 3:O:256:ASP:C    | 2.59                     | 0.46              |
| 2:E:126:TYR:HD1  | 2:E:131:LYS:HG3  | 1.81                     | 0.46              |
| 3:K:285:CYS:HB2  | 3:O:282:CYS:O    | 2.16                     | 0.46              |
| 3:L:147:ARG:HA   | 3:L:155:LEU:HD21 | 1.96                     | 0.46              |
| 3:M:206:HIS:CE1  | 3:N:265:LYS:HG3  | 2.51                     | 0.46              |
| 1:A:48:LYS:HB3   | 1:A:48:LYS:HE2   | 1.77                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:202:MET:HE2  | 1:A:202:MET:HB3  | 1.66                     | 0.46              |
| 2:F:168:ASP:OD1  | 2:F:169:LYS:N    | 2.48                     | 0.46              |
| 3:N:252:PHE:CG   | 3:N:264:ILE:HD11 | 2.51                     | 0.46              |
| 1:A:-35:ILE:HA   | 1:A:-6:PHE:O     | 2.16                     | 0.45              |
| 1:A:26:VAL:HG11  | 1:A:325:LEU:HD21 | 1.98                     | 0.45              |
| 2:F:2:SER:N      | 2:F:5:GLN:HE22   | 2.15                     | 0.45              |
| 2:G:107:PHE:HE2  | 2:G:124:GLY:HA3  | 1.81                     | 0.45              |
| 3:O:210:VAL:HA   | 3:P:261:LYS:HZ1  | 1.81                     | 0.45              |
| 1:A:216:TYR:OH   | 1:D:261:ARG:HD3  | 2.16                     | 0.45              |
| 1:C:77:LEU:HD21  | 1:C:89:LEU:HD23  | 1.98                     | 0.45              |
| 2:H:167:SER:HB2  | 2:H:171:MET:HE2  | 1.99                     | 0.45              |
| 2:H:204:PRO:O    | 2:H:208:ASN:ND2  | 2.38                     | 0.45              |
| 1:A:523:SER:O    | 1:A:527:ILE:HG23 | 2.16                     | 0.45              |
| 1:D:13:ASN:OD1   | 1:D:37:ASN:ND2   | 2.48                     | 0.45              |
| 1:D:362:LEU:HD21 | 1:D:415:HIS:CD2  | 2.52                     | 0.45              |
| 3:M:204:LYS:HA   | 3:M:204:LYS:HD3  | 1.67                     | 0.45              |
| 1:A:2:LYS:O      | 1:A:76:ASP:N     | 2.46                     | 0.45              |
| 1:C:97:ARG:NH2   | 1:C:102:ALA:O    | 2.49                     | 0.45              |
| 2:F:97:ASN:OD1   | 2:F:121:ASN:ND2  | 2.37                     | 0.45              |
| 3:I:146:ASP:CG   | 3:I:158:LYS:HZ1  | 2.24                     | 0.45              |
| 3:J:146:ASP:O    | 3:J:150:THR:HG22 | 2.16                     | 0.45              |
| 3:O:176:LYS:C    | 3:P:185:ARG:HH12 | 2.25                     | 0.45              |
| 1:B:430:LYS:NZ   | 1:B:508:SER:OG   | 2.48                     | 0.45              |
| 1:B:456:LEU:HD23 | 1:B:456:LEU:HA   | 1.86                     | 0.45              |
| 1:C:-58:LYS:HB2  | 1:C:-55:THR:OG1  | 2.16                     | 0.45              |
| 1:C:170:TYR:CE2  | 1:C:277:LYS:HD3  | 2.51                     | 0.45              |
| 2:H:49:PHE:CZ    | 2:H:171:MET:HE1  | 2.51                     | 0.45              |
| 2:H:74:ASP:OD1   | 2:H:102:TYR:OH   | 2.34                     | 0.45              |
| 2:E:48:THR:HA    | 2:E:162:ASP:OD1  | 2.17                     | 0.45              |
| 2:F:380:VAL:HA   | 2:F:383:ASN:HD21 | 1.82                     | 0.45              |
| 2:G:106:GLN:HB3  | 2:G:127:SER:OG   | 2.16                     | 0.45              |
| 3:L:142:TYR:CE2  | 3:L:155:LEU:HB3  | 2.52                     | 0.45              |
| 1:C:54:GLY:HA2   | 1:C:122:ILE:HD12 | 1.98                     | 0.45              |
| 1:C:93:VAL:HG13  | 1:C:96:ALA:HB3   | 1.99                     | 0.45              |
| 2:G:164:TYR:OH   | 2:G:172:HIS:ND1  | 2.44                     | 0.45              |
| 1:C:469:ILE:HD12 | 1:C:469:ILE:O    | 2.16                     | 0.45              |
| 2:G:161:ILE:HB   | 2:G:188:ILE:HG22 | 1.98                     | 0.45              |
| 3:I:279:LEU:HB3  | 3:I:290:VAL:CG2  | 2.47                     | 0.45              |
| 3:L:143:ASN:HB2  | 3:L:146:ASP:CG   | 2.42                     | 0.45              |
| 3:M:252:PHE:CD1  | 3:M:264:ILE:HG22 | 2.52                     | 0.45              |
| 3:N:235:ILE:HD13 | 3:N:275:ILE:HG12 | 1.98                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:72:THR:HG21  | 2:F:350:GLY:HA2  | 1.99                     | 0.45              |
| 3:K:216:TYR:HB2  | 3:K:219:ARG:HD3  | 1.99                     | 0.45              |
| 3:K:284:CYS:SG   | 3:O:284:CYS:N    | 2.85                     | 0.45              |
| 3:L:180:ASN:ND2  | 3:L:276:ASN:OD1  | 2.35                     | 0.45              |
| 3:L:220:LYS:HD3  | 3:L:221:PRO:HD2  | 1.99                     | 0.45              |
| 1:A:131:ASP:N    | 1:A:131:ASP:OD1  | 2.51                     | 0.44              |
| 1:A:229:LYS:HG3  | 1:D:253:TYR:HE1  | 1.82                     | 0.44              |
| 1:C:30:MET:HE2   | 1:C:30:MET:HB2   | 1.79                     | 0.44              |
| 1:C:139:ARG:NH1  | 1:D:135:ASP:OD2  | 2.49                     | 0.44              |
| 1:C:202:MET:O    | 1:C:206:LYS:HB2  | 2.17                     | 0.44              |
| 1:C:337:HIS:NE2  | 1:C:345:SER:OG   | 2.35                     | 0.44              |
| 2:E:107:PHE:HB2  | 2:E:126:TYR:CE2  | 2.52                     | 0.44              |
| 2:E:132:ASN:N    | 2:E:170:ASP:OD2  | 2.45                     | 0.44              |
| 1:D:430:LYS:NZ   | 1:D:508:SER:OG   | 2.44                     | 0.44              |
| 3:I:211:ASP:OD1  | 3:I:223:LEU:HD13 | 2.17                     | 0.44              |
| 3:K:179:ILE:HG22 | 3:K:275:ILE:HG21 | 1.98                     | 0.44              |
| 3:K:278:PRO:HB2  | 3:K:293:ASN:H    | 1.83                     | 0.44              |
| 1:B:232:MET:HE3  | 1:C:232:MET:HE3  | 1.99                     | 0.44              |
| 1:B:469:ILE:HG22 | 1:B:481:ARG:HG2  | 1.99                     | 0.44              |
| 2:F:222:LEU:HD22 | 2:F:226:PHE:CZ   | 2.52                     | 0.44              |
| 2:G:51:ASN:OD1   | 2:G:55:LYS:NZ    | 2.42                     | 0.44              |
| 3:M:166:GLU:O    | 3:M:170:ILE:HG13 | 2.18                     | 0.44              |
| 3:O:177:ALA:HA   | 3:P:185:ARG:HH22 | 1.83                     | 0.44              |
| 3:P:193:CYS:HB2  | 3:P:246:TYR:CE2  | 2.52                     | 0.44              |
| 2:E:130:LYS:HA   | 2:E:130:LYS:HD3  | 1.81                     | 0.44              |
| 2:G:57:ILE:O     | 2:G:61:LEU:HD22  | 2.17                     | 0.44              |
| 3:N:200:LEU:HD11 | 3:N:233:VAL:HG12 | 2.00                     | 0.44              |
| 1:A:177:GLY:O    | 3:I:226:ARG:NH1  | 2.51                     | 0.44              |
| 2:H:23:LYS:HD2   | 2:H:189:VAL:HG11 | 2.00                     | 0.44              |
| 3:J:199:VAL:HG22 | 3:J:232:GLU:HG2  | 1.98                     | 0.44              |
| 3:N:283:LYS:HB3  | 3:N:284:CYS:H    | 1.51                     | 0.44              |
| 1:A:-58:LYS:HA   | 1:A:-58:LYS:HD3  | 1.89                     | 0.44              |
| 1:C:124:LEU:HD12 | 1:C:143:ASN:HD21 | 1.83                     | 0.44              |
| 2:H:334:VAL:HG22 | 2:H:368:LEU:HD23 | 1.99                     | 0.44              |
| 3:N:182:LYS:HE2  | 3:N:203:TYR:HA   | 2.00                     | 0.44              |
| 1:B:124:LEU:HD12 | 1:B:143:ASN:HD21 | 1.83                     | 0.44              |
| 1:B:185:LEU:HD21 | 3:K:215:MET:HG3  | 2.00                     | 0.44              |
| 2:G:324:ALA:HA   | 2:G:327:LEU:HD23 | 1.98                     | 0.44              |
| 2:H:326:LEU:HD12 | 2:H:327:LEU:N    | 2.33                     | 0.44              |
| 2:H:363:ILE:HD11 | 2:H:383:ASN:OD1  | 2.18                     | 0.44              |
| 1:D:432:ASP:HB2  | 1:D:511:ASP:HA   | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:49:PHE:CZ    | 2:E:171:MET:HE1  | 2.52                     | 0.44              |
| 2:F:15:VAL:HB    | 2:F:189:VAL:HG22 | 1.98                     | 0.44              |
| 2:F:49:PHE:CZ    | 2:F:171:MET:HE1  | 2.53                     | 0.44              |
| 2:F:135:PHE:CE2  | 2:F:171:MET:HG2  | 2.53                     | 0.44              |
| 2:G:121:ASN:C    | 2:G:121:ASN:HD22 | 2.25                     | 0.44              |
| 3:J:288:ARG:HB3  | 3:N:231:ARG:NH2  | 2.33                     | 0.44              |
| 3:L:282:CYS:SG   | 3:L:285:CYS:HB2  | 2.57                     | 0.44              |
| 3:N:256:ASP:OD2  | 3:N:259:ASP:N    | 2.30                     | 0.44              |
| 3:K:186:ILE:HD11 | 3:K:189:ASP:HB3  | 2.00                     | 0.44              |
| 3:L:290:VAL:H    | 3:P:288:ARG:C    | 2.26                     | 0.44              |
| 3:P:199:VAL:HG12 | 3:P:201:GLU:HB3  | 1.99                     | 0.44              |
| 1:A:124:LEU:HD12 | 1:A:143:ASN:HD21 | 1.83                     | 0.43              |
| 1:B:201:GLU:OE2  | 1:B:201:GLU:HA   | 2.18                     | 0.43              |
| 2:G:165:GLN:NE2  | 2:G:191:ASP:HB3  | 2.33                     | 0.43              |
| 3:K:282:CYS:HB3  | 3:K:285:CYS:H    | 1.82                     | 0.43              |
| 1:B:-32:ARG:NH2  | 1:B:20:ASN:OD1   | 2.50                     | 0.43              |
| 1:B:229:LYS:HG3  | 1:C:253:TYR:CE1  | 2.53                     | 0.43              |
| 2:E:214:SER:OG   | 2:E:216:ASP:OD1  | 2.35                     | 0.43              |
| 3:I:155:LEU:HD23 | 3:I:158:LYS:HD3  | 1.98                     | 0.43              |
| 3:J:144:LEU:HD23 | 3:J:145:LEU:H    | 1.83                     | 0.43              |
| 3:L:174:HIS:CE1  | 3:L:268:LEU:HB3  | 2.54                     | 0.43              |
| 3:O:182:LYS:HE3  | 3:O:183:PHE:CE1  | 2.53                     | 0.43              |
| 2:H:172:HIS:HD1  | 2:H:176:MET:HE3  | 1.83                     | 0.43              |
| 3:J:278:PRO:HG2  | 3:J:292:LEU:HG   | 1.99                     | 0.43              |
| 1:A:220:LYS:HG2  | 1:A:222:GLU:HB2  | 1.99                     | 0.43              |
| 1:B:281:LYS:HB3  | 1:B:281:LYS:HE2  | 1.77                     | 0.43              |
| 2:E:126:TYR:CZ   | 2:E:133:PHE:HB2  | 2.52                     | 0.43              |
| 2:E:387:LYS:HD3  | 2:E:387:LYS:HA   | 1.92                     | 0.43              |
| 2:F:357:ILE:HA   | 2:F:360:ILE:HB   | 2.00                     | 0.43              |
| 2:H:135:PHE:CE2  | 2:H:171:MET:HG2  | 2.54                     | 0.43              |
| 3:J:174:HIS:CD2  | 3:J:268:LEU:HD23 | 2.54                     | 0.43              |
| 3:K:153:MET:HE3  | 3:K:153:MET:O    | 2.18                     | 0.43              |
| 3:N:204:LYS:HG3  | 3:N:205:PRO:CD   | 2.48                     | 0.43              |
| 1:A:162:LYS:HD2  | 1:A:162:LYS:O    | 2.18                     | 0.43              |
| 3:N:202:LEU:HD12 | 3:N:202:LEU:HA   | 1.90                     | 0.43              |
| 1:A:276:LYS:HE2  | 1:A:276:LYS:HB3  | 1.86                     | 0.43              |
| 1:A:431:THR:OG1  | 1:A:432:ASP:N    | 2.52                     | 0.43              |
| 1:B:13:ASN:HD21  | 1:B:33:ILE:HG22  | 1.84                     | 0.43              |
| 3:K:136:HIS:ND1  | 3:K:138:PHE:O    | 2.52                     | 0.43              |
| 1:A:397:GLU:HB2  | 1:A:400:LEU:HD22 | 2.01                     | 0.43              |
| 1:B:131:ASP:OD1  | 1:B:131:ASP:N    | 2.50                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:362:LEU:HD21 | 1:B:415:HIS:NE2  | 2.33                     | 0.43              |
| 1:C:259:ASP:HA   | 1:C:262:ARG:HG3  | 2.01                     | 0.43              |
| 2:F:327:LEU:HD12 | 2:F:327:LEU:H    | 1.82                     | 0.43              |
| 2:H:12:ASN:HB3   | 2:H:217:PHE:CZ   | 2.54                     | 0.43              |
| 2:H:52:LYS:HB3   | 2:H:52:LYS:HE3   | 1.83                     | 0.43              |
| 3:M:273:ALA:O    | 3:M:277:GLU:HB3  | 2.19                     | 0.43              |
| 3:N:172:ARG:HH21 | 3:N:176:LYS:HZ3  | 1.67                     | 0.43              |
| 1:B:-34:ARG:HB3  | 1:B:-6:PHE:HB3   | 2.01                     | 0.43              |
| 1:C:288:GLU:HG3  | 1:C:289:GLU:HG2  | 2.01                     | 0.43              |
| 2:H:50:THR:HG22  | 2:H:52:LYS:H     | 1.84                     | 0.43              |
| 3:I:146:ASP:OD2  | 3:I:146:ASP:C    | 2.61                     | 0.43              |
| 1:A:172:PHE:HD2  | 1:A:238:PHE:CE1  | 2.31                     | 0.43              |
| 1:A:439:LYS:HD2  | 1:C:528:PHE:O    | 2.18                     | 0.43              |
| 1:D:362:LEU:HD21 | 1:D:415:HIS:NE2  | 2.34                     | 0.43              |
| 2:E:26:ILE:HD13  | 2:E:26:ILE:HA    | 1.85                     | 0.43              |
| 2:F:74:ASP:OD2   | 2:F:74:ASP:C     | 2.62                     | 0.43              |
| 2:G:2:SER:N      | 2:G:5:GLN:HE22   | 2.16                     | 0.43              |
| 2:G:223:THR:OG1  | 2:G:225:ASN:O    | 2.29                     | 0.43              |
| 3:L:241:LYS:HG2  | 3:L:242:ALA:N    | 2.34                     | 0.43              |
| 3:N:167:SER:O    | 3:N:171:ILE:HG13 | 2.18                     | 0.43              |
| 1:A:-49:MET:HG2  | 1:A:-33:PHE:CD2  | 2.54                     | 0.43              |
| 1:A:129:GLU:HB3  | 1:A:131:ASP:OD1  | 2.19                     | 0.43              |
| 1:B:172:PHE:HB3  | 3:K:215:MET:HE1  | 2.01                     | 0.43              |
| 1:B:362:LEU:HD21 | 1:B:415:HIS:CD2  | 2.54                     | 0.43              |
| 1:C:304:LYS:HG3  | 1:C:308:GLU:HG3  | 2.01                     | 0.43              |
| 2:H:364:ILE:HD13 | 2:H:364:ILE:HA   | 1.90                     | 0.43              |
| 3:M:181:PRO:HB2  | 3:N:177:ALA:O    | 2.19                     | 0.43              |
| 3:P:261:LYS:HA   | 3:P:264:ILE:HG22 | 2.00                     | 0.43              |
| 1:A:430:LYS:NZ   | 1:A:508:SER:OG   | 2.48                     | 0.42              |
| 1:A:542:LEU:HD13 | 1:C:409:GLY:HA3  | 2.00                     | 0.42              |
| 2:G:52:LYS:HA    | 2:G:55:LYS:HE2   | 2.01                     | 0.42              |
| 3:K:282:CYS:HB2  | 3:K:285:CYS:HB3  | 2.00                     | 0.42              |
| 1:D:48:LYS:HE2   | 1:D:48:LYS:HB3   | 1.69                     | 0.42              |
| 2:F:24:THR:OG1   | 2:F:60:ARG:NH1   | 2.52                     | 0.42              |
| 3:P:169:LYS:HE3  | 3:P:169:LYS:HB2  | 1.88                     | 0.42              |
| 1:D:162:LYS:HD3  | 1:D:162:LYS:O    | 2.19                     | 0.42              |
| 2:E:98:PHE:H     | 2:E:98:PHE:HD1   | 1.68                     | 0.42              |
| 3:P:167:SER:O    | 3:P:171:ILE:HG13 | 2.19                     | 0.42              |
| 1:A:79:ASN:OD1   | 1:A:79:ASN:N     | 2.49                     | 0.42              |
| 1:A:247:LYS:NZ   | 1:D:222:GLU:OE2  | 2.52                     | 0.42              |
| 1:A:442:LYS:HA   | 1:A:442:LYS:HD3  | 1.74                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:81:GLU:CD    | 1:C:81:GLU:H     | 2.28                     | 0.42              |
| 2:F:27:LEU:HD23  | 2:F:27:LEU:HA    | 1.85                     | 0.42              |
| 2:G:20:GLY:HA2   | 2:G:23:LYS:HG3   | 2.02                     | 0.42              |
| 3:L:282:CYS:HB3  | 3:L:291:ILE:HG13 | 2.01                     | 0.42              |
| 1:A:219:LEU:HD12 | 1:A:219:LEU:HA   | 1.78                     | 0.42              |
| 1:A:447:LEU:HD21 | 1:A:465:ILE:HG12 | 2.01                     | 0.42              |
| 1:D:124:LEU:HD12 | 1:D:143:ASN:HD21 | 1.84                     | 0.42              |
| 2:G:74:ASP:OD1   | 2:G:74:ASP:N     | 2.50                     | 0.42              |
| 2:H:9:ASP:O      | 2:H:30:LYS:NZ    | 2.46                     | 0.42              |
| 3:I:207:GLU:HG3  | 3:I:227:PHE:HE1  | 1.82                     | 0.42              |
| 3:J:184:ALA:HA   | 3:J:199:VAL:HG23 | 2.01                     | 0.42              |
| 3:L:163:SER:O    | 3:L:167:SER:OG   | 2.31                     | 0.42              |
| 1:D:202:MET:HE2  | 1:D:202:MET:HB3  | 1.68                     | 0.42              |
| 2:F:120:GLN:HE21 | 2:F:122:ILE:CG2  | 2.32                     | 0.42              |
| 3:I:146:ASP:OD2  | 3:I:158:LYS:NZ   | 2.52                     | 0.42              |
| 3:I:151:HIS:HB3  | 3:I:154:LEU:HB2  | 2.00                     | 0.42              |
| 3:K:282:CYS:CB   | 3:K:285:CYS:HB3  | 2.50                     | 0.42              |
| 3:N:231:ARG:HH11 | 3:N:233:VAL:HB   | 1.84                     | 0.42              |
| 1:C:101:ASN:HB2  | 1:C:128:SER:HB2  | 2.01                     | 0.42              |
| 1:D:247:LYS:HB3  | 1:D:247:LYS:HE3  | 1.76                     | 0.42              |
| 3:M:242:ALA:N    | 3:M:248:ILE:HD11 | 2.35                     | 0.42              |
| 3:N:202:LEU:HB3  | 3:N:207:GLU:OE2  | 2.19                     | 0.42              |
| 1:C:135:ASP:OD2  | 1:D:139:ARG:NH1  | 2.52                     | 0.42              |
| 1:D:438:LYS:HE2  | 1:D:438:LYS:HB2  | 1.92                     | 0.42              |
| 2:E:52:LYS:HE3   | 2:E:52:LYS:HB3   | 1.86                     | 0.42              |
| 2:F:126:TYR:CD2  | 2:F:131:LYS:HG3  | 2.54                     | 0.42              |
| 2:F:130:LYS:HA   | 2:F:130:LYS:HD3  | 1.83                     | 0.42              |
| 3:K:256:ASP:H    | 3:K:259:ASP:HB3  | 1.84                     | 0.42              |
| 3:O:280:VAL:HG12 | 3:O:282:CYS:H    | 1.85                     | 0.42              |
| 1:A:135:ASP:OD2  | 1:B:139:ARG:NH1  | 2.52                     | 0.42              |
| 1:C:185:LEU:HA   | 1:C:185:LEU:HD12 | 1.86                     | 0.42              |
| 1:C:261:ARG:HB3  | 1:C:261:ARG:CZ   | 2.50                     | 0.42              |
| 1:D:288:GLU:HG3  | 1:D:289:GLU:HG2  | 2.01                     | 0.42              |
| 2:E:352:LEU:HD12 | 2:E:357:ILE:HG12 | 2.02                     | 0.42              |
| 2:G:23:LYS:NZ    | 2:G:191:ASP:HB2  | 2.35                     | 0.42              |
| 2:H:126:TYR:HD1  | 2:H:128:ASN:H    | 1.67                     | 0.42              |
| 3:J:136:HIS:ND1  | 3:J:138:PHE:O    | 2.53                     | 0.42              |
| 1:A:542:LEU:HD23 | 1:A:542:LEU:HA   | 1.85                     | 0.42              |
| 1:C:2:LYS:O      | 1:C:76:ASP:N     | 2.46                     | 0.42              |
| 1:C:432:ASP:HB2  | 1:C:511:ASP:HA   | 2.02                     | 0.42              |
| 2:G:24:THR:HG22  | 2:G:60:ARG:NH1   | 2.35                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:K:158:LYS:HB2  | 3:K:158:LYS:HE3  | 1.97                     | 0.42              |
| 1:A:-4:GLN:NE2   | 1:A:103:ASP:OD2  | 2.37                     | 0.41              |
| 1:B:5:ASN:OD1    | 1:B:18:ASN:ND2   | 2.53                     | 0.41              |
| 1:D:162:LYS:HD3  | 1:D:166:GLN:HE22 | 1.85                     | 0.41              |
| 2:H:176:MET:N    | 2:H:176:MET:HE2  | 2.35                     | 0.41              |
| 3:J:215:MET:HE3  | 3:J:215:MET:HB2  | 1.83                     | 0.41              |
| 3:L:212:LEU:HB2  | 3:L:222:LYS:NZ   | 2.35                     | 0.41              |
| 1:A:288:GLU:HG3  | 1:A:289:GLU:HG2  | 2.02                     | 0.41              |
| 1:C:87:LYS:HE2   | 2:G:153:PHE:HE2  | 1.84                     | 0.41              |
| 1:C:202:MET:HB3  | 1:C:202:MET:HE2  | 1.75                     | 0.41              |
| 3:K:270:ASP:OD2  | 3:K:270:ASP:C    | 2.62                     | 0.41              |
| 3:P:175:ILE:O    | 3:P:179:ILE:HB   | 2.20                     | 0.41              |
| 2:E:341:ILE:HD12 | 2:E:344:LEU:HD21 | 2.01                     | 0.41              |
| 3:I:198:LYS:HB3  | 3:I:233:VAL:HG22 | 2.01                     | 0.41              |
| 3:J:204:LYS:HD3  | 3:J:283:LYS:HE2  | 2.01                     | 0.41              |
| 3:K:228:GLN:HE22 | 3:K:231:ARG:HB2  | 1.85                     | 0.41              |
| 3:L:162:LEU:HB2  | 3:L:252:PHE:HB2  | 2.02                     | 0.41              |
| 3:L:242:ALA:HA   | 3:L:248:ILE:HD11 | 2.01                     | 0.41              |
| 3:O:210:VAL:HA   | 3:P:261:LYS:NZ   | 2.35                     | 0.41              |
| 1:A:470:PRO:HD3  | 1:A:481:ARG:HH12 | 1.85                     | 0.41              |
| 1:D:179:GLU:CD   | 1:D:179:GLU:H    | 2.29                     | 0.41              |
| 2:G:172:HIS:ND1  | 2:G:176:MET:HE3  | 2.35                     | 0.41              |
| 3:I:280:VAL:O    | 3:I:291:ILE:N    | 2.48                     | 0.41              |
| 3:P:179:ILE:HD12 | 3:P:179:ILE:HA   | 1.84                     | 0.41              |
| 1:C:362:LEU:HD21 | 1:C:415:HIS:NE2  | 2.35                     | 0.41              |
| 1:C:470:PRO:HD3  | 1:C:481:ARG:HH12 | 1.85                     | 0.41              |
| 2:E:74:ASP:OD2   | 2:E:74:ASP:C     | 2.63                     | 0.41              |
| 2:G:98:PHE:HB3   | 2:G:121:ASN:HD22 | 1.85                     | 0.41              |
| 2:G:98:PHE:CD1   | 2:G:123:LEU:HB2  | 2.55                     | 0.41              |
| 3:I:133:LEU:HD12 | 3:I:133:LEU:HA   | 1.83                     | 0.41              |
| 3:L:191:ASP:N    | 3:L:191:ASP:OD1  | 2.53                     | 0.41              |
| 3:N:256:ASP:OD2  | 3:N:256:ASP:C    | 2.63                     | 0.41              |
| 3:P:178:ASN:HB2  | 3:P:272:MET:HE2  | 2.01                     | 0.41              |
| 1:A:260:GLY:HA2  | 1:A:263:LYS:NZ   | 2.35                     | 0.41              |
| 1:B:2:LYS:O      | 1:B:76:ASP:N     | 2.45                     | 0.41              |
| 1:B:247:LYS:HD2  | 1:C:224:VAL:HG12 | 2.03                     | 0.41              |
| 2:G:55:LYS:HE2   | 2:G:55:LYS:HB2   | 1.84                     | 0.41              |
| 2:H:49:PHE:HZ    | 2:H:167:SER:HA   | 1.86                     | 0.41              |
| 3:N:165:GLU:C    | 3:N:165:GLU:OE1  | 2.63                     | 0.41              |
| 2:F:50:THR:CG2   | 2:F:52:LYS:HG3   | 2.51                     | 0.41              |
| 3:I:137:ASN:OD1  | 3:I:138:PHE:N    | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:O:161:TYR:N    | 3:O:161:TYR:CD2  | 2.89                     | 0.41              |
| 3:P:265:LYS:HE2  | 3:P:265:LYS:HB2  | 1.74                     | 0.41              |
| 1:D:219:LEU:HD12 | 1:D:219:LEU:HA   | 1.81                     | 0.41              |
| 2:E:5:GLN:HG2    | 2:E:220:TYR:HE2  | 1.86                     | 0.41              |
| 2:G:101:GLU:CD   | 2:G:355:ARG:HH21 | 2.29                     | 0.41              |
| 2:G:374:GLN:O    | 2:G:378:ASN:ND2  | 2.50                     | 0.41              |
| 2:H:74:ASP:OD2   | 2:H:74:ASP:C     | 2.63                     | 0.41              |
| 3:P:198:LYS:HB2  | 3:P:235:ILE:CD1  | 2.50                     | 0.41              |
| 1:A:93:VAL:HG11  | 1:A:97:ARG:HG3   | 2.03                     | 0.41              |
| 1:B:48:LYS:HB3   | 1:B:48:LYS:HE2   | 1.77                     | 0.41              |
| 1:B:431:THR:OG1  | 1:B:432:ASP:N    | 2.54                     | 0.41              |
| 1:C:268:SER:HA   | 1:C:271:ASN:HB2  | 2.03                     | 0.41              |
| 1:C:281:LYS:HE2  | 1:C:281:LYS:HB3  | 1.74                     | 0.41              |
| 1:D:79:ASN:OD1   | 1:D:79:ASN:N     | 2.54                     | 0.41              |
| 1:D:227:GLU:OE2  | 3:I:244:GLN:NE2  | 2.52                     | 0.41              |
| 2:E:2:SER:N      | 2:E:5:GLN:HE22   | 2.19                     | 0.41              |
| 2:E:39:LYS:HB3   | 2:E:39:LYS:HE3   | 1.78                     | 0.41              |
| 2:G:102:TYR:O    | 2:G:125:THR:HG21 | 2.21                     | 0.41              |
| 2:G:179:LYS:HD3  | 2:G:186:LEU:HD12 | 2.03                     | 0.41              |
| 2:H:44:ILE:HG13  | 2:H:68:ASN:OD1   | 2.21                     | 0.41              |
| 3:I:162:LEU:HD12 | 3:I:162:LEU:HA   | 1.76                     | 0.41              |
| 3:J:134:GLN:CD   | 3:J:134:GLN:H    | 2.29                     | 0.41              |
| 3:J:162:LEU:N    | 3:J:252:PHE:O    | 2.46                     | 0.41              |
| 3:J:284:CYS:SG   | 3:N:283:LYS:HB3  | 2.61                     | 0.41              |
| 3:L:152:PRO:HA   | 3:L:155:LEU:HB2  | 2.02                     | 0.41              |
| 3:L:288:ARG:NH2  | 3:P:280:VAL:HB   | 2.36                     | 0.41              |
| 3:M:170:ILE:HD12 | 3:M:171:ILE:N    | 2.35                     | 0.41              |
| 1:C:476:LYS:HE2  | 1:C:476:LYS:HB3  | 1.73                     | 0.41              |
| 1:D:276:LYS:HB3  | 1:D:276:LYS:HE2  | 1.85                     | 0.41              |
| 2:E:126:TYR:CE2  | 2:E:133:PHE:HB2  | 2.56                     | 0.41              |
| 2:H:25:THR:HA    | 2:H:60:ARG:HH22  | 1.86                     | 0.41              |
| 3:J:147:ARG:HD3  | 3:J:148:ILE:N    | 2.36                     | 0.41              |
| 3:L:240:PRO:HA   | 3:L:249:VAL:HG12 | 2.03                     | 0.41              |
| 3:N:171:ILE:HG13 | 3:N:171:ILE:H    | 1.63                     | 0.41              |
| 3:N:234:GLU:C    | 3:N:234:GLU:OE1  | 2.63                     | 0.41              |
| 1:A:281:LYS:HE2  | 1:A:281:LYS:HB3  | 1.74                     | 0.40              |
| 2:F:15:VAL:HG12  | 2:F:17:ALA:H     | 1.86                     | 0.40              |
| 2:F:129:PRO:HD3  | 2:F:200:ARG:HH11 | 1.86                     | 0.40              |
| 2:H:133:PHE:HA   | 2:H:136:GLN:NE2  | 2.36                     | 0.40              |
| 3:K:198:LYS:NZ   | 3:K:277:GLU:HB3  | 2.36                     | 0.40              |
| 3:L:207:GLU:OE1  | 3:L:208:TYR:N    | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:201:GLU:HA   | 1:A:201:GLU:OE1  | 2.21                     | 0.40              |
| 1:B:13:ASN:HD21  | 1:B:33:ILE:CG2   | 2.35                     | 0.40              |
| 1:B:129:GLU:HB3  | 1:B:131:ASP:OD1  | 2.20                     | 0.40              |
| 1:C:430:LYS:NZ   | 1:C:508:SER:OG   | 2.43                     | 0.40              |
| 1:D:-35:ILE:H    | 1:D:-35:ILE:HG13 | 1.72                     | 0.40              |
| 3:I:169:LYS:HE3  | 3:I:169:LYS:HB3  | 1.93                     | 0.40              |
| 3:J:202:LEU:HD12 | 3:J:228:GLN:NE2  | 2.36                     | 0.40              |
| 3:J:252:PHE:HB3  | 3:J:260:LEU:HD11 | 2.03                     | 0.40              |
| 1:A:527:ILE:O    | 1:C:439:LYS:NZ   | 2.50                     | 0.40              |
| 1:B:103:ASP:OD1  | 1:B:103:ASP:N    | 2.40                     | 0.40              |
| 1:C:278:TYR:HB3  | 1:C:281:LYS:HG3  | 2.04                     | 0.40              |
| 1:D:221:LYS:HE2  | 1:D:221:LYS:H    | 1.86                     | 0.40              |
| 2:E:93:ASP:OD1   | 2:E:93:ASP:N     | 2.52                     | 0.40              |
| 2:F:159:ILE:HB   | 2:F:186:LEU:HD23 | 2.02                     | 0.40              |
| 2:F:344:LEU:O    | 2:F:344:LEU:HD12 | 2.20                     | 0.40              |
| 2:G:44:ILE:HG13  | 2:G:68:ASN:OD1   | 2.21                     | 0.40              |
| 2:G:48:THR:O     | 2:G:72:THR:HA    | 2.21                     | 0.40              |
| 2:H:15:VAL:HG12  | 2:H:189:VAL:HG13 | 2.03                     | 0.40              |
| 2:H:329:GLU:HG3  | 2:H:347:GLU:HG3  | 2.03                     | 0.40              |
| 3:K:207:GLU:OE2  | 3:K:225:LYS:NZ   | 2.41                     | 0.40              |
| 3:P:188:SER:HB3  | 3:P:195:THR:HB   | 2.03                     | 0.40              |
| 1:A:77:LEU:HD21  | 1:A:89:LEU:HD23  | 2.03                     | 0.40              |
| 1:B:-61:PHE:CG   | 1:B:-50:LEU:HD11 | 2.56                     | 0.40              |
| 1:C:129:GLU:HB3  | 1:C:131:ASP:OD1  | 2.22                     | 0.40              |
| 2:E:362:LYS:HA   | 2:E:365:ASN:HD21 | 1.85                     | 0.40              |
| 2:G:121:ASN:HB3  | 2:H:122:ILE:CG1  | 2.49                     | 0.40              |
| 2:H:152:ILE:HD13 | 2:H:152:ILE:HA   | 1.98                     | 0.40              |
| 3:I:174:HIS:CE1  | 3:I:268:LEU:HB3  | 2.57                     | 0.40              |
| 1:B:45:LEU:HD11  | 1:B:107:ILE:HG22 | 2.04                     | 0.40              |
| 1:D:470:PRO:HD3  | 1:D:481:ARG:HH12 | 1.87                     | 0.40              |
| 2:E:107:PHE:HB2  | 2:E:126:TYR:HE2  | 1.86                     | 0.40              |
| 2:F:98:PHE:CD2   | 2:F:123:LEU:HB2  | 2.57                     | 0.40              |
| 2:H:327:LEU:HA   | 2:H:330:VAL:HG12 | 2.04                     | 0.40              |
| 3:P:187:THR:OG1  | 3:P:188:SER:N    | 2.54                     | 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     | 618/675 (92%)   | 602 (97%)  | 15 (2%)  | 1 (0%)   | 43          | 63  |
| 1   | B     | 618/675 (92%)   | 602 (97%)  | 15 (2%)  | 1 (0%)   | 43          | 63  |
| 1   | C     | 618/675 (92%)   | 602 (97%)  | 15 (2%)  | 1 (0%)   | 43          | 63  |
| 1   | D     | 618/675 (92%)   | 600 (97%)  | 17 (3%)  | 1 (0%)   | 43          | 63  |
| 2   | E     | 276/494 (56%)   | 271 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | F     | 276/494 (56%)   | 272 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 2   | G     | 276/494 (56%)   | 271 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | H     | 276/494 (56%)   | 271 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 3   | I     | 160/295 (54%)   | 155 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 3   | J     | 160/295 (54%)   | 156 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 3   | K     | 160/295 (54%)   | 153 (96%)  | 7 (4%)   | 0        | 100         | 100 |
| 3   | L     | 160/295 (54%)   | 155 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 3   | M     | 110/295 (37%)   | 104 (94%)  | 6 (6%)   | 0        | 100         | 100 |
| 3   | N     | 110/295 (37%)   | 102 (93%)  | 8 (7%)   | 0        | 100         | 100 |
| 3   | O     | 110/295 (37%)   | 102 (93%)  | 8 (7%)   | 0        | 100         | 100 |
| 3   | P     | 110/295 (37%)   | 101 (92%)  | 9 (8%)   | 0        | 100         | 100 |
| All | All   | 4656/7036 (66%) | 4519 (97%) | 133 (3%) | 4 (0%)   | 49          | 69  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 342 | VAL  |
| 1   | B     | 342 | VAL  |
| 1   | C     | 342 | VAL  |
| 1   | D     | 342 | VAL  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 571/614 (93%)   | 563 (99%)  | 8 (1%)   | 59          | 79 |
| 1   | B     | 571/614 (93%)   | 555 (97%)  | 16 (3%)  | 38          | 64 |
| 1   | C     | 571/614 (93%)   | 559 (98%)  | 12 (2%)  | 47          | 71 |
| 1   | D     | 571/614 (93%)   | 555 (97%)  | 16 (3%)  | 38          | 64 |
| 2   | E     | 253/448 (56%)   | 244 (96%)  | 9 (4%)   | 31          | 56 |
| 2   | F     | 253/448 (56%)   | 242 (96%)  | 11 (4%)  | 26          | 49 |
| 2   | G     | 253/448 (56%)   | 245 (97%)  | 8 (3%)   | 34          | 59 |
| 2   | H     | 253/448 (56%)   | 245 (97%)  | 8 (3%)   | 34          | 59 |
| 3   | I     | 153/276 (55%)   | 148 (97%)  | 5 (3%)   | 33          | 59 |
| 3   | J     | 153/276 (55%)   | 148 (97%)  | 5 (3%)   | 33          | 59 |
| 3   | K     | 153/276 (55%)   | 143 (94%)  | 10 (6%)  | 15          | 33 |
| 3   | L     | 153/276 (55%)   | 143 (94%)  | 10 (6%)  | 15          | 33 |
| 3   | M     | 106/276 (38%)   | 101 (95%)  | 5 (5%)   | 23          | 46 |
| 3   | N     | 106/276 (38%)   | 101 (95%)  | 5 (5%)   | 23          | 46 |
| 3   | O     | 106/276 (38%)   | 100 (94%)  | 6 (6%)   | 18          | 38 |
| 3   | P     | 106/276 (38%)   | 100 (94%)  | 6 (6%)   | 18          | 38 |
| All | All   | 4332/6456 (67%) | 4192 (97%) | 140 (3%) | 35          | 59 |

All (140) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | -71 | VAL  |
| 1   | A     | 218 | SER  |
| 1   | A     | 321 | SER  |
| 1   | A     | 338 | SER  |
| 1   | A     | 407 | GLU  |
| 1   | A     | 428 | ILE  |
| 1   | A     | 452 | ARG  |
| 1   | A     | 549 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | -30 | ASP  |
| 1   | B     | 13  | ASN  |
| 1   | B     | 30  | MET  |
| 1   | B     | 65  | THR  |
| 1   | B     | 116 | LYS  |
| 1   | B     | 118 | LEU  |
| 1   | B     | 157 | LEU  |
| 1   | B     | 218 | SER  |
| 1   | B     | 313 | LYS  |
| 1   | B     | 321 | SER  |
| 1   | B     | 338 | SER  |
| 1   | B     | 346 | SER  |
| 1   | B     | 428 | ILE  |
| 1   | B     | 455 | ASN  |
| 1   | B     | 549 | VAL  |
| 1   | B     | 573 | VAL  |
| 1   | C     | -10 | THR  |
| 1   | C     | -2  | THR  |
| 1   | C     | 32  | ASP  |
| 1   | C     | 213 | THR  |
| 1   | C     | 218 | SER  |
| 1   | C     | 235 | LYS  |
| 1   | C     | 287 | ILE  |
| 1   | C     | 321 | SER  |
| 1   | C     | 338 | SER  |
| 1   | C     | 428 | ILE  |
| 1   | C     | 452 | ARG  |
| 1   | C     | 549 | VAL  |
| 1   | D     | -71 | VAL  |
| 1   | D     | -67 | ASP  |
| 1   | D     | -10 | THR  |
| 1   | D     | 13  | ASN  |
| 1   | D     | 80  | TYR  |
| 1   | D     | 157 | LEU  |
| 1   | D     | 158 | VAL  |
| 1   | D     | 185 | LEU  |
| 1   | D     | 218 | SER  |
| 1   | D     | 224 | VAL  |
| 1   | D     | 313 | LYS  |
| 1   | D     | 321 | SER  |
| 1   | D     | 338 | SER  |
| 1   | D     | 346 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 452 | ARG  |
| 1   | D     | 549 | VAL  |
| 2   | E     | 6   | ILE  |
| 2   | E     | 29  | SER  |
| 2   | E     | 72  | THR  |
| 2   | E     | 126 | TYR  |
| 2   | E     | 154 | SER  |
| 2   | E     | 188 | ILE  |
| 2   | E     | 330 | VAL  |
| 2   | E     | 352 | LEU  |
| 2   | E     | 396 | GLU  |
| 2   | F     | 24  | THR  |
| 2   | F     | 73  | ASN  |
| 2   | F     | 79  | SER  |
| 2   | F     | 126 | TYR  |
| 2   | F     | 154 | SER  |
| 2   | F     | 212 | GLU  |
| 2   | F     | 330 | VAL  |
| 2   | F     | 349 | VAL  |
| 2   | F     | 354 | SER  |
| 2   | F     | 360 | ILE  |
| 2   | F     | 384 | LEU  |
| 2   | G     | 25  | THR  |
| 2   | G     | 55  | LYS  |
| 2   | G     | 61  | LEU  |
| 2   | G     | 72  | THR  |
| 2   | G     | 74  | ASP  |
| 2   | G     | 127 | SER  |
| 2   | G     | 176 | MET  |
| 2   | G     | 323 | ASN  |
| 2   | H     | 7   | ILE  |
| 2   | H     | 77  | VAL  |
| 2   | H     | 107 | PHE  |
| 2   | H     | 188 | ILE  |
| 2   | H     | 323 | ASN  |
| 2   | H     | 352 | LEU  |
| 2   | H     | 354 | SER  |
| 2   | H     | 381 | LEU  |
| 3   | I     | 141 | ASN  |
| 3   | I     | 167 | SER  |
| 3   | I     | 194 | LEU  |
| 3   | I     | 216 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | I     | 222 | LYS  |
| 3   | J     | 162 | LEU  |
| 3   | J     | 164 | GLN  |
| 3   | J     | 167 | SER  |
| 3   | J     | 200 | LEU  |
| 3   | J     | 215 | MET  |
| 3   | K     | 133 | LEU  |
| 3   | K     | 141 | ASN  |
| 3   | K     | 186 | ILE  |
| 3   | K     | 196 | VAL  |
| 3   | K     | 210 | VAL  |
| 3   | K     | 216 | TYR  |
| 3   | K     | 228 | GLN  |
| 3   | K     | 229 | THR  |
| 3   | K     | 253 | SER  |
| 3   | K     | 292 | LEU  |
| 3   | L     | 141 | ASN  |
| 3   | L     | 150 | THR  |
| 3   | L     | 164 | GLN  |
| 3   | L     | 194 | LEU  |
| 3   | L     | 210 | VAL  |
| 3   | L     | 212 | LEU  |
| 3   | L     | 216 | TYR  |
| 3   | L     | 235 | ILE  |
| 3   | L     | 253 | SER  |
| 3   | L     | 291 | ILE  |
| 3   | M     | 164 | GLN  |
| 3   | M     | 196 | VAL  |
| 3   | M     | 233 | VAL  |
| 3   | M     | 256 | ASP  |
| 3   | M     | 279 | LEU  |
| 3   | N     | 196 | VAL  |
| 3   | N     | 210 | VAL  |
| 3   | N     | 231 | ARG  |
| 3   | N     | 233 | VAL  |
| 3   | N     | 257 | VAL  |
| 3   | O     | 163 | SER  |
| 3   | O     | 164 | GLN  |
| 3   | O     | 209 | ILE  |
| 3   | O     | 213 | ASN  |
| 3   | O     | 253 | SER  |
| 3   | O     | 282 | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | P     | 167 | SER  |
| 3   | P     | 170 | ILE  |
| 3   | P     | 178 | ASN  |
| 3   | P     | 196 | VAL  |
| 3   | P     | 264 | ILE  |
| 3   | P     | 285 | CYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 187 | ASN  |
| 1   | A     | 305 | GLN  |
| 1   | A     | 350 | ASN  |
| 1   | A     | 414 | ASN  |
| 1   | A     | 455 | ASN  |
| 1   | A     | 551 | ASN  |
| 1   | B     | 187 | ASN  |
| 1   | B     | 198 | GLN  |
| 1   | B     | 210 | GLN  |
| 1   | B     | 305 | GLN  |
| 1   | B     | 330 | ASN  |
| 1   | B     | 350 | ASN  |
| 1   | C     | -56 | HIS  |
| 1   | C     | -3  | GLN  |
| 1   | C     | 18  | ASN  |
| 1   | C     | 187 | ASN  |
| 1   | C     | 198 | GLN  |
| 1   | C     | 350 | ASN  |
| 1   | C     | 514 | ASN  |
| 1   | D     | 18  | ASN  |
| 1   | D     | 198 | GLN  |
| 1   | D     | 210 | GLN  |
| 1   | D     | 305 | GLN  |
| 1   | D     | 350 | ASN  |
| 2   | E     | 365 | ASN  |
| 2   | F     | 51  | ASN  |
| 2   | F     | 92  | ASN  |
| 2   | G     | 105 | ASN  |
| 2   | G     | 121 | ASN  |
| 2   | H     | 115 | GLN  |
| 3   | I     | 136 | HIS  |
| 3   | I     | 174 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | J     | 164 | GLN  |
| 3   | J     | 174 | HIS  |
| 3   | K     | 141 | ASN  |
| 3   | K     | 149 | GLN  |
| 3   | K     | 178 | ASN  |
| 3   | K     | 276 | ASN  |
| 3   | M     | 173 | ASN  |
| 3   | M     | 174 | HIS  |
| 3   | M     | 178 | ASN  |
| 3   | M     | 206 | HIS  |
| 3   | N     | 174 | HIS  |
| 3   | P     | 173 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

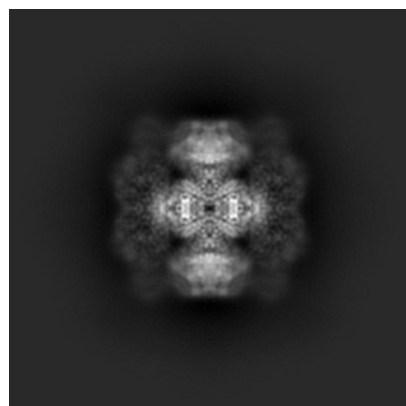
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41983. These allow visual inspection of the internal detail of the map and identification of artifacts.

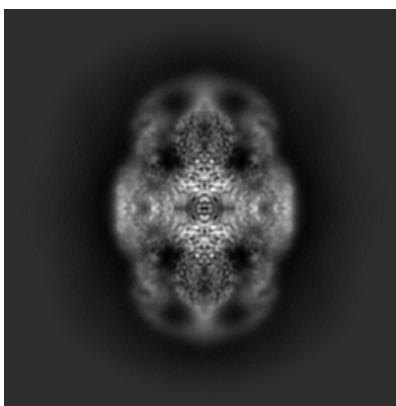
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

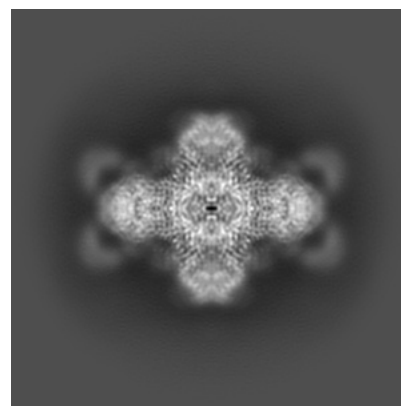
#### 6.1.1 Primary map



X

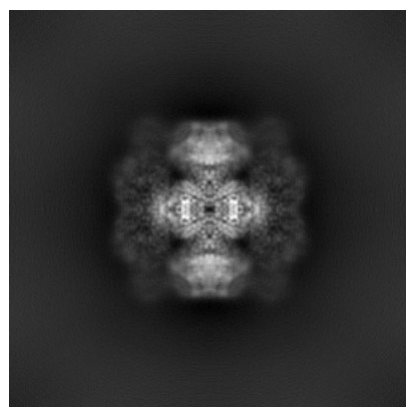


Y

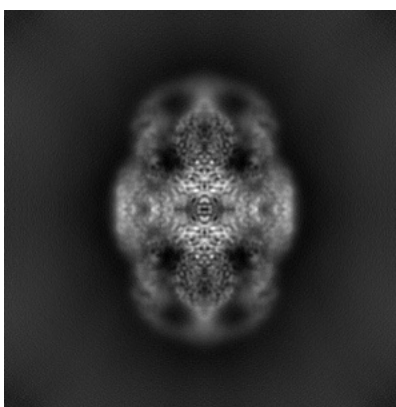


Z

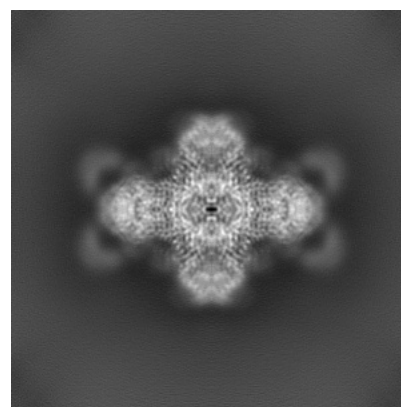
#### 6.1.2 Raw map



X



Y

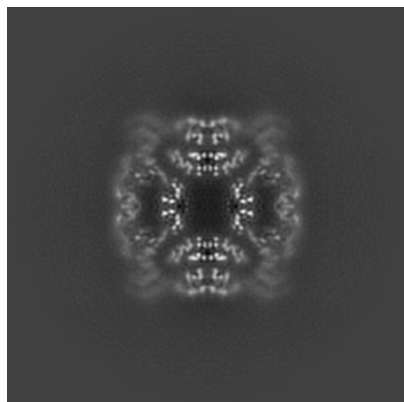


Z

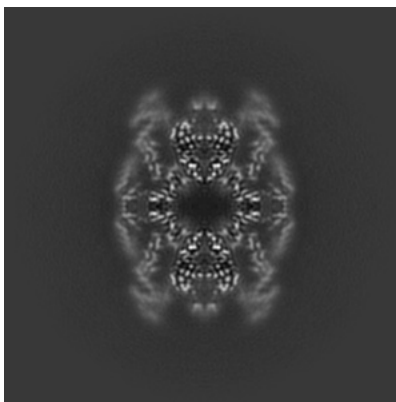
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

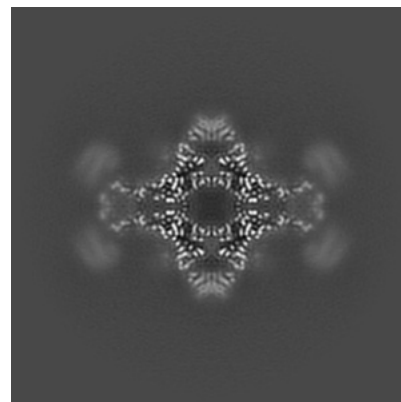
### 6.2.1 Primary map



X Index: 175

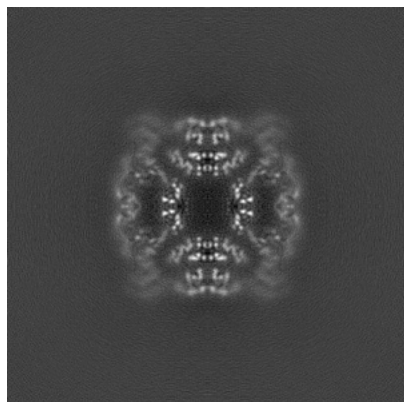


Y Index: 175

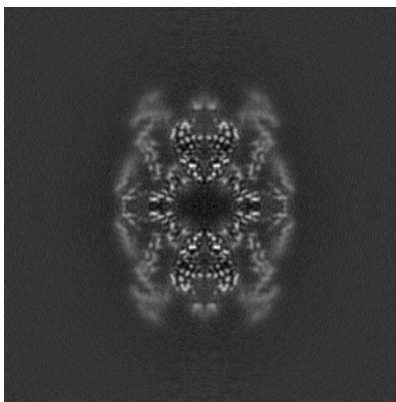


Z Index: 175

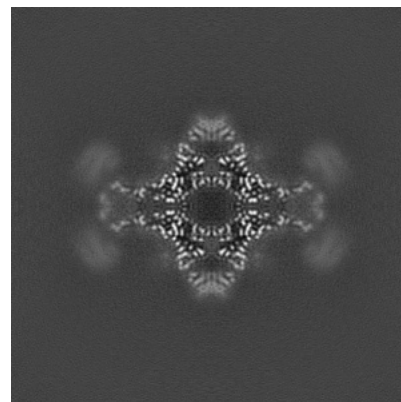
### 6.2.2 Raw map



X Index: 175



Y Index: 175

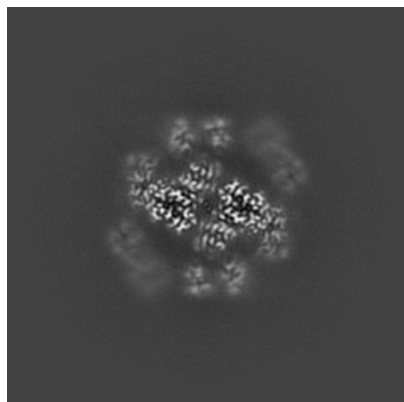


Z Index: 175

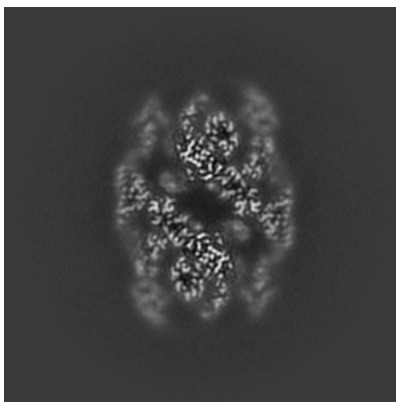
The images above show central slices of the map in three orthogonal directions.

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

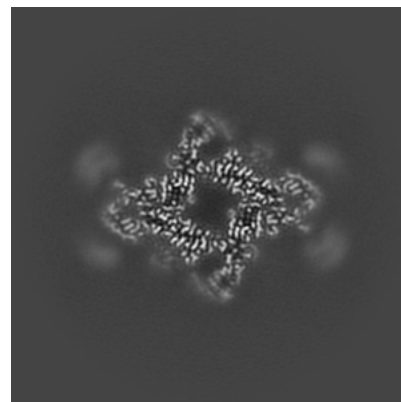
### 6.3.1 Primary map



X Index: 196

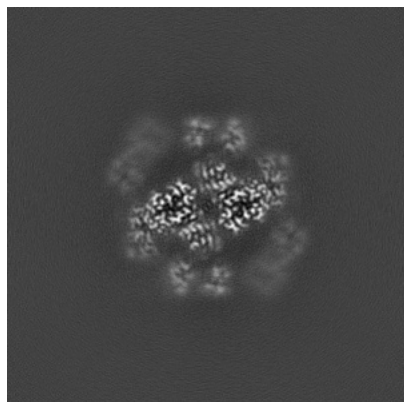


Y Index: 167

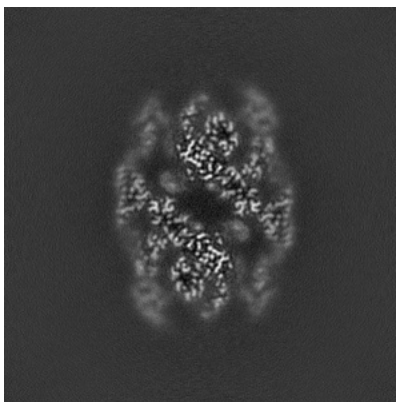


Z Index: 182

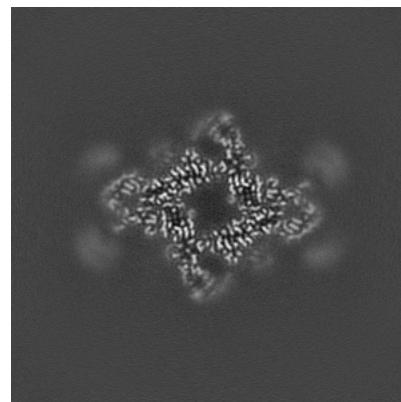
### 6.3.2 Raw map



X Index: 154



Y Index: 167

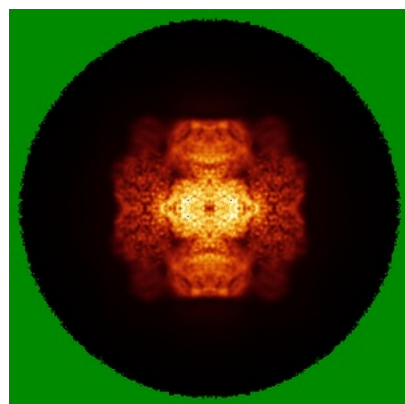


Z Index: 168

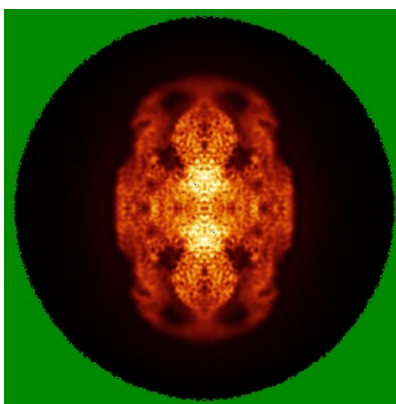
The images above show the largest variance slices of the map in three orthogonal directions.

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

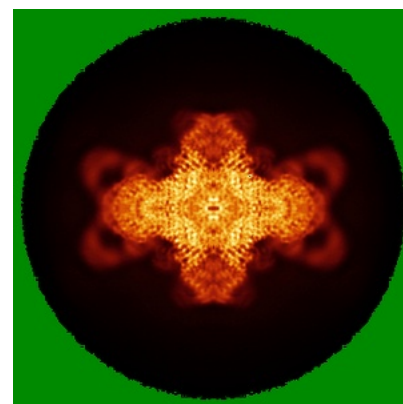
### 6.4.1 Primary map



X

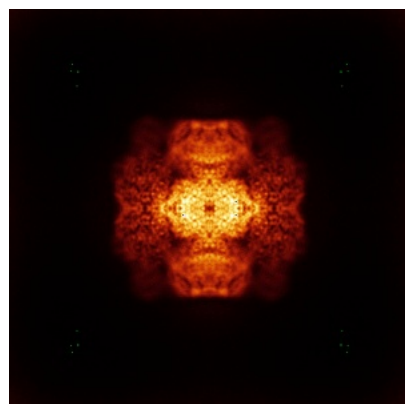


Y

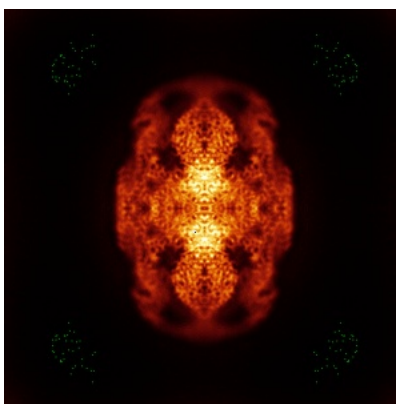


Z

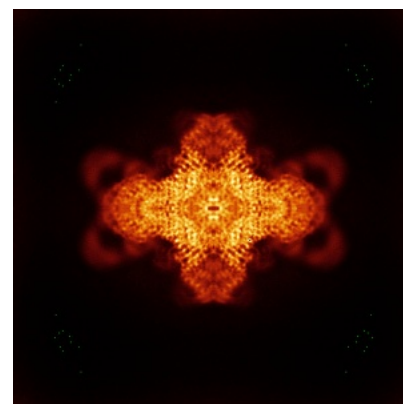
### 6.4.2 Raw map



X



Y



Z

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

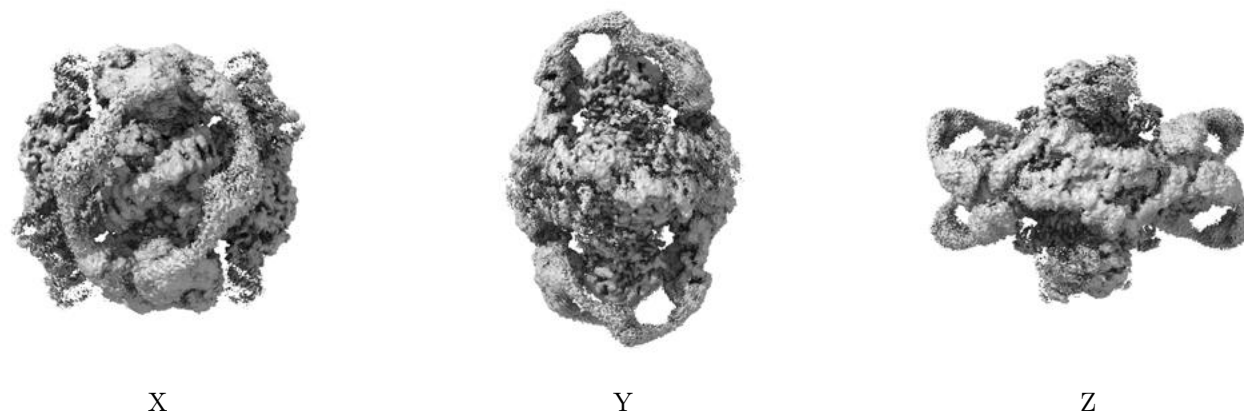
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

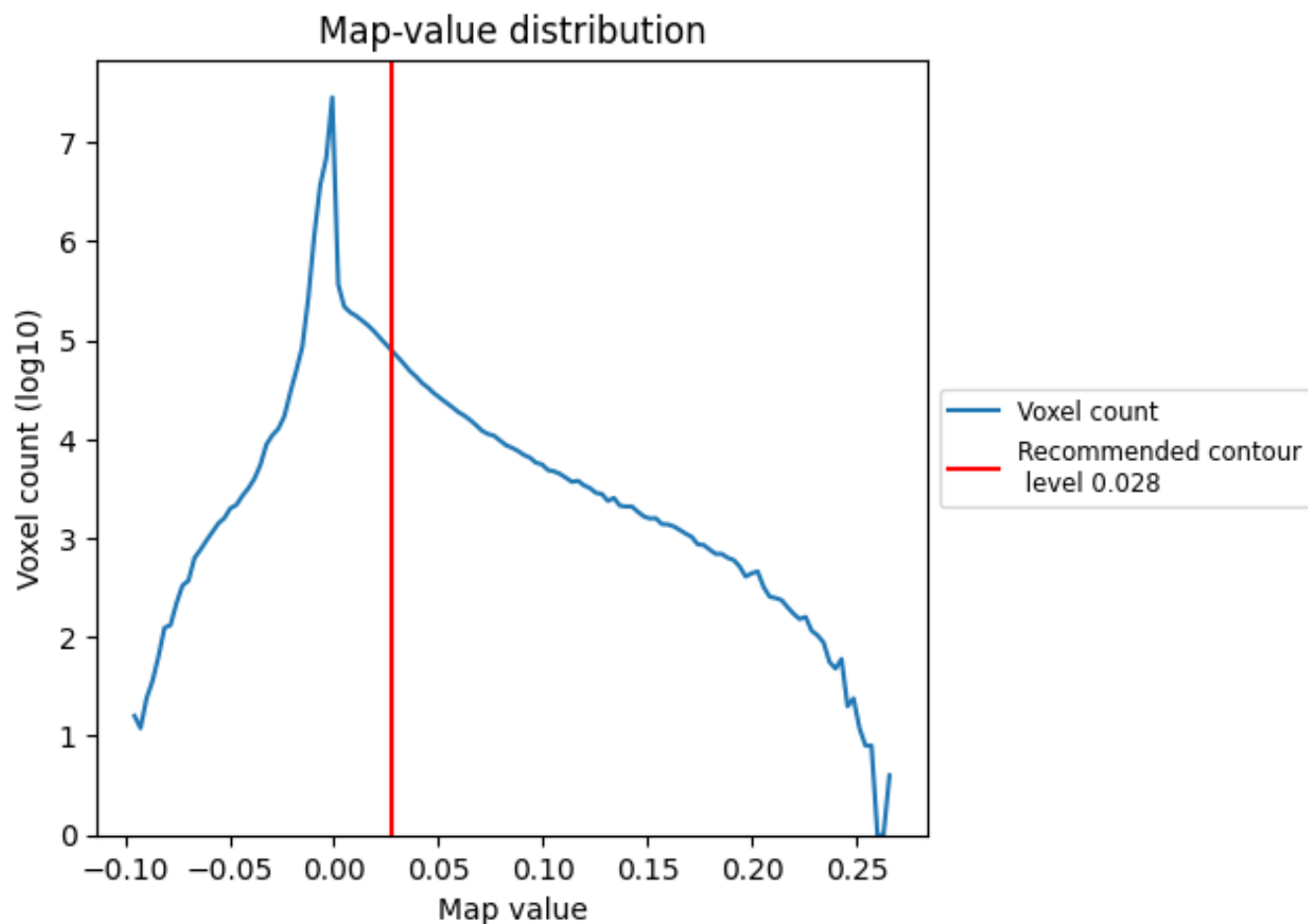
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

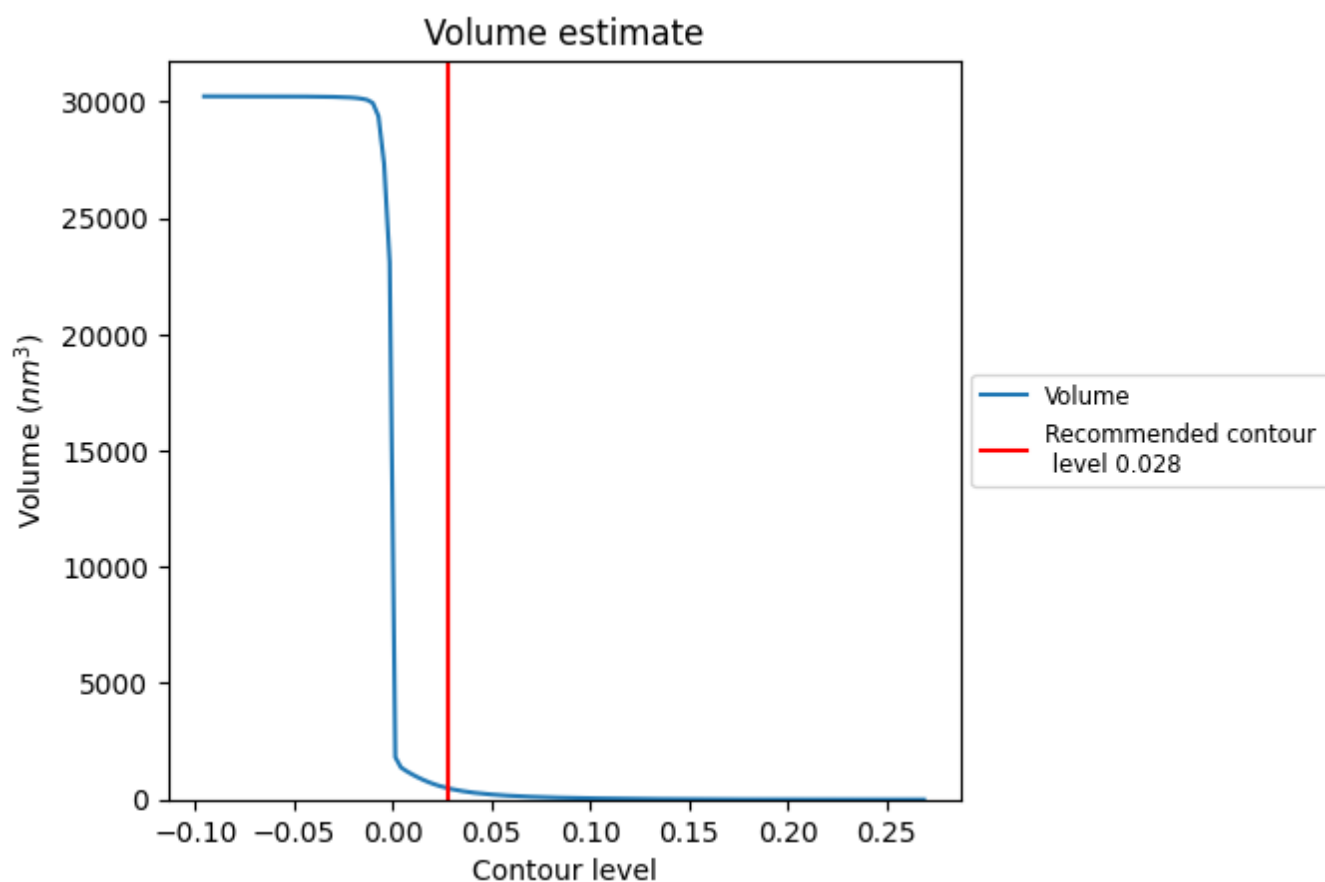
This section contains the results of statistical analysis of the map.

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



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

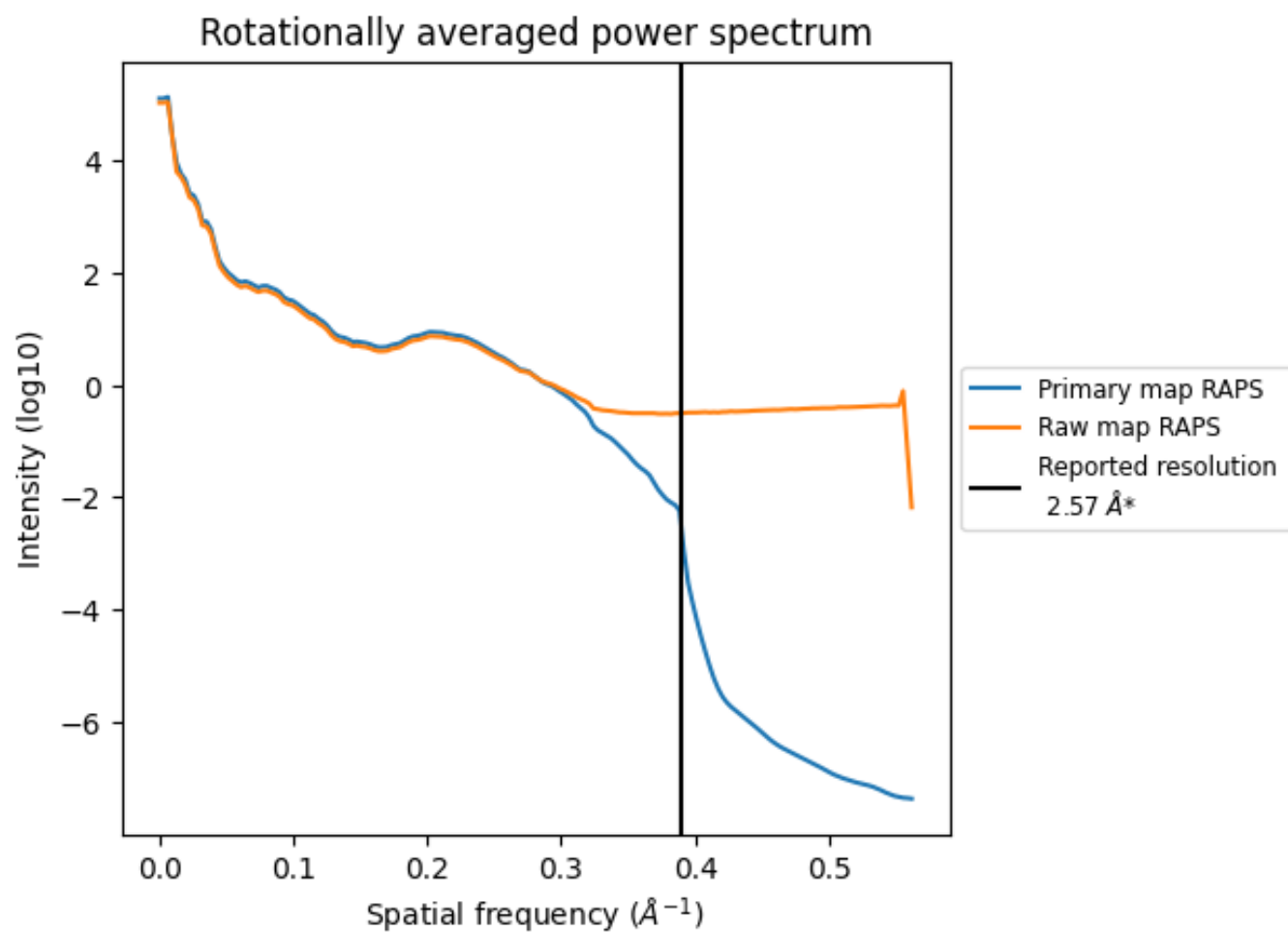
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 487  $\text{nm}^3$ ; this corresponds to an approximate mass of 440 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 ⓘ

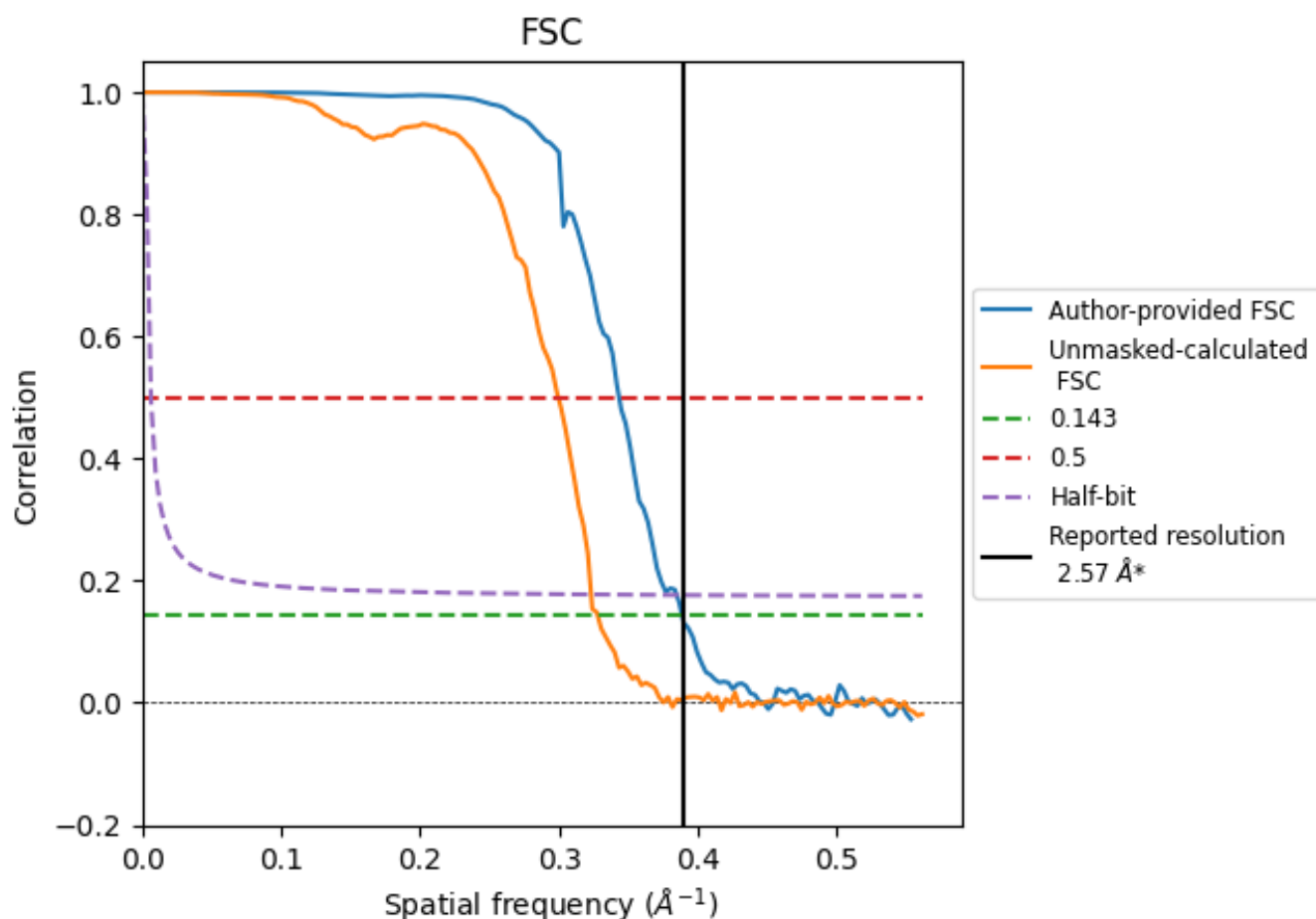


\*Reported resolution corresponds to spatial frequency of 0.389 Å<sup>-1</sup>

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

## 8.2 Resolution estimates

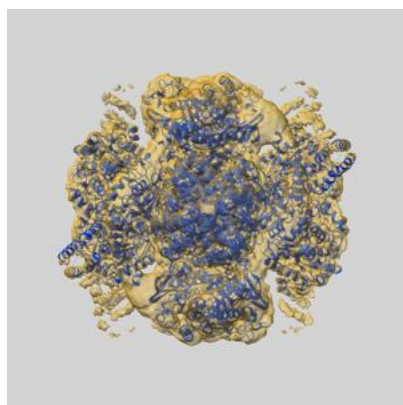
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.57                               | -    | -        |
| Author-provided FSC curve | 2.57                               | 2.91 | 2.60     |
| Unmasked-calculated*      | 3.05                               | 3.34 | 3.09     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.05 differs from the reported value 2.57 by more than 10 %

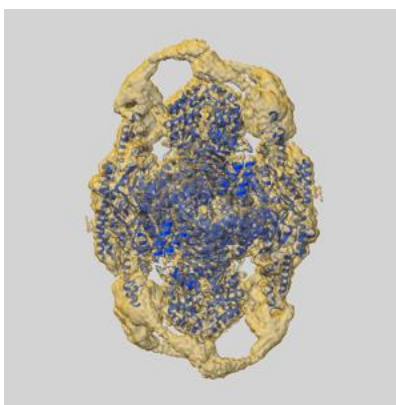
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41983 and PDB model 8U7I. Per-residue inclusion information can be found in section 3 on page 15.

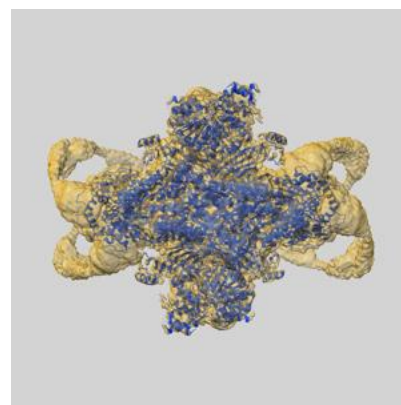
### 9.1 Map-model overlay [i](#)



X



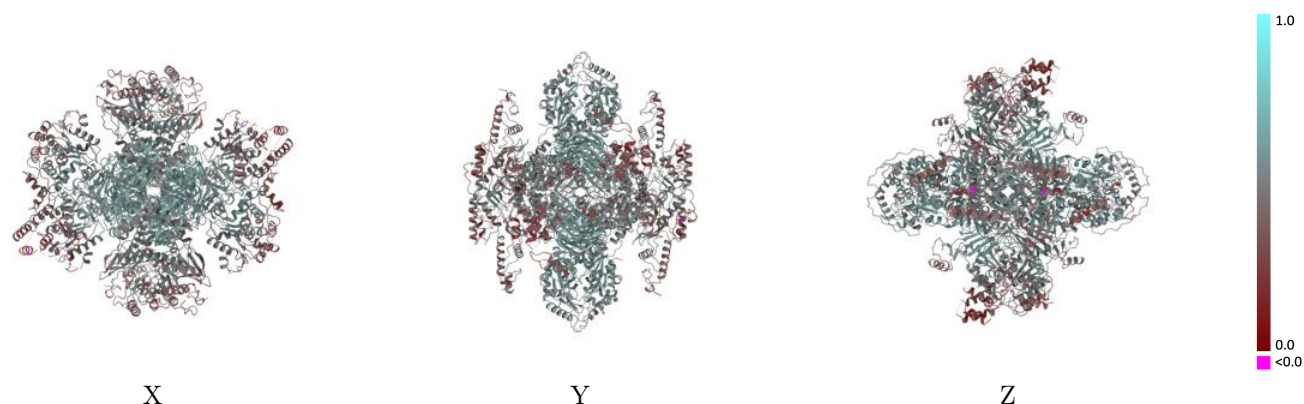
Y



Z

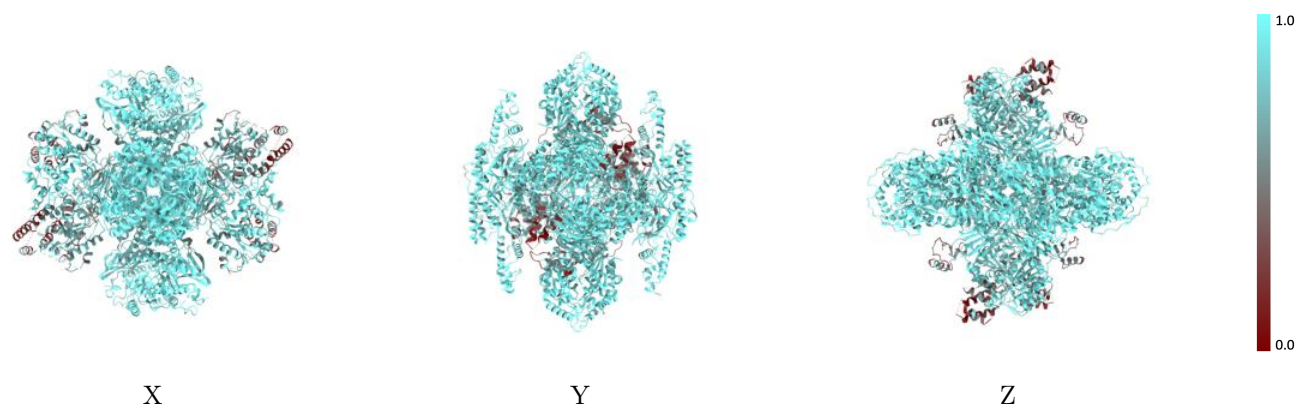
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



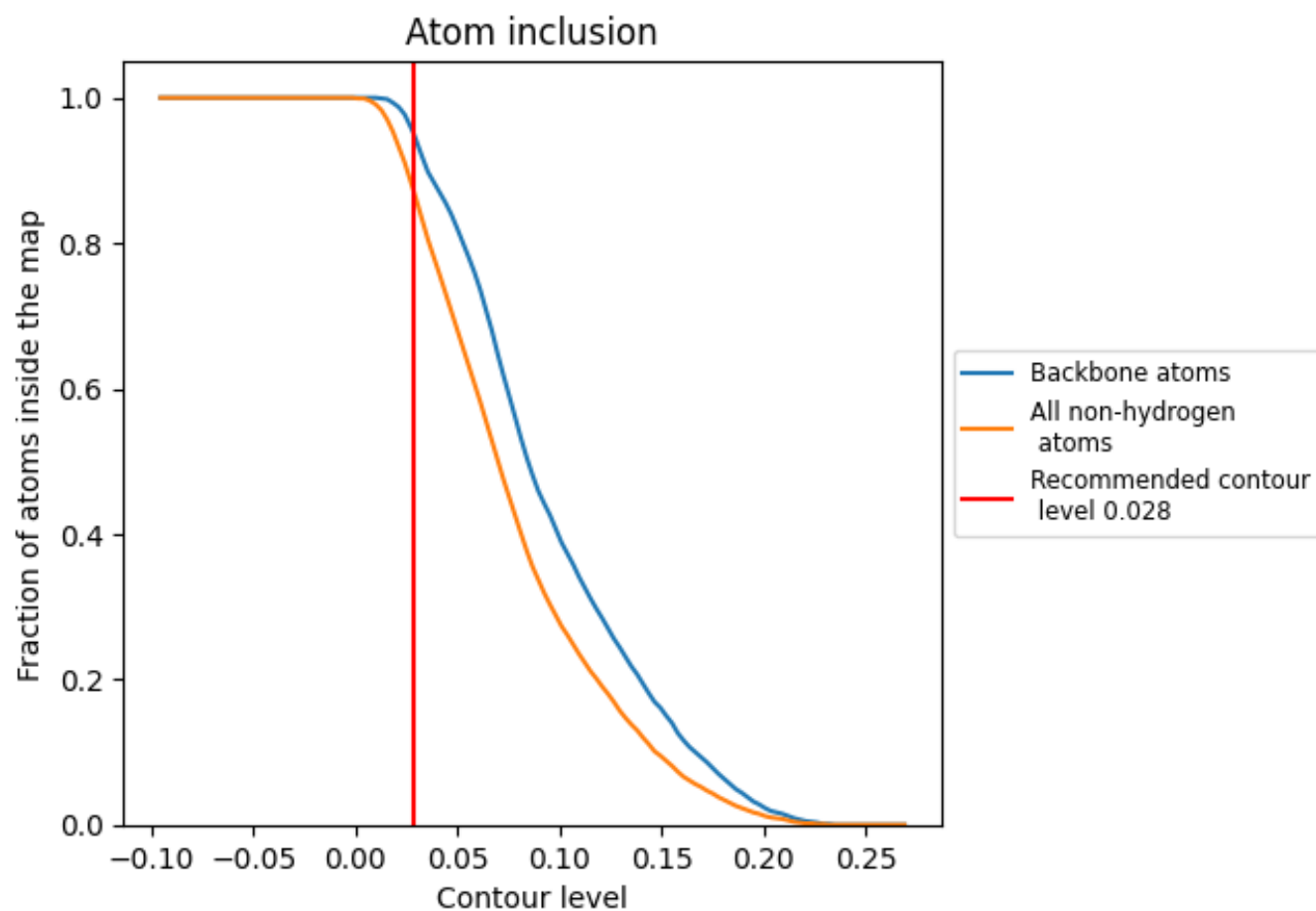
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.028).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.028) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion               | Q-score                      |
|-------|------------------------------|------------------------------|
| All   | <div><div></div>0.8760</div> | <div><div></div>0.4910</div> |
| A     | <div><div></div>0.9100</div> | <div><div></div>0.5540</div> |
| B     | <div><div></div>0.9080</div> | <div><div></div>0.5530</div> |
| C     | <div><div></div>0.9110</div> | <div><div></div>0.5540</div> |
| D     | <div><div></div>0.9100</div> | <div><div></div>0.5550</div> |
| E     | <div><div></div>0.7440</div> | <div><div></div>0.4210</div> |
| F     | <div><div></div>0.7500</div> | <div><div></div>0.4260</div> |
| G     | <div><div></div>0.7460</div> | <div><div></div>0.4240</div> |
| H     | <div><div></div>0.7400</div> | <div><div></div>0.4190</div> |
| I     | <div><div></div>0.9390</div> | <div><div></div>0.4240</div> |
| J     | <div><div></div>0.9390</div> | <div><div></div>0.4250</div> |
| K     | <div><div></div>0.9360</div> | <div><div></div>0.4120</div> |
| L     | <div><div></div>0.9410</div> | <div><div></div>0.4210</div> |
| M     | <div><div></div>0.9280</div> | <div><div></div>0.4080</div> |
| N     | <div><div></div>0.9320</div> | <div><div></div>0.4170</div> |
| O     | <div><div></div>0.9360</div> | <div><div></div>0.4210</div> |
| P     | <div><div></div>0.9350</div> | <div><div></div>0.4190</div> |

1.0

0.0

<0.0