



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:12 PM UTC

PDB ID : 6PEM / pdb\_00006pem  
EMDB ID : EMD-20316  
Title : Focussed refinement of InvGN0N1:SpaPQR:PrgHK from Salmonella SPI-1  
injectisome NC-base  
Authors : Hu, J.; Worrall, L.J.; Strynadka, N.C.J.  
Deposited on : 2019-06-20  
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

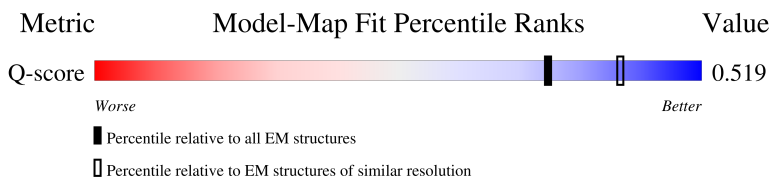
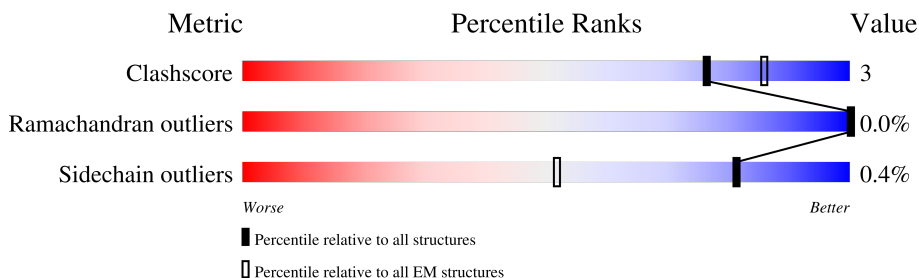
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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                       | 13950 ( 3.00 - 4.00 )                                    |

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   | AA    | 252    |  |
| 1   | AB    | 252    |  |
| 1   | AC    | 252    |  |
| 1   | AD    | 252    |  |

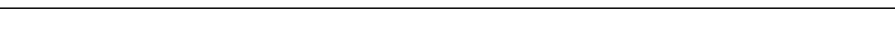
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AE    | 252    |                  |
| 1   | AF    | 252    |                  |
| 1   | AG    | 252    |                  |
| 1   | AH    | 252    |                  |
| 1   | AI    | 252    |                  |
| 1   | AJ    | 252    |                  |
| 1   | AK    | 252    |                  |
| 1   | AL    | 252    |                  |
| 1   | o     | 252    |                  |
| 1   | p     | 252    |                  |
| 1   | q     | 252    |                  |
| 1   | r     | 252    |                  |
| 1   | s     | 252    |                  |
| 1   | t     | 252    |                  |
| 1   | u     | 252    |                  |
| 1   | v     | 252    |                  |
| 1   | w     | 252    |                  |
| 1   | x     | 252    |                  |
| 1   | y     | 252    |                  |
| 1   | z     | 252    |                  |
| 2   | 0     | 224    |                  |
| 2   | 1     | 224    |                  |
| 2   | 2     | 224    |                  |
| 2   | 3     | 224    |                  |
| 2   | 4     | 224    |                  |

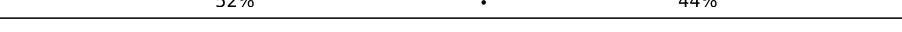
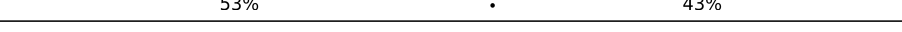
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 3   | 5     | 263    |    |
| 4   | 6     | 86     |    |
| 4   | 7     | 86     |    |
| 4   | 8     | 86     |    |
| 4   | 9     | 86     |    |
| 5   | A     | 562    |    |
| 5   | B     | 562    |    |
| 5   | C     | 562    |    |
| 5   | D     | 562    |    |
| 5   | F     | 562    |    |
| 5   | G     | 562    |    |
| 5   | H     | 562    |    |
| 5   | I     | 562    |  |
| 5   | J     | 562    |  |
| 5   | K     | 562    |  |
| 5   | L     | 562    |  |
| 5   | M     | 562    |  |
| 5   | N     | 562    |  |
| 5   | O     | 562    |  |
| 5   | P     | 562    |  |
| 5   | Q     | 562    |  |
| 6   | E     | 392    |  |
| 6   | R     | 392    |  |
| 6   | S     | 392    |  |
| 6   | T     | 392    |  |

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| Mol | Chain | Length | Quality of chain                                                                              |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 6   | U     | 392    |  51%6%44%   |
| 6   | V     | 392    |  53%.43%    |
| 6   | W     | 392    |  53%.43%    |
| 6   | X     | 392    |  50%7%44%   |
| 6   | Y     | 392    |  50%7%43%   |
| 6   | Z     | 392    |  53%.43%    |
| 6   | a     | 392    |  52%.44%    |
| 6   | b     | 392    |  53%.43%    |
| 6   | c     | 392    |  49%7%43%   |
| 6   | d     | 392    |  51%6%44%   |
| 6   | e     | 392    |  54%.43%    |
| 6   | f     | 392    |  53%.43%    |
| 6   | g     | 392    |  52%.44%  |
| 6   | h     | 392    |  53%.43%  |
| 6   | i     | 392    |  54%.43%  |
| 6   | j     | 392    |  52%.44%  |
| 6   | k     | 392    |  53%.43%  |
| 6   | l     | 392    |  51%6%43% |
| 6   | m     | 392    |  53%.44%  |
| 6   | n     | 392    |  51%5%43% |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 108033 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lipoprotein PrgK.

| Mol | Chain | Residues | Atoms         |          |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|-------|
| 1   | AA    | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | AB    | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | AC    | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | AD    | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | AE    | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | AF    | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | AG    | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | AH    | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | AI    | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | AL    | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | o     | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | p     | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | q     | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | r     | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | s     | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | t     | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |
| 1   | u     | 184      | Total<br>1431 | C<br>901 | N<br>250 | O<br>277 | S<br>3 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | v     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1431  | 901 | 250 | 277 | 3 |         |       |
| 1   | w     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1431  | 901 | 250 | 277 | 3 |         |       |
| 1   | x     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1431  | 901 | 250 | 277 | 3 |         |       |
| 1   | y     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1431  | 901 | 250 | 277 | 3 |         |       |
| 1   | z     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1431  | 901 | 250 | 277 | 3 |         |       |
| 1   | AJ    | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1431  | 901 | 250 | 277 | 3 |         |       |
| 1   | AK    | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1431  | 901 | 250 | 277 | 3 |         |       |

- Molecule 2 is a protein called Surface presentation of antigens protein SpaP.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | 0     | 189      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1468  | 982  | 219 | 256 | 11 |         |       |
| 2   | 1     | 189      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1475  | 988  | 220 | 256 | 11 |         |       |
| 2   | 2     | 187      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1464  | 981  | 219 | 253 | 11 |         |       |
| 2   | 3     | 194      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1520  | 1016 | 227 | 266 | 11 |         |       |
| 2   | 4     | 211      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 1672  | 1108 | 255 | 298 | 11 |         |       |

- Molecule 3 is a protein called Surface presentation of antigens protein SpaR.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | 5     | 228      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1718  | 1136 | 276 | 293 | 13 |         |       |

- Molecule 4 is a protein called Surface presentation of antigens protein SpaQ.

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 4   | 6     | 53       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 405   | 276 | 61 | 67  | 1 |         |       |
| 4   | 7     | 84       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 644   | 436 | 97 | 109 | 2 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 4   | 8     | 84       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 644   | 436 | 97 | 109 | 2 |         |       |
| 4   | 9     | 84       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 647   | 438 | 97 | 109 | 3 |         |       |

- Molecule 5 is a protein called Protein InvG.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | A     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 5   | B     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |
| 5   | C     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 5   | D     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1146  | 736 | 195 | 209 | 6 |         |       |
| 5   | F     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 5   | G     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |
| 5   | H     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 5   | I     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |
| 5   | J     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 5   | K     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |
| 5   | L     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 5   | M     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1146  | 736 | 195 | 209 | 6 |         |       |
| 5   | N     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 5   | O     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |
| 5   | P     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 5   | Q     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |

- Molecule 6 is a protein called Protein PrgH.



| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | E     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1836  | 1170 | 326 | 335 | 5 |         |       |
| 6   | R     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1827  | 1164 | 325 | 333 | 5 |         |       |
| 6   | S     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1831  | 1167 | 326 | 333 | 5 |         |       |
| 6   | T     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1836  | 1170 | 326 | 335 | 5 |         |       |
| 6   | U     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1827  | 1164 | 325 | 333 | 5 |         |       |
| 6   | V     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1831  | 1167 | 326 | 333 | 5 |         |       |
| 6   | W     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1836  | 1170 | 326 | 335 | 5 |         |       |
| 6   | X     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1827  | 1164 | 325 | 333 | 5 |         |       |
| 6   | Y     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1831  | 1167 | 326 | 333 | 5 |         |       |
| 6   | Z     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1836  | 1170 | 326 | 335 | 5 |         |       |
| 6   | a     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1827  | 1164 | 325 | 333 | 5 |         |       |
| 6   | b     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1831  | 1167 | 326 | 333 | 5 |         |       |
| 6   | c     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1836  | 1170 | 326 | 335 | 5 |         |       |
| 6   | d     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1827  | 1164 | 325 | 333 | 5 |         |       |
| 6   | e     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1831  | 1167 | 326 | 333 | 5 |         |       |
| 6   | f     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1836  | 1170 | 326 | 335 | 5 |         |       |
| 6   | g     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1827  | 1164 | 325 | 333 | 5 |         |       |
| 6   | h     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1831  | 1167 | 326 | 333 | 5 |         |       |
| 6   | i     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1836  | 1170 | 326 | 335 | 5 |         |       |
| 6   | j     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1827  | 1164 | 325 | 333 | 5 |         |       |
| 6   | k     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1831  | 1167 | 326 | 333 | 5 |         |       |
| 6   | l     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1836  | 1170 | 326 | 335 | 5 |         |       |

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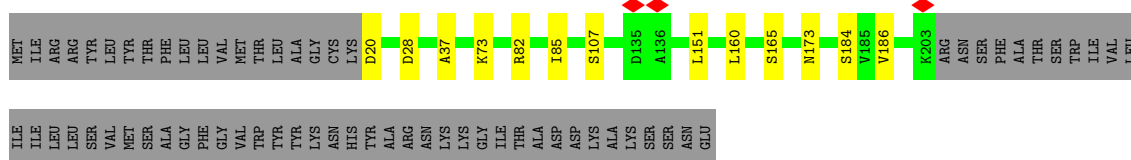
| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | m     | 221      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1827  | 1164 | 325 | 333 | 5 |         |       |
| 6   | n     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1831  | 1167 | 326 | 333 | 5 |         |       |

### 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.

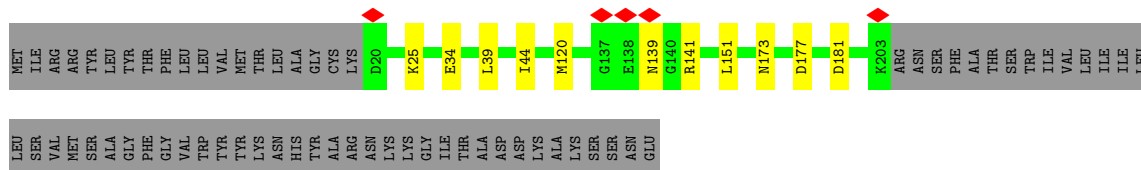
- Molecule 1: Lipoprotein PrgK

Chain AA: 



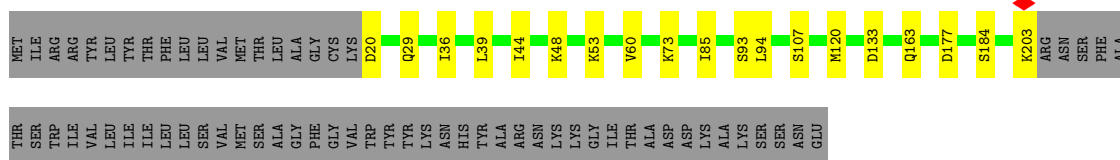
- Molecule 1: Lipoprotein PrgK

Chain AB: 



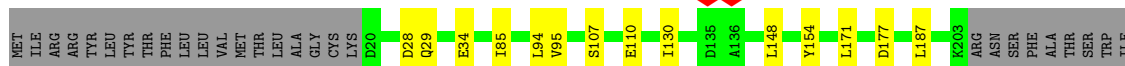
- Molecule 1: Lipoprotein PrgK

Chain AC: 



- Molecule 1: Lipoprotein PrgK

Chain AD: 



VAL  
LEU  
ILE  
ILE  
ARG  
LEU  
LEU  
SER  
VAL  
MET  
SER  
ALA  
PHE  
GLY  
TRP  
TRP  
TYR  
TYR  
LYS  
ASN  
HIS  
TYR  
ALA  
ARG  
ASN  
LYS  
LYS  
GLY  
ILE  
THR  
ALA  
ASP  
LYS  
ALA  
LYS  
SER  
SER  
ASN  
GLU

• Molecule 1: Lipoprotein PrgK



MET  
ILE  
ARG  
ALA  
GLY  
PHE  
TYR  
VAL  
TRP  
TYR  
PHE  
LEU  
LEU  
VAL  
MET  
THR  
ALA  
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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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• Molecule 1: Lipoprotein PrgK



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● Molecule 1: Lipoprotein PrgK



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● Molecule 1: Lipoprotein PrgK



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● Molecule 1: Lipoprotein PrgK



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● Molecule 1: Lipoprotein PrgK



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● Molecule 1: Lipoprotein PrgK



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SER TRP ILE VAL LEU ILE LEU LEU SER MET MET SER ALA GLY PHE LEU VAL CYS LYS TRP TYR TYR LYS ASN HIS TVR ARG ALA ASN LYS LYS ASP ASP ALA LYS LYS ASN ASN GLU

• Molecule 1: Lipoprotein PrgK

Chain x:



MET ILE ARG ARG VAL TYR TYR THR PHE LEU LEU VAL MET THR ALA GLY PHE LEU VAL MET THR TYR TYR LYS ALA GLY ASN CYS LYS D20 Q31 E34 P78 P79 L117 V123 A136 V146 L151 R169 N173 D177 V178 D179 Y180 K203 ARG ASN SER PHE ALA THR THR SER TRP ILE VAL ILE

ILE LEU LEU SER VAL MET SER ALA GLY PHE LEU VAL MET THR TYR TYR LYS ALA GLY ASN CYS LYS TRP TYR TYR LYS ALA GLY ASN GLU

• Molecule 1: Lipoprotein PrgK

Chain y:



MET ILE ARG ARG TYR TYR THR PHE LEU LEU VAL MET THR TYR TYR LYS D20 K21 D22 L23 M43 E62 A68 P78 P79 M120 D135 E138 M139 R141 K172 V178 D179 S184 K203 ARG ASN SER PHE ALA THR THR SER TRP ILE VAL

LEU ILE ILE LEU LEU VAL MET THR PHE LEU VAL MET THR TYR TYR LYS ALA GLY ASN CYS LYS TRP TYR TYR LYS ALA GLY ASN GLU

• Molecule 1: Lipoprotein PrgK

Chain z:



MET ILE ARG ARG TYR TYR THR PHE LEU LEU VAL MET THR TYR TYR LYS D20 K21 L39 L44 E62 V69 N173 S174 D177 Y180 S184 K203 ARG ASN SER PHE ALA THR THR SER TRP ILE VAL LEU ILE ILE LEU LEU LEU VAL MET SER ALA

GLY PHE GLY VAL TYR TYR LYS ASN HIS LEU VAL MET THR TYR TYR LYS ALA GLY PHE LEU VAL MET THR TYR TYR LYS ALA GLY ASN GLU

• Molecule 1: Lipoprotein PrgK

Chain AJ:



MET ILE ARG ARG TYR TYR THR PHE LEU LEU VAL MET THR TYR TYR LYS D20 I36 A37 V38 L39 I44 K48 I49 D50 S51 K73 R99 K102 E110 Q111 R112 I134 G137 E138 Q163 I164 S165 N173 D177 S184 V185 K203

ARG ASN SER PHE ALA SER TRP ILE LEU VAL MET THR TYR TYR LYS ASN HIS TVR ARG ALA ASN LYS LYS GLY ILE THR ALA ASP ASP LYS LYS SER SER ASN GLU

• Molecule 1: Lipoprotein PrgK

Chain AK:

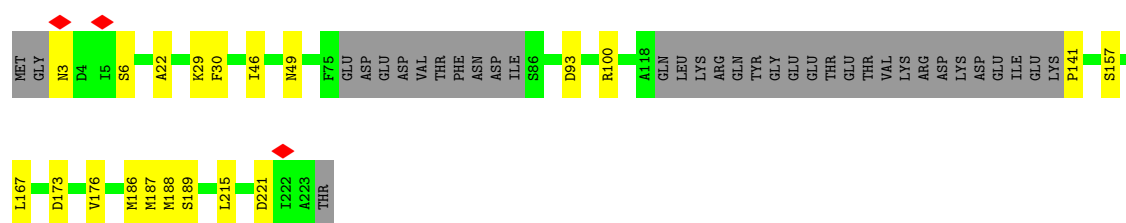


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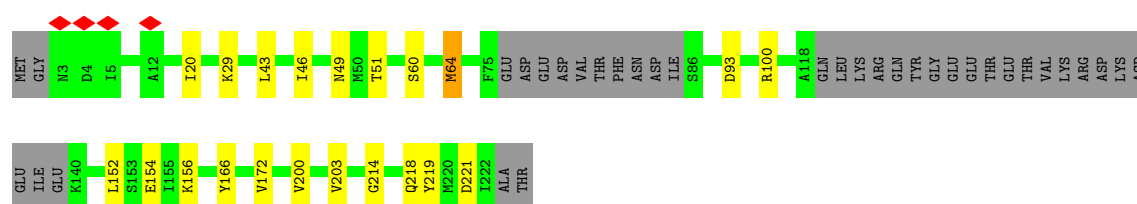
• Molecule 2: Surface presentation of antigens protein SpaP

Chain 0: 



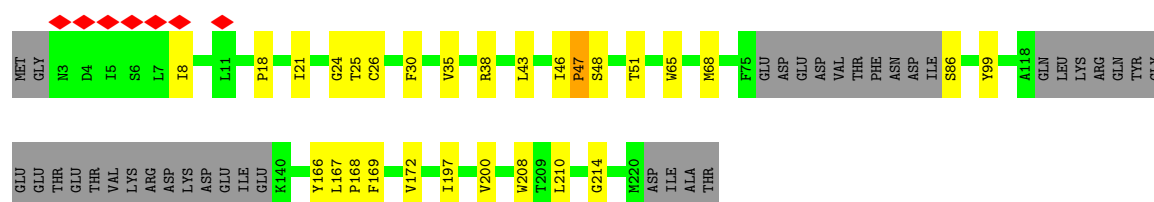
• Molecule 2: Surface presentation of antigens protein SpaP

Chain 1: 



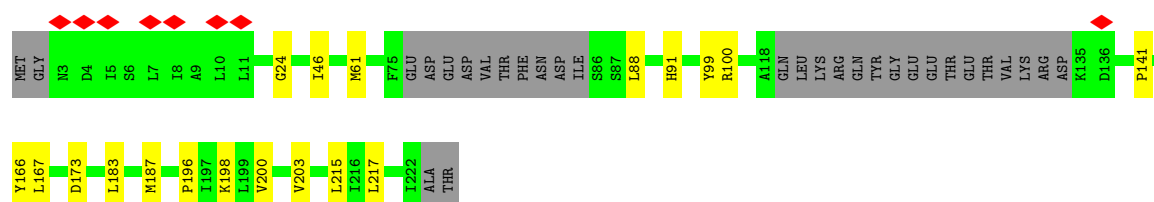
• Molecule 2: Surface presentation of antigens protein SpaP

Chain 2: 

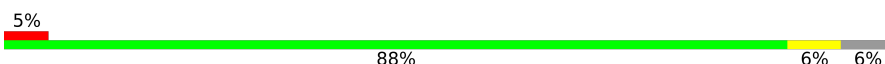


• Molecule 2: Surface presentation of antigens protein SpaP

Chain 3: 



• Molecule 2: Surface presentation of antigens protein SpaP

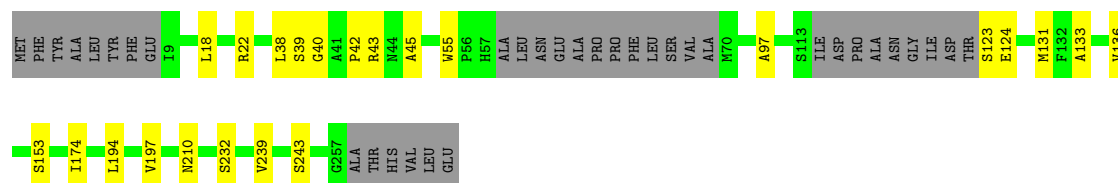
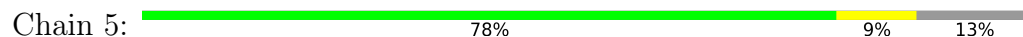
Chain 4: 



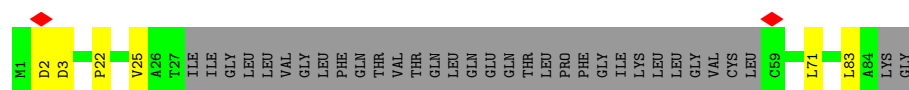




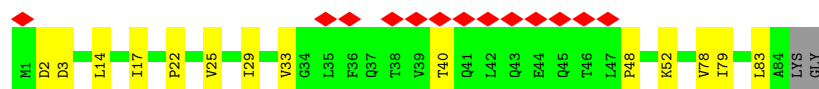
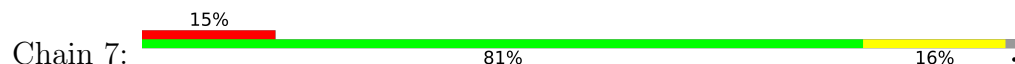
- Molecule 3: Surface presentation of antigens protein SpaR



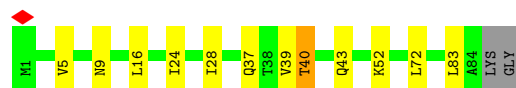
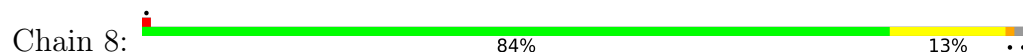
- Molecule 4: Surface presentation of antigens protein SpaQ



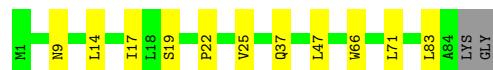
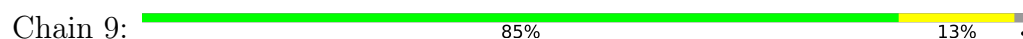
- Molecule 4: Surface presentation of antigens protein SpaQ



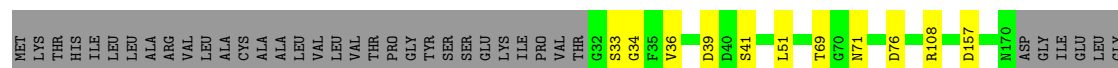
- Molecule 4: Surface presentation of antigens protein SpaQ



- Molecule 4: Surface presentation of antigens protein SpaQ



- Molecule 5: Protein InvG



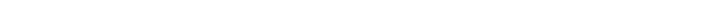
[illegible]

- Molecule 5: Protein InvG

Chain B:  23% 74%

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| TRP | THR | GLY | GLU | ALA | GLY | ILE | GLY | ILE | MET  |
| THR | THR | GLN | GLU | ALA | GLY | GLY | LYS | GLY | LYS  |
| GLY | GLN | ILE | GLY | ARG | VAL | VAL | HIS | VAL | THR  |
| ASP | ILE | MET | GLN | HIS | VAL | LYS | ARG | ARG | ILE  |
| LYS | PRO | SER | ALA | GLU | ALA | ALA | LEU | LEU | LEU  |
| LEU | PHE | LEU | THR | LEU | LEU | ALA | ASN | ASN | LEU  |
| GLN | LEU | ASP | THR | SER | SER | ASN | ASN | ALA | LEU  |
| LYS | GLY | ILE | VAL | LEU | THR | TYR | THR | VAL | VAL  |
| TRP | LYS | GLU | SER | TRP | ALA | GLY | PHE | ARG | VAL  |
| VAL | LEU | ASP | ARG | ILE | GLY | GLY | VAL | LEU | LEU  |
| ARG | PRO | GLY | PRO | VAL | VAL | GLY | ASP | ALA | ALA  |
| VAL | LEU | GLY | VAL | ASP | VAL | MET | GLY | CYS | LYS  |
| THR | ILE | ASP | LEU | VAL | LEU | SER | SER | THR | GLY  |
| LEU | GLY | LYS | LEU | ASN | THR | LEU | ARG | ALA | ALA  |
| ASP | SER | THR | THR | ASN | LYS | GLN | TYR | THR | LEU  |
| ARG | LEU | PRO | GLN | SER | ALA | GLU | ASN | VAL | VAL  |
| GLY | PHE | GLN | GLU | ASP | LEU | LEU | LEU | LEU | LEU  |
| GLN | ARG | ASN | ASN | LEU | ARG | ARG | ARG | ARG | VAL  |
| GLU | TYR | ASP | VAL | GLY | LYS | ASP | THR | THR | THR  |
| ALA | SER | THR | PRO | ARG | GLN | GLN | GLN | PRO | PRO  |
| ILE | SER | THR | ALA | LEU | ASN | LYS | LYS | GLY | GLY  |
| ILE | LYS | THR | ILE | GLY | GLY | ALA | MET | THR | THR  |
| LYS | ASN | SER | PHE | THR | ALA | ALA | VAL | SER | SER  |
|     | LYS | VAL | ASP | SER | ALA | ALA | ALA | ILE | ILE  |
|     | ASN | ASN | ASP | SER | GLY | GLY | GLY | GLY | GLY  |
|     | VAL | VAL | LEU | GLY | ILE | ILE | ASP | PRO | K27  |
|     | VAL | PRO | THR | SER | LYS | ILE | LEU | LEU | V36  |
|     | ARG | GLU | PHE | ILE | THR | ILE | THR | THR | L42  |
|     | PHE | GLY | THR | THR | VAL | ALA | ALA | ILE | K66  |
|     | MET | THR | LYS | ILE | GLY | TYR | GLU | GLU | D76  |
|     | ILE | THR | THR | ASP | ASP | ARG | ARG | ARG | P77  |
|     | GLU | LEU | ILE | LEU | LEU | ASP | LEU | LEU | Q87  |
|     | PRO | ILE | GLY | LYS | GLY | ASN | GLN | GLN | N109 |
|     | VAL | THR | GLY | LEU | VAL | LEU | GLU | GLU | L114 |
|     | ASP | ARG | ALA | ASN | VAL | VAL | GLN | PRO | R115 |
|     | PRO | VAL | LEU | GLN | LEU | GLY | LYS | GLY | N116 |
|     | THR | HIS | GLU | SER | THR | THR | ALA | LEU | V117 |
|     | PRO | GLY | VAL | ILE | ILE | ALA | ASN | ASN | D141 |
|     | ASP | LYS | THR | THR | LYS | ILE | VAL | VAL | K144 |
|     | ALA | SER | TYR | THR | GLN | VAL | SER | SER | N170 |
|     | SER | LEU | GLY | GLY | VAL | HIS | SER | ASP | ASP  |
|     | GLU | LEU | THR | ASP | THR | ILE | GLU | PRO | GLY  |
|     | VAL | VAL | MET | GLY | PHE | GLY | GLU | PRO | ILE  |
|     | ASN | GLY | ARG | ARG | GLY | MET | GLY | PRO | GLY  |
|     | ASN | TYR | VAL | PHE | THR | LEU | GLY | GLY | GLY  |
|     | ILE | THR | LEU | ILE | THR | VAL | ALA | ALA | GLY  |
|     | LEU | ARG | PRO | THR | ARG | VAL | VAL | ALA | GLY  |
|     | LYS | ASP | ARG | LYS | PHE | ALA | ALA | ALA | GLY  |
|     | GLN | ALA | PHE | VAL | VAL | ASN | SER | SER | GLY  |
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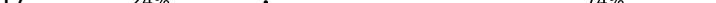
- Molecule 5: Protein InvG

Chain C:  23% 1% 75%

[illegible]

[illegible]

- Molecule 5: Protein InvG

Chain D:  24% . 74%

|     |     |     |     |     |     |     |      |
|-----|-----|-----|-----|-----|-----|-----|------|
| LYS | PRO | SER | ALA | GLU | ALA | LEU | MET  |
| LEU | PHE | LEU | THR | THR | ALA | ASN | THR  |
| GLN | LEU | ASP | VAL | SER | ASN | ASN | LYS  |
| LYS | GLY | ILE | VAL | ILE | VAL | THR | HIS  |
| TRP | LYS | GLU | SER | TRP | ALA | PHE | ILE  |
| VAL | LEU | ASP | ARG | VAL | GLY | VAL | LEU  |
| ARG | PRO | GLY | PRO | VAL | GLY | GLY | LEU  |
| VAL | LEU | ASN | VAL | ASP | MET | ASP | ALA  |
| TYR | ILE | ASP | LEU | LEU | SER | ARG | ARG  |
| LEU | GLY | LYS | LEU | ASN | LEU | THR | VAL  |
| ASP | SER | THR | THR | LYS | GLN | TYR | LEU  |
| ARG | LEU | PRO | GLN | SER | GLU | ASN | ALA  |
| GLY | PHE | GLN | GLU | ASP | ALA | LEU | CYS  |
| GLN | ARG | SER | ASN | GLU | LEU | ARG | ALA  |
| GLU | TYR | ASP | VAL | GLU | LYS | ASP | ALA  |
| ALA | SER | THR | PRO | ARG | GLN | THR | VAL  |
| ILE | SER | THR | ALA | LEU | ASN | LYS | VAL  |
| LYS | ASN | SER | ILE | GLY | ALA | MET | LEU  |
|     |     |     | PHE | THR | ALA | VAL | LEU  |
|     |     |     | ASP | SER | ALA | ILE | THR  |
|     |     |     | ASN | TRP | GLY | PRO | PRO  |
|     |     |     | ASN | SER | ASN | GLY | GLY  |
|     |     |     | ALA | ARG | ILE | ILE | TVR  |
|     |     |     | PRO | SER | LYS | ALA | SER  |
|     |     |     | THR | PHE | ILE | THR | SER  |
|     |     |     | GLU | TYR | VAL | ALA | K27  |
|     |     |     | VAL | GLY | ALA | ILE |      |
|     |     |     | GLY | ILE | TYR | GLU | T24  |
|     |     |     | THR | LYS | PRO | ARG |      |
|     |     |     | ILE | LYS | ASP | LEU | L80  |
|     |     |     | ILE | GLY | THR | LEU |      |
|     |     |     | GLY | GLY | ASN | GLN |      |
|     |     |     | THR | VAL | SER | GLY | S105 |
|     |     |     | ARG | SER | LEU | GLU | E106 |
|     |     |     | ASN | ILE | LEU | GLU | M107 |
|     |     |     | VAL | VAL | LEU | GLN |      |
|     |     |     | ASP | ALA | VAL | PRO | L114 |
|     |     |     | ARG | GLN | LYS | GLY | R115 |
|     |     |     | VAL | LEU | THR | LEU | N116 |
|     |     |     | PRO | SER | THR | GLY | V117 |
|     |     |     | HIS | ILE | ALA | ASN |      |
|     |     |     | VAL | ILE | ALA | ILE |      |
|     |     |     | THR | SER | GLY | VAL | G151 |
|     |     |     | TYR | THR | GLN | VAL |      |
|     |     |     | GLY | LEU | VAL | SER |      |
|     |     |     | THR | GLY | HIS | SER | A163 |
|     |     |     | GLY | GLY | PHE | GLU |      |
|     |     |     | ILE | SER | ILE | PRO | N170 |
|     |     |     | ARG | ARG | GLY | PRO | ASP  |
|     |     |     | VAL | PHE | MET | ALA | GLY  |
|     |     |     | THR | ILE | LEU | MET | ILE  |
|     |     |     | LEU | ALA | VAL | PRO | GLU  |
|     |     |     | PRO | LYS | ALA | ALA | LEU  |
|     |     |     | ARG | VAL | PHE | GLY | GLY  |
|     |     |     | ASP | ASN | VAL | SER | ARG  |
|     |     |     | THR | ALA | LEU | ALA | GLN  |
|     |     |     | ALA | ALA | ASP | ALA | LYS  |
|     |     |     | ASP | VAL | VAL | ASN | LYS  |
|     |     |     | THR | GLY | ALA | GLY | GLY  |
|     |     |     | GLN | GLN | THR | GLY | VAL  |
|     |     |     | ILE | LYS | ARG | LYS | VAL  |
|     |     |     | ILE | THR | GLN | GLY | MET  |
|     |     |     | THR | GLN | VAL | TYR | ARG  |

- Molecule 5: Protein InvG

Chain F:  22% 75%

[illegible]

[illegible]

- Molecule 5: Protein InvG

Chain G:  24% 74%

[illegible]

- Molecule 5: Protein InvG

Chain H:  22% 75%

[illegible]

[illegible]

- Molecule 5: Protein InvG

Chain I:  23% 1% 74%

[illegible]

- Molecule 5: Protein InvG

Chain J:  23% . 75%

[illegible]



- Molecule 5: Protein InvG

[illegible]

- Molecule 5: Protein InvG

[illegible]

[illegible]

- Molecule 5: Protein InvG

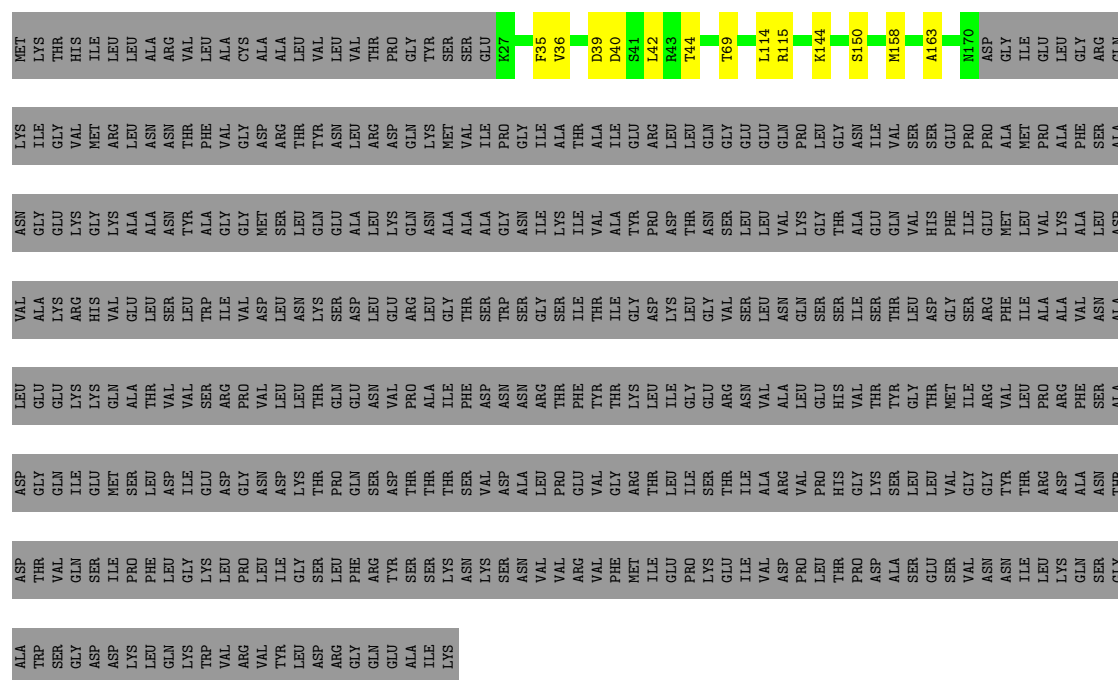
[illegible]

- Molecule 5: Protein InvG

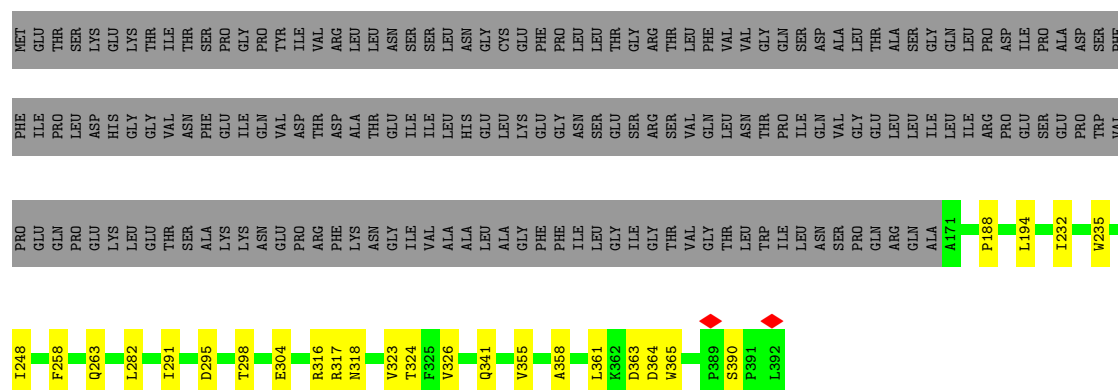
[illegible]



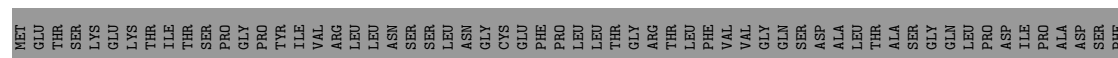
- Molecule 5: Protein InvG



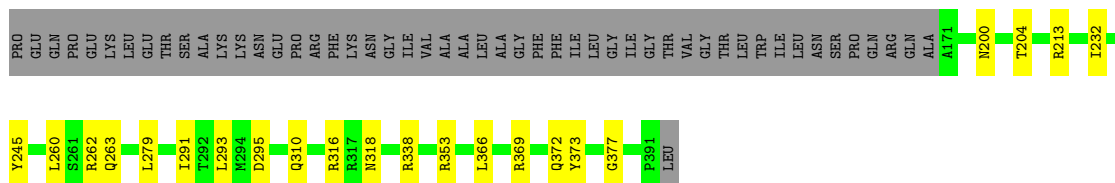
- Molecule 6: Protein PrgH



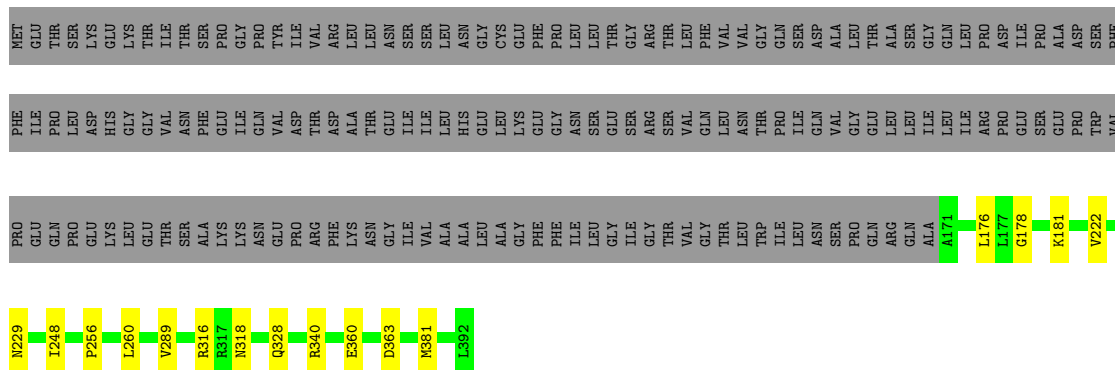
- Molecule 6: Protein PrgH



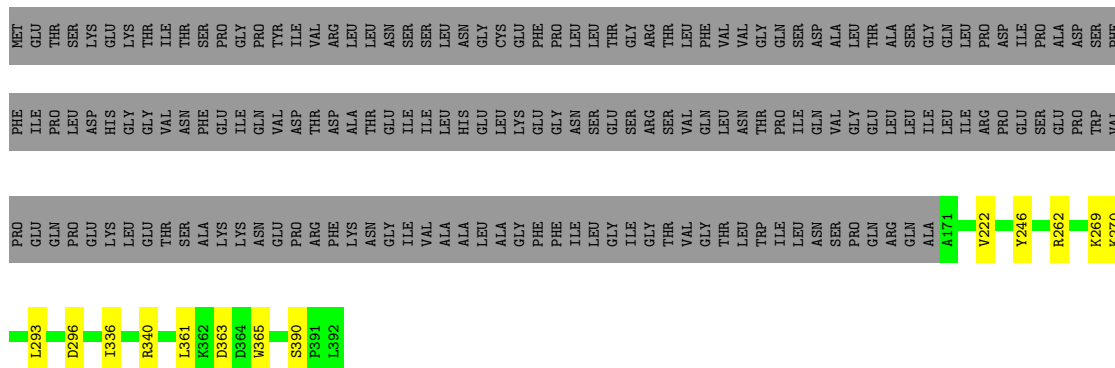




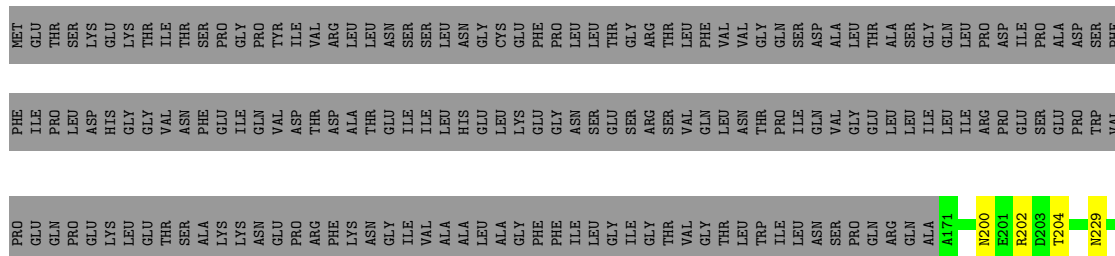
- Molecule 6: Protein PrgH



- Molecule 6: Protein PrgH



- Molecule 6: Protein PrgH





43%

| Letter | Count |
|--------|-------|
| F      | 258   |
| V      | 274   |
| K      | 278   |
| I      | 291   |
| R      | 317   |
| T      | 324   |
| V      | 355   |
| D      | 363   |
| L      | 366   |
| R      | 369   |
| K      | 380   |
| L      | 392   |

## 43%

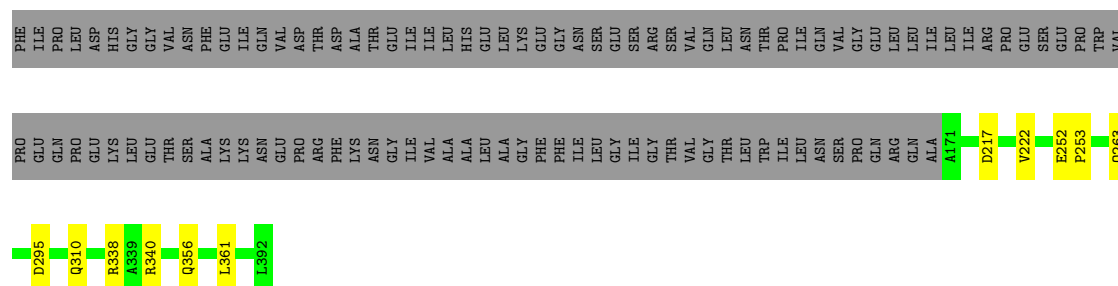
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| E227 | E228 | R231 | L236 | P256 | V257 | F258 | R262 | V274 | K278 | Y285 | A286 | Y289 | N290 | I291 | D295 | A299 | E304 | R316 | Y346 | L361 | K362 | D363 | D364 | W365 | A375 | S390 | P391 | L392 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

## 44%

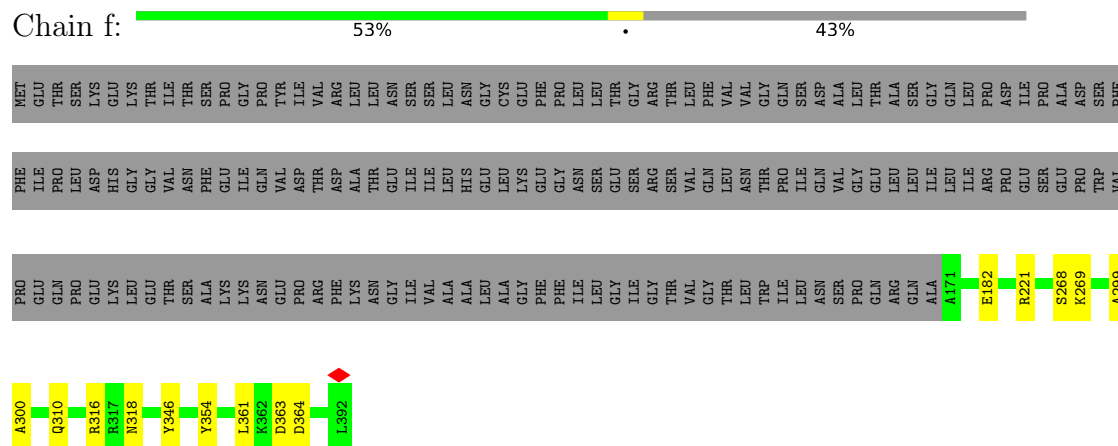
|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|
| R247 | S261 | L282 | T298 | E304 | R316 | R317 | N318 | L337 | Y346 | D363 | W365 | L366 | K380 | P391 | LEU |
| R262 | Q263 | T297 | A299 |      |      |      |      |      | V347 | D364 | W366 |      |      |      |     |
|      |      |      |      |      |      |      |      |      | R348 |      |      |      |      |      |     |

## 43%

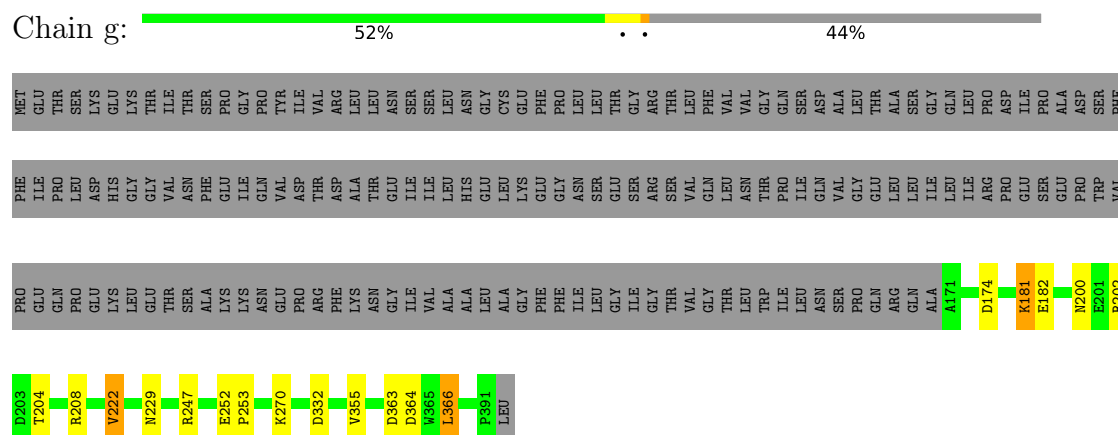
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |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



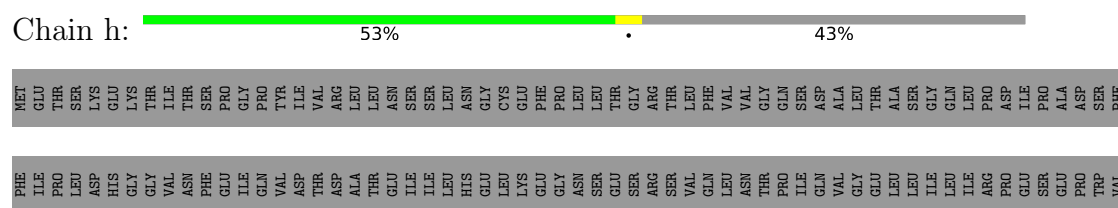
- Molecule 6: Protein PrgH

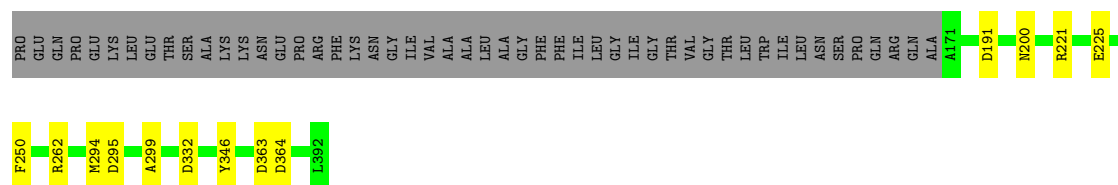


- Molecule 6: Protein PrgH



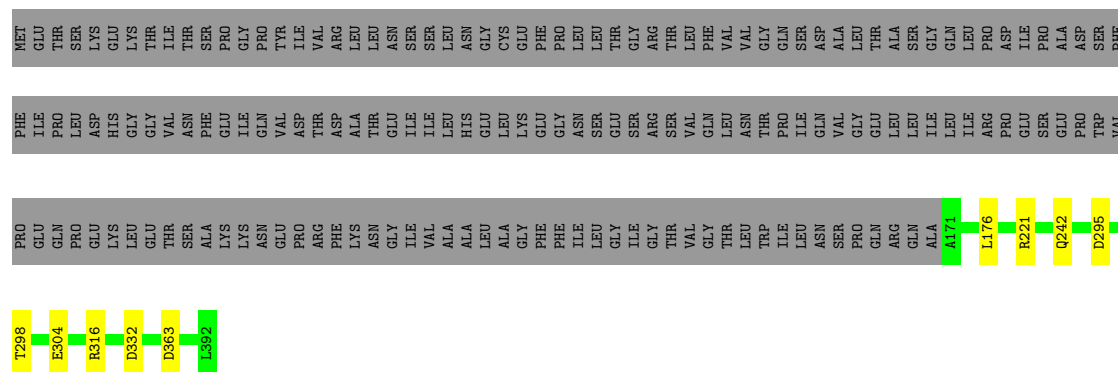
- Molecule 6: Protein PrgH





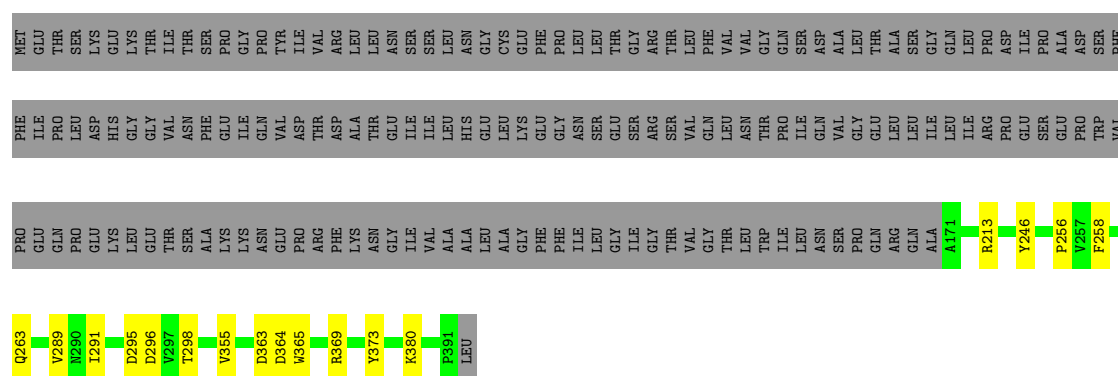
### • Molecule 6: Protein PrgH

Chain i: 54% 43%



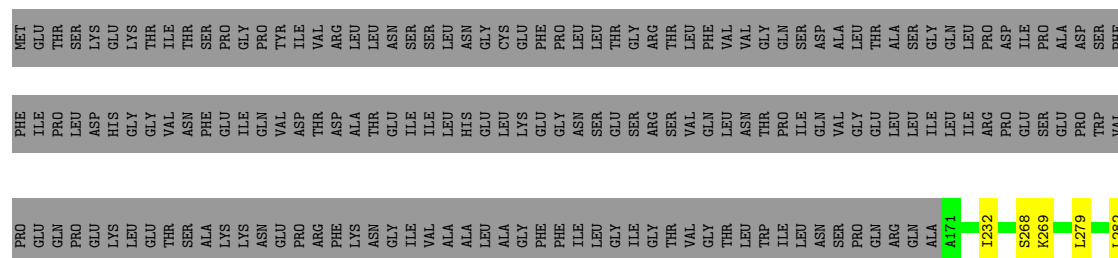
### • Molecule 6: Protein PrgH

Chain j: 52% 44%



### • Molecule 6: Protein PrgH

Chain k: 53% 43%







## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 144097                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 51.3                                    | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.267                                   | Depositor |
| Minimum map value                    | -0.159                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.010                                   | Depositor |
| Recommended contour level            | 0.025                                   | Depositor |
| Map size (Å)                         | 427.5, 427.5, 427.5                     | wwPDB     |
| Map dimensions                       | 250, 250, 250                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.71, 1.71, 1.71                        | Depositor |

## 5 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$   |
| 1   | AA    | 0.33         | 0/1458      | 0.52        | 0/1979        |
| 1   | AB    | 0.34         | 0/1458      | 0.53        | 0/1979        |
| 1   | AC    | 0.32         | 0/1458      | 0.52        | 0/1979        |
| 1   | AD    | 0.33         | 0/1458      | 0.56        | 0/1979        |
| 1   | AE    | 0.33         | 0/1458      | 0.54        | 0/1979        |
| 1   | AF    | 0.34         | 0/1458      | 0.52        | 0/1979        |
| 1   | AG    | 0.33         | 0/1458      | 0.51        | 0/1979        |
| 1   | AH    | 0.32         | 0/1458      | 0.52        | 0/1979        |
| 1   | AI    | 0.33         | 0/1458      | 0.54        | 0/1979        |
| 1   | AJ    | 0.33         | 0/1458      | 0.53        | 0/1979        |
| 1   | AK    | 0.33         | 0/1458      | 0.54        | 0/1979        |
| 1   | AL    | 0.33         | 0/1458      | 0.54        | 0/1979        |
| 1   | o     | 0.32         | 0/1458      | 0.53        | 0/1979        |
| 1   | p     | 0.31         | 0/1458      | 0.50        | 0/1979        |
| 1   | q     | 0.32         | 0/1458      | 0.50        | 0/1979        |
| 1   | r     | 0.32         | 0/1458      | 0.54        | 0/1979        |
| 1   | s     | 0.33         | 0/1458      | 0.53        | 0/1979        |
| 1   | t     | 0.32         | 0/1458      | 0.56        | 0/1979        |
| 1   | u     | 0.32         | 0/1458      | 0.55        | 0/1979        |
| 1   | v     | 0.34         | 0/1458      | 0.55        | 0/1979        |
| 1   | w     | 0.32         | 0/1458      | 0.52        | 0/1979        |
| 1   | x     | 0.33         | 0/1458      | 0.52        | 0/1979        |
| 1   | y     | 0.33         | 0/1458      | 0.52        | 0/1979        |
| 1   | z     | 0.33         | 0/1458      | 0.55        | 0/1979        |
| 2   | 0     | 0.30         | 0/1501      | 0.70        | 0/2040        |
| 2   | 1     | 0.32         | 0/1508      | 0.69        | 0/2049        |
| 2   | 2     | 0.29         | 0/1497      | 0.69        | 1/2032 (0.0%) |
| 2   | 3     | 0.27         | 0/1553      | 0.62        | 0/2107        |
| 2   | 4     | 0.30         | 0/1710      | 0.65        | 0/2318        |
| 3   | 5     | 0.31         | 0/1758      | 0.65        | 0/2402        |
| 4   | 6     | 0.22         | 0/414       | 0.60        | 0/565         |
| 4   | 7     | 0.29         | 0/657       | 0.75        | 1/897 (0.1%)  |
| 4   | 8     | 0.28         | 0/657       | 0.73        | 0/897         |
| 4   | 9     | 0.28         | 0/660       | 0.62        | 0/900         |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 5   | A     | 0.30         | 0/1131   | 0.53        | 0/1525          |
| 5   | B     | 0.31         | 0/1181   | 0.53        | 0/1593          |
| 5   | C     | 0.31         | 0/1131   | 0.54        | 0/1525          |
| 5   | D     | 0.30         | 0/1170   | 0.53        | 0/1579          |
| 5   | F     | 0.31         | 0/1131   | 0.54        | 0/1525          |
| 5   | G     | 0.31         | 0/1181   | 0.57        | 0/1593          |
| 5   | H     | 0.30         | 0/1131   | 0.52        | 0/1525          |
| 5   | I     | 0.30         | 0/1181   | 0.54        | 0/1593          |
| 5   | J     | 0.30         | 0/1131   | 0.55        | 0/1525          |
| 5   | K     | 0.31         | 0/1181   | 0.58        | 0/1593          |
| 5   | L     | 0.32         | 0/1131   | 0.58        | 0/1525          |
| 5   | M     | 0.30         | 0/1170   | 0.52        | 0/1579          |
| 5   | N     | 0.31         | 0/1131   | 0.53        | 0/1525          |
| 5   | O     | 0.31         | 0/1181   | 0.56        | 0/1593          |
| 5   | P     | 0.31         | 0/1131   | 0.53        | 0/1525          |
| 5   | Q     | 0.31         | 0/1181   | 0.57        | 0/1593          |
| 6   | E     | 0.30         | 0/1881   | 0.53        | 0/2541          |
| 6   | R     | 0.30         | 0/1872   | 0.54        | 0/2530          |
| 6   | S     | 0.31         | 0/1876   | 0.56        | 0/2536          |
| 6   | T     | 0.31         | 0/1881   | 0.54        | 0/2541          |
| 6   | U     | 0.30         | 0/1872   | 0.54        | 0/2530          |
| 6   | V     | 0.30         | 0/1876   | 0.52        | 0/2536          |
| 6   | W     | 0.29         | 0/1881   | 0.52        | 0/2541          |
| 6   | X     | 0.29         | 0/1872   | 0.51        | 0/2530          |
| 6   | Y     | 0.31         | 0/1876   | 0.56        | 0/2536          |
| 6   | Z     | 0.30         | 0/1881   | 0.52        | 0/2541          |
| 6   | a     | 0.30         | 0/1872   | 0.51        | 0/2530          |
| 6   | b     | 0.32         | 0/1876   | 0.56        | 0/2536          |
| 6   | c     | 0.31         | 0/1881   | 0.54        | 0/2541          |
| 6   | d     | 0.30         | 0/1872   | 0.50        | 0/2530          |
| 6   | e     | 0.31         | 0/1876   | 0.55        | 0/2536          |
| 6   | f     | 0.31         | 0/1881   | 0.52        | 0/2541          |
| 6   | g     | 0.30         | 0/1872   | 0.54        | 0/2530          |
| 6   | h     | 0.31         | 0/1876   | 0.56        | 0/2536          |
| 6   | i     | 0.30         | 0/1881   | 0.52        | 0/2541          |
| 6   | j     | 0.30         | 0/1872   | 0.55        | 0/2530          |
| 6   | k     | 0.31         | 0/1876   | 0.54        | 0/2536          |
| 6   | l     | 0.31         | 0/1881   | 0.52        | 0/2541          |
| 6   | m     | 0.30         | 0/1872   | 0.50        | 0/2530          |
| 6   | n     | 0.31         | 0/1876   | 0.54        | 0/2536          |
| All | All   | 0.31         | 0/110413 | 0.55        | 2/149475 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 4   | 8     | 0                   | 2                   |
| 6   | b     | 0                   | 1                   |
| 6   | k     | 0                   | 1                   |
| All | All   | 0                   | 4                   |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2   | 2     | 167 | LEU  | N-CA-C    | 5.23 | 121.38      | 109.81   |
| 4   | 7     | 40  | THR  | CA-CB-CG2 | 5.04 | 119.06      | 110.50   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 4   | 8     | 16  | LEU  | Mainchain |
| 4   | 8     | 40  | THR  | Peptide   |
| 6   | b     | 366 | LEU  | Peptide   |
| 6   | k     | 366 | LEU  | Peptide   |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 1431  | 0        | 1424     | 12      | 0            |
| 1   | AB    | 1431  | 0        | 1424     | 9       | 0            |
| 1   | AC    | 1431  | 0        | 1424     | 14      | 0            |
| 1   | AD    | 1431  | 0        | 1424     | 9       | 0            |
| 1   | AE    | 1431  | 0        | 1424     | 8       | 0            |
| 1   | AF    | 1431  | 0        | 1424     | 9       | 0            |
| 1   | AG    | 1431  | 0        | 1424     | 10      | 0            |
| 1   | AH    | 1431  | 0        | 1424     | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AI    | 1431  | 0        | 1424     | 12      | 0            |
| 1   | AJ    | 1431  | 0        | 1424     | 17      | 0            |
| 1   | AK    | 1431  | 0        | 1424     | 7       | 0            |
| 1   | AL    | 1431  | 0        | 1424     | 12      | 0            |
| 1   | o     | 1431  | 0        | 1424     | 11      | 0            |
| 1   | p     | 1431  | 0        | 1424     | 10      | 0            |
| 1   | q     | 1431  | 0        | 1424     | 5       | 0            |
| 1   | r     | 1431  | 0        | 1424     | 11      | 0            |
| 1   | s     | 1431  | 0        | 1424     | 9       | 0            |
| 1   | t     | 1431  | 0        | 1424     | 12      | 0            |
| 1   | u     | 1431  | 0        | 1424     | 16      | 0            |
| 1   | v     | 1431  | 0        | 1424     | 11      | 0            |
| 1   | w     | 1431  | 0        | 1424     | 10      | 0            |
| 1   | x     | 1431  | 0        | 1424     | 10      | 0            |
| 1   | y     | 1431  | 0        | 1424     | 9       | 0            |
| 1   | z     | 1431  | 0        | 1424     | 9       | 0            |
| 2   | 0     | 1468  | 0        | 1509     | 12      | 0            |
| 2   | 1     | 1475  | 0        | 1525     | 13      | 0            |
| 2   | 2     | 1464  | 0        | 1524     | 19      | 0            |
| 2   | 3     | 1520  | 0        | 1577     | 11      | 0            |
| 2   | 4     | 1672  | 0        | 1734     | 10      | 0            |
| 3   | 5     | 1718  | 0        | 1767     | 14      | 0            |
| 4   | 6     | 405   | 0        | 418      | 5       | 0            |
| 4   | 7     | 644   | 0        | 685      | 9       | 0            |
| 4   | 8     | 644   | 0        | 685      | 6       | 0            |
| 4   | 9     | 647   | 0        | 692      | 8       | 0            |
| 5   | A     | 1108  | 0        | 1103     | 7       | 0            |
| 5   | B     | 1154  | 0        | 1163     | 10      | 0            |
| 5   | C     | 1108  | 0        | 1103     | 8       | 0            |
| 5   | D     | 1146  | 0        | 1150     | 8       | 0            |
| 5   | F     | 1108  | 0        | 1103     | 9       | 0            |
| 5   | G     | 1154  | 0        | 1163     | 6       | 0            |
| 5   | H     | 1108  | 0        | 1103     | 9       | 0            |
| 5   | I     | 1154  | 0        | 1163     | 10      | 0            |
| 5   | J     | 1108  | 0        | 1103     | 5       | 0            |
| 5   | K     | 1154  | 0        | 1163     | 10      | 0            |
| 5   | L     | 1108  | 0        | 1103     | 11      | 0            |
| 5   | M     | 1146  | 0        | 1150     | 4       | 0            |
| 5   | N     | 1108  | 0        | 1103     | 10      | 0            |
| 5   | O     | 1154  | 0        | 1163     | 9       | 0            |
| 5   | P     | 1108  | 0        | 1103     | 9       | 0            |
| 5   | Q     | 1154  | 0        | 1163     | 10      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 6   | E     | 1836   | 0        | 1800     | 16      | 0            |
| 6   | R     | 1827   | 0        | 1789     | 10      | 0            |
| 6   | S     | 1831   | 0        | 1788     | 13      | 0            |
| 6   | T     | 1836   | 0        | 1800     | 19      | 0            |
| 6   | U     | 1827   | 0        | 1789     | 13      | 0            |
| 6   | V     | 1831   | 0        | 1788     | 10      | 0            |
| 6   | W     | 1836   | 0        | 1800     | 9       | 0            |
| 6   | X     | 1827   | 0        | 1789     | 17      | 0            |
| 6   | Y     | 1831   | 0        | 1788     | 16      | 0            |
| 6   | Z     | 1836   | 0        | 1800     | 10      | 0            |
| 6   | a     | 1827   | 0        | 1789     | 8       | 0            |
| 6   | b     | 1831   | 0        | 1788     | 12      | 0            |
| 6   | c     | 1836   | 0        | 1800     | 18      | 0            |
| 6   | d     | 1827   | 0        | 1789     | 14      | 0            |
| 6   | e     | 1831   | 0        | 1788     | 6       | 0            |
| 6   | f     | 1836   | 0        | 1800     | 10      | 0            |
| 6   | g     | 1827   | 0        | 1789     | 13      | 0            |
| 6   | h     | 1831   | 0        | 1788     | 10      | 0            |
| 6   | i     | 1836   | 0        | 1800     | 6       | 0            |
| 6   | j     | 1827   | 0        | 1789     | 13      | 0            |
| 6   | k     | 1831   | 0        | 1788     | 8       | 0            |
| 6   | l     | 1836   | 0        | 1800     | 17      | 0            |
| 6   | m     | 1827   | 0        | 1789     | 11      | 0            |
| 6   | n     | 1831   | 0        | 1788     | 11      | 0            |
| All | All   | 108033 | 0        | 107410   | 655     | 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 3.

All (655) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 5:A:39:ASP:H     | 5:A:69:THR:HG22   | 1.51                     | 0.75              |
| 5:Q:39:ASP:H     | 5:Q:69:THR:HG22   | 1.52                     | 0.74              |
| 5:P:39:ASP:H     | 5:P:69:THR:HG22   | 1.61                     | 0.66              |
| 6:E:361:LEU:HD13 | 1:o:165:SER:HB2   | 1.77                     | 0.66              |
| 2:0:187:MET:HE1  | 3:5:210:ASN:HA    | 1.77                     | 0.65              |
| 6:R:316:ARG:HH21 | 6:R:318:ASN:HD21  | 1.45                     | 0.64              |
| 6:l:340:ARG:HH22 | 1:Aj:163:GLN:HE21 | 1.44                     | 0.64              |
| 6:R:261:SER:O    | 6:R:265:ASN:ND2   | 2.31                     | 0.63              |
| 5:G:169:GLN:HE22 | 5:H:115:ARG:HA    | 1.65                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:a:232:ILE:HD11  | 6:a:248:ILE:HG21  | 1.81                     | 0.62              |
| 6:Y:261:SER:O     | 6:Y:265:ASN:ND2   | 2.33                     | 0.61              |
| 2:4:201:LEU:HD11  | 4:9:71:LEU:HB3    | 1.81                     | 0.61              |
| 1:u:139:ASN:HD22  | 1:u:141:ARG:HH11  | 1.48                     | 0.61              |
| 6:S:213:ARG:NH2   | 1:p:43:ASN:O      | 2.34                     | 0.60              |
| 1:AH:123:VAL:HG22 | 1:AH:154:TYR:HE1  | 1.66                     | 0.60              |
| 6:d:263:GLN:HE22  | 6:d:297:VAL:HG23  | 1.66                     | 0.60              |
| 1:AG:99:ARG:HE    | 1:AG:134:ILE:HD12 | 1.66                     | 0.60              |
| 6:T:232:ILE:HG13  | 6:T:282:LEU:HD13  | 1.84                     | 0.60              |
| 5:F:114:LEU:HD21  | 5:F:163:ALA:HB1   | 1.84                     | 0.60              |
| 6:Y:328:GLN:HG2   | 6:Y:360:GLU:HB3   | 1.84                     | 0.59              |
| 6:j:365:TRP:O     | 6:j:369:ARG:NH1   | 2.35                     | 0.59              |
| 6:U:310:GLN:O     | 6:U:338:ARG:NH1   | 2.35                     | 0.59              |
| 6:l:363:ASP:OD1   | 6:l:363:ASP:N     | 2.36                     | 0.59              |
| 2:2:18:PRO:HA     | 2:2:21:ILE:HG22   | 1.84                     | 0.59              |
| 6:e:310:GLN:O     | 6:e:338:ARG:NH1   | 2.36                     | 0.59              |
| 6:V:229:ASN:HD21  | 6:V:248:ILE:H     | 1.49                     | 0.59              |
| 1:t:184:SER:HB3   | 1:u:173:ASN:HD22  | 1.68                     | 0.59              |
| 1:u:85:ILE:HB     | 1:u:107:SER:HB2   | 1.83                     | 0.59              |
| 1:y:179:ASP:OD1   | 1:y:179:ASP:N     | 2.35                     | 0.59              |
| 5:B:114:LEU:HD13  | 5:B:117:VAL:HG23  | 1.84                     | 0.59              |
| 5:L:149:VAL:HG21  | 5:L:159:VAL:HG21  | 1.84                     | 0.59              |
| 5:J:114:LEU:HD21  | 5:J:163:ALA:HB1   | 1.85                     | 0.58              |
| 6:R:310:GLN:O     | 6:R:338:ARG:NH1   | 2.36                     | 0.58              |
| 1:v:139:ASN:HD21  | 1:v:141:ARG:HE    | 1.51                     | 0.58              |
| 4:7:22:PRO:HA     | 4:7:25:VAL:HG12   | 1.85                     | 0.58              |
| 1:AA:165:SER:HB2  | 6:c:361:LEU:HD13  | 1.86                     | 0.58              |
| 6:V:256:PRO:HG2   | 6:V:289:VAL:HG12  | 1.86                     | 0.58              |
| 6:d:316:ARG:HH21  | 6:d:318:ASN:HD21  | 1.52                     | 0.57              |
| 4:6:22:PRO:HA     | 4:6:25:VAL:HB     | 1.86                     | 0.57              |
| 2:1:156:LYS:HE2   | 2:2:208:TRP:HB2   | 1.85                     | 0.57              |
| 1:AL:169:ARG:NH1  | 1:AL:180:TYR:OH   | 2.37                     | 0.57              |
| 1:u:94:LEU:HG     | 1:u:95:VAL:HG23   | 1.87                     | 0.57              |
| 6:W:361:LEU:HD13  | 1:u:165:SER:HB2   | 1.87                     | 0.57              |
| 2:2:210:LEU:HD22  | 4:7:79:ILE:HD12   | 1.86                     | 0.56              |
| 1:AJ:39:LEU:HD22  | 1:AJ:44:ILE:HD11  | 1.86                     | 0.56              |
| 2:3:215:LEU:HD12  | 4:8:83:LEU:HD11   | 1.86                     | 0.56              |
| 5:D:116:ASN:ND2   | 5:D:170:ASN:O     | 2.38                     | 0.56              |
| 6:X:310:GLN:O     | 6:X:338:ARG:NH1   | 2.38                     | 0.56              |
| 6:c:224:ASN:HB3   | 6:c:227:GLU:HG2   | 1.87                     | 0.56              |
| 6:l:361:LEU:HD13  | 1:AJ:165:SER:HB2  | 1.86                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AC:163:GLN:HE21 | 6:e:340:ARG:HH12  | 1.54                     | 0.56              |
| 5:A:36:VAL:HG22   | 5:A:71:ASN:HD22   | 1.70                     | 0.56              |
| 6:V:340:ARG:HH21  | 1:t:163:GLN:HE21  | 1.52                     | 0.55              |
| 1:AD:94:LEU:HG    | 1:AD:95:VAL:HG23  | 1.88                     | 0.55              |
| 5:I:149:VAL:HG21  | 5:I:159:VAL:HG11  | 1.88                     | 0.55              |
| 6:Y:186:VAL:HG22  | 6:Y:196:VAL:HG12  | 1.87                     | 0.55              |
| 5:A:33:SER:OG     | 5:A:34:GLY:N      | 2.39                     | 0.55              |
| 6:S:268:SER:OG    | 6:S:269:LYS:N     | 2.39                     | 0.55              |
| 6:f:221:ARG:NH1   | 6:g:182:GLU:OE2   | 2.40                     | 0.54              |
| 5:C:39:ASP:H      | 5:C:69:THR:HG22   | 1.72                     | 0.54              |
| 6:E:363:ASP:OD1   | 6:E:363:ASP:N     | 2.39                     | 0.54              |
| 5:L:33:SER:OG     | 5:L:34:GLY:N      | 2.40                     | 0.54              |
| 6:U:232:ILE:HD11  | 6:U:279:LEU:HD22  | 1.89                     | 0.54              |
| 6:b:317:ARG:HB2   | 6:b:324:THR:HG23  | 1.89                     | 0.54              |
| 6:l:364:ASP:HA    | 6:l:390:SER:HB3   | 1.89                     | 0.54              |
| 5:P:169:GLN:HE22  | 5:Q:115:ARG:HA    | 1.73                     | 0.54              |
| 1:AJ:112:ARG:NH1  | 1:AK:110:GLU:OE2  | 2.41                     | 0.54              |
| 5:H:116:ASN:ND2   | 5:H:170:ASN:O     | 2.41                     | 0.54              |
| 6:Z:229:ASN:HD21  | 6:Z:247:ARG:HG3   | 1.73                     | 0.54              |
| 1:t:94:LEU:HG     | 1:t:95:VAL:HG23   | 1.90                     | 0.54              |
| 1:AA:173:ASN:HD21 | 1:z:184:SER:HB3   | 1.73                     | 0.54              |
| 1:AC:133:ASP:OD2  | 1:AC:133:ASP:N    | 2.40                     | 0.54              |
| 1:AD:177:ASP:OD1  | 1:AD:177:ASP:N    | 2.40                     | 0.54              |
| 6:X:316:ARG:HE    | 6:X:318:ASN:HD21  | 1.55                     | 0.54              |
| 6:m:310:GLN:O     | 6:m:338:ARG:NH1   | 2.41                     | 0.54              |
| 2:4:175:VAL:HG23  | 4:9:19:SER:HB2    | 1.89                     | 0.54              |
| 1:AJ:99:ARG:HE    | 1:AJ:134:ILE:HD12 | 1.72                     | 0.54              |
| 2:0:221:ASP:OD2   | 1:v:139:ASN:ND2   | 2.41                     | 0.54              |
| 1:AH:34:GLU:OE2   | 1:AI:73:LYS:NZ    | 2.41                     | 0.54              |
| 5:Q:114:LEU:HD21  | 5:Q:163:ALA:HB1   | 1.90                     | 0.54              |
| 6:c:262:ARG:NH1   | 6:c:295:ASP:OD2   | 2.41                     | 0.53              |
| 1:AD:34:GLU:OE1   | 1:AL:73:LYS:NZ    | 2.40                     | 0.53              |
| 1:AG:184:SER:HB3  | 1:AK:173:ASN:HD21 | 1.73                     | 0.53              |
| 6:c:304:GLU:OE1   | 6:c:316:ARG:NH1   | 2.41                     | 0.53              |
| 6:j:256:PRO:HG2   | 6:j:289:VAL:HG12  | 1.89                     | 0.53              |
| 6:k:306:GLY:O     | 6:k:310:GLN:NE2   | 2.40                     | 0.53              |
| 1:s:184:SER:HB3   | 1:t:173:ASN:HD22  | 1.72                     | 0.53              |
| 2:0:100:ARG:NH2   | 2:0:141:PRO:O     | 2.41                     | 0.53              |
| 2:2:24:GLY:O      | 2:2:99:TYR:OH     | 2.27                     | 0.53              |
| 6:a:263:GLN:NE2   | 6:a:295:ASP:OD1   | 2.41                     | 0.53              |
| 6:l:365:TRP:HD1   | 6:l:390:SER:HB2   | 1.73                     | 0.53              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 6:c:363:ASP:OD1  | 6:c:363:ASP:N     | 2.39                     | 0.53              |
| 1:u:148:LEU:HD22 | 1:u:171:LEU:HD13  | 1.91                     | 0.53              |
| 2:0:46:ILE:HD12  | 3:5:97:ALA:HB1    | 1.91                     | 0.53              |
| 1:AC:73:LYS:NZ   | 1:AL:34:GLU:OE2   | 2.40                     | 0.53              |
| 1:u:168:LYS:O    | 1:u:172:LYS:HB2   | 2.08                     | 0.53              |
| 1:AI:169:ARG:NH1 | 1:AI:180:TYR:OH   | 2.42                     | 0.53              |
| 6:X:202:ARG:NH2  | 1:u:41:MET:SD     | 2.80                     | 0.53              |
| 1:AG:28:ASP:OD1  | 1:AG:28:ASP:N     | 2.39                     | 0.53              |
| 6:k:268:SER:OG   | 6:k:269:LYS:N     | 2.42                     | 0.53              |
| 5:F:46:PHE:HB3   | 5:F:57:VAL:HG11   | 1.91                     | 0.52              |
| 6:V:328:GLN:HG2  | 6:V:360:GLU:HB3   | 1.90                     | 0.52              |
| 1:y:139:ASN:HB3  | 1:y:141:ARG:HG3   | 1.90                     | 0.52              |
| 2:0:186:MET:N    | 2:0:186:MET:SD    | 2.82                     | 0.52              |
| 5:F:141:ASP:HB3  | 5:F:144:LYS:HB2   | 1.91                     | 0.52              |
| 6:T:364:ASP:HA   | 6:T:390:SER:HB3   | 1.91                     | 0.52              |
| 1:AH:28:ASP:OD1  | 1:AH:29:GLN:N     | 2.42                     | 0.52              |
| 5:N:60:SER:OG    | 5:N:61:LYS:N      | 2.42                     | 0.52              |
| 6:e:217:ASP:OD1  | 6:e:217:ASP:N     | 2.41                     | 0.52              |
| 3:5:22:ARG:NH1   | 3:5:153:SER:OG    | 2.42                     | 0.52              |
| 5:N:114:LEU:HD21 | 5:N:163:ALA:HB1   | 1.91                     | 0.52              |
| 1:AL:177:ASP:OD1 | 1:AL:177:ASP:N    | 2.40                     | 0.52              |
| 1:v:177:ASP:OD1  | 1:v:177:ASP:N     | 2.43                     | 0.52              |
| 5:D:107:MET:HE2  | 5:D:151:GLY:HA2   | 1.90                     | 0.52              |
| 6:l:326:VAL:HA   | 6:l:358:ALA:HB3   | 1.90                     | 0.52              |
| 1:AC:85:ILE:HB   | 1:AC:107:SER:HB2  | 1.92                     | 0.52              |
| 4:8:39:VAL:HG23  | 4:8:40:THR:HG23   | 1.91                     | 0.52              |
| 1:o:184:SER:HB3  | 1:p:173:ASN:HD21  | 1.75                     | 0.52              |
| 1:s:177:ASP:OD2  | 1:s:177:ASP:N     | 2.42                     | 0.52              |
| 1:AG:85:ILE:HB   | 1:AG:107:SER:HB2  | 1.91                     | 0.52              |
| 6:g:363:ASP:N    | 6:g:363:ASP:OD1   | 2.40                     | 0.52              |
| 6:n:261:SER:O    | 6:n:265:ASN:ND2   | 2.42                     | 0.52              |
| 6:a:316:ARG:HH21 | 6:a:318:ASN:HD21  | 1.56                     | 0.52              |
| 5:G:97:GLN:OE1   | 5:H:150:SER:OG    | 2.28                     | 0.52              |
| 6:T:191:ASP:OD1  | 6:T:191:ASP:N     | 2.40                     | 0.51              |
| 6:c:228:GLU:HG3  | 6:c:231:ARG:HE    | 1.75                     | 0.51              |
| 6:i:304:GLU:OE1  | 6:i:316:ARG:NH1   | 2.41                     | 0.51              |
| 1:AA:184:SER:HB3 | 1:AB:173:ASN:HD21 | 1.75                     | 0.51              |
| 3:5:194:LEU:HA   | 3:5:197:VAL:HG12  | 1.93                     | 0.51              |
| 1:AI:20:ASP:N    | 1:AI:60:VAL:O     | 2.44                     | 0.51              |
| 2:2:65:TRP:HD1   | 2:2:68:MET:HE2    | 1.74                     | 0.51              |
| 6:j:263:GLN:NE2  | 6:j:295:ASP:OD1   | 2.43                     | 0.51              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:0:22:ALA:HB1   | 2:1:51:THR:HG22   | 1.91                     | 0.51              |
| 1:t:150:ALA:HB3  | 1:t:185:VAL:HG12  | 1.91                     | 0.51              |
| 1:t:156:ARG:NH2  | 1:t:190:ARG:O     | 2.43                     | 0.51              |
| 2:1:200:VAL:HA   | 2:1:203:VAL:HG22  | 1.93                     | 0.51              |
| 6:R:363:ASP:OD1  | 6:R:363:ASP:N     | 2.43                     | 0.51              |
| 6:k:232:ILE:HD11 | 6:k:279:LEU:HD22  | 1.92                     | 0.51              |
| 1:s:21:LYS:HD2   | 1:s:62:GLU:HG2    | 1.92                     | 0.51              |
| 1:z:21:LYS:NZ    | 1:z:62:GLU:OE1    | 2.40                     | 0.51              |
| 6:X:246:TYR:OH   | 6:X:296:ASP:OD2   | 2.28                     | 0.51              |
| 6:d:364:ASP:OD1  | 6:d:364:ASP:N     | 2.40                     | 0.51              |
| 6:f:316:ARG:HH21 | 6:f:318:ASN:HD21  | 1.58                     | 0.51              |
| 6:Y:332:ASP:OD1  | 6:Y:332:ASP:N     | 2.43                     | 0.51              |
| 6:c:365:TRP:HD1  | 6:c:390:SER:HB2   | 1.76                     | 0.51              |
| 6:d:363:ASP:OD1  | 6:d:363:ASP:N     | 2.41                     | 0.51              |
| 1:AK:110:GLU:HB3 | 1:AK:130:ILE:HG12 | 1.92                     | 0.51              |
| 6:f:363:ASP:OD1  | 6:f:363:ASP:N     | 2.41                     | 0.51              |
| 2:3:200:VAL:HA   | 2:3:203:VAL:HG22  | 1.93                     | 0.50              |
| 6:R:304:GLU:OE1  | 6:R:316:ARG:NH1   | 2.42                     | 0.50              |
| 5:F:114:LEU:HD13 | 5:F:117:VAL:HG13  | 1.92                     | 0.50              |
| 6:T:340:ARG:HH22 | 1:r:163:GLN:HE21  | 1.59                     | 0.50              |
| 6:c:274:VAL:HG12 | 6:c:278:LYS:HE2   | 1.93                     | 0.50              |
| 6:c:364:ASP:HA   | 6:c:390:SER:HB3   | 1.93                     | 0.50              |
| 6:U:200:ASN:O    | 6:U:204:THR:OG1   | 2.24                     | 0.50              |
| 6:l:228:GLU:OE2  | 6:l:231:ARG:NE    | 2.40                     | 0.50              |
| 1:v:36:ILE:HD11  | 1:v:48:LYS:HB2    | 1.94                     | 0.50              |
| 1:AH:93:SER:OG   | 1:AH:94:LEU:N     | 2.44                     | 0.50              |
| 5:J:33:SER:OG    | 5:J:34:GLY:N      | 2.44                     | 0.50              |
| 5:C:141:ASP:HB3  | 5:C:144:LYS:HB2   | 1.93                     | 0.50              |
| 6:Y:228:GLU:OE2  | 6:Y:231:ARG:NH2   | 2.41                     | 0.50              |
| 6:c:258:PHE:HB3  | 6:c:291:ILE:HG12  | 1.94                     | 0.50              |
| 6:n:363:ASP:OD1  | 6:n:363:ASP:N     | 2.45                     | 0.50              |
| 1:s:39:LEU:HD22  | 1:s:44:ILE:HD11   | 1.93                     | 0.50              |
| 3:5:39:SER:OG    | 3:5:40:GLY:N      | 2.45                     | 0.50              |
| 3:5:133:ALA:HA   | 3:5:136:VAL:HG12  | 1.94                     | 0.50              |
| 5:H:114:LEU:HD21 | 5:H:163:ALA:HB1   | 1.93                     | 0.50              |
| 6:T:364:ASP:N    | 6:T:364:ASP:OD1   | 2.43                     | 0.50              |
| 6:e:263:GLN:NE2  | 6:e:295:ASP:OD1   | 2.45                     | 0.50              |
| 1:AB:177:ASP:OD2 | 1:AB:177:ASP:N    | 2.45                     | 0.50              |
| 1:AC:93:SER:OG   | 1:AC:94:LEU:N     | 2.43                     | 0.49              |
| 2:0:188:MET:HE3  | 2:0:189:SER:H     | 1.77                     | 0.49              |
| 6:E:326:VAL:HA   | 6:E:358:ALA:HB3   | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:T:190:ARG:NH1   | 6:T:286:ALA:O     | 2.44                     | 0.49              |
| 6:T:326:VAL:HA    | 6:T:358:ALA:HB3   | 1.94                     | 0.49              |
| 6:W:246:TYR:OH    | 6:W:296:ASP:OD1   | 2.30                     | 0.49              |
| 6:h:364:ASP:OD1   | 6:h:364:ASP:N     | 2.40                     | 0.49              |
| 6:i:363:ASP:OD1   | 6:i:363:ASP:N     | 2.41                     | 0.49              |
| 2:O:29:LYS:NZ     | 2:O:157:SER:OG    | 2.44                     | 0.49              |
| 6:j:246:TYR:OH    | 6:j:296:ASP:OD2   | 2.30                     | 0.49              |
| 1:v:22:ASP:OD2    | 1:v:25:LYS:NZ     | 2.42                     | 0.49              |
| 5:N:44:THR:HB     | 6:S:380:LYS:HE2   | 1.92                     | 0.49              |
| 6:S:381:MET:HE1   | 6:T:391:PRO:HG2   | 1.93                     | 0.49              |
| 6:T:257:VAL:HG12  | 6:T:290:ASN:HB3   | 1.94                     | 0.49              |
| 6:m:304:GLU:OE1   | 6:m:316:ARG:NH1   | 2.45                     | 0.49              |
| 1:v:20:ASP:N      | 1:v:60:VAL:O      | 2.45                     | 0.49              |
| 1:y:21:LYS:NZ     | 1:y:62:GLU:OE2    | 2.39                     | 0.49              |
| 5:B:116:ASN:ND2   | 5:B:170:ASN:O     | 2.45                     | 0.49              |
| 5:G:114:LEU:HD21  | 5:G:163:ALA:HB1   | 1.95                     | 0.49              |
| 6:X:229:ASN:HD21  | 6:X:248:ILE:H     | 1.60                     | 0.49              |
| 6:g:364:ASP:OD1   | 6:g:364:ASP:N     | 2.42                     | 0.49              |
| 1:AI:99:ARG:HG3   | 1:AI:134:ILE:HD12 | 1.94                     | 0.49              |
| 6:b:217:ASP:OD1   | 6:b:217:ASP:N     | 2.45                     | 0.49              |
| 5:A:108:ARG:NH1   | 5:A:157:ASP:OD1   | 2.46                     | 0.49              |
| 5:K:38:LYS:NZ     | 6:m:369:ARG:O     | 2.40                     | 0.49              |
| 5:D:105:SER:O     | 5:D:105:SER:OG    | 2.31                     | 0.49              |
| 6:d:304:GLU:OE1   | 6:d:316:ARG:NH1   | 2.46                     | 0.49              |
| 1:r:184:SER:HB3   | 1:s:173:ASN:HD21  | 1.77                     | 0.49              |
| 1:w:184:SER:HB3   | 1:x:173:ASN:HD21  | 1.78                     | 0.49              |
| 1:AB:181:ASP:OD1  | 1:AB:181:ASP:N    | 2.46                     | 0.49              |
| 6:U:260:LEU:HD13  | 6:U:291:ILE:HG23  | 1.95                     | 0.49              |
| 6:V:363:ASP:OD2   | 6:V:363:ASP:N     | 2.46                     | 0.49              |
| 6:Y:304:GLU:OE1   | 6:Y:316:ARG:NH1   | 2.42                     | 0.49              |
| 2:2:197:ILE:HA    | 2:2:200:VAL:HG12  | 1.95                     | 0.49              |
| 5:O:169:GLN:NE2   | 5:P:114:LEU:O     | 2.46                     | 0.49              |
| 6:U:372:GLN:O     | 6:U:377:GLY:HA2   | 2.13                     | 0.49              |
| 6:a:304:GLU:OE1   | 6:a:316:ARG:NH1   | 2.46                     | 0.49              |
| 1:AF:173:ASN:HD21 | 1:AJ:184:SER:HB3  | 1.77                     | 0.48              |
| 6:T:232:ILE:HD11  | 6:T:279:LEU:HD22  | 1.95                     | 0.48              |
| 6:n:299:ALA:O     | 6:n:346:TYR:OH    | 2.31                     | 0.48              |
| 1:AC:20:ASP:N     | 1:AC:60:VAL:O     | 2.46                     | 0.48              |
| 1:AI:138:GLU:OE2  | 1:AI:138:GLU:N    | 2.45                     | 0.48              |
| 6:Z:174:ASP:OD1   | 6:Z:174:ASP:N     | 2.42                     | 0.48              |
| 1:AL:164:ILE:HG23 | 1:AL:185:VAL:HB   | 1.96                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:v:184:SER:HB3   | 1:w:173:ASN:HD21  | 1.78                     | 0.48              |
| 1:AE:37:ALA:HB2   | 1:AF:69:VAL:HG12  | 1.96                     | 0.48              |
| 2:1:29:LYS:NZ     | 2:1:218:GLN:OE1   | 2.46                     | 0.48              |
| 1:AH:85:ILE:HB    | 1:AH:107:SER:HB2  | 1.96                     | 0.48              |
| 1:AA:73:LYS:NZ    | 1:AB:34:GLU:OE2   | 2.46                     | 0.48              |
| 2:3:100:ARG:NH2   | 2:3:141:PRO:O     | 2.40                     | 0.48              |
| 6:c:299:ALA:O     | 6:c:346:TYR:OH    | 2.32                     | 0.48              |
| 6:f:268:SER:OG    | 6:f:269:LYS:N     | 2.44                     | 0.48              |
| 1:y:172:LYS:NZ    | 1:y:178:VAL:O     | 2.46                     | 0.48              |
| 4:6:3:ASP:OD1     | 4:6:3:ASP:N       | 2.40                     | 0.48              |
| 1:AE:110:GLU:HG3  | 1:AE:130:ILE:HG12 | 1.96                     | 0.48              |
| 2:2:35:VAL:HB     | 2:3:46:ILE:HD11   | 1.94                     | 0.48              |
| 2:4:214:GLY:HA3   | 4:9:83:LEU:HD13   | 1.94                     | 0.48              |
| 1:AF:34:GLU:OE1   | 1:AJ:73:LYS:NZ    | 2.46                     | 0.48              |
| 1:AG:173:ASN:HD21 | 1:AH:184:SER:HB3  | 1.78                     | 0.48              |
| 5:C:41:SER:O      | 5:C:41:SER:OG     | 2.28                     | 0.48              |
| 2:1:214:GLY:HA3   | 4:6:83:LEU:HD13   | 1.96                     | 0.48              |
| 4:6:2:ASP:N       | 4:6:2:ASP:OD1     | 2.46                     | 0.48              |
| 6:R:247:ARG:NH1   | 6:R:348:ARG:O     | 2.47                     | 0.48              |
| 6:m:364:ASP:OD1   | 6:m:364:ASP:N     | 2.42                     | 0.48              |
| 1:AI:39:LEU:HD22  | 1:AI:44:ILE:HD11  | 1.96                     | 0.48              |
| 5:H:109:ASN:ND2   | 5:H:148:TYR:OH    | 2.43                     | 0.48              |
| 6:U:213:ARG:HD2   | 1:r:201:PRO:HB3   | 1.96                     | 0.48              |
| 1:AL:28:ASP:OD1   | 1:AL:28:ASP:N     | 2.45                     | 0.48              |
| 6:c:228:GLU:OE2   | 6:c:285:TYR:OH    | 2.26                     | 0.48              |
| 1:AE:184:SER:HB3  | 1:o:173:ASN:HD21  | 1.79                     | 0.47              |
| 6:i:242:GLN:NE2   | 6:j:298:THR:OG1   | 2.47                     | 0.47              |
| 1:AG:177:ASP:OD1  | 1:AG:177:ASP:N    | 2.48                     | 0.47              |
| 2:1:221:ASP:OD2   | 2:1:221:ASP:N     | 2.45                     | 0.47              |
| 2:4:180:LEU:HD11  | 2:4:193:ILE:HD12  | 1.96                     | 0.47              |
| 6:E:304:GLU:OE1   | 6:E:316:ARG:NH1   | 2.47                     | 0.47              |
| 5:P:97:GLN:OE1    | 5:Q:150:SER:OG    | 2.30                     | 0.47              |
| 6:d:316:ARG:NE    | 6:d:318:ASN:OD1   | 2.41                     | 0.47              |
| 6:f:364:ASP:OD1   | 6:f:364:ASP:N     | 2.46                     | 0.47              |
| 6:l:364:ASP:OD1   | 6:l:364:ASP:N     | 2.46                     | 0.47              |
| 1:AH:177:ASP:OD2  | 1:AH:177:ASP:N    | 2.47                     | 0.47              |
| 5:C:114:LEU:HD21  | 5:C:163:ALA:HB1   | 1.95                     | 0.47              |
| 6:d:232:ILE:HG22  | 6:d:282:LEU:HD13  | 1.95                     | 0.47              |
| 1:AE:107:SER:O    | 1:AE:111:GLN:NE2  | 2.45                     | 0.47              |
| 5:B:42:LEU:HD22   | 5:B:66:LYS:HB2    | 1.95                     | 0.47              |
| 5:G:169:GLN:NE2   | 5:H:114:LEU:O     | 2.47                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 5:P:113:SER:HB2   | 5:P:146:THR:HG22 | 1.96                     | 0.47              |
| 6:g:181:LYS:HE3   | 6:g:181:LYS:HB2  | 1.54                     | 0.47              |
| 6:h:225:GLU:HG3   | 6:h:250:PHE:HD2  | 1.79                     | 0.47              |
| 1:r:36:ILE:HD11   | 1:r:48:LYS:HB2   | 1.95                     | 0.47              |
| 2:0:30:PHE:HE1    | 2:0:215:LEU:HB3  | 1.78                     | 0.47              |
| 4:9:14:LEU:HA     | 4:9:17:ILE:HG22  | 1.96                     | 0.47              |
| 5:F:168:LYS:HE2   | 5:F:168:LYS:HB2  | 1.73                     | 0.47              |
| 5:M:97:GLN:OE1    | 5:N:150:SER:OG   | 2.32                     | 0.47              |
| 6:W:363:ASP:OD1   | 6:W:363:ASP:N    | 2.41                     | 0.47              |
| 6:W:365:TRP:HD1   | 6:W:390:SER:HB2  | 1.79                     | 0.47              |
| 6:X:363:ASP:OD1   | 6:X:363:ASP:N    | 2.42                     | 0.47              |
| 1:AA:151:LEU:HA   | 1:AA:186:VAL:O   | 2.15                     | 0.47              |
| 2:2:38:ARG:NH1    | 2:2:48:SER:O     | 2.48                     | 0.47              |
| 4:8:37:GLN:O      | 4:8:43:GLN:NE2   | 2.48                     | 0.47              |
| 5:H:90:LEU:HA     | 5:H:103:ASP:HA   | 1.97                     | 0.47              |
| 5:L:57:VAL:HG12   | 5:L:99:ILE:HB    | 1.96                     | 0.47              |
| 6:h:294:MET:HE3   | 6:h:294:MET:HB2  | 1.65                     | 0.47              |
| 1:v:99:ARG:HG3    | 1:v:134:ILE:HB   | 1.96                     | 0.47              |
| 1:AE:160:LEU:HD21 | 6:E:341:GLN:HE22 | 1.80                     | 0.47              |
| 1:AI:85:ILE:HB    | 1:AI:107:SER:HB2 | 1.96                     | 0.47              |
| 6:T:361:LEU:HD13  | 1:r:165:SER:HB2  | 1.96                     | 0.47              |
| 6:W:270:LYS:HD3   | 6:W:270:LYS:HA   | 1.68                     | 0.47              |
| 1:x:151:LEU:HD21  | 1:y:120:MET:HE2  | 1.97                     | 0.47              |
| 1:z:39:LEU:HD22   | 1:z:44:ILE:HD11  | 1.96                     | 0.47              |
| 1:AJ:177:ASP:N    | 1:AJ:177:ASP:OD1 | 2.48                     | 0.47              |
| 2:3:24:GLY:O      | 2:3:99:TYR:OH    | 2.33                     | 0.47              |
| 4:8:5:VAL:O       | 4:8:9:ASN:ND2    | 2.40                     | 0.47              |
| 5:I:158:MET:HE3   | 5:I:158:MET:HB3  | 1.80                     | 0.47              |
| 6:d:228:GLU:OE2   | 6:d:231:ARG:NE   | 2.44                     | 0.47              |
| 5:Q:144:LYS:HD2   | 5:Q:144:LYS:HA   | 1.75                     | 0.47              |
| 6:T:228:GLU:HG3   | 6:T:231:ARG:HE   | 1.80                     | 0.47              |
| 6:V:178:GLY:O     | 6:V:181:LYS:NZ   | 2.48                     | 0.47              |
| 5:L:87:GLN:HE22   | 6:m:376:GLU:HB3  | 1.79                     | 0.46              |
| 6:S:217:ASP:OD2   | 6:S:217:ASP:N    | 2.42                     | 0.46              |
| 6:Y:232:ILE:HG21  | 6:Y:248:ILE:HD12 | 1.97                     | 0.46              |
| 2:4:4:ASP:HA      | 2:4:7:LEU:HD13   | 1.97                     | 0.46              |
| 2:3:183:LEU:HD23  | 4:8:52:LYS:HD2   | 1.97                     | 0.46              |
| 1:AE:173:ASN:HD21 | 1:AF:184:SER:HB3 | 1.81                     | 0.46              |
| 1:v:66:THR:HG21   | 1:w:197:ALA:HA   | 1.97                     | 0.46              |
| 1:AJ:37:ALA:HB2   | 1:AK:69:VAL:HG12 | 1.98                     | 0.46              |
| 2:1:93:ASP:O      | 2:1:100:ARG:NH2  | 2.49                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:2:168:PRO:HD3   | 4:7:78:VAL:HG11  | 1.96                     | 0.46              |
| 4:7:2:ASP:OD2     | 1:AJ:99:ARG:NH1  | 2.49                     | 0.46              |
| 1:AH:39:LEU:HD22  | 1:AH:44:ILE:HD11 | 1.96                     | 0.46              |
| 6:a:299:ALA:O     | 6:a:346:TYR:OH   | 2.33                     | 0.46              |
| 6:E:295:ASP:HB3   | 6:E:298:THR:HG22 | 1.98                     | 0.46              |
| 5:F:144:LYS:HA    | 5:F:144:LYS:HD3  | 1.81                     | 0.46              |
| 5:O:169:GLN:OE1   | 5:P:113:SER:OG   | 2.34                     | 0.46              |
| 6:n:328:GLN:HG2   | 6:n:360:GLU:HB3  | 1.97                     | 0.46              |
| 1:o:173:ASN:OD1   | 1:o:173:ASN:N    | 2.46                     | 0.46              |
| 1:AB:151:LEU:HD21 | 1:AC:120:MET:HE2 | 1.97                     | 0.46              |
| 2:2:169:PHE:HA    | 2:2:172:VAL:HG12 | 1.98                     | 0.46              |
| 5:I:76:ASP:HA     | 5:I:77:PRO:HD3   | 1.75                     | 0.46              |
| 6:X:200:ASN:O     | 6:X:204:THR:OG1  | 2.29                     | 0.46              |
| 6:Y:316:ARG:HE    | 6:Y:318:ASN:HD21 | 1.64                     | 0.46              |
| 6:Z:337:LEU:HD13  | 1:w:164:ILE:HD11 | 1.98                     | 0.46              |
| 1:t:177:ASP:OD1   | 1:t:177:ASP:N    | 2.49                     | 0.46              |
| 1:u:110:GLU:HB3   | 1:u:130:ILE:HG12 | 1.98                     | 0.46              |
| 1:x:169:ARG:NH1   | 1:x:180:TYR:OH   | 2.47                     | 0.46              |
| 2:1:60:SER:O      | 2:1:64:MET:HB2   | 2.16                     | 0.46              |
| 5:I:120:ASN:O     | 5:I:124:ASN:ND2  | 2.44                     | 0.46              |
| 6:b:200:ASN:OD1   | 6:b:200:ASN:N    | 2.48                     | 0.46              |
| 2:0:173:ASP:HA    | 2:0:176:VAL:HG12 | 1.97                     | 0.46              |
| 1:AI:177:ASP:OD1  | 1:AI:177:ASP:N   | 2.47                     | 0.46              |
| 5:F:60:SER:OG     | 5:F:61:LYS:N     | 2.49                     | 0.46              |
| 6:S:299:ALA:O     | 6:S:346:TYR:OH   | 2.33                     | 0.46              |
| 6:Z:258:PHE:HB3   | 6:Z:291:ILE:HG12 | 1.98                     | 0.46              |
| 1:AL:139:ASN:OD1  | 1:AL:141:ARG:NH1 | 2.49                     | 0.46              |
| 1:z:177:ASP:OD2   | 1:z:177:ASP:N    | 2.48                     | 0.46              |
| 1:AB:39:LEU:HD22  | 1:AB:44:ILE:HD11 | 1.97                     | 0.45              |
| 6:m:270:LYS:HD2   | 6:m:270:LYS:HA   | 1.68                     | 0.45              |
| 2:3:173:ASP:OD2   | 2:3:198:LYS:NZ   | 2.34                     | 0.45              |
| 4:7:14:LEU:HD12   | 4:7:17:ILE:HD11  | 1.97                     | 0.45              |
| 6:V:328:GLN:NE2   | 6:V:360:GLU:OE1  | 2.45                     | 0.45              |
| 6:n:262:ARG:HA    | 6:n:293:LEU:HD23 | 1.97                     | 0.45              |
| 1:r:66:THR:HG21   | 1:s:197:ALA:HA   | 1.99                     | 0.45              |
| 1:s:69:VAL:HG12   | 1:t:37:ALA:HB2   | 1.97                     | 0.45              |
| 2:2:86:SER:O      | 2:2:86:SER:OG    | 2.33                     | 0.45              |
| 5:D:114:LEU:HD13  | 5:D:117:VAL:HG23 | 1.98                     | 0.45              |
| 5:H:107:MET:HE2   | 5:H:151:GLY:HA2  | 1.97                     | 0.45              |
| 1:AA:151:LEU:HD21 | 1:AB:120:MET:HE2 | 1.98                     | 0.45              |
| 5:G:108:ARG:HH11  | 5:G:153:PRO:HB3  | 1.80                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 5:K:42:LEU:HD12   | 5:K:66:LYS:HB2    | 1.98                     | 0.45              |
| 5:O:38:LYS:NZ     | 6:U:369:ARG:O     | 2.39                     | 0.45              |
| 6:Y:200:ASN:OD1   | 6:Y:200:ASN:N     | 2.50                     | 0.45              |
| 6:h:191:ASP:OD1   | 6:h:191:ASP:N     | 2.49                     | 0.45              |
| 1:AC:184:SER:HB3  | 1:AL:173:ASN:HD21 | 1.81                     | 0.45              |
| 6:T:248:ILE:HG12  | 6:T:258:PHE:HD1   | 1.80                     | 0.45              |
| 1:o:110:GLU:OE2   | 1:o:132:TYR:OH    | 2.33                     | 0.45              |
| 5:B:76:ASP:HA     | 5:B:77:PRO:HD3    | 1.79                     | 0.45              |
| 6:a:365:TRP:O     | 6:a:369:ARG:NH1   | 2.49                     | 0.45              |
| 6:Y:310:GLN:O     | 6:Y:338:ARG:NH1   | 2.50                     | 0.45              |
| 6:b:191:ASP:OD1   | 6:b:191:ASP:N     | 2.47                     | 0.45              |
| 2:2:214:GLY:HA3   | 4:7:83:LEU:HD13   | 1.98                     | 0.45              |
| 3:5:38:LEU:HD23   | 3:5:43:ARG:HG3    | 1.97                     | 0.45              |
| 5:D:44:THR:HB     | 6:d:380:LYS:HE2   | 1.99                     | 0.45              |
| 5:Q:36:VAL:HG23   | 6:X:373:TYR:HE1   | 1.81                     | 0.45              |
| 6:c:190:ARG:NH1   | 6:c:286:ALA:O     | 2.49                     | 0.45              |
| 6:c:256:PRO:HG2   | 6:c:289:VAL:HG12  | 1.99                     | 0.45              |
| 1:q:153:VAL:HA    | 1:q:188:SER:O     | 2.17                     | 0.45              |
| 1:w:73:LYS:NZ     | 1:x:34:GLU:OE1    | 2.46                     | 0.45              |
| 1:AD:28:ASP:OD2   | 1:AD:29:GLN:N     | 2.46                     | 0.45              |
| 2:4:22:ALA:HB1    | 3:5:42:PRO:HA     | 1.98                     | 0.45              |
| 3:5:123:SER:OG    | 3:5:124:GLU:N     | 2.49                     | 0.45              |
| 5:N:114:LEU:HD13  | 5:N:117:VAL:HG13  | 1.99                     | 0.45              |
| 6:T:356:GLN:NE2   | 6:U:310:GLN:OE1   | 2.50                     | 0.45              |
| 1:AL:85:ILE:HB    | 1:AL:107:SER:HB2  | 1.99                     | 0.45              |
| 1:p:36:ILE:HD11   | 1:p:48:LYS:HB2    | 1.98                     | 0.45              |
| 5:H:97:GLN:OE1    | 5:I:150:SER:OG    | 2.35                     | 0.44              |
| 6:c:200:ASN:O     | 6:c:204:THR:OG1   | 2.31                     | 0.44              |
| 1:x:177:ASP:OD2   | 1:x:177:ASP:N     | 2.47                     | 0.44              |
| 2:1:43:LEU:HD23   | 2:1:46:ILE:HB     | 1.99                     | 0.44              |
| 3:5:232:SER:HB3   | 4:9:9:ASN:HD21    | 1.82                     | 0.44              |
| 5:B:36:VAL:HG23   | 6:a:373:TYR:HE1   | 1.82                     | 0.44              |
| 5:B:144:LYS:HD3   | 5:B:144:LYS:HA    | 1.82                     | 0.44              |
| 1:AL:41:MET:SD    | 6:g:202:ARG:NH2   | 2.84                     | 0.44              |
| 1:AH:173:ASN:HD21 | 1:AI:184:SER:HB3  | 1.81                     | 0.44              |
| 6:E:323:VAL:O     | 6:E:355:VAL:HA    | 2.18                     | 0.44              |
| 5:I:169:GLN:HE22  | 5:J:115:ARG:HA    | 1.83                     | 0.44              |
| 5:K:169:GLN:HE22  | 5:L:115:ARG:HA    | 1.82                     | 0.44              |
| 5:O:42:LEU:HD12   | 5:O:66:LYS:HB2    | 2.00                     | 0.44              |
| 5:Q:40:ASP:OD2    | 5:Q:44:THR:OG1    | 2.33                     | 0.44              |
| 6:T:249:HIS:HB2   | 6:T:257:VAL:HG23  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:n:245:TYR:OH    | 6:n:353:ARG:NH2   | 2.50                     | 0.44              |
| 1:o:129:HIS:HE1   | 1:p:112:ARG:HG2   | 1.83                     | 0.44              |
| 1:p:131:SER:HB3   | 1:p:147:HIS:HB2   | 1.99                     | 0.44              |
| 1:w:28:ASP:H      | 1:w:31:GLN:HB2    | 1.82                     | 0.44              |
| 1:AD:154:TYR:HE2  | 1:AD:187:LEU:HD22 | 1.82                     | 0.44              |
| 1:AF:112:ARG:NE   | 1:AJ:110:GLU:OE2  | 2.51                     | 0.44              |
| 2:3:166:TYR:HB3   | 2:4:196:PRO:HG3   | 1.98                     | 0.44              |
| 1:AH:173:ASN:HB2  | 1:AI:147:HIS:HB3  | 2.00                     | 0.44              |
| 5:B:141:ASP:HB3   | 5:B:144:LYS:HB2   | 1.99                     | 0.44              |
| 6:S:369:ARG:NH2   | 6:T:392:LEU:OXT   | 2.49                     | 0.44              |
| 1:p:39:LEU:HD22   | 1:p:44:ILE:HD11   | 1.99                     | 0.44              |
| 6:n:271:GLU:HA    | 6:n:274:VAL:HG22  | 1.99                     | 0.44              |
| 1:AF:174:SER:O    | 1:AF:174:SER:OG   | 2.35                     | 0.44              |
| 5:Q:35:PHE:HD1    | 6:X:372:GLN:HB2   | 1.83                     | 0.44              |
| 6:T:363:ASP:OD1   | 6:T:363:ASP:N     | 2.50                     | 0.44              |
| 6:g:174:ASP:OD2   | 6:g:174:ASP:N     | 2.46                     | 0.44              |
| 6:g:200:ASN:O     | 6:g:204:THR:OG1   | 2.27                     | 0.44              |
| 6:l:268:SER:OG    | 6:l:271:GLU:OE1   | 2.32                     | 0.44              |
| 1:w:177:ASP:N     | 1:w:177:ASP:OD1   | 2.48                     | 0.44              |
| 2:2:26:CYS:HB2    | 2:2:30:PHE:HE2    | 1.83                     | 0.44              |
| 6:U:263:GLN:NE2   | 6:U:295:ASP:OD1   | 2.50                     | 0.44              |
| 1:AE:168:LYS:NZ   | 1:AE:180:TYR:O    | 2.41                     | 0.44              |
| 5:A:41:SER:O      | 5:A:41:SER:OG     | 2.35                     | 0.44              |
| 5:N:116:ASN:OD1   | 5:N:116:ASN:N     | 2.51                     | 0.44              |
| 6:U:262:ARG:HA    | 6:U:293:LEU:HD23  | 2.00                     | 0.44              |
| 6:Y:340:ARG:NH1   | 1:w:166:ASP:OD1   | 2.51                     | 0.44              |
| 6:j:364:ASP:OD1   | 6:j:364:ASP:N     | 2.43                     | 0.44              |
| 1:u:33:ASN:OD1    | 1:u:48:LYS:NZ     | 2.49                     | 0.44              |
| 1:AD:148:LEU:HD22 | 1:AD:171:LEU:HD13 | 2.00                     | 0.44              |
| 1:AE:173:ASN:OD1  | 1:AE:173:ASN:N    | 2.50                     | 0.44              |
| 6:E:232:ILE:HG21  | 6:E:248:ILE:HD12  | 2.00                     | 0.44              |
| 5:K:38:LYS:HG2    | 6:l:388:PHE:HE1   | 1.83                     | 0.44              |
| 5:L:42:LEU:HD12   | 5:L:66:LYS:HB2    | 2.00                     | 0.44              |
| 6:h:221:ARG:HE    | 6:h:221:ARG:HB3   | 1.69                     | 0.44              |
| 6:l:174:ASP:OD2   | 6:l:174:ASP:N     | 2.51                     | 0.44              |
| 6:l:356:GLN:NE2   | 6:m:310:GLN:OE1   | 2.51                     | 0.44              |
| 4:7:33:VAL:HG11   | 4:7:48:PRO:HB3    | 1.99                     | 0.43              |
| 5:Q:158:MET:HE3   | 5:Q:158:MET:HB3   | 1.95                     | 0.43              |
| 6:e:356:GLN:NE2   | 6:f:310:GLN:OE1   | 2.49                     | 0.43              |
| 6:i:295:ASP:HB3   | 6:i:298:THR:HG22  | 1.99                     | 0.43              |
| 6:n:258:PHE:HB3   | 6:n:291:ILE:HG12  | 1.99                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:0:3:ASN:O       | 2:0:6:SER:OG     | 2.36                     | 0.43              |
| 6:E:263:GLN:NE2   | 6:E:295:ASP:OD1  | 2.51                     | 0.43              |
| 1:q:20:ASP:OD1    | 1:q:20:ASP:N     | 2.50                     | 0.43              |
| 1:AJ:173:ASN:HD21 | 1:AK:184:SER:HB3 | 1.83                     | 0.43              |
| 5:N:109:ASN:OD1   | 5:N:109:ASN:N    | 2.50                     | 0.43              |
| 5:I:38:LYS:NZ     | 6:j:369:ARG:O    | 2.44                     | 0.43              |
| 6:V:316:ARG:HH21  | 6:V:318:ASN:HD21 | 1.66                     | 0.43              |
| 6:j:295:ASP:HB3   | 6:j:298:THR:HG22 | 1.99                     | 0.43              |
| 6:k:363:ASP:OD2   | 6:k:363:ASP:N    | 2.48                     | 0.43              |
| 2:2:38:ARG:HD2    | 2:2:47:PRO:HD2   | 1.98                     | 0.43              |
| 1:AH:201:PRO:HB3  | 6:j:213:ARG:HD3  | 2.01                     | 0.43              |
| 6:Y:213:ARG:NH2   | 1:v:43:ASN:O     | 2.51                     | 0.43              |
| 6:Z:364:ASP:OD1   | 6:Z:364:ASP:N    | 2.51                     | 0.43              |
| 6:b:380:LYS:HE3   | 6:b:380:LYS:HB3  | 1.76                     | 0.43              |
| 6:l:213:ARG:NH2   | 1:AK:43:ASN:O    | 2.52                     | 0.43              |
| 2:1:154:GLU:OE2   | 2:1:219:TYR:OH   | 2.37                     | 0.43              |
| 6:E:258:PHE:HB3   | 6:E:291:ILE:HG12 | 2.00                     | 0.43              |
| 6:S:213:ARG:HD3   | 1:p:201:PRO:HB3  | 2.00                     | 0.43              |
| 6:X:258:PHE:HB3   | 6:X:291:ILE:HG12 | 2.00                     | 0.43              |
| 1:AA:20:ASP:OD1   | 1:AA:20:ASP:N    | 2.51                     | 0.43              |
| 2:3:88:LEU:HA     | 2:3:91:HIS:HB2   | 2.00                     | 0.43              |
| 5:B:116:ASN:OD1   | 5:B:116:ASN:N    | 2.52                     | 0.43              |
| 6:S:363:ASP:OD1   | 6:S:363:ASP:N    | 2.46                     | 0.43              |
| 6:T:252:GLU:HA    | 6:T:253:PRO:HD3  | 1.91                     | 0.43              |
| 6:b:369:ARG:NH1   | 6:c:392:LEU:OXT  | 2.52                     | 0.43              |
| 6:f:299:ALA:O     | 6:f:346:TYR:OH   | 2.37                     | 0.43              |
| 1:AG:94:LEU:HD23  | 1:AG:94:LEU:HA   | 1.88                     | 0.43              |
| 5:C:144:LYS:HD3   | 5:C:144:LYS:HA   | 1.88                     | 0.43              |
| 5:P:116:ASN:OD1   | 5:P:116:ASN:N    | 2.52                     | 0.43              |
| 6:U:245:TYR:OH    | 6:U:353:ARG:NH1  | 2.52                     | 0.43              |
| 6:X:333:ASP:OD1   | 6:X:333:ASP:N    | 2.52                     | 0.43              |
| 6:b:274:VAL:HG12  | 6:b:278:LYS:HE2  | 1.99                     | 0.43              |
| 6:g:208:ARG:HG3   | 6:g:222:VAL:HG11 | 2.01                     | 0.43              |
| 1:r:22:ASP:OD2    | 1:r:22:ASP:N     | 2.50                     | 0.43              |
| 5:J:113:SER:HA    | 5:J:146:THR:HA   | 2.01                     | 0.43              |
| 1:z:39:LEU:HB3    | 1:z:44:ILE:HG13  | 2.01                     | 0.43              |
| 2:2:25:THR:OG1    | 2:2:26:CYS:N     | 2.50                     | 0.43              |
| 5:C:44:THR:HG23   | 6:b:380:LYS:HE2  | 2.00                     | 0.43              |
| 5:F:42:LEU:HD12   | 5:F:66:LYS:HB2   | 2.01                     | 0.43              |
| 5:K:93:TYR:HB2    | 5:K:152:PRO:HG2  | 2.00                     | 0.43              |
| 5:M:28:ILE:HD11   | 6:R:389:PRO:HG3  | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:O:114:LEU:HD12 | 5:O:117:VAL:HB   | 2.01                     | 0.43              |
| 6:W:340:ARG:HH22 | 1:u:163:GLN:HE21 | 1.67                     | 0.43              |
| 6:k:327:ILE:HD12 | 6:k:359:ILE:HG12 | 2.00                     | 0.43              |
| 6:n:235:TRP:HE3  | 6:n:236:LEU:HD12 | 1.84                     | 0.43              |
| 1:s:173:ASN:OD1  | 1:s:173:ASN:N    | 2.48                     | 0.43              |
| 4:7:29:ILE:HD11  | 4:7:52:LYS:HA    | 2.01                     | 0.42              |
| 6:b:363:ASP:HB3  | 1:z:180:TYR:HD2  | 1.84                     | 0.42              |
| 6:d:299:ALA:O    | 6:d:346:TYR:OH   | 2.38                     | 0.42              |
| 6:m:192:LYS:HA   | 6:m:192:LYS:HD3  | 1.74                     | 0.42              |
| 1:AJ:36:ILE:HD11 | 1:AJ:48:LYS:HB2  | 2.01                     | 0.42              |
| 1:AC:53:LYS:HE2  | 1:AC:53:LYS:HB2  | 1.90                     | 0.42              |
| 5:P:114:LEU:HD13 | 5:P:117:VAL:HB   | 2.01                     | 0.42              |
| 6:S:243:LEU:HD12 | 6:S:243:LEU:HA   | 1.89                     | 0.42              |
| 6:U:316:ARG:HH21 | 6:U:318:ASN:HD21 | 1.68                     | 0.42              |
| 6:b:363:ASP:OD1  | 6:b:363:ASP:N    | 2.52                     | 0.42              |
| 2:2:48:SER:OG    | 2:2:51:THR:N     | 2.45                     | 0.42              |
| 1:AI:78:PRO:HA   | 1:AI:79:PRO:HD3  | 1.88                     | 0.42              |
| 5:G:118:SER:OG   | 5:G:119:LEU:N    | 2.53                     | 0.42              |
| 5:N:108:ARG:HD3  | 5:N:153:PRO:HB3  | 2.00                     | 0.42              |
| 6:Y:263:GLN:NE2  | 6:Y:295:ASP:OD1  | 2.53                     | 0.42              |
| 6:l:316:ARG:HH21 | 6:l:318:ASN:HD21 | 1.67                     | 0.42              |
| 1:AA:37:ALA:HB2  | 1:z:69:VAL:HG12  | 2.02                     | 0.42              |
| 6:E:365:TRP:HD1  | 6:E:390:SER:HB2  | 1.84                     | 0.42              |
| 6:V:381:MET:H    | 6:V:381:MET:HG2  | 1.67                     | 0.42              |
| 6:Z:326:VAL:HA   | 6:Z:358:ALA:HB3  | 2.00                     | 0.42              |
| 6:g:270:LYS:HD2  | 6:g:270:LYS:HA   | 1.77                     | 0.42              |
| 6:k:381:MET:HE3  | 6:k:381:MET:HB3  | 1.94                     | 0.42              |
| 1:o:96:SER:O     | 1:o:96:SER:OG    | 2.35                     | 0.42              |
| 1:p:23:LEU:O     | 1:q:48:LYS:NZ    | 2.52                     | 0.42              |
| 1:u:169:ARG:HA   | 1:u:169:ARG:HD2  | 1.89                     | 0.42              |
| 2:1:43:LEU:HD23  | 2:1:46:ILE:HD12  | 2.02                     | 0.42              |
| 2:2:166:TYR:HB3  | 2:3:196:PRO:HG3  | 2.02                     | 0.42              |
| 4:7:3:ASP:OD2    | 4:7:3:ASP:N      | 2.41                     | 0.42              |
| 1:AL:165:SER:HB2 | 6:f:361:LEU:HD13 | 2.02                     | 0.42              |
| 6:g:229:ASN:HD21 | 6:g:247:ARG:HD2  | 1.85                     | 0.42              |
| 6:h:363:ASP:OD1  | 6:h:363:ASP:N    | 2.47                     | 0.42              |
| 6:m:200:ASN:OD1  | 6:m:200:ASN:N    | 2.51                     | 0.42              |
| 1:AJ:50:ASP:OD1  | 1:AJ:51:SER:N    | 2.53                     | 0.42              |
| 1:AA:85:ILE:HB   | 1:AA:107:SER:HB2 | 2.02                     | 0.42              |
| 3:5:131:MET:HE2  | 3:5:131:MET:HB2  | 1.88                     | 0.42              |
| 5:A:76:ASP:OD1   | 5:A:76:ASP:N     | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:N:144:LYS:HD2  | 5:N:144:LYS:HA   | 1.83                     | 0.42              |
| 5:O:39:ASP:H     | 5:O:69:THR:HB    | 1.85                     | 0.42              |
| 6:S:341:GLN:HE22 | 1:p:160:LEU:HD21 | 1.83                     | 0.42              |
| 6:Y:196:VAL:HG23 | 6:Y:222:VAL:HG13 | 2.01                     | 0.42              |
| 6:g:332:ASP:OD1  | 6:g:332:ASP:N    | 2.51                     | 0.42              |
| 6:j:363:ASP:OD1  | 6:j:363:ASP:N    | 2.45                     | 0.42              |
| 6:l:256:PRO:HG2  | 6:l:289:VAL:HG22 | 2.02                     | 0.42              |
| 1:AF:36:ILE:HD11 | 1:AF:48:LYS:HB2  | 2.01                     | 0.42              |
| 5:C:73:GLU:OE1   | 5:C:75:HIS:ND1   | 2.52                     | 0.42              |
| 6:V:260:LEU:HD12 | 6:V:260:LEU:HA   | 1.93                     | 0.42              |
| 6:X:252:GLU:HA   | 6:X:253:PRO:HD3  | 1.90                     | 0.42              |
| 6:f:300:ALA:HB2  | 6:f:354:TYR:HE2  | 1.85                     | 0.42              |
| 1:p:23:LEU:HD21  | 1:p:68:ALA:HB1   | 2.01                     | 0.42              |
| 1:s:78:PRO:HA    | 1:s:79:PRO:HD3   | 1.90                     | 0.42              |
| 1:x:146:VAL:HG13 | 1:x:178:VAL:HG12 | 2.01                     | 0.42              |
| 1:AJ:203:LYS:HD2 | 1:AJ:203:LYS:HA  | 1.86                     | 0.42              |
| 1:AA:82:ARG:H    | 1:AA:82:ARG:HG2  | 1.67                     | 0.42              |
| 1:AG:93:SER:OG   | 1:AG:95:VAL:O    | 2.35                     | 0.42              |
| 5:I:44:THR:HB    | 6:j:380:LYS:HE2  | 2.02                     | 0.42              |
| 5:O:27:LYS:HE3   | 5:O:27:LYS:HB2   | 1.77                     | 0.42              |
| 6:W:336:ILE:HD11 | 6:W:361:LEU:HD21 | 2.01                     | 0.42              |
| 6:b:209:GLN:HG2  | 1:y:43:ASN:HB3   | 2.02                     | 0.42              |
| 6:g:252:GLU:HA   | 6:g:253:PRO:HD3  | 1.88                     | 0.42              |
| 6:j:258:PHE:HB3  | 6:j:291:ILE:HG12 | 2.02                     | 0.42              |
| 1:AB:25:LYS:H    | 1:AC:29:GLN:NE2  | 2.18                     | 0.42              |
| 1:AC:39:LEU:HD22 | 1:AC:44:ILE:HD11 | 2.02                     | 0.42              |
| 6:E:364:ASP:N    | 6:E:364:ASP:OD1  | 2.52                     | 0.42              |
| 5:L:97:GLN:HE22  | 5:M:139:ARG:HE   | 1.68                     | 0.42              |
| 5:L:144:LYS:HA   | 5:L:144:LYS:HD3  | 1.88                     | 0.42              |
| 6:X:337:LEU:HD13 | 1:u:164:ILE:HD11 | 2.00                     | 0.42              |
| 6:Z:248:ILE:HG12 | 6:Z:258:PHE:HD1  | 1.85                     | 0.42              |
| 6:k:232:ILE:HG13 | 6:k:282:LEU:HD23 | 2.01                     | 0.42              |
| 6:l:232:ILE:HG22 | 6:l:282:LEU:HD13 | 2.02                     | 0.42              |
| 1:AF:78:PRO:HA   | 1:AF:79:PRO:HD3  | 1.96                     | 0.41              |
| 5:L:169:GLN:HE22 | 5:M:115:ARG:HA   | 1.85                     | 0.41              |
| 5:N:109:ASN:HB3  | 5:N:150:SER:HB3  | 2.02                     | 0.41              |
| 6:X:235:TRP:CD2  | 6:X:282:LEU:HD11 | 2.55                     | 0.41              |
| 1:t:25:LYS:H     | 1:u:29:GLN:NE2   | 2.18                     | 0.41              |
| 1:u:110:GLU:OE2  | 1:u:132:TYR:OH   | 2.34                     | 0.41              |
| 1:w:160:LEU:HA   | 1:w:163:GLN:HG2  | 2.02                     | 0.41              |
| 1:z:174:SER:O    | 1:z:174:SER:OG   | 2.36                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AB:139:ASN:HB3  | 1:AB:141:ARG:HG2  | 2.01                     | 0.41              |
| 1:AC:177:ASP:OD1  | 1:AC:177:ASP:N    | 2.52                     | 0.41              |
| 1:AG:51:SER:O     | 1:AG:51:SER:OG    | 2.35                     | 0.41              |
| 4:8:24:ILE:O      | 4:8:28:ILE:HG12   | 2.20                     | 0.41              |
| 5:C:93:TYR:HB2    | 5:C:152:PRO:HG2   | 2.00                     | 0.41              |
| 6:R:337:LEU:HD13  | 1:o:164:ILE:HD11  | 2.03                     | 0.41              |
| 6:Z:270:LYS:HE2   | 6:Z:270:LYS:HB2   | 1.91                     | 0.41              |
| 6:h:299:ALA:O     | 6:h:346:TYR:OH    | 2.35                     | 0.41              |
| 1:AJ:102:LYS:HE3  | 1:AJ:102:LYS:HB2  | 1.92                     | 0.41              |
| 1:AJ:164:ILE:HG23 | 1:AJ:185:VAL:HB   | 2.02                     | 0.41              |
| 2:1:152:LEU:HD23  | 2:1:152:LEU:HA    | 1.85                     | 0.41              |
| 5:D:114:LEU:HD21  | 5:D:163:ALA:HB1   | 2.03                     | 0.41              |
| 5:K:152:PRO:HA    | 5:K:153:PRO:HD3   | 1.93                     | 0.41              |
| 5:P:144:LYS:HA    | 5:P:144:LYS:HD3   | 1.86                     | 0.41              |
| 6:X:380:LYS:HE3   | 6:X:380:LYS:HB3   | 1.93                     | 0.41              |
| 1:u:99:ARG:HE     | 1:u:134:ILE:HD12  | 1.85                     | 0.41              |
| 1:AC:203:LYS:HB3  | 1:AC:203:LYS:HE3  | 1.88                     | 0.41              |
| 1:AD:110:GLU:HB3  | 1:AD:130:ILE:HG12 | 2.03                     | 0.41              |
| 1:AH:37:ALA:HB2   | 1:AI:69:VAL:HG12  | 2.02                     | 0.41              |
| 5:D:116:ASN:OD1   | 5:D:116:ASN:N     | 2.52                     | 0.41              |
| 1:y:78:PRO:HA     | 1:y:79:PRO:HD3    | 1.94                     | 0.41              |
| 1:y:184:SER:HB3   | 1:z:173:ASN:HD21  | 1.85                     | 0.41              |
| 1:AF:192:ASP:O    | 6:n:202:ARG:NH1   | 2.51                     | 0.41              |
| 2:0:93:ASP:OD2    | 2:0:93:ASP:N      | 2.54                     | 0.41              |
| 5:F:116:ASN:OD1   | 5:F:116:ASN:N     | 2.53                     | 0.41              |
| 6:S:304:GLU:OE1   | 6:S:316:ARG:NH1   | 2.52                     | 0.41              |
| 1:v:146:VAL:HG13  | 1:v:178:VAL:HG12  | 2.02                     | 0.41              |
| 1:x:31:GLN:HG2    | 1:x:79:PRO:HD2    | 2.02                     | 0.41              |
| 1:AA:28:ASP:OD1   | 1:AA:28:ASP:N     | 2.51                     | 0.41              |
| 6:E:317:ARG:HB2   | 6:E:324:THR:HG23  | 2.02                     | 0.41              |
| 6:R:200:ASN:O     | 6:R:204:THR:OG1   | 2.28                     | 0.41              |
| 6:T:365:TRP:HD1   | 6:T:390:SER:HB2   | 1.85                     | 0.41              |
| 6:e:252:GLU:HA    | 6:e:253:PRO:HD3   | 1.93                     | 0.41              |
| 6:h:262:ARG:NH1   | 6:h:295:ASP:OD1   | 2.49                     | 0.41              |
| 6:l:230:LYS:HB2   | 6:l:230:LYS:HE3   | 1.87                     | 0.41              |
| 1:r:85:ILE:HB     | 1:r:107:SER:HB2   | 2.02                     | 0.41              |
| 1:y:23:LEU:HD11   | 1:y:68:ALA:HB1    | 2.02                     | 0.41              |
| 1:AD:85:ILE:HB    | 1:AD:107:SER:HB2  | 2.03                     | 0.41              |
| 5:O:36:VAL:HG23   | 6:U:373:TYR:HE1   | 1.86                     | 0.41              |
| 5:O:42:LEU:HD23   | 5:O:42:LEU:HA     | 1.92                     | 0.41              |
| 1:AL:99:ARG:HE    | 1:AL:134:ILE:HD12 | 1.86                     | 0.41              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:r:135:ASP:O     | 1:r:139:ASN:ND2  | 2.54                     | 0.41              |
| 2:1:172:VAL:HG22  | 4:6:71:LEU:HD13  | 2.02                     | 0.41              |
| 5:I:114:LEU:HD21  | 5:I:163:ALA:HB1  | 2.03                     | 0.41              |
| 6:X:318:ASN:HD22  | 6:X:323:VAL:HG22 | 1.84                     | 0.41              |
| 6:a:188:PRO:HA    | 6:a:194:LEU:HD12 | 2.02                     | 0.41              |
| 6:m:320:LYS:HE2   | 6:m:320:LYS:HB3  | 1.92                     | 0.41              |
| 1:r:173:ASN:OD1   | 1:r:173:ASN:N    | 2.49                     | 0.41              |
| 1:w:25:LYS:HE2    | 1:w:25:LYS:HB3   | 1.82                     | 0.41              |
| 1:AG:164:ILE:HG23 | 1:AG:185:VAL:HB  | 2.03                     | 0.41              |
| 2:2:43:LEU:HB3    | 2:2:46:ILE:HG12  | 2.03                     | 0.41              |
| 2:3:187:MET:HE3   | 2:3:187:MET:HB3  | 1.81                     | 0.41              |
| 6:E:235:TRP:CD2   | 6:E:282:LEU:HD11 | 2.56                     | 0.41              |
| 5:I:36:VAL:HG23   | 6:j:373:TYR:HE1  | 1.86                     | 0.41              |
| 5:K:97:GLN:HE21   | 5:L:137:PRO:HD2  | 1.85                     | 0.41              |
| 5:Q:42:LEU:HD23   | 5:Q:42:LEU:HA    | 1.91                     | 0.41              |
| 6:X:323:VAL:O     | 6:X:355:VAL:HA   | 2.20                     | 0.41              |
| 6:f:221:ARG:HE    | 6:f:221:ARG:HB3  | 1.76                     | 0.41              |
| 6:h:200:ASN:OD1   | 6:h:200:ASN:N    | 2.54                     | 0.41              |
| 1:o:53:LYS:HA     | 1:o:53:LYS:HD3   | 1.75                     | 0.41              |
| 1:o:135:ASP:OD1   | 1:o:135:ASP:N    | 2.42                     | 0.41              |
| 1:t:24:LEU:HD13   | 1:t:27:LEU:HD11  | 2.03                     | 0.41              |
| 2:4:23:SER:HB3    | 3:5:45:ALA:HB1   | 2.02                     | 0.41              |
| 5:A:51:LEU:HD22   | 5:B:87:GLN:HG2   | 2.03                     | 0.41              |
| 5:K:42:LEU:HD11   | 5:K:88:LEU:HD23  | 2.03                     | 0.41              |
| 6:R:235:TRP:CD2   | 6:R:282:LEU:HD11 | 2.56                     | 0.41              |
| 6:n:200:ASN:OD1   | 6:n:200:ASN:N    | 2.54                     | 0.41              |
| 1:x:117:LEU:O     | 1:x:123:VAL:HG21 | 2.21                     | 0.41              |
| 1:AC:36:ILE:HD11  | 1:AC:48:LYS:HB2  | 2.03                     | 0.40              |
| 2:2:8:ILE:HD12    | 2:2:8:ILE:HA     | 1.94                     | 0.40              |
| 3:5:239:VAL:O     | 3:5:243:SER:OG   | 2.38                     | 0.40              |
| 4:9:22:PRO:HA     | 4:9:25:VAL:HG12  | 2.02                     | 0.40              |
| 5:B:109:ASN:OD1   | 5:B:109:ASN:N    | 2.54                     | 0.40              |
| 6:E:188:PRO:HA    | 6:E:194:LEU:HD12 | 2.02                     | 0.40              |
| 6:d:200:ASN:O     | 6:d:204:THR:OG1  | 2.28                     | 0.40              |
| 6:i:221:ARG:HE    | 6:i:221:ARG:HB3  | 1.73                     | 0.40              |
| 1:t:117:LEU:HD23  | 1:t:117:LEU:HA   | 1.89                     | 0.40              |
| 5:K:76:ASP:HA     | 5:K:77:PRO:HD3   | 1.94                     | 0.40              |
| 6:W:269:LYS:HA    | 6:W:269:LYS:HD2  | 1.98                     | 0.40              |
| 6:Y:272:LEU:HD23  | 6:Y:272:LEU:HA   | 1.90                     | 0.40              |
| 1:r:154:TYR:HE2   | 1:r:187:LEU:HD22 | 1.86                     | 0.40              |
| 1:x:78:PRO:HA     | 1:x:79:PRO:HD3   | 1.94                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AK:160:LEU:HD12 | 1:AK:187:LEU:HD12 | 2.03                     | 0.40              |
| 2:4:34:PHE:HB3    | 2:4:52:LEU:HD23   | 2.03                     | 0.40              |
| 2:4:47:PRO:O      | 2:4:51:THR:OG1    | 2.39                     | 0.40              |
| 5:K:90:LEU:HA     | 5:K:103:ASP:HA    | 2.04                     | 0.40              |
| 6:Z:248:ILE:HG12  | 6:Z:258:PHE:CD1   | 2.56                     | 0.40              |
| 6:Z:256:PRO:HG2   | 6:Z:289:VAL:HG22  | 2.04                     | 0.40              |
| 6:g:366:LEU:H     | 6:g:366:LEU:HG    | 1.82                     | 0.40              |
| 6:m:236:LEU:HD12  | 6:m:236:LEU:HA    | 1.93                     | 0.40              |
| 1:o:177:ASP:N     | 1:o:177:ASP:OD1   | 2.55                     | 0.40              |
| 1:q:85:ILE:HB     | 1:q:107:SER:HB2   | 2.03                     | 0.40              |
| 1:AA:160:LEU:HD12 | 6:d:337:LEU:HD21  | 2.04                     | 0.40              |
| 6:E:316:ARG:NE    | 6:E:318:ASN:OD1   | 2.55                     | 0.40              |
| 6:c:236:LEU:HD12  | 6:c:236:LEU:HA    | 1.93                     | 0.40              |
| 6:d:247:ARG:NH1   | 6:d:348:ARG:O     | 2.54                     | 0.40              |
| 6:h:332:ASP:OD1   | 6:h:332:ASP:N     | 2.37                     | 0.40              |
| 6:k:299:ALA:O     | 6:k:346:TYR:OH    | 2.39                     | 0.40              |
| 1:q:82:ARG:H      | 1:q:82:ARG:HG2    | 1.75                     | 0.40              |
| 1:AD:95:VAL:HG13  | 4:9:66:TRP:HB2    | 2.03                     | 0.40              |
| 3:5:18:LEU:HD23   | 3:5:55:TRP:HH2    | 1.85                     | 0.40              |
| 4:9:37:GLN:HE21   | 4:9:47:LEU:HD23   | 1.86                     | 0.40              |
| 5:D:80:LEU:HD12   | 6:c:375:ALA:HB2   | 2.03                     | 0.40              |
| 5:J:152:PRO:HA    | 5:J:153:PRO:HD3   | 1.91                     | 0.40              |
| 5:L:118:SER:OG    | 5:L:121:GLU:OE1   | 2.29                     | 0.40              |
| 6:S:316:ARG:HH21  | 6:S:318:ASN:HD21  | 1.69                     | 0.40              |
| 6:W:262:ARG:HA    | 6:W:293:LEU:HD23  | 2.04                     | 0.40              |
| 6:Y:299:ALA:O     | 6:Y:346:TYR:OH    | 2.40                     | 0.40              |
| 6:b:258:PHE:HB3   | 6:b:291:ILE:HG12  | 2.03                     | 0.40              |
| 6:d:261:SER:OG    | 6:d:262:ARG:N     | 2.53                     | 0.40              |
| 6:i:332:ASP:OD1   | 6:i:332:ASP:N     | 2.44                     | 0.40              |
| 1:t:53:LYS:HD3    | 1:t:53:LYS:HA     | 1.89                     | 0.40              |
| 1:x:169:ARG:HH11  | 1:x:180:TYR:HH    | 1.65                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | AA    | 182/252 (72%) | 174 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 1   | AB    | 182/252 (72%) | 178 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | AC    | 182/252 (72%) | 175 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AD    | 182/252 (72%) | 175 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AE    | 182/252 (72%) | 177 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | AF    | 182/252 (72%) | 176 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AG    | 182/252 (72%) | 176 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AH    | 182/252 (72%) | 175 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AI    | 182/252 (72%) | 176 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AJ    | 182/252 (72%) | 178 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | AK    | 182/252 (72%) | 175 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AL    | 182/252 (72%) | 177 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | o     | 182/252 (72%) | 176 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | p     | 182/252 (72%) | 172 (94%) | 10 (6%) | 0        | 100         | 100 |
| 1   | q     | 182/252 (72%) | 176 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | r     | 182/252 (72%) | 174 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 1   | s     | 182/252 (72%) | 175 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | t     | 182/252 (72%) | 179 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | u     | 182/252 (72%) | 178 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | v     | 182/252 (72%) | 175 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | w     | 182/252 (72%) | 177 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | x     | 182/252 (72%) | 175 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | y     | 182/252 (72%) | 176 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | z     | 182/252 (72%) | 174 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 2   | 0     | 183/224 (82%) | 178 (97%) | 4 (2%)  | 1 (0%)   | 24          | 57  |
| 2   | 1     | 183/224 (82%) | 176 (96%) | 6 (3%)  | 1 (0%)   | 24          | 57  |
| 2   | 2     | 181/224 (81%) | 174 (96%) | 6 (3%)  | 1 (1%)   | 21          | 54  |
| 2   | 3     | 188/224 (84%) | 185 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 2   | 4     | 208/224 (93%) | 199 (96%) | 9 (4%)  | 0        | 100         | 100 |
| 3   | 5     | 222/263 (84%) | 216 (97%) | 6 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 4   | 6     | 49/86 (57%)   | 48 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 4   | 7     | 82/86 (95%)   | 80 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 4   | 8     | 82/86 (95%)   | 79 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 4   | 9     | 82/86 (95%)   | 81 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 5   | A     | 137/562 (24%) | 136 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 5   | B     | 143/562 (25%) | 139 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 5   | C     | 137/562 (24%) | 134 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 5   | D     | 142/562 (25%) | 138 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 5   | F     | 137/562 (24%) | 135 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 5   | G     | 143/562 (25%) | 137 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 5   | H     | 137/562 (24%) | 134 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 5   | I     | 143/562 (25%) | 141 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 5   | J     | 137/562 (24%) | 135 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 5   | K     | 143/562 (25%) | 139 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 5   | L     | 137/562 (24%) | 135 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 5   | M     | 142/562 (25%) | 137 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 5   | N     | 137/562 (24%) | 134 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 5   | O     | 143/562 (25%) | 140 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 5   | P     | 137/562 (24%) | 136 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 5   | Q     | 143/562 (25%) | 139 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 6   | E     | 220/392 (56%) | 213 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 6   | R     | 219/392 (56%) | 213 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 6   | S     | 220/392 (56%) | 208 (94%) | 12 (6%) | 0        | 100         | 100 |
| 6   | T     | 220/392 (56%) | 210 (96%) | 10 (4%) | 0        | 100         | 100 |
| 6   | U     | 219/392 (56%) | 212 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 6   | V     | 220/392 (56%) | 207 (94%) | 13 (6%) | 0        | 100         | 100 |
| 6   | W     | 220/392 (56%) | 212 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 6   | X     | 219/392 (56%) | 213 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 6   | Y     | 220/392 (56%) | 205 (93%) | 15 (7%) | 0        | 100         | 100 |
| 6   | Z     | 220/392 (56%) | 210 (96%) | 10 (4%) | 0        | 100         | 100 |
| 6   | a     | 219/392 (56%) | 213 (97%) | 6 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 6   | b     | 220/392 (56%)     | 206 (94%)   | 14 (6%)  | 0        | 100         | 100 |
| 6   | c     | 220/392 (56%)     | 211 (96%)   | 9 (4%)   | 0        | 100         | 100 |
| 6   | d     | 219/392 (56%)     | 212 (97%)   | 7 (3%)   | 0        | 100         | 100 |
| 6   | e     | 220/392 (56%)     | 208 (94%)   | 12 (6%)  | 0        | 100         | 100 |
| 6   | f     | 220/392 (56%)     | 209 (95%)   | 11 (5%)  | 0        | 100         | 100 |
| 6   | g     | 219/392 (56%)     | 210 (96%)   | 9 (4%)   | 0        | 100         | 100 |
| 6   | h     | 220/392 (56%)     | 207 (94%)   | 13 (6%)  | 0        | 100         | 100 |
| 6   | i     | 220/392 (56%)     | 212 (96%)   | 8 (4%)   | 0        | 100         | 100 |
| 6   | j     | 219/392 (56%)     | 212 (97%)   | 7 (3%)   | 0        | 100         | 100 |
| 6   | k     | 220/392 (56%)     | 205 (93%)   | 15 (7%)  | 0        | 100         | 100 |
| 6   | l     | 220/392 (56%)     | 210 (96%)   | 10 (4%)  | 0        | 100         | 100 |
| 6   | m     | 219/392 (56%)     | 214 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 6   | n     | 220/392 (56%)     | 207 (94%)   | 13 (6%)  | 0        | 100         | 100 |
| All | All   | 13338/26175 (51%) | 12863 (96%) | 472 (4%) | 3 (0%)   | 100         | 100 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 0     | 49  | ASN  |
| 2   | 2     | 47  | PRO  |
| 2   | 1     | 49  | ASN  |

### 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   | AA    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | AB    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | AC    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | AD    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | AE    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | AF    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | AG    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | AH    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | AI    | 155/215 (72%) | 153 (99%)  | 2 (1%)   | 61          | 72  |
| 1   | AJ    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | AK    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | AL    | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | o     | 155/215 (72%) | 154 (99%)  | 1 (1%)   | 78          | 79  |
| 1   | p     | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | q     | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | r     | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | s     | 155/215 (72%) | 154 (99%)  | 1 (1%)   | 78          | 79  |
| 1   | t     | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | u     | 155/215 (72%) | 154 (99%)  | 1 (1%)   | 78          | 79  |
| 1   | v     | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | w     | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | x     | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | y     | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 1   | z     | 155/215 (72%) | 155 (100%) | 0        | 100         | 100 |
| 2   | 0     | 162/199 (81%) | 161 (99%)  | 1 (1%)   | 78          | 79  |
| 2   | 1     | 164/199 (82%) | 161 (98%)  | 3 (2%)   | 51          | 69  |
| 2   | 2     | 164/199 (82%) | 164 (100%) | 0        | 100         | 100 |
| 2   | 3     | 170/199 (85%) | 167 (98%)  | 3 (2%)   | 51          | 69  |
| 2   | 4     | 187/199 (94%) | 187 (100%) | 0        | 100         | 100 |
| 3   | 5     | 187/219 (85%) | 186 (100%) | 1 (0%)   | 81          | 80  |
| 4   | 6     | 41/71 (58%)   | 41 (100%)  | 0        | 100         | 100 |
| 4   | 7     | 69/71 (97%)   | 69 (100%)  | 0        | 100         | 100 |
| 4   | 8     | 69/71 (97%)   | 68 (99%)   | 1 (1%)   | 59          | 71  |
| 4   | 9     | 70/71 (99%)   | 70 (100%)  | 0        | 100         | 100 |
| 5   | A     | 119/477 (25%) | 119 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 5   | B     | 125/477 (26%) | 125 (100%) | 0        | 100         | 100 |
| 5   | C     | 119/477 (25%) | 119 (100%) | 0        | 100         | 100 |
| 5   | D     | 124/477 (26%) | 124 (100%) | 0        | 100         | 100 |
| 5   | F     | 119/477 (25%) | 118 (99%)  | 1 (1%)   | 73          | 77  |
| 5   | G     | 125/477 (26%) | 125 (100%) | 0        | 100         | 100 |
| 5   | H     | 119/477 (25%) | 119 (100%) | 0        | 100         | 100 |
| 5   | I     | 125/477 (26%) | 125 (100%) | 0        | 100         | 100 |
| 5   | J     | 119/477 (25%) | 119 (100%) | 0        | 100         | 100 |
| 5   | K     | 125/477 (26%) | 125 (100%) | 0        | 100         | 100 |
| 5   | L     | 119/477 (25%) | 119 (100%) | 0        | 100         | 100 |
| 5   | M     | 124/477 (26%) | 124 (100%) | 0        | 100         | 100 |
| 5   | N     | 119/477 (25%) | 118 (99%)  | 1 (1%)   | 73          | 77  |
| 5   | O     | 125/477 (26%) | 125 (100%) | 0        | 100         | 100 |
| 5   | P     | 119/477 (25%) | 118 (99%)  | 1 (1%)   | 73          | 77  |
| 5   | Q     | 125/477 (26%) | 125 (100%) | 0        | 100         | 100 |
| 6   | E     | 190/337 (56%) | 190 (100%) | 0        | 100         | 100 |
| 6   | R     | 189/337 (56%) | 187 (99%)  | 2 (1%)   | 65          | 74  |
| 6   | S     | 188/337 (56%) | 187 (100%) | 1 (0%)   | 81          | 80  |
| 6   | T     | 190/337 (56%) | 188 (99%)  | 2 (1%)   | 65          | 74  |
| 6   | U     | 189/337 (56%) | 188 (100%) | 1 (0%)   | 81          | 80  |
| 6   | V     | 188/337 (56%) | 186 (99%)  | 2 (1%)   | 65          | 74  |
| 6   | W     | 190/337 (56%) | 189 (100%) | 1 (0%)   | 81          | 80  |
| 6   | X     | 189/337 (56%) | 188 (100%) | 1 (0%)   | 81          | 80  |
| 6   | Y     | 188/337 (56%) | 187 (100%) | 1 (0%)   | 81          | 80  |
| 6   | Z     | 190/337 (56%) | 190 (100%) | 0        | 100         | 100 |
| 6   | a     | 189/337 (56%) | 187 (99%)  | 2 (1%)   | 65          | 74  |
| 6   | b     | 188/337 (56%) | 187 (100%) | 1 (0%)   | 81          | 80  |
| 6   | c     | 190/337 (56%) | 190 (100%) | 0        | 100         | 100 |
| 6   | d     | 189/337 (56%) | 188 (100%) | 1 (0%)   | 81          | 80  |
| 6   | e     | 188/337 (56%) | 186 (99%)  | 2 (1%)   | 65          | 74  |
| 6   | f     | 190/337 (56%) | 189 (100%) | 1 (0%)   | 81          | 80  |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 6   | g     | 189/337 (56%)     | 185 (98%)    | 4 (2%)   | 47          | 66  |
| 6   | h     | 188/337 (56%)     | 188 (100%)   | 0        | 100         | 100 |
| 6   | i     | 190/337 (56%)     | 189 (100%)   | 1 (0%)   | 81          | 80  |
| 6   | j     | 189/337 (56%)     | 188 (100%)   | 1 (0%)   | 81          | 80  |
| 6   | k     | 188/337 (56%)     | 187 (100%)   | 1 (0%)   | 81          | 80  |
| 6   | l     | 190/337 (56%)     | 190 (100%)   | 0        | 100         | 100 |
| 6   | m     | 189/337 (56%)     | 187 (99%)    | 2 (1%)   | 65          | 74  |
| 6   | n     | 188/337 (56%)     | 186 (99%)    | 2 (1%)   | 65          | 74  |
| All | All   | 11489/22378 (51%) | 11443 (100%) | 46 (0%)  | 81          | 81  |

All (46) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 0     | 167 | LEU  |
| 2   | 1     | 20  | ILE  |
| 2   | 1     | 64  | MET  |
| 2   | 1     | 166 | TYR  |
| 2   | 3     | 61  | MET  |
| 2   | 3     | 167 | LEU  |
| 2   | 3     | 217 | LEU  |
| 3   | 5     | 174 | ILE  |
| 4   | 8     | 72  | LEU  |
| 1   | AI    | 34  | GLU  |
| 1   | AI    | 133 | ASP  |
| 5   | F     | 111 | VAL  |
| 5   | N     | 111 | VAL  |
| 5   | P     | 111 | VAL  |
| 6   | R     | 355 | VAL  |
| 6   | R     | 366 | LEU  |
| 6   | S     | 355 | VAL  |
| 6   | T     | 222 | VAL  |
| 6   | T     | 355 | VAL  |
| 6   | U     | 366 | LEU  |
| 6   | V     | 176 | LEU  |
| 6   | V     | 222 | VAL  |
| 6   | W     | 222 | VAL  |
| 6   | X     | 366 | LEU  |
| 6   | Y     | 355 | VAL  |
| 6   | a     | 355 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | a     | 366 | LEU  |
| 6   | b     | 355 | VAL  |
| 6   | d     | 366 | LEU  |
| 6   | e     | 222 | VAL  |
| 6   | e     | 361 | LEU  |
| 6   | f     | 182 | GLU  |
| 6   | g     | 181 | LYS  |
| 6   | g     | 222 | VAL  |
| 6   | g     | 355 | VAL  |
| 6   | g     | 366 | LEU  |
| 6   | i     | 176 | LEU  |
| 6   | j     | 355 | VAL  |
| 6   | k     | 355 | VAL  |
| 6   | m     | 355 | VAL  |
| 6   | m     | 366 | LEU  |
| 6   | n     | 333 | ASP  |
| 6   | n     | 355 | VAL  |
| 1   | o     | 202 | VAL  |
| 1   | s     | 60  | VAL  |
| 1   | u     | 177 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 42  | HIS  |
| 1   | AB    | 29  | GLN  |
| 1   | AB    | 33  | ASN  |
| 1   | AC    | 47  | ASN  |
| 1   | AC    | 163 | GLN  |
| 1   | AF    | 47  | ASN  |
| 1   | AG    | 162 | HIS  |
| 2   | 0     | 44  | GLN  |
| 2   | 0     | 53  | ASN  |
| 2   | 1     | 117 | ASN  |
| 2   | 3     | 39  | ASN  |
| 2   | 3     | 113 | GLN  |
| 2   | 4     | 3   | ASN  |
| 2   | 4     | 123 | GLN  |
| 3   | 5     | 175 | ASN  |
| 4   | 7     | 43  | GLN  |
| 4   | 7     | 77  | GLN  |
| 4   | 8     | 37  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | 9     | 9   | ASN  |
| 4   | 9     | 37  | GLN  |
| 4   | 9     | 43  | GLN  |
| 1   | AI    | 162 | HIS  |
| 5   | A     | 71  | ASN  |
| 5   | A     | 87  | GLN  |
| 5   | A     | 109 | ASN  |
| 5   | B     | 87  | GLN  |
| 5   | B     | 135 | ASN  |
| 5   | B     | 169 | GLN  |
| 5   | B     | 170 | ASN  |
| 5   | C     | 123 | ASN  |
| 5   | D     | 87  | GLN  |
| 6   | E     | 199 | GLN  |
| 6   | E     | 263 | GLN  |
| 6   | E     | 341 | GLN  |
| 5   | F     | 71  | ASN  |
| 5   | G     | 123 | ASN  |
| 5   | G     | 124 | ASN  |
| 5   | G     | 169 | GLN  |
| 5   | G     | 170 | ASN  |
| 5   | H     | 97  | GLN  |
| 5   | I     | 87  | GLN  |
| 5   | K     | 87  | GLN  |
| 5   | K     | 97  | GLN  |
| 5   | K     | 123 | ASN  |
| 5   | K     | 169 | GLN  |
| 5   | K     | 170 | ASN  |
| 5   | L     | 87  | GLN  |
| 5   | L     | 169 | GLN  |
| 5   | M     | 123 | ASN  |
| 5   | M     | 142 | ASN  |
| 5   | M     | 161 | ASN  |
| 5   | M     | 169 | GLN  |
| 5   | N     | 97  | GLN  |
| 5   | N     | 123 | ASN  |
| 5   | N     | 170 | ASN  |
| 5   | O     | 109 | ASN  |
| 5   | P     | 87  | GLN  |
| 5   | P     | 124 | ASN  |
| 5   | P     | 169 | GLN  |
| 5   | P     | 170 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | Q     | 87  | GLN  |
| 6   | R     | 229 | ASN  |
| 6   | R     | 318 | ASN  |
| 6   | S     | 209 | GLN  |
| 6   | S     | 219 | ASN  |
| 6   | S     | 265 | ASN  |
| 6   | S     | 318 | ASN  |
| 6   | S     | 341 | GLN  |
| 6   | T     | 249 | HIS  |
| 6   | T     | 341 | GLN  |
| 6   | U     | 263 | GLN  |
| 6   | U     | 318 | ASN  |
| 6   | V     | 229 | ASN  |
| 6   | V     | 318 | ASN  |
| 6   | V     | 319 | HIS  |
| 6   | X     | 229 | ASN  |
| 6   | X     | 318 | ASN  |
| 6   | Y     | 318 | ASN  |
| 6   | Z     | 199 | GLN  |
| 6   | Z     | 209 | GLN  |
| 6   | Z     | 229 | ASN  |
| 6   | Z     | 249 | HIS  |
| 6   | Z     | 265 | ASN  |
| 6   | Z     | 309 | GLN  |
| 6   | Z     | 356 | GLN  |
| 1   | AL    | 162 | HIS  |
| 6   | a     | 209 | GLN  |
| 6   | a     | 263 | GLN  |
| 6   | a     | 290 | ASN  |
| 6   | a     | 310 | GLN  |
| 6   | a     | 318 | ASN  |
| 6   | b     | 199 | GLN  |
| 6   | b     | 219 | ASN  |
| 6   | b     | 249 | HIS  |
| 6   | c     | 219 | ASN  |
| 6   | c     | 263 | GLN  |
| 6   | c     | 318 | ASN  |
| 6   | d     | 263 | GLN  |
| 6   | d     | 265 | ASN  |
| 6   | d     | 356 | GLN  |
| 6   | e     | 219 | ASN  |
| 6   | e     | 310 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | e     | 318 | ASN  |
| 6   | f     | 318 | ASN  |
| 6   | g     | 229 | ASN  |
| 6   | g     | 290 | ASN  |
| 6   | g     | 319 | HIS  |
| 6   | h     | 318 | ASN  |
| 6   | i     | 229 | ASN  |
| 6   | i     | 242 | GLN  |
| 6   | i     | 318 | ASN  |
| 6   | j     | 328 | GLN  |
| 6   | k     | 219 | ASN  |
| 6   | k     | 310 | GLN  |
| 6   | k     | 318 | ASN  |
| 6   | k     | 319 | HIS  |
| 6   | l     | 328 | GLN  |
| 6   | m     | 219 | ASN  |
| 6   | m     | 318 | ASN  |
| 1   | o     | 115 | GLN  |
| 1   | o     | 162 | HIS  |
| 1   | p     | 47  | ASN  |
| 1   | p     | 139 | ASN  |
| 1   | p     | 196 | GLN  |
| 1   | q     | 42  | HIS  |
| 1   | q     | 162 | HIS  |
| 1   | r     | 139 | ASN  |
| 1   | r     | 163 | GLN  |
| 1   | t     | 42  | HIS  |
| 1   | t     | 139 | ASN  |
| 1   | t     | 173 | ASN  |
| 1   | u     | 29  | GLN  |
| 1   | u     | 76  | GLN  |
| 1   | u     | 139 | ASN  |
| 1   | u     | 173 | ASN  |
| 1   | v     | 29  | GLN  |
| 1   | v     | 139 | ASN  |
| 1   | w     | 42  | HIS  |
| 1   | x     | 163 | GLN  |
| 1   | z     | 162 | HIS  |
| 1   | AJ    | 47  | ASN  |
| 1   | AJ    | 129 | HIS  |
| 1   | AJ    | 162 | HIS  |
| 1   | AJ    | 163 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AK    | 47  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

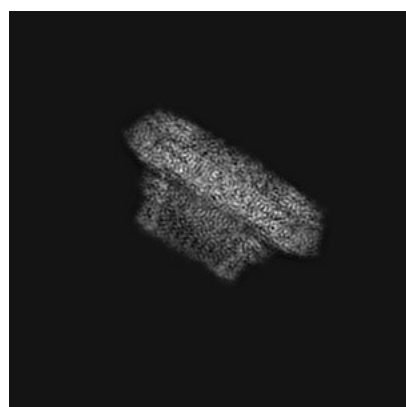
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20316. These allow visual inspection of the internal detail of the map and identification of artifacts.

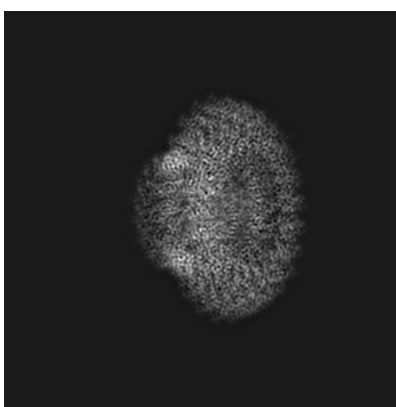
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

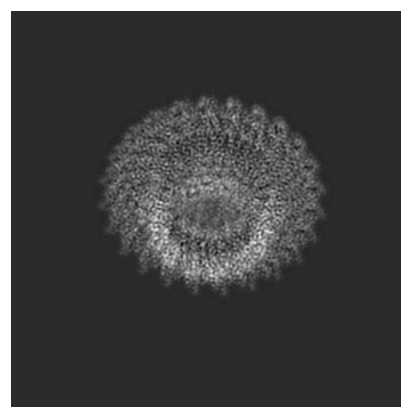
#### 6.1.1 Primary map



X



Y

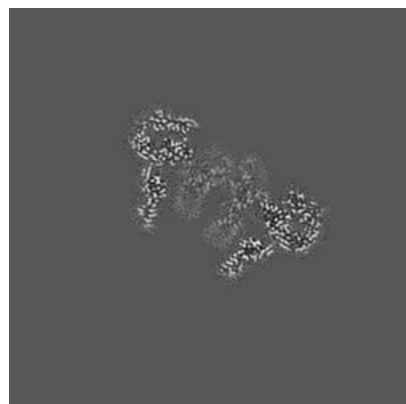


Z

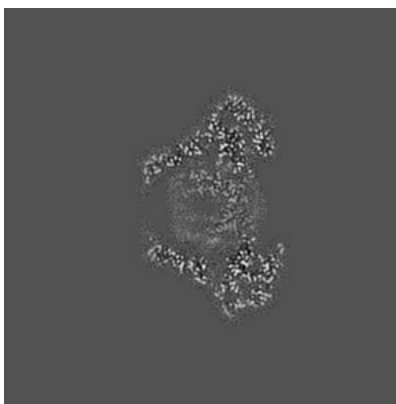
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

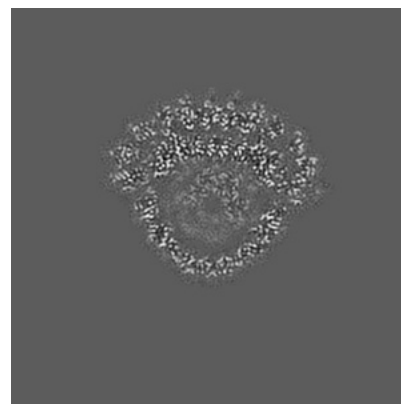
#### 6.2.1 Primary map



X Index: 125



Y Index: 125

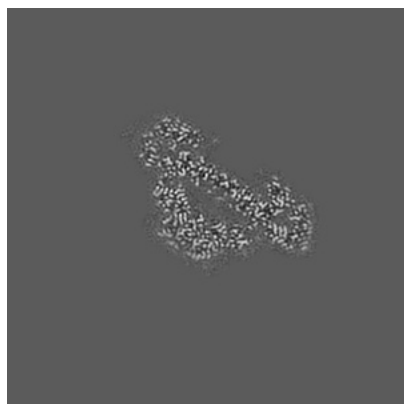


Z Index: 125

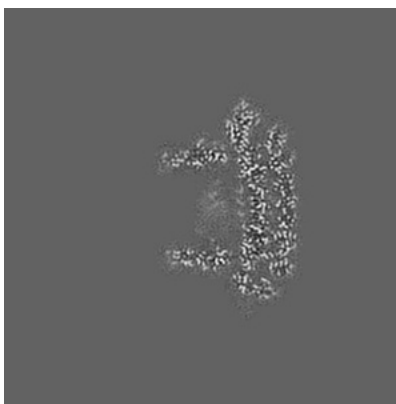
The images above show central slices of the map in three orthogonal directions.

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

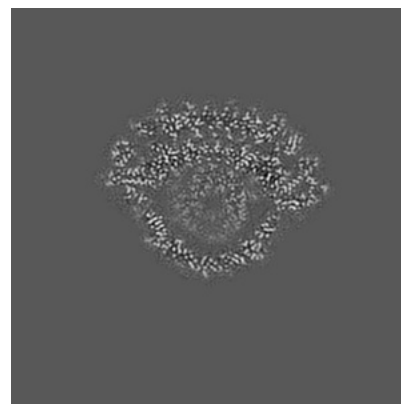
### 6.3.1 Primary map



X Index: 155



Y Index: 107

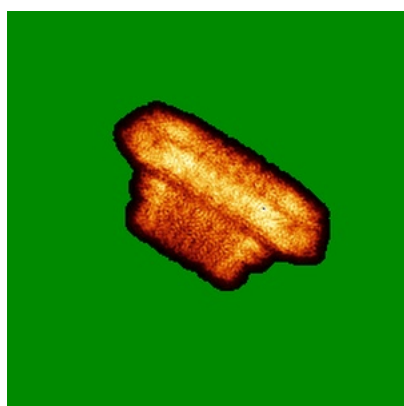


Z Index: 129

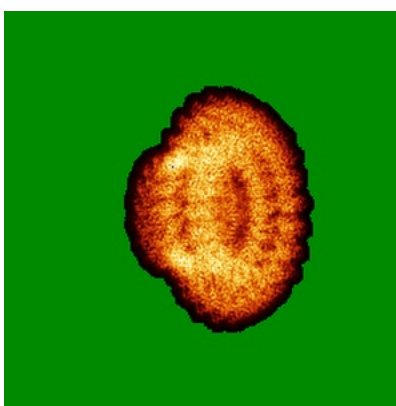
The images above show the largest variance slices of the map in three orthogonal directions.

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

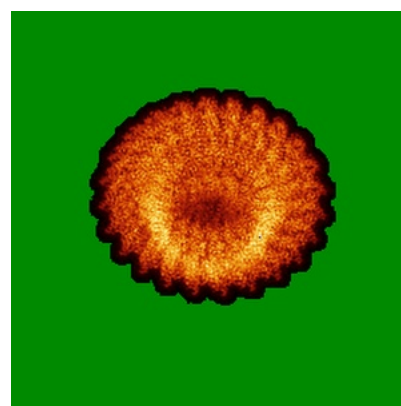
### 6.4.1 Primary map



X



Y

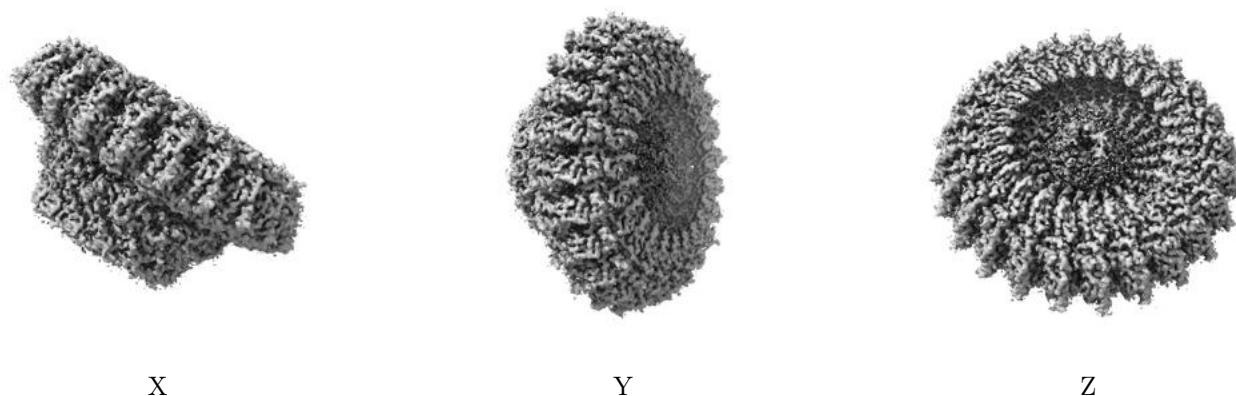


Z

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

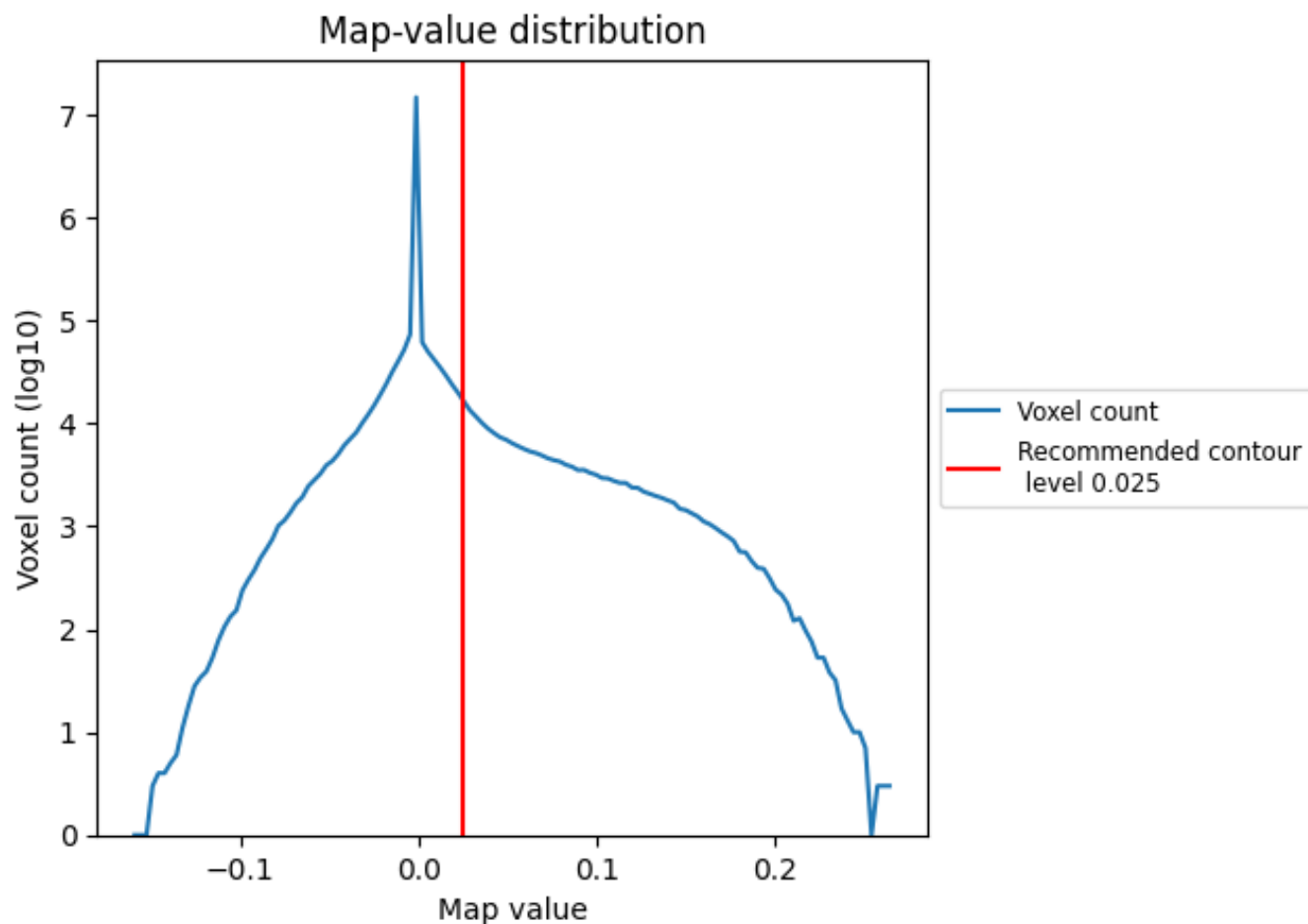
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

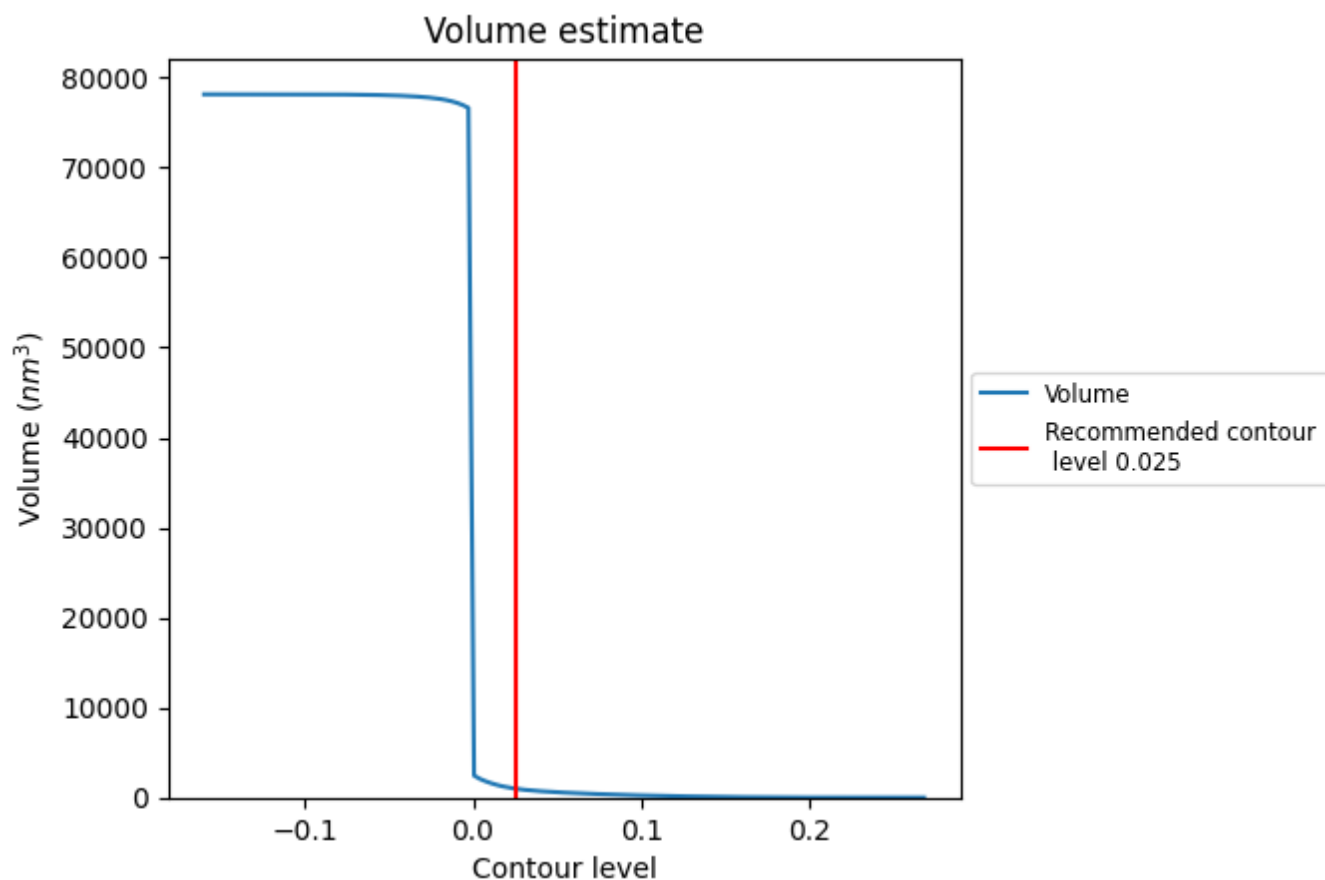
This section contains the results of statistical analysis of the map.

### 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.

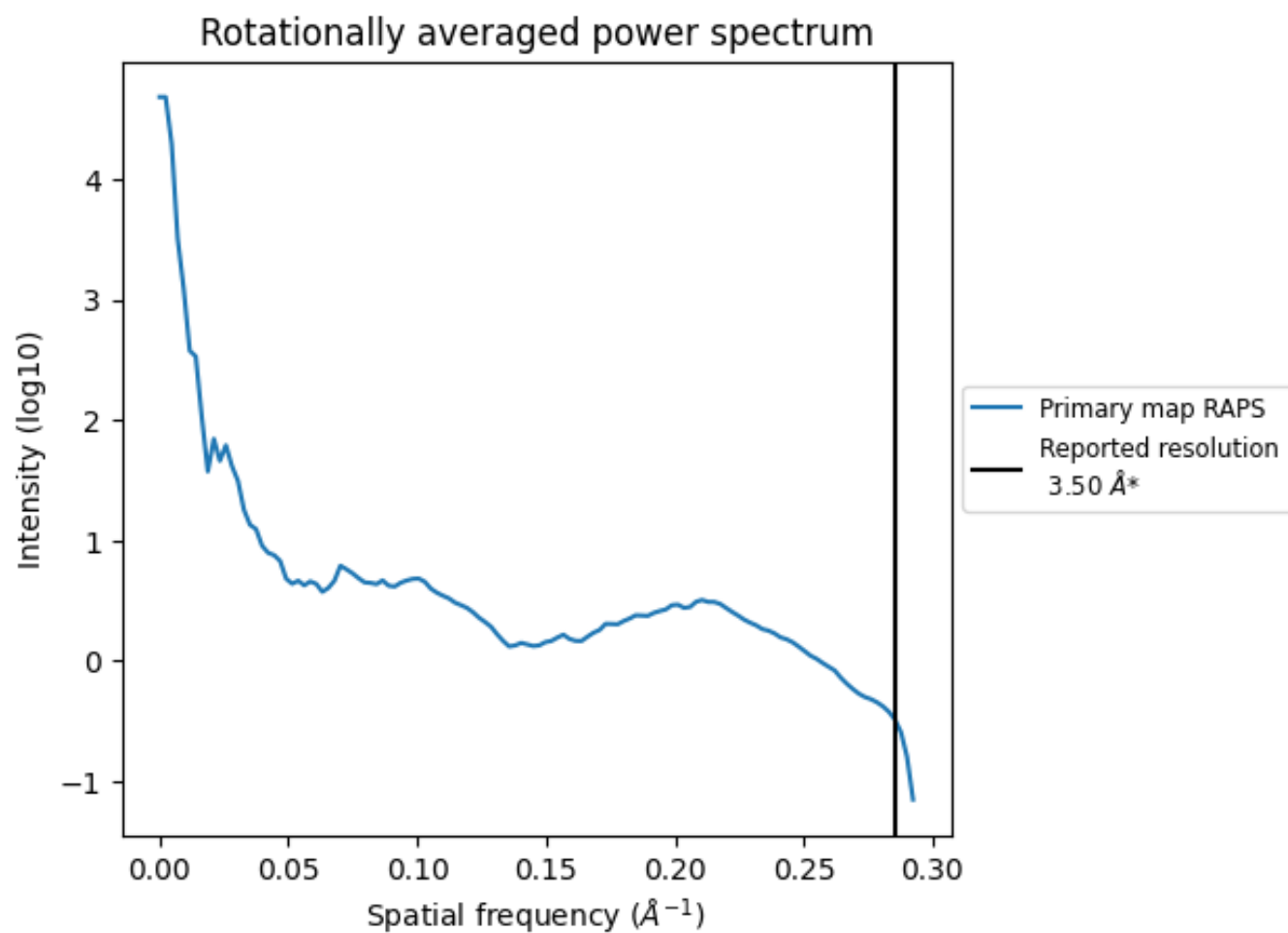
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 996 nm<sup>3</sup>; this corresponds to an approximate mass of 899 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 0.286 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

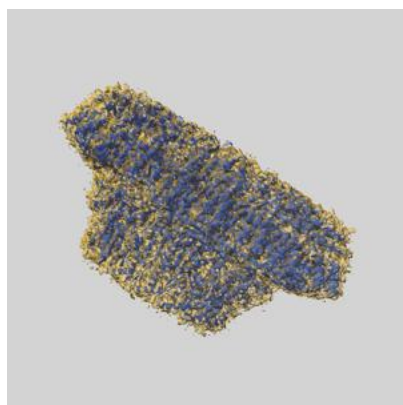
This section was not generated. No FSC curve or half-maps provided.



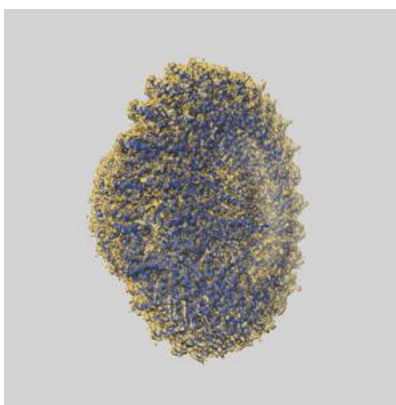
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20316 and PDB model 6PEM. Per-residue inclusion information can be found in section [3](#) on page [11](#).

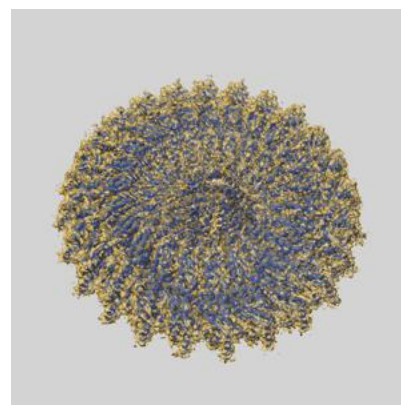
### 9.1 Map-model overlay [i](#)



X



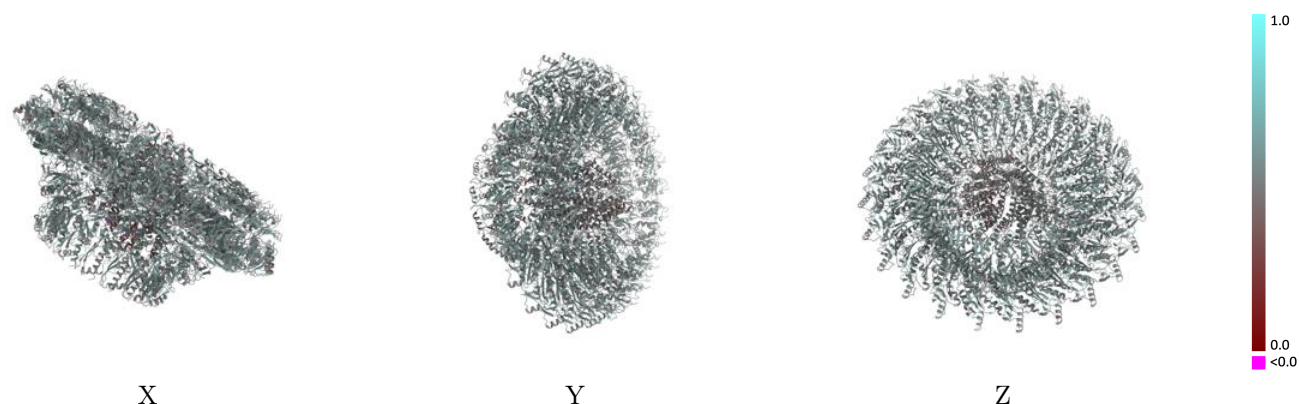
Y



Z

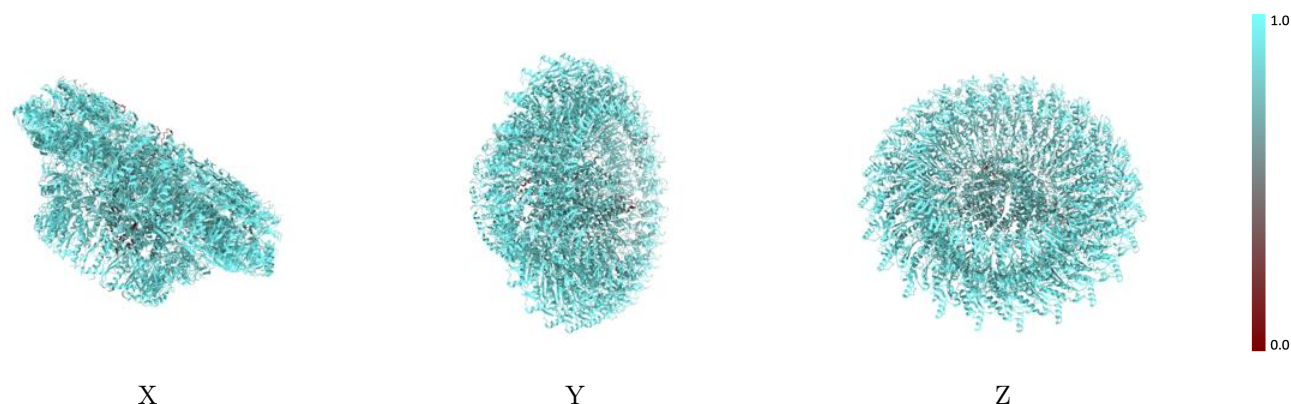
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



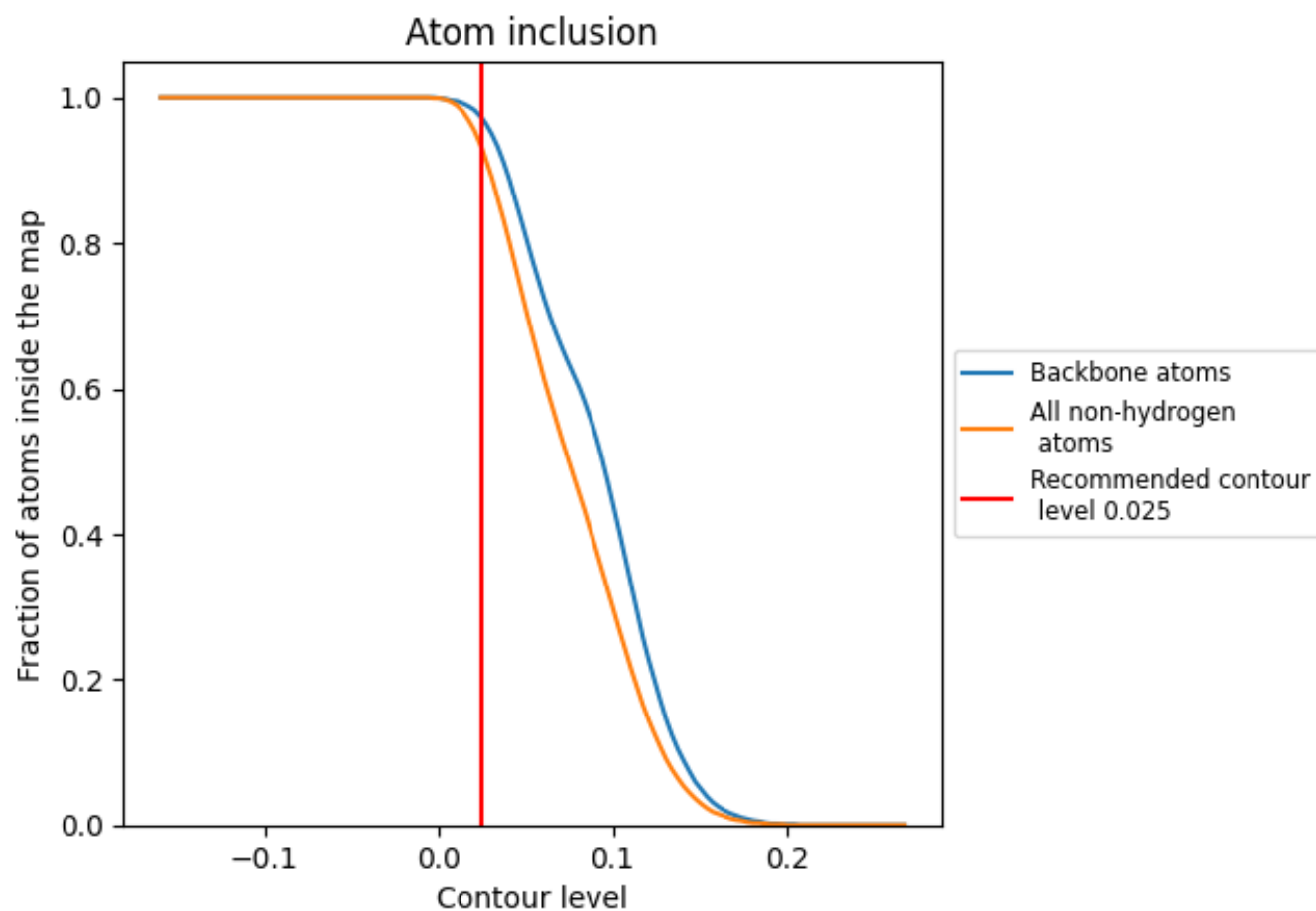
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.025) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9310   |  0.5190   |
| 0     |  0.8550   |  0.4650   |
| 1     |  0.8200   |  0.4340   |
| 2     |  0.8220   |  0.4470   |
| 3     |  0.8440   |  0.4590   |
| 4     |  0.8250   |  0.4700   |
| 5     |  0.9110   |  0.4980   |
| 6     |  0.7410   |  0.4600   |
| 7     |  0.6970   |  0.4290   |
| 8     |  0.8400   |  0.4590   |
| 9     |  0.8700   |  0.4900   |
| A     |  0.9700   |  0.5310   |
| AA    |  0.9280   |  0.5260   |
| AB    |  0.9270   |  0.5270   |
| AC    |  0.9360  |  0.5310  |
| AD    |  0.9360 |  0.5250 |
| AE    |  0.9250 |  0.5260 |
| AF    |  0.9370 |  0.5270 |
| AG    |  0.9270 |  0.5230 |
| AH    |  0.9300 |  0.5290 |
| AI    |  0.9320 |  0.5290 |
| AJ    |  0.9280 |  0.5240 |
| AK    |  0.9170 |  0.5210 |
| AL    |  0.9360 |  0.5240 |
| B     |  0.9570 |  0.5170 |
| C     |  0.9600 |  0.5260 |
| D     |  0.9570 |  0.5150 |
| E     |  0.9370 |  0.5250 |
| F     |  0.9310 |  0.5210 |
| G     |  0.9310 |  0.5180 |
| H     |  0.9550 |  0.5220 |
| I     |  0.9520 |  0.5130 |
| J     |  0.9670 |  0.5260 |
| K     |  0.9470 |  0.5040 |
| L     |  0.9450 |  0.5240 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| M     |  0.9560   |  0.5170   |
| N     |  0.9590   |  0.5220   |
| O     |  0.9410   |  0.5110   |
| P     |  0.9480   |  0.5230   |
| Q     |  0.9620   |  0.5170   |
| R     |  0.9570   |  0.5330   |
| S     |  0.9520   |  0.5330   |
| T     |  0.9420   |  0.5260   |
| U     |  0.9550   |  0.5280   |
| V     |  0.9550   |  0.5290   |
| W     |  0.9450   |  0.5310   |
| X     |  0.9500   |  0.5280   |
| Y     |  0.9490   |  0.5280   |
| Z     |  0.9510   |  0.5250   |
| a     |  0.9550   |  0.5290   |
| b     |  0.9500   |  0.5320   |
| c     |  0.9440   |  0.5290   |
| d     |  0.9590   |  0.5320   |
| e     |  0.9500   |  0.5220   |
| f     |  0.9410  |  0.5280  |
| g     |  0.9510 |  0.5260 |
| h     |  0.9510 |  0.5290 |
| i     |  0.9390 |  0.5310 |
| j     |  0.9580 |  0.5330 |
| k     |  0.9530 |  0.5360 |
| l     |  0.9450 |  0.5310 |
| m     |  0.9530 |  0.5310 |
| n     |  0.9480 |  0.5260 |
| o     |  0.9320 |  0.5320 |
| p     |  0.9220 |  0.5290 |
| q     |  0.9340 |  0.5250 |
| r     |  0.9280 |  0.5270 |
| s     |  0.9220 |  0.5190 |
| t     |  0.9280 |  0.5260 |
| u     |  0.9270 |  0.5220 |
| v     |  0.9310 |  0.5210 |
| w     |  0.9020 |  0.5160 |
| x     |  0.9190 |  0.5200 |
| y     |  0.9240 |  0.5310 |
| z     |  0.9370 |  0.5310 |