



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 06:05 AM UTC

PDB ID : 6E2R / pdb\_00006e2r  
EMDB ID : EMD-8969  
Title : Mechanism of cellular recognition by PCV2  
Authors : Khayat, R.; Dhindwal, S.  
Deposited on : 2018-07-12  
Resolution : 2.80 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

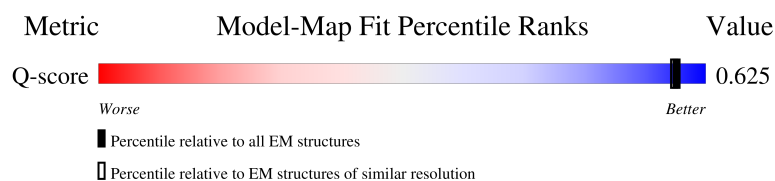
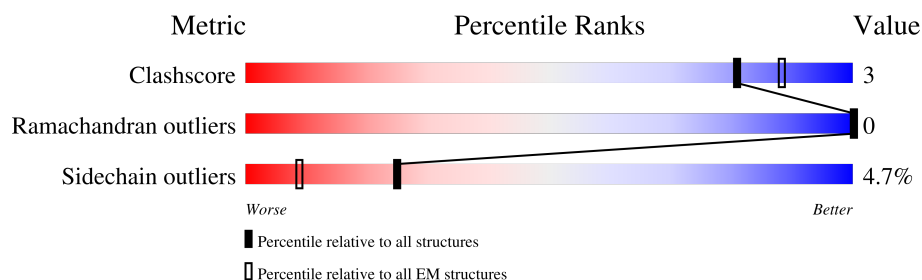
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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                       | 11806 ( 2.30 - 3.30 )                                    |

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   | A1    | 233    | <br>73% 7% • 19% |
| 1   | A2    | 233    | <br>73% 6% • 19% |
| 1   | A3    | 233    | <br>73% 7% • 19% |
| 1   | A4    | 233    | <br>74% 7% 19%   |

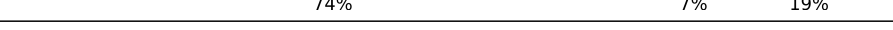
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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 1   | A5    | 233    |  73% 7% 19%   |
| 1   | A6    | 233    |  74% 7% 19%   |
| 1   | A7    | 233    |  73% 7% 19%   |
| 1   | A8    | 233    |  73% 8% 19%   |
| 1   | A9    | 233    |  74% 7% 19%   |
| 1   | AA    | 233    |  74% 7% 19%   |
| 1   | AB    | 233    |  74% 7% 19%   |
| 1   | AC    | 233    |  73% 7% 19%   |
| 1   | AD    | 233    |  73% 7% 19%   |
| 1   | AE    | 233    |  73% 8% 19%   |
| 1   | AF    | 233    |  74% 7% 19%   |
| 1   | AG    | 233    |  73% 7% 19%  |
| 1   | AH    | 233    |  73% 7% 19% |
| 1   | AI    | 233    |  73% 7% 19% |
| 1   | AJ    | 233    |  74% 7% 19% |
| 1   | AK    | 233    |  74% 7% 19% |
| 1   | AL    | 233    |  74% 7% 19% |
| 1   | AM    | 233    |  73% 7% 19% |
| 1   | AN    | 233    |  73% 7% 19% |
| 1   | AO    | 233    |  73% 6% 19% |
| 1   | AP    | 233    |  73% 7% 19% |
| 1   | AQ    | 233    |  74% 7% 19% |
| 1   | AR    | 233    |  73% 7% 19% |
| 1   | AS    | 233    |  73% 7% 19% |
| 1   | AT    | 233    |  73% 7% 19% |

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| Mol | Chain | Length | Quality of chain                                                                                |
|-----|-------|--------|-------------------------------------------------------------------------------------------------|
| 1   | AU    | 233    |  73% 7% 19%   |
| 1   | AV    | 233    |  74% 7% 19%   |
| 1   | AW    | 233    |  73% 7% 19%   |
| 1   | AX    | 233    |  73% 7% 19%   |
| 1   | AY    | 233    |  73% 7% 19%   |
| 1   | AZ    | 233    |  73% 7% 19%   |
| 1   | Aa    | 233    |  74% 6% 19%   |
| 1   | Ab    | 233    |  73% 7% 19%   |
| 1   | Ac    | 233    |  73% 7% 19%   |
| 1   | Ad    | 233    |  73% 7% 19%   |
| 1   | Ae    | 233    |  73% 7% 19%   |
| 1   | Af    | 233    |  74% 7% 19%  |
| 1   | Ag    | 233    |  73% 7% 19% |
| 1   | Ah    | 233    |  74% 7% 19% |
| 1   | Ai    | 233    |  73% 7% 19% |
| 1   | Aj    | 233    |  73% 8% 19% |
| 1   | Ak    | 233    |  74% 7% 19% |
| 1   | Al    | 233    |  73% 7% 19% |
| 1   | Am    | 233    |  73% 7% 19% |
| 1   | An    | 233    |  73% 7% 19% |
| 1   | Ao    | 233    |  73% 7% 19% |
| 1   | Ap    | 233    |  74% 6% 19% |
| 1   | Aq    | 233    |  73% 7% 19% |
| 1   | Ar    | 233    |  74% 7% 19% |
| 1   | As    | 233    |  73% 7% 19% |

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| Mol | Chain | Length | Quality of chain                                                |
|-----|-------|--------|-----------------------------------------------------------------|
| 1   | At    | 233    | <div><div></div><div>74%</div><div>7%</div><div>19%</div></div> |
| 1   | Au    | 233    | <div><div></div><div>74%</div><div>7%</div><div>19%</div></div> |
| 1   | Av    | 233    | <div><div></div><div>73%</div><div>8%</div><div>19%</div></div> |
| 1   | Aw    | 233    | <div><div></div><div>73%</div><div>7%</div><div>19%</div></div> |
| 1   | Ax    | 233    | <div><div></div><div>73%</div><div>7%</div><div>19%</div></div> |
| 1   | Ay    | 233    | <div><div></div><div>73%</div><div>7%</div><div>19%</div></div> |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 183180 atoms, of which 90180 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 Capsid protein of PCV2.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 1   | A1    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | A2    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | A3    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | A4    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | A5    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | A6    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | A7    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | A8    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | A9    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AA    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AB    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AC    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AD    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AE    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AF    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AG    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AH    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |

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| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 1   | AI    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AJ    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AK    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AL    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AM    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AN    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AO    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AP    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AQ    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AR    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AS    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AT    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AU    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AV    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AW    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AX    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AY    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | AZ    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Aa    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ab    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ac    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |

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| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 1   | Ad    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ae    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Af    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ag    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ah    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ai    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Aj    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ak    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Al    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Am    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | An    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ao    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ap    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Aq    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ar    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | As    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | At    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Au    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Av    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Aw    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |
| 1   | Ax    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |

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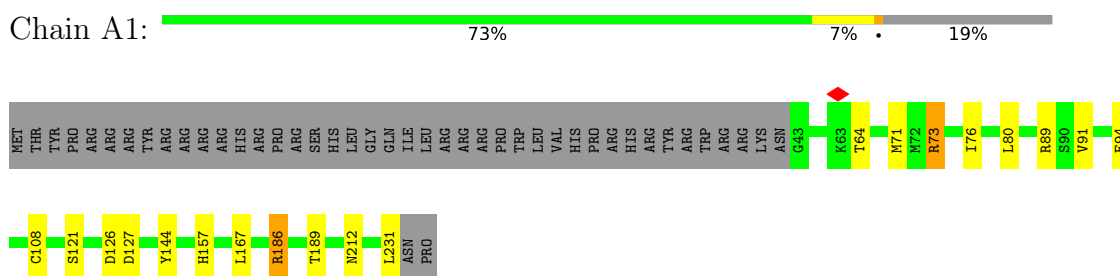
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| Mol | Chain | Residues | Atoms |     |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|-------|
| 1   | Ay    | 189      | Total | C   | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3053  | 995 | 1503 | 268 | 283 | 4 |         |       |

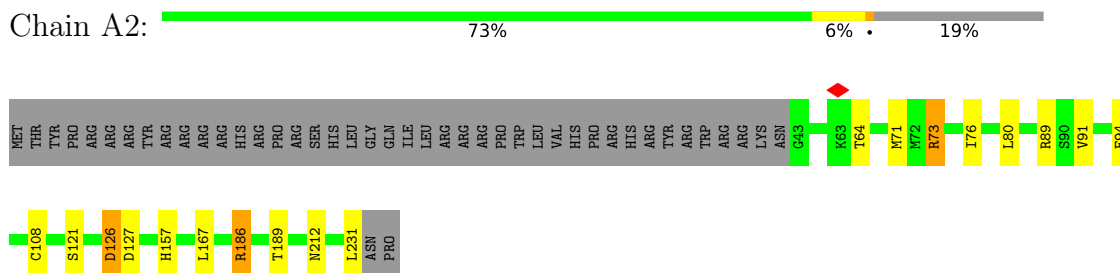
### 3 Residue-property plots

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

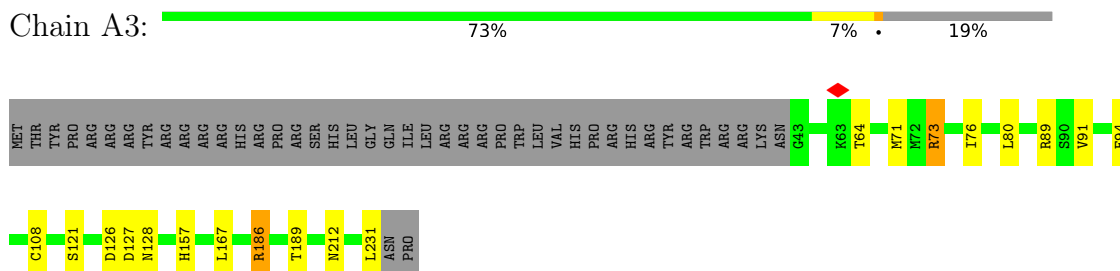
- Molecule 1: Capsid protein of PCV2



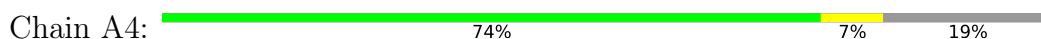
- Molecule 1: Capsid protein of PCV2



- Molecule 1: Capsid protein of PCV2

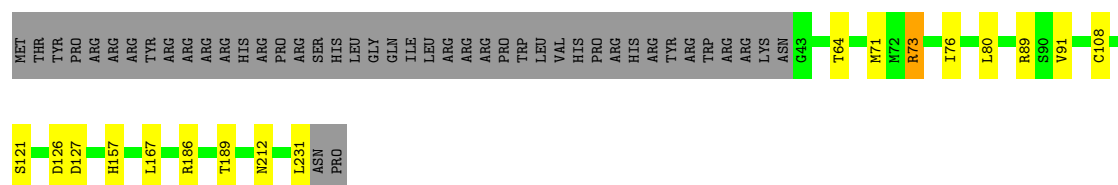


- Molecule 1: Capsid protein of PCV2



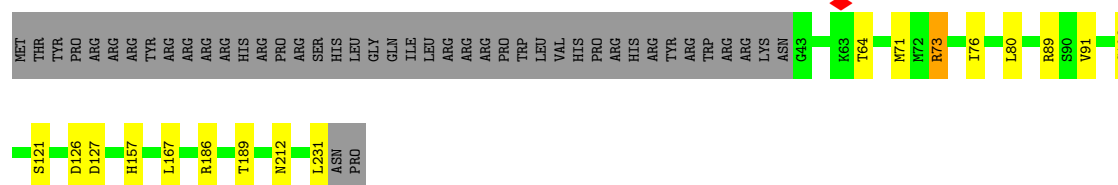


Chain A9:  74% 7% 19%



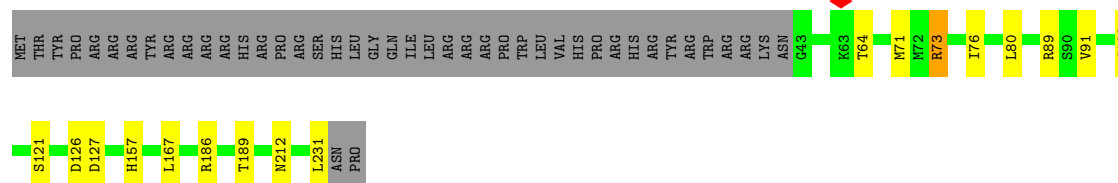
- Molecule 1: Capsid protein of PCV2

Chain AA:  74% 7% 19%



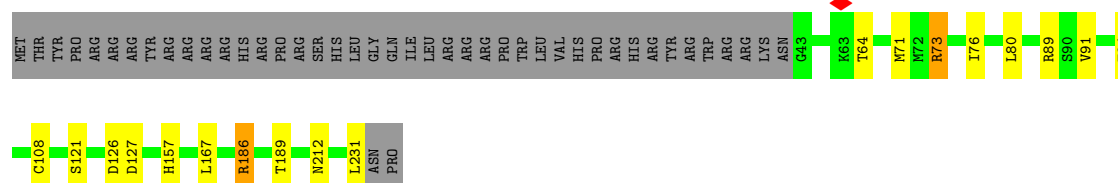
- Molecule 1: Capsid protein of PCV2

Chain AB:  74% 7% 19%



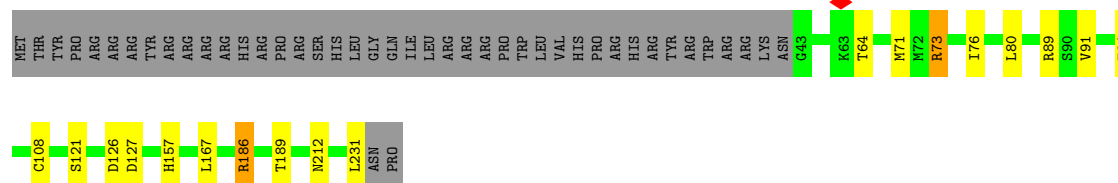
- Molecule 1: Capsid protein of PCV2

Chain AC:  73% 7% 19%



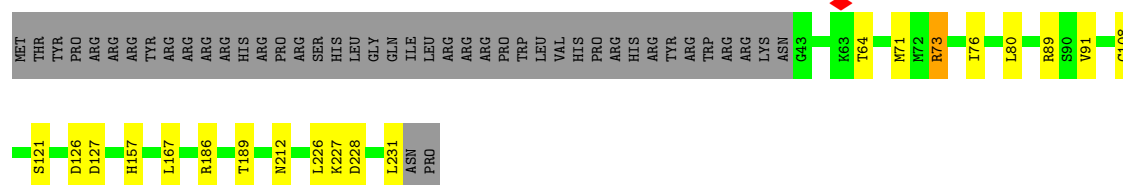
- Molecule 1: Capsid protein of PCV2

Chain AD:  73% 7% 19%



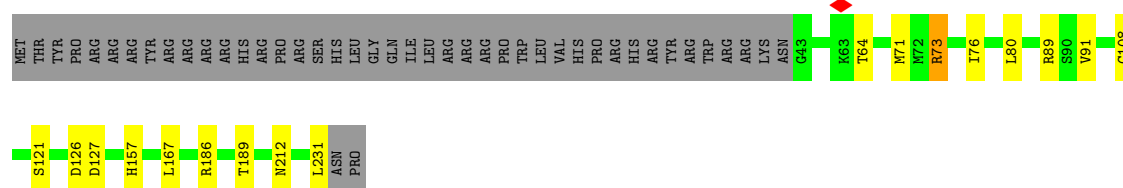
- Molecule 1: Capsid protein of PCV2

Chain AE:  73% 8% 19%



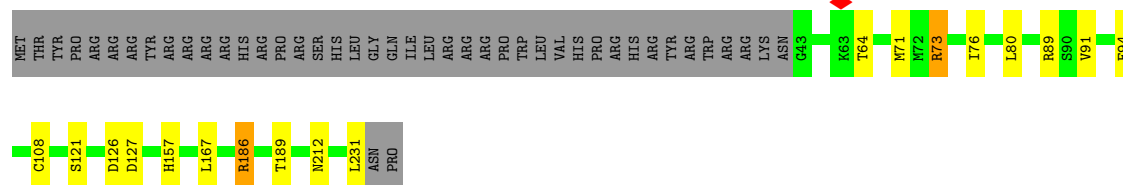
- Molecule 1: Capsid protein of PCV2

Chain AF:  74% 7% 19%



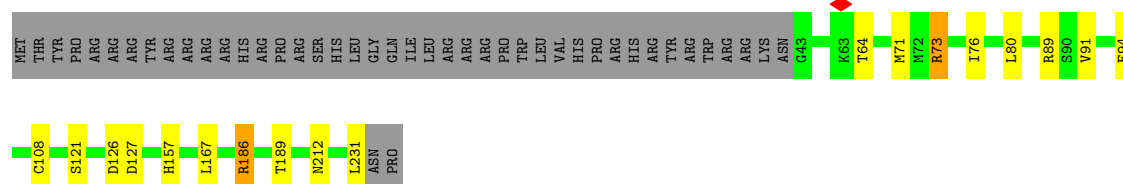
- Molecule 1: Capsid protein of PCV2

Chain AG:  73% 7% 19%



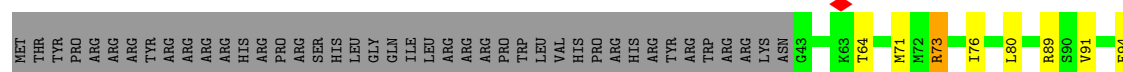
- Molecule 1: Capsid protein of PCV2

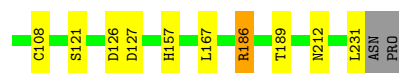
Chain AH:  73% 7% 19%



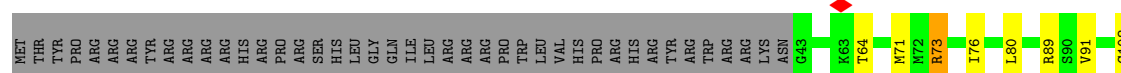
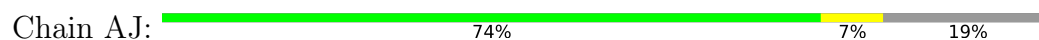
- Molecule 1: Capsid protein of PCV2

Chain AI:  73% 7% 19%

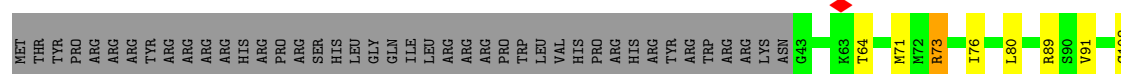




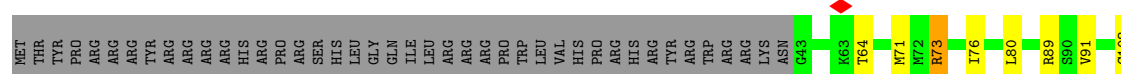
- Molecule 1: Capsid protein of PCV2



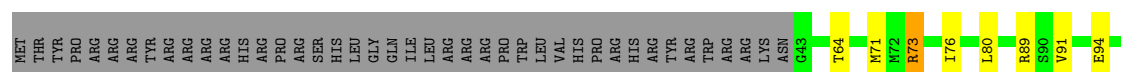
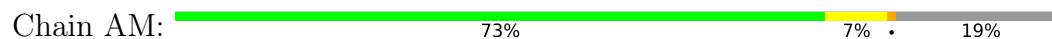
- Molecule 1: Capsid protein of PCV2



- Molecule 1: Capsid protein of PCV2

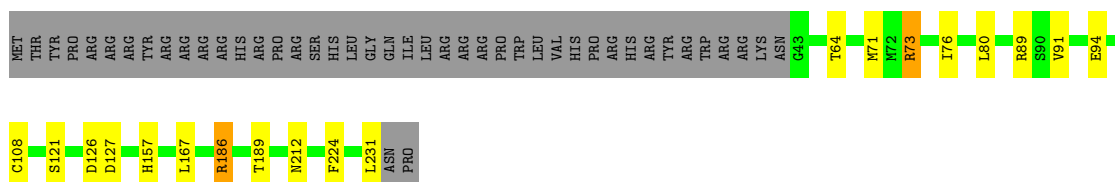


- Molecule 1: Capsid protein of PCV2



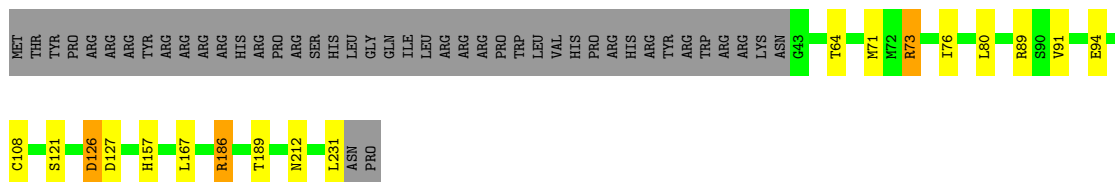
- Molecule 1: Capsid protein of PCV2





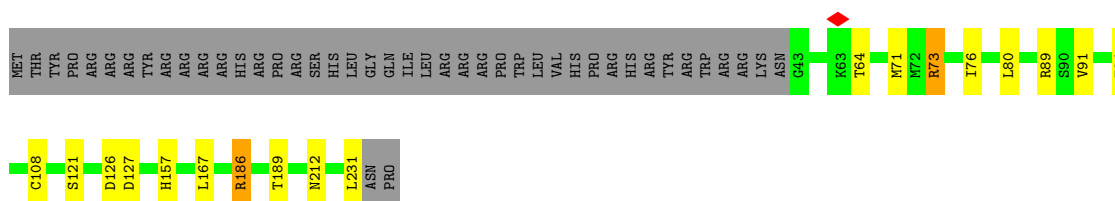
- Molecule 1: Capsid protein of PCV2

Chain AO: 73% 6% 19%



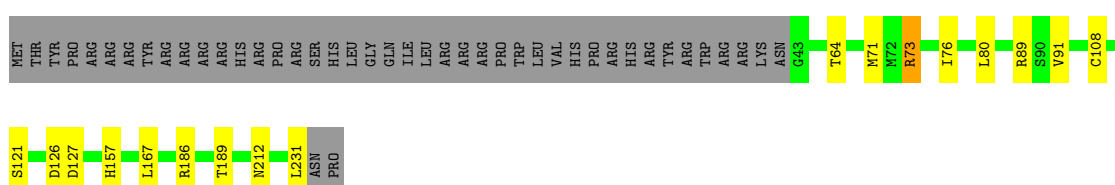
- Molecule 1: Capsid protein of PCV2

Chain AP: 73% 7% 19%



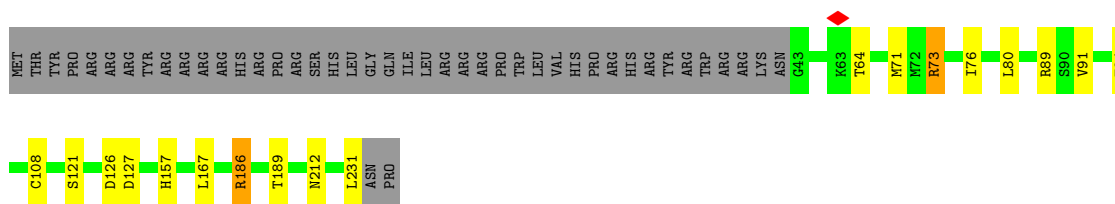
- Molecule 1: Capsid protein of PCV2

Chain AQ: 74% 7% 19%



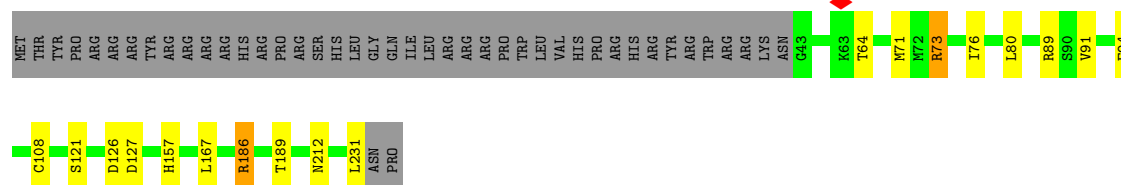
- Molecule 1: Capsid protein of PCV2

Chain AR: 73% 7% 19%



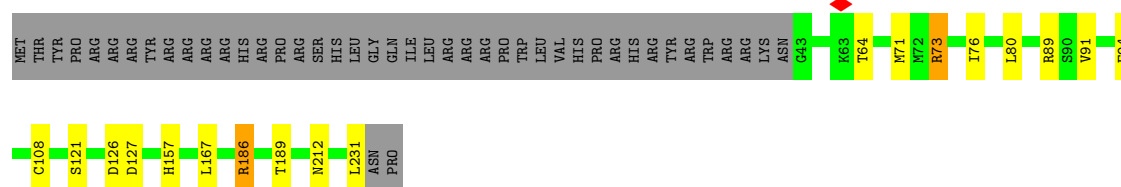
- Molecule 1: Capsid protein of PCV2

Chain AS:  73% 7% 19%



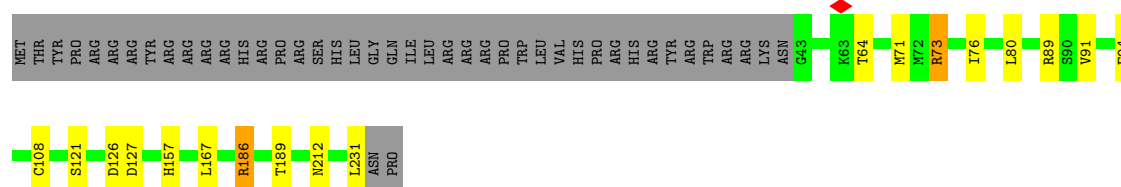
- Molecule 1: Capsid protein of PCV2

Chain AT:  73% 7% 19%



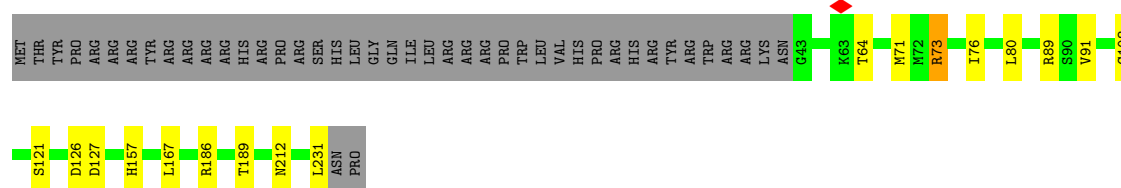
- Molecule 1: Capsid protein of PCV2

Chain AU:  73% 7% 19%



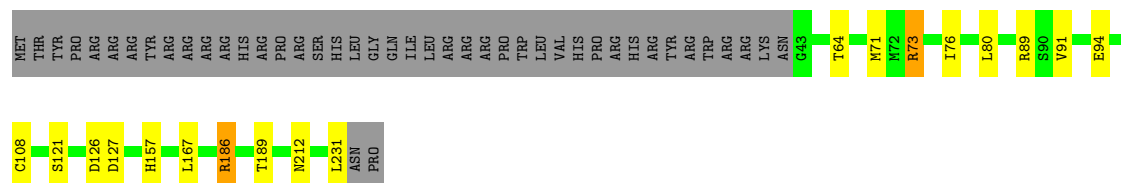
- Molecule 1: Capsid protein of PCV2

Chain AV:  74% 7% 19%

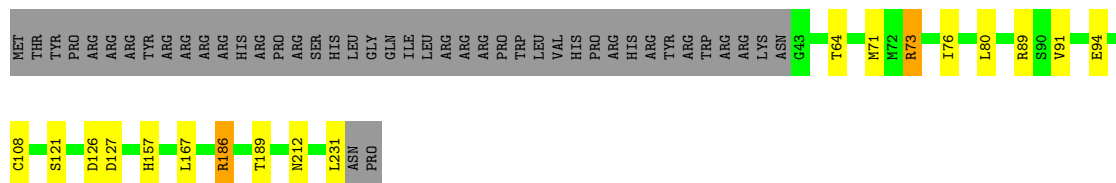


- Molecule 1: Capsid protein of PCV2

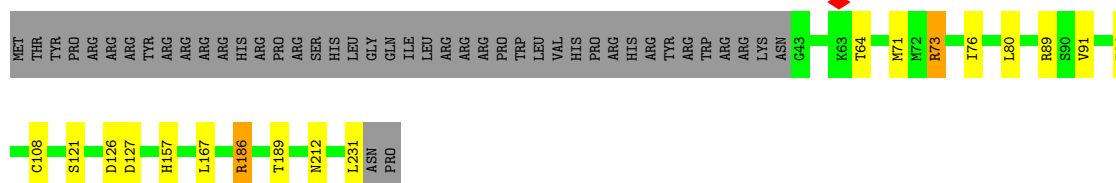
Chain AW:  73% 7% 19%



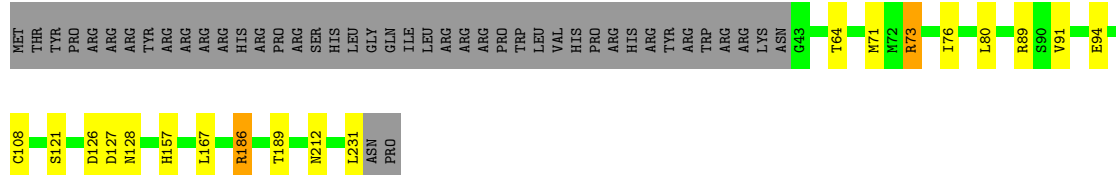
## ● Molecule 1: Capsid protein of PCV2

Chain AX:  73% 7% 19%

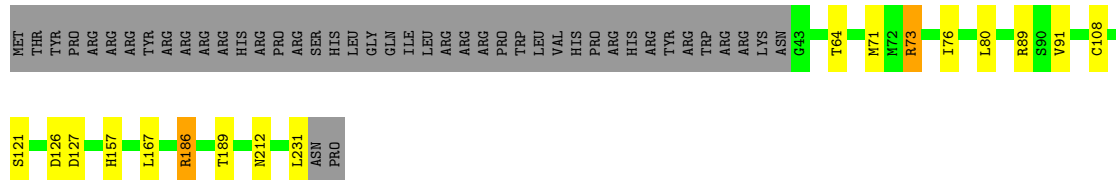
## ● Molecule 1: Capsid protein of PCV2

Chain AY:  73% 7% 19%

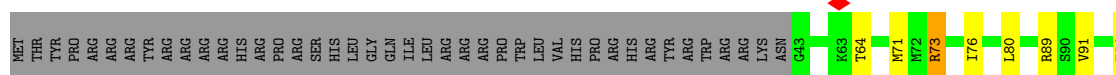
## ● Molecule 1: Capsid protein of PCV2

Chain AZ:  73% 7% 19%

## ● Molecule 1: Capsid protein of PCV2

Chain Aa:  74% 6% 19%

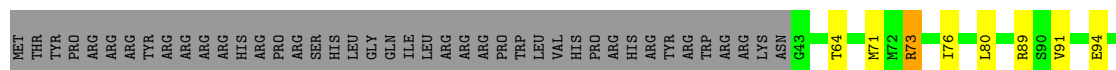
## ● Molecule 1: Capsid protein of PCV2

Chain Ab:  73% 7% 19%



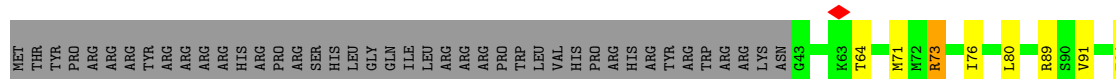
- Molecule 1: Capsid protein of PCV2

Chain Ac: 73% 7% 19%



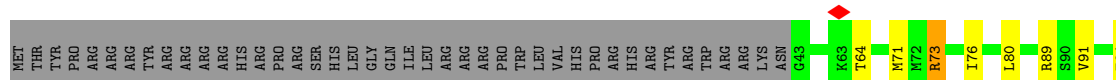
- Molecule 1: Capsid protein of PCV2

Chain Ad: 73% 7% 19%



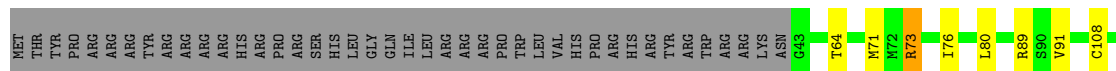
- Molecule 1: Capsid protein of PCV2

Chain Ae: 73% 7% 19%



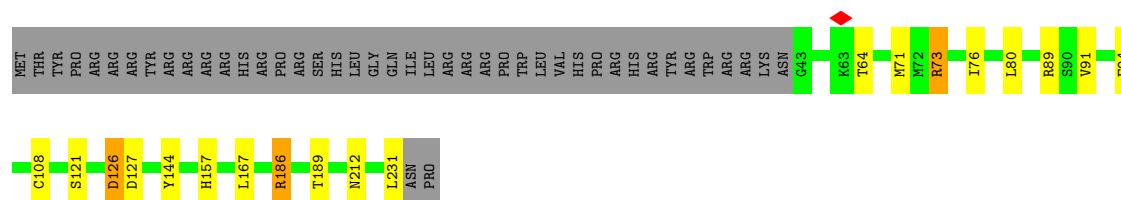
- Molecule 1: Capsid protein of PCV2

Chain Af: 74% 7% 19%



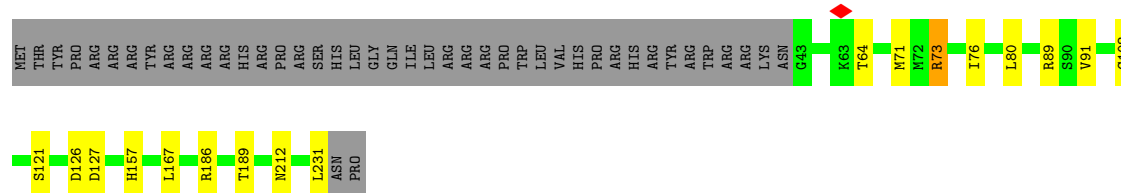
- Molecule 1: Capsid protein of PCV2

Chain Ag: 73% 7% 19%



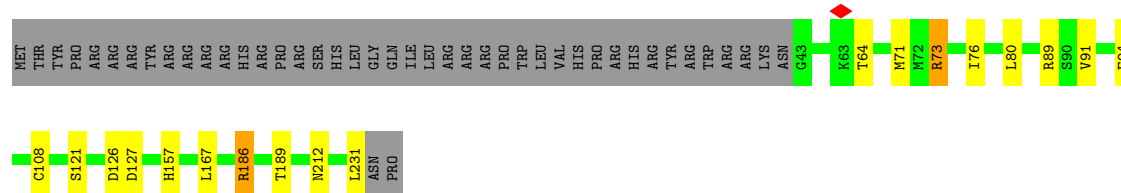
• Molecule 1: Capsid protein of PCV2

Chain Ah: 74% 7% 19%



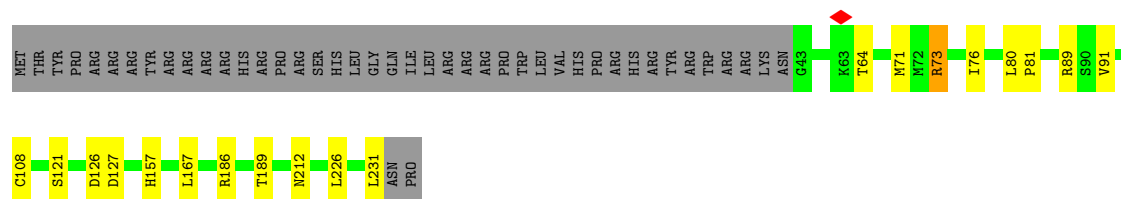
• Molecule 1: Capsid protein of PCV2

Chain Ai: 73% 7% 19%



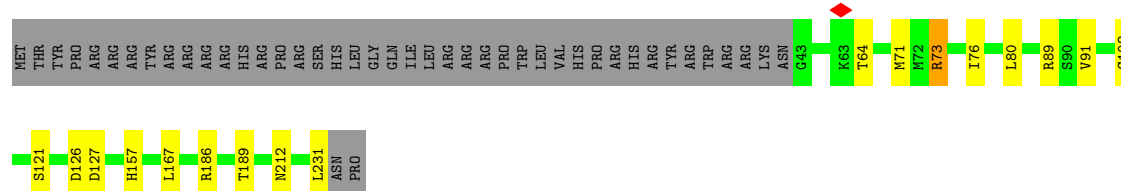
• Molecule 1: Capsid protein of PCV2

Chain Aj: 73% 8% 19%

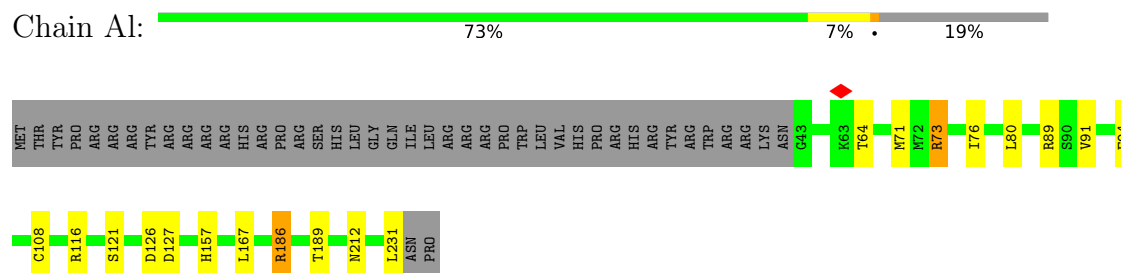


• Molecule 1: Capsid protein of PCV2

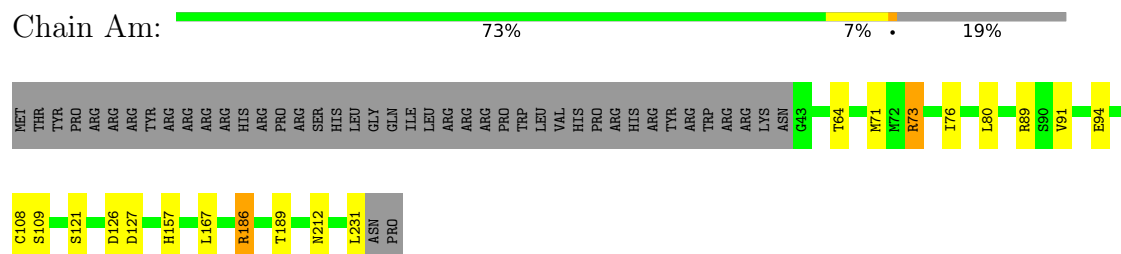
Chain Ak: 74% 7% 19%



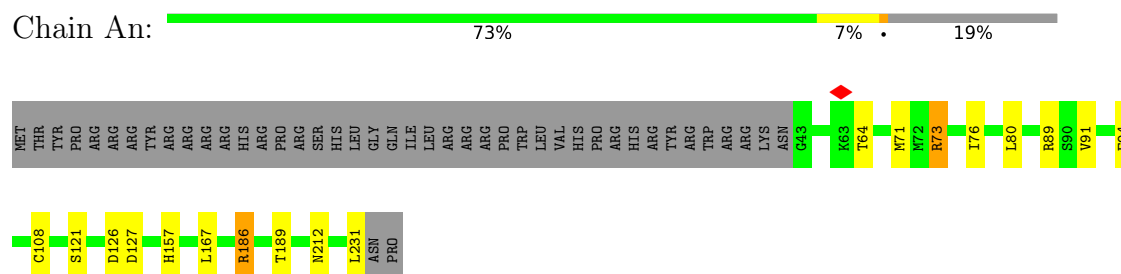
## ● Molecule 1: Capsid protein of PCV2



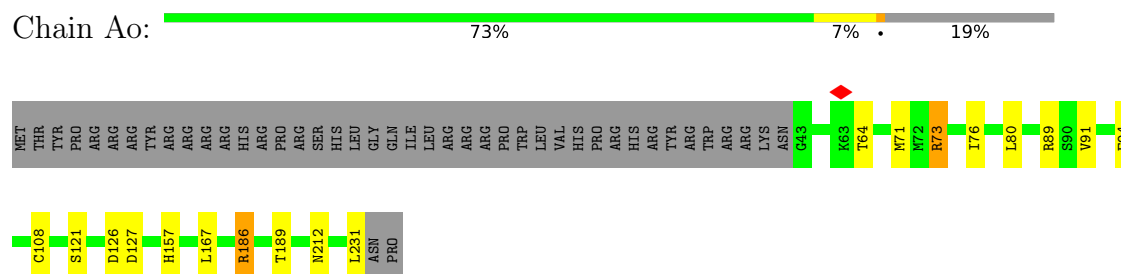
## ● Molecule 1: Capsid protein of PCV2



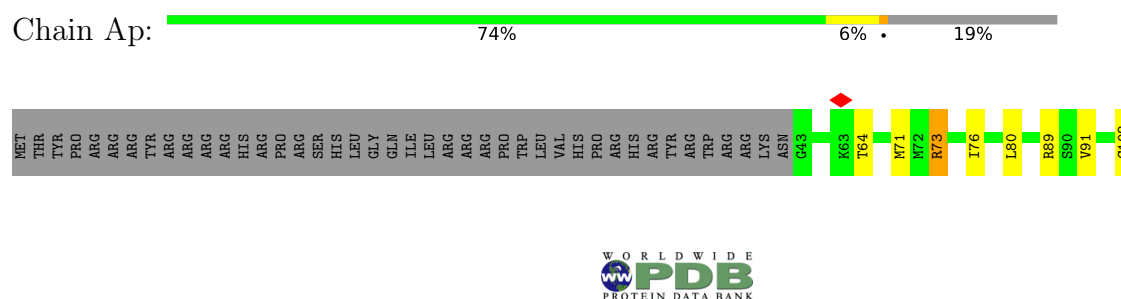
## ● Molecule 1: Capsid protein of PCV2



## ● Molecule 1: Capsid protein of PCV2

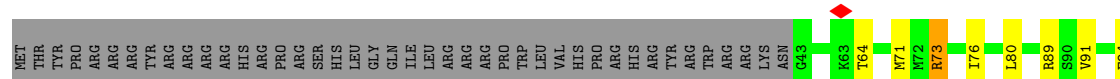


## ● Molecule 1: Capsid protein of PCV2

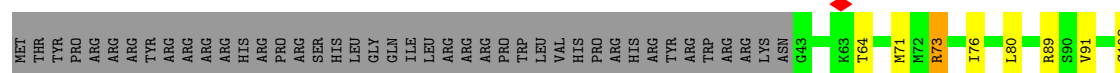




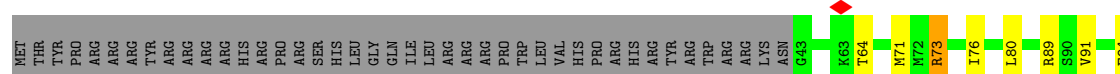
- Molecule 1: Capsid protein of PCV2



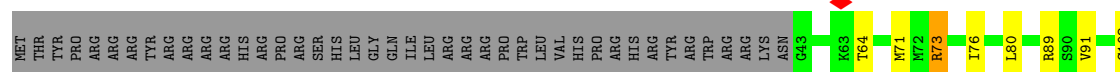
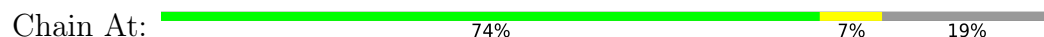
- Molecule 1: Capsid protein of PCV2



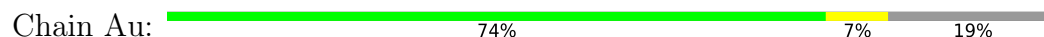
- Molecule 1: Capsid protein of PCV2

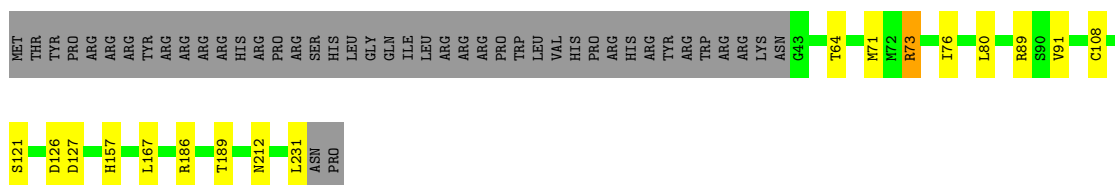


- Molecule 1: Capsid protein of PCV2



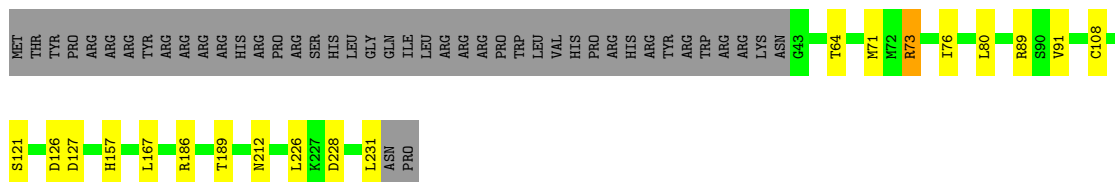
- Molecule 1: Capsid protein of PCV2





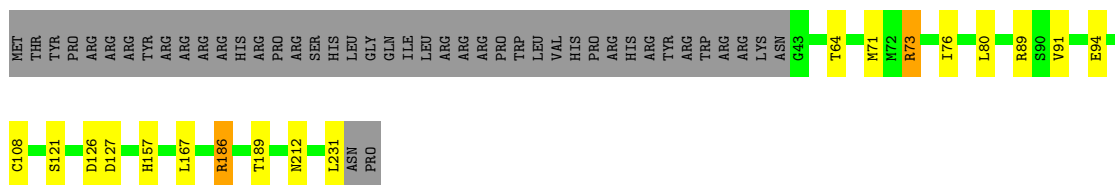
- Molecule 1: Capsid protein of PCV2

Chain Av: 73% 8% 19%



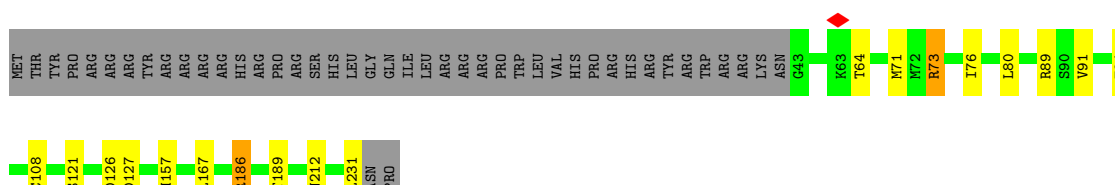
- Molecule 1: Capsid protein of PCV2

Chain Aw: 73% 7% 19%



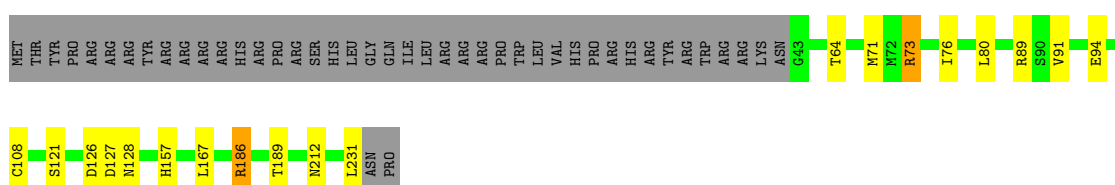
- Molecule 1: Capsid protein of PCV2

Chain Ax: 73% 7% 19%



- Molecule 1: Capsid protein of PCV2

Chain Ay: 73% 7% 19%



## 4 Experimental information

| Property                             | Value                                                            | Source    |
|--------------------------------------|------------------------------------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                                                  | Depositor |
| Imposed symmetry                     | POINT, I                                                         | Depositor |
| Number of particles used             | 93725                                                            | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                                | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION; Per particle estimation | Depositor |
| Microscope                           | FEI TITAN                                                        | Depositor |
| Voltage (kV)                         | 300                                                              | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 35                                                               | Depositor |
| Minimum defocus (nm)                 | 280                                                              | Depositor |
| Maximum defocus (nm)                 | 3200                                                             | Depositor |
| Magnification                        | Not provided                                                     |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)                                        | Depositor |
| Maximum map value                    | 0.338                                                            | Depositor |
| Minimum map value                    | -0.174                                                           | Depositor |
| Average map value                    | 0.002                                                            | Depositor |
| Map value standard deviation         | 0.017                                                            | Depositor |
| Recommended contour level            | 0.04                                                             | Depositor |
| Map size (Å)                         | 327.0, 327.0, 327.0                                              | wwPDB     |
| Map dimensions                       | 300, 300, 300                                                    | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                                                 | wwPDB     |
| Pixel spacing (Å)                    | 1.09, 1.09, 1.09                                                 | Depositor |

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A1    | 0.60         | 0/1597      | 0.51        | 0/2175      |
| 1   | A2    | 0.60         | 0/1597      | 0.50        | 0/2175      |
| 1   | A3    | 0.61         | 0/1597      | 0.51        | 0/2175      |
| 1   | A4    | 0.60         | 0/1597      | 0.50        | 0/2175      |
| 1   | A5    | 0.61         | 0/1597      | 0.50        | 0/2175      |
| 1   | A6    | 0.61         | 0/1597      | 0.50        | 0/2175      |
| 1   | A7    | 0.60         | 0/1597      | 0.50        | 0/2175      |
| 1   | A8    | 0.60         | 0/1597      | 0.50        | 0/2175      |
| 1   | A9    | 0.60         | 0/1597      | 0.50        | 0/2175      |
| 1   | AA    | 0.60         | 0/1597      | 0.51        | 0/2175      |
| 1   | AB    | 0.61         | 0/1597      | 0.50        | 0/2175      |
| 1   | AC    | 0.61         | 0/1597      | 0.51        | 0/2175      |
| 1   | AD    | 0.60         | 0/1597      | 0.51        | 0/2175      |
| 1   | AE    | 0.61         | 0/1597      | 0.51        | 0/2175      |
| 1   | AF    | 0.60         | 0/1597      | 0.50        | 0/2175      |
| 1   | AG    | 0.61         | 0/1597      | 0.50        | 0/2175      |
| 1   | AH    | 0.61         | 0/1597      | 0.51        | 0/2175      |
| 1   | AI    | 0.61         | 0/1597      | 0.51        | 0/2175      |
| 1   | AJ    | 0.61         | 0/1597      | 0.50        | 0/2175      |
| 1   | AK    | 0.61         | 0/1597      | 0.51        | 0/2175      |
| 1   | AL    | 0.60         | 0/1597      | 0.51        | 0/2175      |
| 1   | AM    | 0.60         | 0/1597      | 0.51        | 0/2175      |
| 1   | AN    | 0.60         | 0/1597      | 0.51        | 0/2175      |
| 1   | AO    | 0.60         | 0/1597      | 0.50        | 0/2175      |
| 1   | AP    | 0.60         | 0/1597      | 0.51        | 0/2175      |
| 1   | AQ    | 0.61         | 0/1597      | 0.51        | 0/2175      |
| 1   | AR    | 0.61         | 0/1597      | 0.50        | 0/2175      |
| 1   | AS    | 0.61         | 0/1597      | 0.51        | 0/2175      |
| 1   | AT    | 0.60         | 0/1597      | 0.50        | 0/2175      |
| 1   | AU    | 0.61         | 0/1597      | 0.51        | 0/2175      |
| 1   | AV    | 0.60         | 0/1597      | 0.51        | 0/2175      |
| 1   | AW    | 0.61         | 0/1597      | 0.50        | 0/2175      |
| 1   | AX    | 0.61         | 0/1597      | 0.50        | 0/2175      |
| 1   | AY    | 0.60         | 0/1597      | 0.51        | 0/2175      |

| Mol | Chain | Bond lengths |         | Bond angles |          |
|-----|-------|--------------|---------|-------------|----------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5  |
| 1   | AZ    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | Aa    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | Ab    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | Ac    | 0.61         | 0/1597  | 0.50        | 0/2175   |
| 1   | Ad    | 0.60         | 0/1597  | 0.50        | 0/2175   |
| 1   | Ae    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | Af    | 0.60         | 0/1597  | 0.50        | 0/2175   |
| 1   | Ag    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | Ah    | 0.60         | 0/1597  | 0.51        | 0/2175   |
| 1   | Ai    | 0.60         | 0/1597  | 0.50        | 0/2175   |
| 1   | Aj    | 0.60         | 0/1597  | 0.50        | 0/2175   |
| 1   | Ak    | 0.61         | 0/1597  | 0.50        | 0/2175   |
| 1   | Al    | 0.61         | 0/1597  | 0.50        | 0/2175   |
| 1   | Am    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | An    | 0.60         | 0/1597  | 0.50        | 0/2175   |
| 1   | Ao    | 0.61         | 0/1597  | 0.50        | 0/2175   |
| 1   | Ap    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | Aq    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | Ar    | 0.61         | 0/1597  | 0.50        | 0/2175   |
| 1   | As    | 0.60         | 0/1597  | 0.50        | 0/2175   |
| 1   | At    | 0.61         | 0/1597  | 0.50        | 0/2175   |
| 1   | Au    | 0.60         | 0/1597  | 0.50        | 0/2175   |
| 1   | Av    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | Aw    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | Ax    | 0.61         | 0/1597  | 0.51        | 0/2175   |
| 1   | Ay    | 0.60         | 0/1597  | 0.50        | 0/2175   |
| All | All   | 0.61         | 0/95820 | 0.51        | 0/130500 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A1    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | A2    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | A3    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | A4    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | A5    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | A6    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | A7    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | A8    | 1550  | 1503     | 1503     | 10      | 0            |
| 1   | A9    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | AA    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | AB    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | AC    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AD    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AE    | 1550  | 1503     | 1503     | 11      | 0            |
| 1   | AF    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | AG    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AH    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AI    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | AJ    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | AK    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | AL    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | AM    | 1550  | 1503     | 1503     | 10      | 0            |
| 1   | AN    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | AO    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | AP    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AQ    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | AR    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AS    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AT    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AU    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AV    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | AW    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AX    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | AY    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | AZ    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | Aa    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Ab    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Ac    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Ad    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Ae    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Af    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | Ag    | 1550  | 1503     | 1503     | 11      | 0            |
| 1   | Ah    | 1550  | 1503     | 1503     | 7       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | Ai    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Aj    | 1550  | 1503     | 1503     | 11      | 0            |
| 1   | Ak    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | Al    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | Am    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | An    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Ao    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | Ap    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Aq    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Ar    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | As    | 1550  | 1503     | 1503     | 9       | 0            |
| 1   | At    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | Au    | 1550  | 1503     | 1503     | 7       | 0            |
| 1   | Av    | 1550  | 1503     | 1503     | 10      | 0            |
| 1   | Aw    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Ax    | 1550  | 1503     | 1503     | 8       | 0            |
| 1   | Ay    | 1550  | 1503     | 1503     | 9       | 0            |
| All | All   | 93000 | 90180    | 90180    | 476     | 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 (476) 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) |
|---------------|-----------------|--------------------------|-------------------|
| 1:A4:80:LEU:O | 1:A4:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:A8:80:LEU:O | 1:A8:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:A9:80:LEU:O | 1:A9:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AJ:80:LEU:O | 1:AJ:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Aa:80:LEU:O | 1:Aa:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Ah:80:LEU:O | 1:Ah:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:At:80:LEU:O | 1:At:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AE:80:LEU:O | 1:AE:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Ad:80:LEU:O | 1:Ad:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Am:80:LEU:O | 1:Am:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:An:80:LEU:O | 1:An:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Ar:80:LEU:O | 1:Ar:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:A1:80:LEU:O | 1:A1:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:A5:80:LEU:O | 1:A5:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AG:80:LEU:O | 1:AG:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Aj:80:LEU:O | 1:Aj:89:ARG:NH1 | 2.22                     | 0.73              |

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| Atom-1        | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-----------------|--------------------------|-------------------|
| 1:Ak:80:LEU:O | 1:Ak:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:A7:80:LEU:O | 1:A7:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AB:80:LEU:O | 1:AB:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AQ:80:LEU:O | 1:AQ:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AX:80:LEU:O | 1:AX:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AY:80:LEU:O | 1:AY:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Ap:80:LEU:O | 1:Ap:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Au:80:LEU:O | 1:Au:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AH:80:LEU:O | 1:AH:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AL:80:LEU:O | 1:AL:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AV:80:LEU:O | 1:AV:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Av:80:LEU:O | 1:Av:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Ax:80:LEU:O | 1:Ax:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:A3:80:LEU:O | 1:A3:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AD:80:LEU:O | 1:AD:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AI:80:LEU:O | 1:AI:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AP:80:LEU:O | 1:AP:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AU:80:LEU:O | 1:AU:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Ao:80:LEU:O | 1:Ao:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Aw:80:LEU:O | 1:Aw:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:Ay:80:LEU:O | 1:Ay:89:ARG:NH1 | 2.22                     | 0.73              |
| 1:AC:80:LEU:O | 1:AC:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:AA:80:LEU:O | 1:AA:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:AK:80:LEU:O | 1:AK:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:AM:80:LEU:O | 1:AM:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:Aq:80:LEU:O | 1:Aq:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:Ac:80:LEU:O | 1:Ac:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:As:80:LEU:O | 1:As:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:AO:80:LEU:O | 1:AO:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:AR:80:LEU:O | 1:AR:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:Ab:80:LEU:O | 1:Ab:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:Af:80:LEU:O | 1:Af:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:A2:80:LEU:O | 1:A2:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:A6:80:LEU:O | 1:A6:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:AS:80:LEU:O | 1:AS:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:AW:80:LEU:O | 1:AW:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:Ai:80:LEU:O | 1:Ai:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:AN:80:LEU:O | 1:AN:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:AZ:80:LEU:O | 1:AZ:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:Ae:80:LEU:O | 1:Ae:89:ARG:NH1 | 2.22                     | 0.72              |
| 1:Ag:80:LEU:O | 1:Ag:89:ARG:NH1 | 2.22                     | 0.72              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:AF:80:LEU:O   | 1:AF:89:ARG:NH1  | 2.22                     | 0.72              |
| 1:AT:80:LEU:O   | 1:AT:89:ARG:NH1  | 2.22                     | 0.72              |
| 1:Al:80:LEU:O   | 1:Al:89:ARG:NH1  | 2.22                     | 0.72              |
| 1:AH:108:CYS:SG | 1:AH:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AQ:108:CYS:SG | 1:AQ:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:A6:108:CYS:SG | 1:A6:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AM:108:CYS:SG | 1:AM:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Ac:108:CYS:SG | 1:Ac:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Ar:108:CYS:SG | 1:Ar:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AB:108:CYS:SG | 1:AB:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AR:108:CYS:SG | 1:AR:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Aa:108:CYS:SG | 1:Aa:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Ab:108:CYS:SG | 1:Ab:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Ah:108:CYS:SG | 1:Ah:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Ap:108:CYS:SG | 1:Ap:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:A2:108:CYS:SG | 1:A2:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:A5:108:CYS:SG | 1:A5:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AL:108:CYS:SG | 1:AL:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AO:108:CYS:SG | 1:AO:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AS:108:CYS:SG | 1:AS:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AV:108:CYS:SG | 1:AV:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AW:108:CYS:SG | 1:AW:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AX:108:CYS:SG | 1:AX:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:A7:108:CYS:SG | 1:A7:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:A9:108:CYS:SG | 1:A9:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AT:108:CYS:SG | 1:AT:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AY:108:CYS:SG | 1:AY:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Am:108:CYS:SG | 1:Am:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AD:108:CYS:SG | 1:AD:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AG:108:CYS:SG | 1:AG:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:As:108:CYS:SG | 1:As:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Av:108:CYS:SG | 1:Av:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Ay:108:CYS:SG | 1:Ay:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:A3:108:CYS:SG | 1:A3:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AC:108:CYS:SG | 1:AC:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AK:108:CYS:SG | 1:AK:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AU:108:CYS:SG | 1:AU:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Ak:108:CYS:SG | 1:Ak:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:Ax:108:CYS:SG | 1:Ax:212:ASN:ND2 | 2.73                     | 0.62              |
| 1:AF:108:CYS:SG | 1:AF:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Ai:108:CYS:SG | 1:Ai:212:ASN:ND2 | 2.73                     | 0.61              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A8:108:CYS:SG | 1:A8:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:AI:108:CYS:SG | 1:AI:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:AN:108:CYS:SG | 1:AN:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Ae:108:CYS:SG | 1:Ae:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Ao:108:CYS:SG | 1:Ao:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Au:108:CYS:SG | 1:Au:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:AA:108:CYS:SG | 1:AA:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:AJ:108:CYS:SG | 1:AJ:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:AZ:108:CYS:SG | 1:AZ:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:An:108:CYS:SG | 1:An:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Aq:108:CYS:SG | 1:Aq:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Aw:108:CYS:SG | 1:Aw:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:AE:108:CYS:SG | 1:AE:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Ad:108:CYS:SG | 1:Ad:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Aj:108:CYS:SG | 1:Aj:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:At:108:CYS:SG | 1:At:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Af:108:CYS:SG | 1:Af:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:A1:108:CYS:SG | 1:A1:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:A4:108:CYS:SG | 1:A4:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:AP:108:CYS:SG | 1:AP:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Al:108:CYS:SG | 1:Al:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Ag:108:CYS:SG | 1:Ag:212:ASN:ND2 | 2.73                     | 0.61              |
| 1:Ao:121:SER:OG | 1:Ao:157:HIS:NE2 | 2.31                     | 0.60              |
| 1:AI:121:SER:OG | 1:AI:157:HIS:NE2 | 2.31                     | 0.60              |
| 1:A3:121:SER:OG | 1:A3:157:HIS:NE2 | 2.31                     | 0.60              |
| 1:A5:121:SER:OG | 1:A5:157:HIS:NE2 | 2.31                     | 0.59              |
| 1:AH:121:SER:OG | 1:AH:157:HIS:NE2 | 2.30                     | 0.59              |
| 1:AK:121:SER:OG | 1:AK:157:HIS:NE2 | 2.31                     | 0.59              |
| 1:Ar:121:SER:OG | 1:Ar:157:HIS:NE2 | 2.31                     | 0.59              |
| 1:As:121:SER:OG | 1:As:157:HIS:NE2 | 2.31                     | 0.58              |
| 1:Ax:121:SER:OG | 1:Ax:157:HIS:NE2 | 2.31                     | 0.58              |
| 1:Ah:121:SER:OG | 1:Ah:157:HIS:NE2 | 2.30                     | 0.58              |
| 1:AA:121:SER:OG | 1:AA:157:HIS:NE2 | 2.31                     | 0.58              |
| 1:AR:121:SER:OG | 1:AR:157:HIS:NE2 | 2.31                     | 0.58              |
| 1:AV:121:SER:OG | 1:AV:157:HIS:NE2 | 2.31                     | 0.58              |
| 1:AW:121:SER:OG | 1:AW:157:HIS:NE2 | 2.31                     | 0.57              |
| 1:Ai:121:SER:OG | 1:Ai:157:HIS:NE2 | 2.31                     | 0.57              |
| 1:An:121:SER:OG | 1:An:157:HIS:NE2 | 2.31                     | 0.57              |
| 1:AP:121:SER:OG | 1:AP:157:HIS:NE2 | 2.31                     | 0.57              |
| 1:Aw:121:SER:OG | 1:Aw:157:HIS:NE2 | 2.31                     | 0.57              |
| 1:Aa:121:SER:OG | 1:Aa:157:HIS:NE2 | 2.31                     | 0.57              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A7:121:SER:OG | 1:A7:157:HIS:NE2 | 2.31                     | 0.57              |
| 1:A2:121:SER:OG | 1:A2:157:HIS:NE2 | 2.31                     | 0.57              |
| 1:AM:121:SER:OG | 1:AM:157:HIS:NE2 | 2.31                     | 0.57              |
| 1:Ab:121:SER:OG | 1:Ab:157:HIS:NE2 | 2.31                     | 0.57              |
| 1:AX:121:SER:OG | 1:AX:157:HIS:NE2 | 2.31                     | 0.56              |
| 1:A9:121:SER:OG | 1:A9:157:HIS:NE2 | 2.31                     | 0.56              |
| 1:AY:121:SER:OG | 1:AY:157:HIS:NE2 | 2.31                     | 0.56              |
| 1:Aq:121:SER:OG | 1:Aq:157:HIS:NE2 | 2.31                     | 0.56              |
| 1:AF:121:SER:OG | 1:AF:157:HIS:NE2 | 2.31                     | 0.56              |
| 1:A8:121:SER:OG | 1:A8:157:HIS:NE2 | 2.31                     | 0.56              |
| 1:AU:121:SER:OG | 1:AU:157:HIS:NE2 | 2.31                     | 0.56              |
| 1:Am:121:SER:OG | 1:Am:157:HIS:NE2 | 2.31                     | 0.56              |
| 1:A3:73:ARG:NH1 | 1:A3:127:ASP:OD1 | 2.40                     | 0.56              |
| 1:AB:73:ARG:NH1 | 1:AB:127:ASP:OD1 | 2.39                     | 0.56              |
| 1:AK:73:ARG:NH1 | 1:AK:127:ASP:OD1 | 2.39                     | 0.56              |
| 1:AO:73:ARG:NH1 | 1:AO:127:ASP:OD1 | 2.40                     | 0.56              |
| 1:AW:73:ARG:NH1 | 1:AW:127:ASP:OD1 | 2.39                     | 0.56              |
| 1:A6:73:ARG:NH1 | 1:A6:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:AI:73:ARG:NH1 | 1:AI:127:ASP:OD1 | 2.40                     | 0.55              |
| 1:AT:73:ARG:NH1 | 1:AT:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:AZ:73:ARG:NH1 | 1:AZ:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:Ab:73:ARG:NH1 | 1:Ab:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:Ag:73:ARG:NH1 | 1:Ag:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:A5:73:ARG:NH1 | 1:A5:127:ASP:OD1 | 2.40                     | 0.55              |
| 1:Am:73:ARG:NH1 | 1:Am:127:ASP:OD1 | 2.40                     | 0.55              |
| 1:Ar:73:ARG:NH1 | 1:Ar:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:Au:121:SER:OG | 1:Au:157:HIS:NE2 | 2.31                     | 0.55              |
| 1:AU:73:ARG:NH1 | 1:AU:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:Ad:121:SER:OG | 1:Ad:157:HIS:NE2 | 2.31                     | 0.55              |
| 1:Ah:73:ARG:NH1 | 1:Ah:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:At:73:ARG:NH1 | 1:At:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:A8:73:ARG:NH1 | 1:A8:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:AD:73:ARG:NH1 | 1:AD:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:Aj:73:ARG:NH1 | 1:Aj:127:ASP:OD1 | 2.40                     | 0.55              |
| 1:Aq:73:ARG:NH1 | 1:Aq:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:AL:121:SER:OG | 1:AL:157:HIS:NE2 | 2.31                     | 0.55              |
| 1:Al:73:ARG:NH1 | 1:Al:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:Aw:73:ARG:NH1 | 1:Aw:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:A4:73:ARG:NH1 | 1:A4:127:ASP:OD1 | 2.40                     | 0.55              |
| 1:Ap:121:SER:OG | 1:Ap:157:HIS:NE2 | 2.31                     | 0.55              |
| 1:AJ:73:ARG:NH1 | 1:AJ:127:ASP:OD1 | 2.39                     | 0.55              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:AJ:121:SER:OG | 1:AJ:157:HIS:NE2 | 2.31                     | 0.55              |
| 1:AM:73:ARG:NH1 | 1:AM:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:AR:73:ARG:NH1 | 1:AR:127:ASP:OD1 | 2.40                     | 0.55              |
| 1:Ac:121:SER:OG | 1:Ac:157:HIS:NE2 | 2.31                     | 0.55              |
| 1:A6:121:SER:OG | 1:A6:157:HIS:NE2 | 2.31                     | 0.55              |
| 1:AV:73:ARG:NH1 | 1:AV:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:Au:73:ARG:NH1 | 1:Au:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:AN:73:ARG:NH1 | 1:AN:127:ASP:OD1 | 2.39                     | 0.55              |
| 1:A4:121:SER:OG | 1:A4:157:HIS:NE2 | 2.31                     | 0.54              |
| 1:AP:73:ARG:NH1 | 1:AP:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:AY:73:ARG:NH1 | 1:AY:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:Ag:121:SER:OG | 1:Ag:157:HIS:NE2 | 2.31                     | 0.54              |
| 1:A1:121:SER:OG | 1:A1:157:HIS:NE2 | 2.31                     | 0.54              |
| 1:A7:73:ARG:NH1 | 1:A7:127:ASP:OD1 | 2.40                     | 0.54              |
| 1:AE:121:SER:OG | 1:AE:157:HIS:NE2 | 2.31                     | 0.54              |
| 1:As:73:ARG:NH1 | 1:As:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:Av:73:ARG:NH1 | 1:Av:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:AA:73:ARG:NH1 | 1:AA:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:AC:121:SER:OG | 1:AC:157:HIS:NE2 | 2.31                     | 0.54              |
| 1:AF:73:ARG:NH1 | 1:AF:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:AQ:73:ARG:NH1 | 1:AQ:127:ASP:OD1 | 2.40                     | 0.54              |
| 1:AX:73:ARG:NH1 | 1:AX:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:AZ:121:SER:OG | 1:AZ:157:HIS:NE2 | 2.31                     | 0.54              |
| 1:Ac:73:ARG:NH1 | 1:Ac:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:Ad:73:ARG:NH1 | 1:Ad:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:A2:73:ARG:NH1 | 1:A2:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:At:121:SER:OG | 1:At:157:HIS:NE2 | 2.31                     | 0.54              |
| 1:AC:73:ARG:NH1 | 1:AC:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:AL:73:ARG:NH1 | 1:AL:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:Ae:121:SER:OG | 1:Ae:157:HIS:NE2 | 2.31                     | 0.54              |
| 1:Av:121:SER:OG | 1:Av:157:HIS:NE2 | 2.31                     | 0.54              |
| 1:AQ:121:SER:OG | 1:AQ:157:HIS:NE2 | 2.31                     | 0.54              |
| 1:An:73:ARG:NH1 | 1:An:127:ASP:OD1 | 2.40                     | 0.54              |
| 1:Ap:73:ARG:NH1 | 1:Ap:127:ASP:OD1 | 2.40                     | 0.54              |
| 1:Ax:73:ARG:NH1 | 1:Ax:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:A9:73:ARG:NH1 | 1:A9:127:ASP:OD1 | 2.40                     | 0.54              |
| 1:AH:73:ARG:NH1 | 1:AH:127:ASP:OD1 | 2.40                     | 0.54              |
| 1:Af:73:ARG:NH1 | 1:Af:127:ASP:OD1 | 2.40                     | 0.54              |
| 1:Ai:73:ARG:NH1 | 1:Ai:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:Ak:73:ARG:NH1 | 1:Ak:127:ASP:OD1 | 2.39                     | 0.54              |
| 1:Aa:73:ARG:NH1 | 1:Aa:127:ASP:OD1 | 2.40                     | 0.54              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A1:73:ARG:NH1 | 1:A1:127:ASP:OD1 | 2.39                     | 0.53              |
| 1:AS:73:ARG:NH1 | 1:AS:127:ASP:OD1 | 2.40                     | 0.53              |
| 1:AO:121:SER:OG | 1:AO:157:HIS:NE2 | 2.31                     | 0.53              |
| 1:AT:121:SER:OG | 1:AT:157:HIS:NE2 | 2.31                     | 0.53              |
| 1:AE:73:ARG:NH1 | 1:AE:127:ASP:OD1 | 2.40                     | 0.53              |
| 1:Ak:121:SER:OG | 1:Ak:157:HIS:NE2 | 2.31                     | 0.53              |
| 1:Ay:73:ARG:NH1 | 1:Ay:127:ASP:OD1 | 2.39                     | 0.53              |
| 1:AG:121:SER:OG | 1:AG:157:HIS:NE2 | 2.31                     | 0.53              |
| 1:Ay:121:SER:OG | 1:Ay:157:HIS:NE2 | 2.31                     | 0.53              |
| 1:AG:73:ARG:NH1 | 1:AG:127:ASP:OD1 | 2.40                     | 0.53              |
| 1:Af:121:SER:OG | 1:Af:157:HIS:NE2 | 2.31                     | 0.53              |
| 1:Ao:73:ARG:NH1 | 1:Ao:127:ASP:OD1 | 2.39                     | 0.53              |
| 1:AD:121:SER:OG | 1:AD:157:HIS:NE2 | 2.31                     | 0.53              |
| 1:AB:121:SER:OG | 1:AB:157:HIS:NE2 | 2.31                     | 0.52              |
| 1:Ae:73:ARG:NH1 | 1:Ae:127:ASP:OD1 | 2.39                     | 0.52              |
| 1:AS:121:SER:OG | 1:AS:157:HIS:NE2 | 2.31                     | 0.51              |
| 1:An:89:ARG:NH2 | 1:An:189:THR:O   | 2.42                     | 0.51              |
| 1:AN:121:SER:OG | 1:AN:157:HIS:NE2 | 2.31                     | 0.51              |
| 1:Aj:121:SER:OG | 1:Aj:157:HIS:NE2 | 2.31                     | 0.51              |
| 1:Al:121:SER:OG | 1:Al:157:HIS:NE2 | 2.31                     | 0.51              |
| 1:A7:89:ARG:NH2 | 1:A7:189:THR:O   | 2.42                     | 0.51              |
| 1:A3:89:ARG:NH2 | 1:A3:189:THR:O   | 2.42                     | 0.51              |
| 1:AI:89:ARG:NH2 | 1:AI:189:THR:O   | 2.42                     | 0.51              |
| 1:Ax:89:ARG:NH2 | 1:Ax:189:THR:O   | 2.43                     | 0.51              |
| 1:Ai:89:ARG:NH2 | 1:Ai:189:THR:O   | 2.43                     | 0.51              |
| 1:Ao:89:ARG:NH2 | 1:Ao:189:THR:O   | 2.42                     | 0.51              |
| 1:AU:89:ARG:NH2 | 1:AU:189:THR:O   | 2.42                     | 0.51              |
| 1:AG:89:ARG:NH2 | 1:AG:189:THR:O   | 2.42                     | 0.51              |
| 1:AP:89:ARG:NH2 | 1:AP:189:THR:O   | 2.42                     | 0.51              |
| 1:Aq:89:ARG:NH2 | 1:Aq:189:THR:O   | 2.42                     | 0.50              |
| 1:AJ:89:ARG:NH2 | 1:AJ:189:THR:O   | 2.42                     | 0.50              |
| 1:As:89:ARG:NH2 | 1:As:189:THR:O   | 2.42                     | 0.50              |
| 1:A1:89:ARG:NH2 | 1:A1:189:THR:O   | 2.42                     | 0.50              |
| 1:AA:89:ARG:NH2 | 1:AA:189:THR:O   | 2.42                     | 0.50              |
| 1:Ae:89:ARG:NH2 | 1:Ae:189:THR:O   | 2.42                     | 0.50              |
| 1:A4:89:ARG:NH2 | 1:A4:189:THR:O   | 2.42                     | 0.50              |
| 1:Ay:89:ARG:NH2 | 1:Ay:189:THR:O   | 2.42                     | 0.50              |
| 1:AZ:89:ARG:NH2 | 1:AZ:189:THR:O   | 2.42                     | 0.50              |
| 1:Aj:89:ARG:NH2 | 1:Aj:189:THR:O   | 2.42                     | 0.49              |
| 1:AW:89:ARG:NH2 | 1:AW:189:THR:O   | 2.42                     | 0.49              |
| 1:Ab:89:ARG:NH2 | 1:Ab:189:THR:O   | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A9:89:ARG:NH2  | 1:A9:189:THR:O   | 2.42                     | 0.49              |
| 1:AE:228:ASP:HA  | 1:Aj:81:PRO:HG3  | 1.94                     | 0.48              |
| 1:Al:89:ARG:NH2  | 1:Al:189:THR:O   | 2.42                     | 0.48              |
| 1:At:89:ARG:NH2  | 1:At:189:THR:O   | 2.42                     | 0.48              |
| 1:AB:89:ARG:NH2  | 1:AB:189:THR:O   | 2.42                     | 0.48              |
| 1:Ak:89:ARG:NH2  | 1:Ak:189:THR:O   | 2.42                     | 0.48              |
| 1:Al:80:LEU:HD11 | 1:Al:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Ap:186:ARG:HD3 | 1:Ay:128:ASN:OD1 | 2.13                     | 0.48              |
| 1:Ar:80:LEU:HD11 | 1:Ar:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:At:80:LEU:HD11 | 1:At:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AA:80:LEU:HD11 | 1:AA:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AG:80:LEU:HD11 | 1:AG:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AY:80:LEU:HD11 | 1:AY:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Ac:80:LEU:HD11 | 1:Ac:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Ah:80:LEU:HD11 | 1:Ah:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Ai:80:LEU:HD11 | 1:Ai:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Av:80:LEU:HD11 | 1:Av:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:A5:80:LEU:HD11 | 1:A5:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AF:80:LEU:HD11 | 1:AF:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AO:80:LEU:HD11 | 1:AO:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AP:80:LEU:HD11 | 1:AP:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Af:80:LEU:HD11 | 1:Af:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Aj:80:LEU:HD11 | 1:Aj:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Am:80:LEU:HD11 | 1:Am:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Ap:80:LEU:HD11 | 1:Ap:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Aw:80:LEU:HD11 | 1:Aw:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Ay:80:LEU:HD11 | 1:Ay:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AN:80:LEU:HD11 | 1:AN:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AT:80:LEU:HD11 | 1:AT:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Ao:80:LEU:HD11 | 1:Ao:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:A6:80:LEU:HD11 | 1:A6:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:A7:80:LEU:HD11 | 1:A7:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AK:80:LEU:HD11 | 1:AK:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AM:80:LEU:HD11 | 1:AM:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AS:89:ARG:NH2  | 1:AS:189:THR:O   | 2.43                     | 0.48              |
| 1:Ad:80:LEU:HD11 | 1:Ad:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:As:80:LEU:HD11 | 1:As:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:A1:80:LEU:HD11 | 1:A1:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AB:80:LEU:HD11 | 1:AB:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AS:80:LEU:HD11 | 1:AS:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AV:80:LEU:HD11 | 1:AV:91:VAL:CG2  | 2.44                     | 0.48              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:Ac:89:ARG:NH2   | 1:Ac:189:THR:O   | 2.42                     | 0.48              |
| 1:A9:80:LEU:HD11  | 1:A9:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Aa:80:LEU:HD11  | 1:Aa:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Ag:80:LEU:HD11  | 1:Ag:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Ak:80:LEU:HD11  | 1:Ak:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:An:80:LEU:HD11  | 1:An:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:Au:80:LEU:HD11  | 1:Au:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:A2:80:LEU:HD11  | 1:A2:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AI:80:LEU:HD11  | 1:AI:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AJ:80:LEU:HD11  | 1:AJ:91:VAL:CG2  | 2.44                     | 0.48              |
| 1:AC:80:LEU:HD11  | 1:AC:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AW:80:LEU:HD11  | 1:AW:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AX:80:LEU:HD11  | 1:AX:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AZ:80:LEU:HD11  | 1:AZ:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:Ae:80:LEU:HD11  | 1:Ae:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AE:226:LEU:HD21 | 1:Aj:80:LEU:HD12 | 1.96                     | 0.47              |
| 1:AL:80:LEU:HD11  | 1:AL:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AM:89:ARG:NH2   | 1:AM:189:THR:O   | 2.42                     | 0.47              |
| 1:AU:80:LEU:HD11  | 1:AU:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:Au:89:ARG:NH2   | 1:Au:189:THR:O   | 2.42                     | 0.47              |
| 1:AD:89:ARG:NH2   | 1:AD:189:THR:O   | 2.43                     | 0.47              |
| 1:AE:80:LEU:HD11  | 1:AE:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AQ:80:LEU:HD11  | 1:AQ:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:Af:89:ARG:NH2   | 1:Af:189:THR:O   | 2.42                     | 0.47              |
| 1:A8:80:LEU:HD11  | 1:A8:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AR:80:LEU:HD11  | 1:AR:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AR:89:ARG:NH2   | 1:AR:189:THR:O   | 2.42                     | 0.47              |
| 1:Ax:80:LEU:HD11  | 1:Ax:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AH:80:LEU:HD11  | 1:AH:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AY:89:ARG:NH2   | 1:AY:189:THR:O   | 2.42                     | 0.47              |
| 1:Ab:80:LEU:HD11  | 1:Ab:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:Ag:89:ARG:NH2   | 1:Ag:189:THR:O   | 2.42                     | 0.47              |
| 1:A4:80:LEU:HD11  | 1:A4:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:A3:80:LEU:HD11  | 1:A3:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:AK:89:ARG:NH2   | 1:AK:189:THR:O   | 2.42                     | 0.47              |
| 1:AN:89:ARG:NH2   | 1:AN:189:THR:O   | 2.42                     | 0.47              |
| 1:Al:116:ARG:NH1  | 1:Am:109:SER:O   | 2.40                     | 0.47              |
| 1:Aq:80:LEU:HD11  | 1:Aq:91:VAL:CG2  | 2.44                     | 0.47              |
| 1:A6:89:ARG:NH2   | 1:A6:189:THR:O   | 2.42                     | 0.47              |
| 1:AF:89:ARG:NH2   | 1:AF:189:THR:O   | 2.42                     | 0.47              |
| 1:AD:80:LEU:HD11  | 1:AD:91:VAL:CG2  | 2.44                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A2:89:ARG:NH2   | 1:A2:189:THR:O    | 2.42                     | 0.46              |
| 1:AE:80:LEU:HD12  | 1:Aj:226:LEU:HD21 | 1.96                     | 0.46              |
| 1:AX:89:ARG:NH2   | 1:AX:189:THR:O    | 2.42                     | 0.46              |
| 1:Ap:89:ARG:NH2   | 1:Ap:189:THR:O    | 2.42                     | 0.46              |
| 1:Av:89:ARG:NH2   | 1:Av:189:THR:O    | 2.42                     | 0.46              |
| 1:A5:89:ARG:NH2   | 1:A5:189:THR:O    | 2.42                     | 0.46              |
| 1:Ad:89:ARG:NH2   | 1:Ad:189:THR:O    | 2.42                     | 0.46              |
| 1:Aa:89:ARG:NH2   | 1:Aa:189:THR:O    | 2.42                     | 0.46              |
| 1:AQ:89:ARG:NH2   | 1:AQ:189:THR:O    | 2.42                     | 0.46              |
| 1:Ah:89:ARG:NH2   | 1:Ah:189:THR:O    | 2.42                     | 0.46              |
| 1:AC:89:ARG:NH2   | 1:AC:189:THR:O    | 2.42                     | 0.46              |
| 1:A3:128:ASN:OD1  | 1:Ao:186:ARG:HD3  | 2.17                     | 0.45              |
| 1:A8:89:ARG:NH2   | 1:A8:189:THR:O    | 2.42                     | 0.45              |
| 1:AT:89:ARG:NH2   | 1:AT:189:THR:O    | 2.42                     | 0.45              |
| 1:Ar:89:ARG:NH2   | 1:Ar:189:THR:O    | 2.42                     | 0.45              |
| 1:A8:80:LEU:HD12  | 1:Av:226:LEU:HD21 | 1.97                     | 0.45              |
| 1:AE:89:ARG:NH2   | 1:AE:189:THR:O    | 2.42                     | 0.45              |
| 1:A2:126:ASP:HB2  | 1:Ag:186:ARG:HH11 | 1.81                     | 0.45              |
| 1:AV:89:ARG:NH2   | 1:AV:189:THR:O    | 2.42                     | 0.45              |
| 1:A1:144:TYR:HA   | 1:AN:224:PHE:O    | 2.17                     | 0.45              |
| 1:AH:89:ARG:NH2   | 1:AH:189:THR:O    | 2.42                     | 0.45              |
| 1:A8:78:ASP:O     | 1:Av:228:ASP:OD2  | 2.36                     | 0.44              |
| 1:AL:89:ARG:NH2   | 1:AL:189:THR:O    | 2.42                     | 0.44              |
| 1:AO:89:ARG:NH2   | 1:AO:189:THR:O    | 2.43                     | 0.44              |
| 1:Am:89:ARG:NH2   | 1:Am:189:THR:O    | 2.42                     | 0.44              |
| 1:A8:226:LEU:HD21 | 1:Av:80:LEU:HD12  | 1.99                     | 0.43              |
| 1:Ap:80:LEU:HD11  | 1:Ap:91:VAL:HG23  | 2.01                     | 0.43              |
| 1:AM:186:ARG:HH11 | 1:Ag:126:ASP:HB2  | 1.84                     | 0.43              |
| 1:Af:80:LEU:HD11  | 1:Af:91:VAL:HG23  | 2.01                     | 0.43              |
| 1:Av:80:LEU:HD11  | 1:Av:91:VAL:HG23  | 2.01                     | 0.43              |
| 1:Aw:89:ARG:NH2   | 1:Aw:189:THR:O    | 2.42                     | 0.43              |
| 1:A4:80:LEU:HD11  | 1:A4:91:VAL:HG23  | 2.01                     | 0.43              |
| 1:AG:94:GLU:OE1   | 1:AG:186:ARG:NH1  | 2.52                     | 0.43              |
| 1:AI:80:LEU:HD11  | 1:AI:91:VAL:HG23  | 2.01                     | 0.43              |
| 1:AJ:80:LEU:HD11  | 1:AJ:91:VAL:HG23  | 2.01                     | 0.43              |
| 1:AM:224:PHE:O    | 1:Ag:144:TYR:HA   | 2.19                     | 0.43              |
| 1:Ak:80:LEU:HD11  | 1:Ak:91:VAL:HG23  | 2.01                     | 0.43              |
| 1:A3:80:LEU:HD11  | 1:A3:91:VAL:HG23  | 2.01                     | 0.42              |
| 1:A8:80:LEU:HD11  | 1:A8:91:VAL:HG23  | 2.01                     | 0.42              |
| 1:AD:80:LEU:HD11  | 1:AD:91:VAL:HG23  | 2.01                     | 0.42              |
| 1:AX:80:LEU:HD11  | 1:AX:91:VAL:HG23  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Ae:80:LEU:HD11 | 1:Ae:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:A9:80:LEU:HD11 | 1:A9:91:VAL:HG23 | 2.02                     | 0.42              |
| 1:AL:80:LEU:HD11 | 1:AL:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:AP:80:LEU:HD11 | 1:AP:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:Ag:80:LEU:HD11 | 1:Ag:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:A3:94:GLU:OE1  | 1:A3:186:ARG:NH1 | 2.52                     | 0.42              |
| 1:AE:80:LEU:HD11 | 1:AE:91:VAL:HG23 | 2.02                     | 0.42              |
| 1:AI:94:GLU:OE1  | 1:AI:186:ARG:NH1 | 2.52                     | 0.42              |
| 1:AM:94:GLU:OE1  | 1:AM:186:ARG:NH1 | 2.52                     | 0.42              |
| 1:AQ:80:LEU:HD11 | 1:AQ:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:AU:80:LEU:HD11 | 1:AU:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:Ab:94:GLU:OE1  | 1:Ab:186:ARG:NH1 | 2.52                     | 0.42              |
| 1:Aj:80:LEU:HD11 | 1:Aj:91:VAL:HG23 | 2.02                     | 0.42              |
| 1:Al:80:LEU:HD11 | 1:Al:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:Ao:80:LEU:HD11 | 1:Ao:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:Ay:80:LEU:HD11 | 1:Ay:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:A5:94:GLU:OE1  | 1:A5:186:ARG:NH1 | 2.52                     | 0.42              |
| 1:AZ:80:LEU:HD11 | 1:AZ:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:Ac:80:LEU:HD11 | 1:Ac:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:Au:80:LEU:HD11 | 1:Au:91:VAL:HG23 | 2.02                     | 0.42              |
| 1:AS:80:LEU:HD11 | 1:AS:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:AT:94:GLU:OE1  | 1:AT:186:ARG:NH1 | 2.52                     | 0.42              |
| 1:Aa:80:LEU:HD11 | 1:Aa:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:AN:80:LEU:HD11 | 1:AN:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:AW:80:LEU:HD11 | 1:AW:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:At:80:LEU:HD11 | 1:At:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:A1:94:GLU:OE1  | 1:A1:186:ARG:NH1 | 2.52                     | 0.42              |
| 1:AA:80:LEU:HD11 | 1:AA:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:AC:80:LEU:HD11 | 1:AC:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:AF:80:LEU:HD11 | 1:AF:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:AH:94:GLU:OE1  | 1:AH:186:ARG:NH1 | 2.52                     | 0.42              |
| 1:Ab:80:LEU:HD11 | 1:Ab:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:Ad:80:LEU:HD11 | 1:Ad:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:A7:80:LEU:HD11 | 1:A7:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:AN:94:GLU:OE1  | 1:AN:186:ARG:NH1 | 2.52                     | 0.42              |
| 1:AV:80:LEU:HD11 | 1:AV:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:Aq:80:LEU:HD11 | 1:Aq:91:VAL:HG23 | 2.02                     | 0.42              |
| 1:Aw:80:LEU:HD11 | 1:Aw:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:A1:80:LEU:HD11 | 1:A1:91:VAL:HG23 | 2.01                     | 0.42              |
| 1:AR:94:GLU:OE1  | 1:AR:186:ARG:NH1 | 2.52                     | 0.42              |
| 1:AS:94:GLU:OE1  | 1:AS:186:ARG:NH1 | 2.52                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AW:94:GLU:OE1   | 1:AW:186:ARG:NH1  | 2.52                     | 0.42              |
| 1:AC:94:GLU:OE1   | 1:AC:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:AM:80:LEU:HD11  | 1:AM:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:AO:126:ASP:HB2  | 1:As:186:ARG:HH11 | 1.85                     | 0.41              |
| 1:AY:80:LEU:HD11  | 1:AY:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:Ad:94:GLU:OE1   | 1:Ad:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:Ao:94:GLU:OE1   | 1:Ao:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:A5:80:LEU:HD11  | 1:A5:91:VAL:HG23  | 2.02                     | 0.41              |
| 1:A7:226:LEU:HD21 | 1:AX:80:LEU:HD12  | 2.02                     | 0.41              |
| 1:Am:94:GLU:OE1   | 1:Am:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:Ar:80:LEU:HD11  | 1:Ar:91:VAL:HG23  | 2.02                     | 0.41              |
| 1:AU:94:GLU:OE1   | 1:AU:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:AB:80:LEU:HD11  | 1:AB:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:AO:94:GLU:OE1   | 1:AO:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:AT:80:LEU:HD11  | 1:AT:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:Ah:80:LEU:HD11  | 1:Ah:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:Ai:80:LEU:HD11  | 1:Ai:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:Ai:94:GLU:OE1   | 1:Ai:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:Al:94:GLU:OE1   | 1:Al:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:Am:80:LEU:HD11  | 1:Am:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:Ax:94:GLU:OE1   | 1:Ax:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:Ay:94:GLU:OE1   | 1:Ay:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:A2:94:GLU:OE1   | 1:A2:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:Ax:80:LEU:HD11  | 1:Ax:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:AH:80:LEU:HD11  | 1:AH:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:AR:80:LEU:HD11  | 1:AR:91:VAL:HG23  | 2.02                     | 0.41              |
| 1:An:94:GLU:OE1   | 1:An:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:A2:80:LEU:HD11  | 1:A2:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:A7:94:GLU:OE1   | 1:A7:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:AD:94:GLU:OE1   | 1:AD:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:AE:227:LYS:O    | 1:Aj:81:PRO:HG2   | 2.21                     | 0.41              |
| 1:AG:80:LEU:HD11  | 1:AG:91:VAL:HG23  | 2.01                     | 0.41              |
| 1:AK:80:LEU:HD11  | 1:AK:91:VAL:HG23  | 2.02                     | 0.41              |
| 1:AZ:94:GLU:OE1   | 1:AZ:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:AZ:128:ASN:OD1  | 1:Aa:186:ARG:HD3  | 2.21                     | 0.41              |
| 1:Ag:94:GLU:OE1   | 1:Ag:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:As:94:GLU:OE1   | 1:As:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:AP:94:GLU:OE1   | 1:AP:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:Ae:94:GLU:OE1   | 1:Ae:186:ARG:NH1  | 2.52                     | 0.41              |
| 1:AY:94:GLU:OE1   | 1:AY:186:ARG:NH1  | 2.52                     | 0.40              |
| 1:As:80:LEU:HD11  | 1:As:91:VAL:HG23  | 2.02                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A5:94:GLU:OE1  | 1:A5:186:ARG:NH2 | 2.54                     | 0.40              |
| 1:An:80:LEU:HD11 | 1:An:91:VAL:HG23 | 2.01                     | 0.40              |
| 1:AI:94:GLU:OE1  | 1:AI:186:ARG:NH2 | 2.54                     | 0.40              |
| 1:AO:94:GLU:OE1  | 1:AO:186:ARG:NH2 | 2.54                     | 0.40              |
| 1:AX:94:GLU:OE1  | 1:AX:186:ARG:NH2 | 2.54                     | 0.40              |
| 1:Aq:94:GLU:OE1  | 1:Aq:186:ARG:NH1 | 2.52                     | 0.40              |
| 1:A6:80:LEU:HD11 | 1:A6:91:VAL:HG23 | 2.01                     | 0.40              |
| 1:Ac:94:GLU:OE1  | 1:Ac:186:ARG:NH2 | 2.54                     | 0.40              |
| 1:Aw:94:GLU:OE1  | 1:Aw:186:ARG:NH1 | 2.52                     | 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   | A1    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | A2    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | A3    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | A4    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | A5    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | A6    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | A7    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | A8    | 187/233 (80%) | 180 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | A9    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AA    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AB    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AC    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AD    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | AE    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AF    | 187/233 (80%) | 180 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AG    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AH    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AI    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AJ    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AK    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AL    | 187/233 (80%) | 180 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AM    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AN    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AO    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AP    | 187/233 (80%) | 180 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AQ    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AR    | 187/233 (80%) | 180 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AS    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AT    | 187/233 (80%) | 180 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AU    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AV    | 187/233 (80%) | 180 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AW    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AX    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AY    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | AZ    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Aa    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Ab    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Ac    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Ad    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Ae    | 187/233 (80%) | 180 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | Af    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Ag    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Ah    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Ai    | 187/233 (80%) | 181 (97%) | 6 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | Aj    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Ak    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Al    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Am    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | An    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Ao    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Ap    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Aq    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Ar    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | As    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | At    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Au    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Av    | 187/233 (80%)     | 180 (96%)   | 7 (4%)   | 0        | 100         | 100 |
| 1   | Aw    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Ax    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | Ay    | 187/233 (80%)     | 181 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| All | All   | 11220/13980 (80%) | 10851 (97%) | 369 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A1    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | A2    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | A3    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | A4    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | A5    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | A6    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | A7    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | A8    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | A9    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AA    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AB    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AC    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AD    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AE    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AF    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AG    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AH    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AI    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AJ    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AK    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AL    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AM    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AN    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AO    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AP    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AQ    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AR    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AS    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AT    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AU    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AV    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AW    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AX    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AY    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | AZ    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |
| 1   | Aa    | 172/215 (80%) | 164 (95%) | 8 (5%)   | 23          | 57 |

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| Mol | Chain | Analysed          | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-------------------|------------|----------|-------------|----|
| 1   | Ab    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ac    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ad    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ae    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Af    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ag    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ah    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ai    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Aj    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ak    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Al    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Am    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | An    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ao    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ap    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Aq    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ar    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | As    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | At    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Au    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Av    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Aw    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ax    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| 1   | Ay    | 172/215 (80%)     | 164 (95%)  | 8 (5%)   | 23          | 57 |
| All | All   | 10320/12900 (80%) | 9840 (95%) | 480 (5%) | 25          | 57 |

All (480) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 64  | THR  |
| 1   | A1    | 71  | MET  |
| 1   | A1    | 73  | ARG  |
| 1   | A1    | 76  | ILE  |
| 1   | A1    | 126 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 167 | LEU  |
| 1   | A1    | 186 | ARG  |
| 1   | A1    | 231 | LEU  |
| 1   | A2    | 64  | THR  |
| 1   | A2    | 71  | MET  |
| 1   | A2    | 73  | ARG  |
| 1   | A2    | 76  | ILE  |
| 1   | A2    | 126 | ASP  |
| 1   | A2    | 167 | LEU  |
| 1   | A2    | 186 | ARG  |
| 1   | A2    | 231 | LEU  |
| 1   | A3    | 64  | THR  |
| 1   | A3    | 71  | MET  |
| 1   | A3    | 73  | ARG  |
| 1   | A3    | 76  | ILE  |
| 1   | A3    | 126 | ASP  |
| 1   | A3    | 167 | LEU  |
| 1   | A3    | 186 | ARG  |
| 1   | A3    | 231 | LEU  |
| 1   | A4    | 64  | THR  |
| 1   | A4    | 71  | MET  |
| 1   | A4    | 73  | ARG  |
| 1   | A4    | 76  | ILE  |
| 1   | A4    | 126 | ASP  |
| 1   | A4    | 167 | LEU  |
| 1   | A4    | 186 | ARG  |
| 1   | A4    | 231 | LEU  |
| 1   | A5    | 64  | THR  |
| 1   | A5    | 71  | MET  |
| 1   | A5    | 73  | ARG  |
| 1   | A5    | 76  | ILE  |
| 1   | A5    | 126 | ASP  |
| 1   | A5    | 167 | LEU  |
| 1   | A5    | 186 | ARG  |
| 1   | A5    | 231 | LEU  |
| 1   | A6    | 64  | THR  |
| 1   | A6    | 71  | MET  |
| 1   | A6    | 73  | ARG  |
| 1   | A6    | 76  | ILE  |
| 1   | A6    | 126 | ASP  |
| 1   | A6    | 167 | LEU  |
| 1   | A6    | 186 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A6    | 231 | LEU  |
| 1   | A7    | 64  | THR  |
| 1   | A7    | 71  | MET  |
| 1   | A7    | 73  | ARG  |
| 1   | A7    | 76  | ILE  |
| 1   | A7    | 126 | ASP  |
| 1   | A7    | 167 | LEU  |
| 1   | A7    | 186 | ARG  |
| 1   | A7    | 231 | LEU  |
| 1   | A8    | 64  | THR  |
| 1   | A8    | 71  | MET  |
| 1   | A8    | 73  | ARG  |
| 1   | A8    | 76  | ILE  |
| 1   | A8    | 126 | ASP  |
| 1   | A8    | 167 | LEU  |
| 1   | A8    | 186 | ARG  |
| 1   | A8    | 231 | LEU  |
| 1   | A9    | 64  | THR  |
| 1   | A9    | 71  | MET  |
| 1   | A9    | 73  | ARG  |
| 1   | A9    | 76  | ILE  |
| 1   | A9    | 126 | ASP  |
| 1   | A9    | 167 | LEU  |
| 1   | A9    | 186 | ARG  |
| 1   | A9    | 231 | LEU  |
| 1   | AA    | 64  | THR  |
| 1   | AA    | 71  | MET  |
| 1   | AA    | 73  | ARG  |
| 1   | AA    | 76  | ILE  |
| 1   | AA    | 126 | ASP  |
| 1   | AA    | 167 | LEU  |
| 1   | AA    | 186 | ARG  |
| 1   | AA    | 231 | LEU  |
| 1   | AB    | 64  | THR  |
| 1   | AB    | 71  | MET  |
| 1   | AB    | 73  | ARG  |
| 1   | AB    | 76  | ILE  |
| 1   | AB    | 126 | ASP  |
| 1   | AB    | 167 | LEU  |
| 1   | AB    | 186 | ARG  |
| 1   | AB    | 231 | LEU  |
| 1   | AC    | 64  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AC    | 71  | MET  |
| 1   | AC    | 73  | ARG  |
| 1   | AC    | 76  | ILE  |
| 1   | AC    | 126 | ASP  |
| 1   | AC    | 167 | LEU  |
| 1   | AC    | 186 | ARG  |
| 1   | AC    | 231 | LEU  |
| 1   | AD    | 64  | THR  |
| 1   | AD    | 71  | MET  |
| 1   | AD    | 73  | ARG  |
| 1   | AD    | 76  | ILE  |
| 1   | AD    | 126 | ASP  |
| 1   | AD    | 167 | LEU  |
| 1   | AD    | 186 | ARG  |
| 1   | AD    | 231 | LEU  |
| 1   | AE    | 64  | THR  |
| 1   | AE    | 71  | MET  |
| 1   | AE    | 73  | ARG  |
| 1   | AE    | 76  | ILE  |
| 1   | AE    | 126 | ASP  |
| 1   | AE    | 167 | LEU  |
| 1   | AE    | 186 | ARG  |
| 1   | AE    | 231 | LEU  |
| 1   | AF    | 64  | THR  |
| 1   | AF    | 71  | MET  |
| 1   | AF    | 73  | ARG  |
| 1   | AF    | 76  | ILE  |
| 1   | AF    | 126 | ASP  |
| 1   | AF    | 167 | LEU  |
| 1   | AF    | 186 | ARG  |
| 1   | AF    | 231 | LEU  |
| 1   | AG    | 64  | THR  |
| 1   | AG    | 71  | MET  |
| 1   | AG    | 73  | ARG  |
| 1   | AG    | 76  | ILE  |
| 1   | AG    | 126 | ASP  |
| 1   | AG    | 167 | LEU  |
| 1   | AG    | 186 | ARG  |
| 1   | AG    | 231 | LEU  |
| 1   | AH    | 64  | THR  |
| 1   | AH    | 71  | MET  |
| 1   | AH    | 73  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AH    | 76  | ILE  |
| 1   | AH    | 126 | ASP  |
| 1   | AH    | 167 | LEU  |
| 1   | AH    | 186 | ARG  |
| 1   | AH    | 231 | LEU  |
| 1   | AI    | 64  | THR  |
| 1   | AI    | 71  | MET  |
| 1   | AI    | 73  | ARG  |
| 1   | AI    | 76  | ILE  |
| 1   | AI    | 126 | ASP  |
| 1   | AI    | 167 | LEU  |
| 1   | AI    | 186 | ARG  |
| 1   | AI    | 231 | LEU  |
| 1   | AJ    | 64  | THR  |
| 1   | AJ    | 71  | MET  |
| 1   | AJ    | 73  | ARG  |
| 1   | AJ    | 76  | ILE  |
| 1   | AJ    | 126 | ASP  |
| 1   | AJ    | 167 | LEU  |
| 1   | AJ    | 186 | ARG  |
| 1   | AJ    | 231 | LEU  |
| 1   | AK    | 64  | THR  |
| 1   | AK    | 71  | MET  |
| 1   | AK    | 73  | ARG  |
| 1   | AK    | 76  | ILE  |
| 1   | AK    | 126 | ASP  |
| 1   | AK    | 167 | LEU  |
| 1   | AK    | 186 | ARG  |
| 1   | AK    | 231 | LEU  |
| 1   | AL    | 64  | THR  |
| 1   | AL    | 71  | MET  |
| 1   | AL    | 73  | ARG  |
| 1   | AL    | 76  | ILE  |
| 1   | AL    | 126 | ASP  |
| 1   | AL    | 167 | LEU  |
| 1   | AL    | 186 | ARG  |
| 1   | AL    | 231 | LEU  |
| 1   | AM    | 64  | THR  |
| 1   | AM    | 71  | MET  |
| 1   | AM    | 73  | ARG  |
| 1   | AM    | 76  | ILE  |
| 1   | AM    | 126 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AM    | 167 | LEU  |
| 1   | AM    | 186 | ARG  |
| 1   | AM    | 231 | LEU  |
| 1   | AN    | 64  | THR  |
| 1   | AN    | 71  | MET  |
| 1   | AN    | 73  | ARG  |
| 1   | AN    | 76  | ILE  |
| 1   | AN    | 126 | ASP  |
| 1   | AN    | 167 | LEU  |
| 1   | AN    | 186 | ARG  |
| 1   | AN    | 231 | LEU  |
| 1   | AO    | 64  | THR  |
| 1   | AO    | 71  | MET  |
| 1   | AO    | 73  | ARG  |
| 1   | AO    | 76  | ILE  |
| 1   | AO    | 126 | ASP  |
| 1   | AO    | 167 | LEU  |
| 1   | AO    | 186 | ARG  |
| 1   | AO    | 231 | LEU  |
| 1   | AP    | 64  | THR  |
| 1   | AP    | 71  | MET  |
| 1   | AP    | 73  | ARG  |
| 1   | AP    | 76  | ILE  |
| 1   | AP    | 126 | ASP  |
| 1   | AP    | 167 | LEU  |
| 1   | AP    | 186 | ARG  |
| 1   | AP    | 231 | LEU  |
| 1   | AQ    | 64  | THR  |
| 1   | AQ    | 71  | MET  |
| 1   | AQ    | 73  | ARG  |
| 1   | AQ    | 76  | ILE  |
| 1   | AQ    | 126 | ASP  |
| 1   | AQ    | 167 | LEU  |
| 1   | AQ    | 186 | ARG  |
| 1   | AQ    | 231 | LEU  |
| 1   | AR    | 64  | THR  |
| 1   | AR    | 71  | MET  |
| 1   | AR    | 73  | ARG  |
| 1   | AR    | 76  | ILE  |
| 1   | AR    | 126 | ASP  |
| 1   | AR    | 167 | LEU  |
| 1   | AR    | 186 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AR    | 231 | LEU  |
| 1   | AS    | 64  | THR  |
| 1   | AS    | 71  | MET  |
| 1   | AS    | 73  | ARG  |
| 1   | AS    | 76  | ILE  |
| 1   | AS    | 126 | ASP  |
| 1   | AS    | 167 | LEU  |
| 1   | AS    | 186 | ARG  |
| 1   | AS    | 231 | LEU  |
| 1   | AT    | 64  | THR  |
| 1   | AT    | 71  | MET  |
| 1   | AT    | 73  | ARG  |
| 1   | AT    | 76  | ILE  |
| 1   | AT    | 126 | ASP  |
| 1   | AT    | 167 | LEU  |
| 1   | AT    | 186 | ARG  |
| 1   | AT    | 231 | LEU  |
| 1   | AU    | 64  | THR  |
| 1   | AU    | 71  | MET  |
| 1   | AU    | 73  | ARG  |
| 1   | AU    | 76  | ILE  |
| 1   | AU    | 126 | ASP  |
| 1   | AU    | 167 | LEU  |
| 1   | AU    | 186 | ARG  |
| 1   | AU    | 231 | LEU  |
| 1   | AV    | 64  | THR  |
| 1   | AV    | 71  | MET  |
| 1   | AV    | 73  | ARG  |
| 1   | AV    | 76  | ILE  |
| 1   | AV    | 126 | ASP  |
| 1   | AV    | 167 | LEU  |
| 1   | AV    | 186 | ARG  |
| 1   | AV    | 231 | LEU  |
| 1   | AW    | 64  | THR  |
| 1   | AW    | 71  | MET  |
| 1   | AW    | 73  | ARG  |
| 1   | AW    | 76  | ILE  |
| 1   | AW    | 126 | ASP  |
| 1   | AW    | 167 | LEU  |
| 1   | AW    | 186 | ARG  |
| 1   | AW    | 231 | LEU  |
| 1   | AX    | 64  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AX    | 71  | MET  |
| 1   | AX    | 73  | ARG  |
| 1   | AX    | 76  | ILE  |
| 1   | AX    | 126 | ASP  |
| 1   | AX    | 167 | LEU  |
| 1   | AX    | 186 | ARG  |
| 1   | AX    | 231 | LEU  |
| 1   | AY    | 64  | THR  |
| 1   | AY    | 71  | MET  |
| 1   | AY    | 73  | ARG  |
| 1   | AY    | 76  | ILE  |
| 1   | AY    | 126 | ASP  |
| 1   | AY    | 167 | LEU  |
| 1   | AY    | 186 | ARG  |
| 1   | AY    | 231 | LEU  |
| 1   | AZ    | 64  | THR  |
| 1   | AZ    | 71  | MET  |
| 1   | AZ    | 73  | ARG  |
| 1   | AZ    | 76  | ILE  |
| 1   | AZ    | 126 | ASP  |
| 1   | AZ    | 167 | LEU  |
| 1   | AZ    | 186 | ARG  |
| 1   | AZ    | 231 | LEU  |
| 1   | Aa    | 64  | THR  |
| 1   | Aa    | 71  | MET  |
| 1   | Aa    | 73  | ARG  |
| 1   | Aa    | 76  | ILE  |
| 1   | Aa    | 126 | ASP  |
| 1   | Aa    | 167 | LEU  |
| 1   | Aa    | 186 | ARG  |
| 1   | Aa    | 231 | LEU  |
| 1   | Ab    | 64  | THR  |
| 1   | Ab    | 71  | MET  |
| 1   | Ab    | 73  | ARG  |
| 1   | Ab    | 76  | ILE  |
| 1   | Ab    | 126 | ASP  |
| 1   | Ab    | 167 | LEU  |
| 1   | Ab    | 186 | ARG  |
| 1   | Ab    | 231 | LEU  |
| 1   | Ac    | 64  | THR  |
| 1   | Ac    | 71  | MET  |
| 1   | Ac    | 73  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ac    | 76  | ILE  |
| 1   | Ac    | 126 | ASP  |
| 1   | Ac    | 167 | LEU  |
| 1   | Ac    | 186 | ARG  |
| 1   | Ac    | 231 | LEU  |
| 1   | Ad    | 64  | THR  |
| 1   | Ad    | 71  | MET  |
| 1   | Ad    | 73  | ARG  |
| 1   | Ad    | 76  | ILE  |
| 1   | Ad    | 126 | ASP  |
| 1   | Ad    | 167 | LEU  |
| 1   | Ad    | 186 | ARG  |
| 1   | Ad    | 231 | LEU  |
| 1   | Ae    | 64  | THR  |
| 1   | Ae    | 71  | MET  |
| 1   | Ae    | 73  | ARG  |
| 1   | Ae    | 76  | ILE  |
| 1   | Ae    | 126 | ASP  |
| 1   | Ae    | 167 | LEU  |
| 1   | Ae    | 186 | ARG  |
| 1   | Ae    | 231 | LEU  |
| 1   | Af    | 64  | THR  |
| 1   | Af    | 71  | MET  |
| 1   | Af    | 73  | ARG  |
| 1   | Af    | 76  | ILE  |
| 1   | Af    | 126 | ASP  |
| 1   | Af    | 167 | LEU  |
| 1   | Af    | 186 | ARG  |
| 1   | Af    | 231 | LEU  |
| 1   | Ag    | 64  | THR  |
| 1   | Ag    | 71  | MET  |
| 1   | Ag    | 73  | ARG  |
| 1   | Ag    | 76  | ILE  |
| 1   | Ag    | 126 | ASP  |
| 1   | Ag    | 167 | LEU  |
| 1   | Ag    | 186 | ARG  |
| 1   | Ag    | 231 | LEU  |
| 1   | Ah    | 64  | THR  |
| 1   | Ah    | 71  | MET  |
| 1   | Ah    | 73  | ARG  |
| 1   | Ah    | 76  | ILE  |
| 1   | Ah    | 126 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ah    | 167 | LEU  |
| 1   | Ah    | 186 | ARG  |
| 1   | Ah    | 231 | LEU  |
| 1   | Ai    | 64  | THR  |
| 1   | Ai    | 71  | MET  |
| 1   | Ai    | 73  | ARG  |
| 1   | Ai    | 76  | ILE  |
| 1   | Ai    | 126 | ASP  |
| 1   | Ai    | 167 | LEU  |
| 1   | Ai    | 186 | ARG  |
| 1   | Ai    | 231 | LEU  |
| 1   | Aj    | 64  | THR  |
| 1   | Aj    | 71  | MET  |
| 1   | Aj    | 73  | ARG  |
| 1   | Aj    | 76  | ILE  |
| 1   | Aj    | 126 | ASP  |
| 1   | Aj    | 167 | LEU  |
| 1   | Aj    | 186 | ARG  |
| 1   | Aj    | 231 | LEU  |
| 1   | Ak    | 64  | THR  |
| 1   | Ak    | 71  | MET  |
| 1   | Ak    | 73  | ARG  |
| 1   | Ak    | 76  | ILE  |
| 1   | Ak    | 126 | ASP  |
| 1   | Ak    | 167 | LEU  |
| 1   | Ak    | 186 | ARG  |
| 1   | Ak    | 231 | LEU  |
| 1   | Al    | 64  | THR  |
| 1   | Al    | 71  | MET  |
| 1   | Al    | 73  | ARG  |
| 1   | Al    | 76  | ILE  |
| 1   | Al    | 126 | ASP  |
| 1   | Al    | 167 | LEU  |
| 1   | Al    | 186 | ARG  |
| 1   | Al    | 231 | LEU  |
| 1   | Am    | 64  | THR  |
| 1   | Am    | 71  | MET  |
| 1   | Am    | 73  | ARG  |
| 1   | Am    | 76  | ILE  |
| 1   | Am    | 126 | ASP  |
| 1   | Am    | 167 | LEU  |
| 1   | Am    | 186 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Am    | 231 | LEU  |
| 1   | An    | 64  | THR  |
| 1   | An    | 71  | MET  |
| 1   | An    | 73  | ARG  |
| 1   | An    | 76  | ILE  |
| 1   | An    | 126 | ASP  |
| 1   | An    | 167 | LEU  |
| 1   | An    | 186 | ARG  |
| 1   | An    | 231 | LEU  |
| 1   | Ao    | 64  | THR  |
| 1   | Ao    | 71  | MET  |
| 1   | Ao    | 73  | ARG  |
| 1   | Ao    | 76  | ILE  |
| 1   | Ao    | 126 | ASP  |
| 1   | Ao    | 167 | LEU  |
| 1   | Ao    | 186 | ARG  |
| 1   | Ao    | 231 | LEU  |
| 1   | Ap    | 64  | THR  |
| 1   | Ap    | 71  | MET  |
| 1   | Ap    | 73  | ARG  |
| 1   | Ap    | 76  | ILE  |
| 1   | Ap    | 126 | ASP  |
| 1   | Ap    | 167 | LEU  |
| 1   | Ap    | 186 | ARG  |
| 1   | Ap    | 231 | LEU  |
| 1   | Aq    | 64  | THR  |
| 1   | Aq    | 71  | MET  |
| 1   | Aq    | 73  | ARG  |
| 1   | Aq    | 76  | ILE  |
| 1   | Aq    | 126 | ASP  |
| 1   | Aq    | 167 | LEU  |
| 1   | Aq    | 186 | ARG  |
| 1   | Aq    | 231 | LEU  |
| 1   | Ar    | 64  | THR  |
| 1   | Ar    | 71  | MET  |
| 1   | Ar    | 73  | ARG  |
| 1   | Ar    | 76  | ILE  |
| 1   | Ar    | 126 | ASP  |
| 1   | Ar    | 167 | LEU  |
| 1   | Ar    | 186 | ARG  |
| 1   | Ar    | 231 | LEU  |
| 1   | As    | 64  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | As    | 71  | MET  |
| 1   | As    | 73  | ARG  |
| 1   | As    | 76  | ILE  |
| 1   | As    | 126 | ASP  |
| 1   | As    | 167 | LEU  |
| 1   | As    | 186 | ARG  |
| 1   | As    | 231 | LEU  |
| 1   | At    | 64  | THR  |
| 1   | At    | 71  | MET  |
| 1   | At    | 73  | ARG  |
| 1   | At    | 76  | ILE  |
| 1   | At    | 126 | ASP  |
| 1   | At    | 167 | LEU  |
| 1   | At    | 186 | ARG  |
| 1   | At    | 231 | LEU  |
| 1   | Au    | 64  | THR  |
| 1   | Au    | 71  | MET  |
| 1   | Au    | 73  | ARG  |
| 1   | Au    | 76  | ILE  |
| 1   | Au    | 126 | ASP  |
| 1   | Au    | 167 | LEU  |
| 1   | Au    | 186 | ARG  |
| 1   | Au    | 231 | LEU  |
| 1   | Av    | 64  | THR  |
| 1   | Av    | 71  | MET  |
| 1   | Av    | 73  | ARG  |
| 1   | Av    | 76  | ILE  |
| 1   | Av    | 126 | ASP  |
| 1   | Av    | 167 | LEU  |
| 1   | Av    | 186 | ARG  |
| 1   | Av    | 231 | LEU  |
| 1   | Aw    | 64  | THR  |
| 1   | Aw    | 71  | MET  |
| 1   | Aw    | 73  | ARG  |
| 1   | Aw    | 76  | ILE  |
| 1   | Aw    | 126 | ASP  |
| 1   | Aw    | 167 | LEU  |
| 1   | Aw    | 186 | ARG  |
| 1   | Aw    | 231 | LEU  |
| 1   | Ax    | 64  | THR  |
| 1   | Ax    | 71  | MET  |
| 1   | Ax    | 73  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Ax    | 76  | ILE  |
| 1   | Ax    | 126 | ASP  |
| 1   | Ax    | 167 | LEU  |
| 1   | Ax    | 186 | ARG  |
| 1   | Ax    | 231 | LEU  |
| 1   | Ay    | 64  | THR  |
| 1   | Ay    | 71  | MET  |
| 1   | Ay    | 73  | ARG  |
| 1   | Ay    | 76  | ILE  |
| 1   | Ay    | 126 | ASP  |
| 1   | Ay    | 167 | LEU  |
| 1   | Ay    | 186 | ARG  |
| 1   | Ay    | 231 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (194) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A1    | 77  | ASN  |
| 1   | A1    | 178 | ASN  |
| 1   | A1    | 192 | ASN  |
| 1   | A1    | 212 | ASN  |
| 1   | A2    | 77  | ASN  |
| 1   | A2    | 192 | ASN  |
| 1   | A2    | 212 | ASN  |
| 1   | A3    | 77  | ASN  |
| 1   | A3    | 192 | ASN  |
| 1   | A3    | 212 | ASN  |
| 1   | A4    | 77  | ASN  |
| 1   | A4    | 192 | ASN  |
| 1   | A4    | 212 | ASN  |
| 1   | A5    | 77  | ASN  |
| 1   | A5    | 192 | ASN  |
| 1   | A5    | 212 | ASN  |
| 1   | A6    | 77  | ASN  |
| 1   | A6    | 192 | ASN  |
| 1   | A6    | 212 | ASN  |
| 1   | A7    | 77  | ASN  |
| 1   | A7    | 192 | ASN  |
| 1   | A7    | 212 | ASN  |
| 1   | A8    | 77  | ASN  |
| 1   | A8    | 178 | ASN  |
| 1   | A8    | 192 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A8    | 212 | ASN  |
| 1   | A9    | 77  | ASN  |
| 1   | A9    | 192 | ASN  |
| 1   | A9    | 212 | ASN  |
| 1   | AA    | 77  | ASN  |
| 1   | AA    | 178 | ASN  |
| 1   | AA    | 192 | ASN  |
| 1   | AA    | 212 | ASN  |
| 1   | AB    | 77  | ASN  |
| 1   | AB    | 192 | ASN  |
| 1   | AB    | 212 | ASN  |
| 1   | AC    | 77  | ASN  |
| 1   | AC    | 192 | ASN  |
| 1   | AC    | 212 | ASN  |
| 1   | AD    | 77  | ASN  |
| 1   | AD    | 192 | ASN  |
| 1   | AD    | 212 | ASN  |
| 1   | AE    | 77  | ASN  |
| 1   | AE    | 192 | ASN  |
| 1   | AE    | 212 | ASN  |
| 1   | AF    | 77  | ASN  |
| 1   | AF    | 192 | ASN  |
| 1   | AF    | 212 | ASN  |
| 1   | AG    | 77  | ASN  |
| 1   | AG    | 192 | ASN  |
| 1   | AG    | 212 | ASN  |
| 1   | AH    | 77  | ASN  |
| 1   | AH    | 192 | ASN  |
| 1   | AH    | 212 | ASN  |
| 1   | AI    | 77  | ASN  |
| 1   | AI    | 192 | ASN  |
| 1   | AI    | 212 | ASN  |
| 1   | AJ    | 77  | ASN  |
| 1   | AJ    | 178 | ASN  |
| 1   | AJ    | 192 | ASN  |
| 1   | AJ    | 212 | ASN  |
| 1   | AK    | 77  | ASN  |
| 1   | AK    | 192 | ASN  |
| 1   | AK    | 212 | ASN  |
| 1   | AL    | 77  | ASN  |
| 1   | AL    | 178 | ASN  |
| 1   | AL    | 192 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AL    | 212 | ASN  |
| 1   | AM    | 77  | ASN  |
| 1   | AM    | 192 | ASN  |
| 1   | AM    | 212 | ASN  |
| 1   | AN    | 77  | ASN  |
| 1   | AN    | 192 | ASN  |
| 1   | AN    | 212 | ASN  |
| 1   | AO    | 77  | ASN  |
| 1   | AO    | 192 | ASN  |
| 1   | AO    | 212 | ASN  |
| 1   | AP    | 77  | ASN  |
| 1   | AP    | 192 | ASN  |
| 1   | AP    | 212 | ASN  |
| 1   | AQ    | 77  | ASN  |
| 1   | AQ    | 192 | ASN  |
| 1   | AQ    | 212 | ASN  |
| 1   | AR    | 77  | ASN  |
| 1   | AR    | 192 | ASN  |
| 1   | AR    | 212 | ASN  |
| 1   | AS    | 77  | ASN  |
| 1   | AS    | 192 | ASN  |
| 1   | AS    | 212 | ASN  |
| 1   | AT    | 77  | ASN  |
| 1   | AT    | 192 | ASN  |
| 1   | AT    | 212 | ASN  |
| 1   | AU    | 77  | ASN  |
| 1   | AU    | 178 | ASN  |
| 1   | AU    | 192 | ASN  |
| 1   | AU    | 212 | ASN  |
| 1   | AV    | 77  | ASN  |
| 1   | AV    | 192 | ASN  |
| 1   | AV    | 212 | ASN  |
| 1   | AW    | 77  | ASN  |
| 1   | AW    | 192 | ASN  |
| 1   | AW    | 212 | ASN  |
| 1   | AX    | 77  | ASN  |
| 1   | AX    | 192 | ASN  |
| 1   | AX    | 212 | ASN  |
| 1   | AY    | 77  | ASN  |
| 1   | AY    | 192 | ASN  |
| 1   | AY    | 212 | ASN  |
| 1   | AZ    | 77  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AZ    | 178 | ASN  |
| 1   | AZ    | 192 | ASN  |
| 1   | AZ    | 212 | ASN  |
| 1   | Aa    | 77  | ASN  |
| 1   | Aa    | 178 | ASN  |
| 1   | Aa    | 192 | ASN  |
| 1   | Aa    | 212 | ASN  |
| 1   | Ab    | 77  | ASN  |
| 1   | Ab    | 175 | GLN  |
| 1   | Ab    | 192 | ASN  |
| 1   | Ab    | 212 | ASN  |
| 1   | Ac    | 77  | ASN  |
| 1   | Ac    | 192 | ASN  |
| 1   | Ac    | 212 | ASN  |
| 1   | Ad    | 77  | ASN  |
| 1   | Ad    | 192 | ASN  |
| 1   | Ad    | 212 | ASN  |
| 1   | Ae    | 77  | ASN  |
| 1   | Ae    | 192 | ASN  |
| 1   | Ae    | 212 | ASN  |
| 1   | Af    | 77  | ASN  |
| 1   | Af    | 178 | ASN  |
| 1   | Af    | 192 | ASN  |
| 1   | Af    | 212 | ASN  |
| 1   | Ag    | 77  | ASN  |
| 1   | Ag    | 192 | ASN  |
| 1   | Ag    | 212 | ASN  |
| 1   | Ah    | 77  | ASN  |
| 1   | Ah    | 178 | ASN  |
| 1   | Ah    | 192 | ASN  |
| 1   | Ah    | 212 | ASN  |
| 1   | Ai    | 77  | ASN  |
| 1   | Ai    | 192 | ASN  |
| 1   | Ai    | 212 | ASN  |
| 1   | Aj    | 77  | ASN  |
| 1   | Aj    | 192 | ASN  |
| 1   | Aj    | 212 | ASN  |
| 1   | Ak    | 77  | ASN  |
| 1   | Ak    | 192 | ASN  |
| 1   | Ak    | 212 | ASN  |
| 1   | Al    | 77  | ASN  |
| 1   | Al    | 192 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Al    | 212 | ASN  |
| 1   | Am    | 77  | ASN  |
| 1   | Am    | 178 | ASN  |
| 1   | Am    | 192 | ASN  |
| 1   | Am    | 212 | ASN  |
| 1   | An    | 77  | ASN  |
| 1   | An    | 192 | ASN  |
| 1   | An    | 212 | ASN  |
| 1   | Ao    | 77  | ASN  |
| 1   | Ao    | 178 | ASN  |
| 1   | Ao    | 192 | ASN  |
| 1   | Ao    | 212 | ASN  |
| 1   | Ap    | 77  | ASN  |
| 1   | Ap    | 192 | ASN  |
| 1   | Ap    | 212 | ASN  |
| 1   | Aq    | 77  | ASN  |
| 1   | Aq    | 192 | ASN  |
| 1   | Aq    | 212 | ASN  |
| 1   | Ar    | 77  | ASN  |
| 1   | Ar    | 192 | ASN  |
| 1   | Ar    | 212 | ASN  |
| 1   | As    | 77  | ASN  |
| 1   | As    | 192 | ASN  |
| 1   | As    | 212 | ASN  |
| 1   | At    | 77  | ASN  |
| 1   | At    | 192 | ASN  |
| 1   | At    | 212 | ASN  |
| 1   | Au    | 77  | ASN  |
| 1   | Au    | 192 | ASN  |
| 1   | Au    | 212 | ASN  |
| 1   | Av    | 77  | ASN  |
| 1   | Av    | 192 | ASN  |
| 1   | Av    | 212 | ASN  |
| 1   | Aw    | 77  | ASN  |
| 1   | Aw    | 192 | ASN  |
| 1   | Aw    | 212 | ASN  |
| 1   | Ax    | 77  | ASN  |
| 1   | Ax    | 178 | ASN  |
| 1   | Ax    | 192 | ASN  |
| 1   | Ax    | 212 | ASN  |
| 1   | Ay    | 77  | ASN  |
| 1   | Ay    | 192 | ASN  |

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| Mol | Chain          | Res | Type |
|-----|----------------|-----|------|
| 1   | A <sub>y</sub> | 212 | 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.

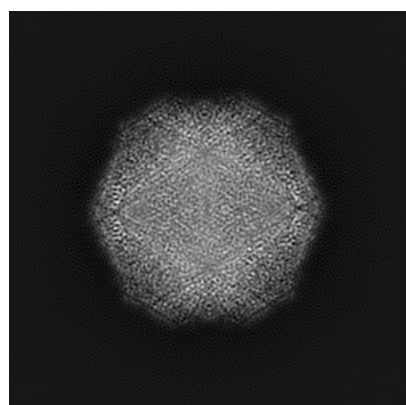
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8969. These allow visual inspection of the internal detail of the map and identification of artifacts.

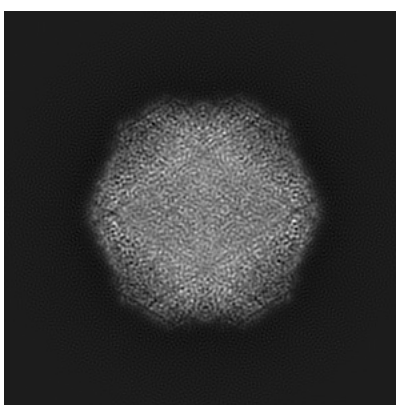
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

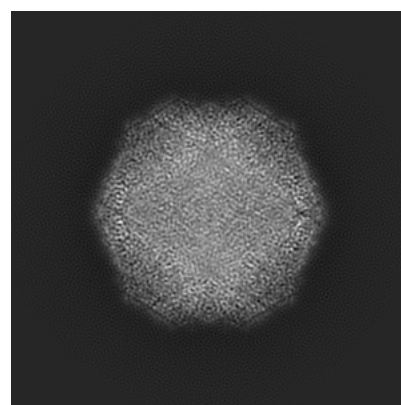
#### 6.1.1 Primary map



X



Y

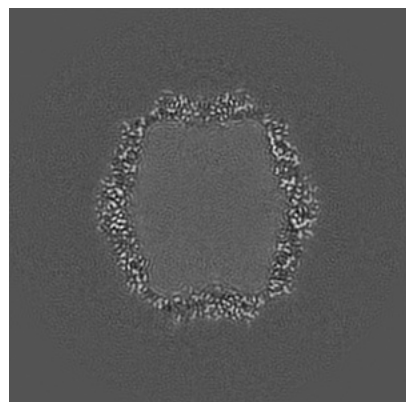


Z

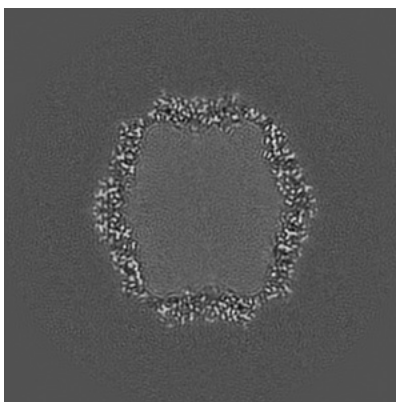
The images above show the map projected in three orthogonal directions.

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

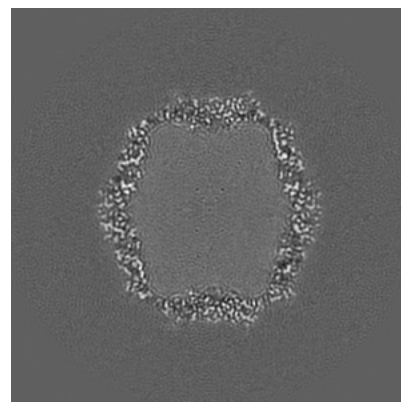
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

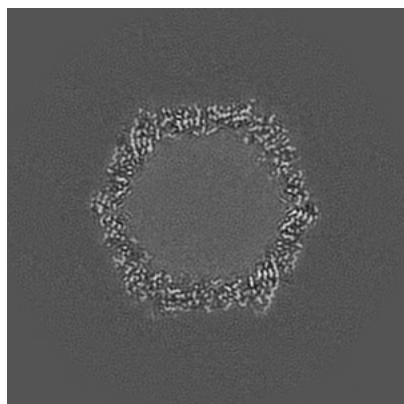


Z Index: 150

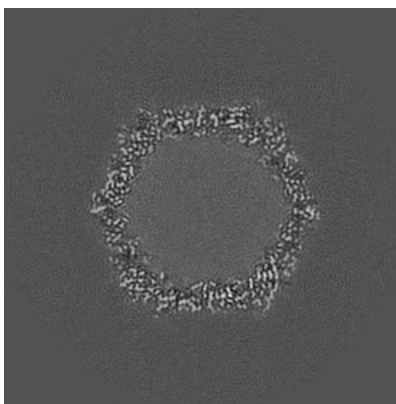
The images above show central slices of the map in three orthogonal directions.

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

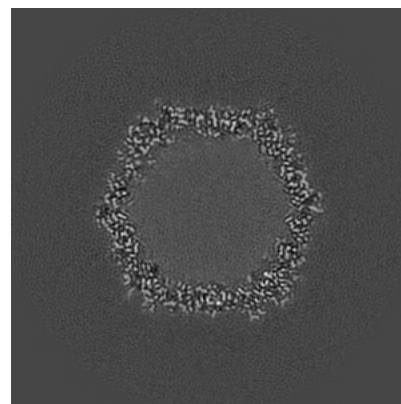
### 6.3.1 Primary map



X Index: 168



Y Index: 167

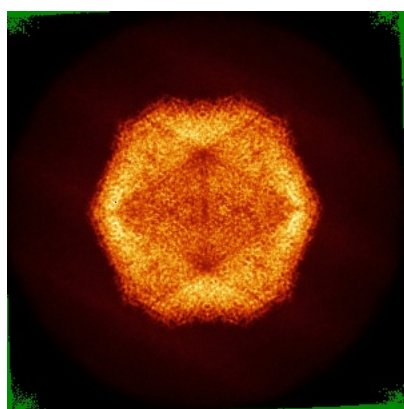


Z Index: 132

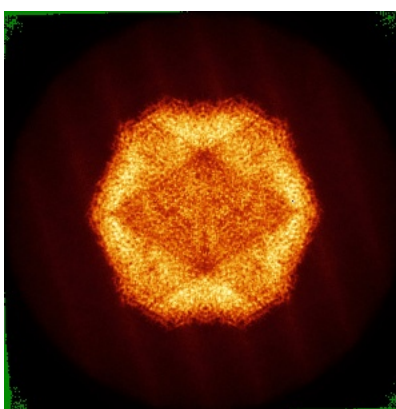
The images above show the largest variance slices of the map in three orthogonal directions.

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

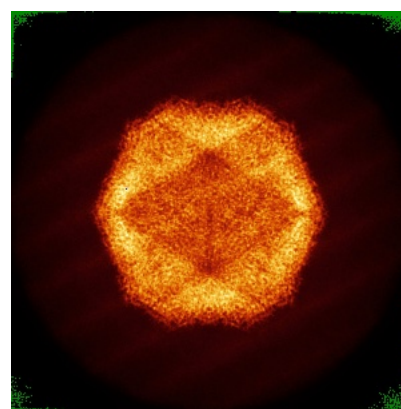
### 6.4.1 Primary map



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](#)

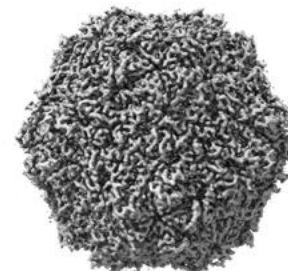
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

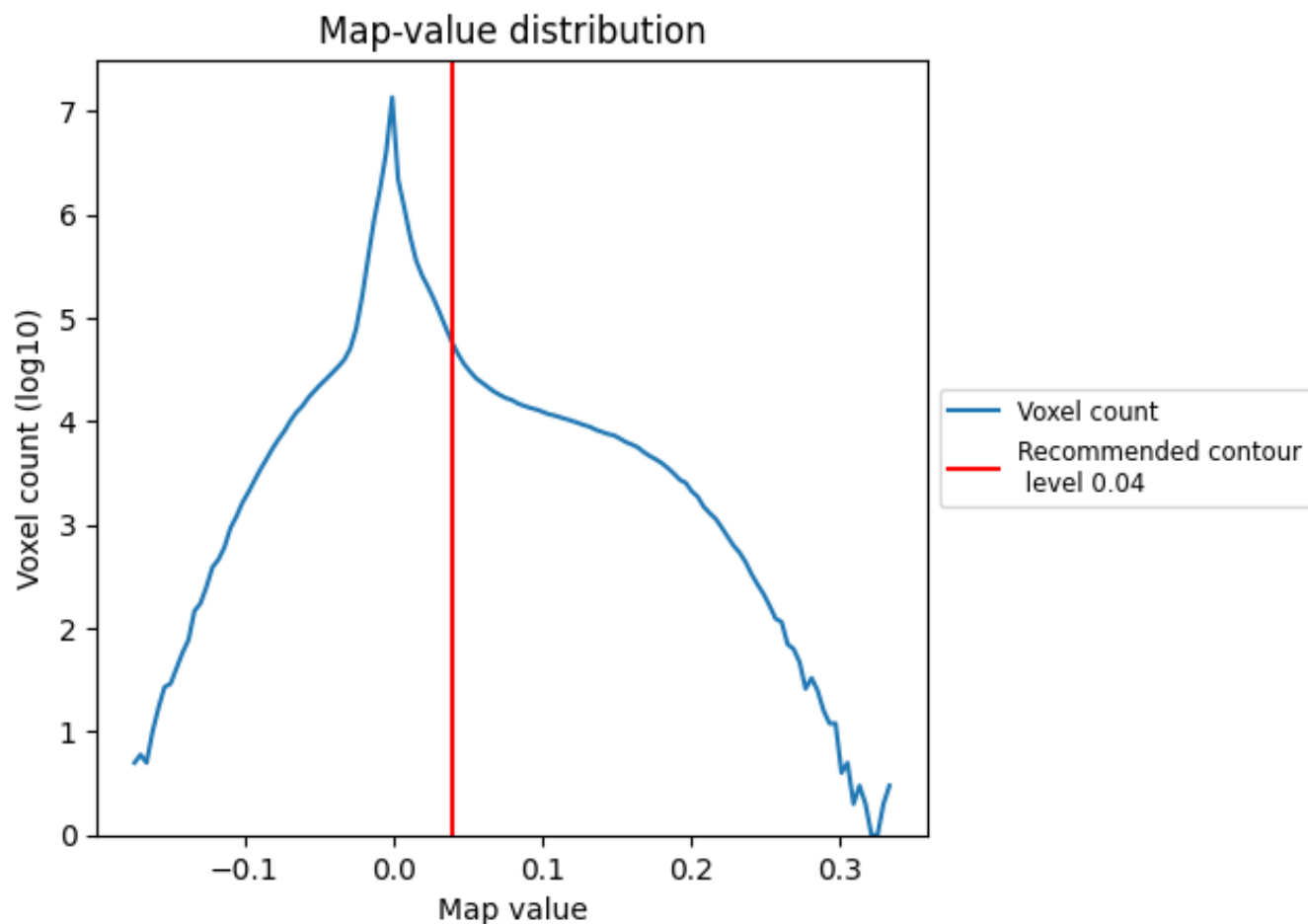
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

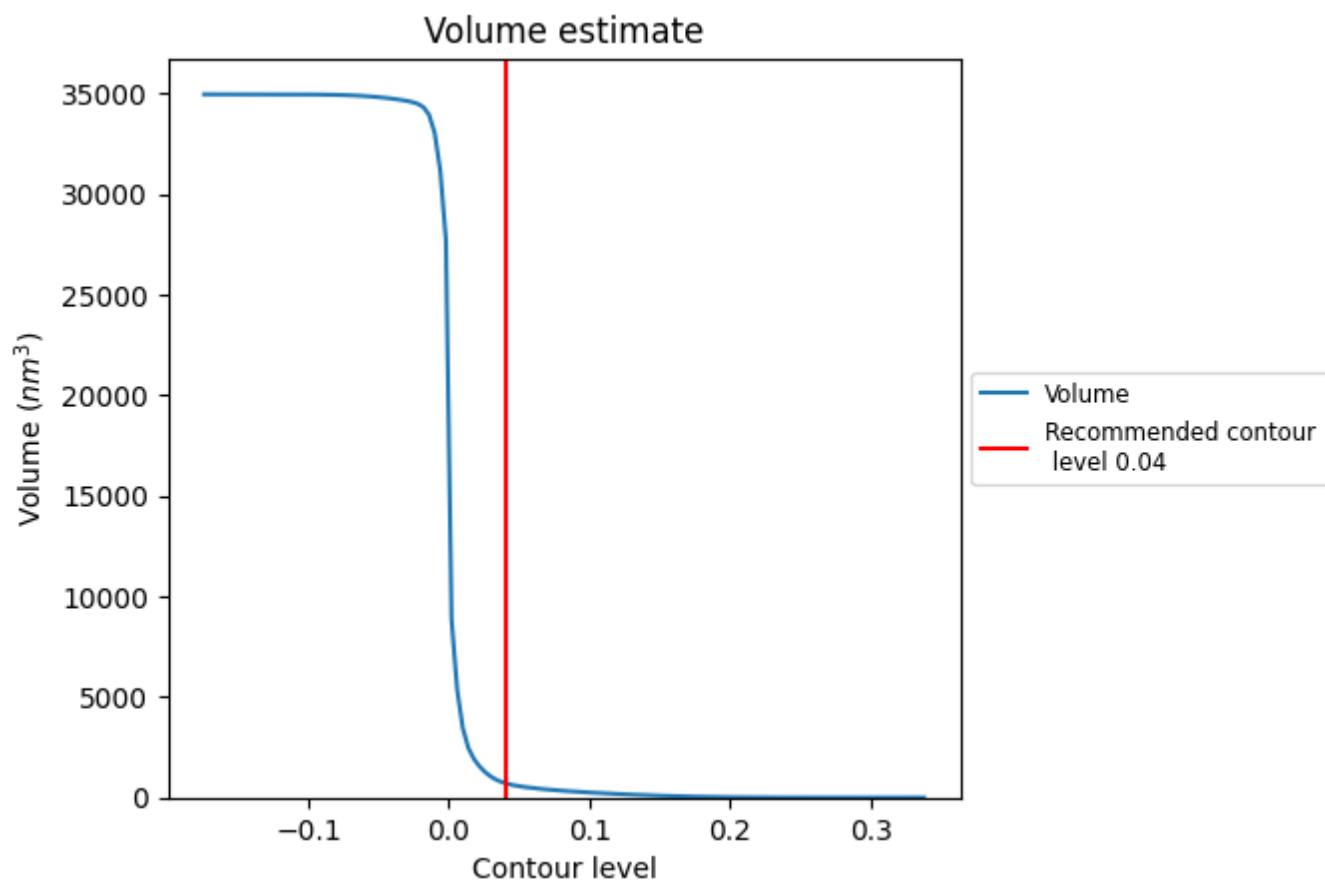
This section contains the results of statistical analysis of the map.

### 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.

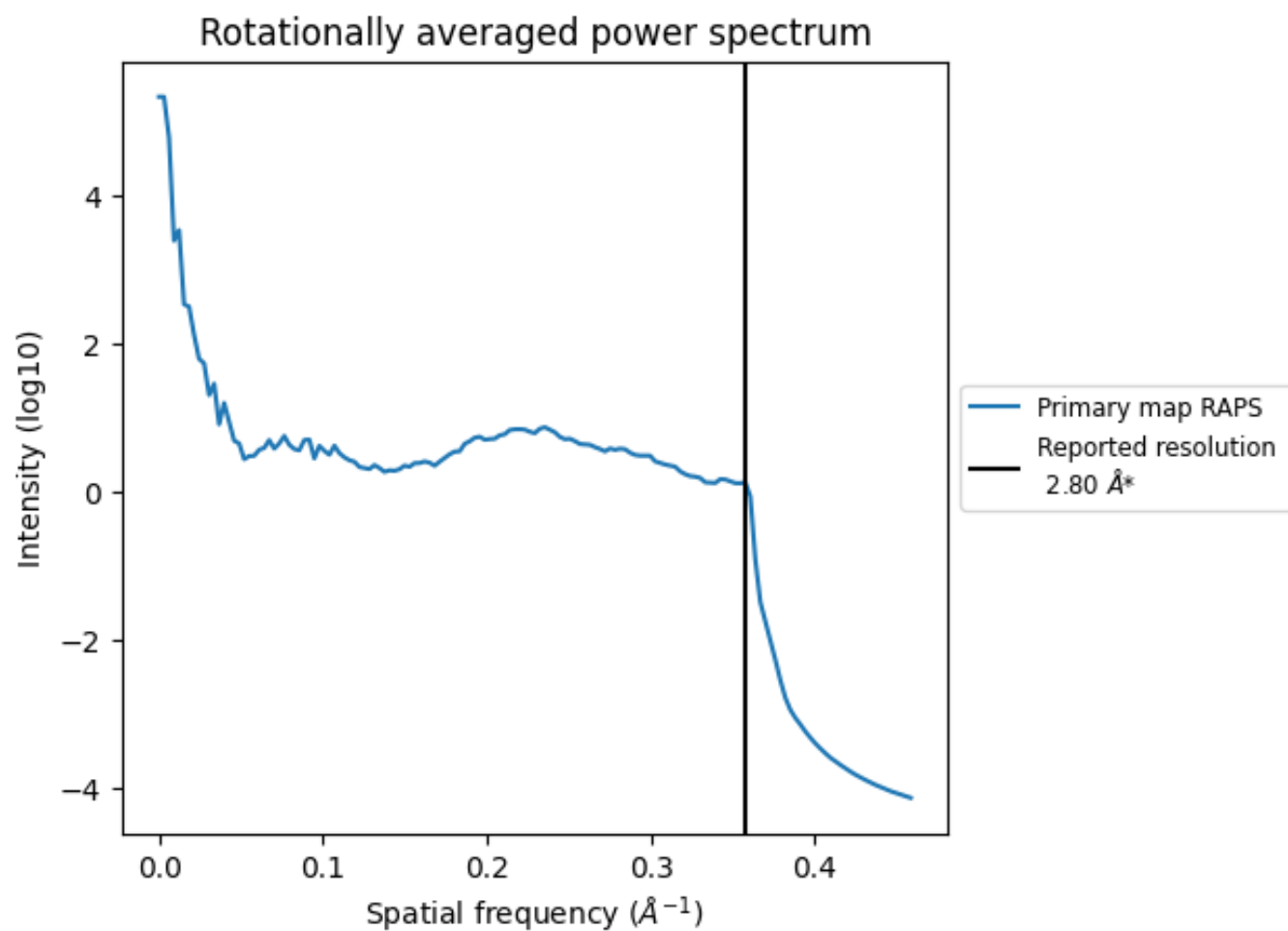
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 719 nm<sup>3</sup>; this corresponds to an approximate mass of 649 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 0.357 Å<sup>-1</sup>

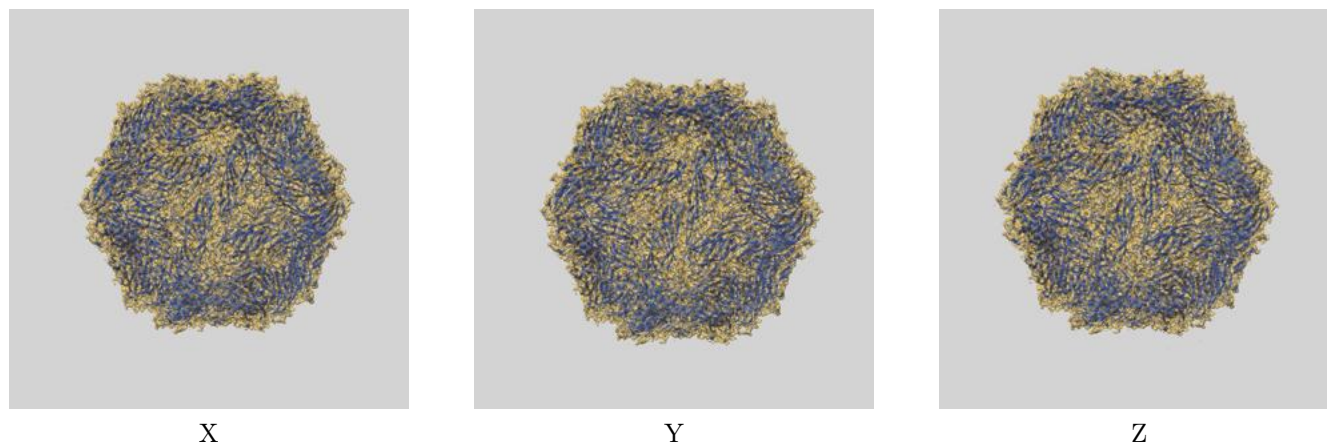
## 8 Fourier-Shell correlation

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

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

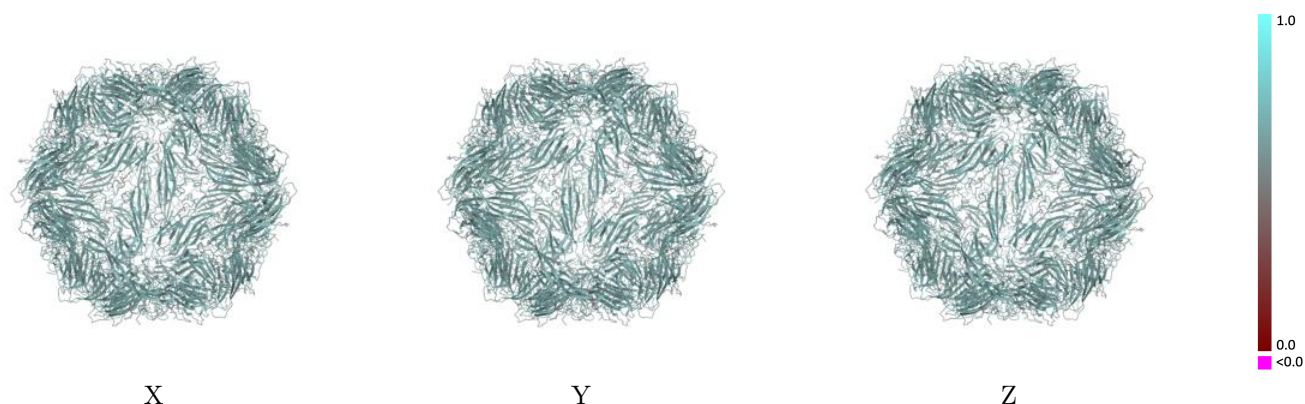
This section contains information regarding the fit between EMDB map EMD-8969 and PDB model 6E2R. Per-residue inclusion information can be found in section 3 on page 10.

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



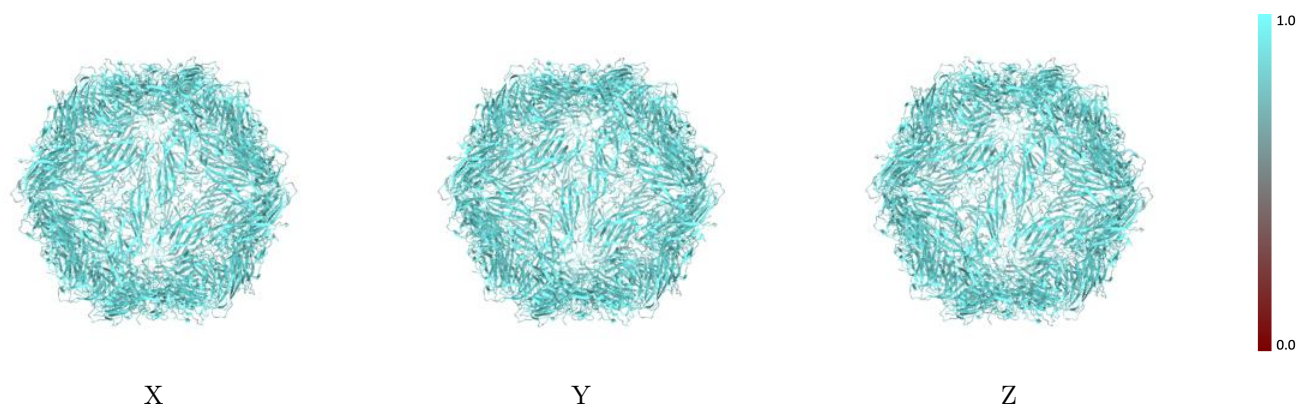
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



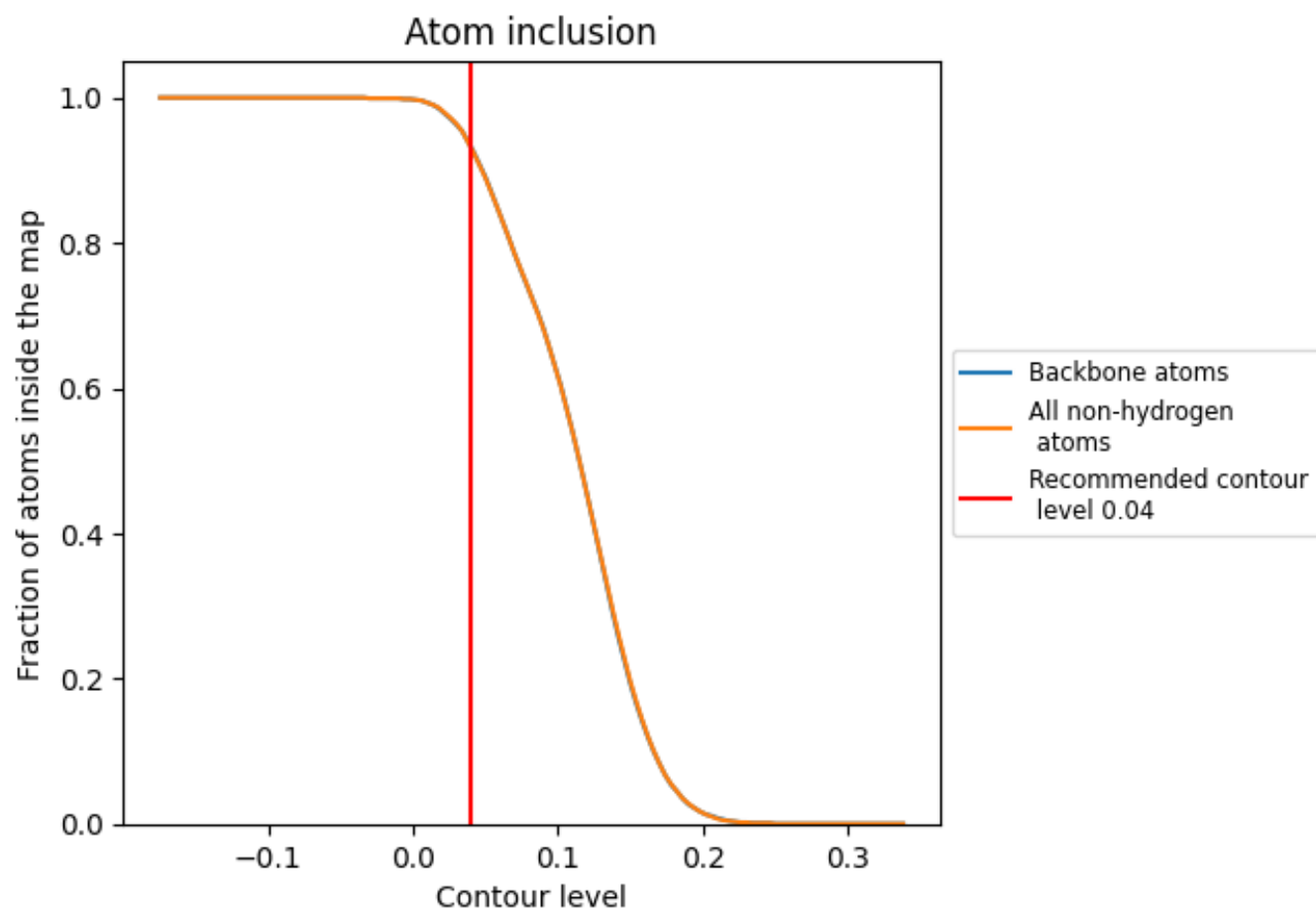
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% 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 (0.04) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9310   |  0.6250   |
| A1    |  0.9370   |  0.6310   |
| A2    |  0.9300   |  0.6210   |
| A3    |  0.9340   |  0.6250   |
| A4    |  0.9360   |  0.6240   |
| A5    |  0.9350   |  0.6270   |
| A6    |  0.9360   |  0.6290   |
| A7    |  0.9340   |  0.6250   |
| A8    |  0.9360   |  0.6260   |
| A9    |  0.9360   |  0.6250   |
| AA    |  0.9360   |  0.6220   |
| AB    |  0.9350   |  0.6230   |
| AC    |  0.9340   |  0.6230   |
| AD    |  0.9360   |  0.6270   |
| AE    |  0.9340  |  0.6200  |
| AF    |  0.9320 |  0.6230 |
| AG    |  0.9310 |  0.6240 |
| AH    |  0.9340 |  0.6180 |
| AI    |  0.9280 |  0.6230 |
| AJ    |  0.9330 |  0.6220 |
| AK    |  0.9380 |  0.6280 |
| AL    |  0.9340 |  0.6240 |
| AM    |  0.9350 |  0.6160 |
| AN    |  0.9360 |  0.6240 |
| AO    |  0.9390 |  0.6260 |
| AP    |  0.9240 |  0.6180 |
| AQ    |  0.9340 |  0.6250 |
| AR    |  0.9360 |  0.6280 |
| AS    |  0.9340 |  0.6240 |
| AT    |  0.9330 |  0.6220 |
| AU    |  0.9400 |  0.6240 |
| AV    |  0.9320 |  0.6270 |
| AW    |  0.9400 |  0.6260 |
| AX    |  0.9290 |  0.6200 |
| AY    |  0.9330 |  0.6270 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| AZ    |  0.9430   |  0.6300   |
| Aa    |  0.9300   |  0.6250   |
| Ab    |  0.9410   |  0.6220   |
| Ac    |  0.9300   |  0.6220   |
| Ad    |  0.9270   |  0.6210   |
| Ae    |  0.9380   |  0.6290   |
| Af    |  0.9360   |  0.6260   |
| Ag    |  0.9340   |  0.6250   |
| Ah    |  0.9330   |  0.6250   |
| Ai    |  0.9300   |  0.6250   |
| Aj    |  0.9400   |  0.6260   |
| Ak    |  0.9380   |  0.6310   |
| Al    |  0.9280   |  0.6180   |
| Am    |  0.9330   |  0.6260   |
| An    |  0.9300   |  0.6270   |
| Ao    |  0.9310   |  0.6250   |
| Ap    |  0.9320   |  0.6260   |
| Aq    |  0.9360  |  0.6260  |
| Ar    |  0.9340 |  0.6250 |
| As    |  0.9330 |  0.6220 |
| At    |  0.9300 |  0.6250 |
| Au    |  0.9360 |  0.6270 |
| Av    |  0.9360 |  0.6260 |
| Aw    |  0.9310 |  0.6250 |
| Ax    |  0.9420 |  0.6280 |
| Ay    |  0.9320 |  0.6260 |