



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:46 AM UTC

PDB ID : 9GB5 / pdb\_00009gb5  
EMDB ID : EMD-51198  
Title : Contracted phiCD508 neck  
Authors : Wilson, J.S.; Fagan, R.P.; Bullough, P.A.  
Deposited on : 2024-07-29  
Resolution : 3.27 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:

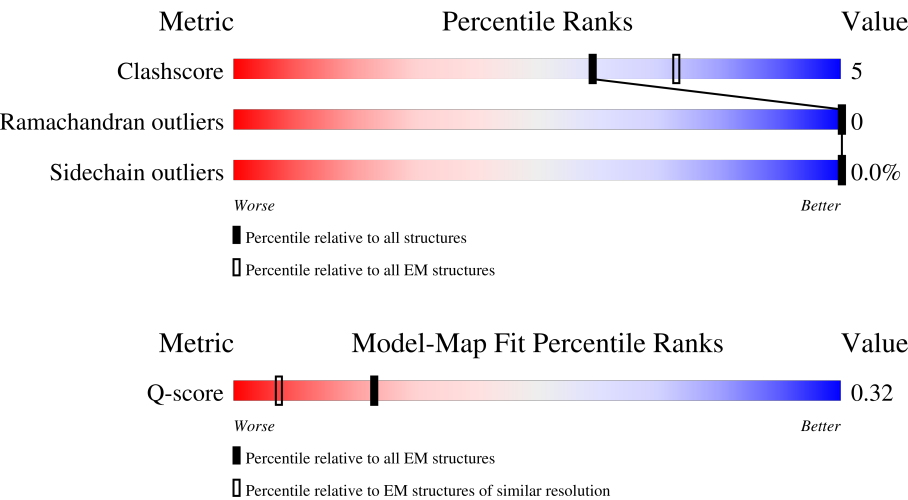
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 3.27 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.



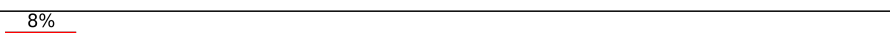
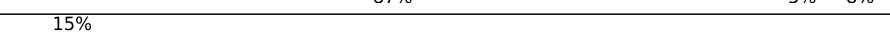
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 14508 ( 2.77 - 3.77 )                                    |

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     | 137    |                  |
| 1   | B     | 137    |                  |
| 1   | C     | 137    |                  |
| 1   | D     | 137    |                  |

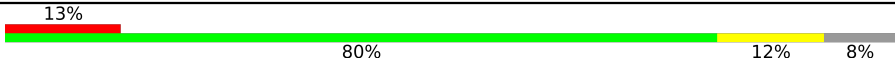
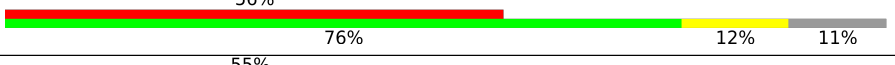
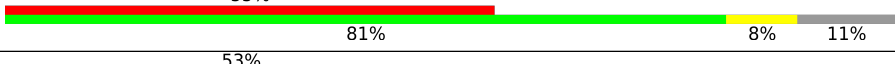
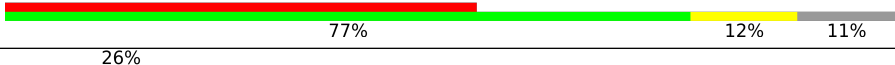
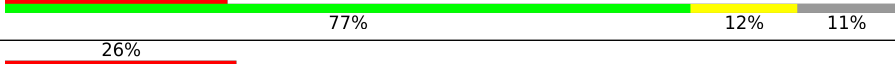
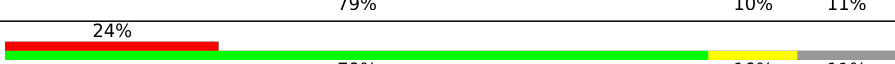
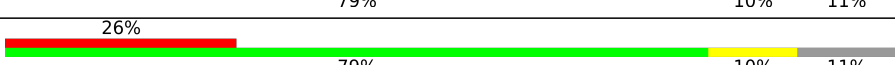
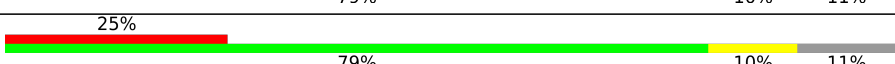
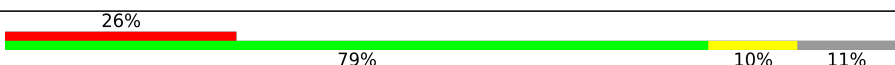
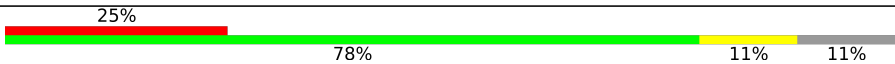
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | E     | 137    |    |
| 1   | F     | 137    |    |
| 2   | G     | 125    |    |
| 2   | K     | 125    |    |
| 2   | M     | 125    |    |
| 2   | O     | 125    |    |
| 2   | Q     | 125    |    |
| 2   | X     | 125    |    |
| 3   | H     | 273    |    |
| 3   | L     | 273    |    |
| 3   | N     | 273    |    |
| 3   | P     | 273    |    |
| 3   | R     | 273    |  |
| 3   | d     | 273    |  |
| 4   | I     | 112    |  |
| 4   | J     | 112    |  |
| 4   | S     | 112    |  |
| 4   | T     | 112    |  |
| 4   | U     | 112    |  |
| 4   | V     | 112    |  |
| 4   | W     | 112    |  |
| 4   | Y     | 112    |  |
| 4   | Z     | 112    |  |
| 4   | a     | 112    |  |
| 4   | b     | 112    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | c     | 112    |    |
| 5   | e     | 473    |    |
| 5   | f     | 473    |    |
| 5   | g     | 473    |    |
| 5   | h     | 473    |    |
| 5   | i     | 473    |    |
| 5   | j     | 473    |    |
| 6   | k     | 500    |    |
| 6   | l     | 500    |    |
| 6   | m     | 500    |    |
| 6   | n     | 500    |    |
| 6   | o     | 500    |   |
| 6   | p     | 500    |  |
| 6   | q     | 500    |  |
| 6   | r     | 500    |  |
| 6   | s     | 500    |  |
| 6   | t     | 500    |  |
| 6   | u     | 500    |  |
| 6   | v     | 500    |  |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 193668 atoms, of which 96480 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 gp56 - Tail tube protein.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 1   | A     | 130      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2060  | 652 | 1031 | 167 | 207 | 3 |         |       |
| 1   | B     | 130      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2060  | 652 | 1031 | 167 | 207 | 3 |         |       |
| 1   | C     | 130      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2060  | 652 | 1031 | 167 | 207 | 3 |         |       |
| 1   | D     | 130      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2060  | 652 | 1031 | 167 | 207 | 3 |         |       |
| 1   | E     | 130      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2060  | 652 | 1031 | 167 | 207 | 3 |         |       |
| 1   | F     | 130      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2060  | 652 | 1031 | 167 | 207 | 3 |         |       |

- Molecule 2 is a protein called gp51 - Neck valve protein.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 2   | G     | 124      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2019  | 623 | 1021 | 172 | 197 | 6 |         |       |
| 2   | K     | 124      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2019  | 623 | 1021 | 172 | 197 | 6 |         |       |
| 2   | M     | 124      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2019  | 623 | 1021 | 172 | 197 | 6 |         |       |
| 2   | O     | 124      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2019  | 623 | 1021 | 172 | 197 | 6 |         |       |
| 2   | Q     | 124      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2019  | 623 | 1021 | 172 | 197 | 6 |         |       |
| 2   | X     | 124      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 2019  | 623 | 1021 | 172 | 197 | 6 |         |       |

- Molecule 3 is a protein called gp53 - Tail adaptor protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 3   | H     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4462  | 1397 | 2247 | 380 | 426 | 12 |         |       |

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| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 3   | L     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4462  | 1397 | 2247 | 380 | 426 | 12 |         |       |
| 3   | N     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4462  | 1397 | 2247 | 380 | 426 | 12 |         |       |
| 3   | P     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4462  | 1397 | 2247 | 380 | 426 | 12 |         |       |
| 3   | R     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4462  | 1397 | 2247 | 380 | 426 | 12 |         |       |
| 3   | d     | 272      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 4462  | 1397 | 2247 | 380 | 426 | 12 |         |       |

- Molecule 4 is a protein called gp50 - Portal adaptor protein.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|---------|-------|
| 4   | I     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | J     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | S     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | T     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | U     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | V     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | W     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | Y     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | Z     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | a     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | b     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |
| 4   | c     | 103      | Total | C   | H   | N   | O   | S | 0       | 0     |
|     |       |          | 1649  | 528 | 816 | 129 | 170 | 6 |         |       |

- Molecule 5 is a protein called gp55 - Tail sheath protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 5   | e     | 420      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6585  | 2089 | 3289 | 529 | 668 | 10 |         |       |
| 5   | f     | 420      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6585  | 2089 | 3289 | 529 | 668 | 10 |         |       |
| 5   | g     | 420      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6585  | 2089 | 3289 | 529 | 668 | 10 |         |       |
| 5   | h     | 420      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6585  | 2089 | 3289 | 529 | 668 | 10 |         |       |
| 5   | i     | 420      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6585  | 2089 | 3289 | 529 | 668 | 10 |         |       |
| 5   | j     | 420      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6585  | 2089 | 3289 | 529 | 668 | 10 |         |       |

- Molecule 6 is a protein called gp45 - Portal protein.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|-------|
| 6   | k     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | l     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | m     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | n     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | o     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | p     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | q     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | r     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | s     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | t     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | u     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |
| 6   | v     | 445      | Total | C    | H    | N   | O   | S  | 0       | 0     |
|     |       |          | 6927  | 2235 | 3430 | 579 | 668 | 15 |         |       |

There are 60 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| k     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| k     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| k     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| k     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| k     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| l     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| l     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| l     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| l     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| l     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| m     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| m     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| m     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| m     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| m     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| n     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| n     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| n     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| n     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| n     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| o     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| o     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| o     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| o     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| o     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| p     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| p     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| p     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| p     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| p     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| q     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| q     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| q     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| q     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| q     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| r     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| r     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| r     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| r     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| r     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| s     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| s     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| s     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| s     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| s     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| t     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| t     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| t     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| t     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| t     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| u     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| u     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| u     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| u     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| u     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |
| v     | 51      | ASN      | LYS    | conflict | UNP A0A069A478 |
| v     | 419     | CYS      | SER    | conflict | UNP A0A069A478 |
| v     | 454     | GLY      | PRO    | conflict | UNP A0A069A478 |
| v     | 456     | ARG      | ILE    | conflict | UNP A0A069A478 |
| v     | 457     | GLU      | VAL    | conflict | UNP A0A069A478 |

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

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

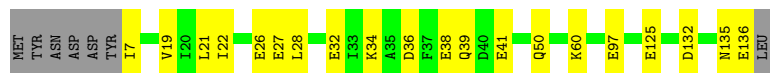
- Molecule 1: gp56 - Tail tube protein

Chain A: 



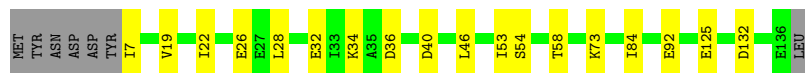
- Molecule 1: gp56 - Tail tube protein

Chain B: 



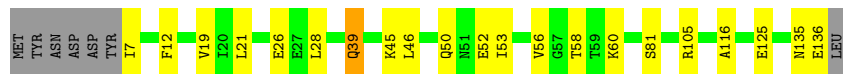
- Molecule 1: gp56 - Tail tube protein

Chain C: 



- Molecule 1: gp56 - Tail tube protein

Chain D: 



- Molecule 1: gp56 - Tail tube protein

Chain E: 



- Molecule 1: gp56 - Tail tube protein

Chain F:  86% 9% 5%



- Molecule 2: gp51 - Neck valve protein

Chain G:  89% 10% .



- Molecule 2: gp51 - Neck valve protein

Chain K:  86% 14% .



- Molecule 2: gp51 - Neck valve protein

Chain M:  85% 14% .



- Molecule 2: gp51 - Neck valve protein

Chain O:  88% 11% .



- Molecule 2: gp51 - Neck valve protein

Chain Q:  90% 9% .



- Molecule 2: gp51 - Neck valve protein

Chain X:  84% 15% .



- Molecule 3: gp53 - Tail adaptor protein

Chain H:  89% 11%



- Molecule 3: gp53 - Tail adaptor protein

Chain L:  86% 13%



- Molecule 3: gp53 - Tail adaptor protein

Chain N:  88% 12%



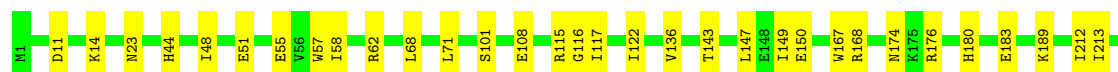
- Molecule 3: gp53 - Tail adaptor protein

Chain P:  86% 14%



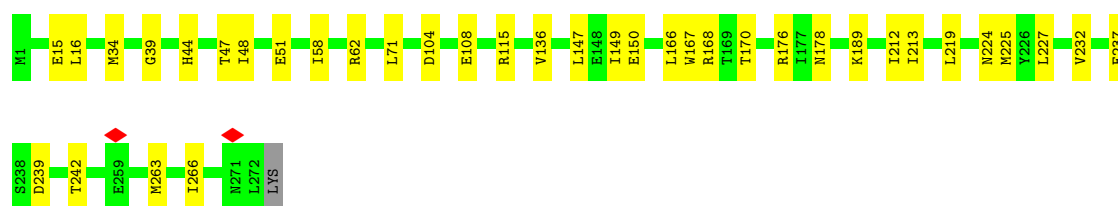
- Molecule 3: gp53 - Tail adaptor protein

Chain R:  86% 14%



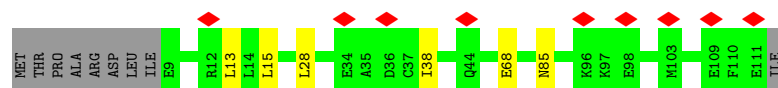
- Molecule 3: gp53 - Tail adaptor protein

Chain d:  86% 14%



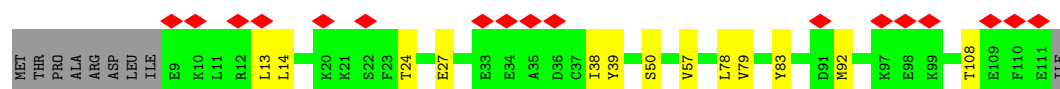
• Molecule 4: gp50 - Portal adaptor protein

Chain I:  8% 87% 5% 8%



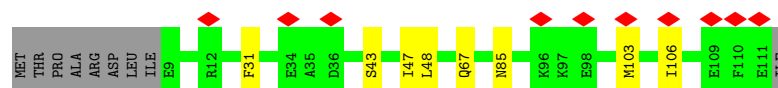
• Molecule 4: gp50 - Portal adaptor protein

Chain J:  15% 80% 12% 8%



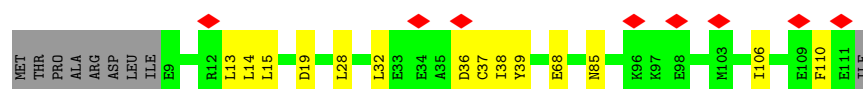
• Molecule 4: gp50 - Portal adaptor protein

Chain S:  9% 85% 7% 8%



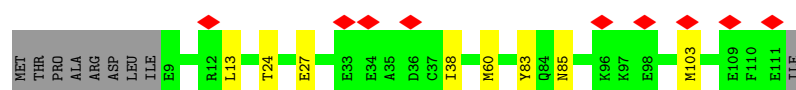
• Molecule 4: gp50 - Portal adaptor protein

Chain T:  7% 79% 12% 8%



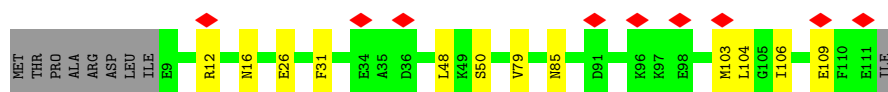
• Molecule 4: gp50 - Portal adaptor protein

Chain U:  8% 85% 7% 8%

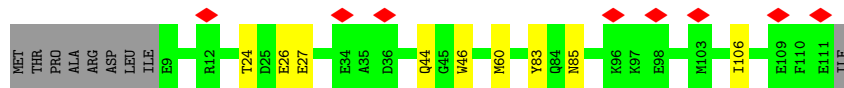
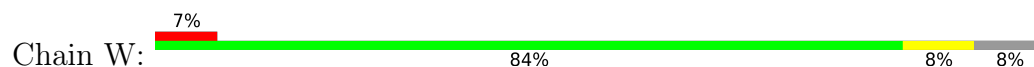


• Molecule 4: gp50 - Portal adaptor protein

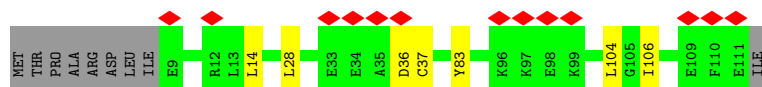
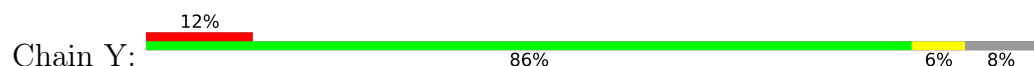
Chain V:  8% 81% 11% 8%



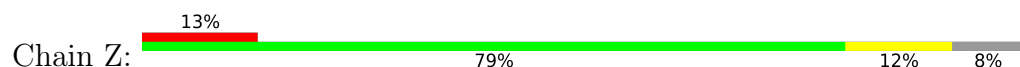
- Molecule 4: gp50 - Portal adaptor protein



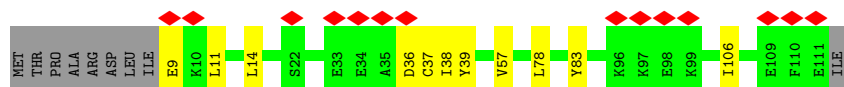
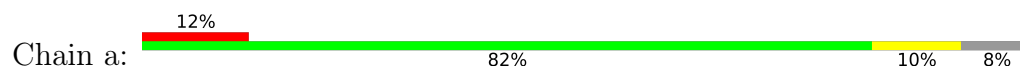
- Molecule 4: gp50 - Portal adaptor protein



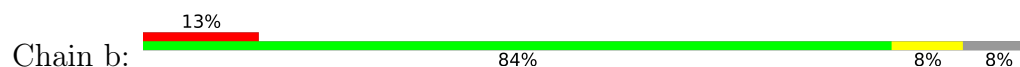
- Molecule 4: gp50 - Portal adaptor protein



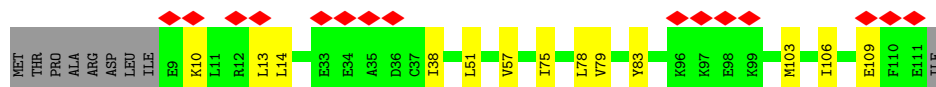
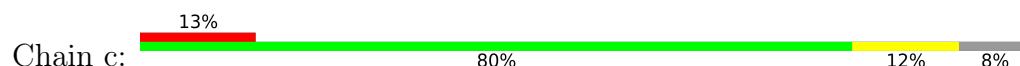
- Molecule 4: gp50 - Portal adaptor protein



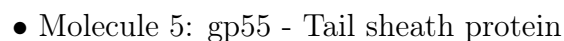
- Molecule 4: gp50 - Portal adaptor protein

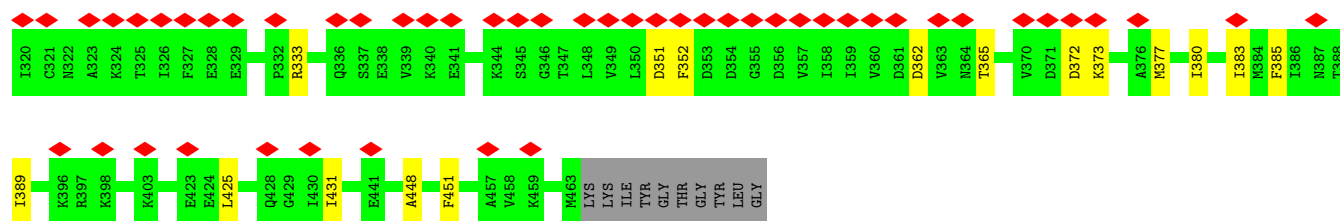


- Molecule 4: gp50 - Portal adaptor protein

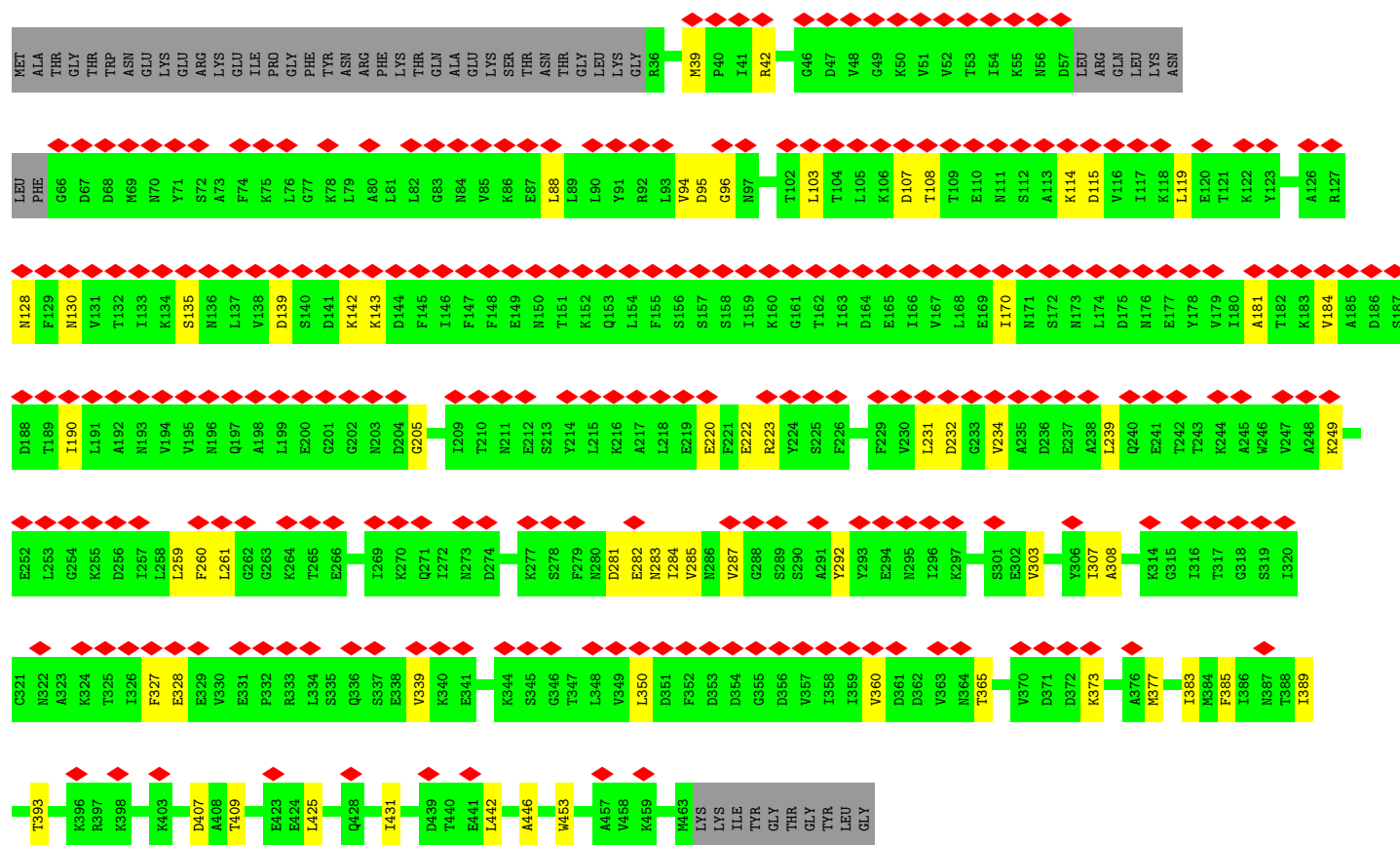
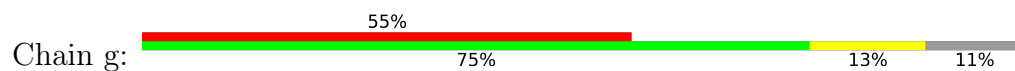


- Molecule 5: gp55 - Tail sheath protein

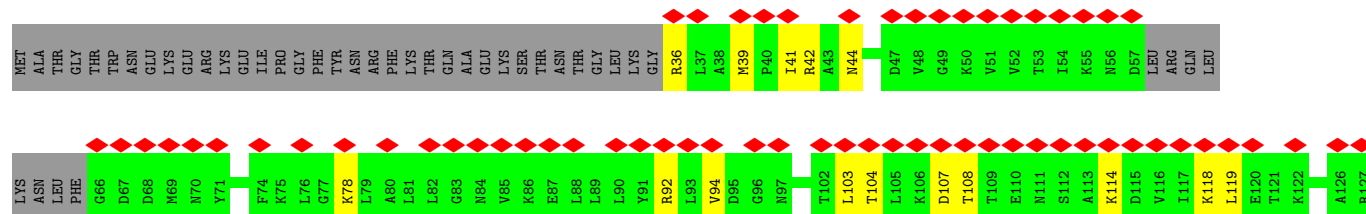
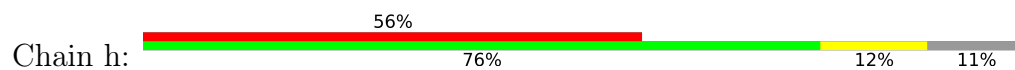


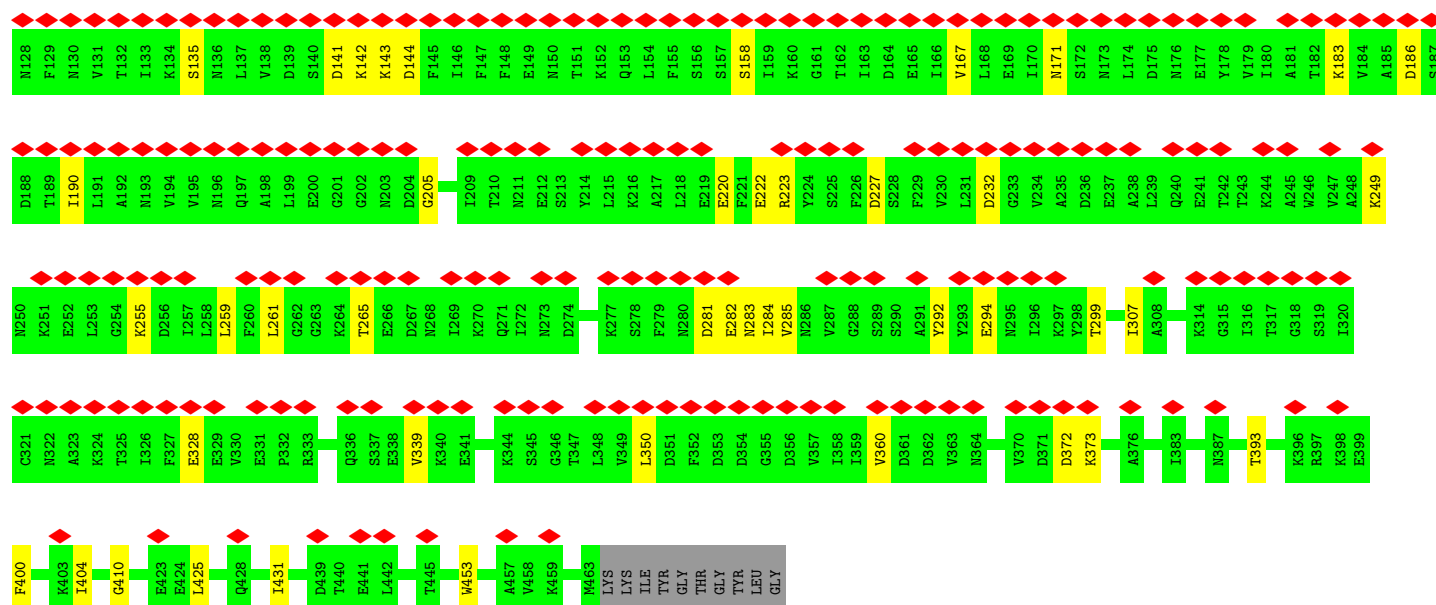


• Molecule 5: gp55 - Tail sheath protein

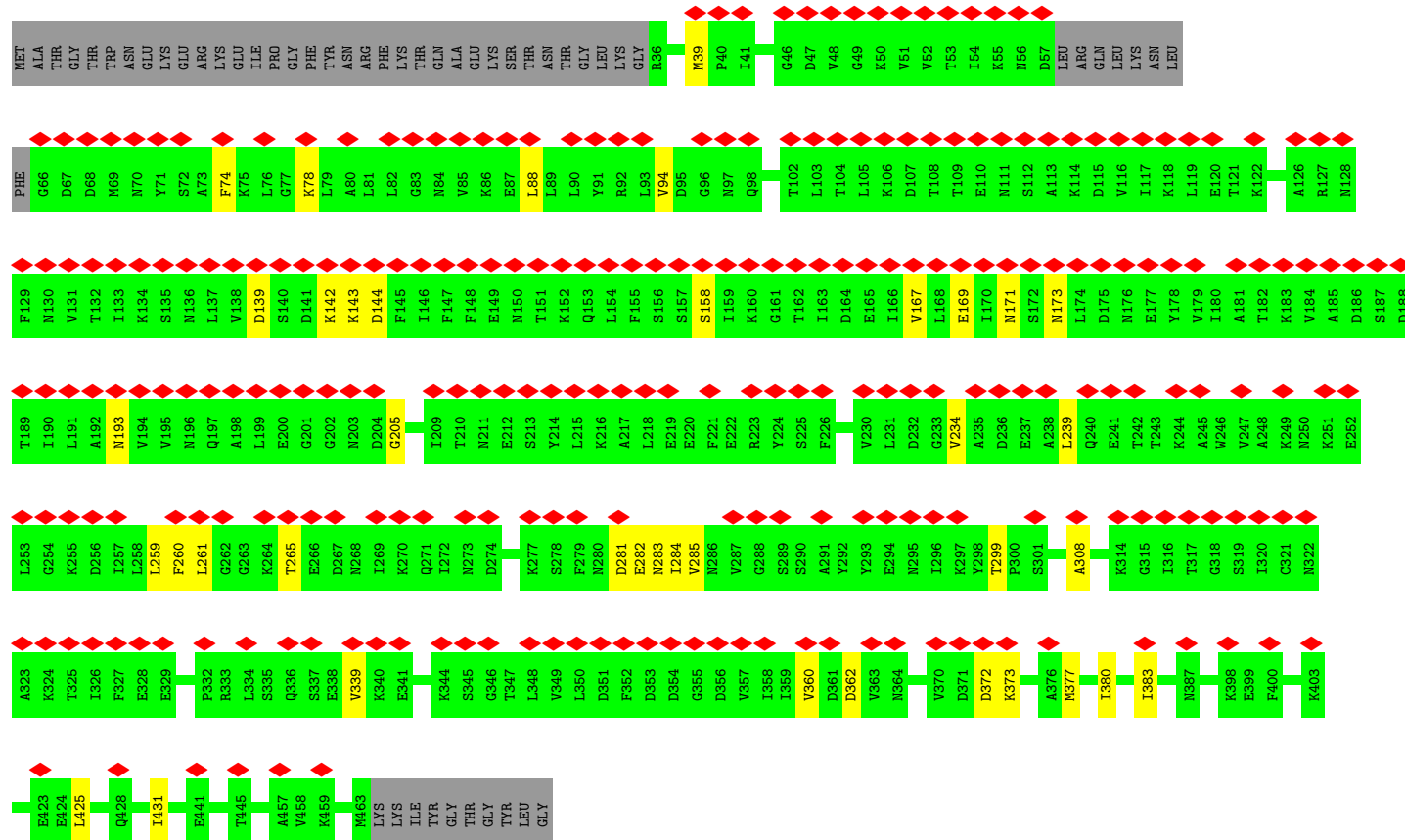
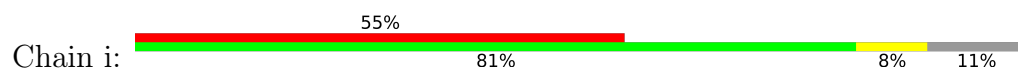


• Molecule 5: gp55 - Tail sheath protein

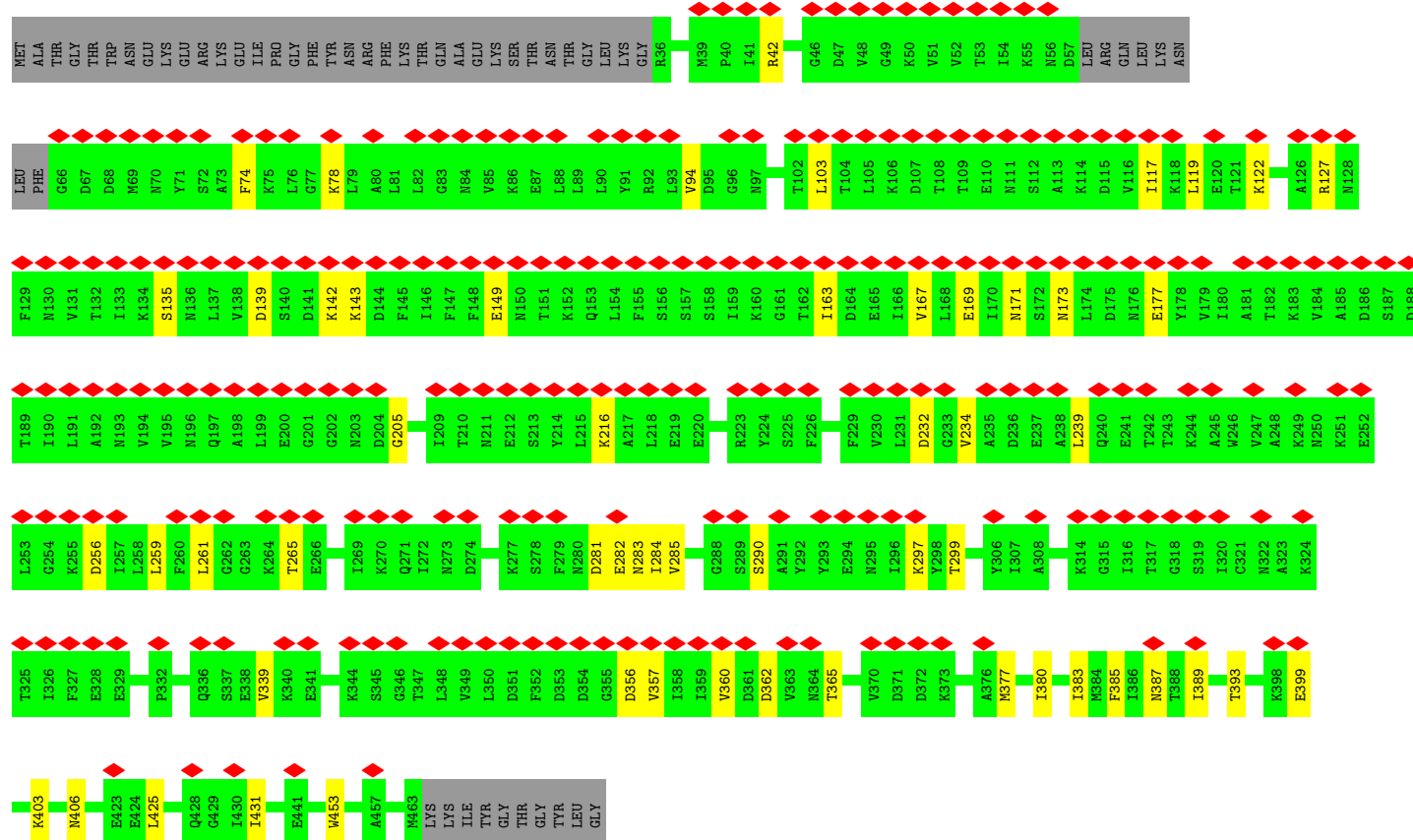
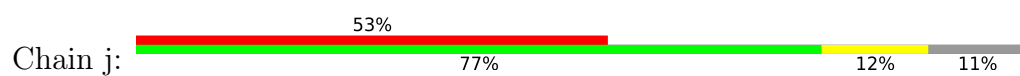




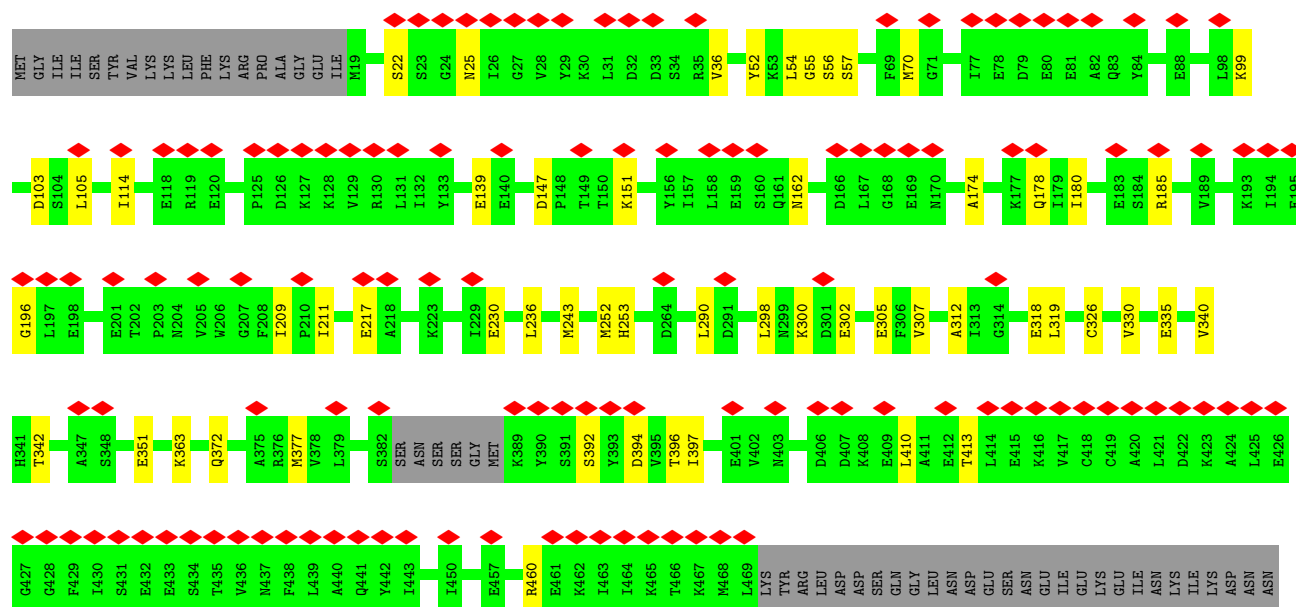
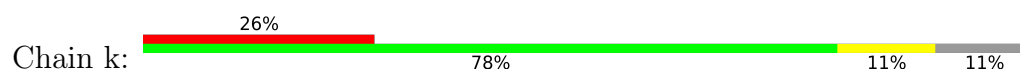
• Molecule 5: gp55 - Tail sheath protein



• Molecule 5: gp55 - Tail sheath protein



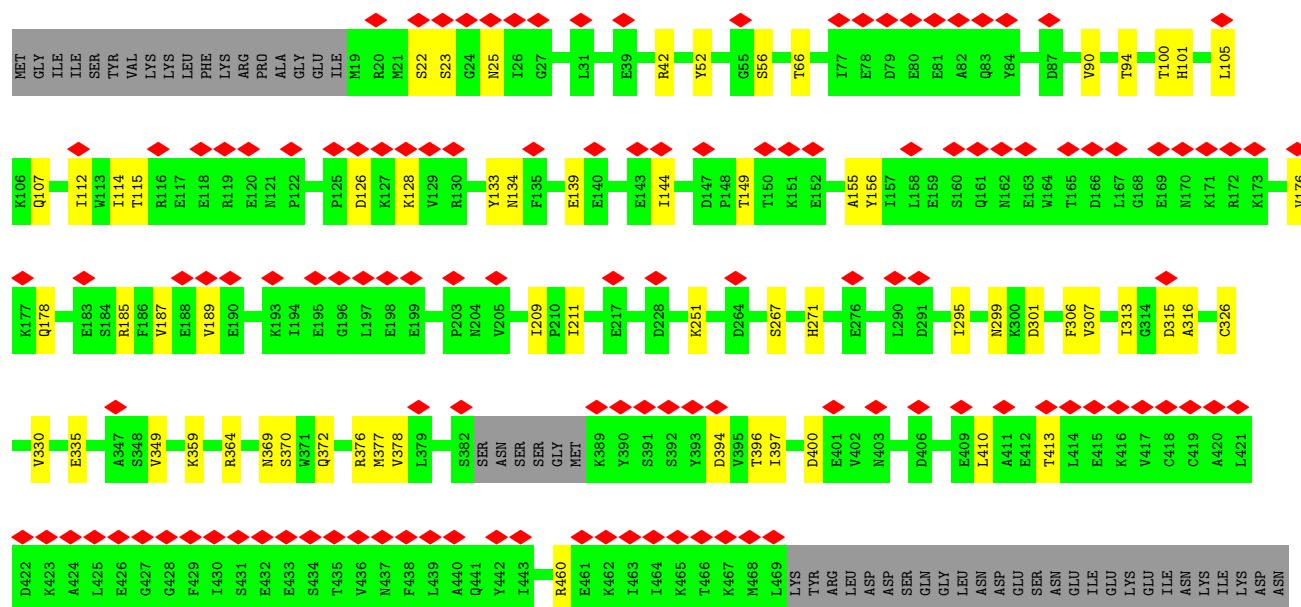
• Molecule 6: gp45 - Portal protein



GLY  
ASN  
GLY

• Molecule 6: gp45 - Portal protein

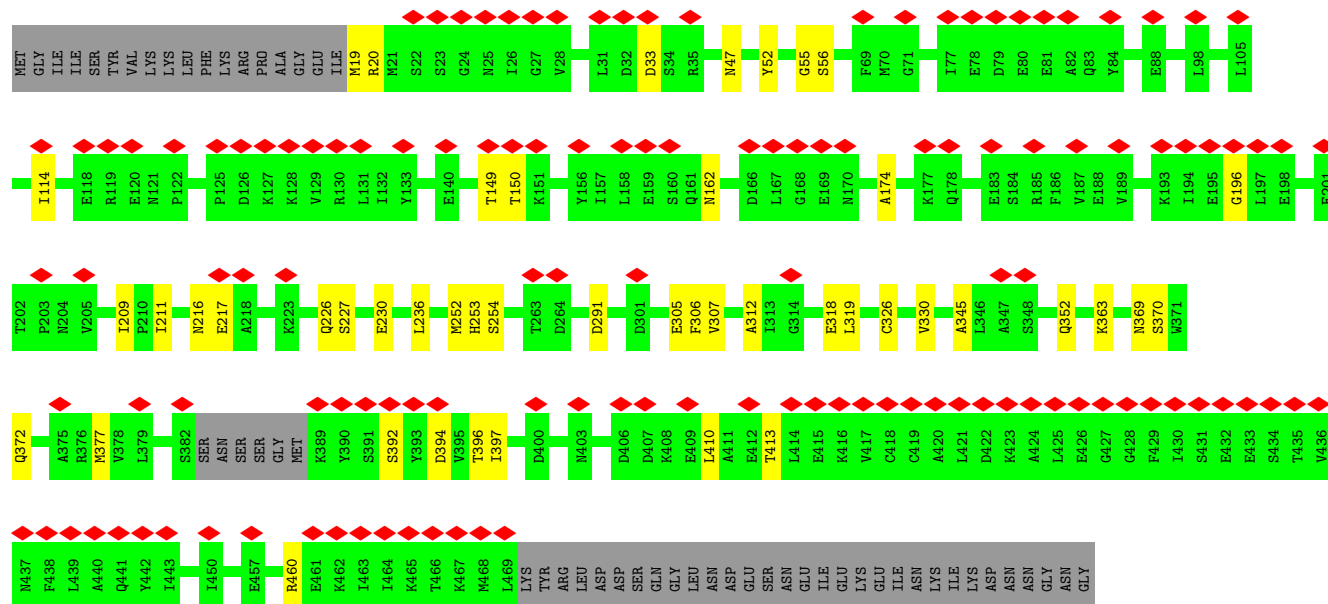
Chain l: 25% 77% 12% 11%



ASN  
GLY  
ASN  
GLY

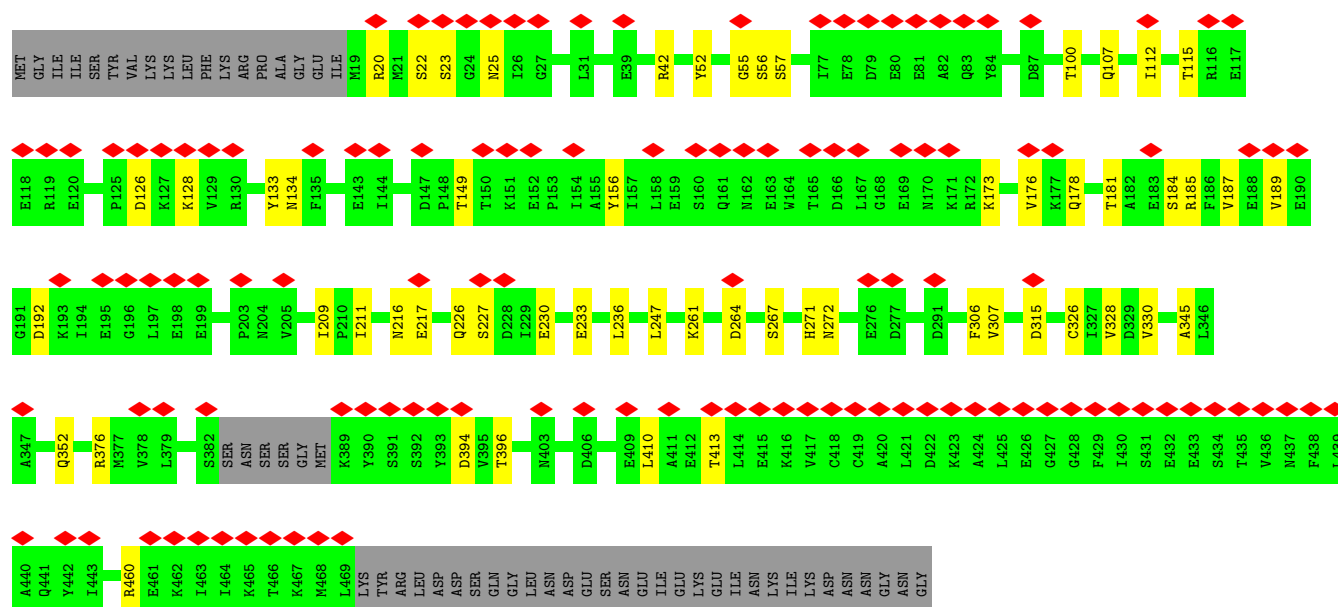
• Molecule 6: gp45 - Portal protein

Chain m: 26% 80% 9% 11%



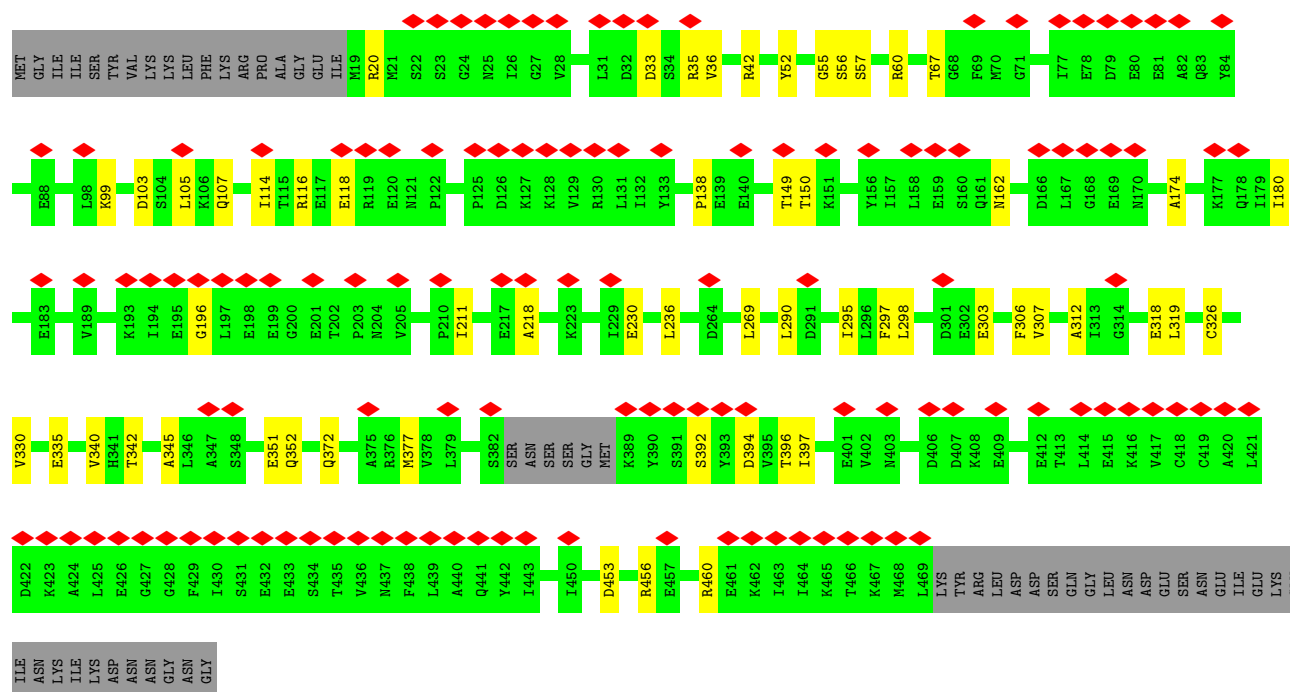
• Molecule 6: gp45 - Portal protein

Chain n: 



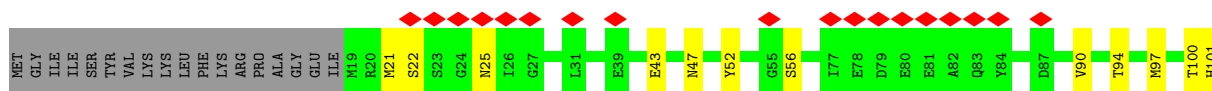
• Molecule 6: gp45 - Portal protein

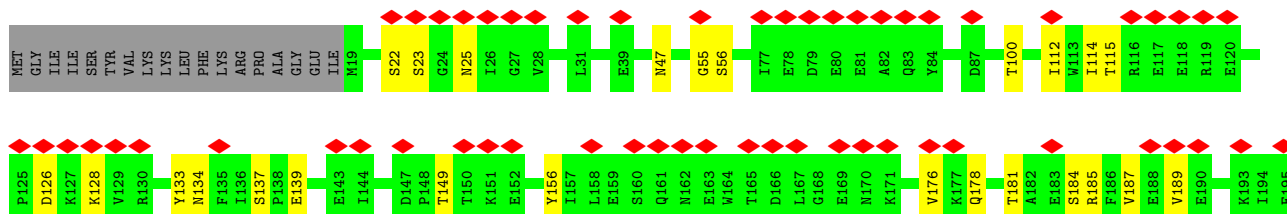
Chain o: 

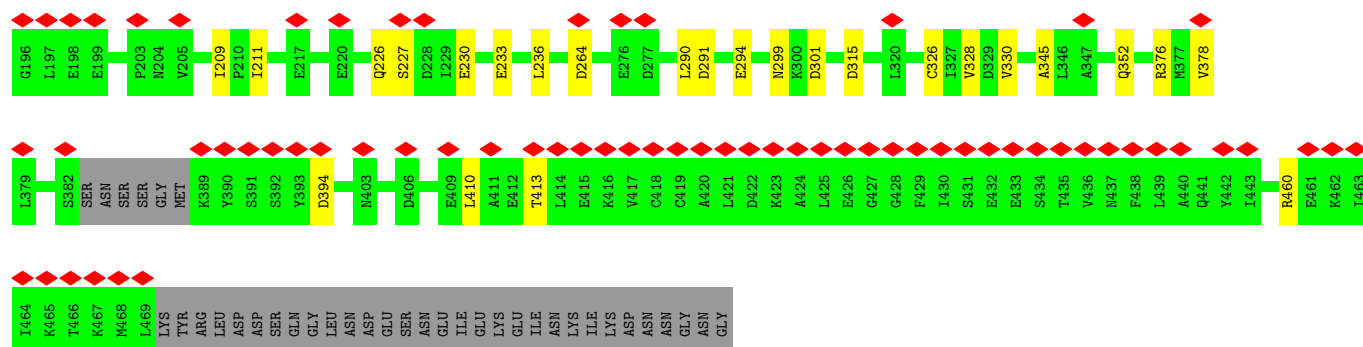


• Molecule 6: gp45 - Portal protein

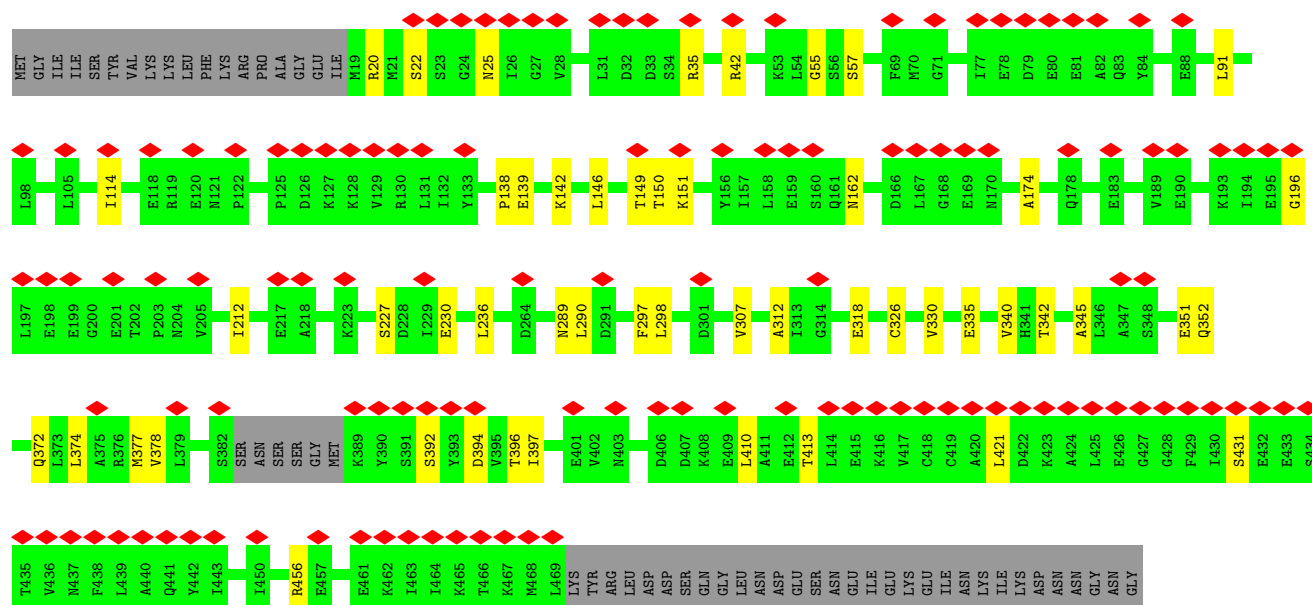
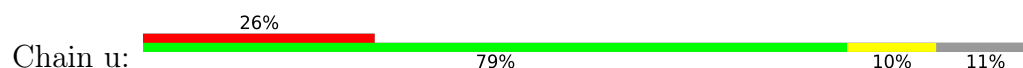
Chain p: 



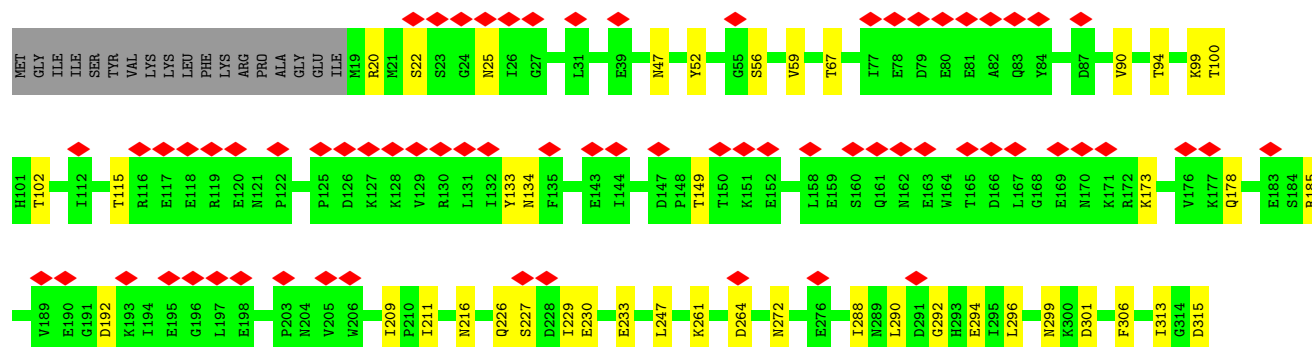
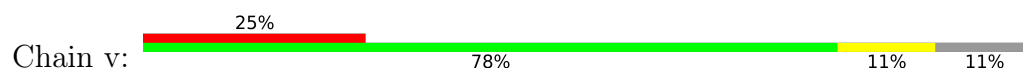


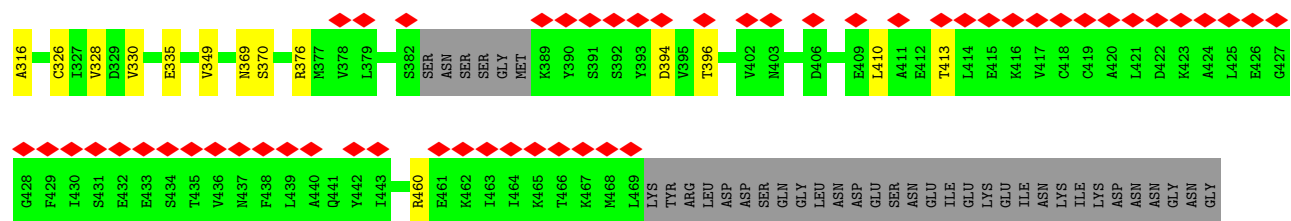


• Molecule 6: gp45 - Portal protein



• Molecule 6: gp45 - Portal protein





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 30325                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 42                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 1.428                                   | Depositor |
| Minimum map value                    | -0.719                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.063                                   | Depositor |
| Recommended contour level            | 0.249                                   | Depositor |
| Map size (Å)                         | 423.99997, 423.99997, 423.99997         | wwPDB     |
| Map dimensions                       | 400, 400, 400                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.06, 1.06, 1.06                        | 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     | 0.23         | 0/1041  | 0.36        | 0/1394  |
| 1   | B     | 0.23         | 0/1041  | 0.36        | 0/1394  |
| 1   | C     | 0.23         | 0/1041  | 0.36        | 0/1394  |
| 1   | D     | 0.22         | 0/1041  | 0.34        | 0/1394  |
| 1   | E     | 0.22         | 0/1041  | 0.36        | 0/1394  |
| 1   | F     | 0.23         | 0/1041  | 0.35        | 0/1394  |
| 2   | G     | 0.24         | 0/1007  | 0.37        | 0/1353  |
| 2   | K     | 0.25         | 0/1007  | 0.38        | 0/1353  |
| 2   | M     | 0.25         | 0/1007  | 0.36        | 0/1353  |
| 2   | O     | 0.25         | 0/1007  | 0.38        | 0/1353  |
| 2   | Q     | 0.25         | 0/1007  | 0.41        | 0/1353  |
| 2   | X     | 0.24         | 0/1007  | 0.39        | 0/1353  |
| 3   | H     | 0.25         | 0/2249  | 0.38        | 0/3030  |
| 3   | L     | 0.25         | 0/2249  | 0.38        | 0/3030  |
| 3   | N     | 0.25         | 0/2249  | 0.37        | 0/3030  |
| 3   | P     | 0.26         | 0/2249  | 0.39        | 0/3030  |
| 3   | R     | 0.25         | 0/2249  | 0.36        | 0/3030  |
| 3   | d     | 0.25         | 0/2249  | 0.38        | 0/3030  |
| 4   | I     | 0.22         | 0/845   | 0.38        | 0/1130  |
| 4   | J     | 0.21         | 0/845   | 0.39        | 0/1130  |
| 4   | S     | 0.23         | 0/845   | 0.42        | 0/1130  |
| 4   | T     | 0.21         | 0/845   | 0.38        | 0/1130  |
| 4   | U     | 0.21         | 0/845   | 0.37        | 0/1130  |
| 4   | V     | 0.21         | 0/845   | 0.35        | 0/1130  |
| 4   | W     | 0.21         | 0/845   | 0.38        | 0/1130  |
| 4   | Y     | 0.21         | 0/845   | 0.37        | 0/1130  |
| 4   | Z     | 0.22         | 0/845   | 0.40        | 0/1130  |
| 4   | a     | 0.21         | 0/845   | 0.39        | 0/1130  |
| 4   | b     | 0.20         | 0/845   | 0.38        | 0/1130  |
| 4   | c     | 0.21         | 0/845   | 0.37        | 0/1130  |
| 5   | e     | 0.15         | 0/3340  | 0.34        | 0/4508  |
| 5   | f     | 0.18         | 0/3340  | 0.37        | 0/4508  |
| 5   | g     | 0.16         | 0/3340  | 0.35        | 0/4508  |
| 5   | h     | 0.16         | 0/3340  | 0.35        | 0/4508  |

| Mol | Chain | Bond lengths |         | Bond angles |          |
|-----|-------|--------------|---------|-------------|----------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5  |
| 5   | i     | 0.17         | 0/3340  | 0.36        | 0/4508   |
| 5   | j     | 0.16         | 0/3340  | 0.34        | 0/4508   |
| 6   | k     | 0.16         | 0/3566  | 0.34        | 0/4820   |
| 6   | l     | 0.16         | 0/3566  | 0.36        | 0/4820   |
| 6   | m     | 0.15         | 0/3566  | 0.34        | 0/4820   |
| 6   | n     | 0.15         | 0/3566  | 0.34        | 0/4820   |
| 6   | o     | 0.15         | 0/3566  | 0.34        | 0/4820   |
| 6   | p     | 0.16         | 0/3566  | 0.34        | 0/4820   |
| 6   | q     | 0.16         | 0/3566  | 0.33        | 0/4820   |
| 6   | r     | 0.15         | 0/3566  | 0.35        | 0/4820   |
| 6   | s     | 0.16         | 0/3566  | 0.35        | 0/4820   |
| 6   | t     | 0.16         | 0/3566  | 0.35        | 0/4820   |
| 6   | u     | 0.16         | 0/3566  | 0.34        | 0/4820   |
| 6   | v     | 0.16         | 0/3566  | 0.34        | 0/4820   |
| All | All   | 0.19         | 0/98754 | 0.36        | 0/133110 |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4   | T     | 0                   | 1                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 4   | T     | 19  | ASP  | Peptide |

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1029  | 1031     | 1030     | 10      | 0            |
| 1   | B     | 1029  | 1031     | 1030     | 16      | 0            |
| 1   | C     | 1029  | 1031     | 1030     | 15      | 0            |
| 1   | D     | 1029  | 1031     | 1030     | 19      | 0            |
| 1   | E     | 1029  | 1031     | 1030     | 14      | 0            |
| 1   | F     | 1029  | 1031     | 1030     | 11      | 0            |
| 2   | G     | 998   | 1021     | 1020     | 8       | 0            |
| 2   | K     | 998   | 1021     | 1020     | 11      | 0            |
| 2   | M     | 998   | 1021     | 1020     | 12      | 0            |
| 2   | O     | 998   | 1021     | 1020     | 10      | 0            |
| 2   | Q     | 998   | 1021     | 1020     | 8       | 0            |
| 2   | X     | 998   | 1021     | 1020     | 13      | 0            |
| 3   | H     | 2215  | 2247     | 2244     | 26      | 0            |
| 3   | L     | 2215  | 2247     | 2244     | 29      | 0            |
| 3   | N     | 2215  | 2247     | 2244     | 24      | 0            |
| 3   | P     | 2215  | 2247     | 2244     | 31      | 0            |
| 3   | R     | 2215  | 2247     | 2244     | 31      | 0            |
| 3   | d     | 2215  | 2247     | 2244     | 29      | 0            |
| 4   | I     | 833   | 816      | 815      | 6       | 0            |
| 4   | J     | 833   | 816      | 815      | 9       | 0            |
| 4   | S     | 833   | 816      | 815      | 7       | 0            |
| 4   | T     | 833   | 816      | 815      | 10      | 0            |
| 4   | U     | 833   | 816      | 815      | 6       | 0            |
| 4   | V     | 833   | 816      | 815      | 11      | 0            |
| 4   | W     | 833   | 816      | 815      | 8       | 0            |
| 4   | Y     | 833   | 816      | 815      | 5       | 0            |
| 4   | Z     | 833   | 816      | 815      | 10      | 0            |
| 4   | a     | 833   | 816      | 815      | 8       | 0            |
| 4   | b     | 833   | 816      | 815      | 9       | 0            |
| 4   | c     | 833   | 816      | 815      | 11      | 0            |
| 5   | e     | 3296  | 3289     | 3287     | 28      | 0            |
| 5   | f     | 3296  | 3289     | 3287     | 36      | 0            |
| 5   | g     | 3296  | 3289     | 3287     | 38      | 0            |
| 5   | h     | 3296  | 3289     | 3287     | 34      | 0            |
| 5   | i     | 3296  | 3289     | 3287     | 24      | 0            |
| 5   | j     | 3296  | 3289     | 3287     | 32      | 0            |
| 6   | k     | 3497  | 3430     | 3424     | 39      | 0            |
| 6   | l     | 3497  | 3430     | 3424     | 42      | 0            |
| 6   | m     | 3497  | 3430     | 3424     | 33      | 0            |
| 6   | n     | 3497  | 3430     | 3424     | 41      | 0            |
| 6   | o     | 3497  | 3430     | 3424     | 43      | 0            |
| 6   | p     | 3497  | 3430     | 3424     | 38      | 0            |
| 6   | q     | 3497  | 3430     | 3424     | 35      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | r     | 3497  | 3430     | 3424     | 37      | 0            |
| 6   | s     | 3497  | 3430     | 3424     | 35      | 0            |
| 6   | t     | 3497  | 3430     | 3424     | 33      | 0            |
| 6   | u     | 3497  | 3430     | 3424     | 34      | 0            |
| 6   | v     | 3497  | 3430     | 3424     | 45      | 0            |
| All | All   | 97188 | 96480    | 96354    | 890     | 0            |

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

All (890) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:U:13:LEU:HD22  | 4:U:38:ILE:HD13  | 1.59                     | 0.82              |
| 4:T:13:LEU:HD22  | 4:T:38:ILE:HD13  | 1.62                     | 0.81              |
| 5:j:234:VAL:HG11 | 5:j:239:LEU:HD12 | 1.61                     | 0.81              |
| 5:f:234:VAL:HG11 | 5:f:239:LEU:HD12 | 1.63                     | 0.79              |
| 6:t:100:THR:HG1  | 6:t:133:TYR:HH   | 1.28                     | 0.76              |
| 6:p:22:SER:OG    | 6:p:25:ASN:OD1   | 2.05                     | 0.74              |
| 5:h:282:GLU:OE2  | 5:h:373:LYS:NZ   | 2.20                     | 0.74              |
| 6:v:22:SER:OG    | 6:v:25:ASN:OD1   | 2.06                     | 0.73              |
| 1:A:46:LEU:HD23  | 1:A:53:ILE:HD13  | 1.68                     | 0.73              |
| 1:D:7:ILE:HD11   | 3:d:213:ILE:HD11 | 1.70                     | 0.73              |
| 6:r:22:SER:OG    | 6:r:25:ASN:OD1   | 2.05                     | 0.73              |
| 4:W:85:ASN:OD1   | 4:c:83:TYR:OH    | 2.06                     | 0.73              |
| 6:t:22:SER:OG    | 6:t:25:ASN:OD1   | 2.06                     | 0.73              |
| 6:m:19:MET:N     | 6:n:233:GLU:OE1  | 2.22                     | 0.73              |
| 6:n:22:SER:OG    | 6:n:25:ASN:OD1   | 2.06                     | 0.73              |
| 4:T:85:ASN:OD1   | 4:Z:83:TYR:OH    | 2.06                     | 0.72              |
| 6:n:216:ASN:ND2  | 6:n:226:GLN:O    | 2.22                     | 0.72              |
| 4:U:24:THR:OG1   | 4:U:27:GLU:OE1   | 2.08                     | 0.72              |
| 2:M:71:ARG:O     | 2:M:71:ARG:NH1   | 2.22                     | 0.72              |
| 1:E:28:LEU:O     | 3:N:178:ASN:ND2  | 2.22                     | 0.72              |
| 6:l:22:SER:OG    | 6:l:25:ASN:OD1   | 2.05                     | 0.71              |
| 6:p:315:ASP:OD2  | 6:q:312:ALA:N    | 2.24                     | 0.71              |
| 2:M:26:SER:OG    | 2:M:41:THR:OG1   | 2.08                     | 0.71              |
| 1:F:7:ILE:HD11   | 3:H:213:ILE:HD11 | 1.71                     | 0.71              |
| 2:K:7:ARG:NH2    | 4:T:68:GLU:OE1   | 2.23                     | 0.71              |
| 6:t:47:ASN:OD1   | 6:t:56:SER:OG    | 2.09                     | 0.71              |
| 4:U:85:ASN:OD1   | 4:a:83:TYR:OH    | 2.07                     | 0.70              |
| 6:p:216:ASN:ND2  | 6:p:226:GLN:O    | 2.24                     | 0.70              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:32:GLU:OE2   | 1:B:34:LYS:NZ    | 2.24                     | 0.70              |
| 5:g:281:ASP:O    | 5:g:365:THR:OG1  | 2.10                     | 0.70              |
| 3:R:62:ARG:NH1   | 3:R:108:GLU:OE1  | 2.24                     | 0.70              |
| 6:n:315:ASP:OD2  | 6:o:312:ALA:N    | 2.24                     | 0.70              |
| 1:A:32:GLU:OE2   | 1:A:66:ASN:ND2   | 2.25                     | 0.69              |
| 6:l:315:ASP:OD2  | 6:m:312:ALA:N    | 2.24                     | 0.69              |
| 6:v:178:GLN:OE1  | 6:v:185:ARG:NH2  | 2.25                     | 0.69              |
| 4:S:85:ASN:OD1   | 4:Y:83:TYR:OH    | 2.10                     | 0.69              |
| 1:E:32:GLU:OE2   | 1:E:34:LYS:NZ    | 2.25                     | 0.69              |
| 5:j:74:PHE:O     | 5:j:78:LYS:NZ    | 2.26                     | 0.69              |
| 6:v:216:ASN:ND2  | 6:v:226:GLN:O    | 2.26                     | 0.69              |
| 2:G:26:SER:OG    | 2:G:41:THR:OG1   | 2.10                     | 0.69              |
| 5:h:220:GLU:OE1  | 5:h:223:ARG:NH2  | 2.26                     | 0.69              |
| 6:p:178:GLN:OE1  | 6:p:185:ARG:NH2  | 2.26                     | 0.69              |
| 6:k:300:LYS:O    | 6:v:261:LYS:NZ   | 2.26                     | 0.69              |
| 5:i:234:VAL:HG11 | 5:i:239:LEU:HD12 | 1.74                     | 0.68              |
| 6:r:315:ASP:OD2  | 6:s:312:ALA:N    | 2.25                     | 0.68              |
| 5:g:220:GLU:OE1  | 5:g:223:ARG:NH2  | 2.27                     | 0.68              |
| 6:k:312:ALA:N    | 6:v:315:ASP:OD2  | 2.25                     | 0.68              |
| 6:q:22:SER:OG    | 6:q:25:ASN:OD1   | 2.11                     | 0.68              |
| 6:l:23:SER:OG    | 6:m:33:ASP:O     | 2.12                     | 0.68              |
| 6:t:376:ARG:NH2  | 6:t:394:ASP:OD1  | 2.27                     | 0.68              |
| 1:B:60:LYS:NZ    | 1:C:54:SER:OG    | 2.27                     | 0.68              |
| 3:P:62:ARG:NH1   | 3:P:108:GLU:OE1  | 2.27                     | 0.68              |
| 1:C:28:LEU:O     | 3:L:178:ASN:ND2  | 2.27                     | 0.67              |
| 3:P:213:ILE:O    | 3:R:176:ARG:NH1  | 2.28                     | 0.67              |
| 5:j:281:ASP:O    | 5:j:365:THR:OG1  | 2.12                     | 0.67              |
| 2:O:71:ARG:O     | 2:O:71:ARG:NH1   | 2.27                     | 0.67              |
| 5:j:127:ARG:NE   | 5:j:149:GLU:OE2  | 2.28                     | 0.67              |
| 1:E:46:LEU:HD23  | 1:E:53:ILE:HD12  | 1.75                     | 0.67              |
| 3:N:62:ARG:NH1   | 3:N:108:GLU:OE1  | 2.28                     | 0.67              |
| 6:l:100:THR:OG1  | 6:l:133:TYR:OH   | 2.13                     | 0.67              |
| 2:Q:6:ARG:NH1    | 4:W:60:MET:O     | 2.27                     | 0.67              |
| 1:D:45:LYS:NZ    | 1:D:52:GLU:OE2   | 2.28                     | 0.67              |
| 4:U:60:MET:O     | 2:X:6:ARG:NH1    | 2.28                     | 0.67              |
| 6:v:47:ASN:OD1   | 6:v:56:SER:OG    | 2.07                     | 0.67              |
| 1:F:28:LEU:O     | 3:P:178:ASN:ND2  | 2.28                     | 0.67              |
| 6:n:376:ARG:NH2  | 6:n:394:ASP:OD1  | 2.28                     | 0.67              |
| 5:e:135:SER:OG   | 5:e:143:LYS:NZ   | 2.28                     | 0.66              |
| 1:F:32:GLU:OE2   | 1:F:34:LYS:NZ    | 2.24                     | 0.66              |
| 6:q:319:LEU:HD11 | 6:r:313:ILE:HD11 | 1.78                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:e:259:LEU:HD23 | 5:e:284:ILE:HG12 | 1.77                     | 0.66              |
| 6:l:178:GLN:OE1  | 6:l:185:ARG:NH2  | 2.28                     | 0.66              |
| 6:o:218:ALA:O    | 6:p:99:LYS:NZ    | 2.19                     | 0.66              |
| 6:t:23:SER:O     | 6:u:142:LYS:NZ   | 2.28                     | 0.66              |
| 1:A:107:LYS:NZ   | 1:B:38:GLU:OE1   | 2.28                     | 0.66              |
| 5:h:307:ILE:HD11 | 5:h:350:LEU:HD21 | 1.78                     | 0.66              |
| 5:h:222:GLU:O    | 5:h:255:LYS:NZ   | 2.29                     | 0.66              |
| 6:t:315:ASP:OD2  | 6:u:312:ALA:N    | 2.28                     | 0.66              |
| 2:G:13:ARG:NH1   | 4:b:60:MET:SD    | 2.68                     | 0.66              |
| 6:u:392:SER:OG   | 6:u:394:ASP:OD1  | 2.14                     | 0.66              |
| 2:Q:26:SER:OG    | 2:Q:41:THR:OG1   | 2.13                     | 0.65              |
| 3:R:213:ILE:O    | 3:d:176:ARG:NH1  | 2.29                     | 0.65              |
| 2:G:71:ARG:O     | 2:G:71:ARG:NH1   | 2.29                     | 0.65              |
| 4:V:31:PHE:HZ    | 4:V:48:LEU:HD12  | 1.62                     | 0.65              |
| 5:j:139:ASP:OD2  | 5:j:142:LYS:NZ   | 2.25                     | 0.65              |
| 6:r:216:ASN:ND2  | 6:r:226:GLN:O    | 2.29                     | 0.65              |
| 4:I:85:ASN:OD1   | 4:J:83:TYR:OH    | 2.15                     | 0.65              |
| 6:l:90:VAL:O     | 6:l:94:THR:HG23  | 1.96                     | 0.65              |
| 2:X:47:VAL:HG11  | 2:X:75:MET:HE2   | 1.80                     | 0.64              |
| 6:q:392:SER:OG   | 6:q:394:ASP:OD1  | 2.15                     | 0.64              |
| 1:F:125:GLU:OE1  | 1:F:125:GLU:N    | 2.31                     | 0.64              |
| 6:k:392:SER:OG   | 6:k:394:ASP:OD1  | 2.14                     | 0.64              |
| 3:N:16:LEU:HD13  | 3:N:34:MET:HE3   | 1.78                     | 0.64              |
| 5:f:44:ASN:OD1   | 5:f:125:THR:OG1  | 2.08                     | 0.64              |
| 5:f:222:GLU:O    | 5:f:255:LYS:NZ   | 2.30                     | 0.64              |
| 6:t:291:ASP:N    | 6:t:294:GLU:OE2  | 2.31                     | 0.64              |
| 3:R:115:ARG:NH2  | 3:d:39:GLY:O     | 2.30                     | 0.64              |
| 6:r:90:VAL:O     | 6:r:94:THR:HG23  | 1.97                     | 0.64              |
| 3:H:115:ARG:NH2  | 3:N:39:GLY:O     | 2.30                     | 0.64              |
| 6:v:100:THR:HG1  | 6:v:133:TYR:HH   | 1.44                     | 0.64              |
| 4:J:24:THR:OG1   | 4:J:27:GLU:OE1   | 2.13                     | 0.63              |
| 5:f:144:ASP:OD1  | 5:f:158:SER:OG   | 2.11                     | 0.63              |
| 6:o:392:SER:OG   | 6:o:394:ASP:OD1  | 2.16                     | 0.63              |
| 5:g:128:ASN:OD1  | 5:g:130:ASN:ND2  | 2.31                     | 0.63              |
| 6:k:319:LEU:HD11 | 6:l:313:ILE:HD11 | 1.81                     | 0.63              |
| 4:a:106:ILE:HD11 | 6:o:295:ILE:HB   | 1.80                     | 0.63              |
| 3:d:62:ARG:NH1   | 3:d:108:GLU:OE1  | 2.30                     | 0.63              |
| 2:Q:62:GLU:N     | 2:Q:62:GLU:OE1   | 2.32                     | 0.62              |
| 6:m:227:SER:N    | 6:m:230:GLU:OE1  | 2.32                     | 0.62              |
| 6:m:392:SER:OG   | 6:m:394:ASP:OD1  | 2.16                     | 0.62              |
| 6:m:20:ARG:NH2   | 6:n:226:GLN:OE1  | 2.33                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:k:252:MET:SD   | 6:k:253:HIS:NE2  | 2.72                     | 0.62              |
| 6:t:227:SER:N    | 6:t:230:GLU:OE1  | 2.32                     | 0.62              |
| 6:k:114:ILE:HB   | 6:k:377:MET:HE1  | 1.82                     | 0.62              |
| 2:O:104:ASN:OD1  | 2:Q:123:ARG:NH2  | 2.32                     | 0.61              |
| 4:V:26:GLU:N     | 4:V:26:GLU:OE1   | 2.31                     | 0.61              |
| 6:l:52:TYR:O     | 6:l:56:SER:OG    | 2.17                     | 0.61              |
| 6:s:47:ASN:OD1   | 6:s:56:SER:OG    | 2.08                     | 0.61              |
| 1:E:125:GLU:N    | 1:E:125:GLU:OE1  | 2.34                     | 0.61              |
| 6:u:351:GLU:OE2  | 6:v:349:VAL:N    | 2.33                     | 0.61              |
| 3:P:208:GLU:OE1  | 3:R:174:ASN:ND2  | 2.33                     | 0.61              |
| 4:V:12:ARG:NH1   | 4:V:16:ASN:OD1   | 2.34                     | 0.61              |
| 5:h:36:ARG:N     | 5:h:227:ASP:OD2  | 2.34                     | 0.61              |
| 5:f:385:PHE:CZ   | 5:f:389:ILE:HD11 | 2.36                     | 0.61              |
| 6:o:351:GLU:OE2  | 6:p:349:VAL:N    | 2.34                     | 0.61              |
| 1:C:125:GLU:OE1  | 1:C:125:GLU:N    | 2.34                     | 0.61              |
| 5:i:259:LEU:HD23 | 5:i:284:ILE:HG12 | 1.82                     | 0.61              |
| 5:j:256:ASP:O    | 5:j:387:ASN:ND2  | 2.33                     | 0.61              |
| 6:u:20:ARG:NH2   | 6:v:226:GLN:OE1  | 2.34                     | 0.60              |
| 4:c:13:LEU:HD22  | 4:c:38:ILE:HD13  | 1.83                     | 0.60              |
| 6:s:392:SER:OG   | 6:s:394:ASP:OD1  | 2.17                     | 0.60              |
| 6:l:376:ARG:NH2  | 6:l:394:ASP:OD1  | 2.34                     | 0.60              |
| 2:K:94:GLU:N     | 2:K:94:GLU:OE1   | 2.35                     | 0.60              |
| 6:k:351:GLU:OE2  | 6:l:349:VAL:N    | 2.35                     | 0.60              |
| 6:o:318:GLU:OE1  | 6:o:318:GLU:N    | 2.35                     | 0.60              |
| 1:B:125:GLU:N    | 1:B:125:GLU:OE1  | 2.35                     | 0.59              |
| 2:G:86:ASN:ND2   | 2:G:89:ASP:OD2   | 2.35                     | 0.59              |
| 3:H:213:ILE:O    | 3:N:176:ARG:NH1  | 2.35                     | 0.59              |
| 1:A:27:GLU:OE1   | 1:A:73:LYS:NZ    | 2.30                     | 0.59              |
| 3:R:212:ILE:HD11 | 3:R:232:VAL:HG12 | 1.83                     | 0.59              |
| 5:e:222:GLU:OE1  | 5:e:249:LYS:NZ   | 2.28                     | 0.59              |
| 5:h:144:ASP:OD1  | 5:h:158:SER:OG   | 2.12                     | 0.59              |
| 6:k:335:GLU:OE2  | 6:k:342:THR:HG21 | 2.02                     | 0.59              |
| 6:q:351:GLU:OE2  | 6:r:349:VAL:N    | 2.35                     | 0.59              |
| 6:n:345:ALA:O    | 6:n:352:GLN:NE2  | 2.35                     | 0.59              |
| 4:W:106:ILE:HD11 | 6:r:295:ILE:HB   | 1.84                     | 0.59              |
| 1:D:28:LEU:O     | 3:H:178:ASN:ND2  | 2.36                     | 0.59              |
| 5:j:385:PHE:CZ   | 5:j:389:ILE:HD11 | 2.37                     | 0.59              |
| 5:i:74:PHE:O     | 5:i:78:LYS:NZ    | 2.33                     | 0.59              |
| 6:r:52:TYR:O     | 6:r:56:SER:OG    | 2.21                     | 0.59              |
| 5:g:385:PHE:CZ   | 5:g:389:ILE:HD11 | 2.37                     | 0.58              |
| 1:D:46:LEU:HD23  | 1:D:53:ILE:HD12  | 1.83                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:119:CYS:SG   | 2:K:120:SER:N    | 2.77                     | 0.58              |
| 5:h:261:LEU:N    | 5:h:285:VAL:O    | 2.36                     | 0.58              |
| 4:a:38:ILE:HG23  | 4:a:39:TYR:HD1   | 1.66                     | 0.58              |
| 6:v:100:THR:OG1  | 6:v:133:TYR:OH   | 2.08                     | 0.58              |
| 6:n:178:GLN:HB3  | 6:n:187:VAL:HG23 | 1.86                     | 0.58              |
| 6:n:227:SER:N    | 6:n:230:GLU:OE1  | 2.36                     | 0.58              |
| 6:r:261:LYS:NZ   | 6:s:303:GLU:OE2  | 2.25                     | 0.58              |
| 3:d:239:ASP:OD2  | 3:d:242:THR:OG1  | 2.17                     | 0.58              |
| 5:g:259:LEU:HD23 | 5:g:284:ILE:HG12 | 1.86                     | 0.58              |
| 5:h:339:VAL:HG11 | 5:h:360:VAL:HG11 | 1.86                     | 0.58              |
| 6:n:181:THR:OG1  | 6:n:184:SER:O    | 2.09                     | 0.58              |
| 2:X:8:ARG:NE     | 2:X:115:CYS:SG   | 2.75                     | 0.58              |
| 6:o:345:ALA:O    | 6:o:352:GLN:NE2  | 2.37                     | 0.58              |
| 6:q:149:THR:HG23 | 6:q:150:THR:HG23 | 1.84                     | 0.58              |
| 2:Q:47:VAL:HG11  | 2:Q:75:MET:HE2   | 1.85                     | 0.58              |
| 5:j:282:GLU:OE1  | 5:j:282:GLU:N    | 2.36                     | 0.58              |
| 6:u:318:GLU:N    | 6:u:318:GLU:OE1  | 2.36                     | 0.57              |
| 6:n:23:SER:OG    | 6:o:33:ASP:O     | 2.22                     | 0.57              |
| 6:v:52:TYR:O     | 6:v:56:SER:OG    | 2.22                     | 0.57              |
| 3:d:16:LEU:HD13  | 3:d:34:MET:HE3   | 1.87                     | 0.57              |
| 6:r:396:THR:HG21 | 6:s:460:ARG:CB   | 2.34                     | 0.57              |
| 4:S:43:SER:O     | 4:S:47:ILE:HD12  | 2.04                     | 0.57              |
| 5:j:135:SER:OG   | 5:j:143:LYS:NZ   | 2.37                     | 0.57              |
| 5:f:333:ARG:NH2  | 5:f:351:ASP:OD2  | 2.37                     | 0.57              |
| 6:n:20:ARG:NH2   | 6:o:230:GLU:OE2  | 2.37                     | 0.57              |
| 6:n:52:TYR:O     | 6:n:56:SER:OG    | 2.22                     | 0.57              |
| 1:D:58:THR:OG1   | 1:E:50:GLN:O     | 2.11                     | 0.57              |
| 5:g:307:ILE:HD11 | 5:g:350:LEU:HD21 | 1.86                     | 0.57              |
| 6:o:67:THR:HB    | 6:o:105:LEU:HD12 | 1.85                     | 0.57              |
| 1:D:12:PHE:HD1   | 3:L:253:ILE:HD12 | 1.69                     | 0.57              |
| 4:S:31:PHE:HZ    | 4:S:48:LEU:HD22  | 1.70                     | 0.57              |
| 5:f:183:LYS:NZ   | 5:f:186:ASP:OD1  | 2.29                     | 0.57              |
| 1:C:58:THR:OG1   | 1:D:50:GLN:O     | 2.13                     | 0.57              |
| 3:d:147:LEU:HD23 | 3:d:149:ILE:HD11 | 1.87                     | 0.57              |
| 5:g:292:TYR:O    | 5:g:328:GLU:N    | 2.37                     | 0.57              |
| 5:f:94:VAL:HG13  | 5:f:205:GLY:HA2  | 1.86                     | 0.56              |
| 2:G:53:LYS:O     | 2:G:72:THR:HG23  | 2.05                     | 0.56              |
| 2:K:108:GLN:NE2  | 2:K:118:GLN:OE1  | 2.38                     | 0.56              |
| 5:e:385:PHE:CZ   | 5:e:389:ILE:HD11 | 2.40                     | 0.56              |
| 6:k:22:SER:OG    | 6:k:25:ASN:OD1   | 2.23                     | 0.56              |
| 6:o:20:ARG:NH2   | 6:p:226:GLN:OE1  | 2.38                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:i:259:LEU:N    | 5:i:283:ASN:O    | 2.36                     | 0.56              |
| 6:k:396:THR:HG21 | 6:l:460:ARG:CB   | 2.36                     | 0.56              |
| 1:D:60:LYS:NZ    | 1:E:54:SER:OG    | 2.38                     | 0.56              |
| 5:i:261:LEU:N    | 5:i:285:VAL:O    | 2.37                     | 0.56              |
| 6:l:396:THR:HG21 | 6:m:460:ARG:CB   | 2.36                     | 0.56              |
| 6:s:396:THR:HG21 | 6:t:460:ARG:CB   | 2.36                     | 0.56              |
| 6:u:227:SER:N    | 6:u:230:GLU:OE1  | 2.39                     | 0.56              |
| 3:L:1:MET:CE     | 3:L:54:ILE:HD11  | 2.36                     | 0.56              |
| 3:L:147:LEU:HD23 | 3:L:149:ILE:HD11 | 1.88                     | 0.56              |
| 4:V:85:ASN:OD1   | 4:b:83:TYR:OH    | 2.22                     | 0.56              |
| 5:f:259:LEU:HD11 | 5:f:261:LEU:HD21 | 1.87                     | 0.56              |
| 6:m:396:THR:HG21 | 6:n:460:ARG:CB   | 2.36                     | 0.56              |
| 1:C:92:GLU:OE1   | 1:C:92:GLU:N     | 2.39                     | 0.55              |
| 6:t:126:ASP:O    | 6:t:128:LYS:NZ   | 2.39                     | 0.55              |
| 4:c:75:ILE:O     | 4:c:79:VAL:HG22  | 2.05                     | 0.55              |
| 6:s:305:GLU:N    | 6:s:305:GLU:OE1  | 2.39                     | 0.55              |
| 1:D:46:LEU:CD2   | 1:D:53:ILE:HD12  | 2.37                     | 0.55              |
| 5:e:261:LEU:N    | 5:e:285:VAL:O    | 2.37                     | 0.55              |
| 5:h:393:THR:HG21 | 5:h:453:TRP:CZ2  | 2.40                     | 0.55              |
| 6:m:114:ILE:HB   | 6:m:377:MET:HE1  | 1.87                     | 0.55              |
| 3:N:1:MET:CE     | 3:N:54:ILE:HD11  | 2.36                     | 0.55              |
| 3:d:212:ILE:HD11 | 3:d:232:VAL:HG12 | 1.88                     | 0.55              |
| 6:p:90:VAL:O     | 6:p:94:THR:OG1   | 2.17                     | 0.55              |
| 4:W:24:THR:OG1   | 4:W:27:GLU:OE1   | 2.23                     | 0.55              |
| 4:I:15:LEU:HD13  | 4:I:28:LEU:HD11  | 1.88                     | 0.55              |
| 5:e:282:GLU:OE1  | 5:e:282:GLU:N    | 2.39                     | 0.55              |
| 6:k:460:ARG:CB   | 6:v:396:THR:HG21 | 2.37                     | 0.55              |
| 5:i:139:ASP:OD2  | 5:i:142:LYS:NZ   | 2.39                     | 0.55              |
| 3:P:1:MET:CE     | 3:P:54:ILE:HD11  | 2.36                     | 0.55              |
| 4:Z:14:LEU:HB2   | 4:Z:38:ILE:HD11  | 1.89                     | 0.55              |
| 5:f:261:LEU:N    | 5:f:285:VAL:O    | 2.39                     | 0.55              |
| 6:u:162:ASN:N    | 6:u:174:ALA:O    | 2.39                     | 0.55              |
| 1:B:28:LEU:O     | 3:d:178:ASN:ND2  | 2.40                     | 0.55              |
| 6:n:126:ASP:O    | 6:n:128:LYS:NZ   | 2.39                     | 0.55              |
| 3:R:183:GLU:OE2  | 3:R:251:LYS:NZ   | 2.40                     | 0.54              |
| 6:m:47:ASN:OD1   | 6:m:56:SER:OG    | 2.12                     | 0.54              |
| 6:s:55:GLY:O     | 6:s:236:LEU:HD22 | 2.07                     | 0.54              |
| 5:j:265:THR:OG1  | 5:j:299:THR:HG22 | 2.06                     | 0.54              |
| 6:v:90:VAL:O     | 6:v:94:THR:OG1   | 2.22                     | 0.54              |
| 6:o:396:THR:HG21 | 6:p:460:ARG:CB   | 2.38                     | 0.54              |
| 6:q:396:THR:HG21 | 6:r:460:ARG:CB   | 2.37                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:q:20:ARG:NH2   | 6:r:226:GLN:OE1  | 2.41                     | 0.54              |
| 5:h:39:MET:HG3   | 5:h:41:ILE:HG23  | 1.90                     | 0.54              |
| 4:c:109:GLU:N    | 4:c:109:GLU:OE1  | 2.41                     | 0.54              |
| 6:p:21:MET:HE1   | 6:p:26:ILE:HB    | 1.89                     | 0.54              |
| 6:p:47:ASN:OD1   | 6:p:56:SER:OG    | 2.08                     | 0.54              |
| 5:i:144:ASP:OD1  | 5:i:158:SER:OG   | 2.21                     | 0.54              |
| 1:D:7:ILE:HD11   | 3:d:213:ILE:CD1  | 2.37                     | 0.54              |
| 1:F:92:GLU:N     | 1:F:92:GLU:OE1   | 2.40                     | 0.54              |
| 3:H:39:GLY:O     | 3:L:115:ARG:NH2  | 2.40                     | 0.54              |
| 2:M:114:LEU:HD21 | 2:M:117:TYR:CZ   | 2.43                     | 0.54              |
| 6:p:376:ARG:NH2  | 6:p:394:ASP:OD1  | 2.41                     | 0.54              |
| 6:p:227:SER:N    | 6:p:230:GLU:OE1  | 2.41                     | 0.53              |
| 4:a:9:GLU:OE1    | 4:a:11:LEU:N     | 2.41                     | 0.53              |
| 3:P:16:LEU:HD13  | 3:P:34:MET:HE3   | 1.89                     | 0.53              |
| 4:c:57:VAL:HG21  | 4:c:78:LEU:HD22  | 1.91                     | 0.53              |
| 5:j:399:GLU:O    | 5:j:403:LYS:NZ   | 2.30                     | 0.53              |
| 2:G:114:LEU:HD21 | 2:G:117:TYR:CZ   | 2.43                     | 0.53              |
| 2:M:102:ILE:HG23 | 2:M:119:CYS:SG   | 2.49                     | 0.53              |
| 3:N:147:LEU:HD23 | 3:N:149:ILE:HD11 | 1.90                     | 0.53              |
| 5:g:261:LEU:N    | 5:g:285:VAL:O    | 2.42                     | 0.53              |
| 6:r:178:GLN:OE1  | 6:r:185:ARG:NH2  | 2.41                     | 0.53              |
| 6:u:55:GLY:O     | 6:u:236:LEU:HD22 | 2.08                     | 0.53              |
| 1:C:22:ILE:HD11  | 1:C:73:LYS:HD3   | 1.90                     | 0.53              |
| 5:f:287:VAL:HG11 | 5:f:303:VAL:HG13 | 1.90                     | 0.53              |
| 6:k:52:TYR:O     | 6:k:56:SER:N     | 2.41                     | 0.53              |
| 6:v:227:SER:N    | 6:v:230:GLU:OE1  | 2.40                     | 0.53              |
| 5:e:259:LEU:N    | 5:e:283:ASN:O    | 2.41                     | 0.53              |
| 6:r:335:GLU:N    | 6:r:335:GLU:OE1  | 2.41                     | 0.53              |
| 1:D:135:ASN:OD1  | 1:D:136:GLU:N    | 2.39                     | 0.53              |
| 3:R:147:LEU:HD23 | 3:R:149:ILE:HD11 | 1.91                     | 0.53              |
| 4:b:106:ILE:HD12 | 6:p:290:LEU:HD23 | 1.90                     | 0.53              |
| 5:e:231:LEU:HD21 | 5:e:234:VAL:O    | 2.07                     | 0.53              |
| 1:E:92:GLU:OE1   | 1:E:92:GLU:N     | 2.41                     | 0.53              |
| 6:n:42:ARG:NH1   | 6:n:107:GLN:OE1  | 2.42                     | 0.53              |
| 5:f:36:ARG:N     | 5:f:227:ASP:OD2  | 2.42                     | 0.53              |
| 5:i:362:ASP:OD2  | 5:i:380:ILE:N    | 2.41                     | 0.53              |
| 6:k:55:GLY:O     | 6:k:236:LEU:HD22 | 2.09                     | 0.53              |
| 6:k:180:ILE:HG21 | 6:k:211:ILE:CD1  | 2.39                     | 0.53              |
| 6:l:176:VAL:HG23 | 6:l:189:VAL:HG12 | 1.91                     | 0.53              |
| 6:p:396:THR:HG21 | 6:q:460:ARG:CB   | 2.38                     | 0.53              |
| 6:s:369:ASN:OD1  | 6:s:370:SER:N    | 2.42                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:e:265:THR:OG1  | 5:e:266:GLU:OE1  | 2.24                     | 0.53              |
| 6:l:335:GLU:OE1  | 6:l:335:GLU:N    | 2.42                     | 0.52              |
| 6:t:137:SER:OG   | 6:t:139:GLU:OE1  | 2.26                     | 0.52              |
| 1:B:135:ASN:OD1  | 1:B:136:GLU:N    | 2.41                     | 0.52              |
| 3:R:237:GLU:OE2  | 3:d:168:ARG:NH2  | 2.42                     | 0.52              |
| 5:f:281:ASP:O    | 5:f:365:THR:OG1  | 2.26                     | 0.52              |
| 5:j:356:ASP:OD1  | 5:j:357:VAL:N    | 2.42                     | 0.52              |
| 6:m:55:GLY:O     | 6:m:236:LEU:HD22 | 2.09                     | 0.52              |
| 4:Z:39:TYR:CE2   | 4:Z:92:MET:HE3   | 2.44                     | 0.52              |
| 5:f:362:ASP:OD2  | 5:f:380:ILE:N    | 2.42                     | 0.52              |
| 2:K:114:LEU:HD21 | 2:K:117:TYR:CZ   | 2.44                     | 0.52              |
| 5:f:42:ARG:NH2   | 5:f:232:ASP:O    | 2.41                     | 0.52              |
| 6:v:376:ARG:NH2  | 6:v:394:ASP:OD1  | 2.41                     | 0.52              |
| 1:C:32:GLU:OE2   | 1:C:34:LYS:NZ    | 2.42                     | 0.52              |
| 4:V:31:PHE:CZ    | 4:V:48:LEU:HD12  | 2.43                     | 0.52              |
| 4:b:14:LEU:HB2   | 4:b:38:ILE:HD11  | 1.91                     | 0.52              |
| 3:d:168:ARG:NH1  | 3:d:170:THR:HG22 | 2.24                     | 0.52              |
| 4:c:14:LEU:HB2   | 4:c:38:ILE:HD11  | 1.91                     | 0.52              |
| 5:h:183:LYS:NZ   | 5:h:186:ASP:OD1  | 2.31                     | 0.52              |
| 5:j:259:LEU:HD23 | 5:j:284:ILE:HG12 | 1.92                     | 0.52              |
| 6:q:55:GLY:O     | 6:q:236:LEU:HD22 | 2.09                     | 0.52              |
| 5:h:259:LEU:N    | 5:h:283:ASN:O    | 2.41                     | 0.52              |
| 5:h:265:THR:OG1  | 5:h:299:THR:HG22 | 2.09                     | 0.52              |
| 1:A:92:GLU:N     | 1:A:92:GLU:OE1   | 2.42                     | 0.52              |
| 1:B:22:ILE:HD12  | 1:B:27:GLU:HG3   | 1.92                     | 0.52              |
| 3:d:263:MET:HB3  | 3:d:266:ILE:HD11 | 1.91                     | 0.52              |
| 5:h:94:VAL:HG13  | 5:h:205:GLY:HA2  | 1.92                     | 0.52              |
| 6:n:100:THR:OG1  | 6:n:133:TYR:OH   | 2.09                     | 0.52              |
| 6:s:114:ILE:CG1  | 6:s:377:MET:HE1  | 2.39                     | 0.52              |
| 1:A:38:GLU:OE2   | 1:F:107:LYS:NZ   | 2.24                     | 0.52              |
| 5:h:259:LEU:HD23 | 5:h:284:ILE:HG12 | 1.91                     | 0.52              |
| 6:n:178:GLN:OE1  | 6:n:185:ARG:NH2  | 2.43                     | 0.52              |
| 2:M:4:ILE:HD11   | 2:M:115:CYS:HB3  | 1.92                     | 0.52              |
| 4:T:39:TYR:OH    | 4:Z:44:GLN:OE1   | 2.10                     | 0.52              |
| 6:m:369:ASN:OD1  | 6:m:370:SER:N    | 2.43                     | 0.52              |
| 6:n:267:SER:OG   | 6:n:271:HIS:NE2  | 2.42                     | 0.52              |
| 6:q:305:GLU:N    | 6:q:305:GLU:OE1  | 2.43                     | 0.52              |
| 6:t:115:THR:OG1  | 6:t:134:ASN:OD1  | 2.12                     | 0.52              |
| 3:H:1:MET:HE1    | 3:H:52:ARG:HD2   | 1.92                     | 0.51              |
| 4:V:109:GLU:OE1  | 4:V:109:GLU:N    | 2.41                     | 0.51              |
| 4:b:13:LEU:HD22  | 4:b:38:ILE:HD13  | 1.91                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:g:139:ASP:OD2  | 5:g:142:LYS:NZ   | 2.43                     | 0.51              |
| 5:f:36:ARG:NH1   | 5:f:225:SER:O    | 2.44                     | 0.51              |
| 5:i:94:VAL:HG13  | 5:i:205:GLY:HA2  | 1.92                     | 0.51              |
| 5:i:265:THR:OG1  | 5:i:299:THR:HG22 | 2.10                     | 0.51              |
| 6:r:139:GLU:N    | 6:r:139:GLU:OE1  | 2.42                     | 0.51              |
| 4:W:83:TYR:OH    | 4:b:85:ASN:OD1   | 2.24                     | 0.51              |
| 5:i:167:VAL:HG22 | 5:i:171:ASN:ND2  | 2.25                     | 0.51              |
| 6:n:396:THR:HG21 | 6:o:460:ARG:CB   | 2.40                     | 0.51              |
| 6:o:55:GLY:O     | 6:o:236:LEU:HD22 | 2.10                     | 0.51              |
| 5:h:404:ILE:HD11 | 5:h:410:GLY:HA2  | 1.92                     | 0.51              |
| 6:s:162:ASN:N    | 6:s:174:ALA:O    | 2.41                     | 0.51              |
| 1:C:22:ILE:HG22  | 1:C:84:ILE:HG12  | 1.91                     | 0.51              |
| 4:a:38:ILE:HG23  | 4:a:39:TYR:CD1   | 2.46                     | 0.51              |
| 5:g:42:ARG:NH2   | 5:g:232:ASP:O    | 2.42                     | 0.51              |
| 5:g:234:VAL:HG11 | 5:g:239:LEU:HD12 | 1.93                     | 0.51              |
| 5:j:261:LEU:N    | 5:j:285:VAL:O    | 2.40                     | 0.51              |
| 6:m:318:GLU:OE1  | 6:m:318:GLU:N    | 2.43                     | 0.51              |
| 3:H:237:GLU:OE2  | 3:N:168:ARG:NH2  | 2.43                     | 0.51              |
| 3:R:150:GLU:OE1  | 3:R:150:GLU:N    | 2.44                     | 0.51              |
| 5:h:167:VAL:HG22 | 5:h:171:ASN:ND2  | 2.26                     | 0.51              |
| 6:n:326:CYS:O    | 6:n:330:VAL:HG23 | 2.11                     | 0.51              |
| 6:s:212:ILE:HG12 | 6:s:373:LEU:HD22 | 1.93                     | 0.51              |
| 3:L:58:ILE:CG2   | 3:L:71:LEU:HD23  | 2.41                     | 0.51              |
| 6:m:217:GLU:OE2  | 6:m:363:LYS:NZ   | 2.31                     | 0.50              |
| 6:n:149:THR:HG21 | 6:o:196:GLY:HA3  | 1.93                     | 0.50              |
| 6:u:149:THR:HG23 | 6:u:150:THR:HG23 | 1.94                     | 0.50              |
| 4:J:13:LEU:HD22  | 4:J:38:ILE:HD13  | 1.94                     | 0.50              |
| 2:Q:102:ILE:HG23 | 2:Q:119:CYS:SG   | 2.51                     | 0.50              |
| 6:o:326:CYS:O    | 6:o:330:VAL:HG23 | 2.11                     | 0.50              |
| 4:J:39:TYR:CD1   | 4:J:92:MET:HE1   | 2.46                     | 0.50              |
| 3:L:15:GLU:OE1   | 3:L:15:GLU:N     | 2.44                     | 0.50              |
| 2:X:102:ILE:HG23 | 2:X:119:CYS:SG   | 2.51                     | 0.50              |
| 2:X:119:CYS:SG   | 2:X:120:SER:N    | 2.85                     | 0.50              |
| 6:k:196:GLY:HA3  | 6:v:149:THR:HG21 | 1.93                     | 0.50              |
| 6:o:52:TYR:O     | 6:o:56:SER:N     | 2.44                     | 0.50              |
| 1:B:36:ASP:OD1   | 1:B:36:ASP:N     | 2.42                     | 0.50              |
| 5:j:167:VAL:HG22 | 5:j:171:ASN:ND2  | 2.26                     | 0.50              |
| 3:H:55:GLU:OE1   | 3:H:57:TRP:NE1   | 2.43                     | 0.50              |
| 5:h:104:THR:OG1  | 5:h:118:LYS:NZ   | 2.42                     | 0.50              |
| 6:m:252:MET:SD   | 6:m:253:HIS:NE2  | 2.84                     | 0.50              |
| 6:s:19:MET:N     | 6:t:233:GLU:OE2  | 2.44                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:u:35:ARG:NH2   | 6:u:138:PRO:O    | 2.42                     | 0.50              |
| 2:M:22:ILE:HD12  | 2:M:93:PHE:CD2   | 2.47                     | 0.50              |
| 3:N:212:ILE:HD11 | 3:N:232:VAL:HG12 | 1.94                     | 0.50              |
| 6:m:326:CYS:O    | 6:m:330:VAL:HG23 | 2.11                     | 0.50              |
| 6:r:21:MET:HE3   | 6:s:37:ASP:HA    | 1.93                     | 0.50              |
| 6:u:22:SER:OG    | 6:u:25:ASN:OD1   | 2.24                     | 0.50              |
| 5:h:107:ASP:OD1  | 5:h:114:LYS:N    | 2.42                     | 0.50              |
| 6:k:300:LYS:NZ   | 6:v:301:ASP:O    | 2.32                     | 0.50              |
| 6:p:149:THR:HG21 | 6:q:196:GLY:HA3  | 1.92                     | 0.50              |
| 6:s:52:TYR:O     | 6:s:56:SER:N     | 2.44                     | 0.50              |
| 2:K:102:ILE:HG23 | 2:K:119:CYS:SG   | 2.52                     | 0.50              |
| 6:t:178:GLN:OE1  | 6:t:185:ARG:NH2  | 2.45                     | 0.50              |
| 6:k:326:CYS:O    | 6:k:330:VAL:HG23 | 2.12                     | 0.50              |
| 6:m:162:ASN:N    | 6:m:174:ALA:O    | 2.42                     | 0.50              |
| 6:p:259:LYS:C    | 6:p:260:LEU:HD12 | 2.37                     | 0.50              |
| 6:q:162:ASN:N    | 6:q:174:ALA:O    | 2.44                     | 0.50              |
| 1:C:36:ASP:N     | 1:C:36:ASP:OD1   | 2.45                     | 0.49              |
| 1:C:132:ASP:N    | 1:C:132:ASP:OD1  | 2.43                     | 0.49              |
| 2:G:102:ILE:HG23 | 2:G:119:CYS:SG   | 2.52                     | 0.49              |
| 4:a:36:ASP:OD1   | 4:a:37:CYS:N     | 2.45                     | 0.49              |
| 5:e:393:THR:HG21 | 5:e:453:TRP:HH2  | 1.76                     | 0.49              |
| 5:g:393:THR:HG21 | 5:g:453:TRP:HH2  | 1.76                     | 0.49              |
| 5:h:108:THR:N    | 5:h:190:ILE:O    | 2.44                     | 0.49              |
| 5:j:389:ILE:O    | 5:j:393:THR:HG23 | 2.12                     | 0.49              |
| 6:k:305:GLU:N    | 6:k:305:GLU:OE1  | 2.45                     | 0.49              |
| 6:o:114:ILE:HB   | 6:o:377:MET:HE1  | 1.95                     | 0.49              |
| 6:q:292:GLY:N    | 6:q:294:GLU:OE1  | 2.44                     | 0.49              |
| 6:u:345:ALA:O    | 6:u:352:GLN:NE2  | 2.42                     | 0.49              |
| 1:E:116:ALA:N    | 1:F:31:GLU:O     | 2.45                     | 0.49              |
| 5:g:222:GLU:OE1  | 5:g:249:LYS:NZ   | 2.41                     | 0.49              |
| 6:p:52:TYR:O     | 6:p:56:SER:OG    | 2.30                     | 0.49              |
| 5:e:94:VAL:HG13  | 5:e:205:GLY:HA2  | 1.93                     | 0.49              |
| 5:g:287:VAL:HG11 | 5:g:303:VAL:HG13 | 1.94                     | 0.49              |
| 6:m:149:THR:HG23 | 6:m:150:THR:HG23 | 1.94                     | 0.49              |
| 6:u:326:CYS:O    | 6:u:330:VAL:HG23 | 2.13                     | 0.49              |
| 3:P:237:GLU:OE2  | 3:R:168:ARG:NH2  | 2.46                     | 0.49              |
| 6:k:162:ASN:N    | 6:k:174:ALA:O    | 2.44                     | 0.49              |
| 6:s:20:ARG:NH2   | 6:t:226:GLN:OE1  | 2.45                     | 0.49              |
| 6:v:335:GLU:OE1  | 6:v:335:GLU:N    | 2.46                     | 0.49              |
| 3:H:147:LEU:HD23 | 3:H:149:ILE:HD11 | 1.94                     | 0.49              |
| 5:j:339:VAL:HG11 | 5:j:360:VAL:HG11 | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:p:139:GLU:OE1  | 6:p:139:GLU:N    | 2.45                     | 0.49              |
| 6:q:19:MET:N     | 6:r:233:GLU:OE1  | 2.45                     | 0.49              |
| 6:t:114:ILE:CD1  | 6:t:378:VAL:HG22 | 2.43                     | 0.49              |
| 1:B:39:GLN:NE2   | 1:B:41:GLU:OE1   | 2.44                     | 0.49              |
| 2:O:102:ILE:HG23 | 2:O:119:CYS:SG   | 2.52                     | 0.49              |
| 6:k:99:LYS:NZ    | 6:k:103:ASP:OD1  | 2.45                     | 0.49              |
| 6:k:318:GLU:OE1  | 6:k:318:GLU:N    | 2.43                     | 0.49              |
| 6:v:326:CYS:O    | 6:v:330:VAL:HG23 | 2.13                     | 0.49              |
| 3:H:1:MET:HE1    | 3:H:52:ARG:CD    | 2.42                     | 0.49              |
| 5:i:339:VAL:HG11 | 5:i:360:VAL:HG11 | 1.95                     | 0.49              |
| 6:k:178:GLN:OE1  | 6:k:185:ARG:NH2  | 2.46                     | 0.49              |
| 6:l:251:LYS:NZ   | 6:m:291:ASP:OD1  | 2.45                     | 0.49              |
| 6:m:305:GLU:OE1  | 6:m:305:GLU:N    | 2.46                     | 0.49              |
| 6:n:330:VAL:HG22 | 6:o:57:SER:HA    | 1.95                     | 0.49              |
| 6:o:162:ASN:N    | 6:o:174:ALA:O    | 2.46                     | 0.49              |
| 1:B:132:ASP:OD1  | 1:B:132:ASP:N    | 2.41                     | 0.49              |
| 3:H:1:MET:HE3    | 3:H:54:ILE:HD11  | 1.95                     | 0.49              |
| 3:H:168:ARG:NH2  | 3:L:237:GLU:OE2  | 2.46                     | 0.49              |
| 4:I:13:LEU:HD23  | 4:I:38:ILE:HD13  | 1.95                     | 0.49              |
| 4:J:50:SER:OG    | 4:J:79:VAL:HG23  | 2.13                     | 0.49              |
| 5:f:167:VAL:HG22 | 5:f:171:ASN:ND2  | 2.28                     | 0.49              |
| 6:u:396:THR:HG21 | 6:v:460:ARG:CB   | 2.42                     | 0.49              |
| 1:E:43:SER:OG    | 1:E:52:GLU:OE1   | 2.30                     | 0.49              |
| 3:L:48:ILE:HD12  | 3:L:242:THR:HG22 | 1.95                     | 0.49              |
| 5:j:362:ASP:OD2  | 5:j:380:ILE:N    | 2.45                     | 0.49              |
| 2:M:114:LEU:HD22 | 2:O:97:TYR:OH    | 2.12                     | 0.49              |
| 3:d:48:ILE:HD12  | 3:d:242:THR:HG22 | 1.94                     | 0.49              |
| 5:e:167:VAL:HG22 | 5:e:171:ASN:HD21 | 1.78                     | 0.49              |
| 5:g:377:MET:O    | 5:g:383:ILE:HD11 | 2.13                     | 0.49              |
| 5:h:425:LEU:HB2  | 5:h:431:ILE:HD12 | 1.94                     | 0.49              |
| 6:l:100:THR:HG23 | 6:l:112:ILE:HD11 | 1.93                     | 0.49              |
| 6:l:114:ILE:CG2  | 6:l:377:MET:HE2  | 2.42                     | 0.49              |
| 1:B:7:ILE:HD11   | 3:P:213:ILE:HD11 | 1.95                     | 0.48              |
| 1:F:7:ILE:HD11   | 3:H:213:ILE:CD1  | 2.40                     | 0.48              |
| 3:N:55:GLU:OE1   | 3:N:57:TRP:NE1   | 2.46                     | 0.48              |
| 3:P:48:ILE:HD12  | 3:P:242:THR:HG22 | 1.95                     | 0.48              |
| 4:U:83:TYR:OH    | 4:Z:85:ASN:OD1   | 2.26                     | 0.48              |
| 5:f:333:ARG:NH1  | 5:f:352:PHE:O    | 2.46                     | 0.48              |
| 6:v:115:THR:OG1  | 6:v:134:ASN:OD1  | 2.12                     | 0.48              |
| 4:J:57:VAL:HG21  | 4:J:78:LEU:HD12  | 1.94                     | 0.48              |
| 4:Y:36:ASP:OD1   | 4:Y:37:CYS:N     | 2.45                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:P:136:VAL:HG13 | 3:P:167:TRP:O    | 2.13                     | 0.48              |
| 3:P:239:ASP:OD2  | 3:P:242:THR:OG1  | 2.17                     | 0.48              |
| 2:X:85:VAL:HG23  | 2:X:91:LEU:HD12  | 1.95                     | 0.48              |
| 6:r:176:VAL:HG23 | 6:r:189:VAL:HG12 | 1.95                     | 0.48              |
| 3:d:224:ASN:OD1  | 3:d:225:MET:N    | 2.46                     | 0.48              |
| 5:f:425:LEU:HB2  | 5:f:431:ILE:HD12 | 1.96                     | 0.48              |
| 5:i:169:GLU:OE2  | 5:i:173:ASN:ND2  | 2.46                     | 0.48              |
| 6:l:267:SER:OG   | 6:l:271:HIS:NE2  | 2.46                     | 0.48              |
| 6:m:372:GLN:HG3  | 6:m:397:ILE:HD12 | 1.95                     | 0.48              |
| 6:n:55:GLY:O     | 6:n:236:LEU:HD22 | 2.13                     | 0.48              |
| 4:T:15:LEU:HD21  | 4:T:28:LEU:HD11  | 1.94                     | 0.48              |
| 5:e:287:VAL:HG22 | 5:e:348:LEU:HD22 | 1.96                     | 0.48              |
| 6:l:115:THR:OG1  | 6:l:134:ASN:OD1  | 2.16                     | 0.48              |
| 6:o:42:ARG:NH1   | 6:o:107:GLN:OE1  | 2.45                     | 0.48              |
| 3:L:212:ILE:HD11 | 3:L:232:VAL:HG12 | 1.95                     | 0.48              |
| 3:N:166:LEU:HD23 | 3:N:168:ARG:H    | 1.78                     | 0.48              |
| 3:P:168:ARG:NH1  | 3:P:170:THR:HG22 | 2.28                     | 0.48              |
| 4:W:44:GLN:NE2   | 4:b:92:MET:SD    | 2.86                     | 0.48              |
| 5:i:372:ASP:OD1  | 5:i:373:LYS:N    | 2.46                     | 0.48              |
| 6:t:264:ASP:OD1  | 6:t:264:ASP:N    | 2.46                     | 0.48              |
| 4:J:14:LEU:HB2   | 4:J:38:ILE:HD11  | 1.95                     | 0.48              |
| 5:f:281:ASP:OD1  | 5:f:282:GLU:N    | 2.46                     | 0.48              |
| 6:n:328:VAL:HG11 | 6:o:340:VAL:HG11 | 1.96                     | 0.48              |
| 6:r:252:MET:HE1  | 6:s:290:LEU:HB2  | 1.95                     | 0.48              |
| 6:t:330:VAL:HG22 | 6:u:57:SER:HA    | 1.95                     | 0.48              |
| 3:R:189:LYS:NZ   | 3:R:247:THR:OG1  | 2.47                     | 0.48              |
| 5:f:259:LEU:HD23 | 5:f:284:ILE:HG12 | 1.95                     | 0.48              |
| 6:q:99:LYS:NZ    | 6:q:103:ASP:OD1  | 2.44                     | 0.48              |
| 6:q:326:CYS:O    | 6:q:330:VAL:HG23 | 2.14                     | 0.48              |
| 5:h:78:LYS:NZ    | 5:h:294:GLU:OE1  | 2.47                     | 0.48              |
| 6:l:313:ILE:HG23 | 6:l:316:ALA:HB3  | 1.96                     | 0.48              |
| 6:q:410:LEU:O    | 6:q:413:THR:OG1  | 2.29                     | 0.48              |
| 5:i:143:LYS:NZ   | 5:i:193:ASN:OD1  | 2.40                     | 0.48              |
| 6:l:149:THR:HG21 | 6:m:196:GLY:HA3  | 1.96                     | 0.48              |
| 6:o:180:ILE:HG21 | 6:o:211:ILE:HD11 | 1.96                     | 0.48              |
| 6:u:335:GLU:CG   | 6:u:342:THR:HG21 | 2.43                     | 0.48              |
| 3:H:168:ARG:NH1  | 3:H:170:THR:HG22 | 2.29                     | 0.47              |
| 5:g:260:PHE:HD2  | 5:g:308:ALA:HB2  | 1.78                     | 0.47              |
| 5:j:94:VAL:HG13  | 5:j:205:GLY:HA2  | 1.95                     | 0.47              |
| 5:g:389:ILE:O    | 5:g:393:THR:HG23 | 2.14                     | 0.47              |
| 5:j:94:VAL:O     | 5:j:216:LYS:NZ   | 2.34                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:o:372:GLN:HG3  | 6:o:397:ILE:HD12 | 1.96                     | 0.47              |
| 6:r:326:CYS:O    | 6:r:330:VAL:HG23 | 2.14                     | 0.47              |
| 6:t:326:CYS:O    | 6:t:330:VAL:HG23 | 2.14                     | 0.47              |
| 5:h:135:SER:OG   | 5:h:143:LYS:NZ   | 2.47                     | 0.47              |
| 6:k:230:GLU:OE2  | 6:v:20:ARG:NH2   | 2.48                     | 0.47              |
| 3:R:68:LEU:HD21  | 3:R:115:ARG:HB2  | 1.97                     | 0.47              |
| 5:e:141:ASP:OD1  | 5:e:142:LYS:N    | 2.47                     | 0.47              |
| 5:e:222:GLU:O    | 5:e:255:LYS:NZ   | 2.44                     | 0.47              |
| 5:h:292:TYR:O    | 5:h:328:GLU:N    | 2.48                     | 0.47              |
| 6:n:264:ASP:OD1  | 6:n:264:ASP:N    | 2.47                     | 0.47              |
| 6:s:372:GLN:HG3  | 6:s:397:ILE:HD12 | 1.96                     | 0.47              |
| 6:t:328:VAL:HG11 | 6:u:340:VAL:HG11 | 1.95                     | 0.47              |
| 3:P:219:LEU:HD13 | 3:P:227:LEU:HD11 | 1.95                     | 0.47              |
| 4:Z:103:MET:C    | 4:Z:104:LEU:HD12 | 2.39                     | 0.47              |
| 4:c:10:LYS:HG3   | 4:c:38:ILE:HD12  | 1.95                     | 0.47              |
| 5:i:234:VAL:CG1  | 5:i:239:LEU:HD12 | 2.43                     | 0.47              |
| 6:l:126:ASP:O    | 6:l:128:LYS:NZ   | 2.47                     | 0.47              |
| 6:m:52:TYR:O     | 6:m:56:SER:OG    | 2.32                     | 0.47              |
| 6:q:209:ILE:HG22 | 6:q:211:ILE:H    | 1.80                     | 0.47              |
| 6:q:318:GLU:OE1  | 6:q:318:GLU:N    | 2.43                     | 0.47              |
| 6:v:292:GLY:N    | 6:v:294:GLU:OE1  | 2.47                     | 0.47              |
| 1:C:7:ILE:HD11   | 3:R:213:ILE:HD11 | 1.97                     | 0.47              |
| 4:I:15:LEU:HD13  | 4:I:28:LEU:CD1   | 2.44                     | 0.47              |
| 6:k:57:SER:HA    | 6:v:330:VAL:HG22 | 1.96                     | 0.47              |
| 6:k:209:ILE:HG22 | 6:k:211:ILE:H    | 1.79                     | 0.47              |
| 1:D:81:SER:OG    | 1:D:105:ARG:NH1  | 2.48                     | 0.47              |
| 3:H:176:ARG:NH1  | 3:L:213:ILE:O    | 2.48                     | 0.47              |
| 5:h:42:ARG:NH2   | 5:h:232:ASP:O    | 2.44                     | 0.47              |
| 5:h:281:ASP:OD1  | 5:h:282:GLU:N    | 2.48                     | 0.47              |
| 5:i:281:ASP:OD1  | 5:i:282:GLU:N    | 2.48                     | 0.47              |
| 5:j:425:LEU:HB2  | 5:j:431:ILE:HD12 | 1.96                     | 0.47              |
| 6:l:139:GLU:OE1  | 6:l:139:GLU:N    | 2.43                     | 0.47              |
| 6:n:217:GLU:OE2  | 6:o:60:ARG:NH2   | 2.48                     | 0.47              |
| 6:p:330:VAL:HG22 | 6:q:57:SER:HA    | 1.96                     | 0.47              |
| 6:q:178:GLN:OE1  | 6:q:185:ARG:NH2  | 2.46                     | 0.47              |
| 4:b:39:TYR:CG    | 4:b:92:MET:HE3   | 2.50                     | 0.47              |
| 5:i:425:LEU:HB2  | 5:i:431:ILE:HD12 | 1.96                     | 0.47              |
| 3:N:237:GLU:OE2  | 3:P:168:ARG:NH2  | 2.47                     | 0.47              |
| 3:d:58:ILE:CG2   | 3:d:71:LEU:HD23  | 2.45                     | 0.47              |
| 6:n:307:VAL:HG12 | 6:o:306:PHE:CE2  | 2.49                     | 0.47              |
| 1:D:12:PHE:CD1   | 3:L:253:ILE:HD12 | 2.50                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:o:307:VAL:HG12 | 6:p:306:PHE:CD2  | 2.50                     | 0.47              |
| 6:p:326:CYS:O    | 6:p:330:VAL:HG23 | 2.15                     | 0.47              |
| 6:q:139:GLU:N    | 6:q:139:GLU:OE1  | 2.47                     | 0.47              |
| 6:r:149:THR:HG21 | 6:s:196:GLY:HA3  | 1.96                     | 0.47              |
| 6:t:149:THR:HG21 | 6:u:196:GLY:HA3  | 1.96                     | 0.47              |
| 1:B:21:LEU:HD23  | 1:B:26:GLU:HA    | 1.97                     | 0.46              |
| 4:V:103:MET:HG2  | 6:p:296:LEU:HD13 | 1.98                     | 0.46              |
| 4:Y:106:ILE:HG23 | 6:v:290:LEU:HD23 | 1.97                     | 0.46              |
| 5:e:265:THR:CG2  | 5:e:299:THR:HG22 | 2.45                     | 0.46              |
| 6:k:54:LEU:HD13  | 6:k:243:MET:HG2  | 1.97                     | 0.46              |
| 1:F:41:GLU:OE1   | 1:F:41:GLU:N     | 2.42                     | 0.46              |
| 2:X:52:GLU:OE2   | 2:X:71:ARG:NH1   | 2.48                     | 0.46              |
| 5:e:167:VAL:HG22 | 5:e:171:ASN:ND2  | 2.30                     | 0.46              |
| 6:t:345:ALA:O    | 6:t:352:GLN:NE2  | 2.48                     | 0.46              |
| 4:V:106:ILE:HG23 | 6:o:290:LEU:HD23 | 1.96                     | 0.46              |
| 6:k:217:GLU:OE2  | 6:k:363:LYS:NZ   | 2.37                     | 0.46              |
| 5:h:222:GLU:OE1  | 5:h:249:LYS:NZ   | 2.38                     | 0.46              |
| 1:B:7:ILE:HD11   | 3:P:213:ILE:CD1  | 2.45                     | 0.46              |
| 4:S:103:MET:HE2  | 6:v:296:LEU:HD21 | 1.98                     | 0.46              |
| 3:d:150:GLU:OE1  | 3:d:150:GLU:N    | 2.49                     | 0.46              |
| 3:d:263:MET:HE2  | 5:j:406:ASN:HA   | 1.98                     | 0.46              |
| 5:g:259:LEU:N    | 5:g:283:ASN:O    | 2.43                     | 0.46              |
| 6:o:149:THR:HG23 | 6:o:150:THR:HG23 | 1.97                     | 0.46              |
| 6:s:99:LYS:NZ    | 6:s:103:ASP:OD1  | 2.47                     | 0.46              |
| 1:D:39:GLN:NE2   | 1:D:56:VAL:O     | 2.46                     | 0.46              |
| 3:H:68:LEU:HD21  | 3:H:115:ARG:HB2  | 1.97                     | 0.46              |
| 3:L:168:ARG:NH2  | 3:d:237:GLU:OE2  | 2.47                     | 0.46              |
| 5:e:95:ASP:OD1   | 5:e:96:GLY:N     | 2.49                     | 0.46              |
| 6:k:410:LEU:O    | 6:k:413:THR:OG1  | 2.29                     | 0.46              |
| 6:l:410:LEU:O    | 6:l:413:THR:OG1  | 2.34                     | 0.46              |
| 6:q:372:GLN:HG3  | 6:q:397:ILE:HD12 | 1.98                     | 0.46              |
| 6:v:52:TYR:OH    | 6:v:233:GLU:OE2  | 2.27                     | 0.46              |
| 3:H:261:PRO:HB3  | 5:f:448:ALA:HB1  | 1.98                     | 0.46              |
| 3:d:136:VAL:HG13 | 3:d:167:TRP:O    | 2.15                     | 0.46              |
| 5:g:259:LEU:HD11 | 5:g:261:LEU:HD21 | 1.96                     | 0.46              |
| 6:o:35:ARG:NH2   | 6:o:138:PRO:O    | 2.43                     | 0.46              |
| 6:t:181:THR:OG1  | 6:t:184:SER:O    | 2.13                     | 0.46              |
| 6:v:410:LEU:O    | 6:v:413:THR:OG1  | 2.30                     | 0.46              |
| 3:L:68:LEU:HD21  | 3:L:115:ARG:HB2  | 1.96                     | 0.46              |
| 5:f:282:GLU:N    | 5:f:282:GLU:OE1  | 2.47                     | 0.46              |
| 2:O:53:LYS:O     | 2:O:72:THR:HG23  | 2.16                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:X:22:ILE:HD12  | 2:X:93:PHE:CD2   | 2.50                     | 0.46              |
| 6:n:410:LEU:O    | 6:n:413:THR:OG1  | 2.30                     | 0.46              |
| 3:H:15:GLU:OE1   | 3:H:15:GLU:N     | 2.49                     | 0.46              |
| 5:g:231:LEU:HD21 | 5:g:234:VAL:O    | 2.16                     | 0.46              |
| 6:o:453:ASP:O    | 6:o:456:ARG:NE   | 2.49                     | 0.46              |
| 6:q:52:TYR:O     | 6:q:56:SER:N     | 2.48                     | 0.46              |
| 3:R:239:ASP:OD2  | 3:R:242:THR:OG1  | 2.22                     | 0.45              |
| 4:W:46:TRP:CZ2   | 4:c:51:LEU:HD22  | 2.50                     | 0.45              |
| 5:j:103:LEU:O    | 5:j:119:LEU:N    | 2.47                     | 0.45              |
| 4:Z:13:LEU:HD22  | 4:Z:38:ILE:HD13  | 1.97                     | 0.45              |
| 5:h:141:ASP:OD1  | 5:h:142:LYS:N    | 2.48                     | 0.45              |
| 5:h:372:ASP:OD1  | 5:h:373:LYS:N    | 2.49                     | 0.45              |
| 6:s:43:GLU:O     | 6:s:47:ASN:N     | 2.49                     | 0.45              |
| 6:t:100:THR:OG1  | 6:t:133:TYR:OH   | 2.04                     | 0.45              |
| 6:u:372:GLN:HG3  | 6:u:397:ILE:HD12 | 1.98                     | 0.45              |
| 2:M:43:ILE:HD12  | 2:M:81:VAL:HG11  | 1.99                     | 0.45              |
| 4:W:24:THR:OG1   | 4:W:26:GLU:OE1   | 2.34                     | 0.45              |
| 4:Y:104:LEU:HD22 | 6:v:288:ILE:HD11 | 1.98                     | 0.45              |
| 4:Z:109:GLU:N    | 4:Z:109:GLU:OE1  | 2.49                     | 0.45              |
| 6:l:364:ARG:NH2  | 6:l:400:ASP:O    | 2.49                     | 0.45              |
| 3:H:136:VAL:HG13 | 3:H:167:TRP:O    | 2.15                     | 0.45              |
| 3:N:136:VAL:HG13 | 3:N:167:TRP:O    | 2.17                     | 0.45              |
| 5:f:95:ASP:OD1   | 5:f:96:GLY:N     | 2.49                     | 0.45              |
| 5:h:103:LEU:N    | 5:h:119:LEU:O    | 2.50                     | 0.45              |
| 5:j:42:ARG:NH2   | 5:j:232:ASP:O    | 2.48                     | 0.45              |
| 6:s:410:LEU:O    | 6:s:413:THR:OG1  | 2.29                     | 0.45              |
| 1:F:135:ASN:OD1  | 1:F:136:GLU:N    | 2.49                     | 0.45              |
| 6:u:114:ILE:CG1  | 6:u:377:MET:HE1  | 2.46                     | 0.45              |
| 1:E:46:LEU:CD2   | 1:E:53:ILE:HD12  | 2.45                     | 0.45              |
| 3:N:104:ASP:OD2  | 3:P:2:ARG:NH2    | 2.47                     | 0.45              |
| 3:P:147:LEU:HD23 | 3:P:149:ILE:HD11 | 1.97                     | 0.45              |
| 4:V:103:MET:N    | 6:p:272:ASN:OD1  | 2.45                     | 0.45              |
| 5:g:108:THR:N    | 5:g:190:ILE:O    | 2.48                     | 0.45              |
| 5:j:377:MET:O    | 5:j:383:ILE:HD11 | 2.17                     | 0.45              |
| 6:k:372:GLN:HG3  | 6:k:397:ILE:HD12 | 1.99                     | 0.45              |
| 3:P:58:ILE:CG2   | 3:P:71:LEU:HD23  | 2.47                     | 0.45              |
| 3:d:47:THR:HG21  | 3:d:242:THR:O    | 2.17                     | 0.45              |
| 6:l:326:CYS:O    | 6:l:330:VAL:HG23 | 2.17                     | 0.45              |
| 6:r:313:ILE:HG23 | 6:r:316:ALA:HB3  | 1.98                     | 0.45              |
| 3:N:150:GLU:N    | 3:N:150:GLU:OE1  | 2.49                     | 0.45              |
| 2:Q:75:MET:HE1   | 2:Q:93:PHE:CE1   | 2.51                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:R:212:ILE:HD11 | 3:R:232:VAL:CG1  | 2.47                     | 0.45              |
| 5:f:222:GLU:OE1  | 5:f:249:LYS:NZ   | 2.40                     | 0.45              |
| 5:f:234:VAL:HG12 | 5:f:236:ASP:H    | 1.82                     | 0.45              |
| 6:n:261:LYS:NZ   | 6:o:303:GLU:OE2  | 2.30                     | 0.45              |
| 6:s:209:ILE:HG22 | 6:s:211:ILE:H    | 1.82                     | 0.45              |
| 6:s:318:GLU:OE1  | 6:s:318:GLU:N    | 2.47                     | 0.45              |
| 1:C:7:ILE:HD11   | 3:R:213:ILE:CD1  | 2.47                     | 0.45              |
| 3:N:48:ILE:HD12  | 3:N:242:THR:HG22 | 1.98                     | 0.45              |
| 3:P:68:LEU:HD21  | 3:P:115:ARG:HB2  | 1.98                     | 0.45              |
| 3:P:218:ARG:NH2  | 3:P:221:GLU:O    | 2.49                     | 0.45              |
| 6:n:209:ILE:HG22 | 6:n:211:ILE:H    | 1.81                     | 0.45              |
| 6:r:307:VAL:HG12 | 6:s:306:PHE:CD2  | 2.52                     | 0.45              |
| 6:s:19:MET:HG2   | 6:s:21:MET:HE2   | 1.99                     | 0.45              |
| 6:t:209:ILE:HG22 | 6:t:211:ILE:H    | 1.82                     | 0.45              |
| 3:R:55:GLU:OE1   | 3:R:57:TRP:NE1   | 2.50                     | 0.45              |
| 4:T:14:LEU:HD22  | 4:T:32:LEU:HD21  | 1.99                     | 0.45              |
| 5:g:407:ASP:OD1  | 5:g:409:THR:OG1  | 2.17                     | 0.45              |
| 5:j:259:LEU:N    | 5:j:283:ASN:O    | 2.46                     | 0.45              |
| 6:l:101:HIS:O    | 6:l:105:LEU:HD23 | 2.17                     | 0.45              |
| 6:r:100:THR:HG23 | 6:r:112:ILE:HD11 | 1.99                     | 0.45              |
| 6:r:101:HIS:O    | 6:r:105:LEU:HD23 | 2.16                     | 0.45              |
| 6:v:299:ASN:OD1  | 6:v:301:ASP:N    | 2.46                     | 0.45              |
| 5:e:281:ASP:OD1  | 5:e:282:GLU:N    | 2.50                     | 0.44              |
| 5:f:377:MET:O    | 5:f:383:ILE:HD11 | 2.17                     | 0.44              |
| 6:o:319:LEU:HD22 | 6:p:247:LEU:HD22 | 1.99                     | 0.44              |
| 6:u:410:LEU:O    | 6:u:413:THR:OG1  | 2.31                     | 0.44              |
| 1:C:46:LEU:HD23  | 1:C:53:ILE:HD12  | 1.99                     | 0.44              |
| 6:o:335:GLU:CG   | 6:o:342:THR:HG21 | 2.47                     | 0.44              |
| 6:r:410:LEU:O    | 6:r:413:THR:OG1  | 2.32                     | 0.44              |
| 3:L:212:ILE:HD11 | 3:L:232:VAL:CG1  | 2.48                     | 0.44              |
| 6:l:209:ILE:HG22 | 6:l:211:ILE:H    | 1.82                     | 0.44              |
| 1:A:7:ILE:HD11   | 3:P:256:ILE:HA   | 2.00                     | 0.44              |
| 5:e:169:GLU:OE2  | 5:e:173:ASN:ND2  | 2.46                     | 0.44              |
| 5:f:76:LEU:HD21  | 5:f:302:GLU:HG2  | 1.99                     | 0.44              |
| 5:i:377:MET:O    | 5:i:383:ILE:HD11 | 2.17                     | 0.44              |
| 6:o:335:GLU:CD   | 6:o:342:THR:HG21 | 2.43                     | 0.44              |
| 2:K:61:SER:O     | 3:R:23:ASN:ND2   | 2.50                     | 0.44              |
| 3:N:68:LEU:HD21  | 3:N:115:ARG:HB2  | 1.99                     | 0.44              |
| 5:g:39:MET:CG    | 5:g:88:LEU:HD11  | 2.47                     | 0.44              |
| 6:k:342:THR:HG23 | 6:k:342:THR:O    | 2.17                     | 0.44              |
| 6:l:313:ILE:O    | 6:m:254:SER:OG   | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:r:97:MET:O     | 6:r:101:HIS:ND1  | 2.51                     | 0.44              |
| 6:t:156:TYR:CE1  | 6:t:209:ILE:HG21 | 2.53                     | 0.44              |
| 6:k:36:VAL:HG22  | 6:v:20:ARG:HH22  | 1.81                     | 0.44              |
| 6:l:156:TYR:CD1  | 6:l:209:ILE:HG21 | 2.53                     | 0.44              |
| 6:q:276:GLU:OE1  | 6:q:276:GLU:N    | 2.44                     | 0.44              |
| 1:C:40:ASP:OD2   | 1:D:45:LYS:NZ    | 2.50                     | 0.44              |
| 1:D:116:ALA:N    | 1:E:31:GLU:O     | 2.50                     | 0.44              |
| 5:f:44:ASN:O     | 5:f:92:ARG:NH2   | 2.50                     | 0.44              |
| 5:i:282:GLU:HB3  | 5:i:383:ILE:HD12 | 2.00                     | 0.44              |
| 6:k:298:LEU:HD12 | 6:k:302:GLU:CB   | 2.48                     | 0.44              |
| 6:p:173:LYS:N    | 6:p:192:ASP:OD2  | 2.49                     | 0.44              |
| 6:r:264:ASP:OD1  | 6:r:264:ASP:N    | 2.48                     | 0.44              |
| 6:u:374:LEU:O    | 6:u:378:VAL:HG23 | 2.17                     | 0.44              |
| 1:E:26:GLU:OE2   | 3:N:180:HIS:NE2  | 2.45                     | 0.44              |
| 3:L:136:VAL:HG13 | 3:L:167:TRP:O    | 2.17                     | 0.44              |
| 4:T:36:ASP:OD1   | 4:T:37:CYS:N     | 2.50                     | 0.44              |
| 4:c:106:ILE:HG21 | 6:q:252:MET:HE3  | 1.98                     | 0.44              |
| 5:j:117:ILE:CG1  | 5:j:163:ILE:HG23 | 2.48                     | 0.44              |
| 6:l:307:VAL:HG12 | 6:m:306:PHE:CD2  | 2.52                     | 0.44              |
| 6:p:23:SER:OG    | 6:q:33:ASP:O     | 2.36                     | 0.44              |
| 3:N:101:SER:N    | 3:N:116:GLY:O    | 2.48                     | 0.44              |
| 5:f:372:ASP:OD1  | 5:f:373:LYS:N    | 2.51                     | 0.44              |
| 5:j:393:THR:HG21 | 5:j:453:TRP:HH2  | 1.83                     | 0.44              |
| 6:v:209:ILE:HG22 | 6:v:211:ILE:H    | 1.82                     | 0.44              |
| 3:R:44:HIS:ND1   | 3:R:51:GLU:OE1   | 2.50                     | 0.43              |
| 4:Z:75:ILE:O     | 4:Z:79:VAL:HG12  | 2.18                     | 0.43              |
| 5:g:234:VAL:CG1  | 5:g:239:LEU:HD12 | 2.48                     | 0.43              |
| 6:r:453:ASP:OD1  | 6:r:454:GLY:N    | 2.51                     | 0.43              |
| 3:L:101:SER:N    | 3:L:116:GLY:O    | 2.46                     | 0.43              |
| 5:g:94:VAL:HG13  | 5:g:205:GLY:HA2  | 1.98                     | 0.43              |
| 3:L:2:ARG:NH2    | 3:d:104:ASP:OD2  | 2.49                     | 0.43              |
| 3:N:58:ILE:CG2   | 3:N:71:LEU:HD23  | 2.47                     | 0.43              |
| 4:T:106:ILE:HD11 | 6:l:295:ILE:HB   | 2.00                     | 0.43              |
| 4:U:103:MET:N    | 6:n:272:ASN:OD1  | 2.44                     | 0.43              |
| 4:Z:50:SER:OG    | 4:Z:79:VAL:HG23  | 2.19                     | 0.43              |
| 3:d:170:THR:HG21 | 3:d:189:LYS:HD3  | 2.00                     | 0.43              |
| 5:g:339:VAL:HG11 | 5:g:360:VAL:HG11 | 2.01                     | 0.43              |
| 5:i:39:MET:CG    | 5:i:88:LEU:HD11  | 2.48                     | 0.43              |
| 6:o:297:PHE:C    | 6:o:298:LEU:HD22 | 2.43                     | 0.43              |
| 5:g:281:ASP:OD1  | 5:g:283:ASN:N    | 2.47                     | 0.43              |
| 5:h:44:ASN:O     | 5:h:92:ARG:NH2   | 2.51                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:l:114:ILE:CD1  | 6:l:378:VAL:HG22 | 2.48                     | 0.43              |
| 1:E:19:VAL:HG13  | 1:E:26:GLU:OE2   | 2.19                     | 0.43              |
| 3:L:16:LEU:HD13  | 3:L:34:MET:HE3   | 2.00                     | 0.43              |
| 2:M:52:GLU:OE1   | 4:S:67:GLN:NE2   | 2.47                     | 0.43              |
| 3:P:5:ILE:HD11   | 3:P:54:ILE:HD13  | 2.00                     | 0.43              |
| 3:d:44:HIS:ND1   | 3:d:51:GLU:OE1   | 2.50                     | 0.43              |
| 5:e:204:ASP:O    | 5:e:207:THR:OG1  | 2.31                     | 0.43              |
| 5:e:440:THR:O    | 5:e:444:ALA:N    | 2.49                     | 0.43              |
| 6:k:139:GLU:OE1  | 6:k:139:GLU:N    | 2.48                     | 0.43              |
| 6:r:369:ASN:OD1  | 6:r:370:SER:N    | 2.51                     | 0.43              |
| 6:s:449:TYR:N    | 6:s:457:GLU:OE2  | 2.51                     | 0.43              |
| 6:u:42:ARG:NH1   | 6:u:139:GLU:OE2  | 2.46                     | 0.43              |
| 2:K:47:VAL:HG22  | 2:K:77:VAL:HG23  | 1.99                     | 0.43              |
| 5:f:39:MET:HE3   | 5:f:232:ASP:OD1  | 2.18                     | 0.43              |
| 6:m:307:VAL:HG12 | 6:n:306:PHE:CD2  | 2.53                     | 0.43              |
| 6:q:180:ILE:HG21 | 6:q:211:ILE:CD1  | 2.48                     | 0.43              |
| 6:s:66:THR:HG22  | 6:s:359:LYS:HE3  | 2.01                     | 0.43              |
| 6:v:369:ASN:OD1  | 6:v:370:SER:N    | 2.52                     | 0.43              |
| 4:V:50:SER:HB2   | 4:V:79:VAL:HG23  | 2.01                     | 0.43              |
| 5:e:37:LEU:HD12  | 5:e:228:SER:O    | 2.18                     | 0.43              |
| 5:i:260:PHE:CG   | 5:i:308:ALA:HB2  | 2.54                     | 0.43              |
| 6:n:20:ARG:HH22  | 6:o:36:VAL:HG22  | 1.84                     | 0.43              |
| 1:B:19:VAL:HG13  | 1:B:26:GLU:OE2   | 2.18                     | 0.43              |
| 3:H:263:MET:HE1  | 5:f:451:PHE:CD2  | 2.54                     | 0.43              |
| 3:N:47:THR:HG21  | 3:N:242:THR:O    | 2.19                     | 0.43              |
| 3:N:115:ARG:NH2  | 3:P:39:GLY:O     | 2.50                     | 0.43              |
| 3:P:1:MET:SD     | 3:P:52:ARG:NH1   | 2.91                     | 0.43              |
| 5:e:42:ARG:NH2   | 5:e:232:ASP:O    | 2.48                     | 0.43              |
| 5:e:266:GLU:OE1  | 5:e:266:GLU:N    | 2.46                     | 0.43              |
| 5:g:135:SER:OG   | 5:g:143:LYS:NZ   | 2.52                     | 0.43              |
| 6:p:59:VAL:HG13  | 6:p:229:ILE:HG22 | 2.01                     | 0.43              |
| 6:p:209:ILE:HG22 | 6:p:211:ILE:H    | 1.83                     | 0.43              |
| 6:q:70:MET:HE1   | 6:q:105:LEU:HD21 | 1.99                     | 0.43              |
| 6:r:43:GLU:O     | 6:r:47:ASN:N     | 2.52                     | 0.43              |
| 2:K:52:GLU:OE2   | 2:K:71:ARG:NH1   | 2.52                     | 0.43              |
| 3:N:58:ILE:HG21  | 3:N:71:LEU:HD23  | 2.01                     | 0.43              |
| 3:P:47:THR:HG21  | 3:P:242:THR:O    | 2.19                     | 0.43              |
| 3:P:101:SER:N    | 3:P:116:GLY:O    | 2.48                     | 0.43              |
| 3:R:136:VAL:HG13 | 3:R:167:TRP:O    | 2.17                     | 0.43              |
| 5:f:92:ARG:NH1   | 5:f:124:PRO:O    | 2.48                     | 0.43              |
| 5:g:282:GLU:OE2  | 5:g:373:LYS:NZ   | 2.46                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:l:299:ASN:OD1  | 6:l:301:ASP:N    | 2.50                     | 0.43              |
| 6:p:267:SER:OG   | 6:p:271:HIS:NE2  | 2.51                     | 0.43              |
| 6:q:335:GLU:OE1  | 6:q:342:THR:HG21 | 2.19                     | 0.43              |
| 3:L:219:LEU:HD13 | 3:L:227:LEU:HD11 | 1.99                     | 0.43              |
| 4:S:106:ILE:HG23 | 6:u:290:LEU:HD23 | 2.00                     | 0.43              |
| 5:f:231:LEU:HD11 | 5:f:240:GLN:HG2  | 2.01                     | 0.43              |
| 6:l:372:GLN:HG3  | 6:l:397:ILE:HD12 | 2.01                     | 0.43              |
| 6:n:100:THR:HG23 | 6:n:112:ILE:HD11 | 2.01                     | 0.43              |
| 6:n:156:TYR:CE1  | 6:n:209:ILE:HG21 | 2.54                     | 0.43              |
| 6:p:328:VAL:HG11 | 6:q:340:VAL:HG11 | 2.00                     | 0.43              |
| 3:P:166:LEU:HD23 | 3:P:168:ARG:H    | 1.83                     | 0.42              |
| 5:g:115:ASP:HB3  | 5:g:184:VAL:HG11 | 2.01                     | 0.42              |
| 6:k:147:ASP:O    | 6:k:151:LYS:N    | 2.48                     | 0.42              |
| 6:m:216:ASN:O    | 6:m:226:GLN:N    | 2.52                     | 0.42              |
| 6:p:264:ASP:OD1  | 6:p:264:ASP:N    | 2.50                     | 0.42              |
| 6:p:335:GLU:OE2  | 6:p:342:THR:OG1  | 2.27                     | 0.42              |
| 6:r:209:ILE:HG22 | 6:r:211:ILE:H    | 1.84                     | 0.42              |
| 3:L:176:ARG:NH1  | 3:d:213:ILE:O    | 2.52                     | 0.42              |
| 2:X:75:MET:HE3   | 2:X:121:LEU:HD11 | 2.00                     | 0.42              |
| 5:g:103:LEU:N    | 5:g:119:LEU:O    | 2.51                     | 0.42              |
| 6:l:42:ARG:NH1   | 6:l:107:GLN:OE1  | 2.51                     | 0.42              |
| 6:o:342:THR:O    | 6:o:342:THR:HG23 | 2.19                     | 0.42              |
| 6:v:264:ASP:N    | 6:v:264:ASP:OD1  | 2.51                     | 0.42              |
| 1:B:97:GLU:OE1   | 1:B:97:GLU:N     | 2.52                     | 0.42              |
| 4:a:14:LEU:HB2   | 4:a:38:ILE:HD11  | 2.00                     | 0.42              |
| 6:u:212:ILE:HD11 | 6:u:377:MET:HE3  | 2.02                     | 0.42              |
| 1:C:19:VAL:HG13  | 1:C:26:GLU:OE2   | 2.20                     | 0.42              |
| 3:L:5:ILE:HD11   | 3:L:54:ILE:HD13  | 2.01                     | 0.42              |
| 6:l:144:ILE:HD12 | 6:l:155:ALA:O    | 2.20                     | 0.42              |
| 6:u:91:LEU:HD23  | 6:u:456:ARG:HG3  | 2.01                     | 0.42              |
| 6:l:369:ASN:OD1  | 6:l:370:SER:N    | 2.51                     | 0.42              |
| 6:r:372:GLN:HG3  | 6:r:397:ILE:HD12 | 2.01                     | 0.42              |
| 6:u:114:ILE:HB   | 6:u:377:MET:HE1  | 2.01                     | 0.42              |
| 6:u:307:VAL:HG12 | 6:v:306:PHE:CD2  | 2.55                     | 0.42              |
| 4:J:39:TYR:CE1   | 4:J:92:MET:HE1   | 2.55                     | 0.42              |
| 3:R:11:ASP:O     | 3:R:14:LYS:NZ    | 2.47                     | 0.42              |
| 3:d:15:GLU:OE1   | 3:d:15:GLU:N     | 2.51                     | 0.42              |
| 3:d:166:LEU:HD23 | 3:d:168:ARG:H    | 1.84                     | 0.42              |
| 5:g:442:LEU:O    | 5:g:446:ALA:N    | 2.52                     | 0.42              |
| 1:E:135:ASN:OD1  | 1:E:136:GLU:N    | 2.51                     | 0.42              |
| 2:O:104:ASN:OD1  | 2:O:105:ILE:N    | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:R:58:ILE:HD11  | 3:R:117:ILE:CD1  | 2.50                     | 0.42              |
| 4:S:103:MET:N    | 6:v:272:ASN:OD1  | 2.46                     | 0.42              |
| 5:g:107:ASP:OD1  | 5:g:114:LYS:N    | 2.46                     | 0.42              |
| 5:j:290:SER:OG   | 5:j:297:LYS:NZ   | 2.31                     | 0.42              |
| 6:o:180:ILE:HG21 | 6:o:211:ILE:CD1  | 2.50                     | 0.42              |
| 6:o:335:GLU:OE2  | 6:o:342:THR:HG21 | 2.19                     | 0.42              |
| 6:u:297:PHE:C    | 6:u:298:LEU:HD22 | 2.44                     | 0.42              |
| 1:A:58:THR:OG1   | 1:B:50:GLN:O     | 2.11                     | 0.42              |
| 3:H:58:ILE:CG2   | 3:H:71:LEU:HD23  | 2.49                     | 0.42              |
| 3:L:44:HIS:ND1   | 3:L:51:GLU:OE1   | 2.52                     | 0.42              |
| 2:M:114:LEU:HD21 | 2:M:117:TYR:OH   | 2.20                     | 0.42              |
| 6:q:298:LEU:HD12 | 6:q:302:GLU:CB   | 2.49                     | 0.42              |
| 6:v:313:ILE:HG23 | 6:v:316:ALA:HB3  | 2.01                     | 0.42              |
| 1:D:21:LEU:HD23  | 1:D:26:GLU:HA    | 2.01                     | 0.42              |
| 2:X:104:ASN:OD1  | 2:X:105:ILE:N    | 2.53                     | 0.42              |
| 5:g:39:MET:HG3   | 5:g:88:LEU:HD11  | 2.02                     | 0.42              |
| 6:l:66:THR:HG22  | 6:l:359:LYS:HE3  | 2.02                     | 0.42              |
| 6:n:176:VAL:HG23 | 6:n:189:VAL:HG12 | 2.02                     | 0.42              |
| 3:H:104:ASP:OD2  | 3:N:2:ARG:NH2    | 2.50                     | 0.42              |
| 2:M:85:VAL:HG23  | 2:M:91:LEU:HD12  | 2.01                     | 0.42              |
| 2:O:20:THR:N     | 2:O:47:VAL:O     | 2.52                     | 0.42              |
| 3:P:266:ILE:HD11 | 5:h:400:PHE:O    | 2.19                     | 0.42              |
| 5:g:425:LEU:HB2  | 5:g:431:ILE:HD12 | 2.02                     | 0.42              |
| 6:m:345:ALA:O    | 6:m:352:GLN:NE2  | 2.48                     | 0.42              |
| 1:A:28:LEU:H     | 1:A:28:LEU:HD23  | 1.85                     | 0.41              |
| 2:X:43:ILE:HD12  | 2:X:81:VAL:HG11  | 2.01                     | 0.41              |
| 4:a:57:VAL:HG21  | 4:a:78:LEU:HD12  | 2.02                     | 0.41              |
| 5:f:130:ASN:O    | 5:f:148:PHE:N    | 2.52                     | 0.41              |
| 5:h:282:GLU:N    | 5:h:282:GLU:OE1  | 2.48                     | 0.41              |
| 6:r:173:LYS:N    | 6:r:192:ASP:OD2  | 2.51                     | 0.41              |
| 6:v:99:LYS:HA    | 6:v:102:THR:HG22 | 2.02                     | 0.41              |
| 3:P:150:GLU:OE1  | 3:P:150:GLU:N    | 2.53                     | 0.41              |
| 6:k:307:VAL:HG12 | 6:l:306:PHE:CD2  | 2.55                     | 0.41              |
| 6:t:55:GLY:O     | 6:t:236:LEU:HD22 | 2.19                     | 0.41              |
| 1:F:9:GLU:OE1    | 1:F:9:GLU:N      | 2.49                     | 0.41              |
| 4:V:104:LEU:HD11 | 6:o:269:LEU:HD21 | 2.02                     | 0.41              |
| 5:e:131:VAL:HG22 | 5:e:147:PHE:CD2  | 2.56                     | 0.41              |
| 5:g:95:ASP:OD1   | 5:g:96:GLY:N     | 2.53                     | 0.41              |
| 6:m:410:LEU:O    | 6:m:413:THR:OG1  | 2.31                     | 0.41              |
| 6:n:115:THR:OG1  | 6:n:134:ASN:OD1  | 2.14                     | 0.41              |
| 6:p:301:ASP:O    | 6:q:300:LYS:NZ   | 2.50                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 6:t:178:GLN:HB3  | 6:t:187:VAL:HG23 | 2.03                     | 0.41              |
| 6:u:146:LEU:HD22 | 6:u:151:LYS:O    | 2.20                     | 0.41              |
| 6:v:173:LYS:N    | 6:v:192:ASP:OD2  | 2.48                     | 0.41              |
| 2:K:104:ASN:OD1  | 2:K:105:ILE:N    | 2.53                     | 0.41              |
| 3:L:39:GLY:O     | 3:d:115:ARG:NH2  | 2.53                     | 0.41              |
| 6:n:173:LYS:N    | 6:n:192:ASP:OD2  | 2.50                     | 0.41              |
| 6:u:342:THR:HG23 | 6:u:342:THR:O    | 2.20                     | 0.41              |
| 4:I:68:GLU:OE2   | 2:O:76:LEU:HD13  | 2.20                     | 0.41              |
| 3:L:5:ILE:CD1    | 3:L:54:ILE:HD13  | 2.50                     | 0.41              |
| 3:L:47:THR:HG21  | 3:L:242:THR:O    | 2.21                     | 0.41              |
| 6:s:116:ARG:NH1  | 6:s:118:GLU:OE2  | 2.53                     | 0.41              |
| 3:L:68:LEU:HD21  | 3:L:115:ARG:CB   | 2.50                     | 0.41              |
| 3:R:48:ILE:HG23  | 3:R:122:ILE:HG23 | 2.03                     | 0.41              |
| 4:T:110:PHE:CZ   | 6:v:247:LEU:HD23 | 2.56                     | 0.41              |
| 5:g:170:ILE:HG21 | 5:g:181:ALA:HB2  | 2.03                     | 0.41              |
| 5:h:259:LEU:HD11 | 5:h:261:LEU:HD21 | 2.03                     | 0.41              |
| 5:i:167:VAL:HG22 | 5:i:171:ASN:HD21 | 1.86                     | 0.41              |
| 6:k:70:MET:HE1   | 6:k:105:LEU:HD21 | 2.02                     | 0.41              |
| 6:p:20:ARG:NH2   | 6:q:230:GLU:OE2  | 2.50                     | 0.41              |
| 6:s:137:SER:OG   | 6:s:139:GLU:OE1  | 2.36                     | 0.41              |
| 6:v:67:THR:HG21  | 6:v:102:THR:HA   | 2.03                     | 0.41              |
| 4:J:108:THR:OG1  | 6:t:290:LEU:O    | 2.37                     | 0.41              |
| 4:b:106:ILE:HG23 | 6:p:290:LEU:HD23 | 2.03                     | 0.41              |
| 5:g:303:VAL:HG23 | 5:g:327:PHE:CE2  | 2.56                     | 0.41              |
| 1:A:26:GLU:OE2   | 3:R:180:HIS:NE2  | 2.53                     | 0.41              |
| 1:D:125:GLU:N    | 1:D:125:GLU:OE1  | 2.54                     | 0.41              |
| 3:P:5:ILE:CD1    | 3:P:54:ILE:HD13  | 2.51                     | 0.41              |
| 3:R:101:SER:N    | 3:R:116:GLY:O    | 2.50                     | 0.41              |
| 4:Y:14:LEU:HD22  | 4:Y:28:LEU:HB3   | 2.03                     | 0.41              |
| 5:e:339:VAL:CG1  | 5:e:360:VAL:HG11 | 2.51                     | 0.41              |
| 5:f:126:ALA:HB2  | 5:f:203:ASN:CA   | 2.51                     | 0.41              |
| 5:j:169:GLU:OE2  | 5:j:173:ASN:ND2  | 2.50                     | 0.41              |
| 6:m:319:LEU:HD22 | 6:n:247:LEU:HD22 | 2.03                     | 0.41              |
| 6:t:176:VAL:HG23 | 6:t:189:VAL:HG12 | 2.03                     | 0.41              |
| 6:v:59:VAL:HG13  | 6:v:229:ILE:CG2  | 2.51                     | 0.41              |
| 2:G:56:GLU:OE2   | 2:Q:71:ARG:NE    | 2.54                     | 0.41              |
| 3:H:44:HIS:ND1   | 3:H:51:GLU:OE1   | 2.50                     | 0.41              |
| 3:H:101:SER:N    | 3:H:116:GLY:O    | 2.50                     | 0.41              |
| 4:I:68:GLU:OE1   | 2:O:7:ARG:NH2    | 2.49                     | 0.41              |
| 2:K:70:ILE:HD13  | 2:X:104:ASN:ND2  | 2.35                     | 0.41              |
| 2:O:75:MET:HE1   | 2:O:93:PHE:CE2   | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:R:48:ILE:HD12  | 3:R:242:THR:HG22 | 2.03                     | 0.41              |
| 5:e:282:GLU:HB3  | 5:e:383:ILE:HD12 | 2.02                     | 0.41              |
| 5:i:39:MET:HG3   | 5:i:88:LEU:HD11  | 2.03                     | 0.41              |
| 5:j:122:LYS:NZ   | 5:j:177:GLU:OE2  | 2.52                     | 0.41              |
| 6:k:340:VAL:HG11 | 6:v:328:VAL:HG11 | 2.03                     | 0.41              |
| 6:l:178:GLN:HB3  | 6:l:187:VAL:HG23 | 2.03                     | 0.41              |
| 6:l:307:VAL:HG12 | 6:m:306:PHE:HD2  | 1.86                     | 0.41              |
| 6:p:369:ASN:OD1  | 6:p:370:SER:N    | 2.52                     | 0.41              |
| 6:s:91:LEU:HD23  | 6:s:456:ARG:HG3  | 2.02                     | 0.41              |
| 6:s:421:LEU:HD22 | 6:s:431:SER:OG   | 2.21                     | 0.41              |
| 6:t:100:THR:HG23 | 6:t:112:ILE:HD11 | 2.03                     | 0.41              |
| 6:t:410:LEU:O    | 6:t:413:THR:OG1  | 2.31                     | 0.41              |
| 1:D:19:VAL:HG13  | 1:D:26:GLU:OE2   | 2.21                     | 0.41              |
| 3:L:86:ASP:O     | 3:L:90:ASN:N     | 2.55                     | 0.41              |
| 4:c:103:MET:HE1  | 6:s:290:LEU:HD21 | 2.03                     | 0.41              |
| 4:c:106:ILE:HD11 | 6:s:295:ILE:CG2  | 2.51                     | 0.41              |
| 6:t:299:ASN:OD1  | 6:t:301:ASP:N    | 2.53                     | 0.41              |
| 6:v:59:VAL:HG13  | 6:v:229:ILE:HG22 | 2.02                     | 0.41              |
| 3:H:2:ARG:NH2    | 3:L:104:ASP:OD2  | 2.50                     | 0.40              |
| 3:R:58:ILE:HG21  | 3:R:71:LEU:HD23  | 2.03                     | 0.40              |
| 3:R:58:ILE:CG2   | 3:R:71:LEU:HD23  | 2.51                     | 0.40              |
| 4:T:106:ILE:HG23 | 6:k:290:LEU:HD23 | 2.02                     | 0.40              |
| 3:d:219:LEU:HD13 | 3:d:227:LEU:HD11 | 2.02                     | 0.40              |
| 6:o:116:ARG:NH1  | 6:o:118:GLU:OE2  | 2.52                     | 0.40              |
| 6:r:313:ILE:CG2  | 6:r:316:ALA:HB3  | 2.51                     | 0.40              |
| 6:r:330:VAL:HG22 | 6:s:57:SER:HA    | 2.03                     | 0.40              |
| 6:v:313:ILE:CG2  | 6:v:316:ALA:HB3  | 2.51                     | 0.40              |
| 6:m:209:ILE:HG22 | 6:m:211:ILE:H    | 1.86                     | 0.40              |
| 6:u:289:ASN:O    | 6:u:290:LEU:HD22 | 2.22                     | 0.40              |
| 3:P:68:LEU:HD21  | 3:P:115:ARG:CB   | 2.51                     | 0.40              |
| 6:m:330:VAL:HG22 | 6:n:57:SER:HA    | 2.04                     | 0.40              |
| 6:p:410:LEU:O    | 6:p:413:THR:OG1  | 2.30                     | 0.40              |
| 2:M:5:ASP:OD1    | 2:M:6:ARG:N      | 2.54                     | 0.40              |
| 3:R:68:LEU:HD21  | 3:R:115:ARG:CB   | 2.51                     | 0.40              |
| 3:R:143:THR:OG1  | 3:R:167:TRP:NE1  | 2.55                     | 0.40              |
| 5:j:167:VAL:HG22 | 5:j:171:ASN:HD21 | 1.86                     | 0.40              |
| 6:k:54:LEU:HD13  | 6:k:243:MET:CG   | 2.51                     | 0.40              |
| 3:H:143:THR:OG1  | 3:H:167:TRP:NE1  | 2.54                     | 0.40              |
| 2:X:75:MET:HE1   | 2:X:93:PHE:CZ    | 2.56                     | 0.40              |
| 6:o:99:LYS:NZ    | 6:o:103:ASP:OD1  | 2.50                     | 0.40              |
| 6:r:376:ARG:NH2  | 6:r:394:ASP:OD1  | 2.52                     | 0.40              |

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| Atom-1           | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|----------------|--------------------------|-------------------|
| 6:u:421:LEU:HD22 | 6:u:431:SER:OG | 2.22                     | 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     | 128/137 (93%) | 124 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | B     | 128/137 (93%) | 123 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 1   | C     | 128/137 (93%) | 124 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | D     | 128/137 (93%) | 124 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | E     | 128/137 (93%) | 122 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 1   | F     | 128/137 (93%) | 126 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 2   | G     | 122/125 (98%) | 118 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 2   | K     | 122/125 (98%) | 117 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 2   | M     | 122/125 (98%) | 120 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 2   | O     | 122/125 (98%) | 121 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 2   | Q     | 122/125 (98%) | 117 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 2   | X     | 122/125 (98%) | 120 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 3   | H     | 270/273 (99%) | 255 (94%) | 15 (6%) | 0        | 100         | 100 |
| 3   | L     | 270/273 (99%) | 258 (96%) | 12 (4%) | 0        | 100         | 100 |
| 3   | N     | 270/273 (99%) | 259 (96%) | 11 (4%) | 0        | 100         | 100 |
| 3   | P     | 270/273 (99%) | 256 (95%) | 14 (5%) | 0        | 100         | 100 |
| 3   | R     | 270/273 (99%) | 254 (94%) | 16 (6%) | 0        | 100         | 100 |
| 3   | d     | 270/273 (99%) | 255 (94%) | 15 (6%) | 0        | 100         | 100 |
| 4   | I     | 101/112 (90%) | 99 (98%)  | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 4   | J     | 101/112 (90%)     | 98 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 4   | S     | 101/112 (90%)     | 99 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 4   | T     | 101/112 (90%)     | 98 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 4   | U     | 101/112 (90%)     | 98 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 4   | V     | 101/112 (90%)     | 99 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 4   | W     | 101/112 (90%)     | 97 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| 4   | Y     | 101/112 (90%)     | 100 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 4   | Z     | 101/112 (90%)     | 97 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| 4   | a     | 101/112 (90%)     | 98 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 4   | b     | 101/112 (90%)     | 98 (97%)    | 3 (3%)   | 0        | 100         | 100 |
| 4   | c     | 101/112 (90%)     | 99 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 5   | e     | 416/473 (88%)     | 394 (95%)   | 22 (5%)  | 0        | 100         | 100 |
| 5   | f     | 416/473 (88%)     | 392 (94%)   | 24 (6%)  | 0        | 100         | 100 |
| 5   | g     | 416/473 (88%)     | 392 (94%)   | 24 (6%)  | 0        | 100         | 100 |
| 5   | h     | 416/473 (88%)     | 393 (94%)   | 23 (6%)  | 0        | 100         | 100 |
| 5   | i     | 416/473 (88%)     | 392 (94%)   | 24 (6%)  | 0        | 100         | 100 |
| 5   | j     | 416/473 (88%)     | 389 (94%)   | 27 (6%)  | 0        | 100         | 100 |
| 6   | k     | 441/500 (88%)     | 433 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 6   | l     | 441/500 (88%)     | 424 (96%)   | 17 (4%)  | 0        | 100         | 100 |
| 6   | m     | 441/500 (88%)     | 432 (98%)   | 9 (2%)   | 0        | 100         | 100 |
| 6   | n     | 441/500 (88%)     | 431 (98%)   | 10 (2%)  | 0        | 100         | 100 |
| 6   | o     | 441/500 (88%)     | 432 (98%)   | 9 (2%)   | 0        | 100         | 100 |
| 6   | p     | 441/500 (88%)     | 430 (98%)   | 11 (2%)  | 0        | 100         | 100 |
| 6   | q     | 441/500 (88%)     | 431 (98%)   | 10 (2%)  | 0        | 100         | 100 |
| 6   | r     | 441/500 (88%)     | 429 (97%)   | 12 (3%)  | 0        | 100         | 100 |
| 6   | s     | 441/500 (88%)     | 431 (98%)   | 10 (2%)  | 0        | 100         | 100 |
| 6   | t     | 441/500 (88%)     | 434 (98%)   | 7 (2%)   | 0        | 100         | 100 |
| 6   | u     | 441/500 (88%)     | 433 (98%)   | 8 (2%)   | 0        | 100         | 100 |
| 6   | v     | 441/500 (88%)     | 431 (98%)   | 10 (2%)  | 0        | 100         | 100 |
| All | All   | 12120/13392 (90%) | 11696 (96%) | 424 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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     | 115/122 (94%)  | 115 (100%) | 0        | 100         | 100 |
| 1   | B     | 115/122 (94%)  | 115 (100%) | 0        | 100         | 100 |
| 1   | C     | 115/122 (94%)  | 115 (100%) | 0        | 100         | 100 |
| 1   | D     | 115/122 (94%)  | 114 (99%)  | 1 (1%)   | 70          | 78  |
| 1   | E     | 115/122 (94%)  | 115 (100%) | 0        | 100         | 100 |
| 1   | F     | 115/122 (94%)  | 115 (100%) | 0        | 100         | 100 |
| 2   | G     | 116/117 (99%)  | 116 (100%) | 0        | 100         | 100 |
| 2   | K     | 116/117 (99%)  | 116 (100%) | 0        | 100         | 100 |
| 2   | M     | 116/117 (99%)  | 116 (100%) | 0        | 100         | 100 |
| 2   | O     | 116/117 (99%)  | 116 (100%) | 0        | 100         | 100 |
| 2   | Q     | 116/117 (99%)  | 116 (100%) | 0        | 100         | 100 |
| 2   | X     | 116/117 (99%)  | 116 (100%) | 0        | 100         | 100 |
| 3   | H     | 249/250 (100%) | 249 (100%) | 0        | 100         | 100 |
| 3   | L     | 249/250 (100%) | 249 (100%) | 0        | 100         | 100 |
| 3   | N     | 249/250 (100%) | 249 (100%) | 0        | 100         | 100 |
| 3   | P     | 249/250 (100%) | 249 (100%) | 0        | 100         | 100 |
| 3   | R     | 249/250 (100%) | 249 (100%) | 0        | 100         | 100 |
| 3   | d     | 249/250 (100%) | 249 (100%) | 0        | 100         | 100 |
| 4   | I     | 93/101 (92%)   | 93 (100%)  | 0        | 100         | 100 |
| 4   | J     | 93/101 (92%)   | 93 (100%)  | 0        | 100         | 100 |
| 4   | S     | 93/101 (92%)   | 93 (100%)  | 0        | 100         | 100 |
| 4   | T     | 93/101 (92%)   | 93 (100%)  | 0        | 100         | 100 |
| 4   | U     | 93/101 (92%)   | 93 (100%)  | 0        | 100         | 100 |
| 4   | V     | 93/101 (92%)   | 93 (100%)  | 0        | 100         | 100 |
| 4   | W     | 93/101 (92%)   | 93 (100%)  | 0        | 100         | 100 |
| 4   | Y     | 93/101 (92%)   | 93 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 4   | Z     | 93/101 (92%)      | 93 (100%)    | 0        | 100         | 100 |
| 4   | a     | 93/101 (92%)      | 93 (100%)    | 0        | 100         | 100 |
| 4   | b     | 93/101 (92%)      | 93 (100%)    | 0        | 100         | 100 |
| 4   | c     | 93/101 (92%)      | 93 (100%)    | 0        | 100         | 100 |
| 5   | e     | 369/413 (89%)     | 369 (100%)   | 0        | 100         | 100 |
| 5   | f     | 369/413 (89%)     | 369 (100%)   | 0        | 100         | 100 |
| 5   | g     | 369/413 (89%)     | 369 (100%)   | 0        | 100         | 100 |
| 5   | h     | 369/413 (89%)     | 369 (100%)   | 0        | 100         | 100 |
| 5   | i     | 369/413 (89%)     | 369 (100%)   | 0        | 100         | 100 |
| 5   | j     | 369/413 (89%)     | 369 (100%)   | 0        | 100         | 100 |
| 6   | k     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | l     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | m     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | n     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | o     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | p     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | q     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | r     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | s     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | t     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | u     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| 6   | v     | 374/447 (84%)     | 374 (100%)   | 0        | 100         | 100 |
| All | All   | 10698/11988 (89%) | 10697 (100%) | 1 (0%)   | 100         | 100 |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 39  | GLN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 39  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 51  | ASN  |
| 1   | F     | 42  | GLN  |
| 2   | G     | 86  | ASN  |
| 3   | H     | 38  | GLN  |
| 3   | H     | 42  | ASN  |
| 3   | L     | 42  | ASN  |
| 3   | L     | 191 | HIS  |
| 3   | N     | 38  | GLN  |
| 3   | N     | 42  | ASN  |
| 2   | O     | 51  | ASN  |
| 3   | P     | 191 | HIS  |
| 3   | R     | 42  | ASN  |
| 3   | R     | 224 | ASN  |
| 4   | T     | 52  | GLN  |
| 4   | W     | 52  | GLN  |
| 4   | Y     | 44  | GLN  |
| 3   | d     | 42  | ASN  |
| 5   | e     | 295 | ASN  |
| 5   | g     | 211 | ASN  |
| 5   | g     | 240 | GLN  |
| 5   | h     | 240 | GLN  |
| 5   | j     | 56  | ASN  |
| 5   | j     | 286 | ASN  |
| 6   | o     | 366 | GLN  |
| 6   | p     | 289 | ASN  |
| 6   | q     | 245 | HIS  |
| 6   | r     | 216 | ASN  |
| 6   | r     | 253 | HIS  |
| 6   | r     | 289 | ASN  |
| 6   | u     | 161 | GLN  |
| 6   | u     | 253 | HIS  |
| 6   | v     | 216 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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.

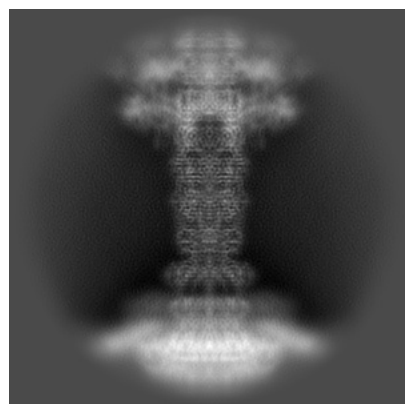
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51198. These allow visual inspection of the internal detail of the map and identification of artifacts.

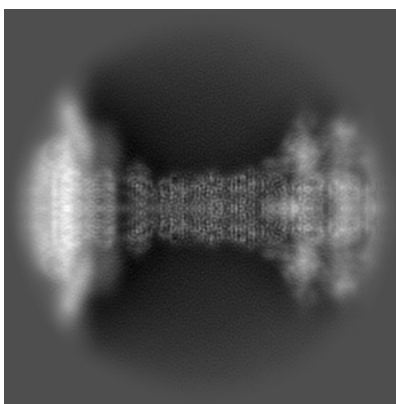
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

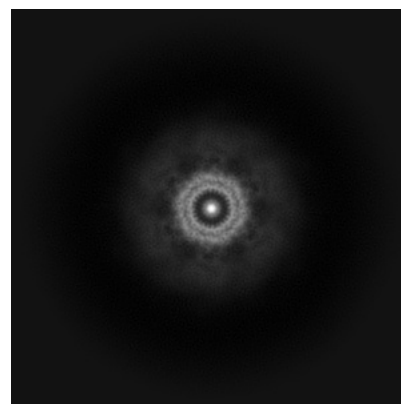
#### 6.1.1 Primary map



X

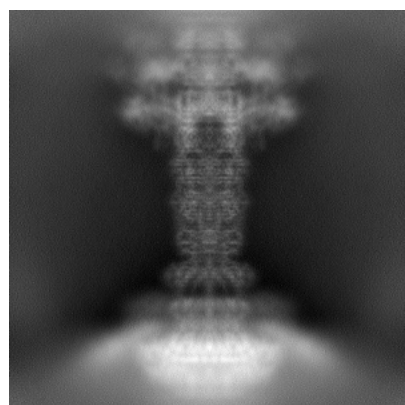


Y

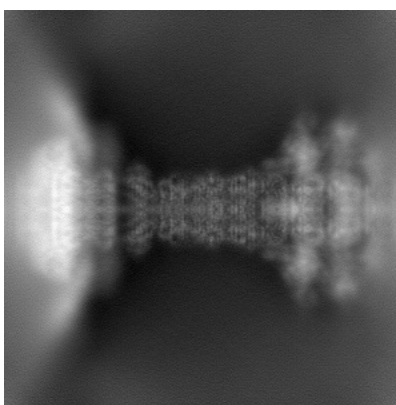


Z

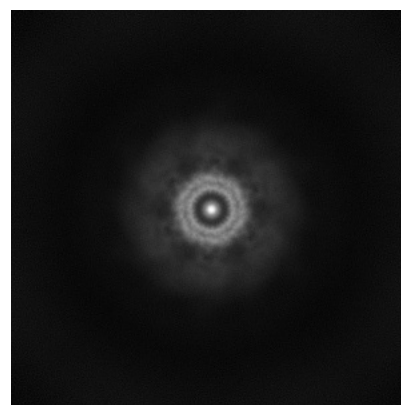
#### 6.1.2 Raw map



X



Y

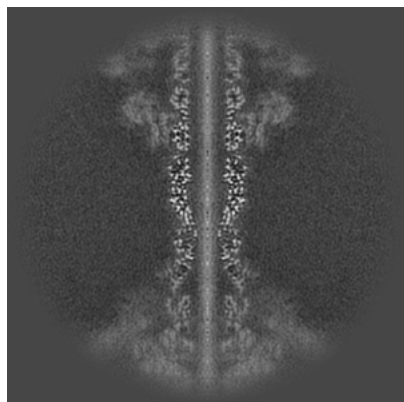


Z

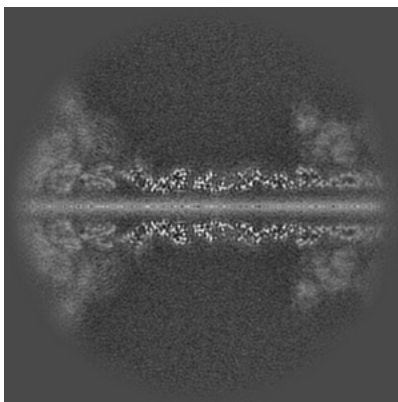
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

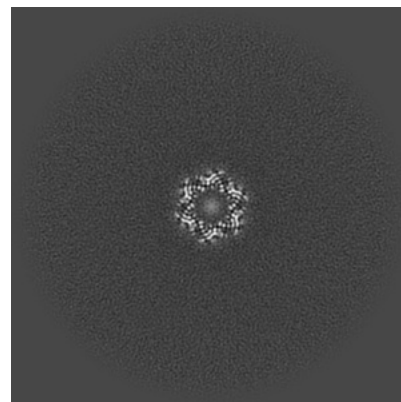
### 6.2.1 Primary map



X Index: 200

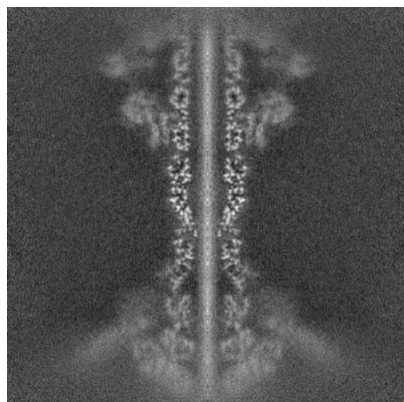


Y Index: 200

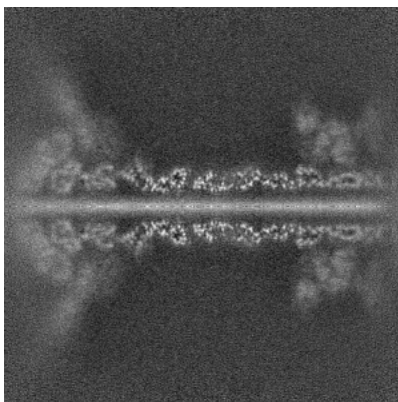


Z Index: 200

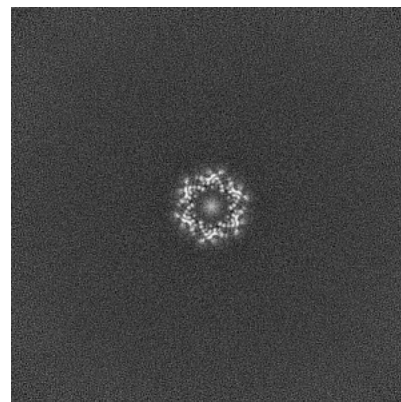
### 6.2.2 Raw map



X Index: 200



Y Index: 200

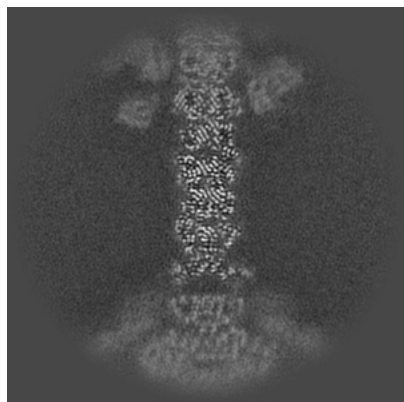


Z Index: 200

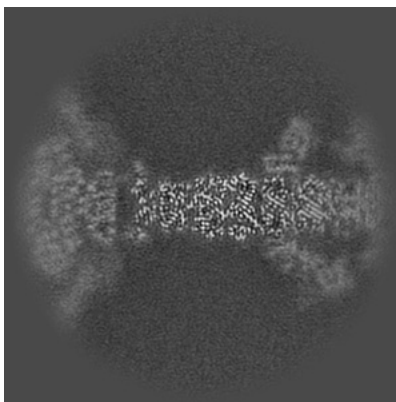
The images above show central slices of the map in three orthogonal directions.

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

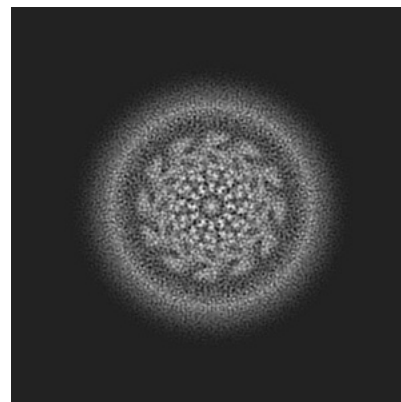
### 6.3.1 Primary map



X Index: 180

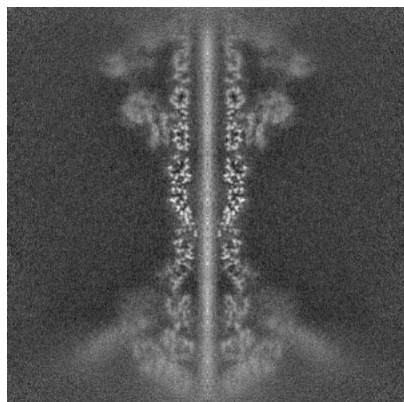


Y Index: 220

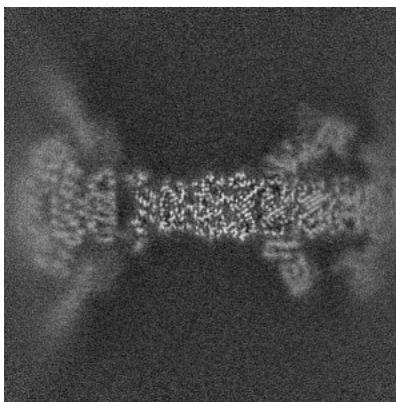


Z Index: 63

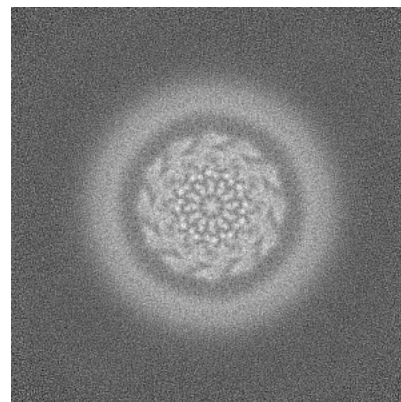
### 6.3.2 Raw map



X Index: 200



Y Index: 180

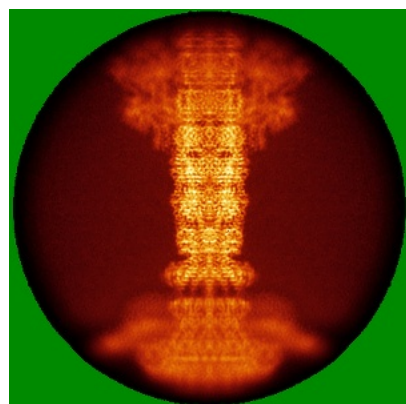


Z Index: 61

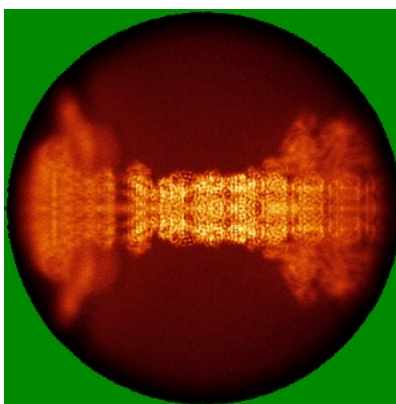
The images above show the largest variance slices of the map in three orthogonal directions.

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

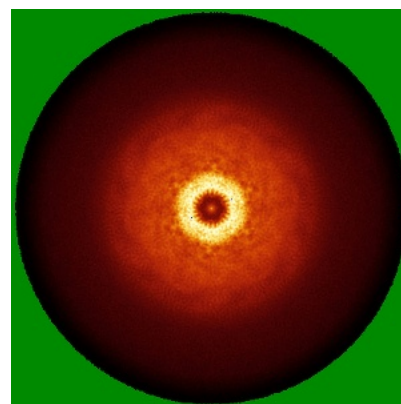
### 6.4.1 Primary map



X

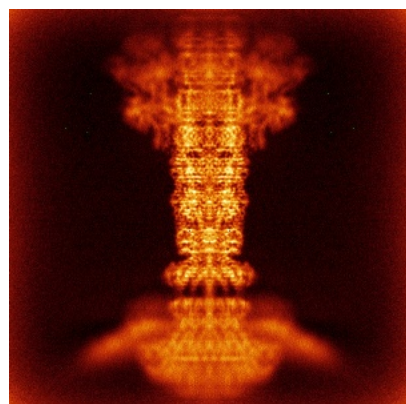


Y

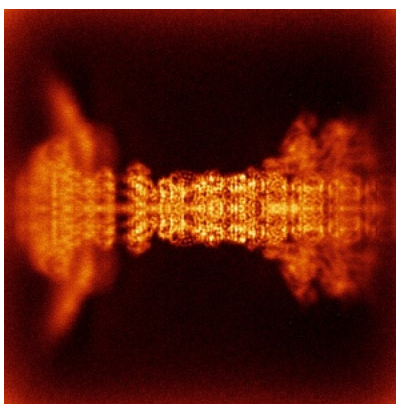


Z

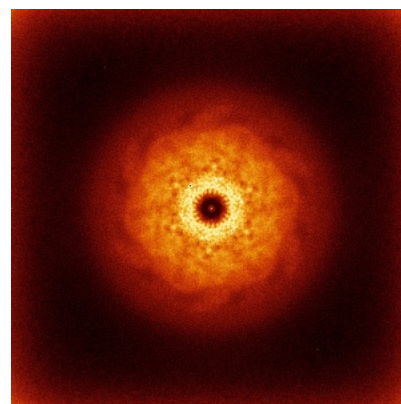
### 6.4.2 Raw map



X



Y

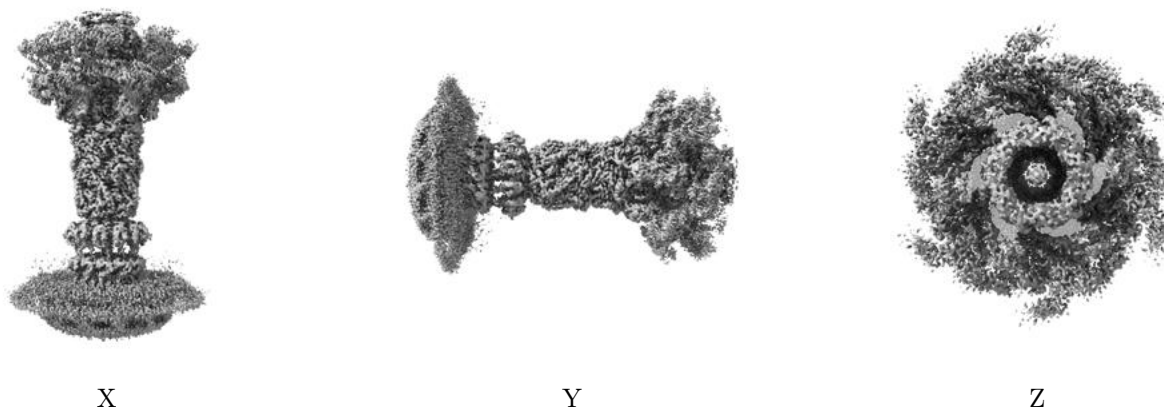


Z

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

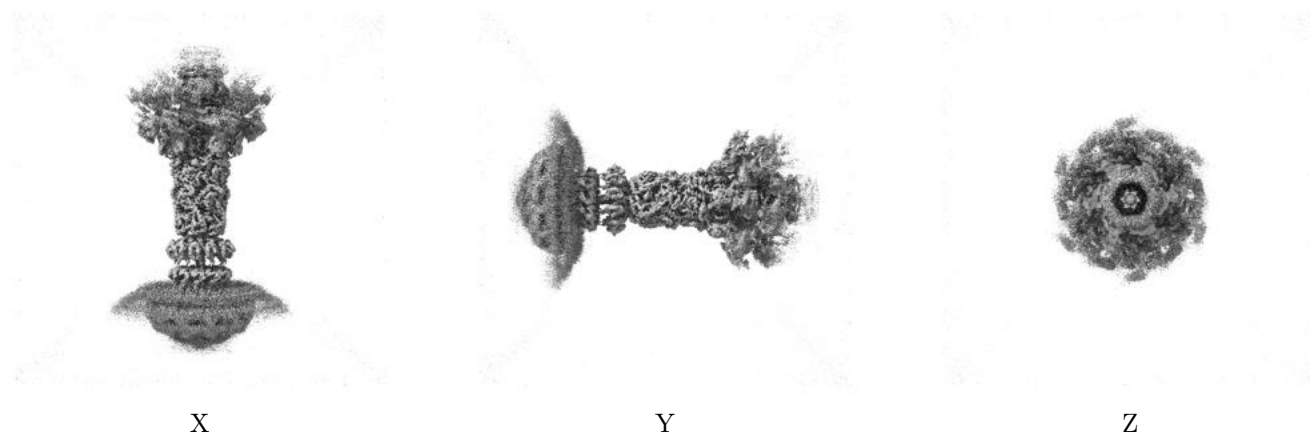
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.249. 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.

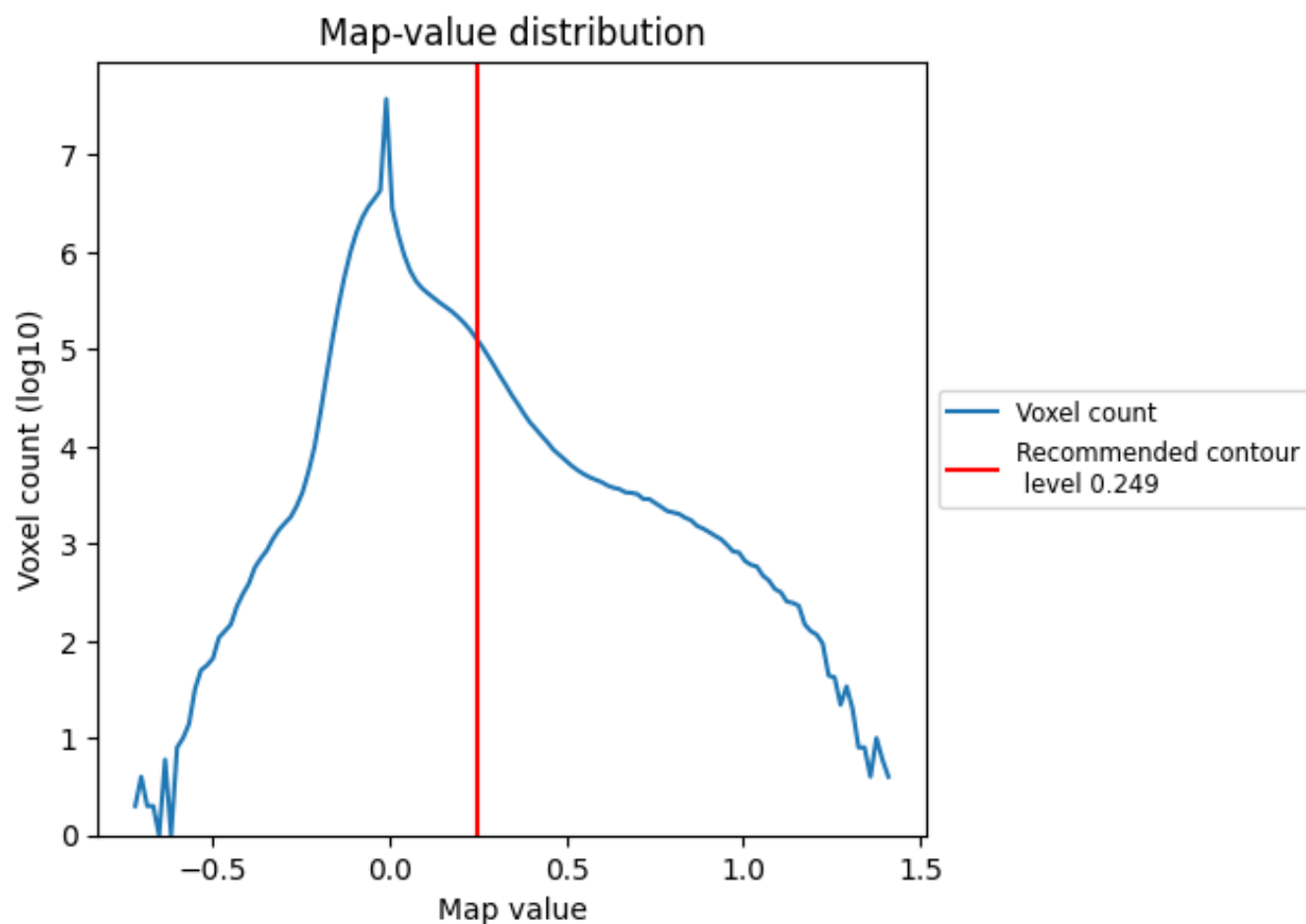
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

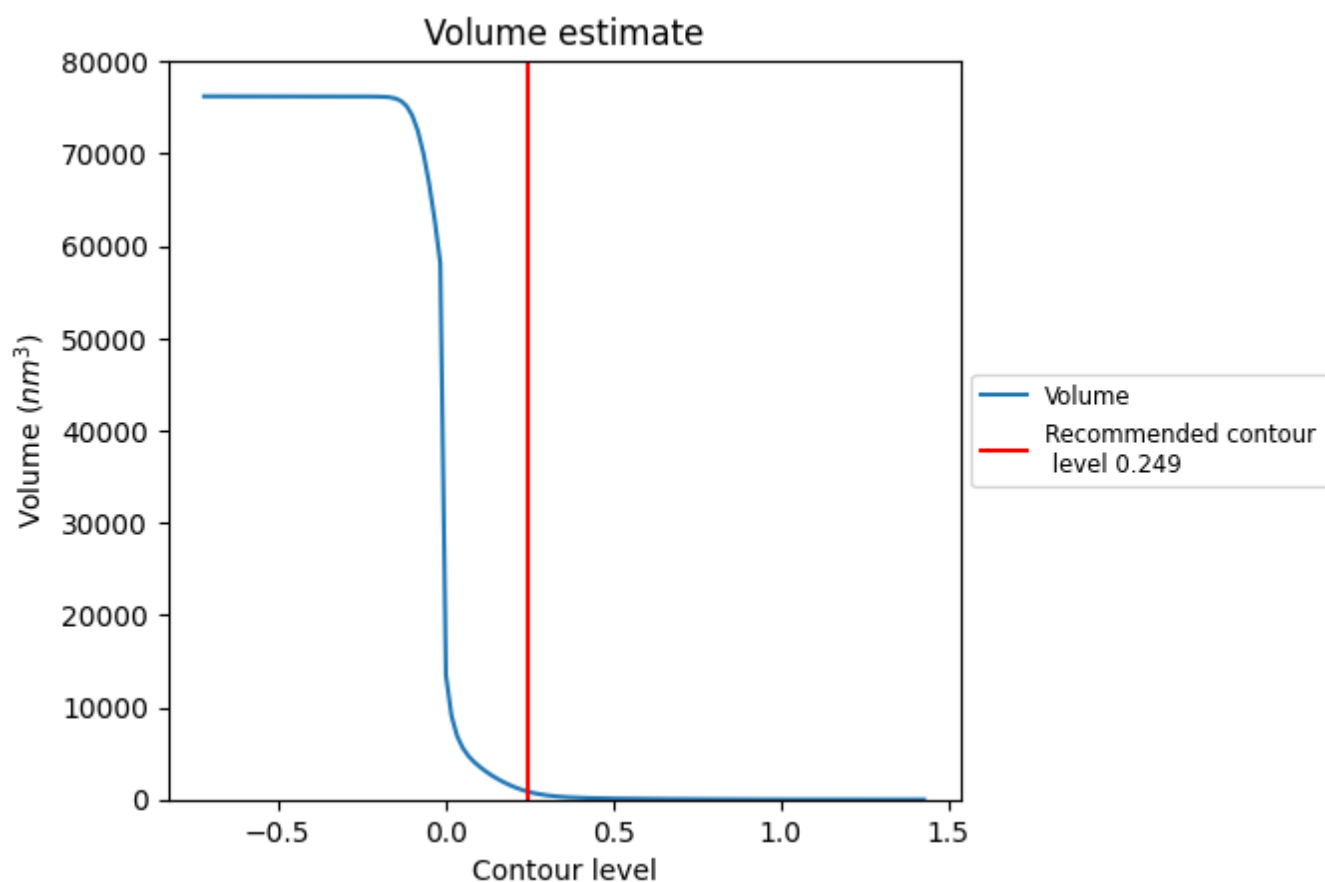
This section contains the results of statistical analysis of the map.

### 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.

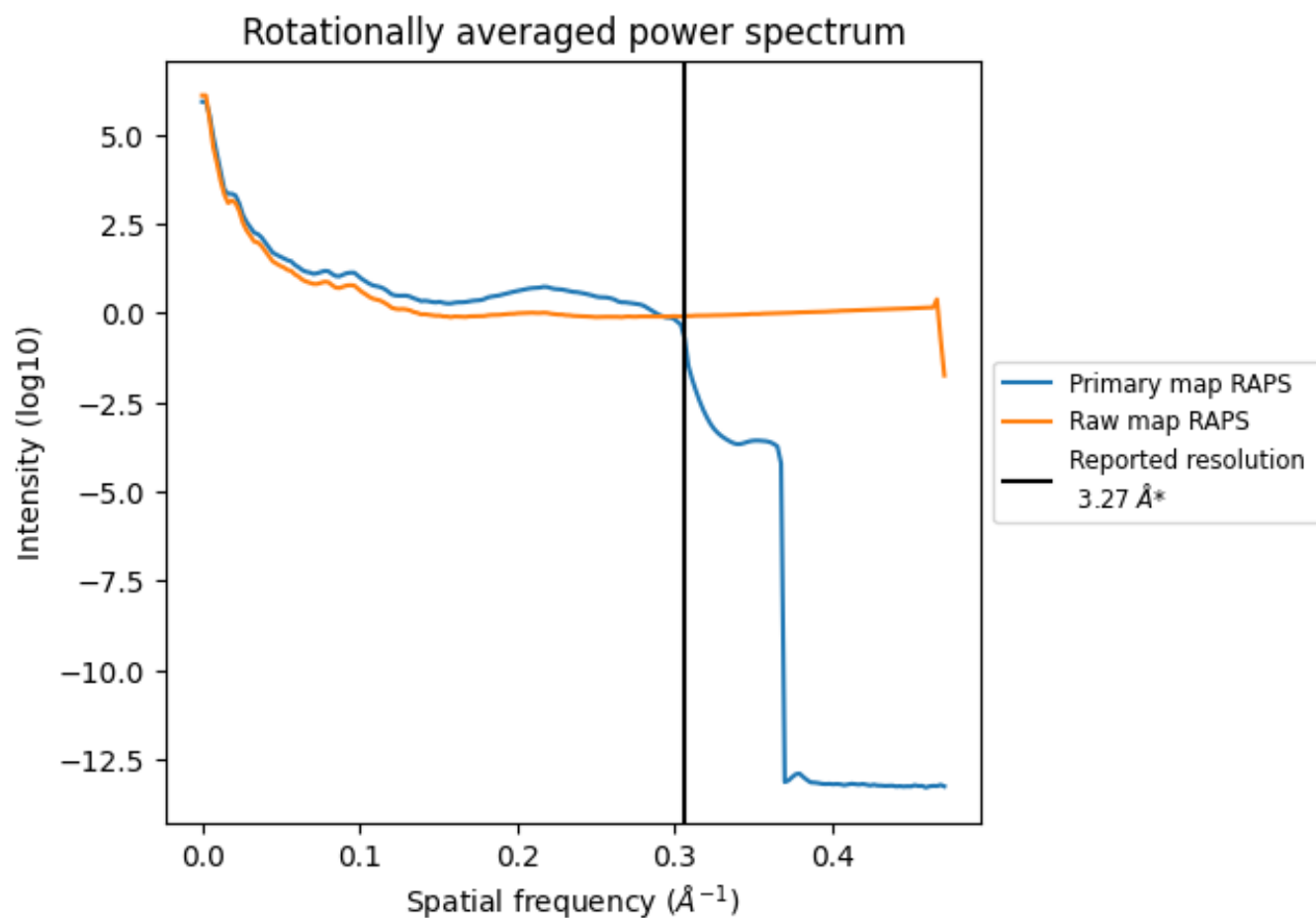
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 839 nm<sup>3</sup>; this corresponds to an approximate mass of 758 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 ⓘ

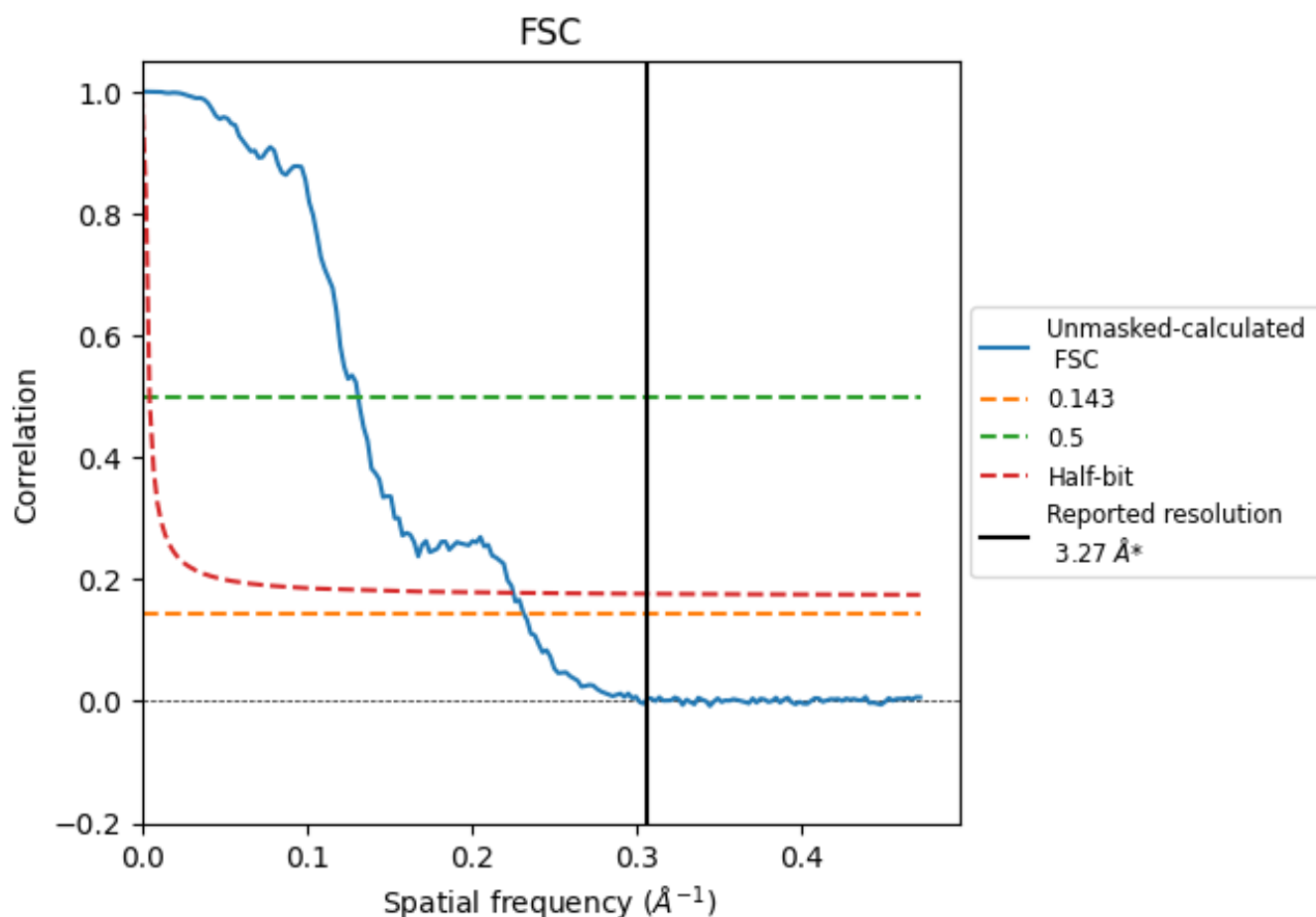


\*Reported resolution corresponds to spatial frequency of 0.306  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.306 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

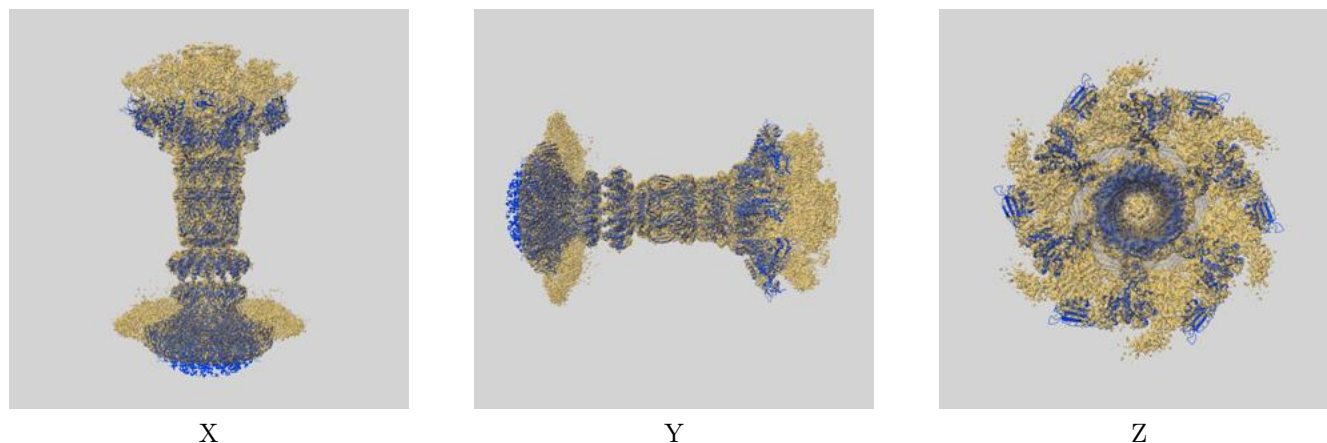
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.27                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.32                               | 7.63 | 4.44     |

\*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 4.32 differs from the reported value 3.27 by more than 10 %

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

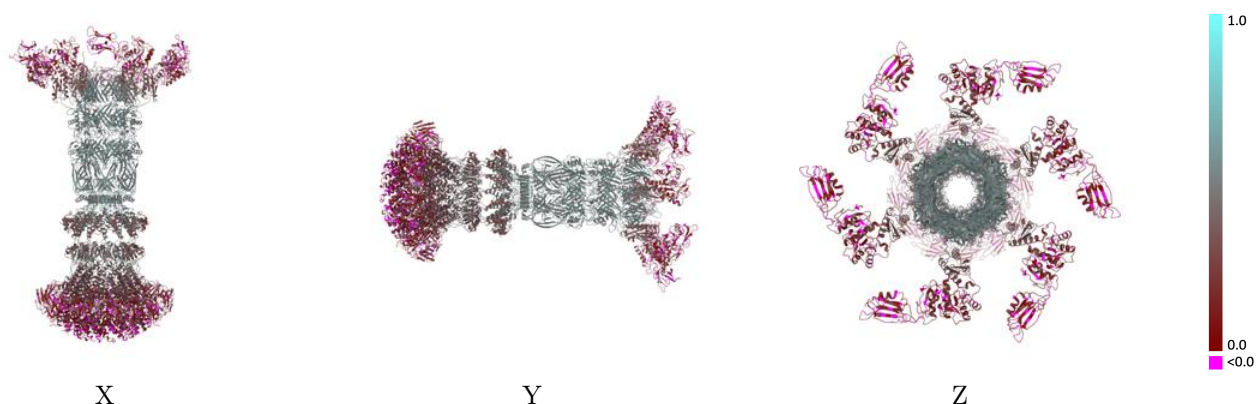
This section contains information regarding the fit between EMDB map EMD-51198 and PDB model 9GB5. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



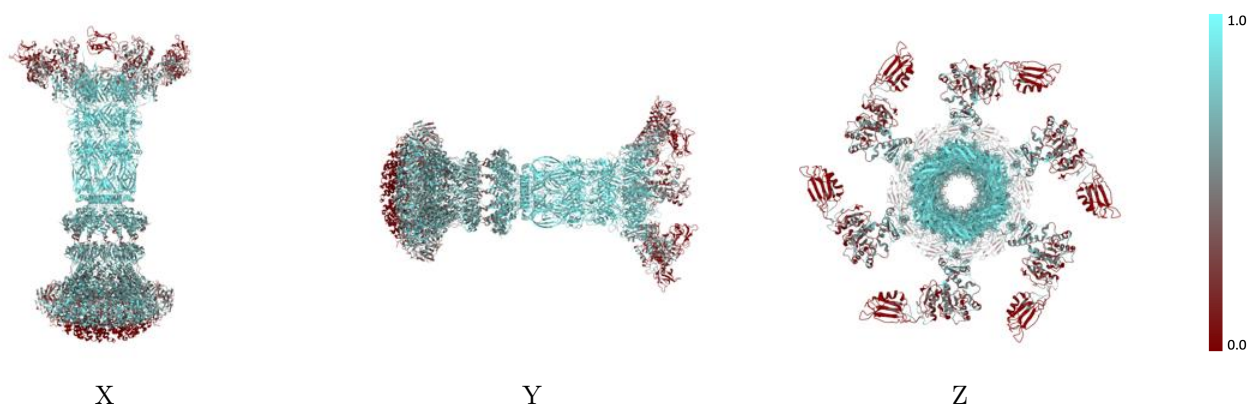
The images above show the 3D surface view of the map at the recommended contour level 0.249 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



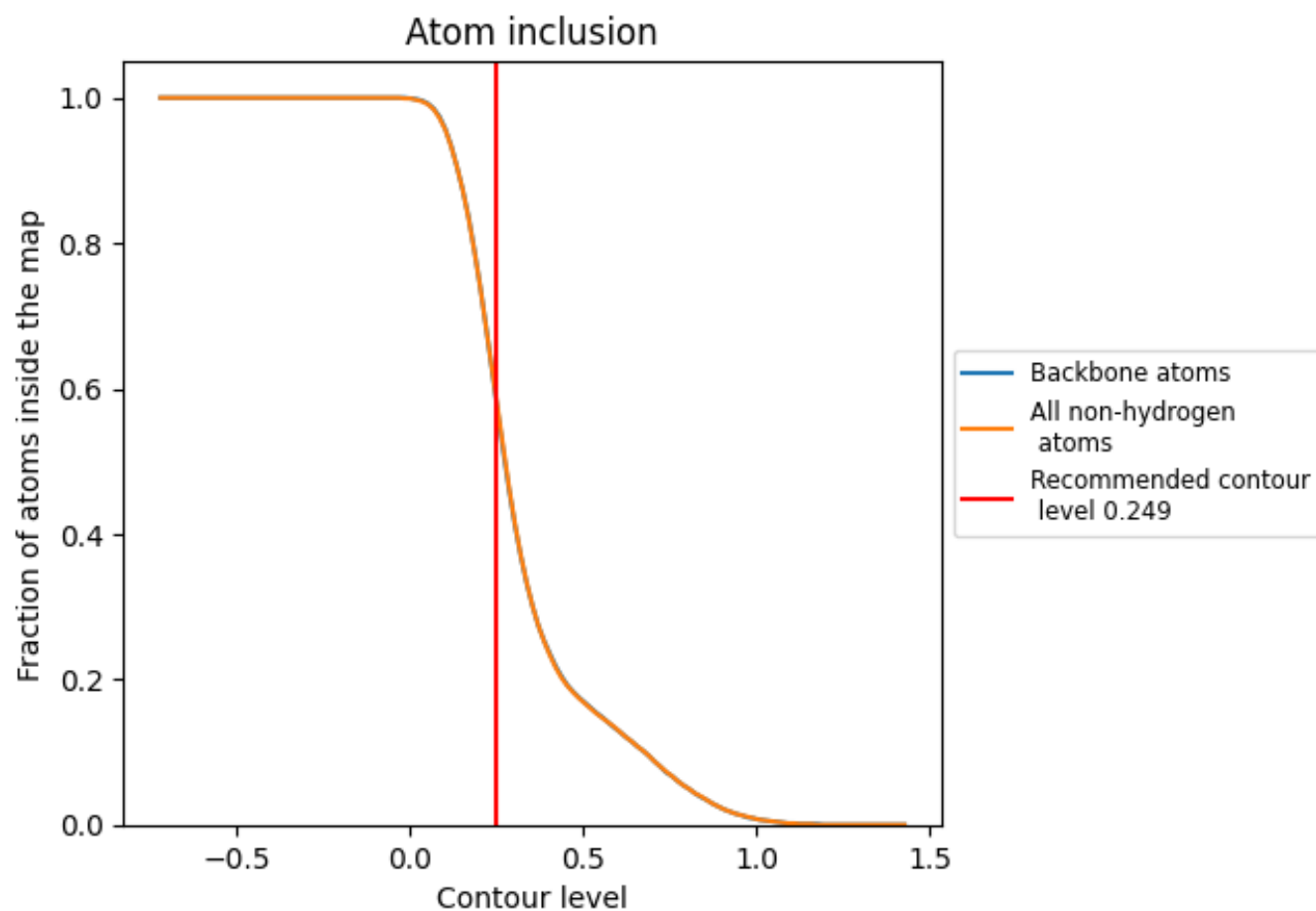
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.249).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 59% 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 (0.249) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.5860   |  0.3200   |
| A     |  0.8190   |  0.5250   |
| B     |  0.8320   |  0.5320   |
| C     |  0.8230   |  0.5290   |
| D     |  0.8250   |  0.5230   |
| E     |  0.8350   |  0.5270   |
| F     |  0.8180   |  0.5290   |
| G     |  0.8550   |  0.5230   |
| H     |  0.8550   |  0.5190   |
| I     |  0.7150   |  0.4490   |
| J     |  0.6660   |  0.4220   |
| K     |  0.8500   |  0.5180   |
| L     |  0.8500   |  0.5210   |
| M     |  0.8530   |  0.5220   |
| N     |  0.8570  |  0.5230  |
| O     |  0.8610 |  0.5220 |
| P     |  0.8520 |  0.5210 |
| Q     |  0.8550 |  0.5180 |
| R     |  0.8510 |  0.5200 |
| S     |  0.6910 |  0.4390 |
| T     |  0.7040 |  0.4420 |
| U     |  0.6980 |  0.4450 |
| V     |  0.6890 |  0.4360 |
| W     |  0.7060 |  0.4460 |
| X     |  0.8600 |  0.5210 |
| Y     |  0.6750 |  0.4260 |
| Z     |  0.6580 |  0.4160 |
| a     |  0.6720 |  0.4270 |
| b     |  0.6660 |  0.4300 |
| c     |  0.6670 |  0.4280 |
| d     |  0.8550 |  0.5220 |
| e     |  0.3170 |  0.1920 |
| f     |  0.3210 |  0.1960 |
| g     |  0.3150 |  0.1900 |
| h     |  0.3140 |  0.1900 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| i     |  0.3150 |  0.1890 |
| j     |  0.3210 |  0.1910 |
| k     |  0.5520 |  0.2370 |
| l     |  0.5300 |  0.2210 |
| m     |  0.5570 |  0.2350 |
| n     |  0.5340 |  0.2250 |
| o     |  0.5530 |  0.2360 |
| p     |  0.5320 |  0.2230 |
| q     |  0.5540 |  0.2340 |
| r     |  0.5360 |  0.2230 |
| s     |  0.5520 |  0.2370 |
| t     |  0.5370 |  0.2260 |
| u     |  0.5540 |  0.2350 |
| v     |  0.5330 |  0.2240 |