



## wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 01:21 PM UTC

PDB ID : 6PEP / pdb\_00006pep  
EMDB ID : EMD-20317  
Title : Focussed refinement of InvGN0N1:SpaPQR:PrgIJ from the Salmonella SPI-1  
injectisome needle complex  
Authors : Hu, J.; Worrall, L.J.; Strynadka, N.C.J.  
Deposited on : 2019-06-20  
Resolution : 3.80 Å(reported)

This is a wwPDB EM Validation Summary 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

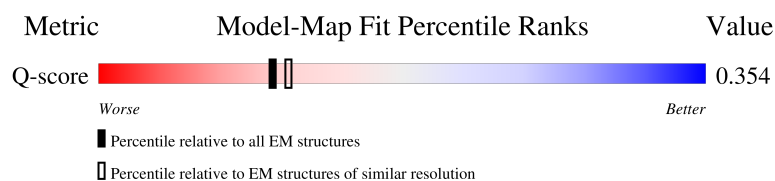
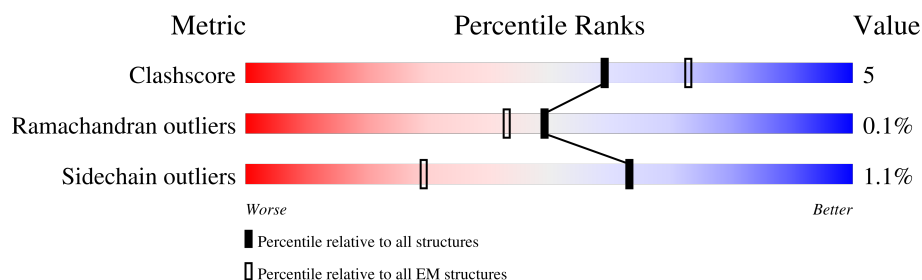
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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                       | 10198 ( 3.30 - 4.30 )                                    |

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   | 0     | 224    | <div> <div>7%</div> <div>77%</div> <div>11%</div> <div>11%</div> </div> |
| 1   | 1     | 224    | <div> <div>6%</div> <div>81%</div> <div>8%</div> <div>11%</div> </div>  |
| 1   | 2     | 224    | <div> <div>5%</div> <div>74%</div> <div>14%</div> <div>12%</div> </div> |
| 1   | 3     | 224    | <div> <div>74%</div> <div>17%</div> <div>9%</div> </div>                |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 4     | 224    |                  |
| 2   | 5     | 263    |                  |
| 3   | 6     | 86     |                  |
| 3   | 7     | 86     |                  |
| 3   | 8     | 86     |                  |
| 3   | 9     | 86     |                  |
| 4   | A     | 562    |                  |
| 4   | B     | 562    |                  |
| 4   | C     | 562    |                  |
| 4   | D     | 562    |                  |
| 4   | F     | 562    |                  |
| 4   | G     | 562    |                  |
| 4   | H     | 562    |                  |
| 4   | I     | 562    |                  |
| 4   | J     | 562    |                  |
| 4   | K     | 562    |                  |
| 4   | L     | 562    |                  |
| 4   | M     | 562    |                  |
| 4   | N     | 562    |                  |
| 4   | O     | 562    |                  |
| 4   | P     | 562    |                  |
| 4   | Q     | 562    |                  |
| 5   | AM    | 101    |                  |
| 5   | AN    | 101    |                  |
| 5   | AO    | 101    |                  |

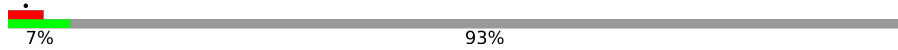
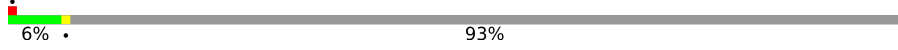
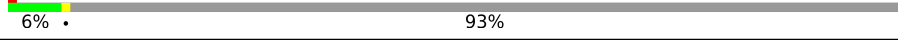
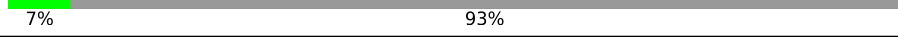
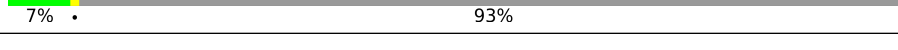
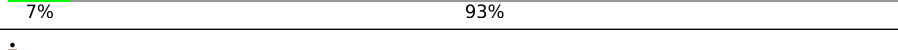
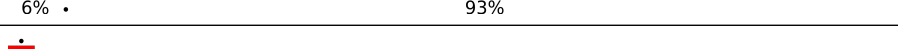
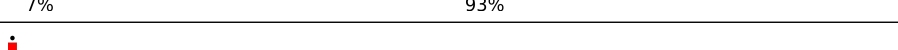
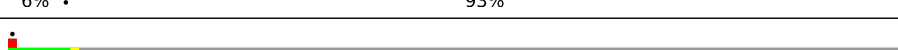
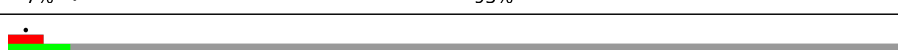
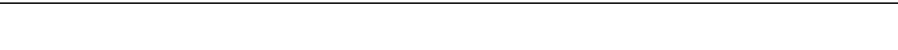
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 5   | AP    | 101    |                  |
| 5   | AQ    | 101    |                  |
| 5   | AR    | 101    |                  |
| 6   | AS    | 80     |                  |
| 6   | AT    | 80     |                  |
| 6   | AU    | 80     |                  |
| 6   | AV    | 80     |                  |
| 6   | AW    | 80     |                  |
| 6   | AX    | 80     |                  |
| 6   | AY    | 80     |                  |
| 6   | AZ    | 80     |                  |
| 6   | BA    | 80     |                  |
| 6   | BB    | 80     |                  |
| 6   | BC    | 80     |                  |
| 6   | BD    | 80     |                  |
| 6   | BE    | 80     |                  |
| 7   | E     | 392    |                  |
| 7   | R     | 392    |                  |
| 7   | S     | 392    |                  |
| 7   | T     | 392    |                  |
| 7   | U     | 392    |                  |
| 7   | V     | 392    |                  |
| 7   | W     | 392    |                  |
| 7   | X     | 392    |                  |
| 7   | Y     | 392    |                  |

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| Mol | Chain | Length | Quality of chain                                                                            |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 7   | Z     | 392    |  7% 93%   |
| 7   | a     | 392    |  6% 93%   |
| 7   | b     | 392    |  7% 93%   |
| 7   | c     | 392    |  7% 93%   |
| 7   | d     | 392    |  6% 93%   |
| 7   | e     | 392    |  7% 93%   |
| 7   | f     | 392    |  7% 93%   |
| 7   | g     | 392    |  7% 93%   |
| 7   | h     | 392    |  6% 93%   |
| 7   | i     | 392    |  7% 93%   |
| 7   | j     | 392    |  6% 93%   |
| 7   | k     | 392    |  7% 93% |
| 7   | l     | 392    |  7% 93% |
| 7   | m     | 392    |  6% 93% |
| 7   | n     | 392    |  7% 93% |

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 45454 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 Surface presentation of antigens protein SpaP.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 0     | 199      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1562  | 1041 | 231 | 279 | 11 |         |       |
| 1   | 1     | 199      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1569  | 1047 | 232 | 279 | 11 |         |       |
| 1   | 2     | 197      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1553  | 1037 | 230 | 275 | 11 |         |       |
| 1   | 3     | 204      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1606  | 1071 | 238 | 286 | 11 |         |       |
| 1   | 4     | 221      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 1758  | 1163 | 266 | 318 | 11 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | 5     | 247      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1885  | 1252 | 300 | 320 | 13 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|-------|
| 3   | 6     | 53       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 405   | 276 | 61 | 67  | 1 |         |       |
| 3   | 7     | 84       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 644   | 436 | 97 | 109 | 2 |         |       |
| 3   | 8     | 84       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 644   | 436 | 97 | 109 | 2 |         |       |
| 3   | 9     | 84       | Total | C   | N  | O   | S | 0       | 0     |
|     |       |          | 647   | 438 | 97 | 109 | 3 |         |       |

- Molecule 4 is a protein called Protein InvG.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | A     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 4   | B     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |
| 4   | C     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 4   | D     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1146  | 736 | 195 | 209 | 6 |         |       |
| 4   | F     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 4   | G     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |
| 4   | H     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 4   | I     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |
| 4   | J     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 4   | K     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |
| 4   | L     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 4   | M     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1146  | 736 | 195 | 209 | 6 |         |       |
| 4   | N     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 4   | O     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |
| 4   | P     | 139      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1108  | 710 | 189 | 203 | 6 |         |       |
| 4   | Q     | 144      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1154  | 741 | 198 | 209 | 6 |         |       |

- Molecule 5 is a protein called Protein PrgJ.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | AM    | 39       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 298   | 187 | 49  | 60  | 2 |         |       |
| 5   | AN    | 78       | Total | C   | N   | O   | S | 7       | 0     |
|     |       |          | 644   | 396 | 116 | 130 | 2 |         |       |
| 5   | AO    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 667   | 410 | 114 | 140 | 3 |         |       |
| 5   | AP    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 675   | 416 | 115 | 141 | 3 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | AQ    | 89       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 675   | 416 | 115 | 141 | 3 |         |       |
| 5   | AR    | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 667   | 410 | 114 | 140 | 3 |         |       |

- Molecule 6 is a protein called Protein PrgI.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 6   | AS    | 59       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 466   | 294 | 80  | 92  |  |         |       |
| 6   | AT    | 59       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 466   | 294 | 80  | 92  |  |         |       |
| 6   | AU    | 59       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 466   | 294 | 80  | 92  |  |         |       |
| 6   | AV    | 59       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 466   | 294 | 80  | 92  |  |         |       |
| 6   | AW    | 59       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 466   | 294 | 80  | 92  |  |         |       |
| 6   | AX    | 73       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 574   | 362 | 95  | 117 |  |         |       |
| 6   | AY    | 78       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 612   | 387 | 101 | 124 |  |         |       |
| 6   | AZ    | 57       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 460   | 289 | 76  | 95  |  |         |       |
| 6   | BA    | 54       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 437   | 275 | 73  | 89  |  |         |       |
| 6   | BB    | 48       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 388   | 247 | 64  | 77  |  |         |       |
| 6   | BC    | 48       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 388   | 247 | 64  | 77  |  |         |       |
| 6   | BD    | 48       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 388   | 247 | 64  | 77  |  |         |       |
| 6   | BE    | 43       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 346   | 219 | 59  | 68  |  |         |       |

- Molecule 7 is a protein called Protein PrgH.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | E     | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 236   | 159 | 38 | 38 | 1 |         |       |
| 7   | R     | 27       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 227   | 153 | 37 | 36 | 1 |         |       |

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| Mol | Chain | Residues | Atoms        |          |         |         |        | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 7   | S     | 28       | Total<br>231 | C<br>156 | N<br>38 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | T     | 28       | Total<br>236 | C<br>159 | N<br>38 | O<br>38 | S<br>1 | 0       | 0     |
| 7   | U     | 27       | Total<br>227 | C<br>153 | N<br>37 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | V     | 28       | Total<br>231 | C<br>156 | N<br>38 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | W     | 28       | Total<br>236 | C<br>159 | N<br>38 | O<br>38 | S<br>1 | 0       | 0     |
| 7   | X     | 27       | Total<br>227 | C<br>153 | N<br>37 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | Y     | 28       | Total<br>231 | C<br>156 | N<br>38 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | Z     | 28       | Total<br>236 | C<br>159 | N<br>38 | O<br>38 | S<br>1 | 0       | 0     |
| 7   | a     | 27       | Total<br>227 | C<br>153 | N<br>37 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | b     | 28       | Total<br>231 | C<br>156 | N<br>38 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | c     | 28       | Total<br>236 | C<br>159 | N<br>38 | O<br>38 | S<br>1 | 0       | 0     |
| 7   | d     | 27       | Total<br>227 | C<br>153 | N<br>37 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | e     | 28       | Total<br>231 | C<br>156 | N<br>38 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | f     | 28       | Total<br>236 | C<br>159 | N<br>38 | O<br>38 | S<br>1 | 0       | 0     |
| 7   | g     | 27       | Total<br>227 | C<br>153 | N<br>37 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | h     | 28       | Total<br>231 | C<br>156 | N<br>38 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | i     | 28       | Total<br>236 | C<br>159 | N<br>38 | O<br>38 | S<br>1 | 0       | 0     |
| 7   | j     | 27       | Total<br>227 | C<br>153 | N<br>37 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | k     | 28       | Total<br>231 | C<br>156 | N<br>38 | O<br>36 | S<br>1 | 0       | 0     |
| 7   | l     | 28       | Total<br>236 | C<br>159 | N<br>38 | O<br>38 | S<br>1 | 0       | 0     |
| 7   | m     | 27       | Total<br>227 | C<br>153 | N<br>37 | O<br>36 | S<br>1 | 0       | 0     |

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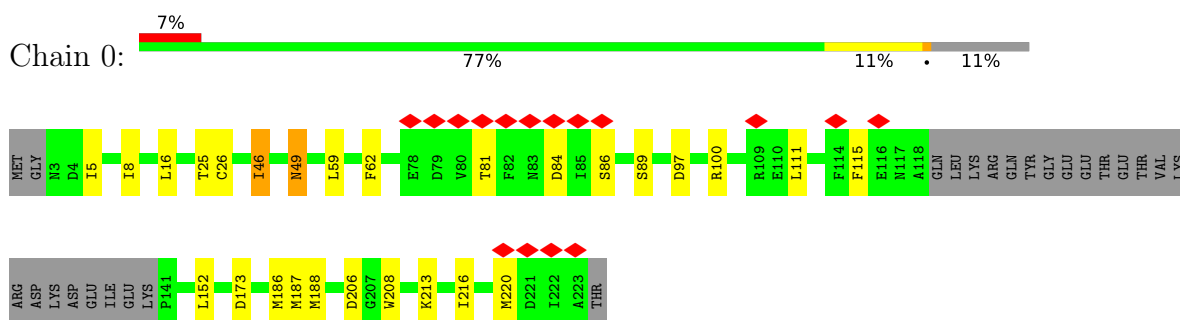
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| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | n     | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 231   | 156 | 38 | 36 | 1 |         |       |

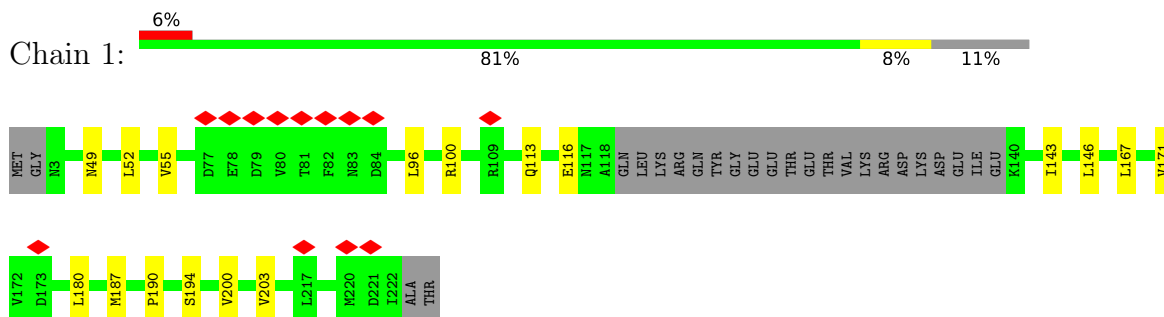
### 3 Residue-property plots [i](#)

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.

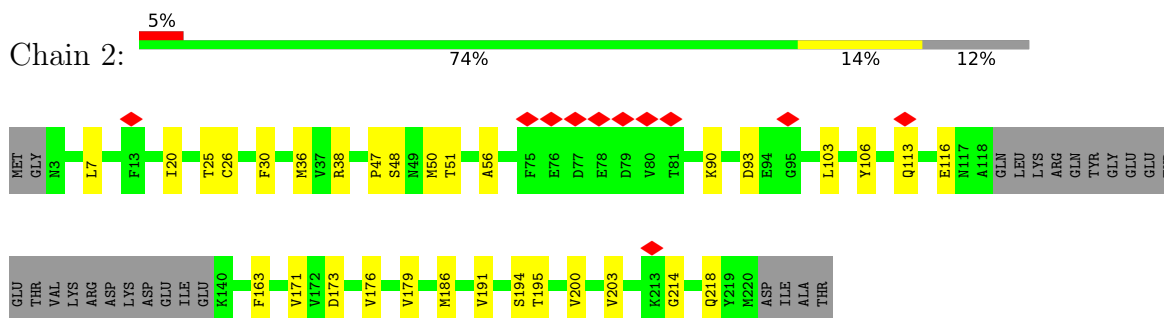
- Molecule 1: Surface presentation of antigens protein SpaP



- Molecule 1: Surface presentation of antigens protein SpaP



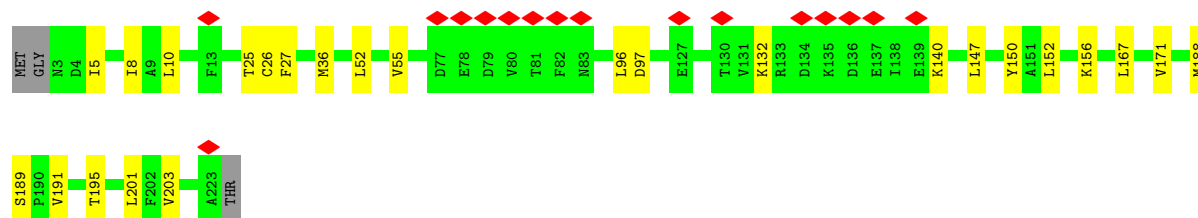
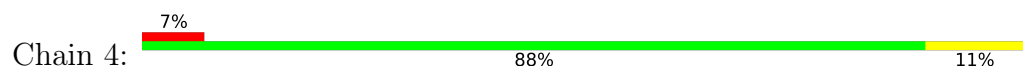
- Molecule 1: Surface presentation of antigens protein SpaP



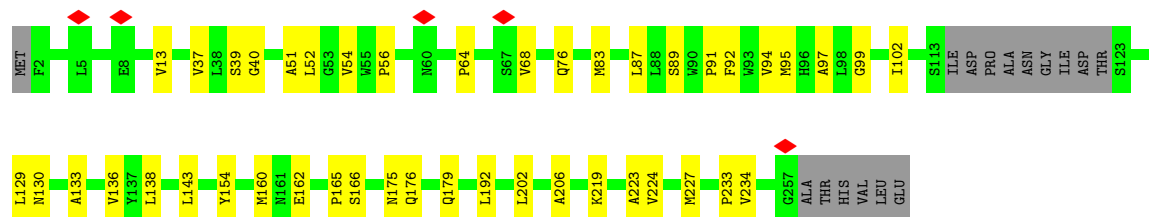
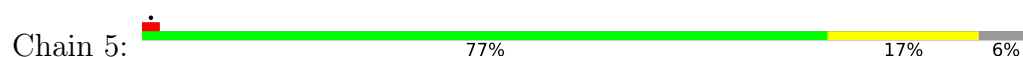
- Molecule 1: Surface presentation of antigens protein SpaP



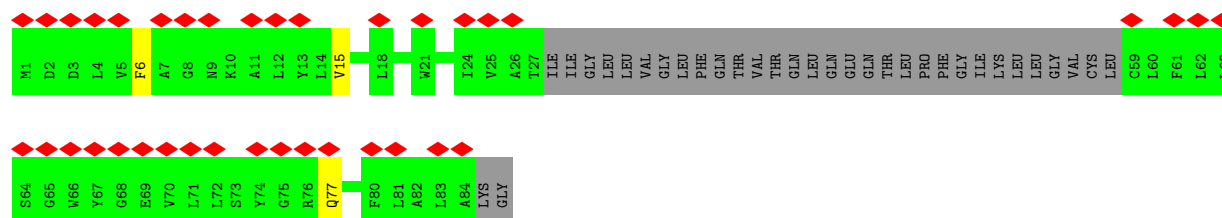
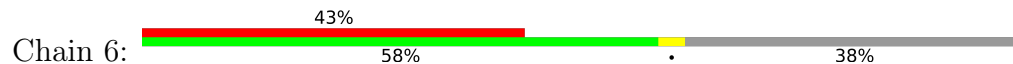
- Molecule 1: Surface presentation of antigens protein SpaP



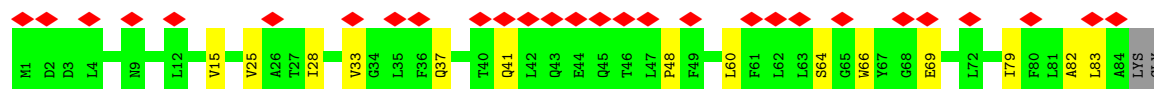
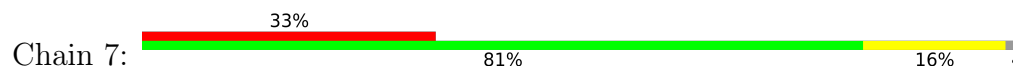
- Molecule 2: Surface presentation of antigens protein SpaR



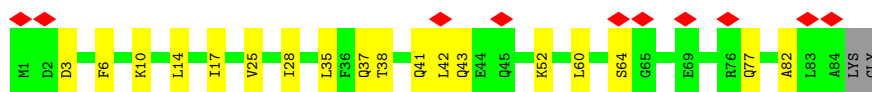
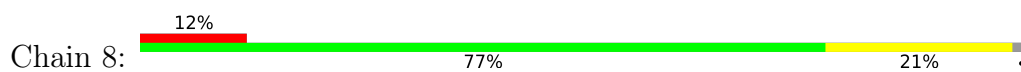
- Molecule 3: Surface presentation of antigens protein SpaQ



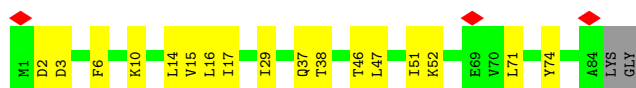
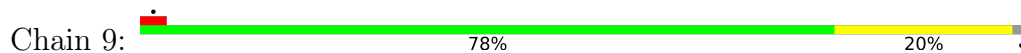
- Molecule 3: Surface presentation of antigens protein SpaQ



- Molecule 3: Surface presentation of antigens protein SpaQ



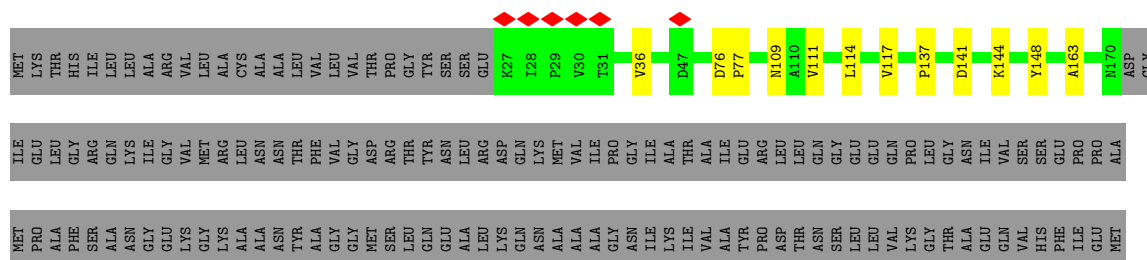
• Molecule 3: Surface presentation of antigens protein SpaQ



• Molecule 4: Protein InvG



• Molecule 4: Protein InvG



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

- Molecule 4: Protein InvG

Chain C:  21% . 75%

[illegible]

- Molecule 4: Protein InvG

Chain D:  23% 74%

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |                                                                    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|--------------------------------------------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|-----|-----|-----|
| PRO | ALA | PHE | SER | ASN | GLY | GLU | LYS | GLY | ALA | ASN | TYR | ALA | GLY | GLY | LYS | ALA | ASN | LYS | ASN | GLN | LYS | <div><div></div><div></div><div></div><div></div><div></div></div> | K27 | D28 | P29 | V30 | T31 | G32 | K38 | D39 | D40 | T44 | Q52 | S60 | K61 | T69 | F74 | Q87  | Q97  | M158 | K168 | Q169 | N170 | ASP | GLY | TYR |
| LEU | MET | THR | ILE | LEU | ALA | VAL | ARG | CYS | LEU | ALA | VAL | THR | GLY | THR | PRO | GLY | SER | SER | GLU | K27 | D28 |                                                                    | P29 | V30 | T31 | G32 | K38 | D39 | D40 | T44 | Q52 | S60 | K61 | T69 | F74 | Q87 | Q97 | M158 | K168 | Q169 | N170 | ASP  | GLY  | TYR |     |     |
| GLU | LEU | GLY | ARG | GLN | LYS | TYL | GLY | VAL | MET | ARG | LEU | ASN | THR | PHE | VAL | GLY | ASP | ARG | THR | TYR | ASN |                                                                    | GLN | MET | VAL | ILE | PRO | GLY | ALA | ILE | GLU | ARG | LEU | GLN | GLY | ASN | ILE | VAL  | SER  | SER  | GLU  | PRO  | PRO  | ALA | MET |     |
| ASN | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY |                                                                    | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY | GLY  | GLY  | GLY  | GLY  | GLY  | GLY  | GLY |     |     |
| THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR |                                                                    | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR | THR  | THR  | THR  | THR  | THR  | THR  | THR | THR |     |



[illegible]

- Molecule 4: Protein InvG

Chain H:  22% . 75%

[illegible]

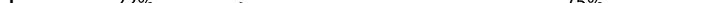
- Molecule 4: Protein InvG

Chain I:  23% 1% 74%

[illegible]

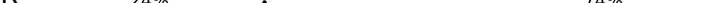
[illegible]

- Molecule 4: Protein InvG

Chain J:  22% . 75%

[illegible]

- Molecule 4: Protein InvG

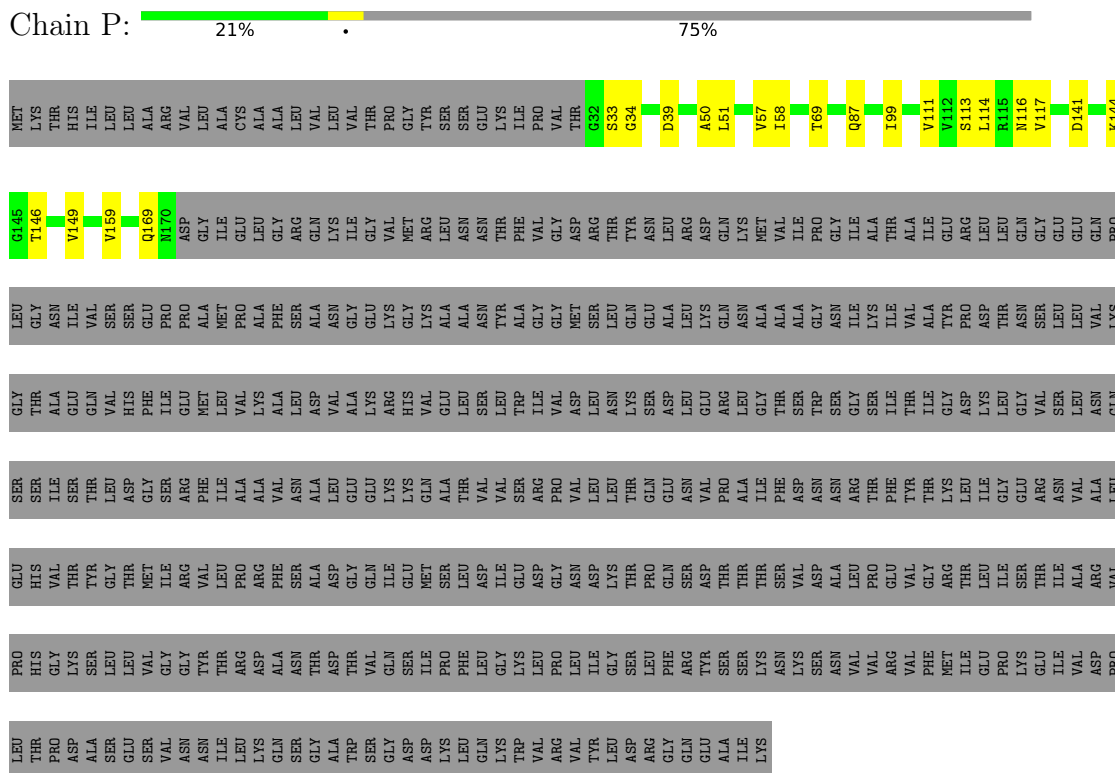
Chain K:  24% 74%

[illegible]

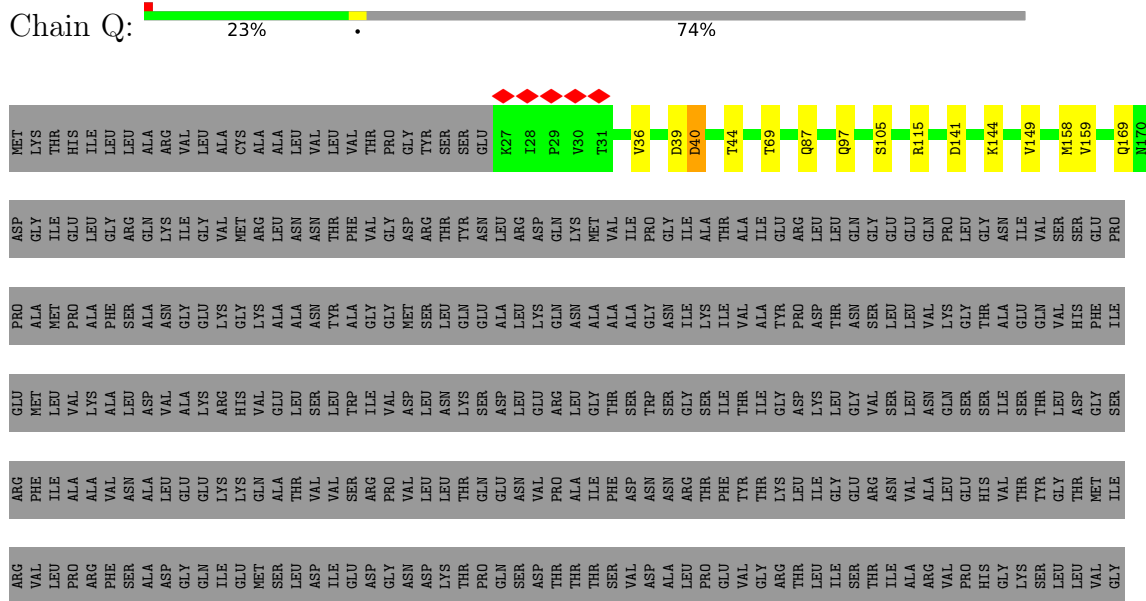




- Molecule 4: Protein InvG



- Molecule 4: Protein InvG



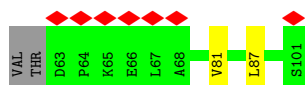
GLY TYR ASN THR ARG ASP ALA THR ASN ASP THR THR VAL GLN SER GLY ASP ILE PRO LYS PHE LEU GLN LYS GLY LEU LEU PRO ARG MET LEU ILE GLY SER ASP LEU PHE GLY ARG TYR SER ASP LYS ASN LYS SER ASN VAL VAL ARG VAL MET PHE MET ILE GLU PRO LYS ASP GLU ILE VAL ASP PRO THR THR ASP ALA SER GLU ASN SER VAL

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

### • Molecule 5: Protein PrgJ



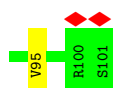
MET SER ILE ALA THR ILE VAL PRO GLU ASN ALA VAL ILE GLY GLN VAL ASN ILE ARG SER MET LEU THR ASP ILE VAL SER LEU ASP ARG LEU ASN GLN ALA PHE SER GLY ILE ALA THR VAL ASP GLU THR ASN THR ARG ILE ASP PRO ASN SER LEU



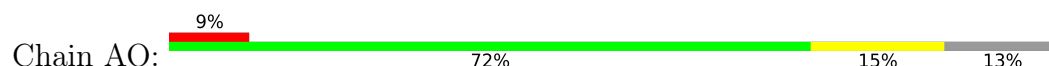
### • Molecule 5: Protein PrgJ



MET SER ILE ALA THR ILE VAL PRO GLU ASN ALA VAL ILE G14 Q15 A16 I19 E20 MET THR ASP ILE VAL SER LEU ASP D31 R32 A41 V46 D47 K48 I51 T52 N53 R54 T55 E56 D63 P64 K65 E66 L67 A68 I69 S75 V81 V84 S85 T86

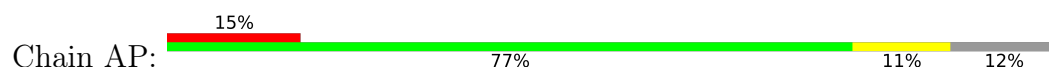


### • Molecule 5: Protein PrgJ



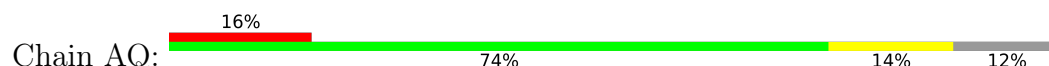
MET SER ILE ALA THR ILE VAL PRO GLU ASN ALA VAL ILE G14 Q15 M22 E23 T24 D25 I26 V27 S28 L29 D30 D31 D47 K48 Q49 T50 T52 N53 D63 P64 K65 E66 L67 A68 I69 M73 M83 K90 R100 S101

### • Molecule 5: Protein PrgJ



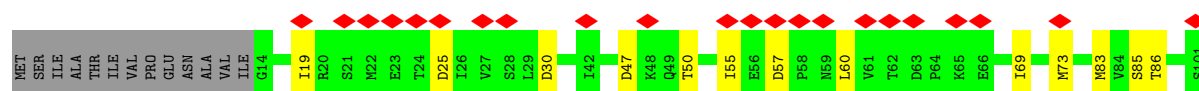
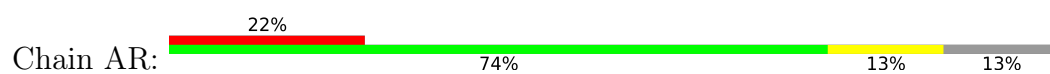
MET SER ILE ALA THR ILE VAL PRO GLU ASN ALA VAL I113 A16 M22 E23 T24 D25 I26 V27 S28 L29 D30 D31 R32 Q35 E56 D57 K65 M73 I74 S75 T86 R89 K90 L98 L99 R100 S101

### • Molecule 5: Protein PrgJ

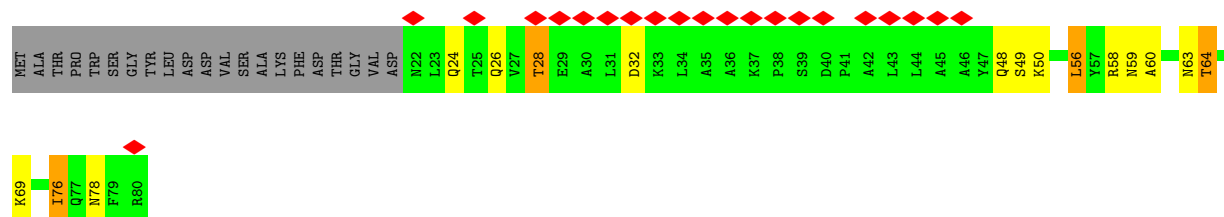


MET SER ILE ALA THR ILE VAL PRO GLU ASN ALA VAL I113 G14 Q15 R20 S21 M22 E23 T24 D25 S28 D31 I42 A43 T44 N53 R54 I55 E56 D57 P58 T62 D63 P64 K65 E72 S75 S76 L87 R100 S101

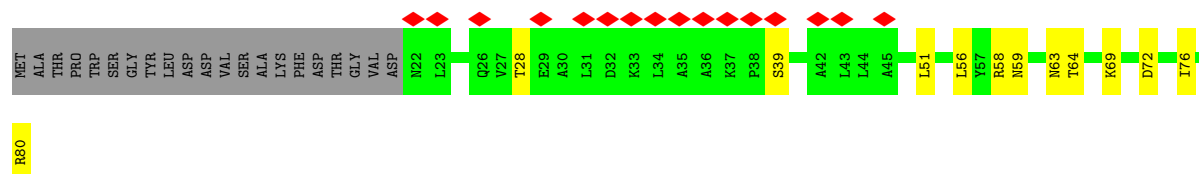
### • Molecule 5: Protein PrgJ



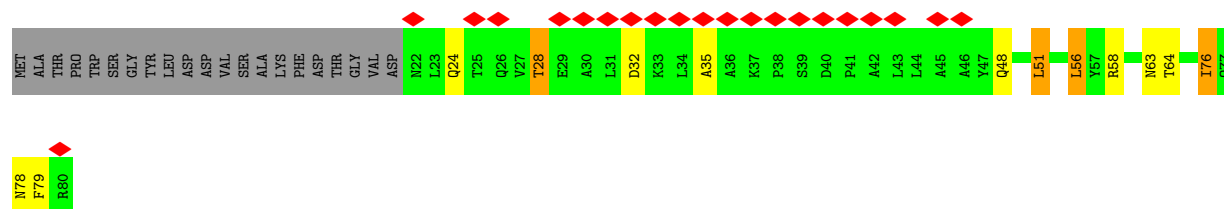
• Molecule 6: Protein PrgI



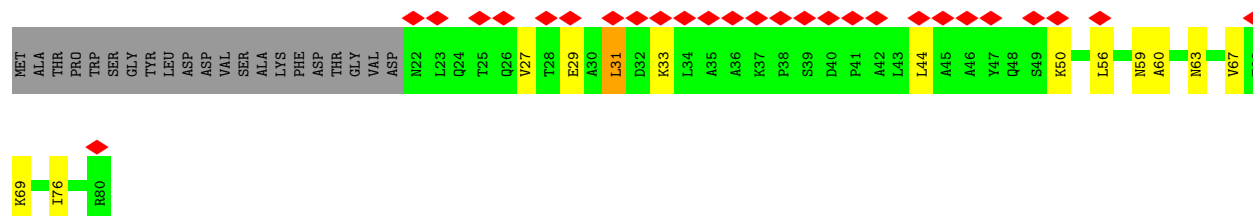
• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



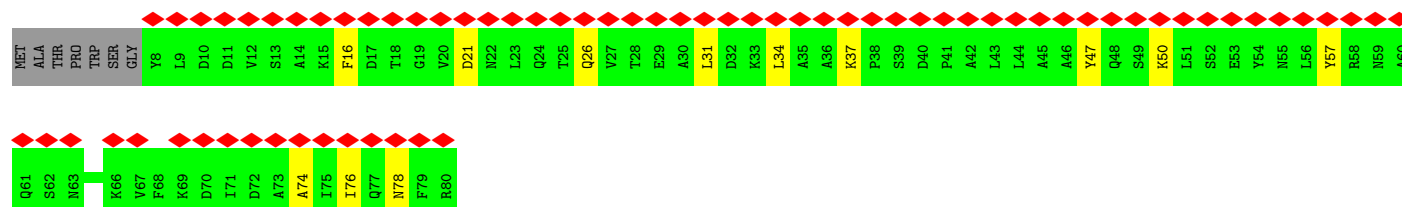
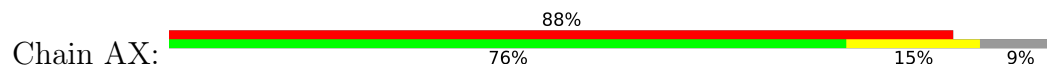
• Molecule 6: Protein PrgI



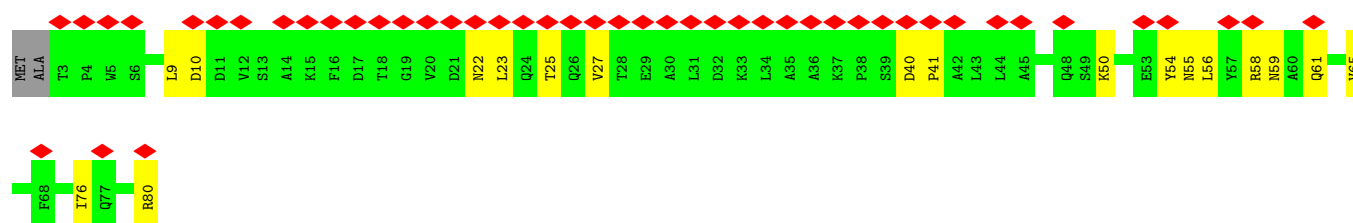
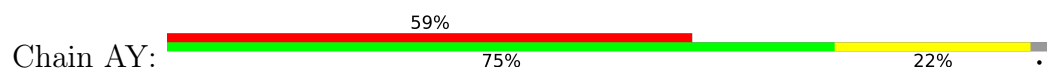
• Molecule 6: Protein PrgI



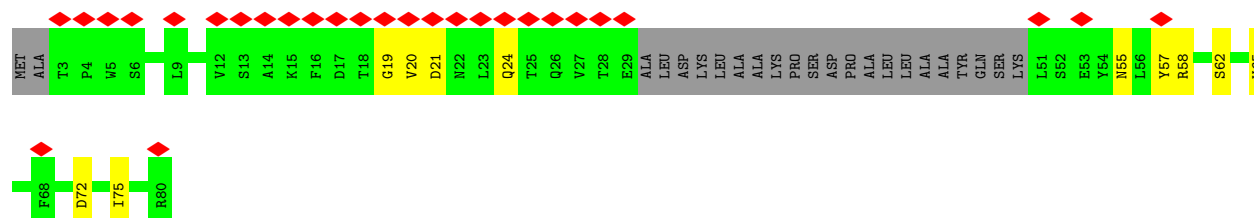
- Molecule 6: Protein PrgI



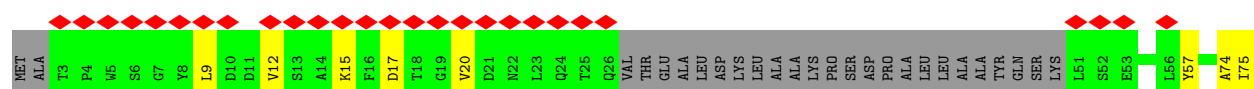
- Molecule 6: Protein PrgI



- Molecule 6: Protein PrgI

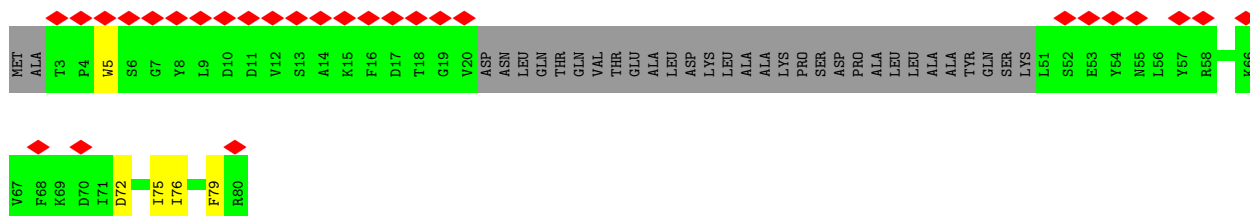


- Molecule 6: Protein PrgI

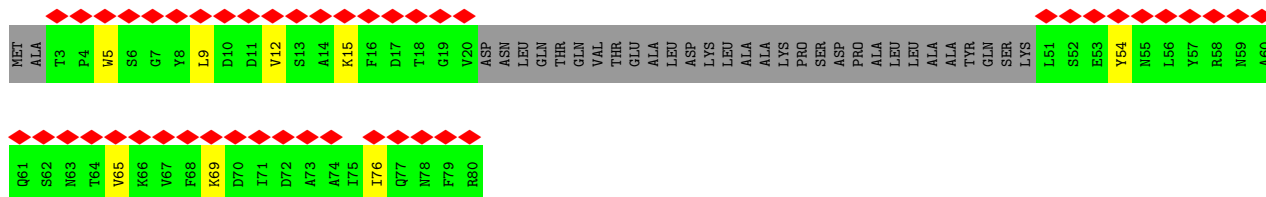




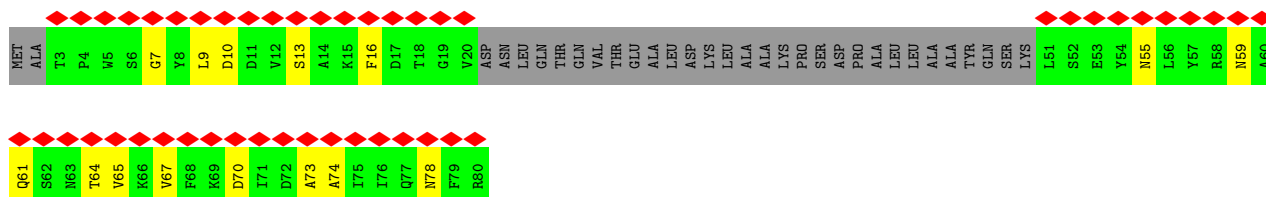
• Molecule 6: Protein PrgI



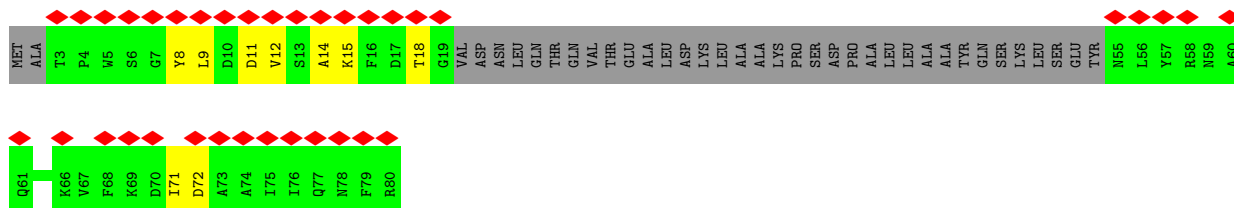
• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



• Molecule 6: Protein PrgI



• Molecule 7: Protein PrgH





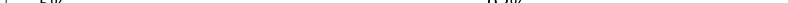
[illegible]

- Molecule 7: Protein PrgH

Chain T:  7% 93%

[illegible]

- Molecule 7: Protein PrgH

Chain U:  5% 93%

[illegible]

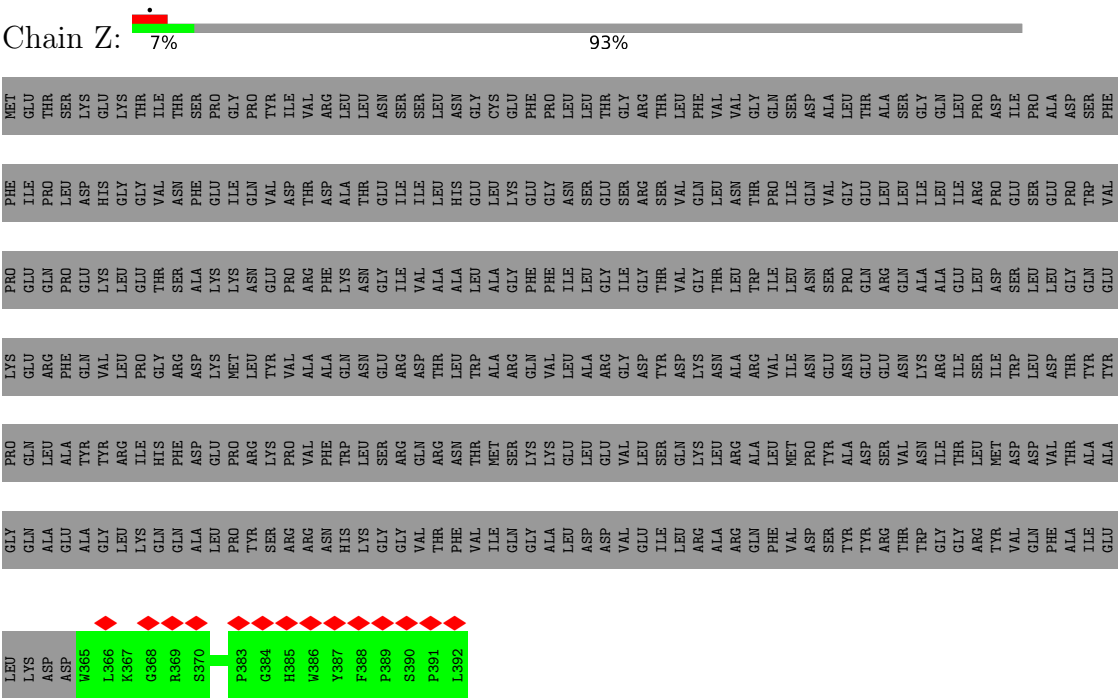
LEU LYS ASP ASP W365 L366 R369 Q372 Y373 E376 G377 K380 P391 LEU

Chain V:  7% 93%

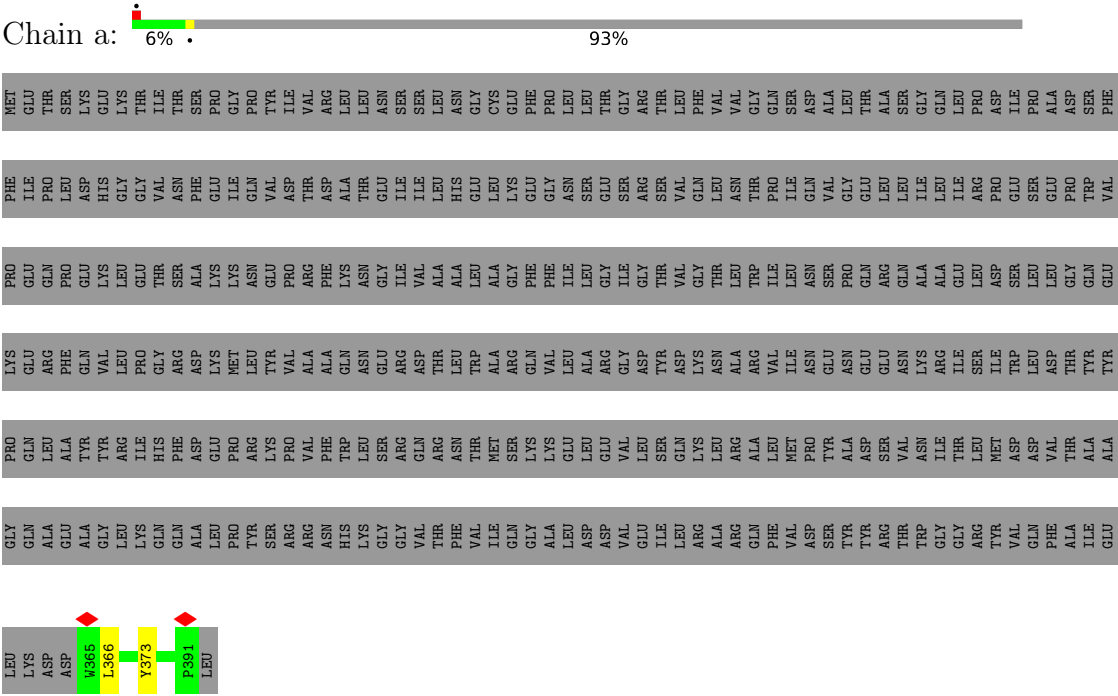
Chain W:  6% 93%

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | GLN | ALA | ALA | ALA | LEU | GLN | GLN | ALA | LEU | PRO | TYR | SER | ARG | ARG | ASN | HIS | LYS | GLY | GLY | VAL | THR | PHE | VAL | ILE | GLN | GLN | ALA | LEU | ASP | ASP | VAL | GLU | ILE | LEU | ARG | ALA | ARG | GLN | PHE | VAL | ASP | SER | TYR | TYR | THR | TRP | GLY | GLY | ARG | TYR | VAL | GLN | PHE | ALA | ILE | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

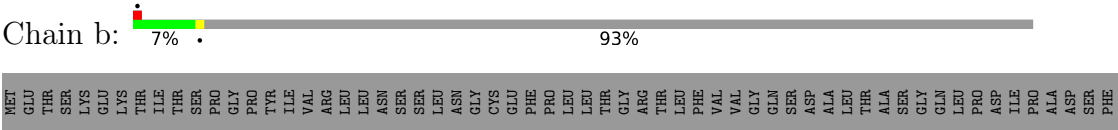




● Molecule 7: Protein PrgH



● Molecule 7: Protein PrgH



LEU  
LYS  
ASP  
ASP  
W365  
L366  
K367  
M381  
L392

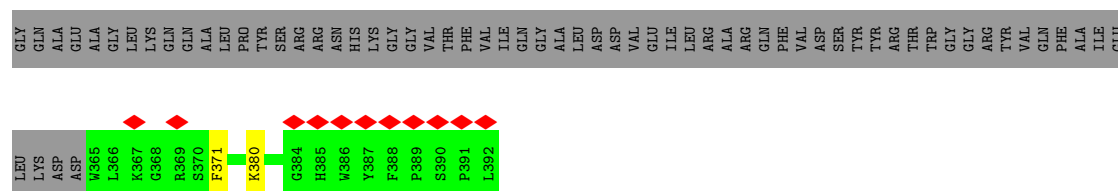
Chain c:  7% 93%

[illegible]

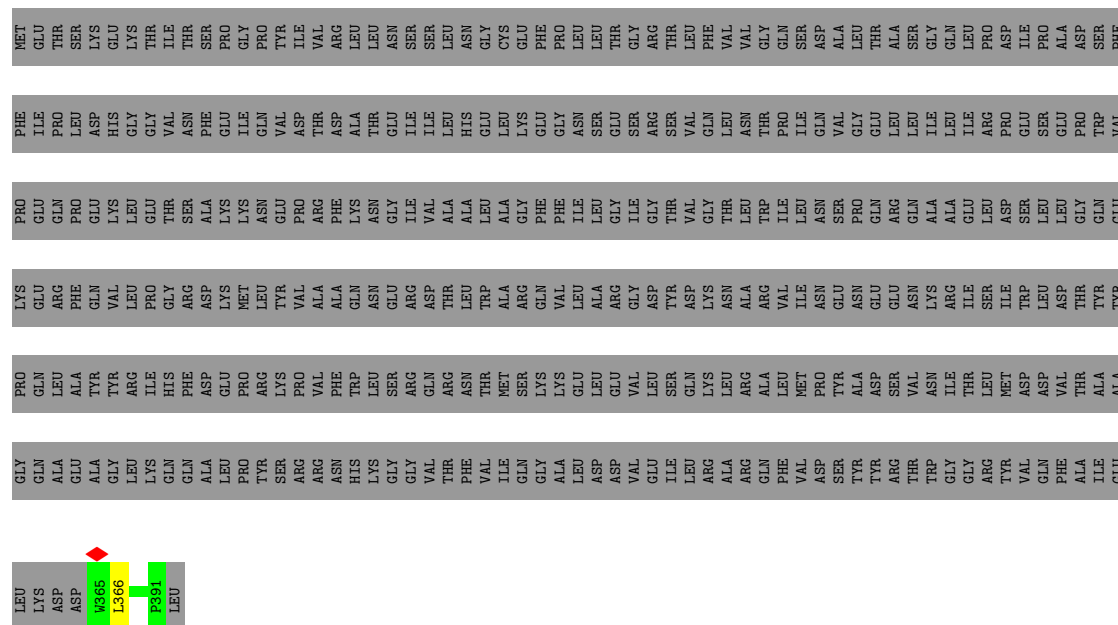
Chain d:  6% 93%

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PRO | GLU | GLN | PRO | PRO | GLU | LYS | LEU | GLU | THR | SER | ALA | LYS | LYS | ASN | GLU | ARG | PHE | LYS | ASN | GLY | ILE | VAL | ALA | ALA | LEU | GLY | PHE | PHE | ILE | LEU | GLY | ILE | GLY | THR | VAL | GLY | THR | THR | TRP | ILE | LEU | ASN | SER | PRO | PRO | GLN | ARG | GLN | ALA | ALA | ALA | GLU | GLU | LEU | ASP | SER | LEU | LEU | GLY | GLN | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

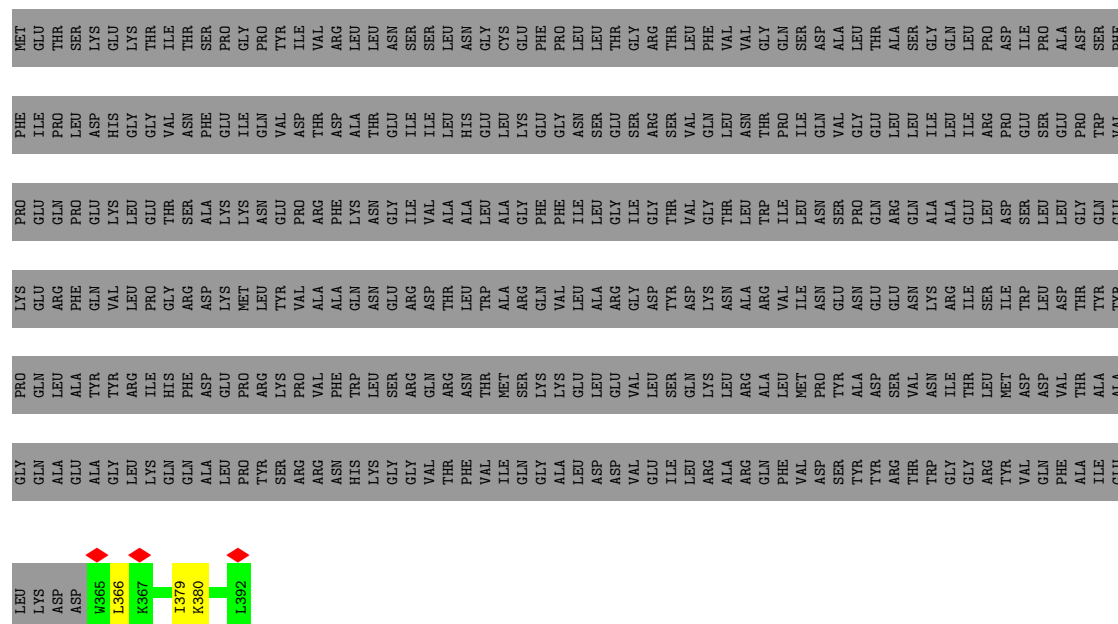




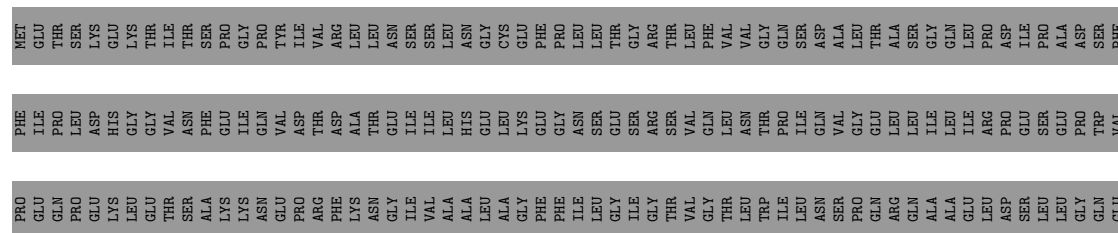
- Molecule 7: Protein PrgH



- Molecule 7: Protein PrgH









## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 25666                                   | 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                    | 5.972                                   | Depositor |
| Minimum map value                    | -2.765                                  | Depositor |
| Average map value                    | -0.012                                  | Depositor |
| Map value standard deviation         | 0.211                                   | Depositor |
| Recommended contour level            | 1.1                                     | Depositor |
| Map size ( $\text{\AA}$ )            | 427.5, 427.5, 427.5                     | wwPDB     |
| Map dimensions                       | 250, 250, 250                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 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   | 0     | 0.34         | 0/1598  | 0.67        | 0/2172        |
| 1   | 1     | 0.32         | 0/1605  | 0.68        | 1/2181 (0.0%) |
| 1   | 2     | 0.30         | 0/1589  | 0.67        | 0/2159        |
| 1   | 3     | 0.33         | 0/1642  | 0.62        | 0/2230        |
| 1   | 4     | 0.34         | 0/1799  | 0.65        | 0/2441        |
| 2   | 5     | 0.34         | 0/1935  | 0.72        | 0/2647        |
| 3   | 6     | 0.27         | 0/414   | 0.71        | 0/565         |
| 3   | 7     | 0.30         | 0/657   | 0.70        | 0/897         |
| 3   | 8     | 0.32         | 0/657   | 0.74        | 0/897         |
| 3   | 9     | 0.32         | 0/660   | 0.66        | 0/900         |
| 4   | A     | 0.33         | 0/1131  | 0.64        | 1/1525 (0.1%) |
| 4   | B     | 0.33         | 0/1181  | 0.63        | 0/1593        |
| 4   | C     | 0.33         | 0/1131  | 0.62        | 0/1525        |
| 4   | D     | 0.34         | 0/1170  | 0.61        | 0/1579        |
| 4   | F     | 0.34         | 0/1131  | 0.64        | 0/1525        |
| 4   | G     | 0.34         | 0/1181  | 0.66        | 2/1593 (0.1%) |
| 4   | H     | 0.37         | 0/1131  | 0.65        | 1/1525 (0.1%) |
| 4   | I     | 0.33         | 0/1181  | 0.60        | 0/1593        |
| 4   | J     | 0.35         | 0/1131  | 0.62        | 0/1525        |
| 4   | K     | 0.35         | 0/1181  | 0.65        | 0/1593        |
| 4   | L     | 0.34         | 0/1131  | 0.64        | 0/1525        |
| 4   | M     | 0.32         | 0/1170  | 0.62        | 0/1579        |
| 4   | N     | 0.35         | 0/1131  | 0.63        | 0/1525        |
| 4   | O     | 0.34         | 0/1181  | 0.62        | 0/1593        |
| 4   | P     | 0.33         | 0/1131  | 0.61        | 0/1525        |
| 4   | Q     | 0.34         | 0/1181  | 0.65        | 0/1593        |
| 5   | AM    | 0.37         | 0/300   | 0.87        | 0/403         |
| 5   | AN    | 0.28         | 0/646   | 0.63        | 0/870         |
| 5   | AO    | 0.31         | 0/671   | 0.65        | 0/908         |
| 5   | AP    | 0.31         | 0/679   | 0.71        | 0/919         |
| 5   | AQ    | 0.28         | 0/679   | 0.64        | 0/919         |
| 5   | AR    | 0.29         | 0/671   | 0.71        | 0/908         |
| 6   | AS    | 0.31         | 0/472   | 0.65        | 0/638         |
| 6   | AT    | 0.29         | 0/472   | 0.61        | 0/638         |

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 6   | AU    | 0.32         | 0/472   | 0.61        | 0/638          |
| 6   | AV    | 0.33         | 0/472   | 0.73        | 0/638          |
| 6   | AW    | 0.30         | 0/472   | 0.59        | 0/638          |
| 6   | AX    | 0.27         | 0/582   | 0.61        | 0/788          |
| 6   | AY    | 0.32         | 0/623   | 0.67        | 0/846          |
| 6   | AZ    | 0.24         | 0/467   | 0.51        | 0/632          |
| 6   | BA    | 0.24         | 0/444   | 0.50        | 0/600          |
| 6   | BB    | 0.28         | 0/395   | 0.67        | 0/533          |
| 6   | BC    | 0.25         | 0/395   | 0.56        | 0/533          |
| 6   | BD    | 0.26         | 0/395   | 0.58        | 0/533          |
| 6   | BE    | 0.27         | 0/352   | 0.69        | 0/474          |
| 7   | E     | 0.27         | 0/248   | 0.52        | 0/334          |
| 7   | R     | 0.32         | 0/239   | 0.61        | 0/323          |
| 7   | S     | 0.35         | 0/243   | 0.74        | 0/329          |
| 7   | T     | 0.26         | 0/248   | 0.52        | 0/334          |
| 7   | U     | 0.31         | 0/239   | 0.56        | 0/323          |
| 7   | V     | 0.33         | 0/243   | 0.74        | 0/329          |
| 7   | W     | 0.26         | 0/248   | 0.52        | 0/334          |
| 7   | X     | 0.32         | 0/239   | 0.58        | 0/323          |
| 7   | Y     | 0.34         | 0/243   | 0.71        | 0/329          |
| 7   | Z     | 0.26         | 0/248   | 0.52        | 0/334          |
| 7   | a     | 0.30         | 0/239   | 0.55        | 0/323          |
| 7   | b     | 0.35         | 0/243   | 0.67        | 0/329          |
| 7   | c     | 0.27         | 0/248   | 0.55        | 0/334          |
| 7   | d     | 0.29         | 0/239   | 0.50        | 0/323          |
| 7   | e     | 0.37         | 0/243   | 0.72        | 0/329          |
| 7   | f     | 0.29         | 0/248   | 0.59        | 0/334          |
| 7   | g     | 0.28         | 0/239   | 0.48        | 0/323          |
| 7   | h     | 0.34         | 0/243   | 0.77        | 0/329          |
| 7   | i     | 0.26         | 0/248   | 0.56        | 0/334          |
| 7   | j     | 0.30         | 0/239   | 0.50        | 0/323          |
| 7   | k     | 0.31         | 0/243   | 0.73        | 0/329          |
| 7   | l     | 0.30         | 0/248   | 0.56        | 0/334          |
| 7   | m     | 0.30         | 0/239   | 0.59        | 0/323          |
| 7   | n     | 0.34         | 0/243   | 0.70        | 0/329          |
| All | All   | 0.32         | 0/46529 | 0.64        | 5/62949 (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 |
|-----|-------|---------------------|---------------------|
| 3   | 8     | 0                   | 1                   |
| 7   | b     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 4   | A     | 90  | LEU  | CA-CB-CG | 5.32 | 134.93      | 116.30   |
| 1   | 1     | 167 | LEU  | N-CA-C   | 5.20 | 121.31      | 109.81   |
| 4   | H     | 143 | ARG  | CA-CB-CG | 5.19 | 124.47      | 114.10   |
| 4   | G     | 29  | PRO  | CA-C-N   | 5.11 | 131.18      | 121.97   |
| 4   | G     | 29  | PRO  | C-N-CA   | 5.11 | 131.18      | 121.97   |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | 8     | 41  | GLN  | Peptide |
| 7   | b     | 366 | LEU  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 1562  | 0        | 1597     | 20      | 0            |
| 1   | 1     | 1569  | 0        | 1613     | 9       | 0            |
| 1   | 2     | 1553  | 0        | 1598     | 24      | 0            |
| 1   | 3     | 1606  | 0        | 1649     | 22      | 0            |
| 1   | 4     | 1758  | 0        | 1806     | 19      | 0            |
| 2   | 5     | 1885  | 0        | 1931     | 31      | 0            |
| 3   | 6     | 405   | 0        | 418      | 2       | 0            |
| 3   | 7     | 644   | 0        | 685      | 9       | 0            |
| 3   | 8     | 644   | 0        | 685      | 9       | 0            |
| 3   | 9     | 647   | 0        | 692      | 13      | 0            |
| 4   | A     | 1108  | 0        | 1103     | 11      | 0            |
| 4   | B     | 1154  | 0        | 1163     | 8       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | C     | 1108  | 0        | 1103     | 11      | 0            |
| 4   | D     | 1146  | 0        | 1150     | 9       | 0            |
| 4   | F     | 1108  | 0        | 1103     | 10      | 0            |
| 4   | G     | 1154  | 0        | 1163     | 8       | 0            |
| 4   | H     | 1108  | 0        | 1103     | 6       | 0            |
| 4   | I     | 1154  | 0        | 1163     | 12      | 0            |
| 4   | J     | 1108  | 0        | 1103     | 8       | 0            |
| 4   | K     | 1154  | 0        | 1163     | 10      | 0            |
| 4   | L     | 1108  | 0        | 1103     | 13      | 0            |
| 4   | M     | 1146  | 0        | 1150     | 11      | 0            |
| 4   | N     | 1108  | 0        | 1103     | 10      | 0            |
| 4   | O     | 1154  | 0        | 1163     | 10      | 0            |
| 4   | P     | 1108  | 0        | 1103     | 13      | 0            |
| 4   | Q     | 1154  | 0        | 1163     | 11      | 0            |
| 5   | AM    | 298   | 0        | 307      | 1       | 0            |
| 5   | AN    | 644   | 0        | 654      | 11      | 0            |
| 5   | AO    | 667   | 0        | 672      | 10      | 0            |
| 5   | AP    | 675   | 0        | 683      | 8       | 0            |
| 5   | AQ    | 675   | 0        | 683      | 10      | 0            |
| 5   | AR    | 667   | 0        | 672      | 9       | 0            |
| 6   | AS    | 466   | 0        | 470      | 14      | 0            |
| 6   | AT    | 466   | 0        | 470      | 5       | 0            |
| 6   | AU    | 466   | 0        | 470      | 10      | 0            |
| 6   | AV    | 466   | 0        | 470      | 7       | 0            |
| 6   | AW    | 466   | 0        | 470      | 9       | 0            |
| 6   | AX    | 574   | 0        | 566      | 8       | 0            |
| 6   | AY    | 612   | 0        | 598      | 11      | 0            |
| 6   | AZ    | 460   | 0        | 435      | 9       | 0            |
| 6   | BA    | 437   | 0        | 413      | 6       | 0            |
| 6   | BB    | 388   | 0        | 369      | 4       | 0            |
| 6   | BC    | 388   | 0        | 369      | 7       | 0            |
| 6   | BD    | 388   | 0        | 369      | 9       | 0            |
| 6   | BE    | 346   | 0        | 329      | 7       | 0            |
| 7   | E     | 236   | 0        | 219      | 1       | 0            |
| 7   | R     | 227   | 0        | 208      | 1       | 0            |
| 7   | S     | 231   | 0        | 207      | 1       | 0            |
| 7   | T     | 236   | 0        | 219      | 0       | 0            |
| 7   | U     | 227   | 0        | 208      | 5       | 0            |
| 7   | V     | 231   | 0        | 207      | 1       | 0            |
| 7   | W     | 236   | 0        | 219      | 2       | 0            |
| 7   | X     | 227   | 0        | 208      | 2       | 0            |
| 7   | Y     | 231   | 0        | 207      | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | Z     | 236   | 0        | 219      | 0       | 0            |
| 7   | a     | 227   | 0        | 208      | 1       | 0            |
| 7   | b     | 231   | 0        | 207      | 1       | 0            |
| 7   | c     | 236   | 0        | 219      | 2       | 0            |
| 7   | d     | 227   | 0        | 208      | 2       | 0            |
| 7   | e     | 231   | 0        | 207      | 1       | 0            |
| 7   | f     | 236   | 0        | 219      | 1       | 0            |
| 7   | g     | 227   | 0        | 208      | 0       | 0            |
| 7   | h     | 231   | 0        | 207      | 3       | 0            |
| 7   | i     | 236   | 0        | 219      | 0       | 0            |
| 7   | j     | 227   | 0        | 208      | 5       | 0            |
| 7   | k     | 231   | 0        | 207      | 2       | 0            |
| 7   | l     | 236   | 0        | 219      | 1       | 0            |
| 7   | m     | 227   | 0        | 208      | 2       | 0            |
| 7   | n     | 231   | 0        | 207      | 0       | 0            |
| All | All   | 45454 | 0        | 45317    | 421     | 0            |

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

The worst 5 of 421 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 4:Q:39:ASP:H     | 4:Q:69:THR:HG22 | 1.55                     | 0.72              |
| 4:I:169:GLN:HE22 | 4:J:115:ARG:HA  | 1.57                     | 0.69              |
| 4:A:39:ASP:H     | 4:A:69:THR:HG22 | 1.59                     | 0.68              |
| 1:O:46:ILE:HD12  | 2:5:97:ALA:HB1  | 1.77                     | 0.65              |
| 6:AW:52:SER:HB2  | 6:BC:69:LYS:HD3 | 1.78                     | 0.64              |

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   | 0     | 195/224 (87%) | 189 (97%) | 5 (3%)  | 1 (0%)   | 24          | 57  |
| 1   | 1     | 195/224 (87%) | 186 (95%) | 8 (4%)  | 1 (0%)   | 24          | 57  |
| 1   | 2     | 193/224 (86%) | 187 (97%) | 5 (3%)  | 1 (0%)   | 24          | 57  |
| 1   | 3     | 200/224 (89%) | 195 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | 4     | 220/224 (98%) | 209 (95%) | 11 (5%) | 0        | 100         | 100 |
| 2   | 5     | 243/263 (92%) | 224 (92%) | 19 (8%) | 0        | 100         | 100 |
| 3   | 6     | 49/86 (57%)   | 46 (94%)  | 3 (6%)  | 0        | 100         | 100 |
| 3   | 7     | 82/86 (95%)   | 80 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 3   | 8     | 82/86 (95%)   | 80 (98%)  | 1 (1%)  | 1 (1%)   | 10          | 40  |
| 3   | 9     | 82/86 (95%)   | 81 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 4   | A     | 137/562 (24%) | 136 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 4   | B     | 143/562 (25%) | 139 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 4   | C     | 137/562 (24%) | 134 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 4   | D     | 142/562 (25%) | 138 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 4   | F     | 137/562 (24%) | 135 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 4   | G     | 143/562 (25%) | 137 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 4   | H     | 137/562 (24%) | 134 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 4   | I     | 143/562 (25%) | 141 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 4   | J     | 137/562 (24%) | 134 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 4   | K     | 143/562 (25%) | 139 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 4   | L     | 137/562 (24%) | 135 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 4   | M     | 142/562 (25%) | 137 (96%) | 5 (4%)  | 0        | 100         | 100 |
| 4   | N     | 137/562 (24%) | 134 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 4   | O     | 143/562 (25%) | 140 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 4   | P     | 137/562 (24%) | 136 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 4   | Q     | 143/562 (25%) | 139 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 5   | AM    | 37/101 (37%)  | 37 (100%) | 0       | 0        | 100         | 100 |
| 5   | AN    | 79/101 (78%)  | 79 (100%) | 0       | 0        | 100         | 100 |
| 5   | AO    | 86/101 (85%)  | 84 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 5   | AP    | 87/101 (86%)  | 87 (100%) | 0       | 0        | 100         | 100 |
| 5   | AQ    | 87/101 (86%)  | 87 (100%) | 0       | 0        | 100         | 100 |
| 5   | AR    | 86/101 (85%)  | 83 (96%)  | 3 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed    | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------|-----------|---------|----------|-------------|-----|
| 6   | AS    | 57/80 (71%) | 55 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 6   | AT    | 57/80 (71%) | 55 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 6   | AU    | 57/80 (71%) | 55 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 6   | AV    | 57/80 (71%) | 55 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 6   | AW    | 57/80 (71%) | 55 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 6   | AX    | 71/80 (89%) | 68 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 6   | AY    | 76/80 (95%) | 73 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 6   | AZ    | 53/80 (66%) | 52 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 6   | BA    | 50/80 (62%) | 47 (94%)  | 3 (6%)  | 0        | 100         | 100 |
| 6   | BB    | 44/80 (55%) | 43 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 6   | BC    | 44/80 (55%) | 44 (100%) | 0       | 0        | 100         | 100 |
| 6   | BD    | 44/80 (55%) | 43 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 6   | BE    | 39/80 (49%) | 37 (95%)  | 2 (5%)  | 0        | 100         | 100 |
| 7   | E     | 26/392 (7%) | 22 (85%)  | 4 (15%) | 0        | 100         | 100 |
| 7   | R     | 25/392 (6%) | 25 (100%) | 0       | 0        | 100         | 100 |
| 7   | S     | 26/392 (7%) | 20 (77%)  | 6 (23%) | 0        | 100         | 100 |
| 7   | T     | 26/392 (7%) | 22 (85%)  | 4 (15%) | 0        | 100         | 100 |
| 7   | U     | 25/392 (6%) | 24 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 7   | V     | 26/392 (7%) | 19 (73%)  | 7 (27%) | 0        | 100         | 100 |
| 7   | W     | 26/392 (7%) | 23 (88%)  | 3 (12%) | 0        | 100         | 100 |
| 7   | X     | 25/392 (6%) | 24 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 7   | Y     | 26/392 (7%) | 19 (73%)  | 7 (27%) | 0        | 100         | 100 |
| 7   | Z     | 26/392 (7%) | 22 (85%)  | 4 (15%) | 0        | 100         | 100 |
| 7   | a     | 25/392 (6%) | 24 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 7   | b     | 26/392 (7%) | 19 (73%)  | 7 (27%) | 0        | 100         | 100 |
| 7   | c     | 26/392 (7%) | 22 (85%)  | 4 (15%) | 0        | 100         | 100 |
| 7   | d     | 25/392 (6%) | 25 (100%) | 0       | 0        | 100         | 100 |
| 7   | e     | 26/392 (7%) | 18 (69%)  | 8 (31%) | 0        | 100         | 100 |
| 7   | f     | 26/392 (7%) | 22 (85%)  | 4 (15%) | 0        | 100         | 100 |
| 7   | g     | 25/392 (6%) | 25 (100%) | 0       | 0        | 100         | 100 |
| 7   | h     | 26/392 (7%) | 19 (73%)  | 7 (27%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 7   | i     | 26/392 (7%)      | 22 (85%)   | 4 (15%)  | 0        | 100         | 100 |
| 7   | j     | 25/392 (6%)      | 25 (100%)  | 0        | 0        | 100         | 100 |
| 7   | k     | 26/392 (7%)      | 19 (73%)   | 7 (27%)  | 0        | 100         | 100 |
| 7   | l     | 26/392 (7%)      | 22 (85%)   | 4 (15%)  | 0        | 100         | 100 |
| 7   | m     | 25/392 (6%)      | 24 (96%)   | 1 (4%)   | 0        | 100         | 100 |
| 7   | n     | 26/392 (7%)      | 19 (73%)   | 7 (27%)  | 0        | 100         | 100 |
| All | All   | 5563/21773 (26%) | 5329 (96%) | 230 (4%) | 4 (0%)   | 49          | 79  |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 8     | 42  | LEU  |
| 1   | 0     | 49  | ASN  |
| 1   | 1     | 49  | ASN  |
| 1   | 2     | 47  | PRO  |

### 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   | 0     | 175/199 (88%) | 172 (98%)  | 3 (2%)   | 53          | 67  |
| 1   | 1     | 177/199 (89%) | 177 (100%) | 0        | 100         | 100 |
| 1   | 2     | 175/199 (88%) | 175 (100%) | 0        | 100         | 100 |
| 1   | 3     | 180/199 (90%) | 179 (99%)  | 1 (1%)   | 78          | 79  |
| 1   | 4     | 197/199 (99%) | 197 (100%) | 0        | 100         | 100 |
| 2   | 5     | 205/219 (94%) | 204 (100%) | 1 (0%)   | 81          | 81  |
| 3   | 6     | 41/71 (58%)   | 41 (100%)  | 0        | 100         | 100 |
| 3   | 7     | 69/71 (97%)   | 69 (100%)  | 0        | 100         | 100 |
| 3   | 8     | 69/71 (97%)   | 69 (100%)  | 0        | 100         | 100 |
| 3   | 9     | 70/71 (99%)   | 70 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 4   | A     | 119/477 (25%) | 118 (99%)  | 1 (1%)   | 73          | 76  |
| 4   | B     | 125/477 (26%) | 125 (100%) | 0        | 100         | 100 |
| 4   | C     | 119/477 (25%) | 119 (100%) | 0        | 100         | 100 |
| 4   | D     | 124/477 (26%) | 123 (99%)  | 1 (1%)   | 73          | 76  |
| 4   | F     | 119/477 (25%) | 118 (99%)  | 1 (1%)   | 73          | 76  |
| 4   | G     | 125/477 (26%) | 124 (99%)  | 1 (1%)   | 73          | 76  |
| 4   | H     | 119/477 (25%) | 118 (99%)  | 1 (1%)   | 73          | 76  |
| 4   | I     | 125/477 (26%) | 125 (100%) | 0        | 100         | 100 |
| 4   | J     | 119/477 (25%) | 118 (99%)  | 1 (1%)   | 73          | 76  |
| 4   | K     | 125/477 (26%) | 125 (100%) | 0        | 100         | 100 |
| 4   | L     | 119/477 (25%) | 118 (99%)  | 1 (1%)   | 73          | 76  |
| 4   | M     | 124/477 (26%) | 123 (99%)  | 1 (1%)   | 73          | 76  |
| 4   | N     | 119/477 (25%) | 118 (99%)  | 1 (1%)   | 73          | 76  |
| 4   | O     | 125/477 (26%) | 125 (100%) | 0        | 100         | 100 |
| 4   | P     | 119/477 (25%) | 118 (99%)  | 1 (1%)   | 73          | 76  |
| 4   | Q     | 125/477 (26%) | 124 (99%)  | 1 (1%)   | 73          | 76  |
| 5   | AM    | 34/88 (39%)   | 33 (97%)   | 1 (3%)   | 37          | 58  |
| 5   | AN    | 71/88 (81%)   | 71 (100%)  | 0        | 100         | 100 |
| 5   | AO    | 76/88 (86%)   | 76 (100%)  | 0        | 100         | 100 |
| 5   | AP    | 77/88 (88%)   | 76 (99%)   | 1 (1%)   | 61          | 71  |
| 5   | AQ    | 77/88 (88%)   | 77 (100%)  | 0        | 100         | 100 |
| 5   | AR    | 76/88 (86%)   | 76 (100%)  | 0        | 100         | 100 |
| 6   | AS    | 50/67 (75%)   | 46 (92%)   | 4 (8%)   | 11          | 36  |
| 6   | AT    | 50/67 (75%)   | 44 (88%)   | 6 (12%)  | 5           | 21  |
| 6   | AU    | 50/67 (75%)   | 45 (90%)   | 5 (10%)  | 7           | 28  |
| 6   | AV    | 50/67 (75%)   | 45 (90%)   | 5 (10%)  | 7           | 28  |
| 6   | AW    | 50/67 (75%)   | 44 (88%)   | 6 (12%)  | 5           | 21  |
| 6   | AX    | 62/67 (92%)   | 62 (100%)  | 0        | 100         | 100 |
| 6   | AY    | 66/67 (98%)   | 66 (100%)  | 0        | 100         | 100 |
| 6   | AZ    | 51/67 (76%)   | 51 (100%)  | 0        | 100         | 100 |
| 6   | BA    | 48/67 (72%)   | 47 (98%)   | 1 (2%)   | 47          | 64  |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|-------------|-----|
| 6   | BB    | 42/67 (63%)      | 42 (100%)  | 0        | 100         | 100 |
| 6   | BC    | 42/67 (63%)      | 42 (100%)  | 0        | 100         | 100 |
| 6   | BD    | 42/67 (63%)      | 42 (100%)  | 0        | 100         | 100 |
| 6   | BE    | 37/67 (55%)      | 37 (100%)  | 0        | 100         | 100 |
| 7   | E     | 23/337 (7%)      | 23 (100%)  | 0        | 100         | 100 |
| 7   | R     | 22/337 (6%)      | 21 (96%)   | 1 (4%)   | 24          | 48  |
| 7   | S     | 21/337 (6%)      | 21 (100%)  | 0        | 100         | 100 |
| 7   | T     | 23/337 (7%)      | 23 (100%)  | 0        | 100         | 100 |
| 7   | U     | 22/337 (6%)      | 21 (96%)   | 1 (4%)   | 24          | 48  |
| 7   | V     | 21/337 (6%)      | 20 (95%)   | 1 (5%)   | 23          | 47  |
| 7   | W     | 23/337 (7%)      | 23 (100%)  | 0        | 100         | 100 |
| 7   | X     | 22/337 (6%)      | 21 (96%)   | 1 (4%)   | 24          | 48  |
| 7   | Y     | 21/337 (6%)      | 21 (100%)  | 0        | 100         | 100 |
| 7   | Z     | 23/337 (7%)      | 23 (100%)  | 0        | 100         | 100 |
| 7   | a     | 22/337 (6%)      | 21 (96%)   | 1 (4%)   | 24          | 48  |
| 7   | b     | 21/337 (6%)      | 21 (100%)  | 0        | 100         | 100 |
| 7   | c     | 23/337 (7%)      | 23 (100%)  | 0        | 100         | 100 |
| 7   | d     | 22/337 (6%)      | 21 (96%)   | 1 (4%)   | 24          | 48  |
| 7   | e     | 21/337 (6%)      | 21 (100%)  | 0        | 100         | 100 |
| 7   | f     | 23/337 (7%)      | 23 (100%)  | 0        | 100         | 100 |
| 7   | g     | 22/337 (6%)      | 21 (96%)   | 1 (4%)   | 24          | 48  |
| 7   | h     | 21/337 (6%)      | 21 (100%)  | 0        | 100         | 100 |
| 7   | i     | 23/337 (7%)      | 23 (100%)  | 0        | 100         | 100 |
| 7   | j     | 22/337 (6%)      | 22 (100%)  | 0        | 100         | 100 |
| 7   | k     | 21/337 (6%)      | 21 (100%)  | 0        | 100         | 100 |
| 7   | l     | 23/337 (7%)      | 23 (100%)  | 0        | 100         | 100 |
| 7   | m     | 22/337 (6%)      | 21 (96%)   | 1 (4%)   | 24          | 48  |
| 7   | n     | 21/337 (6%)      | 21 (100%)  | 0        | 100         | 100 |
| All | All   | 4887/18617 (26%) | 4834 (99%) | 53 (1%)  | 63          | 73  |

5 of 53 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AW    | 28  | THR  |
| 4   | D     | 40  | ASP  |
| 7   | a     | 366 | LEU  |
| 6   | AW    | 44  | LEU  |
| 6   | AW    | 64  | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | C     | 161 | ASN  |
| 4   | L     | 71  | ASN  |
| 4   | F     | 71  | ASN  |
| 4   | H     | 97  | GLN  |
| 4   | M     | 78  | 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.

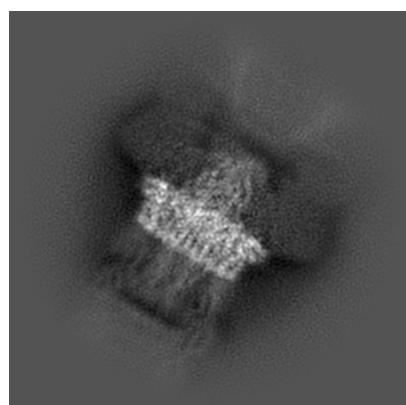
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20317. These allow visual inspection of the internal detail of the map and identification of artifacts.

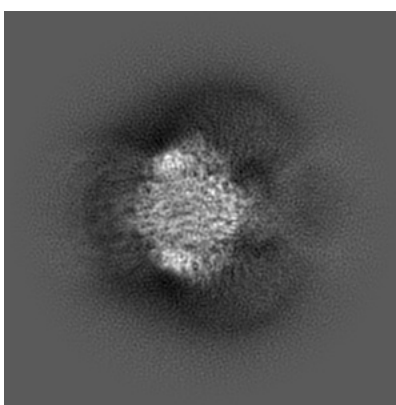
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

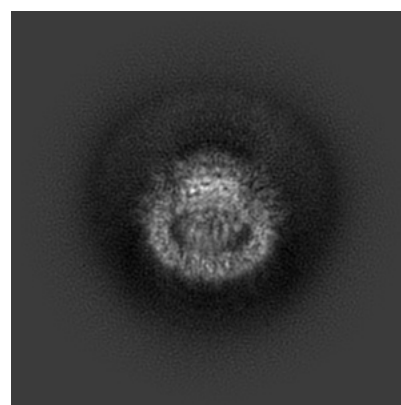
#### 6.1.1 Primary map



X



Y

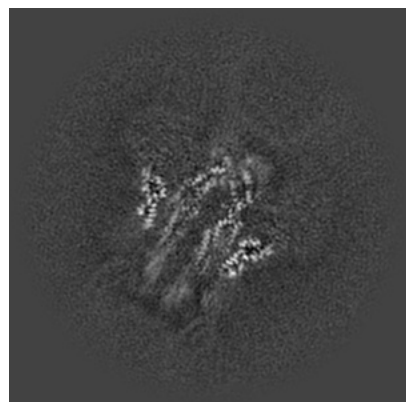


Z

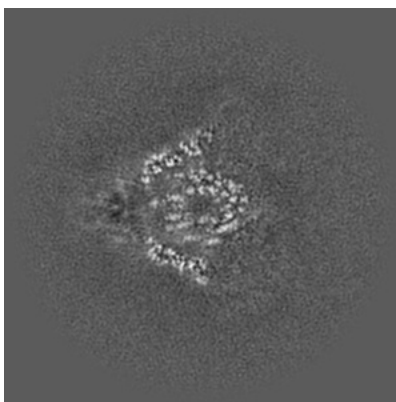
The images above show the map projected in three orthogonal directions.

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

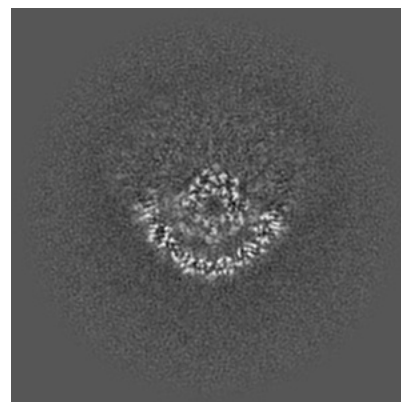
#### 6.2.1 Primary map



X Index: 125



Y Index: 125

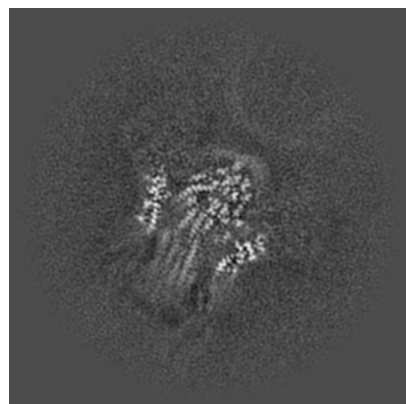


Z Index: 125

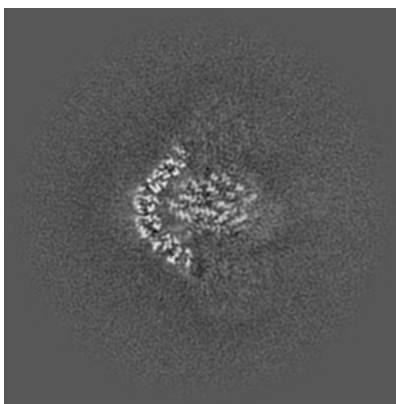
The images above show central slices of the map in three orthogonal directions.

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

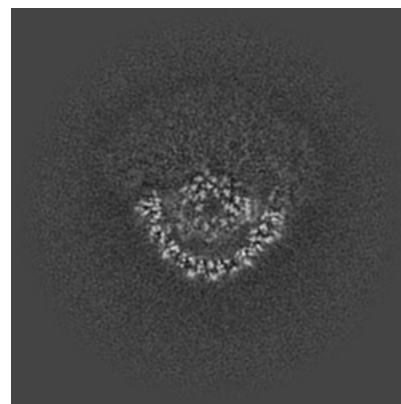
### 6.3.1 Primary map



X Index: 134



Y Index: 139

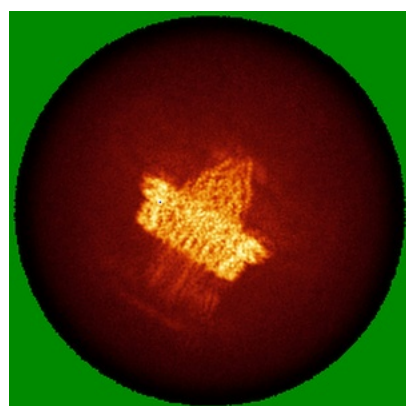


Z Index: 123

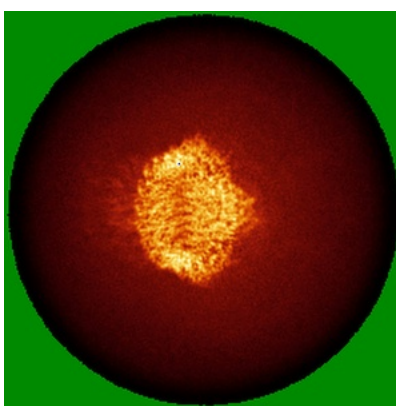
The images above show the largest variance slices of the map in three orthogonal directions.

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

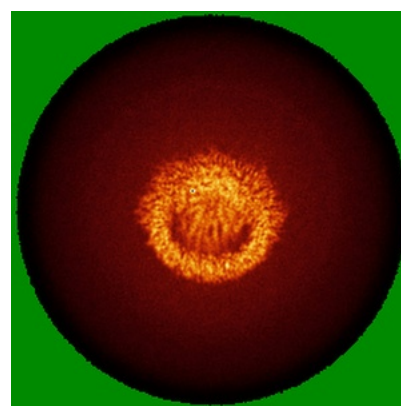
### 6.4.1 Primary map



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

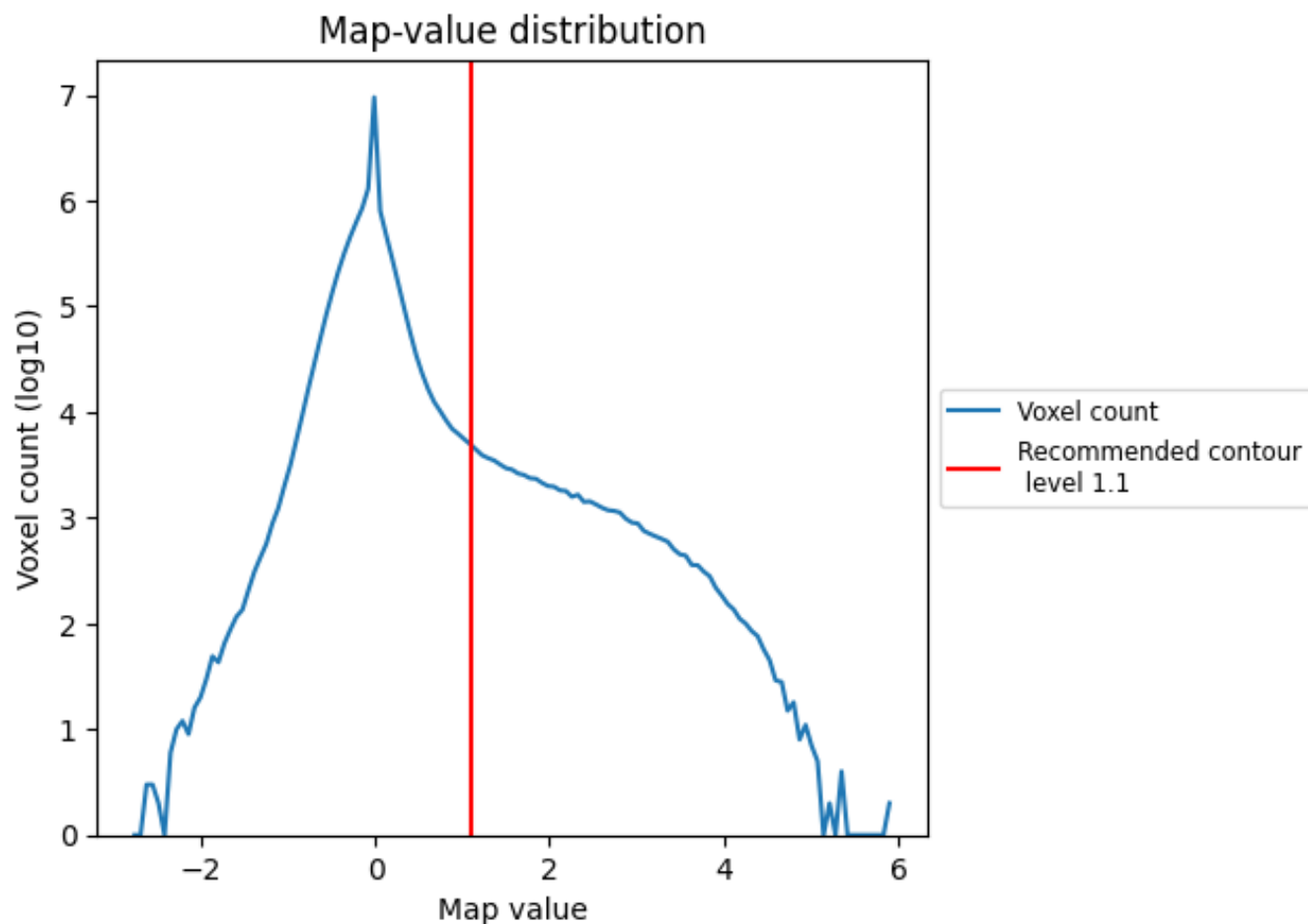
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

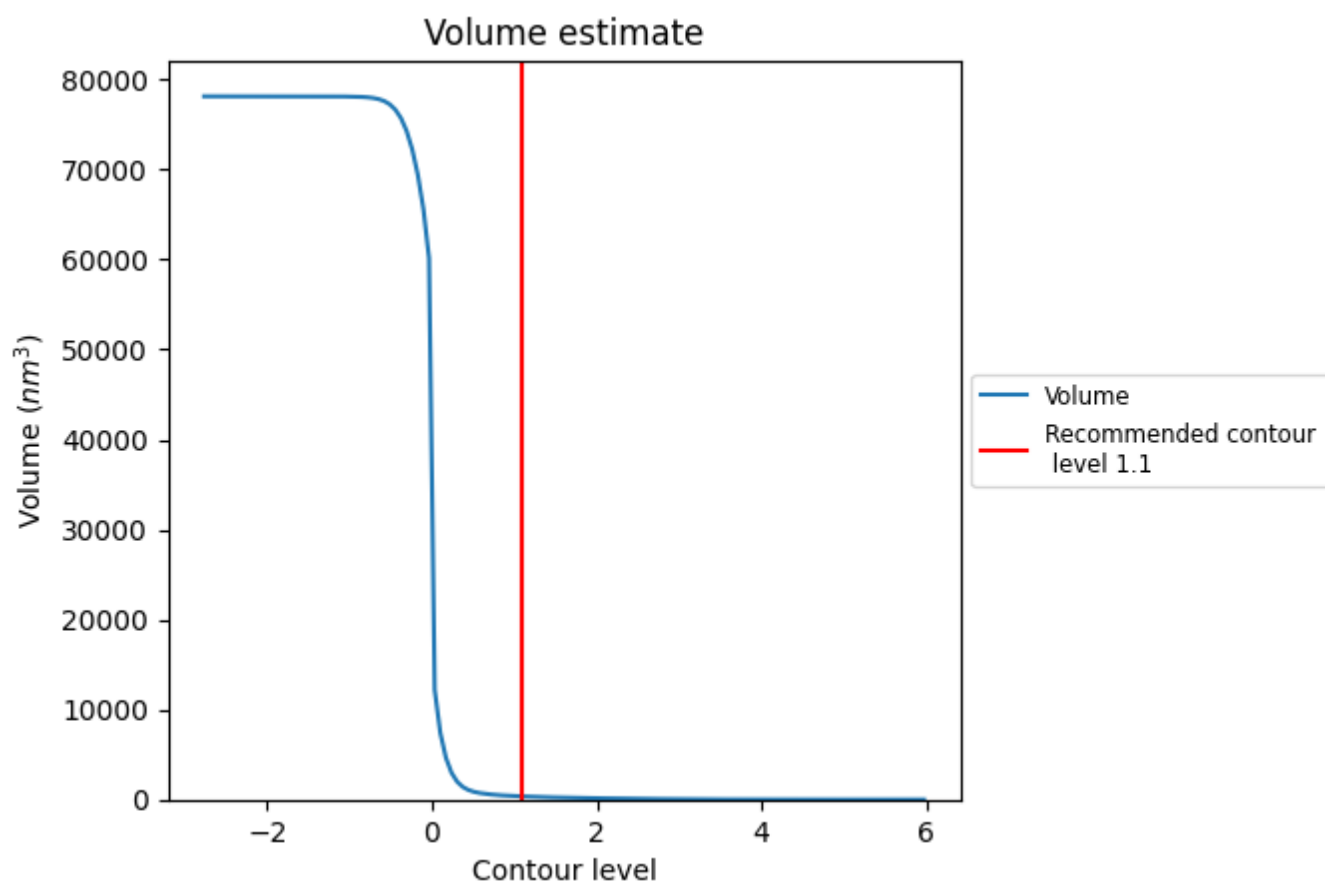
This section contains the results of statistical analysis of the map.

### 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.

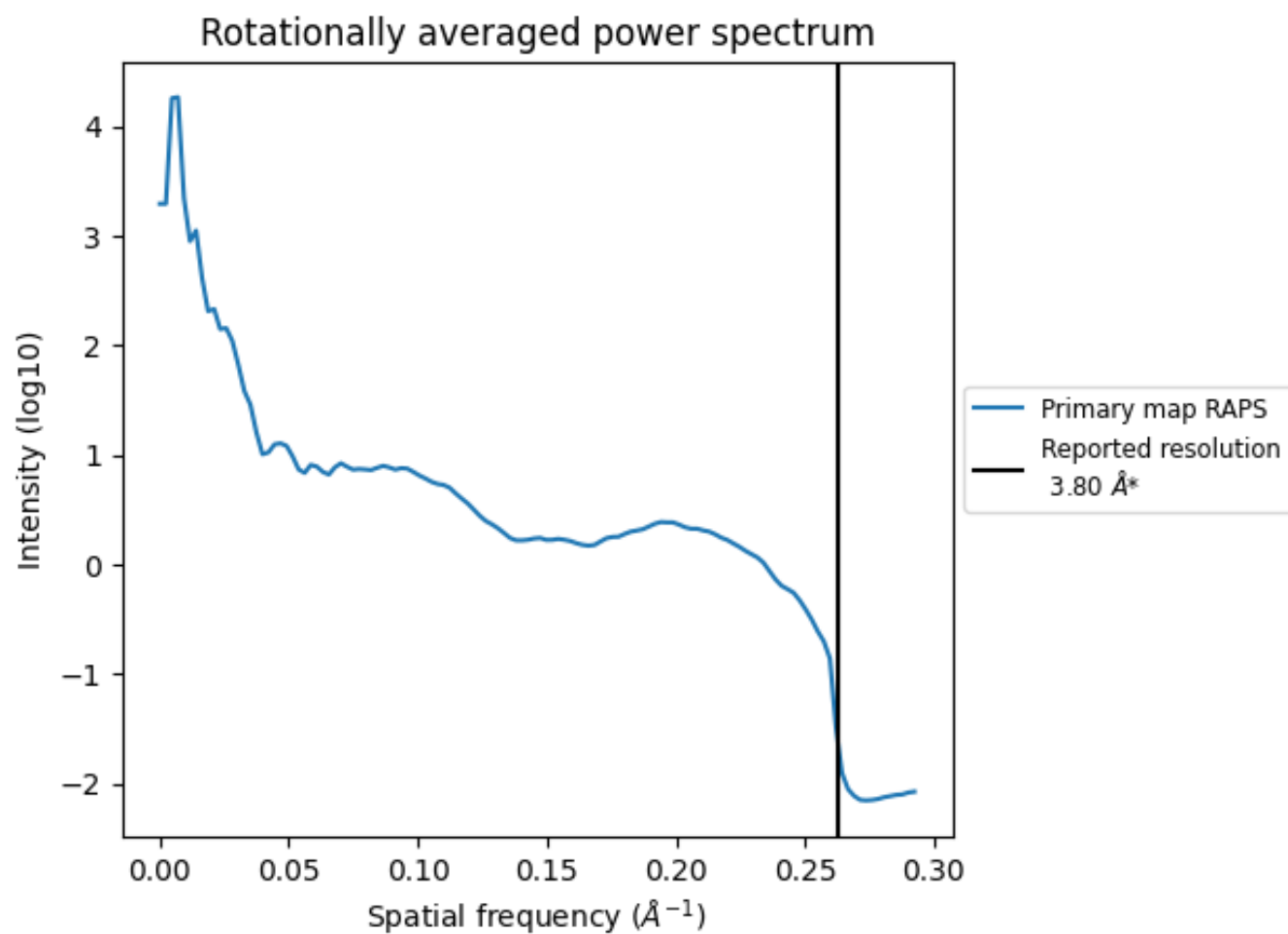
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352  $\text{nm}^3$ ; this corresponds to an approximate mass of 318 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 0.263 Å<sup>-1</sup>

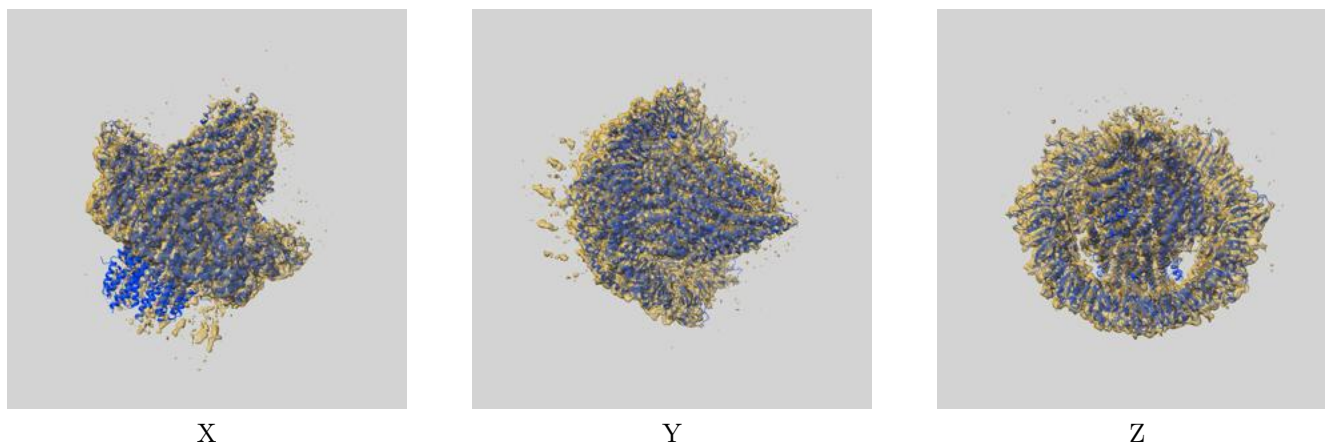
## 8 Fourier-Shell correlation

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

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

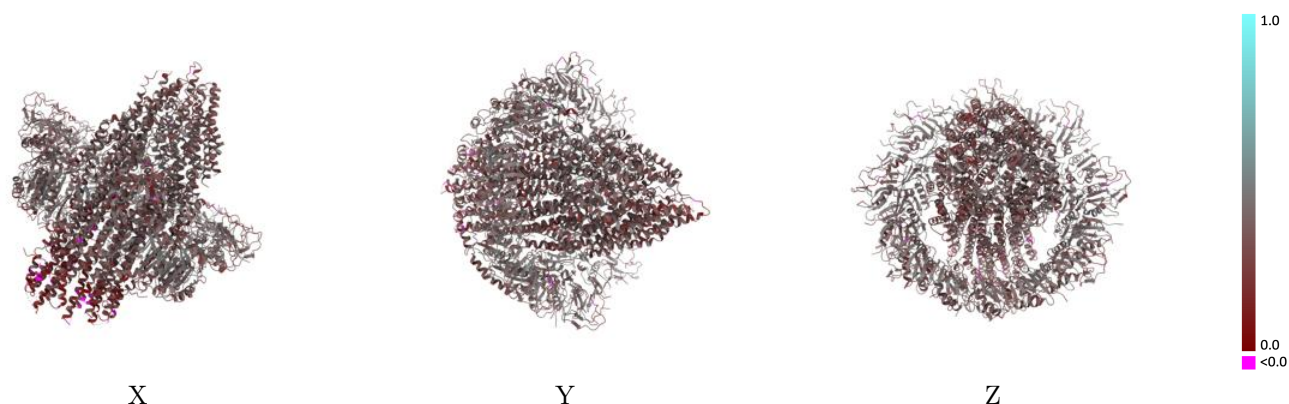
This section contains information regarding the fit between EMDB map EMD-20317 and PDB model 6PEP. Per-residue inclusion information can be found in section [3](#) on page [11](#).

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



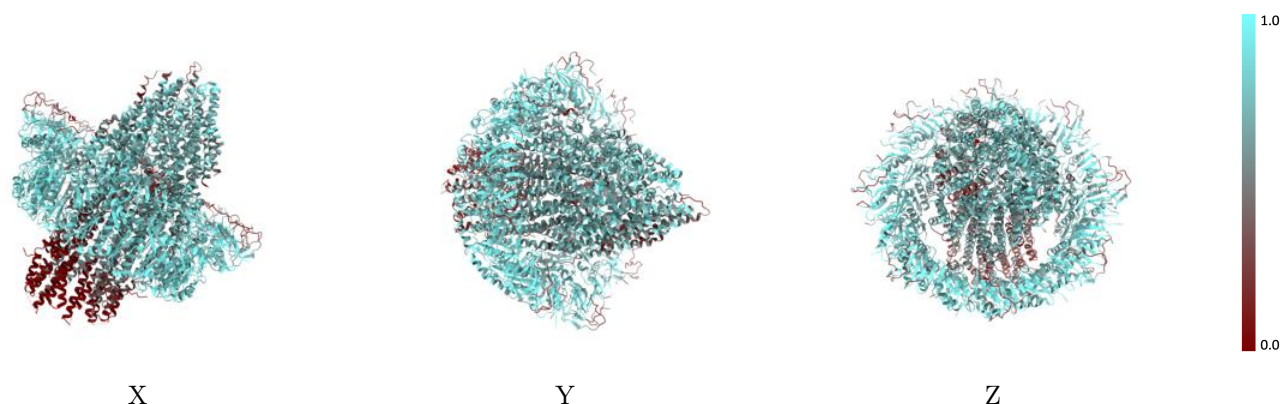
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



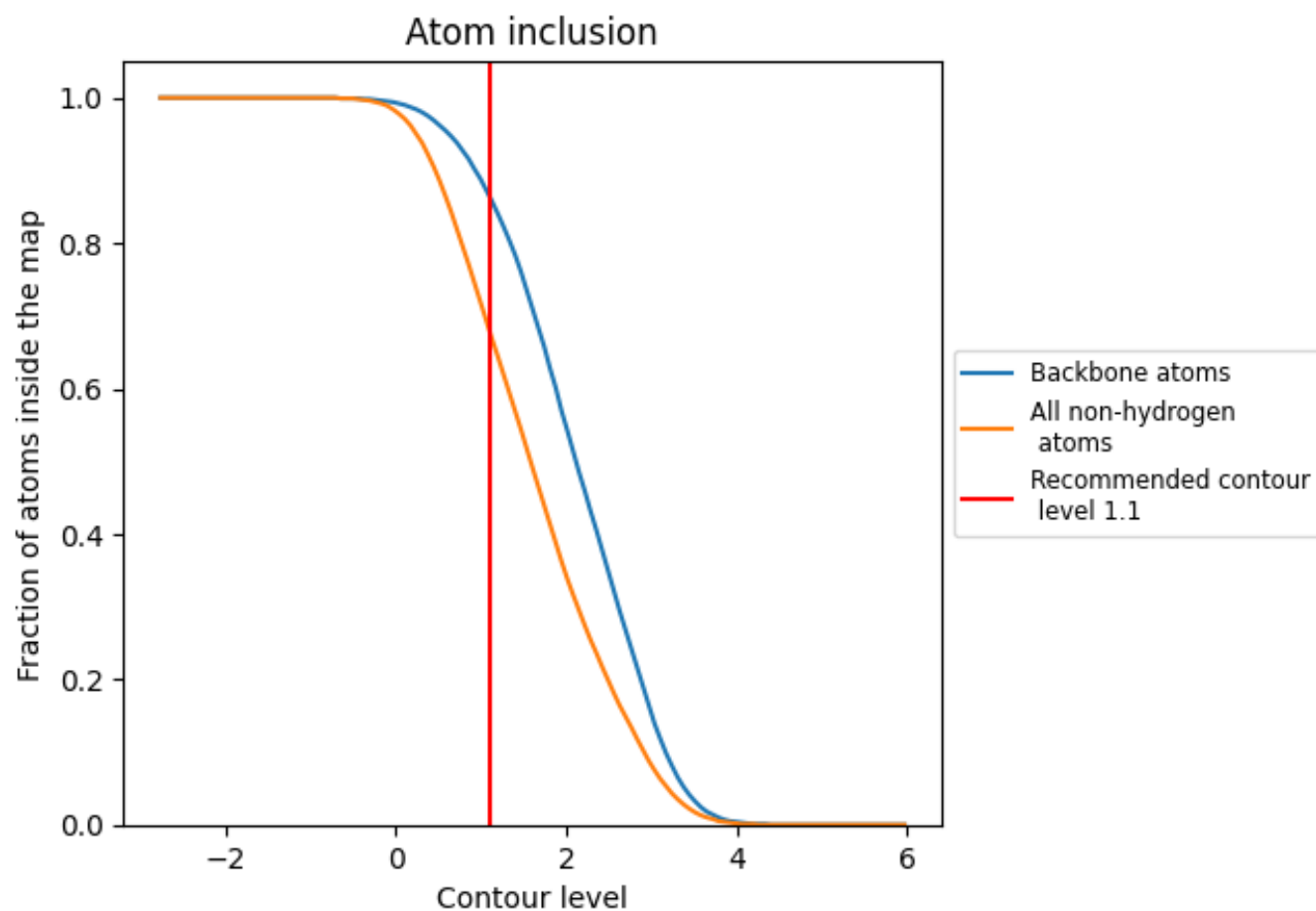
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 68% 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 (1.1) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6780   |  0.3540   |
| 0     |  0.6950   |  0.3510   |
| 1     |  0.6950   |  0.3290   |
| 2     |  0.7060   |  0.3440   |
| 3     |  0.7160   |  0.3590   |
| 4     |  0.7060   |  0.3560   |
| 5     |  0.7550   |  0.3840   |
| 6     |  0.2890   |  0.3300   |
| 7     |  0.4720   |  0.3090   |
| 8     |  0.6190   |  0.3280   |
| 9     |  0.6780   |  0.3490   |
| A     |  0.8350   |  0.3860   |
| AM    |  0.5990   |  0.3480   |
| AN    |  0.6120   |  0.3240   |
| AO    |  0.6120  |  0.3230  |
| AP    |  0.5880 |  0.3370 |
| AQ    |  0.6090 |  0.3310 |
| AR    |  0.4980 |  0.3180 |
| AS    |  0.4470 |  0.2930 |
| AT    |  0.5320 |  0.2710 |
| AU    |  0.4620 |  0.2840 |
| AV    |  0.4380 |  0.2750 |
| AW    |  0.3440 |  0.2710 |
| AX    |  0.0760 |  0.2480 |
| AY    |  0.2770 |  0.2410 |
| AZ    |  0.3540 |  0.2470 |
| B     |  0.8140 |  0.3820 |
| BA    |  0.3290 |  0.2260 |
| BB    |  0.3030 |  0.2240 |
| BC    |  0.0320 |  0.2120 |
| BD    |  0.0450 |  0.1870 |
| BE    |  0.1390 |  0.1860 |
| C     |  0.8340 |  0.3870 |
| D     |  0.8170 |  0.3970 |
| E     |  0.4280 |  0.3170 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| F     |  0.8330   |  0.3990   |
| G     |  0.8110   |  0.3940   |
| H     |  0.8340   |  0.4010   |
| I     |  0.8050   |  0.3970   |
| J     |  0.8420   |  0.4020   |
| K     |  0.8280   |  0.3860   |
| L     |  0.8420   |  0.3980   |
| M     |  0.8230   |  0.3880   |
| N     |  0.8480   |  0.3920   |
| O     |  0.8180   |  0.3800   |
| P     |  0.8420   |  0.3770   |
| Q     |  0.8140   |  0.3840   |
| R     |  0.7640   |  0.3900   |
| S     |  0.7770   |  0.3880   |
| T     |  0.3840   |  0.3150   |
| U     |  0.7680   |  0.3880   |
| V     |  0.7630   |  0.3920   |
| W     |  0.3760  |  0.3230  |
| X     |  0.7910 |  0.4040 |
| Y     |  0.7900 |  0.4020 |
| Z     |  0.4060 |  0.3170 |
| a     |  0.7860 |  0.3920 |
| b     |  0.8040 |  0.4070 |
| c     |  0.4500 |  0.3230 |
| d     |  0.7730 |  0.3920 |
| e     |  0.7900 |  0.4020 |
| f     |  0.4540 |  0.3200 |
| g     |  0.7680 |  0.3970 |
| h     |  0.7950 |  0.4130 |
| i     |  0.4280 |  0.3170 |
| j     |  0.8090 |  0.4170 |
| k     |  0.8040 |  0.4220 |
| l     |  0.4150 |  0.3190 |
| m     |  0.7680 |  0.4210 |
| n     |  0.7590 |  0.3930 |