



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:59 PM UTC

PDB ID : 8GTD / pdb\_00008gtd  
EMDB ID : EMD-34250  
Title : Cryo-EM model of the marine siphophage vB\_DshS-R4C portal-adaptor complex  
Authors : Huang, Y.; Sun, H.; Wei, S.; Zheng, Q.; Li, S.; Zhang, R.; Xia, N.  
Deposited on : 2022-09-08  
Resolution : 4.70 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:

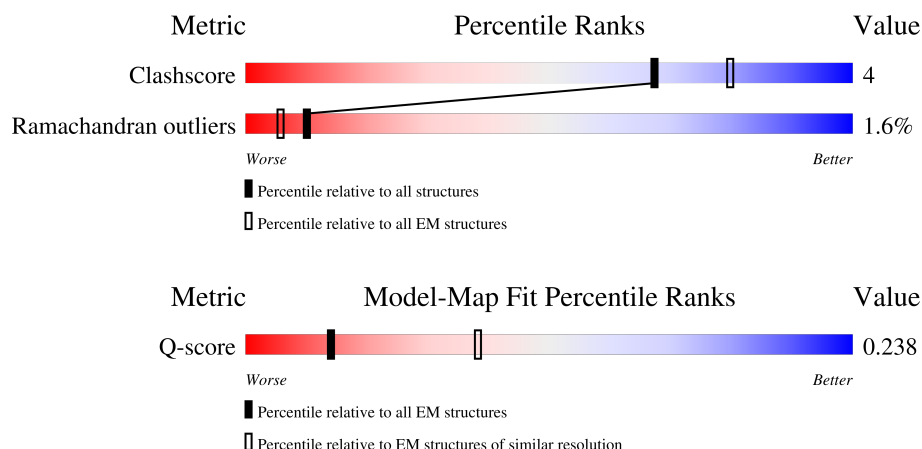
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 4.70 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                       | -                                                        |
| Q-score               | -                           | 25397                       | 1989 ( 4.20 - 5.20 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 551    |                  |
| 1   | B     | 551    |                  |
| 1   | C     | 551    |                  |
| 1   | D     | 551    |                  |
| 1   | E     | 551    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | F     | 551    |                  |
| 1   | G     | 551    |                  |
| 1   | H     | 551    |                  |
| 1   | I     | 551    |                  |
| 1   | J     | 551    |                  |
| 1   | K     | 551    |                  |
| 1   | L     | 551    |                  |
| 2   | M     | 178    |                  |
| 2   | N     | 178    |                  |
| 2   | O     | 178    |                  |
| 2   | P     | 178    |                  |
| 2   | Q     | 178    |                  |
| 2   | R     | 178    |                  |
| 2   | S     | 178    |                  |
| 2   | T     | 178    |                  |
| 2   | U     | 178    |                  |
| 2   | V     | 178    |                  |
| 2   | W     | 178    |                  |
| 2   | X     | 178    |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29580 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Portal protein.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 1   | A     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | B     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | C     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | D     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | E     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | F     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | G     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | H     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | I     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | J     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | K     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |
| 1   | L     | 438      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1752  | 876 | 438 | 438 |         |       |

- Molecule 2 is a protein called Head-to-tail joining protein.

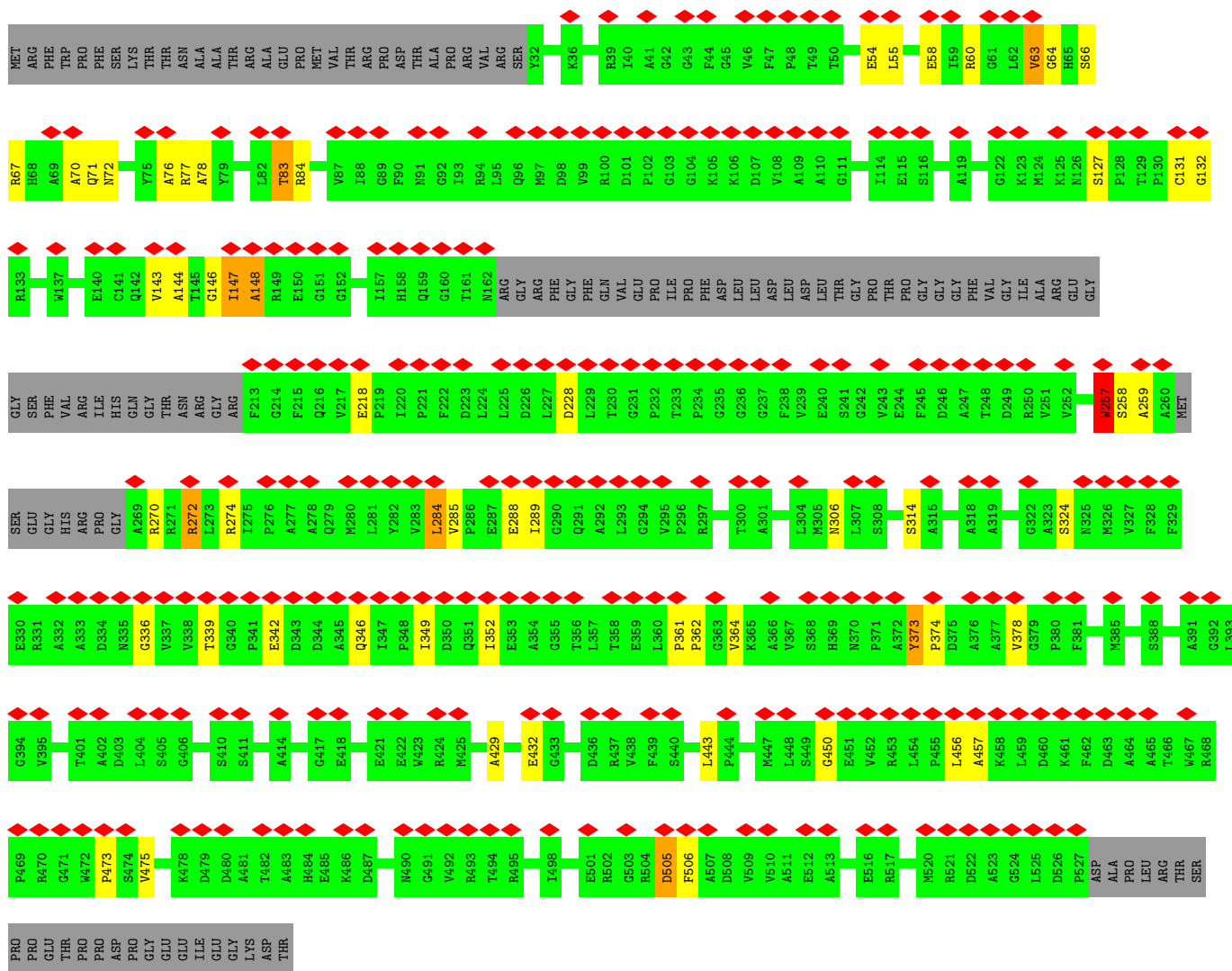
| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 2   | M     | 178      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 713   | 356 | 178 | 179 |         |       |
| 2   | N     | 178      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 713   | 356 | 178 | 179 |         |       |
| 2   | O     | 178      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 713   | 356 | 178 | 179 |         |       |

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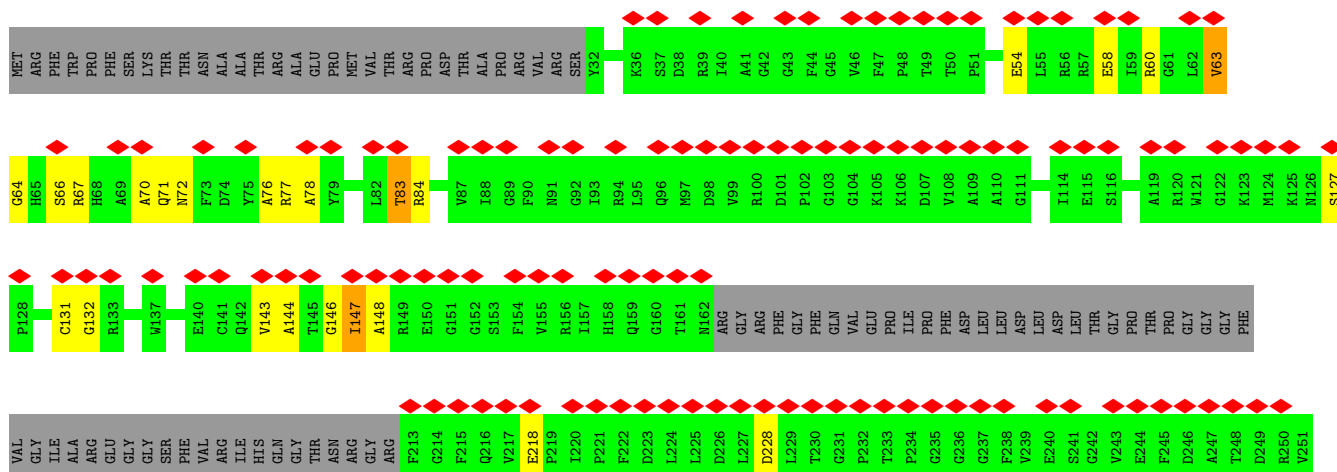
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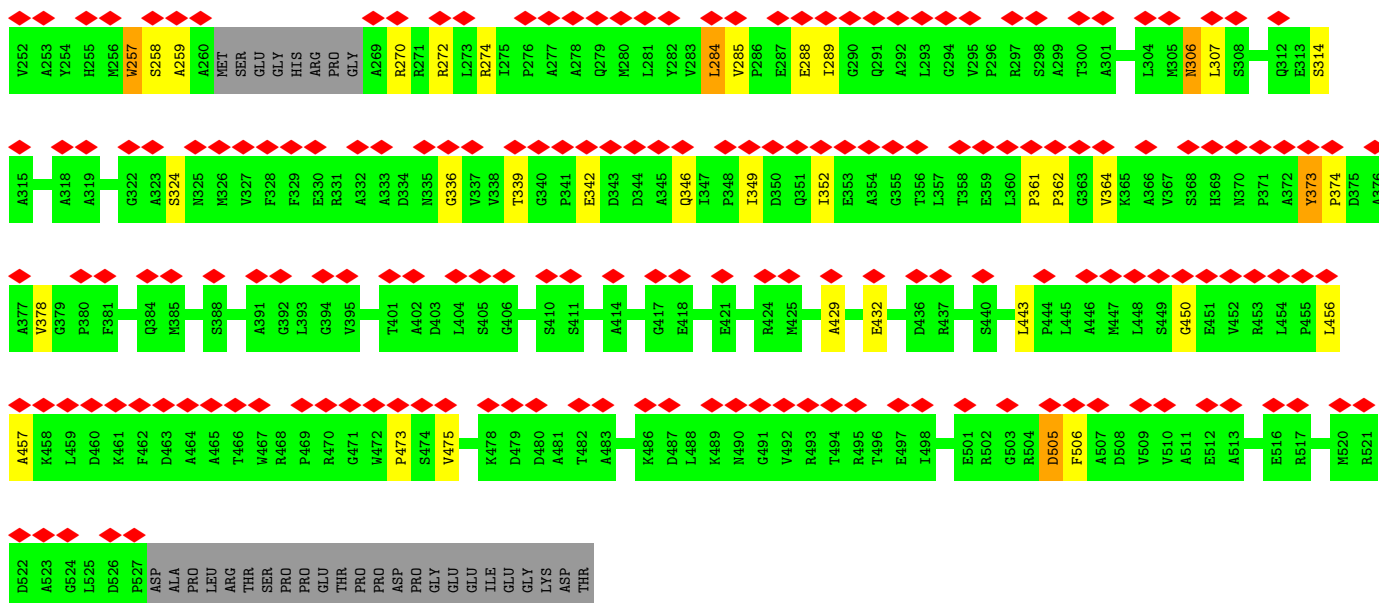
| Mol | Chain | Residues | Atoms        |          |          |          | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|
| 2   | P     | 178      | Total<br>713 | C<br>356 | N<br>178 | O<br>179 | 0       | 0     |
| 2   | Q     | 178      | Total<br>713 | C<br>356 | N<br>178 | O<br>179 | 0       | 0     |
| 2   | R     | 178      | Total<br>713 | C<br>356 | N<br>178 | O<br>179 | 0       | 0     |
| 2   | S     | 178      | Total<br>713 | C<br>356 | N<br>178 | O<br>179 | 0       | 0     |
| 2   | T     | 178      | Total<br>713 | C<br>356 | N<br>178 | O<br>179 | 0       | 0     |
| 2   | U     | 178      | Total<br>713 | C<br>356 | N<br>178 | O<br>179 | 0       | 0     |
| 2   | V     | 178      | Total<br>713 | C<br>356 | N<br>178 | O<br>179 | 0       | 0     |
| 2   | W     | 178      | Total<br>713 | C<br>356 | N<br>178 | O<br>179 | 0       | 0     |
| 2   | X     | 178      | Total<br>713 | C<br>356 | N<br>178 | O<br>179 | 0       | 0     |



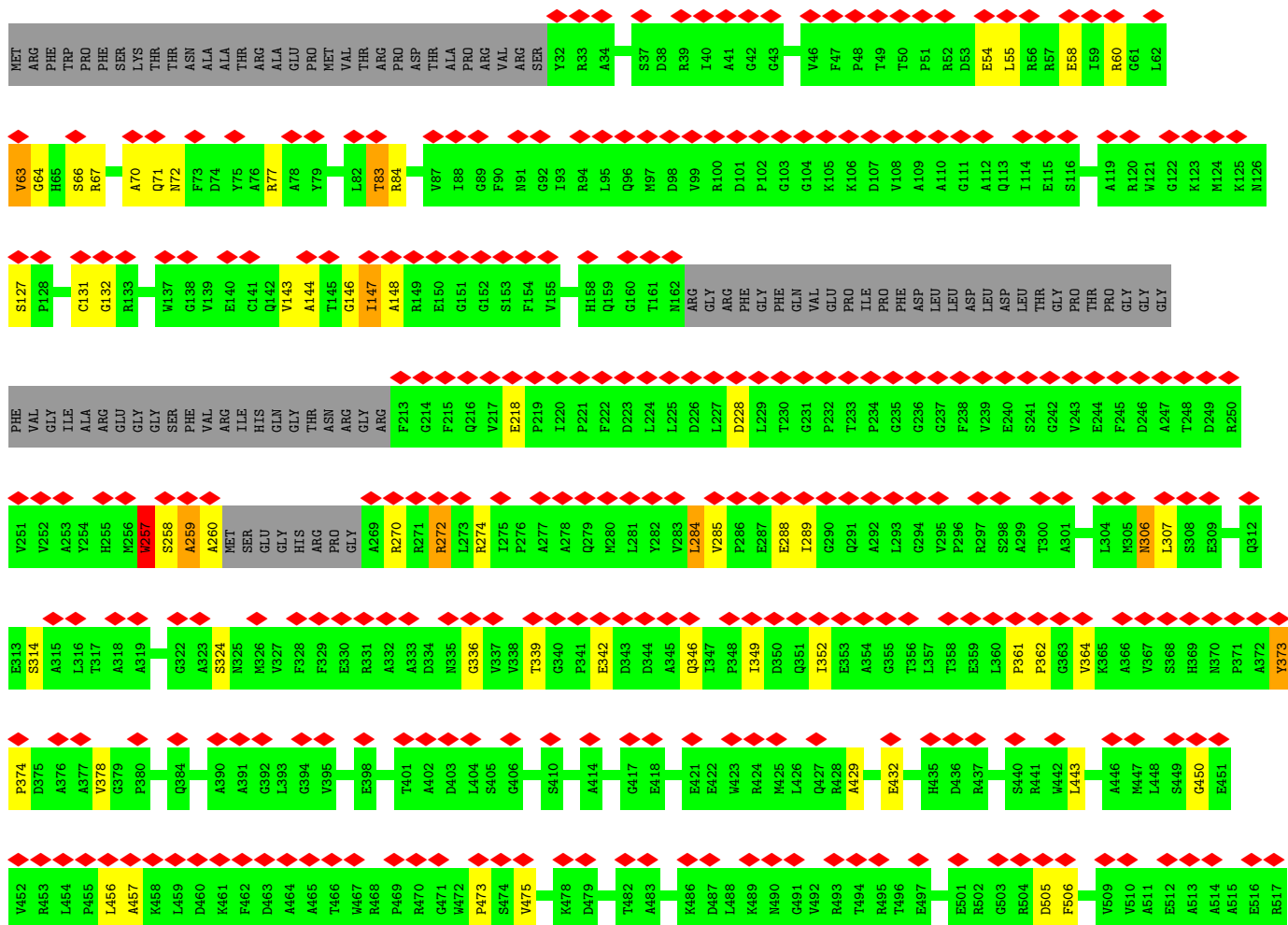


- Molecule 1: Portal protein

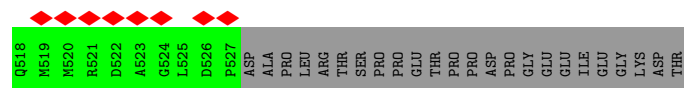




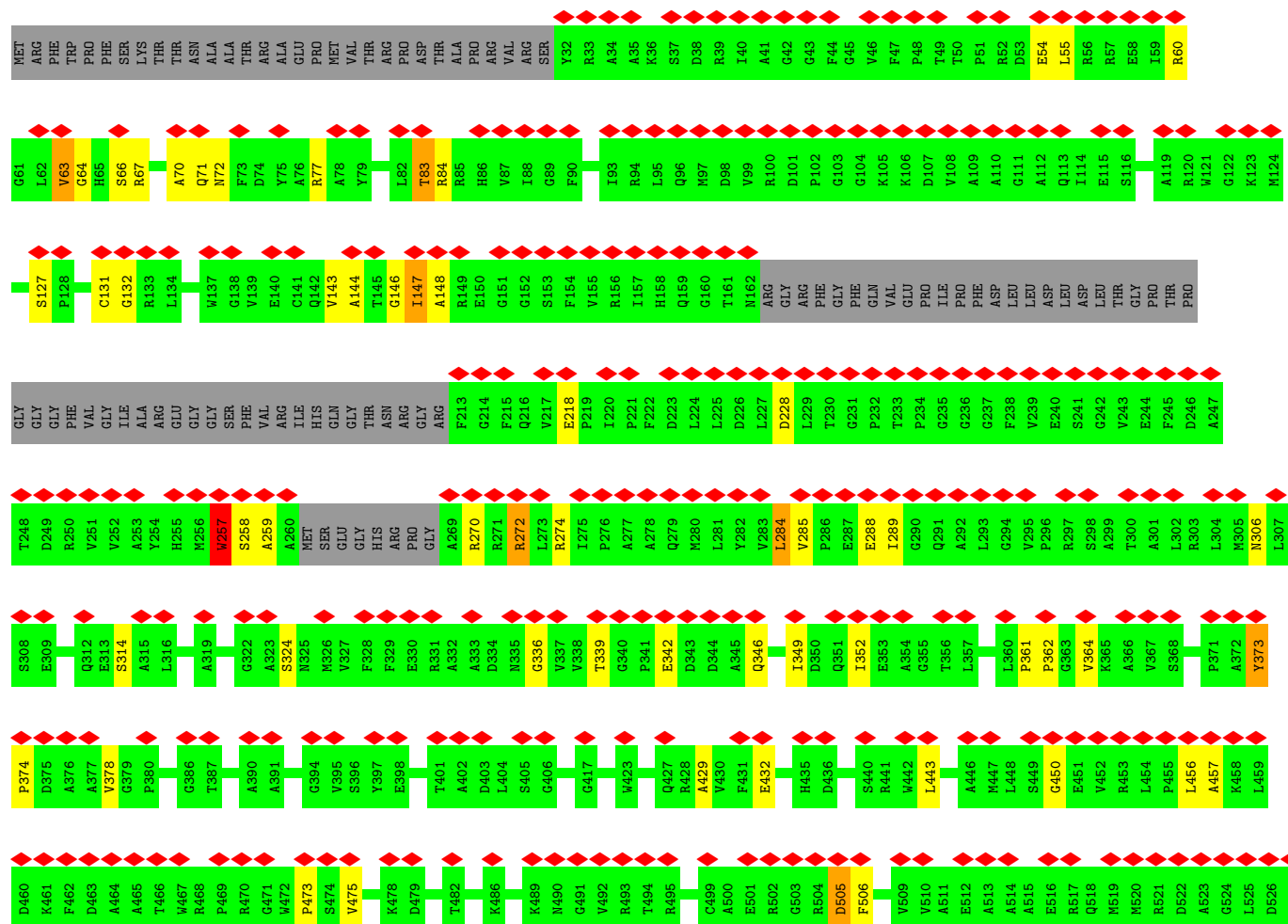
• Molecule 1: Portal protein





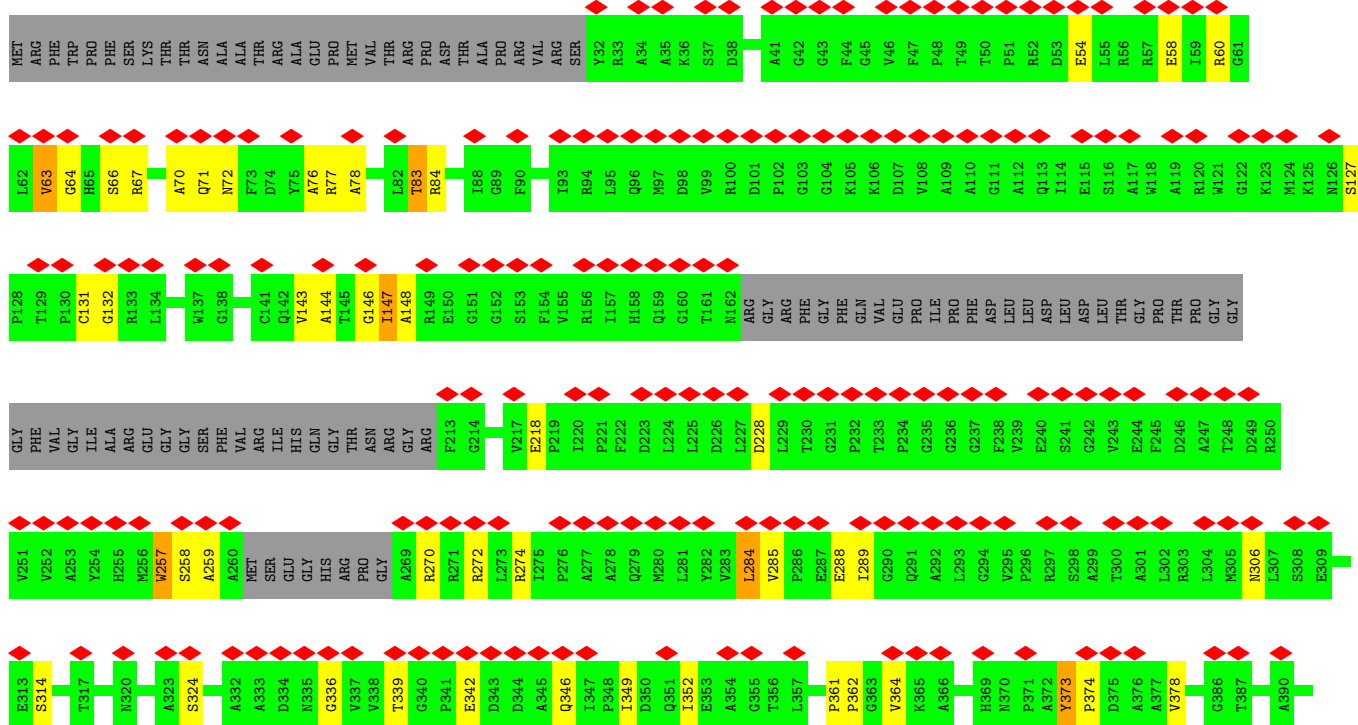
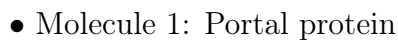


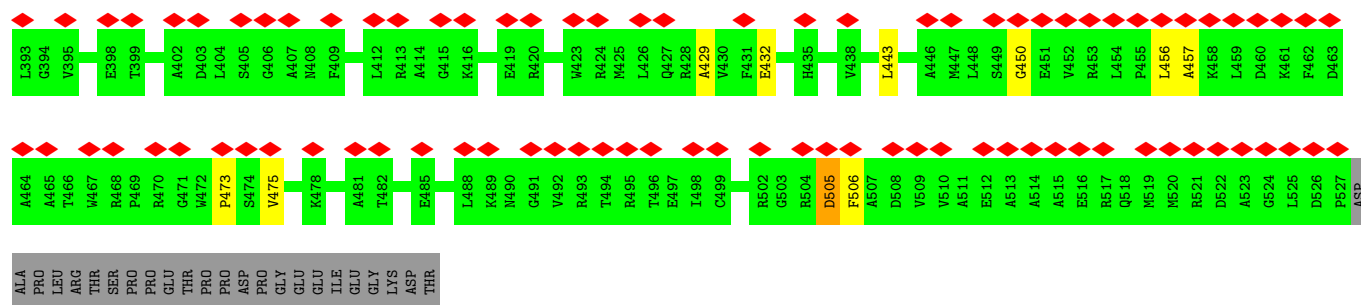
• Molecule 1: Portal protein



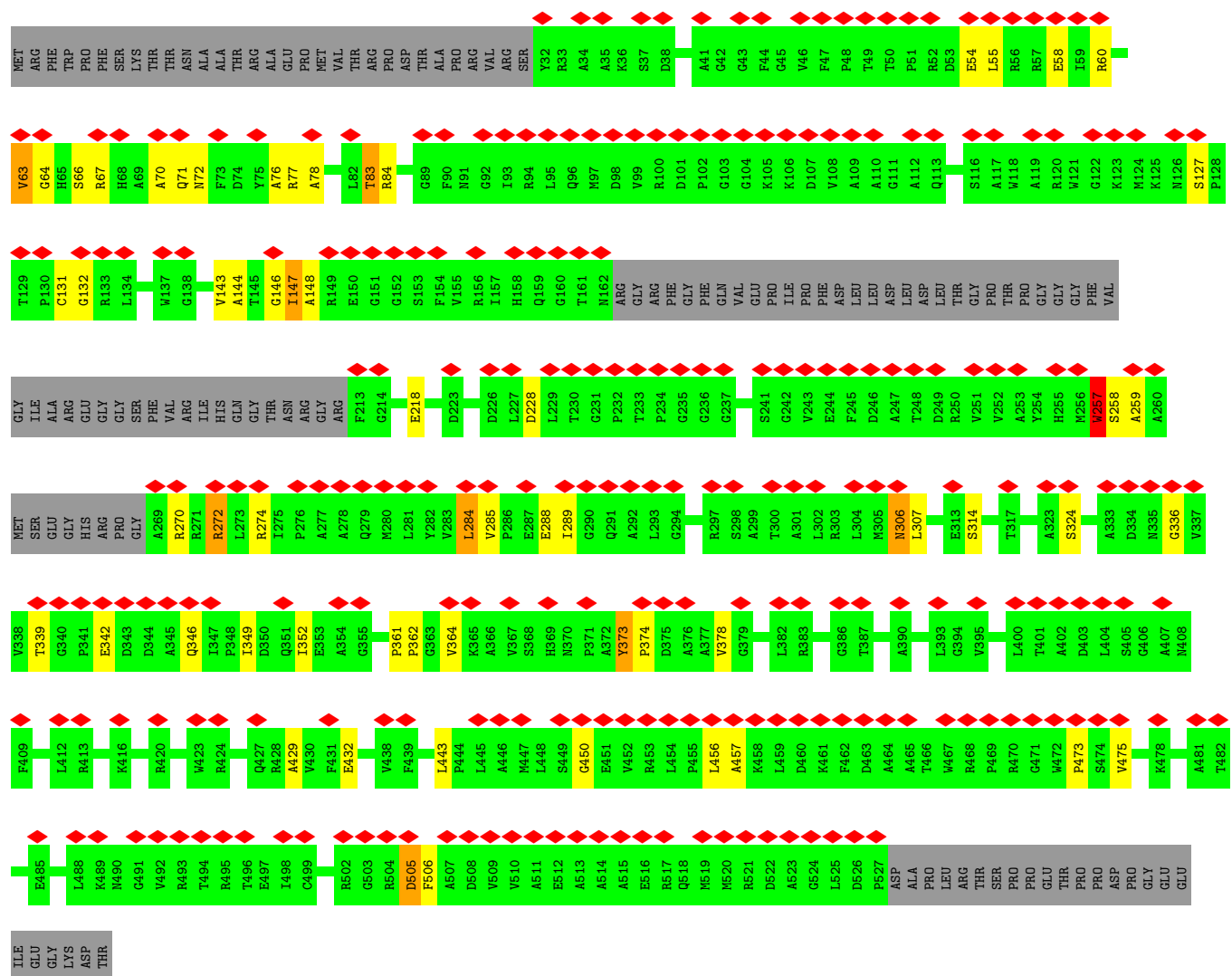
• Molecule 1: Portal protein



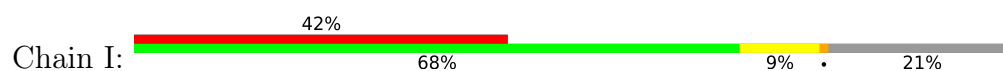


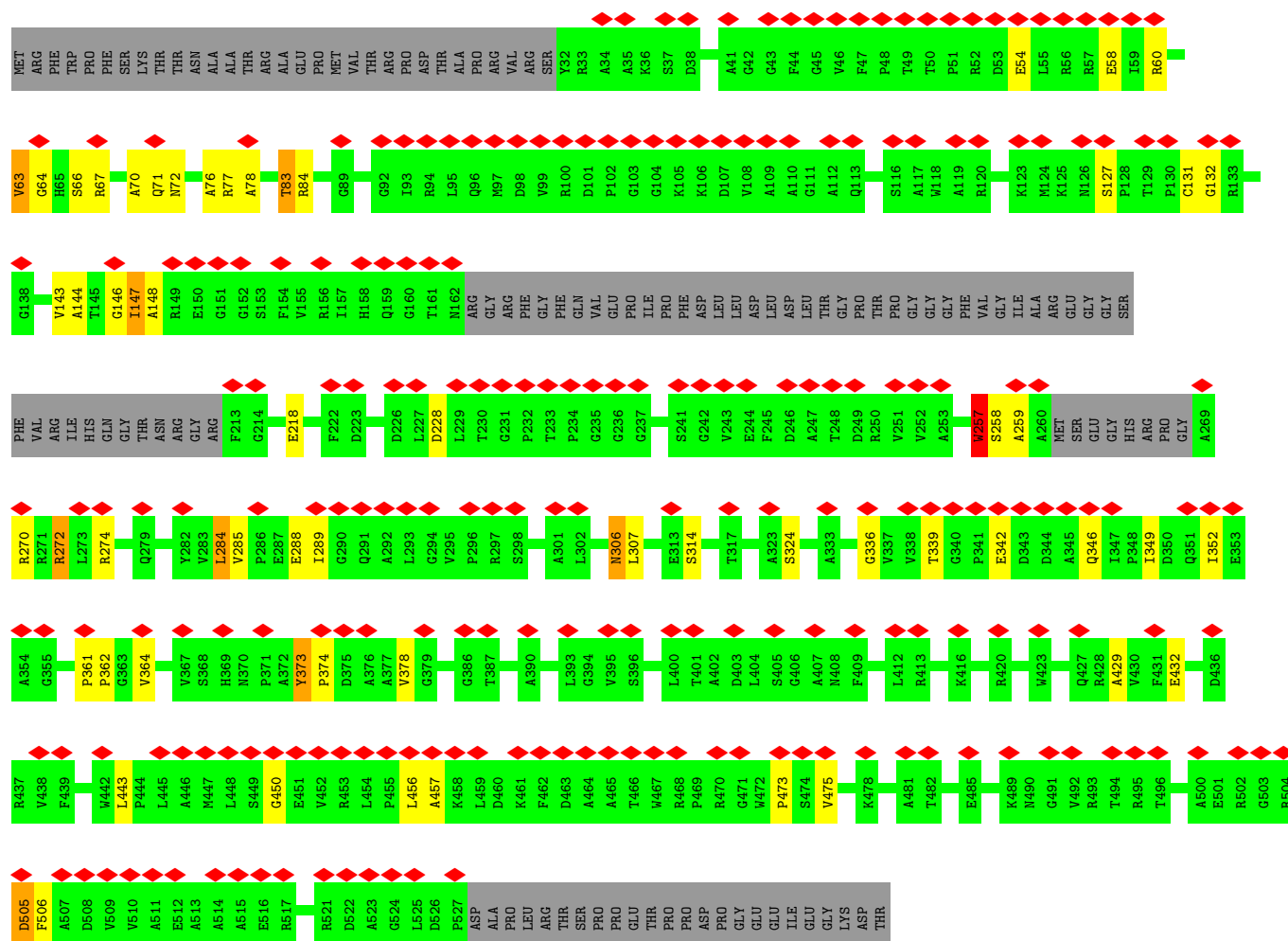


• Molecule 1: Portal protein

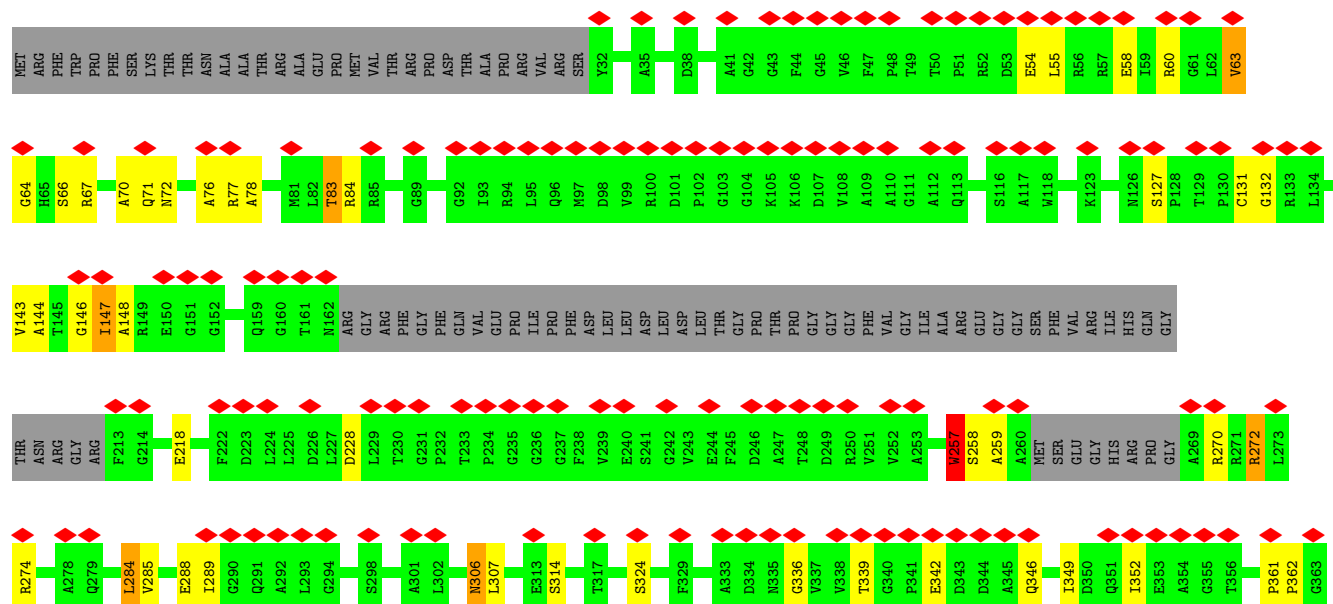
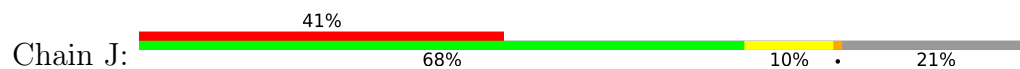


• Molecule 1: Portal protein

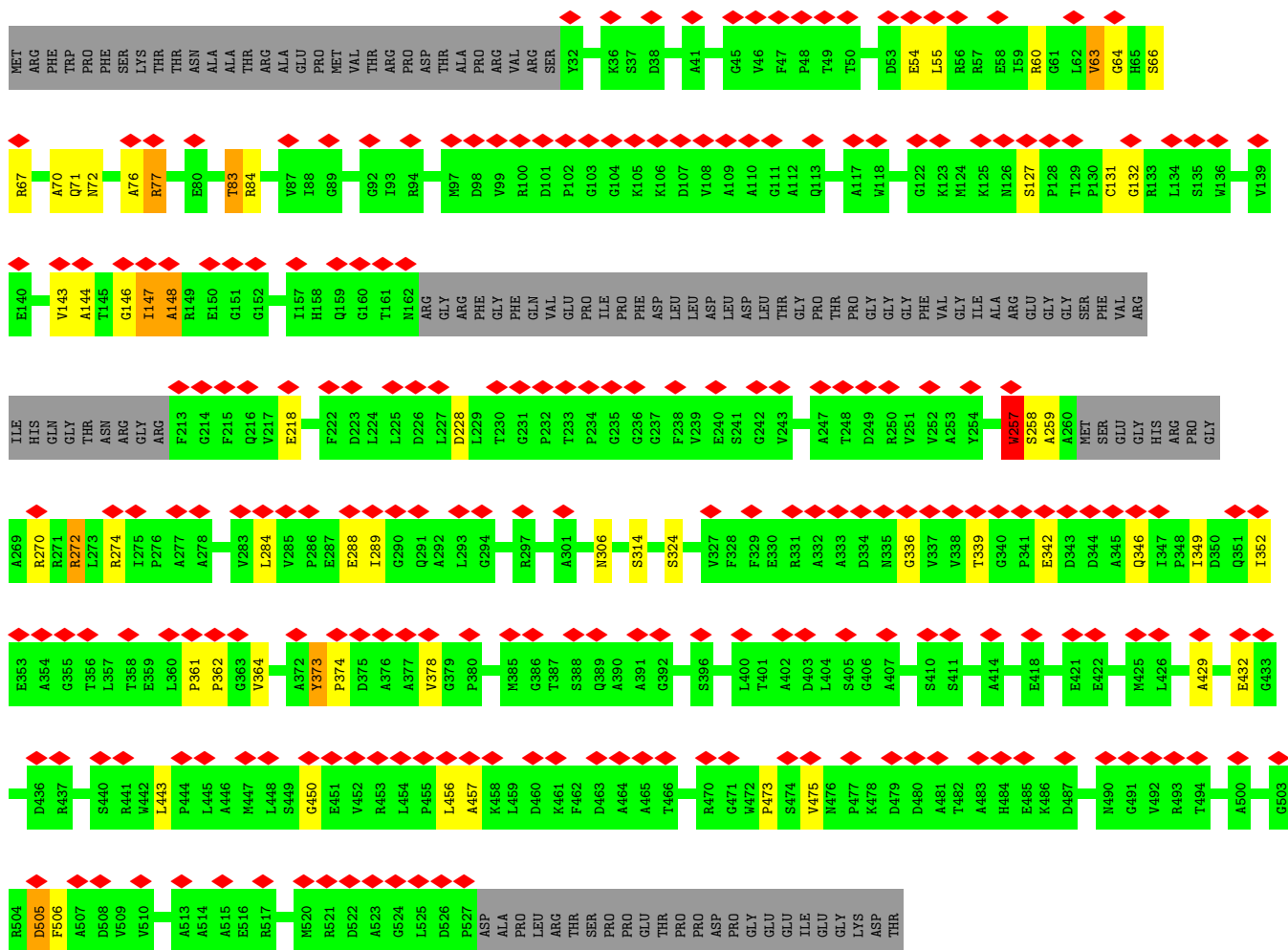




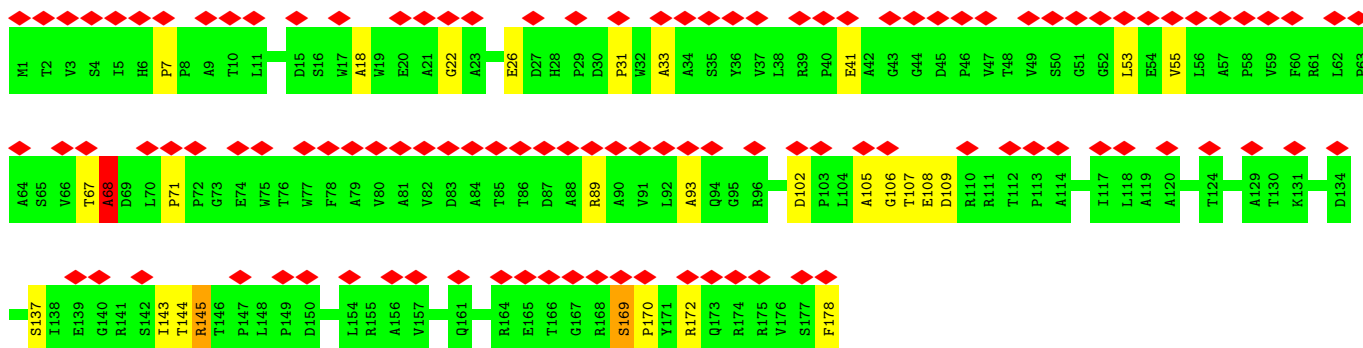
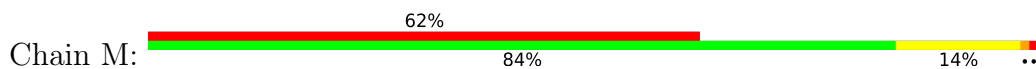
### • Molecule 1: Portal protein



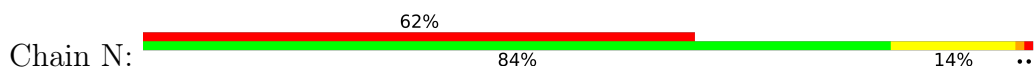


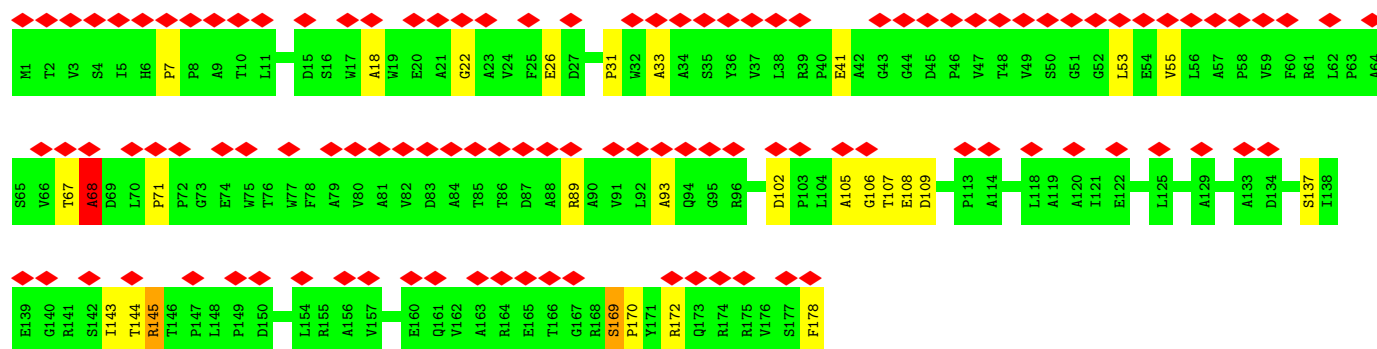


• Molecule 2: Head-to-tail joining protein

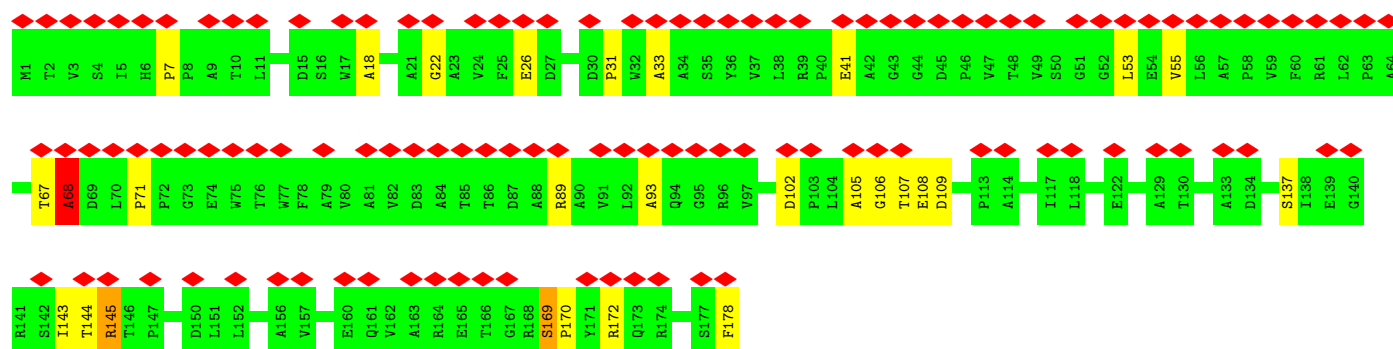
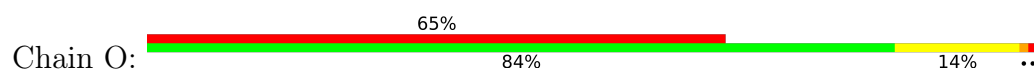


• Molecule 2: Head-to-tail joining protein

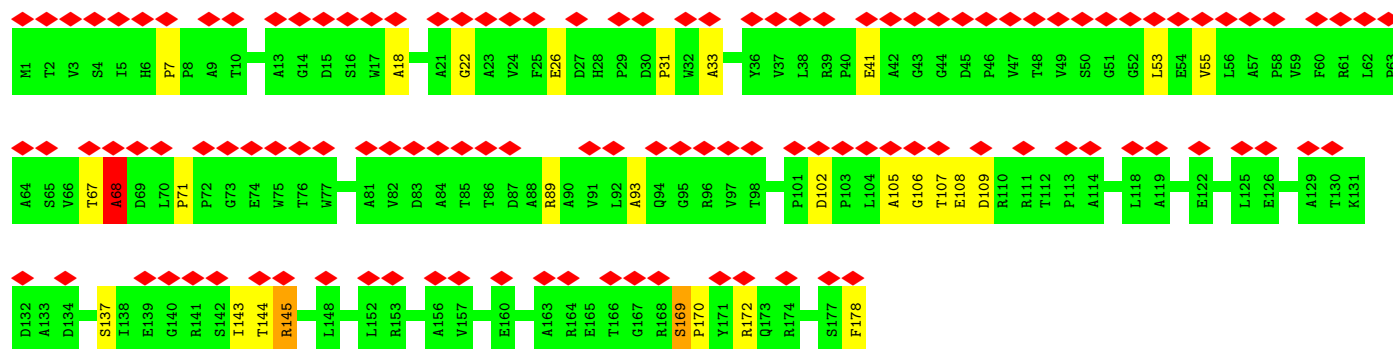
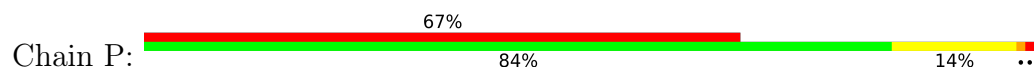




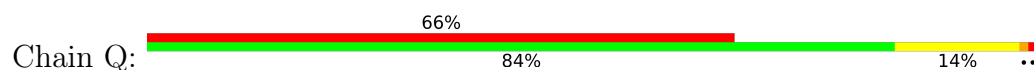
• Molecule 2: Head-to-tail joining protein

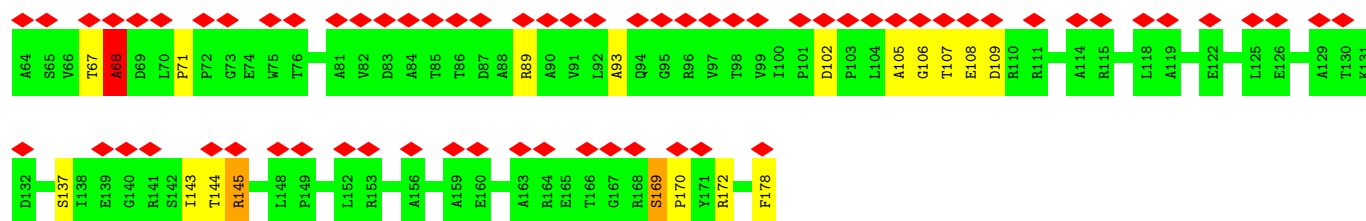


• Molecule 2: Head-to-tail joining protein

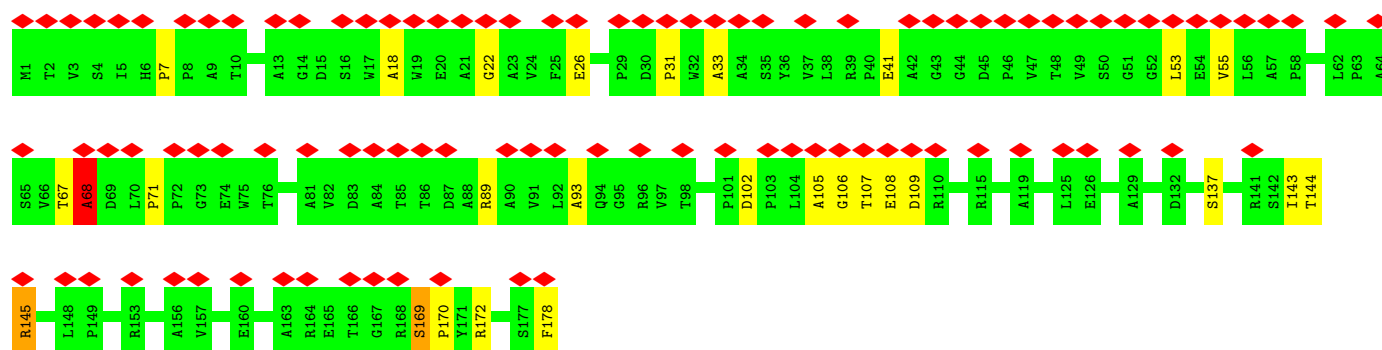
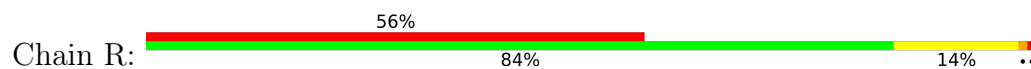


• Molecule 2: Head-to-tail joining protein

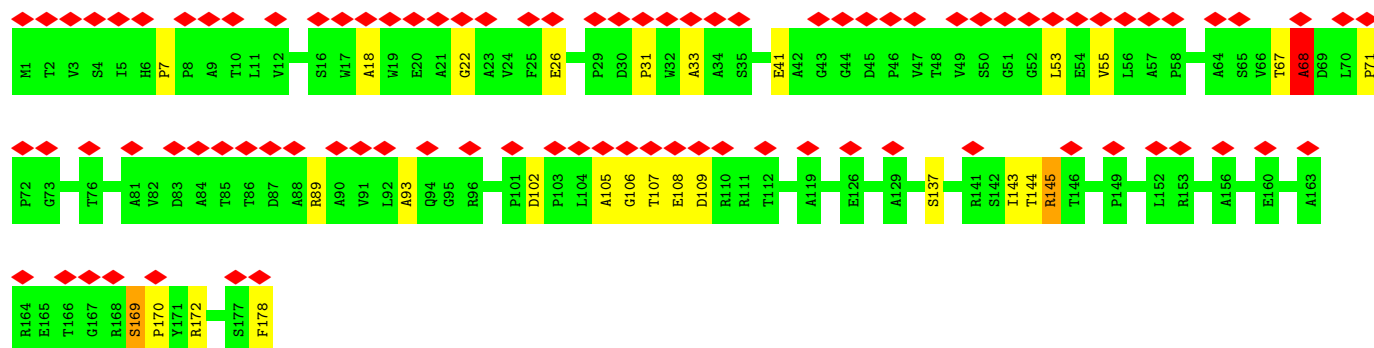
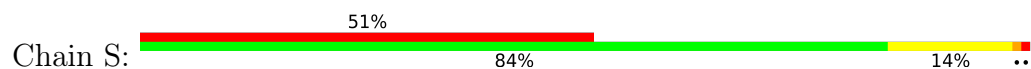




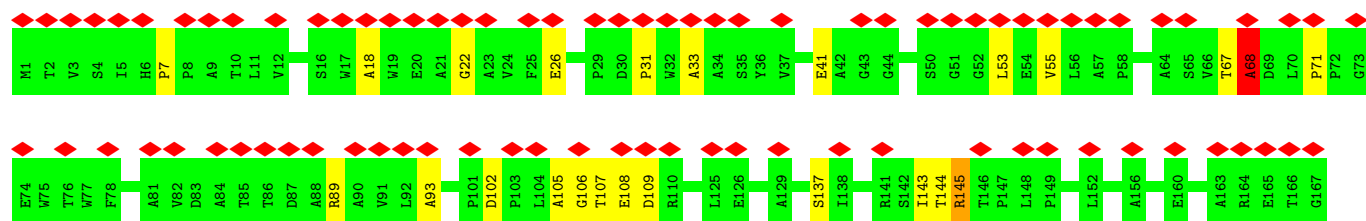
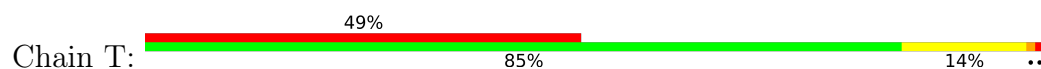
• Molecule 2: Head-to-tail joining protein



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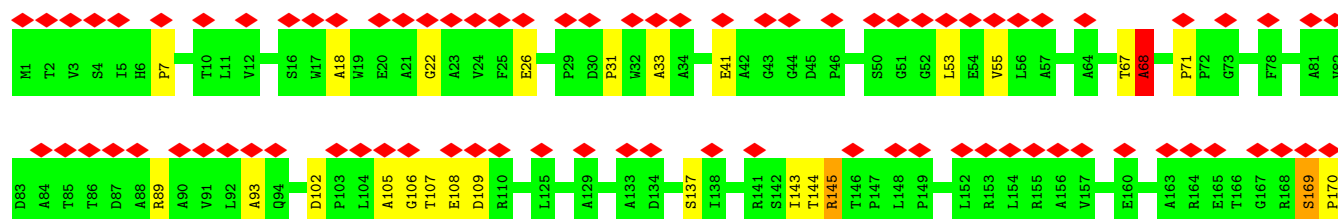
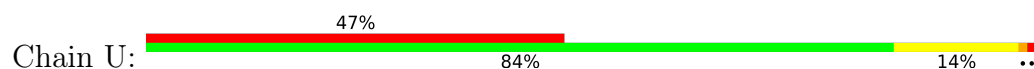
• Molecule 2: Head-to-tail joining protein



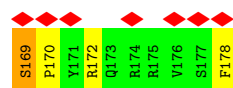
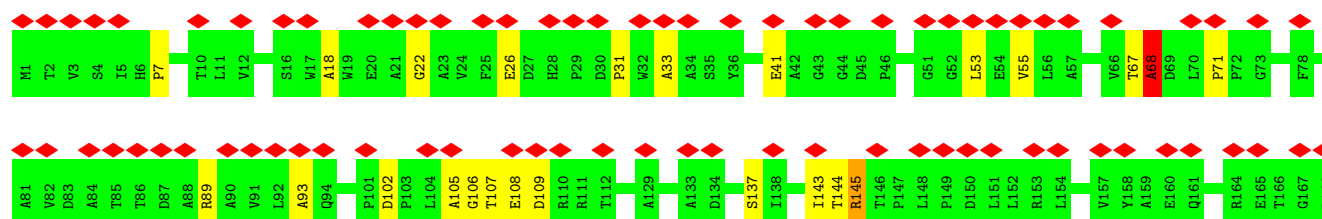
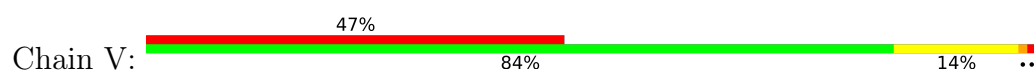




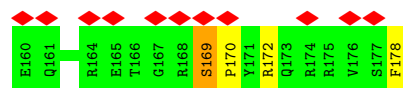
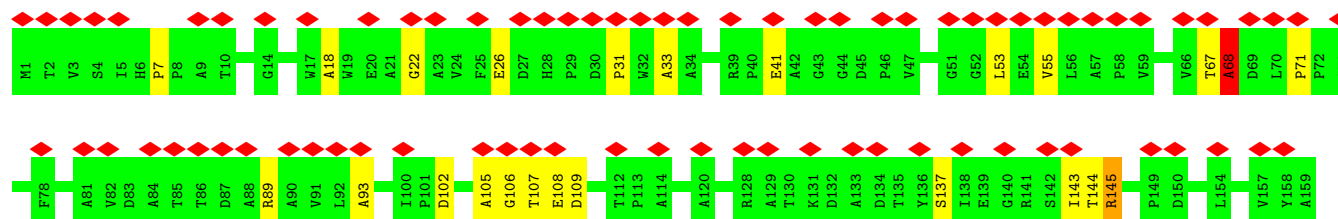
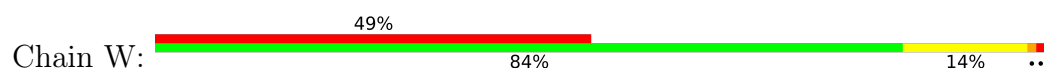
- Molecule 2: Head-to-tail joining protein



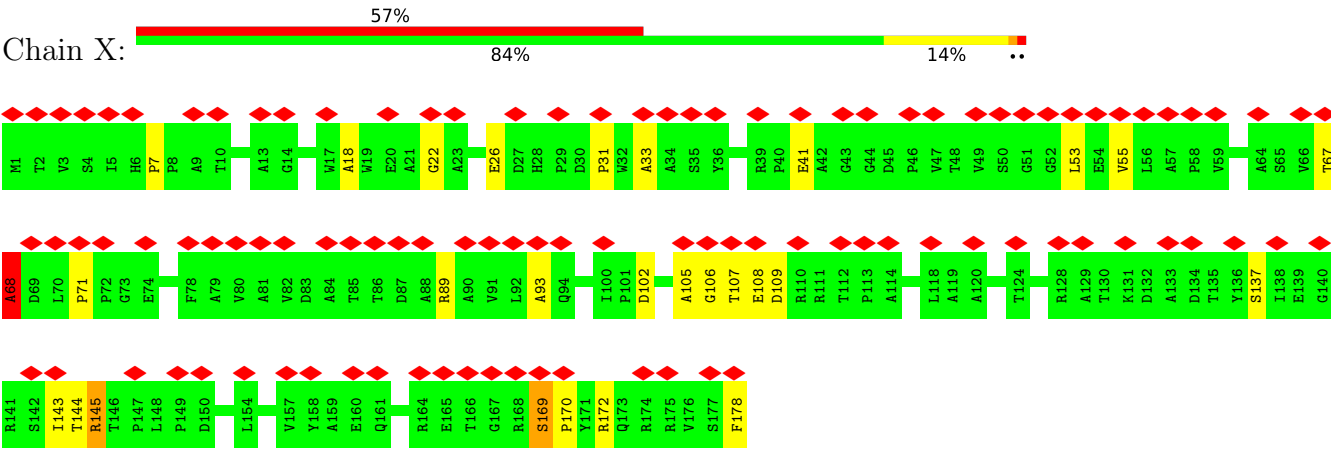
- Molecule 2: Head-to-tail joining protein



- Molecule 2: Head-to-tail joining protein



- Molecule 2: Head-to-tail joining protein



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C12                              | Depositor |
| Number of particles used             | 5844                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TECNAI F30                          | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.102                                   | Depositor |
| Minimum map value                    | -0.053                                  | Depositor |
| Average map value                    | -0.000                                  | Depositor |
| Map value standard deviation         | 0.008                                   | Depositor |
| Recommended contour level            | 0.0302                                  | Depositor |
| Map size (Å)                         | 270.72, 270.72, 270.72                  | wwPDB     |
| Map dimensions                       | 240, 240, 240                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.128, 1.128, 1.128                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |                  | Bond angles |                  |
|-----|-------|--------------|------------------|-------------|------------------|
|     |       | RMSZ         | $\# Z  > 5$      | RMSZ        | $\# Z  > 5$      |
| 1   | A     | 1.21         | 10/1749 (0.6%)   | 1.67        | 42/2181 (1.9%)   |
| 1   | B     | 1.21         | 11/1749 (0.6%)   | 1.67        | 42/2181 (1.9%)   |
| 1   | C     | 1.21         | 9/1749 (0.5%)    | 1.67        | 42/2181 (1.9%)   |
| 1   | D     | 1.21         | 10/1749 (0.6%)   | 1.67        | 41/2181 (1.9%)   |
| 1   | E     | 1.21         | 9/1749 (0.5%)    | 1.67        | 42/2181 (1.9%)   |
| 1   | F     | 1.21         | 10/1749 (0.6%)   | 1.67        | 42/2181 (1.9%)   |
| 1   | G     | 1.21         | 9/1749 (0.5%)    | 1.67        | 42/2181 (1.9%)   |
| 1   | H     | 1.21         | 10/1749 (0.6%)   | 1.67        | 42/2181 (1.9%)   |
| 1   | I     | 1.21         | 9/1749 (0.5%)    | 1.67        | 42/2181 (1.9%)   |
| 1   | J     | 1.21         | 10/1749 (0.6%)   | 1.67        | 41/2181 (1.9%)   |
| 1   | K     | 1.21         | 9/1749 (0.5%)    | 1.67        | 42/2181 (1.9%)   |
| 1   | L     | 1.21         | 10/1749 (0.6%)   | 1.67        | 42/2181 (1.9%)   |
| 2   | M     | 0.93         | 0/712            | 1.76        | 26/887 (2.9%)    |
| 2   | N     | 0.93         | 0/712            | 1.76        | 26/887 (2.9%)    |
| 2   | O     | 0.93         | 0/712            | 1.76        | 26/887 (2.9%)    |
| 2   | P     | 0.93         | 0/712            | 1.77        | 26/887 (2.9%)    |
| 2   | Q     | 0.93         | 0/712            | 1.76        | 26/887 (2.9%)    |
| 2   | R     | 0.93         | 0/712            | 1.77        | 26/887 (2.9%)    |
| 2   | S     | 0.93         | 0/712            | 1.77        | 26/887 (2.9%)    |
| 2   | T     | 0.93         | 0/712            | 1.77        | 26/887 (2.9%)    |
| 2   | U     | 0.93         | 0/712            | 1.76        | 26/887 (2.9%)    |
| 2   | V     | 0.93         | 0/712            | 1.77        | 26/887 (2.9%)    |
| 2   | W     | 0.93         | 0/712            | 1.76        | 26/887 (2.9%)    |
| 2   | X     | 0.93         | 0/712            | 1.77        | 26/887 (2.9%)    |
| All | All   | 1.14         | 116/29532 (0.4%) | 1.70        | 814/36816 (2.2%) |

All (116) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | E     | 147 | ILE  | C-O   | -8.86 | 1.14        | 1.24     |
| 1   | K     | 147 | ILE  | C-O   | -8.86 | 1.14        | 1.24     |
| 1   | C     | 147 | ILE  | C-O   | -8.85 | 1.14        | 1.24     |
| 1   | I     | 147 | ILE  | C-O   | -8.85 | 1.14        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | G     | 147 | ILE  | C-O   | -8.83 | 1.14        | 1.24     |
| 1   | A     | 147 | ILE  | C-O   | -8.76 | 1.14        | 1.24     |
| 1   | D     | 147 | ILE  | C-O   | -8.76 | 1.14        | 1.24     |
| 1   | J     | 147 | ILE  | C-O   | -8.76 | 1.14        | 1.24     |
| 1   | B     | 147 | ILE  | C-O   | -8.74 | 1.14        | 1.24     |
| 1   | H     | 147 | ILE  | C-O   | -8.74 | 1.14        | 1.24     |
| 1   | F     | 147 | ILE  | C-O   | -8.73 | 1.14        | 1.24     |
| 1   | L     | 147 | ILE  | C-O   | -8.73 | 1.14        | 1.24     |
| 1   | E     | 258 | SER  | CA-C  | -8.45 | 1.42        | 1.53     |
| 1   | K     | 258 | SER  | CA-C  | -8.45 | 1.42        | 1.53     |
| 1   | B     | 258 | SER  | CA-C  | -8.41 | 1.42        | 1.53     |
| 1   | C     | 258 | SER  | CA-C  | -8.39 | 1.42        | 1.53     |
| 1   | I     | 258 | SER  | CA-C  | -8.39 | 1.42        | 1.53     |
| 1   | A     | 258 | SER  | CA-C  | -8.38 | 1.42        | 1.53     |
| 1   | H     | 258 | SER  | CA-C  | -8.39 | 1.42        | 1.53     |
| 1   | D     | 258 | SER  | CA-C  | -8.37 | 1.42        | 1.53     |
| 1   | G     | 258 | SER  | CA-C  | -8.37 | 1.42        | 1.53     |
| 1   | J     | 258 | SER  | CA-C  | -8.37 | 1.42        | 1.53     |
| 1   | F     | 258 | SER  | CA-C  | -8.36 | 1.42        | 1.53     |
| 1   | L     | 258 | SER  | CA-C  | -8.36 | 1.42        | 1.53     |
| 1   | B     | 270 | ARG  | CA-C  | -8.33 | 1.42        | 1.52     |
| 1   | G     | 270 | ARG  | CA-C  | -8.30 | 1.42        | 1.52     |
| 1   | C     | 270 | ARG  | CA-C  | -8.29 | 1.42        | 1.52     |
| 1   | F     | 270 | ARG  | CA-C  | -8.29 | 1.42        | 1.52     |
| 1   | I     | 270 | ARG  | CA-C  | -8.29 | 1.42        | 1.52     |
| 1   | L     | 270 | ARG  | CA-C  | -8.29 | 1.42        | 1.52     |
| 1   | A     | 270 | ARG  | CA-C  | -8.27 | 1.42        | 1.52     |
| 1   | E     | 270 | ARG  | CA-C  | -8.27 | 1.42        | 1.52     |
| 1   | H     | 270 | ARG  | CA-C  | -8.27 | 1.42        | 1.52     |
| 1   | K     | 270 | ARG  | CA-C  | -8.27 | 1.42        | 1.52     |
| 1   | D     | 270 | ARG  | CA-C  | -8.23 | 1.42        | 1.52     |
| 1   | J     | 270 | ARG  | CA-C  | -8.23 | 1.42        | 1.52     |
| 1   | B     | 60  | ARG  | C-O   | 6.59  | 1.31        | 1.24     |
| 1   | H     | 60  | ARG  | C-O   | 6.54  | 1.31        | 1.24     |
| 1   | A     | 60  | ARG  | C-O   | 6.50  | 1.31        | 1.24     |
| 1   | G     | 60  | ARG  | C-O   | 6.50  | 1.31        | 1.24     |
| 1   | E     | 60  | ARG  | C-O   | 6.50  | 1.31        | 1.24     |
| 1   | K     | 60  | ARG  | C-O   | 6.50  | 1.31        | 1.24     |
| 1   | F     | 60  | ARG  | C-O   | 6.49  | 1.31        | 1.24     |
| 1   | L     | 60  | ARG  | C-O   | 6.49  | 1.31        | 1.24     |
| 1   | C     | 60  | ARG  | C-O   | 6.49  | 1.31        | 1.24     |
| 1   | I     | 60  | ARG  | C-O   | 6.49  | 1.31        | 1.24     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | D     | 60  | ARG  | C-O   | 6.47  | 1.31        | 1.24     |
| 1   | J     | 60  | ARG  | C-O   | 6.47  | 1.31        | 1.24     |
| 1   | F     | 257 | TRP  | CA-C  | -6.07 | 1.44        | 1.52     |
| 1   | L     | 257 | TRP  | CA-C  | -6.07 | 1.44        | 1.52     |
| 1   | D     | 257 | TRP  | CA-C  | -6.06 | 1.44        | 1.52     |
| 1   | J     | 257 | TRP  | CA-C  | -6.06 | 1.44        | 1.52     |
| 1   | E     | 257 | TRP  | CA-C  | -6.01 | 1.44        | 1.52     |
| 1   | K     | 257 | TRP  | CA-C  | -6.01 | 1.44        | 1.52     |
| 1   | B     | 257 | TRP  | CA-C  | -6.00 | 1.44        | 1.52     |
| 1   | H     | 257 | TRP  | CA-C  | -6.00 | 1.44        | 1.52     |
| 1   | A     | 257 | TRP  | CA-C  | -6.00 | 1.44        | 1.52     |
| 1   | C     | 257 | TRP  | CA-C  | -5.98 | 1.44        | 1.52     |
| 1   | I     | 257 | TRP  | CA-C  | -5.98 | 1.44        | 1.52     |
| 1   | G     | 257 | TRP  | CA-C  | -5.97 | 1.44        | 1.52     |
| 1   | B     | 83  | THR  | CA-C  | -5.21 | 1.46        | 1.52     |
| 1   | E     | 83  | THR  | CA-C  | -5.21 | 1.46        | 1.52     |
| 1   | K     | 83  | THR  | CA-C  | -5.21 | 1.46        | 1.52     |
| 1   | F     | 83  | THR  | CA-C  | -5.20 | 1.46        | 1.52     |
| 1   | L     | 83  | THR  | CA-C  | -5.20 | 1.46        | 1.52     |
| 1   | H     | 83  | THR  | CA-C  | -5.19 | 1.46        | 1.52     |
| 1   | A     | 83  | THR  | CA-C  | -5.19 | 1.46        | 1.52     |
| 1   | D     | 83  | THR  | CA-C  | -5.19 | 1.46        | 1.52     |
| 1   | G     | 83  | THR  | CA-C  | -5.19 | 1.46        | 1.52     |
| 1   | J     | 83  | THR  | CA-C  | -5.19 | 1.46        | 1.52     |
| 1   | C     | 83  | THR  | CA-C  | -5.16 | 1.46        | 1.52     |
| 1   | I     | 83  | THR  | CA-C  | -5.16 | 1.46        | 1.52     |
| 1   | D     | 55  | LEU  | C-O   | -5.10 | 1.18        | 1.24     |
| 1   | J     | 55  | LEU  | C-O   | -5.10 | 1.18        | 1.24     |
| 1   | H     | 55  | LEU  | C-O   | -5.09 | 1.18        | 1.24     |
| 1   | D     | 58  | GLU  | C-O   | -5.08 | 1.18        | 1.24     |
| 1   | G     | 58  | GLU  | C-O   | -5.08 | 1.18        | 1.24     |
| 1   | J     | 58  | GLU  | C-O   | -5.08 | 1.18        | 1.24     |
| 1   | C     | 259 | ALA  | CA-C  | -5.07 | 1.46        | 1.52     |
| 1   | I     | 259 | ALA  | CA-C  | -5.07 | 1.46        | 1.52     |
| 1   | C     | 58  | GLU  | C-O   | -5.07 | 1.18        | 1.24     |
| 1   | I     | 58  | GLU  | C-O   | -5.07 | 1.18        | 1.24     |
| 1   | A     | 259 | ALA  | CA-C  | -5.06 | 1.46        | 1.52     |
| 1   | E     | 55  | LEU  | C-O   | -5.06 | 1.18        | 1.24     |
| 1   | K     | 55  | LEU  | C-O   | -5.06 | 1.18        | 1.24     |
| 1   | F     | 373 | TYR  | CA-C  | -5.05 | 1.48        | 1.53     |
| 1   | L     | 373 | TYR  | CA-C  | -5.05 | 1.48        | 1.53     |
| 1   | D     | 373 | TYR  | CA-C  | -5.05 | 1.48        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | F     | 55  | LEU  | C-O   | -5.04 | 1.18        | 1.24     |
| 1   | L     | 55  | LEU  | C-O   | -5.04 | 1.18        | 1.24     |
| 1   | B     | 259 | ALA  | CA-C  | -5.04 | 1.46        | 1.52     |
| 1   | E     | 259 | ALA  | CA-C  | -5.04 | 1.46        | 1.52     |
| 1   | K     | 259 | ALA  | CA-C  | -5.04 | 1.46        | 1.52     |
| 1   | B     | 373 | TYR  | CA-C  | -5.04 | 1.48        | 1.53     |
| 1   | E     | 373 | TYR  | CA-C  | -5.04 | 1.48        | 1.53     |
| 1   | H     | 373 | TYR  | CA-C  | -5.04 | 1.48        | 1.53     |
| 1   | K     | 373 | TYR  | CA-C  | -5.04 | 1.48        | 1.53     |
| 1   | A     | 373 | TYR  | CA-C  | -5.04 | 1.48        | 1.53     |
| 1   | G     | 373 | TYR  | CA-C  | -5.04 | 1.48        | 1.53     |
| 1   | J     | 373 | TYR  | CA-C  | -5.04 | 1.48        | 1.53     |
| 1   | A     | 55  | LEU  | C-O   | -5.03 | 1.18        | 1.24     |
| 1   | H     | 259 | ALA  | CA-C  | -5.02 | 1.46        | 1.52     |
| 1   | A     | 58  | GLU  | C-O   | -5.02 | 1.18        | 1.24     |
| 1   | D     | 259 | ALA  | CA-C  | -5.02 | 1.46        | 1.52     |
| 1   | G     | 259 | ALA  | CA-C  | -5.02 | 1.46        | 1.52     |
| 1   | J     | 259 | ALA  | CA-C  | -5.02 | 1.46        | 1.52     |
| 1   | B     | 148 | ALA  | C-O   | 5.02  | 1.30        | 1.24     |
| 1   | B     | 58  | GLU  | C-O   | -5.01 | 1.18        | 1.24     |
| 1   | H     | 58  | GLU  | C-O   | -5.01 | 1.18        | 1.24     |
| 1   | F     | 259 | ALA  | CA-C  | -5.01 | 1.46        | 1.52     |
| 1   | L     | 259 | ALA  | CA-C  | -5.01 | 1.46        | 1.52     |
| 1   | B     | 55  | LEU  | C-O   | -5.01 | 1.18        | 1.24     |
| 1   | F     | 148 | ALA  | C-O   | 5.01  | 1.30        | 1.24     |
| 1   | L     | 148 | ALA  | C-O   | 5.01  | 1.30        | 1.24     |
| 1   | C     | 373 | TYR  | CA-C  | -5.00 | 1.48        | 1.53     |
| 1   | I     | 373 | TYR  | CA-C  | -5.00 | 1.48        | 1.53     |

All (814) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | P     | 143 | ILE  | N-CA-C | 12.26 | 123.10      | 110.72   |
| 2   | V     | 143 | ILE  | N-CA-C | 12.24 | 123.08      | 110.72   |
| 2   | R     | 143 | ILE  | N-CA-C | 12.24 | 123.08      | 110.72   |
| 2   | X     | 143 | ILE  | N-CA-C | 12.24 | 123.08      | 110.72   |
| 2   | Q     | 143 | ILE  | N-CA-C | 12.23 | 123.07      | 110.72   |
| 2   | W     | 143 | ILE  | N-CA-C | 12.23 | 123.07      | 110.72   |
| 2   | N     | 143 | ILE  | N-CA-C | 12.23 | 123.07      | 110.72   |
| 2   | S     | 143 | ILE  | N-CA-C | 12.22 | 123.07      | 110.72   |
| 2   | M     | 143 | ILE  | N-CA-C | 12.21 | 123.05      | 110.72   |
| 2   | T     | 143 | ILE  | N-CA-C | 12.20 | 123.04      | 110.72   |

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| Mol | Chain | Res | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 2   | O     | 143 | ILE  | N-CA-C | 12.19  | 123.03      | 110.72   |
| 2   | U     | 143 | ILE  | N-CA-C | 12.19  | 123.03      | 110.72   |
| 1   | E     | 63  | VAL  | N-CA-C | -10.86 | 100.33      | 110.53   |
| 1   | K     | 63  | VAL  | N-CA-C | -10.82 | 100.35      | 110.53   |
| 1   | B     | 63  | VAL  | N-CA-C | -10.82 | 100.36      | 110.53   |
| 1   | F     | 63  | VAL  | N-CA-C | -10.82 | 100.36      | 110.53   |
| 1   | L     | 63  | VAL  | N-CA-C | -10.82 | 100.36      | 110.53   |
| 1   | A     | 63  | VAL  | N-CA-C | -10.81 | 100.37      | 110.53   |
| 1   | C     | 63  | VAL  | N-CA-C | -10.81 | 100.37      | 110.53   |
| 1   | H     | 63  | VAL  | N-CA-C | -10.81 | 100.37      | 110.53   |
| 1   | I     | 63  | VAL  | N-CA-C | -10.81 | 100.37      | 110.53   |
| 1   | D     | 63  | VAL  | N-CA-C | -10.80 | 100.38      | 110.53   |
| 1   | G     | 63  | VAL  | N-CA-C | -10.80 | 100.38      | 110.53   |
| 1   | J     | 63  | VAL  | N-CA-C | -10.80 | 100.38      | 110.53   |
| 2   | R     | 144 | THR  | N-CA-C | 9.49   | 124.48      | 111.39   |
| 2   | X     | 144 | THR  | N-CA-C | 9.49   | 124.48      | 111.39   |
| 2   | N     | 144 | THR  | N-CA-C | 9.48   | 124.48      | 111.39   |
| 2   | M     | 144 | THR  | N-CA-C | 9.46   | 124.45      | 111.39   |
| 2   | S     | 144 | THR  | N-CA-C | 9.46   | 124.45      | 111.39   |
| 2   | O     | 144 | THR  | N-CA-C | 9.46   | 124.44      | 111.39   |
| 2   | U     | 144 | THR  | N-CA-C | 9.46   | 124.44      | 111.39   |
| 2   | P     | 144 | THR  | N-CA-C | 9.45   | 124.43      | 111.39   |
| 2   | Q     | 144 | THR  | N-CA-C | 9.45   | 124.43      | 111.39   |
| 2   | V     | 144 | THR  | N-CA-C | 9.45   | 124.43      | 111.39   |
| 2   | W     | 144 | THR  | N-CA-C | 9.45   | 124.43      | 111.39   |
| 2   | T     | 144 | THR  | N-CA-C | 9.44   | 124.41      | 111.39   |
| 1   | D     | 324 | SER  | N-CA-C | 9.05   | 121.23      | 111.36   |
| 1   | J     | 324 | SER  | N-CA-C | 9.05   | 121.23      | 111.36   |
| 1   | F     | 324 | SER  | N-CA-C | 9.04   | 121.21      | 111.36   |
| 1   | H     | 324 | SER  | N-CA-C | 9.04   | 121.21      | 111.36   |
| 1   | L     | 324 | SER  | N-CA-C | 9.04   | 121.21      | 111.36   |
| 1   | A     | 324 | SER  | N-CA-C | 9.01   | 121.18      | 111.36   |
| 1   | B     | 324 | SER  | N-CA-C | 9.01   | 121.18      | 111.36   |
| 1   | E     | 324 | SER  | N-CA-C | 9.01   | 121.18      | 111.36   |
| 1   | G     | 324 | SER  | N-CA-C | 9.01   | 121.18      | 111.36   |
| 1   | K     | 324 | SER  | N-CA-C | 9.01   | 121.18      | 111.36   |
| 1   | C     | 324 | SER  | N-CA-C | 9.00   | 121.17      | 111.36   |
| 1   | I     | 324 | SER  | N-CA-C | 9.00   | 121.17      | 111.36   |
| 2   | P     | 53  | LEU  | N-CA-C | 8.46   | 122.75      | 109.81   |
| 2   | V     | 53  | LEU  | N-CA-C | 8.46   | 122.75      | 109.81   |
| 2   | M     | 53  | LEU  | N-CA-C | 8.45   | 122.73      | 109.81   |
| 2   | S     | 53  | LEU  | N-CA-C | 8.45   | 122.73      | 109.81   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | T     | 53  | LEU  | N-CA-C | 8.45  | 122.73      | 109.81   |
| 2   | O     | 53  | LEU  | N-CA-C | 8.44  | 122.72      | 109.81   |
| 2   | U     | 53  | LEU  | N-CA-C | 8.44  | 122.72      | 109.81   |
| 2   | Q     | 53  | LEU  | N-CA-C | 8.44  | 122.72      | 109.81   |
| 2   | R     | 53  | LEU  | N-CA-C | 8.44  | 122.72      | 109.81   |
| 2   | W     | 53  | LEU  | N-CA-C | 8.44  | 122.72      | 109.81   |
| 2   | X     | 53  | LEU  | N-CA-C | 8.44  | 122.72      | 109.81   |
| 2   | N     | 53  | LEU  | N-CA-C | 8.43  | 122.70      | 109.81   |
| 1   | F     | 346 | GLN  | N-CA-C | 8.30  | 119.95      | 111.07   |
| 1   | L     | 346 | GLN  | N-CA-C | 8.30  | 119.95      | 111.07   |
| 1   | B     | 346 | GLN  | N-CA-C | 8.30  | 119.95      | 111.07   |
| 1   | D     | 346 | GLN  | N-CA-C | 8.29  | 119.94      | 111.07   |
| 1   | J     | 346 | GLN  | N-CA-C | 8.29  | 119.94      | 111.07   |
| 1   | E     | 346 | GLN  | N-CA-C | 8.27  | 119.92      | 111.07   |
| 1   | A     | 346 | GLN  | N-CA-C | 8.26  | 119.91      | 111.07   |
| 1   | G     | 346 | GLN  | N-CA-C | 8.26  | 119.91      | 111.07   |
| 1   | H     | 346 | GLN  | N-CA-C | 8.24  | 119.89      | 111.07   |
| 1   | C     | 346 | GLN  | N-CA-C | 8.23  | 119.88      | 111.07   |
| 1   | I     | 346 | GLN  | N-CA-C | 8.23  | 119.88      | 111.07   |
| 1   | K     | 346 | GLN  | N-CA-C | 8.21  | 119.86      | 111.07   |
| 1   | C     | 77  | ARG  | N-CA-C | -7.76 | 102.79      | 111.71   |
| 1   | I     | 77  | ARG  | N-CA-C | -7.76 | 102.79      | 111.71   |
| 1   | G     | 77  | ARG  | N-CA-C | -7.75 | 102.80      | 111.71   |
| 1   | E     | 77  | ARG  | N-CA-C | -7.74 | 102.81      | 111.71   |
| 1   | K     | 77  | ARG  | N-CA-C | -7.74 | 102.81      | 111.71   |
| 1   | B     | 77  | ARG  | N-CA-C | -7.74 | 102.81      | 111.71   |
| 1   | A     | 77  | ARG  | N-CA-C | -7.72 | 102.83      | 111.71   |
| 1   | F     | 77  | ARG  | N-CA-C | -7.71 | 102.85      | 111.71   |
| 1   | L     | 77  | ARG  | N-CA-C | -7.71 | 102.85      | 111.71   |
| 1   | D     | 77  | ARG  | N-CA-C | -7.70 | 102.85      | 111.71   |
| 1   | J     | 77  | ARG  | N-CA-C | -7.70 | 102.85      | 111.71   |
| 1   | H     | 77  | ARG  | N-CA-C | -7.68 | 102.88      | 111.71   |
| 1   | D     | 506 | PHE  | N-CA-C | 7.67  | 119.65      | 111.28   |
| 1   | J     | 506 | PHE  | N-CA-C | 7.67  | 119.65      | 111.28   |
| 1   | B     | 506 | PHE  | N-CA-C | 7.66  | 119.63      | 111.28   |
| 1   | A     | 506 | PHE  | N-CA-C | 7.66  | 119.63      | 111.28   |
| 1   | G     | 506 | PHE  | N-CA-C | 7.66  | 119.63      | 111.28   |
| 1   | C     | 506 | PHE  | N-CA-C | 7.65  | 119.62      | 111.28   |
| 1   | I     | 506 | PHE  | N-CA-C | 7.65  | 119.62      | 111.28   |
| 1   | F     | 506 | PHE  | N-CA-C | 7.64  | 119.61      | 111.28   |
| 1   | L     | 506 | PHE  | N-CA-C | 7.64  | 119.61      | 111.28   |
| 1   | H     | 506 | PHE  | N-CA-C | 7.64  | 119.61      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 432 | GLU  | N-CA-C | -7.63 | 102.96      | 111.28   |
| 1   | K     | 432 | GLU  | N-CA-C | -7.63 | 102.96      | 111.28   |
| 1   | E     | 506 | PHE  | N-CA-C | 7.63  | 119.59      | 111.28   |
| 1   | K     | 506 | PHE  | N-CA-C | 7.63  | 119.59      | 111.28   |
| 1   | G     | 432 | GLU  | N-CA-C | -7.62 | 102.97      | 111.28   |
| 1   | B     | 432 | GLU  | N-CA-C | -7.62 | 102.98      | 111.28   |
| 1   | C     | 432 | GLU  | N-CA-C | -7.61 | 102.99      | 111.28   |
| 1   | F     | 432 | GLU  | N-CA-C | -7.61 | 102.99      | 111.28   |
| 1   | I     | 432 | GLU  | N-CA-C | -7.61 | 102.99      | 111.28   |
| 1   | L     | 432 | GLU  | N-CA-C | -7.61 | 102.99      | 111.28   |
| 1   | J     | 432 | GLU  | N-CA-C | -7.60 | 103.00      | 111.28   |
| 1   | A     | 432 | GLU  | N-CA-C | -7.60 | 103.00      | 111.28   |
| 1   | D     | 432 | GLU  | N-CA-C | -7.57 | 103.03      | 111.28   |
| 1   | H     | 432 | GLU  | N-CA-C | -7.57 | 103.03      | 111.28   |
| 2   | P     | 22  | GLY  | N-CA-C | 7.44  | 122.30      | 112.77   |
| 2   | V     | 22  | GLY  | N-CA-C | 7.44  | 122.30      | 112.77   |
| 1   | F     | 54  | GLU  | N-CA-C | -7.43 | 103.18      | 111.28   |
| 1   | L     | 54  | GLU  | N-CA-C | -7.43 | 103.18      | 111.28   |
| 1   | A     | 54  | GLU  | N-CA-C | -7.43 | 103.19      | 111.28   |
| 1   | G     | 54  | GLU  | N-CA-C | -7.43 | 103.19      | 111.28   |
| 2   | T     | 22  | GLY  | N-CA-C | 7.42  | 122.27      | 112.77   |
| 1   | D     | 54  | GLU  | N-CA-C | -7.42 | 103.19      | 111.28   |
| 1   | J     | 54  | GLU  | N-CA-C | -7.42 | 103.19      | 111.28   |
| 1   | B     | 54  | GLU  | N-CA-C | -7.42 | 103.19      | 111.28   |
| 1   | C     | 54  | GLU  | N-CA-C | -7.42 | 103.19      | 111.28   |
| 1   | I     | 54  | GLU  | N-CA-C | -7.42 | 103.19      | 111.28   |
| 1   | H     | 54  | GLU  | N-CA-C | -7.41 | 103.20      | 111.28   |
| 2   | N     | 22  | GLY  | N-CA-C | 7.41  | 122.25      | 112.77   |
| 2   | M     | 22  | GLY  | N-CA-C | 7.40  | 122.25      | 112.77   |
| 1   | E     | 54  | GLU  | N-CA-C | -7.40 | 103.21      | 111.28   |
| 1   | K     | 54  | GLU  | N-CA-C | -7.40 | 103.21      | 111.28   |
| 2   | O     | 22  | GLY  | N-CA-C | 7.40  | 122.24      | 112.77   |
| 2   | U     | 22  | GLY  | N-CA-C | 7.40  | 122.24      | 112.77   |
| 2   | Q     | 22  | GLY  | N-CA-C | 7.39  | 122.23      | 112.77   |
| 2   | S     | 22  | GLY  | N-CA-C | 7.39  | 122.24      | 112.77   |
| 2   | W     | 22  | GLY  | N-CA-C | 7.39  | 122.23      | 112.77   |
| 2   | R     | 22  | GLY  | N-CA-C | 7.39  | 122.23      | 112.77   |
| 2   | X     | 22  | GLY  | N-CA-C | 7.39  | 122.23      | 112.77   |
| 1   | C     | 336 | GLY  | N-CA-C | -7.39 | 105.03      | 115.30   |
| 1   | I     | 336 | GLY  | N-CA-C | -7.39 | 105.03      | 115.30   |
| 1   | H     | 336 | GLY  | N-CA-C | -7.38 | 105.04      | 115.30   |
| 1   | B     | 336 | GLY  | N-CA-C | -7.37 | 105.05      | 115.30   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 336 | GLY  | N-CA-C | -7.37 | 105.05      | 115.30   |
| 1   | F     | 336 | GLY  | N-CA-C | -7.37 | 105.06      | 115.30   |
| 1   | L     | 336 | GLY  | N-CA-C | -7.37 | 105.06      | 115.30   |
| 1   | D     | 336 | GLY  | N-CA-C | -7.37 | 105.06      | 115.30   |
| 1   | J     | 336 | GLY  | N-CA-C | -7.37 | 105.06      | 115.30   |
| 1   | E     | 336 | GLY  | N-CA-C | -7.37 | 105.06      | 115.30   |
| 1   | K     | 336 | GLY  | N-CA-C | -7.37 | 105.06      | 115.30   |
| 1   | G     | 336 | GLY  | N-CA-C | -7.36 | 105.06      | 115.30   |
| 2   | T     | 7   | PRO  | CA-C-N | -7.27 | 112.27      | 119.76   |
| 2   | T     | 7   | PRO  | C-N-CA | -7.27 | 112.27      | 119.76   |
| 2   | S     | 7   | PRO  | CA-C-N | -7.24 | 112.31      | 119.76   |
| 2   | S     | 7   | PRO  | C-N-CA | -7.24 | 112.31      | 119.76   |
| 2   | P     | 7   | PRO  | CA-C-N | -7.23 | 112.31      | 119.76   |
| 2   | P     | 7   | PRO  | C-N-CA | -7.23 | 112.31      | 119.76   |
| 2   | V     | 7   | PRO  | CA-C-N | -7.23 | 112.31      | 119.76   |
| 2   | V     | 7   | PRO  | C-N-CA | -7.23 | 112.31      | 119.76   |
| 2   | M     | 7   | PRO  | CA-C-N | -7.21 | 112.34      | 119.76   |
| 2   | M     | 7   | PRO  | C-N-CA | -7.21 | 112.34      | 119.76   |
| 2   | Q     | 7   | PRO  | CA-C-N | -7.21 | 112.34      | 119.76   |
| 2   | Q     | 7   | PRO  | C-N-CA | -7.21 | 112.34      | 119.76   |
| 2   | W     | 7   | PRO  | CA-C-N | -7.21 | 112.34      | 119.76   |
| 2   | W     | 7   | PRO  | C-N-CA | -7.21 | 112.34      | 119.76   |
| 2   | R     | 7   | PRO  | CA-C-N | -7.20 | 112.35      | 119.76   |
| 2   | R     | 7   | PRO  | C-N-CA | -7.20 | 112.35      | 119.76   |
| 2   | X     | 7   | PRO  | CA-C-N | -7.20 | 112.35      | 119.76   |
| 2   | X     | 7   | PRO  | C-N-CA | -7.20 | 112.35      | 119.76   |
| 2   | N     | 7   | PRO  | CA-C-N | -7.18 | 112.37      | 119.76   |
| 2   | N     | 7   | PRO  | C-N-CA | -7.18 | 112.37      | 119.76   |
| 2   | O     | 7   | PRO  | CA-C-N | -7.18 | 112.37      | 119.76   |
| 2   | O     | 7   | PRO  | C-N-CA | -7.18 | 112.37      | 119.76   |
| 2   | U     | 7   | PRO  | CA-C-N | -7.18 | 112.37      | 119.76   |
| 2   | U     | 7   | PRO  | C-N-CA | -7.18 | 112.37      | 119.76   |
| 1   | C     | 289 | ILE  | N-CA-C | 6.94  | 117.72      | 110.72   |
| 1   | I     | 289 | ILE  | N-CA-C | 6.94  | 117.72      | 110.72   |
| 1   | E     | 289 | ILE  | N-CA-C | 6.93  | 117.72      | 110.72   |
| 1   | K     | 289 | ILE  | N-CA-C | 6.93  | 117.72      | 110.72   |
| 1   | F     | 378 | VAL  | N-CA-C | 6.93  | 117.69      | 110.62   |
| 1   | L     | 378 | VAL  | N-CA-C | 6.93  | 117.69      | 110.62   |
| 1   | H     | 289 | ILE  | N-CA-C | 6.93  | 117.72      | 110.72   |
| 1   | A     | 289 | ILE  | N-CA-C | 6.92  | 117.71      | 110.72   |
| 1   | F     | 289 | ILE  | N-CA-C | 6.91  | 117.70      | 110.72   |
| 1   | L     | 289 | ILE  | N-CA-C | 6.91  | 117.70      | 110.72   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 289 | ILE  | N-CA-C | 6.91  | 117.70      | 110.72   |
| 1   | D     | 289 | ILE  | N-CA-C | 6.91  | 117.70      | 110.72   |
| 1   | G     | 289 | ILE  | N-CA-C | 6.91  | 117.70      | 110.72   |
| 1   | J     | 289 | ILE  | N-CA-C | 6.91  | 117.70      | 110.72   |
| 1   | B     | 378 | VAL  | N-CA-C | 6.89  | 117.65      | 110.62   |
| 1   | E     | 378 | VAL  | N-CA-C | 6.89  | 117.65      | 110.62   |
| 1   | H     | 378 | VAL  | N-CA-C | 6.89  | 117.65      | 110.62   |
| 1   | K     | 378 | VAL  | N-CA-C | 6.89  | 117.65      | 110.62   |
| 2   | O     | 93  | ALA  | N-CA-C | 6.88  | 120.19      | 109.52   |
| 2   | U     | 93  | ALA  | N-CA-C | 6.88  | 120.19      | 109.52   |
| 1   | A     | 378 | VAL  | N-CA-C | 6.88  | 117.64      | 110.62   |
| 2   | N     | 93  | ALA  | N-CA-C | 6.88  | 120.18      | 109.52   |
| 1   | C     | 378 | VAL  | N-CA-C | 6.87  | 117.63      | 110.62   |
| 1   | I     | 378 | VAL  | N-CA-C | 6.87  | 117.63      | 110.62   |
| 1   | D     | 378 | VAL  | N-CA-C | 6.87  | 117.62      | 110.62   |
| 1   | G     | 378 | VAL  | N-CA-C | 6.87  | 117.62      | 110.62   |
| 1   | J     | 378 | VAL  | N-CA-C | 6.87  | 117.62      | 110.62   |
| 2   | M     | 93  | ALA  | N-CA-C | 6.86  | 120.16      | 109.52   |
| 2   | Q     | 93  | ALA  | N-CA-C | 6.86  | 120.15      | 109.52   |
| 2   | W     | 93  | ALA  | N-CA-C | 6.86  | 120.15      | 109.52   |
| 2   | P     | 93  | ALA  | N-CA-C | 6.85  | 120.14      | 109.52   |
| 2   | V     | 93  | ALA  | N-CA-C | 6.85  | 120.14      | 109.52   |
| 2   | T     | 93  | ALA  | N-CA-C | 6.85  | 120.14      | 109.52   |
| 2   | R     | 93  | ALA  | N-CA-C | 6.85  | 120.14      | 109.52   |
| 2   | X     | 93  | ALA  | N-CA-C | 6.85  | 120.14      | 109.52   |
| 2   | S     | 93  | ALA  | N-CA-C | 6.84  | 120.12      | 109.52   |
| 1   | D     | 339 | THR  | N-CA-C | -6.72 | 99.95       | 109.96   |
| 1   | J     | 339 | THR  | N-CA-C | -6.72 | 99.95       | 109.96   |
| 1   | F     | 339 | THR  | N-CA-C | -6.71 | 99.96       | 109.96   |
| 1   | L     | 339 | THR  | N-CA-C | -6.71 | 99.96       | 109.96   |
| 1   | A     | 339 | THR  | N-CA-C | -6.71 | 99.97       | 109.96   |
| 1   | G     | 339 | THR  | N-CA-C | -6.71 | 99.97       | 109.96   |
| 1   | E     | 339 | THR  | N-CA-C | -6.70 | 99.98       | 109.96   |
| 1   | K     | 339 | THR  | N-CA-C | -6.70 | 99.98       | 109.96   |
| 1   | H     | 339 | THR  | N-CA-C | -6.70 | 99.98       | 109.96   |
| 1   | C     | 339 | THR  | N-CA-C | -6.69 | 99.99       | 109.96   |
| 1   | I     | 339 | THR  | N-CA-C | -6.69 | 99.99       | 109.96   |
| 1   | B     | 339 | THR  | N-CA-C | -6.68 | 100.00      | 109.96   |
| 2   | Q     | 71  | PRO  | N-CA-C | 6.64  | 118.80      | 110.70   |
| 2   | W     | 71  | PRO  | N-CA-C | 6.64  | 118.80      | 110.70   |
| 2   | O     | 71  | PRO  | N-CA-C | 6.62  | 118.77      | 110.70   |
| 2   | U     | 71  | PRO  | N-CA-C | 6.62  | 118.77      | 110.70   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | S     | 71  | PRO  | N-CA-C | 6.61  | 118.77      | 110.70   |
| 2   | P     | 71  | PRO  | N-CA-C | 6.59  | 118.74      | 110.70   |
| 2   | V     | 71  | PRO  | N-CA-C | 6.59  | 118.74      | 110.70   |
| 2   | R     | 71  | PRO  | N-CA-C | 6.58  | 118.73      | 110.70   |
| 2   | X     | 71  | PRO  | N-CA-C | 6.58  | 118.73      | 110.70   |
| 2   | M     | 71  | PRO  | N-CA-C | 6.58  | 118.73      | 110.70   |
| 2   | N     | 71  | PRO  | N-CA-C | 6.58  | 118.73      | 110.70   |
| 1   | D     | 63  | VAL  | CA-C-N | -6.58 | 112.68      | 119.98   |
| 1   | D     | 63  | VAL  | C-N-CA | -6.58 | 112.68      | 119.98   |
| 2   | T     | 71  | PRO  | N-CA-C | 6.58  | 118.73      | 110.70   |
| 1   | J     | 63  | VAL  | CA-C-N | -6.58 | 112.68      | 119.98   |
| 1   | J     | 63  | VAL  | C-N-CA | -6.58 | 112.68      | 119.98   |
| 1   | H     | 63  | VAL  | CA-C-N | -6.56 | 112.70      | 119.98   |
| 1   | H     | 63  | VAL  | C-N-CA | -6.56 | 112.70      | 119.98   |
| 1   | A     | 63  | VAL  | CA-C-N | -6.55 | 112.70      | 119.98   |
| 1   | A     | 63  | VAL  | C-N-CA | -6.55 | 112.70      | 119.98   |
| 1   | F     | 63  | VAL  | CA-C-N | -6.55 | 112.71      | 119.98   |
| 1   | F     | 63  | VAL  | C-N-CA | -6.55 | 112.71      | 119.98   |
| 1   | L     | 63  | VAL  | CA-C-N | -6.55 | 112.71      | 119.98   |
| 1   | L     | 63  | VAL  | C-N-CA | -6.55 | 112.71      | 119.98   |
| 1   | B     | 63  | VAL  | CA-C-N | -6.53 | 112.73      | 119.98   |
| 1   | B     | 63  | VAL  | C-N-CA | -6.53 | 112.73      | 119.98   |
| 1   | G     | 63  | VAL  | CA-C-N | -6.53 | 112.73      | 119.98   |
| 1   | G     | 63  | VAL  | C-N-CA | -6.53 | 112.73      | 119.98   |
| 1   | C     | 63  | VAL  | CA-C-N | -6.53 | 112.73      | 119.98   |
| 1   | C     | 63  | VAL  | C-N-CA | -6.53 | 112.73      | 119.98   |
| 1   | I     | 63  | VAL  | CA-C-N | -6.53 | 112.73      | 119.98   |
| 1   | I     | 63  | VAL  | C-N-CA | -6.53 | 112.73      | 119.98   |
| 1   | E     | 63  | VAL  | CA-C-N | -6.52 | 112.74      | 119.98   |
| 1   | E     | 63  | VAL  | C-N-CA | -6.52 | 112.74      | 119.98   |
| 1   | F     | 284 | LEU  | N-CA-C | 6.52  | 124.20      | 113.89   |
| 1   | L     | 284 | LEU  | N-CA-C | 6.52  | 124.20      | 113.89   |
| 1   | H     | 284 | LEU  | N-CA-C | 6.52  | 124.19      | 113.89   |
| 1   | B     | 284 | LEU  | N-CA-C | 6.52  | 124.19      | 113.89   |
| 1   | C     | 284 | LEU  | N-CA-C | 6.51  | 124.18      | 113.89   |
| 1   | I     | 284 | LEU  | N-CA-C | 6.51  | 124.18      | 113.89   |
| 1   | K     | 63  | VAL  | CA-C-N | -6.51 | 112.75      | 119.98   |
| 1   | K     | 63  | VAL  | C-N-CA | -6.51 | 112.75      | 119.98   |
| 1   | A     | 284 | LEU  | N-CA-C | 6.51  | 124.17      | 113.89   |
| 1   | E     | 284 | LEU  | N-CA-C | 6.50  | 124.17      | 113.89   |
| 1   | K     | 284 | LEU  | N-CA-C | 6.50  | 124.17      | 113.89   |
| 1   | D     | 284 | LEU  | N-CA-C | 6.50  | 124.16      | 113.89   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | J     | 284 | LEU  | N-CA-C | 6.50 | 124.16      | 113.89   |
| 2   | N     | 106 | GLY  | N-CA-C | 6.49 | 120.22      | 111.72   |
| 2   | P     | 106 | GLY  | N-CA-C | 6.49 | 120.22      | 111.72   |
| 2   | V     | 106 | GLY  | N-CA-C | 6.49 | 120.22      | 111.72   |
| 1   | G     | 284 | LEU  | N-CA-C | 6.49 | 124.14      | 113.89   |
| 2   | W     | 106 | GLY  | N-CA-C | 6.48 | 120.21      | 111.72   |
| 2   | R     | 106 | GLY  | N-CA-C | 6.47 | 120.20      | 111.72   |
| 2   | X     | 106 | GLY  | N-CA-C | 6.47 | 120.20      | 111.72   |
| 2   | Q     | 106 | GLY  | N-CA-C | 6.47 | 120.20      | 111.72   |
| 2   | S     | 106 | GLY  | N-CA-C | 6.47 | 120.19      | 111.72   |
| 2   | O     | 106 | GLY  | N-CA-C | 6.47 | 120.19      | 111.72   |
| 2   | U     | 106 | GLY  | N-CA-C | 6.47 | 120.19      | 111.72   |
| 2   | M     | 106 | GLY  | N-CA-C | 6.46 | 120.18      | 111.72   |
| 1   | F     | 342 | GLU  | N-CA-C | 6.45 | 118.31      | 111.28   |
| 2   | T     | 106 | GLY  | N-CA-C | 6.45 | 120.17      | 111.72   |
| 1   | L     | 342 | GLU  | N-CA-C | 6.45 | 118.31      | 111.28   |
| 1   | B     | 342 | GLU  | N-CA-C | 6.44 | 118.30      | 111.28   |
| 1   | E     | 342 | GLU  | N-CA-C | 6.44 | 118.30      | 111.28   |
| 1   | K     | 342 | GLU  | N-CA-C | 6.44 | 118.30      | 111.28   |
| 1   | F     | 127 | SER  | N-CA-C | 6.44 | 122.30      | 113.16   |
| 1   | L     | 127 | SER  | N-CA-C | 6.44 | 122.30      | 113.16   |
| 1   | C     | 127 | SER  | N-CA-C | 6.43 | 122.28      | 113.16   |
| 1   | I     | 127 | SER  | N-CA-C | 6.43 | 122.28      | 113.16   |
| 1   | D     | 127 | SER  | N-CA-C | 6.42 | 122.28      | 113.16   |
| 1   | J     | 127 | SER  | N-CA-C | 6.42 | 122.28      | 113.16   |
| 1   | B     | 127 | SER  | N-CA-C | 6.42 | 122.28      | 113.16   |
| 1   | A     | 127 | SER  | N-CA-C | 6.42 | 122.27      | 113.16   |
| 1   | A     | 342 | GLU  | N-CA-C | 6.41 | 118.26      | 111.28   |
| 1   | H     | 127 | SER  | N-CA-C | 6.41 | 122.26      | 113.16   |
| 1   | E     | 127 | SER  | N-CA-C | 6.41 | 122.26      | 113.16   |
| 1   | K     | 127 | SER  | N-CA-C | 6.41 | 122.26      | 113.16   |
| 1   | C     | 342 | GLU  | N-CA-C | 6.40 | 118.25      | 111.28   |
| 1   | G     | 342 | GLU  | N-CA-C | 6.40 | 118.25      | 111.28   |
| 1   | I     | 342 | GLU  | N-CA-C | 6.40 | 118.25      | 111.28   |
| 1   | H     | 342 | GLU  | N-CA-C | 6.39 | 118.25      | 111.28   |
| 1   | D     | 342 | GLU  | N-CA-C | 6.39 | 118.24      | 111.28   |
| 1   | J     | 342 | GLU  | N-CA-C | 6.39 | 118.24      | 111.28   |
| 1   | G     | 127 | SER  | N-CA-C | 6.37 | 122.20      | 113.16   |
| 1   | C     | 456 | LEU  | N-CA-C | 6.30 | 118.14      | 111.28   |
| 1   | I     | 456 | LEU  | N-CA-C | 6.30 | 118.14      | 111.28   |
| 1   | B     | 456 | LEU  | N-CA-C | 6.29 | 118.13      | 111.28   |
| 1   | D     | 456 | LEU  | N-CA-C | 6.29 | 118.13      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | J     | 456 | LEU  | N-CA-C | 6.29  | 118.13      | 111.28   |
| 1   | E     | 456 | LEU  | N-CA-C | 6.29  | 118.13      | 111.28   |
| 1   | K     | 456 | LEU  | N-CA-C | 6.29  | 118.13      | 111.28   |
| 1   | G     | 456 | LEU  | N-CA-C | 6.28  | 118.13      | 111.28   |
| 1   | A     | 456 | LEU  | N-CA-C | 6.28  | 118.12      | 111.28   |
| 2   | O     | 145 | ARG  | N-CA-C | 6.27  | 124.16      | 110.80   |
| 2   | U     | 145 | ARG  | N-CA-C | 6.27  | 124.16      | 110.80   |
| 1   | H     | 456 | LEU  | N-CA-C | 6.27  | 118.11      | 111.28   |
| 1   | F     | 456 | LEU  | N-CA-C | 6.27  | 118.11      | 111.28   |
| 1   | G     | 146 | GLY  | N-CA-C | -6.27 | 105.21      | 112.73   |
| 1   | L     | 456 | LEU  | N-CA-C | 6.27  | 118.11      | 111.28   |
| 2   | N     | 145 | ARG  | N-CA-C | 6.27  | 124.15      | 110.80   |
| 2   | Q     | 145 | ARG  | N-CA-C | 6.27  | 124.15      | 110.80   |
| 2   | W     | 145 | ARG  | N-CA-C | 6.27  | 124.15      | 110.80   |
| 1   | E     | 146 | GLY  | N-CA-C | -6.25 | 105.22      | 112.73   |
| 2   | R     | 145 | ARG  | N-CA-C | 6.25  | 124.12      | 110.80   |
| 1   | K     | 146 | GLY  | N-CA-C | -6.25 | 105.22      | 112.73   |
| 2   | X     | 145 | ARG  | N-CA-C | 6.25  | 124.12      | 110.80   |
| 2   | M     | 145 | ARG  | N-CA-C | 6.25  | 124.12      | 110.80   |
| 2   | S     | 145 | ARG  | N-CA-C | 6.25  | 124.12      | 110.80   |
| 1   | D     | 146 | GLY  | N-CA-C | -6.25 | 105.24      | 112.73   |
| 1   | J     | 146 | GLY  | N-CA-C | -6.25 | 105.24      | 112.73   |
| 1   | A     | 146 | GLY  | N-CA-C | -6.23 | 105.25      | 112.73   |
| 1   | C     | 146 | GLY  | N-CA-C | -6.23 | 105.25      | 112.73   |
| 1   | I     | 146 | GLY  | N-CA-C | -6.23 | 105.25      | 112.73   |
| 2   | P     | 145 | ARG  | N-CA-C | 6.23  | 124.07      | 110.80   |
| 1   | F     | 146 | GLY  | N-CA-C | -6.23 | 105.25      | 112.73   |
| 2   | V     | 145 | ARG  | N-CA-C | 6.23  | 124.07      | 110.80   |
| 2   | T     | 145 | ARG  | N-CA-C | 6.23  | 124.07      | 110.80   |
| 1   | L     | 146 | GLY  | N-CA-C | -6.21 | 105.28      | 112.73   |
| 1   | B     | 146 | GLY  | N-CA-C | -6.21 | 105.28      | 112.73   |
| 1   | H     | 146 | GLY  | N-CA-C | -6.21 | 105.28      | 112.73   |
| 2   | P     | 102 | ASP  | CA-C-N | -6.05 | 114.00      | 120.47   |
| 2   | P     | 102 | ASP  | C-N-CA | -6.05 | 114.00      | 120.47   |
| 2   | R     | 102 | ASP  | CA-C-N | -6.05 | 114.00      | 120.47   |
| 2   | R     | 102 | ASP  | C-N-CA | -6.05 | 114.00      | 120.47   |
| 2   | V     | 102 | ASP  | CA-C-N | -6.05 | 114.00      | 120.47   |
| 2   | V     | 102 | ASP  | C-N-CA | -6.05 | 114.00      | 120.47   |
| 2   | X     | 102 | ASP  | CA-C-N | -6.05 | 114.00      | 120.47   |
| 2   | X     | 102 | ASP  | C-N-CA | -6.05 | 114.00      | 120.47   |
| 2   | T     | 108 | GLU  | N-CA-C | 6.02  | 118.30      | 108.55   |
| 2   | O     | 108 | GLU  | N-CA-C | 6.01  | 118.29      | 108.55   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | T     | 102 | ASP  | CA-C-N | -6.01 | 114.03      | 120.47   |
| 2   | T     | 102 | ASP  | C-N-CA | -6.01 | 114.03      | 120.47   |
| 2   | U     | 108 | GLU  | N-CA-C | 6.01  | 118.29      | 108.55   |
| 2   | S     | 108 | GLU  | N-CA-C | 6.01  | 118.28      | 108.55   |
| 2   | S     | 102 | ASP  | CA-C-N | -6.00 | 114.05      | 120.47   |
| 2   | S     | 102 | ASP  | C-N-CA | -6.00 | 114.05      | 120.47   |
| 2   | P     | 108 | GLU  | N-CA-C | 6.00  | 118.27      | 108.55   |
| 2   | V     | 108 | GLU  | N-CA-C | 6.00  | 118.27      | 108.55   |
| 2   | M     | 108 | GLU  | N-CA-C | 6.00  | 118.27      | 108.55   |
| 2   | Q     | 108 | GLU  | N-CA-C | 6.00  | 118.27      | 108.55   |
| 2   | W     | 108 | GLU  | N-CA-C | 6.00  | 118.27      | 108.55   |
| 2   | M     | 102 | ASP  | CA-C-N | -5.99 | 114.06      | 120.47   |
| 2   | M     | 102 | ASP  | C-N-CA | -5.99 | 114.06      | 120.47   |
| 2   | R     | 108 | GLU  | N-CA-C | 5.99  | 118.26      | 108.55   |
| 2   | X     | 108 | GLU  | N-CA-C | 5.99  | 118.26      | 108.55   |
| 2   | Q     | 102 | ASP  | CA-C-N | -5.99 | 114.06      | 120.47   |
| 2   | Q     | 102 | ASP  | C-N-CA | -5.99 | 114.06      | 120.47   |
| 2   | N     | 102 | ASP  | CA-C-N | -5.98 | 114.07      | 120.47   |
| 2   | N     | 102 | ASP  | C-N-CA | -5.98 | 114.07      | 120.47   |
| 2   | N     | 108 | GLU  | N-CA-C | 5.98  | 118.23      | 108.55   |
| 2   | W     | 102 | ASP  | CA-C-N | -5.97 | 114.08      | 120.47   |
| 2   | W     | 102 | ASP  | C-N-CA | -5.97 | 114.08      | 120.47   |
| 2   | P     | 55  | VAL  | N-CA-C | 5.97  | 116.71      | 110.62   |
| 2   | V     | 55  | VAL  | N-CA-C | 5.97  | 116.71      | 110.62   |
| 1   | E     | 450 | GLY  | N-CA-C | -5.97 | 106.71      | 115.30   |
| 1   | K     | 450 | GLY  | N-CA-C | -5.97 | 106.71      | 115.30   |
| 1   | A     | 450 | GLY  | N-CA-C | -5.96 | 106.71      | 115.30   |
| 1   | C     | 450 | GLY  | N-CA-C | -5.96 | 106.71      | 115.30   |
| 1   | G     | 450 | GLY  | N-CA-C | -5.96 | 106.71      | 115.30   |
| 1   | I     | 450 | GLY  | N-CA-C | -5.96 | 106.71      | 115.30   |
| 1   | B     | 450 | GLY  | N-CA-C | -5.96 | 106.71      | 115.30   |
| 1   | H     | 450 | GLY  | N-CA-C | -5.96 | 106.72      | 115.30   |
| 2   | S     | 55  | VAL  | N-CA-C | 5.95  | 116.69      | 110.62   |
| 2   | O     | 102 | ASP  | CA-C-N | -5.95 | 114.10      | 120.47   |
| 2   | O     | 102 | ASP  | C-N-CA | -5.95 | 114.10      | 120.47   |
| 2   | U     | 102 | ASP  | CA-C-N | -5.95 | 114.10      | 120.47   |
| 2   | U     | 102 | ASP  | C-N-CA | -5.95 | 114.10      | 120.47   |
| 1   | D     | 450 | GLY  | N-CA-C | -5.95 | 106.73      | 115.30   |
| 1   | F     | 450 | GLY  | N-CA-C | -5.95 | 106.73      | 115.30   |
| 2   | T     | 55  | VAL  | N-CA-C | 5.95  | 116.69      | 110.62   |
| 1   | J     | 450 | GLY  | N-CA-C | -5.95 | 106.73      | 115.30   |
| 2   | W     | 55  | VAL  | N-CA-C | 5.95  | 116.69      | 110.62   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | L     | 450 | GLY  | N-CA-C | -5.95 | 106.73      | 115.30   |
| 2   | X     | 55  | VAL  | N-CA-C | 5.95  | 116.69      | 110.62   |
| 2   | M     | 55  | VAL  | N-CA-C | 5.94  | 116.68      | 110.62   |
| 2   | O     | 55  | VAL  | N-CA-C | 5.94  | 116.68      | 110.62   |
| 2   | U     | 55  | VAL  | N-CA-C | 5.94  | 116.68      | 110.62   |
| 2   | Q     | 55  | VAL  | N-CA-C | 5.92  | 116.66      | 110.62   |
| 2   | N     | 55  | VAL  | N-CA-C | 5.92  | 116.66      | 110.62   |
| 1   | C     | 306 | ASN  | CA-C-N | -5.92 | 112.34      | 120.28   |
| 1   | C     | 306 | ASN  | C-N-CA | -5.92 | 112.34      | 120.28   |
| 1   | I     | 306 | ASN  | CA-C-N | -5.92 | 112.34      | 120.28   |
| 1   | I     | 306 | ASN  | C-N-CA | -5.92 | 112.34      | 120.28   |
| 2   | R     | 55  | VAL  | N-CA-C | 5.91  | 116.65      | 110.62   |
| 1   | F     | 306 | ASN  | CA-C-N | -5.91 | 112.36      | 120.28   |
| 1   | F     | 306 | ASN  | C-N-CA | -5.91 | 112.36      | 120.28   |
| 1   | L     | 306 | ASN  | CA-C-N | -5.91 | 112.36      | 120.28   |
| 1   | L     | 306 | ASN  | C-N-CA | -5.91 | 112.36      | 120.28   |
| 1   | H     | 306 | ASN  | CA-C-N | -5.90 | 112.38      | 120.28   |
| 1   | H     | 306 | ASN  | C-N-CA | -5.90 | 112.38      | 120.28   |
| 1   | A     | 306 | ASN  | CA-C-N | -5.90 | 112.38      | 120.28   |
| 1   | A     | 306 | ASN  | C-N-CA | -5.90 | 112.38      | 120.28   |
| 1   | G     | 306 | ASN  | CA-C-N | -5.90 | 112.38      | 120.28   |
| 1   | G     | 306 | ASN  | C-N-CA | -5.90 | 112.38      | 120.28   |
| 1   | E     | 306 | ASN  | CA-C-N | -5.89 | 112.38      | 120.28   |
| 1   | E     | 306 | ASN  | C-N-CA | -5.89 | 112.38      | 120.28   |
| 1   | K     | 306 | ASN  | CA-C-N | -5.89 | 112.38      | 120.28   |
| 1   | K     | 306 | ASN  | C-N-CA | -5.89 | 112.38      | 120.28   |
| 1   | D     | 306 | ASN  | CA-C-N | -5.89 | 112.39      | 120.28   |
| 1   | D     | 306 | ASN  | C-N-CA | -5.89 | 112.39      | 120.28   |
| 1   | J     | 306 | ASN  | CA-C-N | -5.89 | 112.39      | 120.28   |
| 1   | J     | 306 | ASN  | C-N-CA | -5.89 | 112.39      | 120.28   |
| 1   | C     | 457 | ALA  | N-CA-C | 5.88  | 117.69      | 111.28   |
| 1   | I     | 457 | ALA  | N-CA-C | 5.88  | 117.69      | 111.28   |
| 1   | B     | 306 | ASN  | CA-C-N | -5.88 | 112.40      | 120.28   |
| 1   | B     | 306 | ASN  | C-N-CA | -5.88 | 112.40      | 120.28   |
| 1   | E     | 72  | ASN  | N-CA-C | 5.88  | 120.73      | 113.50   |
| 1   | K     | 72  | ASN  | N-CA-C | 5.88  | 120.73      | 113.50   |
| 2   | M     | 137 | SER  | N-CA-C | 5.87  | 118.32      | 107.99   |
| 2   | P     | 137 | SER  | N-CA-C | 5.87  | 118.32      | 107.99   |
| 2   | V     | 137 | SER  | N-CA-C | 5.87  | 118.32      | 107.99   |
| 2   | O     | 137 | SER  | N-CA-C | 5.87  | 118.32      | 107.99   |
| 2   | R     | 137 | SER  | N-CA-C | 5.87  | 118.32      | 107.99   |
| 1   | G     | 218 | GLU  | CA-C-N | -5.87 | 113.92      | 120.14   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 218 | GLU  | C-N-CA | -5.87 | 113.92      | 120.14   |
| 2   | U     | 137 | SER  | N-CA-C | 5.87  | 118.32      | 107.99   |
| 2   | W     | 137 | SER  | N-CA-C | 5.87  | 118.32      | 107.99   |
| 2   | X     | 137 | SER  | N-CA-C | 5.87  | 118.32      | 107.99   |
| 2   | N     | 137 | SER  | N-CA-C | 5.87  | 118.31      | 107.99   |
| 2   | Q     | 137 | SER  | N-CA-C | 5.87  | 118.31      | 107.99   |
| 1   | H     | 218 | GLU  | CA-C-N | -5.87 | 113.92      | 120.14   |
| 1   | H     | 218 | GLU  | C-N-CA | -5.87 | 113.92      | 120.14   |
| 2   | T     | 137 | SER  | N-CA-C | 5.87  | 118.31      | 107.99   |
| 1   | C     | 72  | ASN  | N-CA-C | 5.86  | 120.71      | 113.50   |
| 1   | F     | 72  | ASN  | N-CA-C | 5.86  | 120.71      | 113.50   |
| 1   | I     | 72  | ASN  | N-CA-C | 5.86  | 120.71      | 113.50   |
| 1   | L     | 72  | ASN  | N-CA-C | 5.86  | 120.71      | 113.50   |
| 1   | G     | 72  | ASN  | N-CA-C | 5.86  | 120.70      | 113.50   |
| 2   | S     | 137 | SER  | N-CA-C | 5.85  | 118.29      | 107.99   |
| 1   | B     | 72  | ASN  | N-CA-C | 5.85  | 120.70      | 113.50   |
| 1   | G     | 457 | ALA  | N-CA-C | 5.85  | 117.65      | 111.28   |
| 1   | C     | 218 | GLU  | CA-C-N | -5.84 | 113.95      | 120.14   |
| 1   | C     | 218 | GLU  | C-N-CA | -5.84 | 113.95      | 120.14   |
| 1   | F     | 218 | GLU  | CA-C-N | -5.84 | 113.95      | 120.14   |
| 1   | F     | 218 | GLU  | C-N-CA | -5.84 | 113.95      | 120.14   |
| 1   | I     | 218 | GLU  | CA-C-N | -5.84 | 113.95      | 120.14   |
| 1   | I     | 218 | GLU  | C-N-CA | -5.84 | 113.95      | 120.14   |
| 1   | L     | 218 | GLU  | CA-C-N | -5.84 | 113.95      | 120.14   |
| 1   | L     | 218 | GLU  | C-N-CA | -5.84 | 113.95      | 120.14   |
| 1   | A     | 72  | ASN  | N-CA-C | 5.84  | 120.68      | 113.50   |
| 1   | D     | 218 | GLU  | CA-C-N | -5.84 | 113.95      | 120.14   |
| 1   | D     | 218 | GLU  | C-N-CA | -5.84 | 113.95      | 120.14   |
| 1   | J     | 218 | GLU  | CA-C-N | -5.84 | 113.95      | 120.14   |
| 1   | J     | 218 | GLU  | C-N-CA | -5.84 | 113.95      | 120.14   |
| 1   | A     | 218 | GLU  | CA-C-N | -5.83 | 113.96      | 120.14   |
| 1   | A     | 218 | GLU  | C-N-CA | -5.83 | 113.96      | 120.14   |
| 1   | D     | 72  | ASN  | N-CA-C | 5.83  | 120.67      | 113.50   |
| 1   | H     | 457 | ALA  | N-CA-C | 5.83  | 117.64      | 111.28   |
| 1   | J     | 72  | ASN  | N-CA-C | 5.83  | 120.67      | 113.50   |
| 1   | E     | 218 | GLU  | CA-C-N | -5.83 | 113.96      | 120.14   |
| 1   | E     | 218 | GLU  | C-N-CA | -5.83 | 113.96      | 120.14   |
| 1   | K     | 218 | GLU  | CA-C-N | -5.83 | 113.96      | 120.14   |
| 1   | K     | 218 | GLU  | C-N-CA | -5.83 | 113.96      | 120.14   |
| 1   | B     | 218 | GLU  | CA-C-N | -5.82 | 113.97      | 120.14   |
| 1   | B     | 218 | GLU  | C-N-CA | -5.82 | 113.97      | 120.14   |
| 1   | E     | 457 | ALA  | N-CA-C | 5.82  | 117.63      | 111.28   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | K     | 457 | ALA  | N-CA-C | 5.82  | 117.63      | 111.28   |
| 1   | A     | 457 | ALA  | N-CA-C | 5.82  | 117.62      | 111.28   |
| 1   | D     | 457 | ALA  | N-CA-C | 5.82  | 117.62      | 111.28   |
| 1   | J     | 457 | ALA  | N-CA-C | 5.82  | 117.62      | 111.28   |
| 1   | F     | 457 | ALA  | N-CA-C | 5.81  | 117.62      | 111.28   |
| 1   | L     | 457 | ALA  | N-CA-C | 5.81  | 117.62      | 111.28   |
| 1   | H     | 72  | ASN  | N-CA-C | 5.80  | 120.64      | 113.50   |
| 1   | B     | 457 | ALA  | N-CA-C | 5.79  | 117.60      | 111.28   |
| 2   | P     | 89  | ARG  | N-CA-C | -5.77 | 100.58      | 109.52   |
| 2   | R     | 89  | ARG  | N-CA-C | -5.77 | 100.58      | 109.52   |
| 2   | V     | 89  | ARG  | N-CA-C | -5.77 | 100.58      | 109.52   |
| 2   | X     | 89  | ARG  | N-CA-C | -5.77 | 100.58      | 109.52   |
| 2   | N     | 89  | ARG  | N-CA-C | -5.76 | 100.58      | 109.52   |
| 2   | T     | 89  | ARG  | N-CA-C | -5.76 | 100.58      | 109.52   |
| 2   | O     | 89  | ARG  | N-CA-C | -5.76 | 100.59      | 109.52   |
| 2   | U     | 89  | ARG  | N-CA-C | -5.76 | 100.59      | 109.52   |
| 2   | M     | 89  | ARG  | N-CA-C | -5.76 | 100.59      | 109.52   |
| 2   | S     | 89  | ARG  | N-CA-C | -5.76 | 100.59      | 109.52   |
| 2   | Q     | 89  | ARG  | N-CA-C | -5.74 | 100.62      | 109.52   |
| 2   | W     | 89  | ARG  | N-CA-C | -5.74 | 100.62      | 109.52   |
| 1   | B     | 143 | VAL  | N-CA-C | -5.72 | 104.79      | 110.62   |
| 1   | E     | 143 | VAL  | N-CA-C | -5.68 | 104.83      | 110.62   |
| 1   | K     | 143 | VAL  | N-CA-C | -5.68 | 104.83      | 110.62   |
| 2   | O     | 105 | ALA  | N-CA-C | 5.67  | 116.88      | 108.60   |
| 1   | D     | 143 | VAL  | N-CA-C | -5.67 | 104.83      | 110.62   |
| 2   | U     | 105 | ALA  | N-CA-C | 5.67  | 116.88      | 108.60   |
| 1   | J     | 143 | VAL  | N-CA-C | -5.67 | 104.83      | 110.62   |
| 1   | A     | 143 | VAL  | N-CA-C | -5.67 | 104.84      | 110.62   |
| 2   | N     | 105 | ALA  | N-CA-C | 5.66  | 116.87      | 108.60   |
| 1   | F     | 143 | VAL  | N-CA-C | -5.66 | 104.84      | 110.62   |
| 1   | L     | 143 | VAL  | N-CA-C | -5.66 | 104.84      | 110.62   |
| 1   | C     | 143 | VAL  | N-CA-C | -5.66 | 104.85      | 110.62   |
| 1   | I     | 143 | VAL  | N-CA-C | -5.66 | 104.85      | 110.62   |
| 2   | T     | 105 | ALA  | N-CA-C | 5.65  | 116.85      | 108.60   |
| 1   | G     | 144 | ALA  | N-CA-C | 5.65  | 117.44      | 111.28   |
| 1   | B     | 144 | ALA  | N-CA-C | 5.65  | 117.44      | 111.28   |
| 1   | H     | 144 | ALA  | N-CA-C | 5.65  | 117.44      | 111.28   |
| 2   | Q     | 105 | ALA  | N-CA-C | 5.65  | 116.84      | 108.60   |
| 2   | M     | 105 | ALA  | N-CA-C | 5.64  | 116.84      | 108.60   |
| 2   | S     | 105 | ALA  | N-CA-C | 5.64  | 116.84      | 108.60   |
| 1   | G     | 143 | VAL  | N-CA-C | -5.64 | 104.86      | 110.62   |
| 2   | W     | 105 | ALA  | N-CA-C | 5.64  | 116.84      | 108.60   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | R     | 105 | ALA  | N-CA-C | 5.64  | 116.83      | 108.60   |
| 2   | X     | 105 | ALA  | N-CA-C | 5.64  | 116.83      | 108.60   |
| 1   | B     | 70  | ALA  | N-CA-C | -5.64 | 105.14      | 111.28   |
| 2   | P     | 105 | ALA  | N-CA-C | 5.63  | 116.83      | 108.60   |
| 2   | V     | 105 | ALA  | N-CA-C | 5.63  | 116.83      | 108.60   |
| 1   | D     | 144 | ALA  | N-CA-C | 5.63  | 117.42      | 111.28   |
| 1   | J     | 144 | ALA  | N-CA-C | 5.63  | 117.42      | 111.28   |
| 1   | H     | 143 | VAL  | N-CA-C | -5.63 | 104.88      | 110.62   |
| 1   | A     | 144 | ALA  | N-CA-C | 5.62  | 117.41      | 111.28   |
| 1   | C     | 144 | ALA  | N-CA-C | 5.62  | 117.41      | 111.28   |
| 1   | I     | 144 | ALA  | N-CA-C | 5.62  | 117.41      | 111.28   |
| 1   | G     | 70  | ALA  | N-CA-C | -5.62 | 105.16      | 111.28   |
| 1   | A     | 70  | ALA  | N-CA-C | -5.61 | 105.17      | 111.28   |
| 1   | C     | 70  | ALA  | N-CA-C | -5.60 | 105.17      | 111.28   |
| 1   | I     | 70  | ALA  | N-CA-C | -5.60 | 105.17      | 111.28   |
| 1   | E     | 144 | ALA  | N-CA-C | 5.60  | 117.39      | 111.28   |
| 1   | F     | 144 | ALA  | N-CA-C | 5.60  | 117.39      | 111.28   |
| 1   | K     | 144 | ALA  | N-CA-C | 5.60  | 117.39      | 111.28   |
| 1   | L     | 144 | ALA  | N-CA-C | 5.60  | 117.39      | 111.28   |
| 1   | D     | 70  | ALA  | N-CA-C | -5.59 | 105.18      | 111.28   |
| 1   | F     | 70  | ALA  | N-CA-C | -5.59 | 105.18      | 111.28   |
| 1   | J     | 70  | ALA  | N-CA-C | -5.59 | 105.18      | 111.28   |
| 1   | L     | 70  | ALA  | N-CA-C | -5.59 | 105.18      | 111.28   |
| 1   | A     | 274 | ARG  | N-CA-C | -5.59 | 101.57      | 109.96   |
| 1   | D     | 274 | ARG  | N-CA-C | -5.59 | 101.57      | 109.96   |
| 1   | H     | 70  | ALA  | N-CA-C | -5.59 | 105.19      | 111.28   |
| 1   | J     | 274 | ARG  | N-CA-C | -5.59 | 101.57      | 109.96   |
| 1   | C     | 274 | ARG  | N-CA-C | -5.59 | 101.58      | 109.96   |
| 1   | I     | 274 | ARG  | N-CA-C | -5.59 | 101.58      | 109.96   |
| 1   | B     | 306 | ASN  | N-CA-C | -5.58 | 105.09      | 111.07   |
| 1   | E     | 71  | GLN  | N-CA-C | 5.58  | 117.44      | 111.36   |
| 1   | K     | 71  | GLN  | N-CA-C | 5.58  | 117.44      | 111.36   |
| 1   | E     | 70  | ALA  | N-CA-C | -5.58 | 105.19      | 111.28   |
| 1   | K     | 70  | ALA  | N-CA-C | -5.58 | 105.19      | 111.28   |
| 1   | G     | 274 | ARG  | N-CA-C | -5.58 | 101.59      | 109.96   |
| 1   | E     | 274 | ARG  | N-CA-C | -5.58 | 101.59      | 109.96   |
| 1   | F     | 443 | LEU  | CA-C-N | -5.58 | 112.86      | 119.05   |
| 1   | F     | 443 | LEU  | C-N-CA | -5.58 | 112.86      | 119.05   |
| 1   | K     | 274 | ARG  | N-CA-C | -5.58 | 101.59      | 109.96   |
| 1   | L     | 443 | LEU  | CA-C-N | -5.58 | 112.86      | 119.05   |
| 1   | L     | 443 | LEU  | C-N-CA | -5.58 | 112.86      | 119.05   |
| 1   | E     | 429 | ALA  | N-CA-C | 5.58  | 117.44      | 111.36   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 274 | ARG  | N-CA-C | -5.58 | 101.60      | 109.96   |
| 1   | G     | 71  | GLN  | N-CA-C | 5.58  | 117.44      | 111.36   |
| 1   | K     | 429 | ALA  | N-CA-C | 5.58  | 117.44      | 111.36   |
| 1   | L     | 274 | ARG  | N-CA-C | -5.58 | 101.60      | 109.96   |
| 1   | B     | 274 | ARG  | N-CA-C | -5.57 | 101.60      | 109.96   |
| 1   | H     | 274 | ARG  | N-CA-C | -5.57 | 101.60      | 109.96   |
| 1   | C     | 71  | GLN  | N-CA-C | 5.57  | 117.43      | 111.36   |
| 1   | I     | 71  | GLN  | N-CA-C | 5.57  | 117.43      | 111.36   |
| 1   | J     | 443 | LEU  | CA-C-N | -5.56 | 112.88      | 119.05   |
| 1   | J     | 443 | LEU  | C-N-CA | -5.56 | 112.88      | 119.05   |
| 1   | G     | 429 | ALA  | N-CA-C | 5.56  | 117.42      | 111.36   |
| 1   | C     | 443 | LEU  | CA-C-N | -5.56 | 112.88      | 119.05   |
| 1   | C     | 443 | LEU  | C-N-CA | -5.56 | 112.88      | 119.05   |
| 1   | I     | 443 | LEU  | CA-C-N | -5.56 | 112.88      | 119.05   |
| 1   | I     | 443 | LEU  | C-N-CA | -5.56 | 112.88      | 119.05   |
| 1   | G     | 306 | ASN  | N-CA-C | -5.55 | 105.13      | 111.07   |
| 1   | A     | 429 | ALA  | N-CA-C | 5.55  | 117.41      | 111.36   |
| 1   | C     | 429 | ALA  | N-CA-C | 5.55  | 117.41      | 111.36   |
| 1   | I     | 429 | ALA  | N-CA-C | 5.55  | 117.41      | 111.36   |
| 1   | B     | 429 | ALA  | N-CA-C | 5.55  | 117.41      | 111.36   |
| 1   | F     | 429 | ALA  | N-CA-C | 5.55  | 117.41      | 111.36   |
| 1   | H     | 429 | ALA  | N-CA-C | 5.55  | 117.41      | 111.36   |
| 1   | L     | 429 | ALA  | N-CA-C | 5.55  | 117.41      | 111.36   |
| 1   | B     | 71  | GLN  | N-CA-C | 5.54  | 117.40      | 111.36   |
| 1   | F     | 306 | ASN  | N-CA-C | -5.54 | 105.14      | 111.07   |
| 1   | L     | 306 | ASN  | N-CA-C | -5.54 | 105.14      | 111.07   |
| 1   | A     | 71  | GLN  | N-CA-C | 5.54  | 117.40      | 111.36   |
| 1   | A     | 443 | LEU  | CA-C-N | -5.54 | 112.90      | 119.05   |
| 1   | A     | 443 | LEU  | C-N-CA | -5.54 | 112.90      | 119.05   |
| 1   | D     | 429 | ALA  | N-CA-C | 5.53  | 117.39      | 111.36   |
| 1   | J     | 429 | ALA  | N-CA-C | 5.53  | 117.39      | 111.36   |
| 1   | A     | 306 | ASN  | N-CA-C | -5.53 | 105.16      | 111.07   |
| 1   | B     | 443 | LEU  | CA-C-N | -5.53 | 112.91      | 119.05   |
| 1   | B     | 443 | LEU  | C-N-CA | -5.53 | 112.91      | 119.05   |
| 1   | D     | 71  | GLN  | N-CA-C | 5.53  | 117.39      | 111.36   |
| 1   | E     | 306 | ASN  | N-CA-C | -5.53 | 105.16      | 111.07   |
| 1   | E     | 443 | LEU  | CA-C-N | -5.53 | 112.91      | 119.05   |
| 1   | E     | 443 | LEU  | C-N-CA | -5.53 | 112.91      | 119.05   |
| 1   | H     | 306 | ASN  | N-CA-C | -5.53 | 105.16      | 111.07   |
| 1   | J     | 71  | GLN  | N-CA-C | 5.53  | 117.39      | 111.36   |
| 1   | K     | 306 | ASN  | N-CA-C | -5.53 | 105.16      | 111.07   |
| 1   | K     | 443 | LEU  | CA-C-N | -5.53 | 112.91      | 119.05   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | K     | 443 | LEU  | C-N-CA | -5.53 | 112.91      | 119.05   |
| 1   | F     | 71  | GLN  | N-CA-C | 5.53  | 117.38      | 111.36   |
| 1   | H     | 71  | GLN  | N-CA-C | 5.53  | 117.38      | 111.36   |
| 1   | L     | 71  | GLN  | N-CA-C | 5.53  | 117.38      | 111.36   |
| 2   | W     | 169 | SER  | N-CA-C | 5.52  | 122.01      | 109.81   |
| 2   | O     | 169 | SER  | N-CA-C | 5.52  | 122.00      | 109.81   |
| 2   | T     | 169 | SER  | N-CA-C | 5.52  | 122.00      | 109.81   |
| 2   | U     | 169 | SER  | N-CA-C | 5.52  | 122.00      | 109.81   |
| 1   | D     | 443 | LEU  | CA-C-N | -5.51 | 112.93      | 119.05   |
| 1   | D     | 443 | LEU  | C-N-CA | -5.51 | 112.93      | 119.05   |
| 1   | G     | 443 | LEU  | CA-C-N | -5.51 | 112.93      | 119.05   |
| 1   | G     | 443 | LEU  | C-N-CA | -5.51 | 112.93      | 119.05   |
| 1   | D     | 306 | ASN  | N-CA-C | -5.51 | 105.17      | 111.07   |
| 1   | J     | 306 | ASN  | N-CA-C | -5.51 | 105.17      | 111.07   |
| 2   | M     | 169 | SER  | N-CA-C | 5.51  | 121.99      | 109.81   |
| 2   | N     | 169 | SER  | N-CA-C | 5.51  | 121.99      | 109.81   |
| 2   | Q     | 169 | SER  | N-CA-C | 5.51  | 121.98      | 109.81   |
| 2   | P     | 169 | SER  | N-CA-C | 5.51  | 121.98      | 109.81   |
| 2   | R     | 169 | SER  | N-CA-C | 5.51  | 121.98      | 109.81   |
| 2   | S     | 169 | SER  | N-CA-C | 5.51  | 121.98      | 109.81   |
| 1   | H     | 443 | LEU  | CA-C-N | -5.51 | 112.94      | 119.05   |
| 1   | H     | 443 | LEU  | C-N-CA | -5.51 | 112.94      | 119.05   |
| 2   | V     | 169 | SER  | N-CA-C | 5.51  | 121.98      | 109.81   |
| 2   | X     | 169 | SER  | N-CA-C | 5.51  | 121.98      | 109.81   |
| 1   | C     | 306 | ASN  | N-CA-C | -5.50 | 105.18      | 111.07   |
| 1   | I     | 306 | ASN  | N-CA-C | -5.50 | 105.18      | 111.07   |
| 2   | R     | 169 | SER  | CA-C-N | -5.41 | 114.38      | 119.90   |
| 2   | R     | 169 | SER  | C-N-CA | -5.41 | 114.38      | 119.90   |
| 2   | X     | 169 | SER  | CA-C-N | -5.41 | 114.38      | 119.90   |
| 2   | X     | 169 | SER  | C-N-CA | -5.41 | 114.38      | 119.90   |
| 1   | E     | 475 | VAL  | N-CA-C | 5.41  | 116.18      | 110.72   |
| 1   | K     | 475 | VAL  | N-CA-C | 5.41  | 116.18      | 110.72   |
| 1   | C     | 475 | VAL  | N-CA-C | 5.40  | 116.17      | 110.72   |
| 1   | I     | 475 | VAL  | N-CA-C | 5.40  | 116.17      | 110.72   |
| 2   | N     | 169 | SER  | CA-C-N | -5.40 | 114.39      | 119.90   |
| 2   | N     | 169 | SER  | C-N-CA | -5.40 | 114.39      | 119.90   |
| 2   | T     | 169 | SER  | CA-C-N | -5.40 | 114.39      | 119.90   |
| 2   | T     | 169 | SER  | C-N-CA | -5.40 | 114.39      | 119.90   |
| 1   | A     | 475 | VAL  | N-CA-C | 5.39  | 116.16      | 110.72   |
| 2   | O     | 169 | SER  | CA-C-N | -5.38 | 114.41      | 119.90   |
| 2   | O     | 169 | SER  | C-N-CA | -5.38 | 114.41      | 119.90   |
| 2   | U     | 169 | SER  | CA-C-N | -5.38 | 114.41      | 119.90   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | U     | 169 | SER  | C-N-CA | -5.38 | 114.41      | 119.90   |
| 2   | Q     | 169 | SER  | CA-C-N | -5.38 | 114.41      | 119.90   |
| 2   | Q     | 169 | SER  | C-N-CA | -5.38 | 114.41      | 119.90   |
| 2   | W     | 169 | SER  | CA-C-N | -5.38 | 114.41      | 119.90   |
| 2   | W     | 169 | SER  | C-N-CA | -5.38 | 114.41      | 119.90   |
| 1   | D     | 475 | VAL  | N-CA-C | 5.37  | 116.15      | 110.72   |
| 1   | J     | 475 | VAL  | N-CA-C | 5.37  | 116.15      | 110.72   |
| 1   | G     | 475 | VAL  | N-CA-C | 5.37  | 116.14      | 110.72   |
| 2   | M     | 169 | SER  | CA-C-N | -5.37 | 114.43      | 119.90   |
| 2   | M     | 169 | SER  | C-N-CA | -5.37 | 114.43      | 119.90   |
| 2   | P     | 169 | SER  | CA-C-N | -5.37 | 114.43      | 119.90   |
| 2   | P     | 169 | SER  | C-N-CA | -5.37 | 114.43      | 119.90   |
| 1   | H     | 475 | VAL  | N-CA-C | 5.37  | 116.14      | 110.72   |
| 2   | V     | 169 | SER  | CA-C-N | -5.37 | 114.43      | 119.90   |
| 2   | V     | 169 | SER  | C-N-CA | -5.37 | 114.43      | 119.90   |
| 1   | B     | 475 | VAL  | N-CA-C | 5.36  | 116.14      | 110.72   |
| 1   | F     | 475 | VAL  | N-CA-C | 5.36  | 116.13      | 110.72   |
| 1   | L     | 475 | VAL  | N-CA-C | 5.36  | 116.13      | 110.72   |
| 1   | B     | 349 | ILE  | N-CA-C | 5.36  | 117.34      | 109.63   |
| 2   | S     | 169 | SER  | CA-C-N | -5.35 | 114.44      | 119.90   |
| 2   | S     | 169 | SER  | C-N-CA | -5.35 | 114.44      | 119.90   |
| 1   | C     | 349 | ILE  | N-CA-C | 5.35  | 117.33      | 109.63   |
| 1   | I     | 349 | ILE  | N-CA-C | 5.35  | 117.33      | 109.63   |
| 1   | A     | 349 | ILE  | N-CA-C | 5.34  | 117.32      | 109.63   |
| 1   | E     | 349 | ILE  | N-CA-C | 5.33  | 117.31      | 109.63   |
| 1   | K     | 349 | ILE  | N-CA-C | 5.33  | 117.31      | 109.63   |
| 1   | D     | 349 | ILE  | N-CA-C | 5.33  | 117.30      | 109.63   |
| 1   | J     | 349 | ILE  | N-CA-C | 5.33  | 117.30      | 109.63   |
| 1   | G     | 349 | ILE  | N-CA-C | 5.33  | 117.30      | 109.63   |
| 1   | H     | 349 | ILE  | N-CA-C | 5.33  | 117.30      | 109.63   |
| 1   | F     | 349 | ILE  | N-CA-C | 5.32  | 117.29      | 109.63   |
| 1   | L     | 349 | ILE  | N-CA-C | 5.32  | 117.29      | 109.63   |
| 1   | G     | 314 | SER  | N-CA-C | 5.29  | 116.86      | 111.14   |
| 1   | A     | 314 | SER  | N-CA-C | 5.29  | 116.85      | 111.14   |
| 1   | B     | 314 | SER  | N-CA-C | 5.29  | 116.85      | 111.14   |
| 1   | F     | 314 | SER  | N-CA-C | 5.29  | 116.85      | 111.14   |
| 1   | L     | 314 | SER  | N-CA-C | 5.29  | 116.85      | 111.14   |
| 1   | C     | 314 | SER  | N-CA-C | 5.29  | 116.85      | 111.14   |
| 1   | I     | 314 | SER  | N-CA-C | 5.29  | 116.85      | 111.14   |
| 1   | H     | 314 | SER  | N-CA-C | 5.27  | 116.83      | 111.14   |
| 1   | E     | 314 | SER  | N-CA-C | 5.27  | 116.83      | 111.14   |
| 1   | K     | 314 | SER  | N-CA-C | 5.27  | 116.83      | 111.14   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | D     | 314 | SER  | N-CA-C | 5.26  | 116.82      | 111.14   |
| 1   | J     | 314 | SER  | N-CA-C | 5.26  | 116.82      | 111.14   |
| 2   | T     | 26  | GLU  | N-CA-C | -5.24 | 105.62      | 112.23   |
| 2   | O     | 107 | THR  | N-CA-C | 5.24  | 116.80      | 111.14   |
| 2   | U     | 107 | THR  | N-CA-C | 5.24  | 116.80      | 111.14   |
| 2   | S     | 26  | GLU  | N-CA-C | -5.24 | 105.63      | 112.23   |
| 2   | S     | 107 | THR  | N-CA-C | 5.24  | 116.80      | 111.14   |
| 1   | D     | 364 | VAL  | N-CA-C | 5.23  | 120.22      | 109.34   |
| 1   | F     | 364 | VAL  | N-CA-C | 5.23  | 120.22      | 109.34   |
| 1   | L     | 364 | VAL  | N-CA-C | 5.23  | 120.22      | 109.34   |
| 2   | N     | 26  | GLU  | N-CA-C | -5.23 | 105.64      | 112.23   |
| 2   | N     | 107 | THR  | N-CA-C | 5.22  | 116.78      | 111.14   |
| 2   | T     | 107 | THR  | N-CA-C | 5.22  | 116.78      | 111.14   |
| 2   | M     | 26  | GLU  | N-CA-C | -5.22 | 105.65      | 112.23   |
| 1   | B     | 364 | VAL  | N-CA-C | 5.22  | 120.20      | 109.34   |
| 1   | A     | 364 | VAL  | N-CA-C | 5.22  | 120.19      | 109.34   |
| 1   | G     | 364 | VAL  | N-CA-C | 5.22  | 120.19      | 109.34   |
| 1   | H     | 364 | VAL  | N-CA-C | 5.22  | 120.20      | 109.34   |
| 1   | E     | 364 | VAL  | N-CA-C | 5.22  | 120.19      | 109.34   |
| 2   | S     | 172 | ARG  | N-CA-C | 5.22  | 117.44      | 110.35   |
| 1   | K     | 364 | VAL  | N-CA-C | 5.22  | 120.19      | 109.34   |
| 1   | C     | 364 | VAL  | N-CA-C | 5.21  | 120.19      | 109.34   |
| 2   | Q     | 107 | THR  | N-CA-C | 5.21  | 116.77      | 111.14   |
| 1   | I     | 364 | VAL  | N-CA-C | 5.21  | 120.19      | 109.34   |
| 2   | W     | 107 | THR  | N-CA-C | 5.21  | 116.77      | 111.14   |
| 2   | M     | 107 | THR  | N-CA-C | 5.21  | 116.77      | 111.14   |
| 2   | O     | 26  | GLU  | N-CA-C | -5.21 | 105.66      | 112.23   |
| 1   | H     | 473 | PRO  | N-CA-C | 5.21  | 119.67      | 111.38   |
| 2   | U     | 26  | GLU  | N-CA-C | -5.21 | 105.66      | 112.23   |
| 1   | C     | 473 | PRO  | N-CA-C | 5.21  | 119.66      | 111.38   |
| 2   | P     | 107 | THR  | N-CA-C | 5.21  | 116.77      | 111.14   |
| 2   | Q     | 172 | ARG  | N-CA-C | 5.21  | 117.43      | 110.35   |
| 1   | I     | 473 | PRO  | N-CA-C | 5.21  | 119.66      | 111.38   |
| 2   | V     | 107 | THR  | N-CA-C | 5.21  | 116.77      | 111.14   |
| 2   | W     | 172 | ARG  | N-CA-C | 5.21  | 117.43      | 110.35   |
| 1   | E     | 473 | PRO  | N-CA-C | 5.21  | 119.66      | 111.38   |
| 1   | K     | 473 | PRO  | N-CA-C | 5.21  | 119.66      | 111.38   |
| 1   | A     | 473 | PRO  | N-CA-C | 5.21  | 119.66      | 111.38   |
| 2   | R     | 107 | THR  | N-CA-C | 5.20  | 116.76      | 111.14   |
| 1   | J     | 364 | VAL  | N-CA-C | 5.20  | 120.17      | 109.34   |
| 2   | X     | 107 | THR  | N-CA-C | 5.20  | 116.76      | 111.14   |
| 1   | B     | 473 | PRO  | N-CA-C | 5.20  | 119.65      | 111.38   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | F     | 473 | PRO  | N-CA-C | 5.20  | 119.65      | 111.38   |
| 2   | T     | 172 | ARG  | N-CA-C | 5.20  | 117.42      | 110.35   |
| 1   | L     | 473 | PRO  | N-CA-C | 5.20  | 119.65      | 111.38   |
| 2   | M     | 172 | ARG  | N-CA-C | 5.20  | 117.42      | 110.35   |
| 2   | Q     | 26  | GLU  | N-CA-C | -5.20 | 105.68      | 112.23   |
| 2   | R     | 26  | GLU  | N-CA-C | -5.20 | 105.68      | 112.23   |
| 2   | W     | 26  | GLU  | N-CA-C | -5.20 | 105.68      | 112.23   |
| 2   | X     | 26  | GLU  | N-CA-C | -5.20 | 105.68      | 112.23   |
| 2   | O     | 172 | ARG  | N-CA-C | 5.19  | 117.41      | 110.35   |
| 2   | P     | 26  | GLU  | N-CA-C | -5.19 | 105.69      | 112.23   |
| 2   | P     | 172 | ARG  | N-CA-C | 5.19  | 117.41      | 110.35   |
| 2   | U     | 172 | ARG  | N-CA-C | 5.19  | 117.41      | 110.35   |
| 2   | V     | 26  | GLU  | N-CA-C | -5.19 | 105.69      | 112.23   |
| 2   | V     | 172 | ARG  | N-CA-C | 5.19  | 117.41      | 110.35   |
| 1   | D     | 473 | PRO  | N-CA-C | 5.19  | 119.63      | 111.38   |
| 1   | G     | 473 | PRO  | N-CA-C | 5.19  | 119.63      | 111.38   |
| 1   | J     | 473 | PRO  | N-CA-C | 5.19  | 119.63      | 111.38   |
| 2   | N     | 172 | ARG  | N-CA-C | 5.19  | 117.41      | 110.35   |
| 2   | P     | 33  | ALA  | N-CA-C | 5.19  | 117.22      | 110.53   |
| 2   | V     | 33  | ALA  | N-CA-C | 5.19  | 117.22      | 110.53   |
| 1   | F     | 288 | GLU  | N-CA-C | -5.18 | 102.61      | 110.28   |
| 2   | R     | 172 | ARG  | N-CA-C | 5.18  | 117.39      | 110.35   |
| 1   | L     | 288 | GLU  | N-CA-C | -5.18 | 102.61      | 110.28   |
| 2   | X     | 172 | ARG  | N-CA-C | 5.18  | 117.39      | 110.35   |
| 1   | C     | 288 | GLU  | N-CA-C | -5.18 | 102.62      | 110.28   |
| 1   | E     | 288 | GLU  | N-CA-C | -5.18 | 102.62      | 110.28   |
| 1   | I     | 288 | GLU  | N-CA-C | -5.18 | 102.62      | 110.28   |
| 1   | K     | 288 | GLU  | N-CA-C | -5.18 | 102.62      | 110.28   |
| 1   | G     | 288 | GLU  | N-CA-C | -5.18 | 102.62      | 110.28   |
| 2   | S     | 33  | ALA  | N-CA-C | 5.17  | 117.21      | 110.53   |
| 2   | R     | 33  | ALA  | N-CA-C | 5.17  | 117.20      | 110.53   |
| 2   | X     | 33  | ALA  | N-CA-C | 5.17  | 117.20      | 110.53   |
| 1   | H     | 288 | GLU  | N-CA-C | -5.17 | 102.63      | 110.28   |
| 2   | M     | 33  | ALA  | N-CA-C | 5.17  | 117.20      | 110.53   |
| 1   | D     | 288 | GLU  | N-CA-C | -5.17 | 102.64      | 110.28   |
| 1   | J     | 288 | GLU  | N-CA-C | -5.17 | 102.64      | 110.28   |
| 1   | A     | 288 | GLU  | N-CA-C | -5.16 | 102.64      | 110.28   |
| 1   | B     | 228 | ASP  | N-CA-C | 5.16  | 118.73      | 112.23   |
| 1   | C     | 228 | ASP  | N-CA-C | 5.16  | 118.73      | 112.23   |
| 2   | O     | 33  | ALA  | N-CA-C | 5.16  | 117.18      | 110.53   |
| 1   | E     | 228 | ASP  | N-CA-C | 5.16  | 118.73      | 112.23   |
| 1   | I     | 228 | ASP  | N-CA-C | 5.16  | 118.73      | 112.23   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | U     | 33  | ALA  | N-CA-C | 5.16  | 117.18      | 110.53   |
| 1   | K     | 228 | ASP  | N-CA-C | 5.16  | 118.73      | 112.23   |
| 1   | D     | 228 | ASP  | N-CA-C | 5.15  | 118.72      | 112.23   |
| 1   | J     | 228 | ASP  | N-CA-C | 5.15  | 118.72      | 112.23   |
| 1   | A     | 228 | ASP  | N-CA-C | 5.15  | 118.72      | 112.23   |
| 2   | N     | 33  | ALA  | N-CA-C | 5.15  | 117.17      | 110.53   |
| 1   | G     | 228 | ASP  | N-CA-C | 5.15  | 118.72      | 112.23   |
| 2   | T     | 33  | ALA  | N-CA-C | 5.15  | 117.17      | 110.53   |
| 1   | F     | 228 | ASP  | N-CA-C | 5.14  | 118.71      | 112.23   |
| 1   | L     | 228 | ASP  | N-CA-C | 5.14  | 118.71      | 112.23   |
| 1   | H     | 228 | ASP  | N-CA-C | 5.14  | 118.71      | 112.23   |
| 1   | B     | 288 | GLU  | N-CA-C | -5.14 | 102.68      | 110.28   |
| 2   | Q     | 33  | ALA  | N-CA-C | 5.13  | 117.15      | 110.53   |
| 2   | W     | 33  | ALA  | N-CA-C | 5.13  | 117.15      | 110.53   |
| 2   | N     | 68  | ALA  | N-CA-C | 5.06  | 121.58      | 110.80   |
| 2   | Q     | 68  | ALA  | N-CA-C | 5.06  | 121.58      | 110.80   |
| 2   | S     | 68  | ALA  | N-CA-C | 5.06  | 121.58      | 110.80   |
| 2   | W     | 68  | ALA  | N-CA-C | 5.06  | 121.58      | 110.80   |
| 2   | M     | 68  | ALA  | N-CA-C | 5.05  | 121.56      | 110.80   |
| 2   | O     | 68  | ALA  | N-CA-C | 5.05  | 121.56      | 110.80   |
| 2   | R     | 68  | ALA  | N-CA-C | 5.05  | 121.56      | 110.80   |
| 2   | U     | 68  | ALA  | N-CA-C | 5.05  | 121.56      | 110.80   |
| 2   | X     | 68  | ALA  | N-CA-C | 5.05  | 121.56      | 110.80   |
| 2   | R     | 18  | ALA  | N-CA-C | 5.04  | 117.56      | 108.48   |
| 2   | T     | 68  | ALA  | N-CA-C | 5.04  | 121.55      | 110.80   |
| 2   | X     | 18  | ALA  | N-CA-C | 5.04  | 117.56      | 108.48   |
| 1   | H     | 505 | ASP  | N-CA-C | 5.04  | 121.53      | 110.80   |
| 2   | P     | 68  | ALA  | N-CA-C | 5.03  | 121.52      | 110.80   |
| 2   | V     | 68  | ALA  | N-CA-C | 5.03  | 121.52      | 110.80   |
| 2   | Q     | 18  | ALA  | N-CA-C | 5.03  | 117.54      | 108.48   |
| 2   | W     | 18  | ALA  | N-CA-C | 5.03  | 117.54      | 108.48   |
| 2   | T     | 18  | ALA  | N-CA-C | 5.03  | 117.53      | 108.48   |
| 2   | M     | 18  | ALA  | N-CA-C | 5.03  | 117.53      | 108.48   |
| 2   | P     | 18  | ALA  | N-CA-C | 5.03  | 117.53      | 108.48   |
| 2   | V     | 18  | ALA  | N-CA-C | 5.03  | 117.53      | 108.48   |
| 1   | B     | 505 | ASP  | N-CA-C | 5.03  | 121.50      | 110.80   |
| 1   | A     | 505 | ASP  | N-CA-C | 5.02  | 121.50      | 110.80   |
| 2   | N     | 18  | ALA  | N-CA-C | 5.02  | 117.52      | 108.48   |
| 2   | O     | 18  | ALA  | N-CA-C | 5.02  | 117.52      | 108.48   |
| 1   | G     | 505 | ASP  | N-CA-C | 5.02  | 121.50      | 110.80   |
| 2   | U     | 18  | ALA  | N-CA-C | 5.02  | 117.52      | 108.48   |
| 1   | C     | 505 | ASP  | N-CA-C | 5.02  | 121.50      | 110.80   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | F     | 505 | ASP  | N-CA-C | 5.02 | 121.50      | 110.80   |
| 1   | I     | 505 | ASP  | N-CA-C | 5.02 | 121.50      | 110.80   |
| 1   | L     | 505 | ASP  | N-CA-C | 5.02 | 121.50      | 110.80   |
| 2   | S     | 18  | ALA  | N-CA-C | 5.01 | 117.50      | 108.48   |
| 1   | E     | 505 | ASP  | N-CA-C | 5.01 | 121.47      | 110.80   |
| 1   | K     | 505 | ASP  | N-CA-C | 5.01 | 121.47      | 110.80   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1752  | 0        | 496      | 8       | 0            |
| 1   | B     | 1752  | 0        | 496      | 9       | 0            |
| 1   | C     | 1752  | 0        | 496      | 9       | 0            |
| 1   | D     | 1752  | 0        | 496      | 10      | 0            |
| 1   | E     | 1752  | 0        | 496      | 8       | 0            |
| 1   | F     | 1752  | 0        | 496      | 8       | 0            |
| 1   | G     | 1752  | 0        | 496      | 8       | 0            |
| 1   | H     | 1752  | 0        | 496      | 10      | 0            |
| 1   | I     | 1752  | 0        | 496      | 10      | 0            |
| 1   | J     | 1752  | 0        | 496      | 10      | 0            |
| 1   | K     | 1752  | 0        | 496      | 9       | 0            |
| 1   | L     | 1752  | 0        | 496      | 8       | 0            |
| 2   | M     | 713   | 0        | 188      | 5       | 0            |
| 2   | N     | 713   | 0        | 188      | 5       | 0            |
| 2   | O     | 713   | 0        | 188      | 5       | 0            |
| 2   | P     | 713   | 0        | 188      | 5       | 0            |
| 2   | Q     | 713   | 0        | 188      | 5       | 0            |
| 2   | R     | 713   | 0        | 188      | 5       | 0            |
| 2   | S     | 713   | 0        | 188      | 5       | 0            |
| 2   | T     | 713   | 0        | 188      | 4       | 0            |
| 2   | U     | 713   | 0        | 188      | 5       | 0            |
| 2   | V     | 713   | 0        | 188      | 5       | 0            |
| 2   | W     | 713   | 0        | 188      | 5       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | X     | 713   | 0        | 188      | 5       | 0            |
| All | All   | 29580 | 0        | 8208     | 142     | 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 4.

All (142) 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:A:147:ILE:O   | 1:A:148:ALA:C   | 2.35                     | 0.67              |
| 1:L:147:ILE:O   | 1:L:148:ALA:C   | 2.35                     | 0.67              |
| 1:H:147:ILE:O   | 1:H:148:ALA:C   | 2.35                     | 0.67              |
| 1:K:147:ILE:O   | 1:K:148:ALA:C   | 2.35                     | 0.67              |
| 1:J:147:ILE:O   | 1:J:148:ALA:C   | 2.35                     | 0.66              |
| 1:B:147:ILE:O   | 1:B:148:ALA:C   | 2.35                     | 0.66              |
| 1:I:147:ILE:O   | 1:I:148:ALA:C   | 2.35                     | 0.66              |
| 1:F:147:ILE:O   | 1:F:148:ALA:C   | 2.35                     | 0.65              |
| 1:C:147:ILE:O   | 1:C:148:ALA:C   | 2.35                     | 0.64              |
| 1:G:147:ILE:O   | 1:G:148:ALA:C   | 2.35                     | 0.61              |
| 1:D:147:ILE:O   | 1:D:148:ALA:C   | 2.35                     | 0.61              |
| 1:E:147:ILE:O   | 1:E:148:ALA:C   | 2.35                     | 0.60              |
| 1:A:373:TYR:O   | 1:A:374:PRO:C   | 2.50                     | 0.53              |
| 1:E:373:TYR:O   | 1:E:374:PRO:C   | 2.50                     | 0.53              |
| 1:D:373:TYR:O   | 1:D:374:PRO:C   | 2.50                     | 0.53              |
| 1:G:373:TYR:O   | 1:G:374:PRO:C   | 2.50                     | 0.52              |
| 1:F:373:TYR:O   | 1:F:374:PRO:C   | 2.50                     | 0.52              |
| 1:C:373:TYR:O   | 1:C:374:PRO:C   | 2.50                     | 0.52              |
| 1:H:373:TYR:O   | 1:H:374:PRO:C   | 2.50                     | 0.52              |
| 1:A:352:ILE:CA  | 2:X:178:PHE:OXT | 2.58                     | 0.52              |
| 1:K:373:TYR:O   | 1:K:374:PRO:C   | 2.50                     | 0.52              |
| 2:N:109:ASP:O   | 2:O:41:GLU:O    | 2.29                     | 0.51              |
| 1:B:373:TYR:O   | 1:B:374:PRO:C   | 2.50                     | 0.51              |
| 1:I:373:TYR:O   | 1:I:374:PRO:C   | 2.50                     | 0.51              |
| 2:P:109:ASP:O   | 2:Q:41:GLU:O    | 2.30                     | 0.50              |
| 2:N:178:PHE:OXT | 1:C:352:ILE:CA  | 2.60                     | 0.50              |
| 2:R:109:ASP:O   | 2:S:41:GLU:O    | 2.30                     | 0.50              |
| 1:J:373:TYR:O   | 1:J:374:PRO:C   | 2.50                     | 0.50              |
| 2:T:109:ASP:O   | 2:U:41:GLU:O    | 2.30                     | 0.49              |
| 2:M:41:GLU:O    | 2:X:109:ASP:O   | 2.29                     | 0.49              |
| 2:V:178:PHE:OXT | 1:K:352:ILE:CA  | 2.60                     | 0.49              |
| 2:P:178:PHE:OXT | 1:E:352:ILE:CA  | 2.60                     | 0.49              |

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| Atom-1          | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|----------------|--------------------------|-------------------|
| 2:Q:178:PHE:OXT | 1:F:352:ILE:CA | 2.61                     | 0.49              |
| 2:O:178:PHE:OXT | 1:D:352:ILE:CA | 2.61                     | 0.49              |
| 2:T:178:PHE:OXT | 1:I:352:ILE:CA | 2.60                     | 0.49              |
| 1:L:373:TYR:O   | 1:L:374:PRO:C  | 2.50                     | 0.49              |
| 2:V:109:ASP:O   | 2:W:41:GLU:O   | 2.30                     | 0.49              |
| 1:A:63:VAL:O    | 1:A:64:GLY:C   | 2.56                     | 0.49              |
| 2:U:178:PHE:OXT | 1:J:352:ILE:CA | 2.61                     | 0.49              |
| 2:R:178:PHE:OXT | 1:G:352:ILE:CA | 2.60                     | 0.48              |
| 2:W:178:PHE:OXT | 1:L:352:ILE:CA | 2.61                     | 0.48              |
| 2:S:178:PHE:OXT | 1:H:352:ILE:CA | 2.61                     | 0.48              |
| 1:J:63:VAL:O    | 1:J:64:GLY:C   | 2.56                     | 0.48              |
| 1:C:63:VAL:O    | 1:C:64:GLY:C   | 2.56                     | 0.48              |
| 1:H:63:VAL:O    | 1:H:64:GLY:C   | 2.56                     | 0.48              |
| 1:L:63:VAL:O    | 1:L:64:GLY:C   | 2.56                     | 0.47              |
| 1:G:63:VAL:O    | 1:G:64:GLY:C   | 2.56                     | 0.47              |
| 1:E:63:VAL:O    | 1:E:64:GLY:C   | 2.56                     | 0.47              |
| 1:I:63:VAL:O    | 1:I:64:GLY:C   | 2.56                     | 0.47              |
| 2:O:109:ASP:O   | 2:P:41:GLU:O   | 2.33                     | 0.46              |
| 2:Q:109:ASP:O   | 2:R:41:GLU:O   | 2.33                     | 0.46              |
| 1:F:63:VAL:O    | 1:F:64:GLY:C   | 2.56                     | 0.46              |
| 1:B:63:VAL:O    | 1:B:64:GLY:C   | 2.56                     | 0.46              |
| 2:S:109:ASP:O   | 2:T:41:GLU:O   | 2.33                     | 0.46              |
| 1:C:83:THR:O    | 1:C:84:ARG:C   | 2.59                     | 0.46              |
| 1:K:83:THR:O    | 1:K:84:ARG:C   | 2.59                     | 0.46              |
| 2:W:109:ASP:O   | 2:X:41:GLU:O   | 2.33                     | 0.46              |
| 1:J:83:THR:O    | 1:J:84:ARG:C   | 2.59                     | 0.46              |
| 1:D:63:VAL:O    | 1:D:64:GLY:C   | 2.56                     | 0.45              |
| 1:L:83:THR:O    | 1:L:84:ARG:C   | 2.59                     | 0.45              |
| 1:K:63:VAL:O    | 1:K:64:GLY:C   | 2.56                     | 0.45              |
| 2:U:109:ASP:O   | 2:V:41:GLU:O   | 2.33                     | 0.45              |
| 1:D:83:THR:O    | 1:D:84:ARG:C   | 2.59                     | 0.45              |
| 2:M:178:PHE:OXT | 1:B:352:ILE:CA | 2.64                     | 0.45              |
| 1:A:83:THR:O    | 1:A:84:ARG:C   | 2.59                     | 0.44              |
| 1:G:83:THR:O    | 1:G:84:ARG:C   | 2.59                     | 0.44              |
| 1:F:83:THR:O    | 1:F:84:ARG:C   | 2.59                     | 0.44              |
| 1:H:83:THR:O    | 1:H:84:ARG:C   | 2.59                     | 0.44              |
| 2:Q:169:SER:O   | 2:Q:170:PRO:C  | 2.61                     | 0.44              |
| 1:D:66:SER:O    | 1:D:67:ARG:C   | 2.60                     | 0.44              |
| 1:B:66:SER:O    | 1:B:67:ARG:C   | 2.60                     | 0.43              |
| 2:M:109:ASP:O   | 2:N:41:GLU:O   | 2.36                     | 0.43              |
| 1:C:76:ALA:C    | 1:C:78:ALA:N   | 2.73                     | 0.43              |

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| Atom-1        | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|---------------|--------------------------|-------------------|
| 1:H:66:SER:O  | 1:H:67:ARG:C  | 2.60                     | 0.43              |
| 1:E:83:THR:O  | 1:E:84:ARG:C  | 2.59                     | 0.43              |
| 1:L:66:SER:O  | 1:L:67:ARG:C  | 2.60                     | 0.43              |
| 2:S:169:SER:O | 2:S:170:PRO:C | 2.61                     | 0.43              |
| 1:I:83:THR:O  | 1:I:84:ARG:C  | 2.59                     | 0.43              |
| 2:P:169:SER:O | 2:P:170:PRO:C | 2.61                     | 0.43              |
| 1:H:76:ALA:C  | 1:H:78:ALA:N  | 2.73                     | 0.43              |
| 1:B:83:THR:O  | 1:B:84:ARG:C  | 2.59                     | 0.43              |
| 2:N:169:SER:O | 2:N:170:PRO:C | 2.61                     | 0.43              |
| 1:I:66:SER:O  | 1:I:67:ARG:C  | 2.60                     | 0.43              |
| 1:G:66:SER:O  | 1:G:67:ARG:C  | 2.60                     | 0.42              |
| 1:G:76:ALA:C  | 1:G:78:ALA:N  | 2.73                     | 0.42              |
| 1:H:284:LEU:O | 1:H:285:VAL:C | 2.62                     | 0.42              |
| 1:I:76:ALA:C  | 1:I:78:ALA:N  | 2.73                     | 0.42              |
| 1:J:306:ASN:O | 1:J:307:LEU:C | 2.62                     | 0.42              |
| 1:J:284:LEU:O | 1:J:285:VAL:C | 2.62                     | 0.42              |
| 2:M:169:SER:O | 2:M:170:PRO:C | 2.61                     | 0.42              |
| 1:G:284:LEU:O | 1:G:285:VAL:C | 2.62                     | 0.42              |
| 2:X:169:SER:O | 2:X:170:PRO:C | 2.61                     | 0.42              |
| 1:I:306:ASN:O | 1:I:307:LEU:C | 2.62                     | 0.42              |
| 1:J:76:ALA:C  | 1:J:78:ALA:N  | 2.73                     | 0.42              |
| 1:K:76:ALA:C  | 1:K:78:ALA:N  | 2.73                     | 0.42              |
| 1:K:284:LEU:O | 1:K:285:VAL:C | 2.62                     | 0.42              |
| 1:E:284:LEU:O | 1:E:285:VAL:C | 2.62                     | 0.42              |
| 1:F:66:SER:O  | 1:F:67:ARG:C  | 2.60                     | 0.42              |
| 1:E:66:SER:O  | 1:E:67:ARG:C  | 2.60                     | 0.42              |
| 1:F:284:LEU:O | 1:F:285:VAL:C | 2.62                     | 0.42              |
| 1:D:306:ASN:O | 1:D:307:LEU:C | 2.62                     | 0.42              |
| 2:U:169:SER:O | 2:U:170:PRO:C | 2.61                     | 0.42              |
| 2:W:67:THR:O  | 2:W:68:ALA:C  | 2.63                     | 0.42              |
| 1:A:284:LEU:O | 1:A:285:VAL:C | 2.62                     | 0.41              |
| 2:O:67:THR:O  | 2:O:68:ALA:C  | 2.63                     | 0.41              |
| 1:I:284:LEU:O | 1:I:285:VAL:C | 2.62                     | 0.41              |
| 1:J:66:SER:O  | 1:J:67:ARG:C  | 2.60                     | 0.41              |
| 2:V:67:THR:O  | 2:V:68:ALA:C  | 2.63                     | 0.41              |
| 1:K:66:SER:O  | 1:K:67:ARG:C  | 2.60                     | 0.41              |
| 1:B:76:ALA:C  | 1:B:78:ALA:N  | 2.73                     | 0.41              |
| 1:F:76:ALA:C  | 1:F:78:ALA:N  | 2.73                     | 0.41              |
| 2:R:169:SER:O | 2:R:170:PRO:C | 2.61                     | 0.41              |
| 2:S:67:THR:O  | 2:S:68:ALA:C  | 2.63                     | 0.41              |
| 2:X:67:THR:O  | 2:X:68:ALA:C  | 2.63                     | 0.41              |

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| Atom-1        | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|---------------|--------------------------|-------------------|
| 1:C:284:LEU:O | 1:C:285:VAL:C | 2.62                     | 0.41              |
| 2:R:67:THR:O  | 2:R:68:ALA:C  | 2.63                     | 0.41              |
| 2:T:67:THR:O  | 2:T:68:ALA:C  | 2.63                     | 0.41              |
| 1:A:306:ASN:O | 1:A:307:LEU:C | 2.62                     | 0.41              |
| 1:B:284:LEU:O | 1:B:285:VAL:C | 2.62                     | 0.41              |
| 2:U:67:THR:O  | 2:U:68:ALA:C  | 2.63                     | 0.41              |
| 2:W:169:SER:O | 2:W:170:PRO:C | 2.61                     | 0.41              |
| 2:N:67:THR:O  | 2:N:68:ALA:C  | 2.63                     | 0.41              |
| 1:H:306:ASN:O | 1:H:307:LEU:C | 2.62                     | 0.41              |
| 1:L:76:ALA:O  | 1:L:77:ARG:C  | 2.64                     | 0.41              |
| 2:V:169:SER:O | 2:V:170:PRO:C | 2.61                     | 0.41              |
| 1:J:257:TRP:O | 1:J:272:ARG:N | 2.54                     | 0.41              |
| 1:A:76:ALA:O  | 1:A:77:ARG:C  | 2.64                     | 0.41              |
| 1:I:257:TRP:O | 1:I:272:ARG:N | 2.54                     | 0.41              |
| 1:K:257:TRP:O | 1:K:272:ARG:N | 2.54                     | 0.41              |
| 1:D:284:LEU:O | 1:D:285:VAL:C | 2.62                     | 0.41              |
| 2:P:67:THR:O  | 2:P:68:ALA:C  | 2.63                     | 0.40              |
| 2:Q:67:THR:O  | 2:Q:68:ALA:C  | 2.63                     | 0.40              |
| 1:E:257:TRP:O | 1:E:272:ARG:N | 2.54                     | 0.40              |
| 1:C:306:ASN:O | 1:C:307:LEU:C | 2.62                     | 0.40              |
| 1:D:257:TRP:O | 1:D:272:ARG:N | 2.54                     | 0.40              |
| 1:H:257:TRP:O | 1:H:272:ARG:N | 2.54                     | 0.40              |
| 1:L:257:TRP:O | 1:L:272:ARG:N | 2.54                     | 0.40              |
| 2:M:67:THR:O  | 2:M:68:ALA:C  | 2.63                     | 0.40              |
| 1:C:66:SER:O  | 1:C:67:ARG:C  | 2.60                     | 0.40              |
| 2:O:169:SER:O | 2:O:170:PRO:C | 2.61                     | 0.40              |
| 1:D:259:ALA:O | 1:D:260:ALA:C | 2.63                     | 0.40              |
| 1:B:257:TRP:O | 1:B:272:ARG:N | 2.54                     | 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   | A     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | B     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | C     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | D     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | E     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | F     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | G     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | H     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | I     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | J     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | K     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 1   | L     | 432/551 (78%)   | 387 (90%)  | 38 (9%)  | 7 (2%)   | 7           | 37 |
| 2   | M     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | N     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | O     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | P     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | Q     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | R     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | S     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | T     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | U     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | V     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | W     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| 2   | X     | 176/178 (99%)   | 160 (91%)  | 13 (7%)  | 3 (2%)   | 7           | 35 |
| All | All   | 7296/8748 (83%) | 6564 (90%) | 612 (8%) | 120 (2%) | 10          | 37 |

All (120) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | M     | 68  | ALA  |
| 2   | N     | 68  | ALA  |
| 2   | O     | 68  | ALA  |
| 2   | P     | 68  | ALA  |
| 2   | Q     | 68  | ALA  |
| 2   | R     | 68  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | S     | 68  | ALA  |
| 2   | T     | 68  | ALA  |
| 2   | U     | 68  | ALA  |
| 2   | V     | 68  | ALA  |
| 2   | W     | 68  | ALA  |
| 2   | X     | 68  | ALA  |
| 1   | A     | 257 | TRP  |
| 2   | M     | 145 | ARG  |
| 1   | B     | 257 | TRP  |
| 2   | N     | 145 | ARG  |
| 1   | C     | 257 | TRP  |
| 2   | O     | 145 | ARG  |
| 1   | D     | 257 | TRP  |
| 2   | P     | 145 | ARG  |
| 1   | E     | 257 | TRP  |
| 2   | Q     | 145 | ARG  |
| 1   | F     | 257 | TRP  |
| 2   | R     | 145 | ARG  |
| 1   | G     | 257 | TRP  |
| 2   | S     | 145 | ARG  |
| 1   | H     | 257 | TRP  |
| 2   | T     | 145 | ARG  |
| 1   | I     | 257 | TRP  |
| 2   | U     | 145 | ARG  |
| 1   | J     | 257 | TRP  |
| 2   | V     | 145 | ARG  |
| 1   | K     | 257 | TRP  |
| 2   | W     | 145 | ARG  |
| 1   | L     | 257 | TRP  |
| 2   | X     | 145 | ARG  |
| 1   | A     | 131 | CYS  |
| 1   | A     | 272 | ARG  |
| 1   | B     | 131 | CYS  |
| 1   | B     | 272 | ARG  |
| 1   | C     | 131 | CYS  |
| 1   | C     | 272 | ARG  |
| 1   | D     | 131 | CYS  |
| 1   | D     | 272 | ARG  |
| 1   | E     | 131 | CYS  |
| 1   | E     | 272 | ARG  |
| 1   | F     | 131 | CYS  |
| 1   | F     | 272 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 131 | CYS  |
| 1   | G     | 272 | ARG  |
| 1   | H     | 131 | CYS  |
| 1   | H     | 272 | ARG  |
| 1   | I     | 131 | CYS  |
| 1   | I     | 272 | ARG  |
| 1   | J     | 131 | CYS  |
| 1   | J     | 272 | ARG  |
| 1   | K     | 131 | CYS  |
| 1   | K     | 272 | ARG  |
| 1   | L     | 131 | CYS  |
| 1   | L     | 272 | ARG  |
| 1   | D     | 505 | ASP  |
| 1   | J     | 505 | ASP  |
| 1   | A     | 505 | ASP  |
| 2   | M     | 31  | PRO  |
| 1   | B     | 505 | ASP  |
| 2   | N     | 31  | PRO  |
| 1   | C     | 505 | ASP  |
| 2   | O     | 31  | PRO  |
| 2   | P     | 31  | PRO  |
| 1   | E     | 505 | ASP  |
| 2   | Q     | 31  | PRO  |
| 1   | F     | 505 | ASP  |
| 2   | R     | 31  | PRO  |
| 1   | G     | 505 | ASP  |
| 2   | S     | 31  | PRO  |
| 1   | H     | 505 | ASP  |
| 2   | T     | 31  | PRO  |
| 1   | I     | 505 | ASP  |
| 2   | U     | 31  | PRO  |
| 2   | V     | 31  | PRO  |
| 1   | K     | 505 | ASP  |
| 2   | W     | 31  | PRO  |
| 1   | L     | 505 | ASP  |
| 2   | X     | 31  | PRO  |
| 1   | A     | 132 | GLY  |
| 1   | B     | 132 | GLY  |
| 1   | C     | 132 | GLY  |
| 1   | D     | 132 | GLY  |
| 1   | E     | 132 | GLY  |
| 1   | F     | 132 | GLY  |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 132 | GLY  |
| 1   | H     | 132 | GLY  |
| 1   | I     | 132 | GLY  |
| 1   | J     | 132 | GLY  |
| 1   | K     | 132 | GLY  |
| 1   | L     | 132 | GLY  |
| 1   | A     | 361 | PRO  |
| 1   | B     | 361 | PRO  |
| 1   | C     | 361 | PRO  |
| 1   | D     | 361 | PRO  |
| 1   | E     | 361 | PRO  |
| 1   | F     | 361 | PRO  |
| 1   | G     | 361 | PRO  |
| 1   | H     | 361 | PRO  |
| 1   | I     | 361 | PRO  |
| 1   | J     | 361 | PRO  |
| 1   | K     | 361 | PRO  |
| 1   | L     | 361 | PRO  |
| 1   | A     | 362 | PRO  |
| 1   | B     | 362 | PRO  |
| 1   | C     | 362 | PRO  |
| 1   | D     | 362 | PRO  |
| 1   | E     | 362 | PRO  |
| 1   | F     | 362 | PRO  |
| 1   | G     | 362 | PRO  |
| 1   | H     | 362 | PRO  |
| 1   | I     | 362 | PRO  |
| 1   | J     | 362 | PRO  |
| 1   | K     | 362 | PRO  |
| 1   | L     | 362 | PRO  |

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

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.

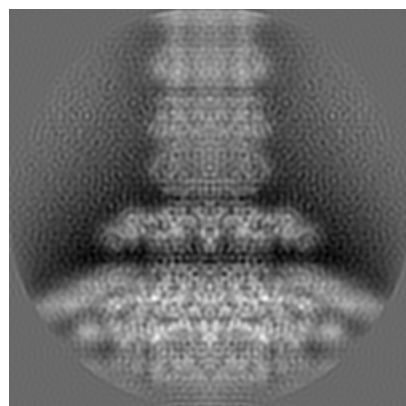
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34250. These allow visual inspection of the internal detail of the map and identification of artifacts.

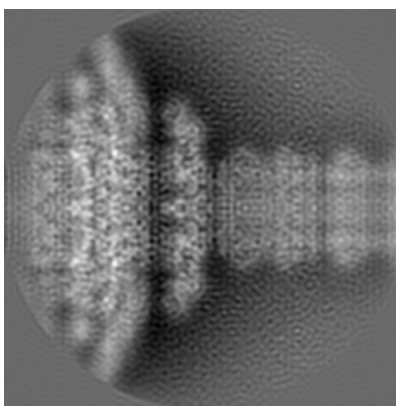
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

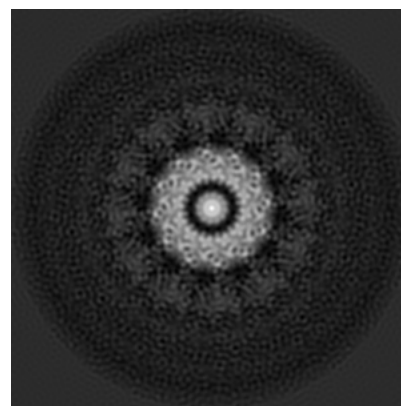
#### 6.1.1 Primary map



X

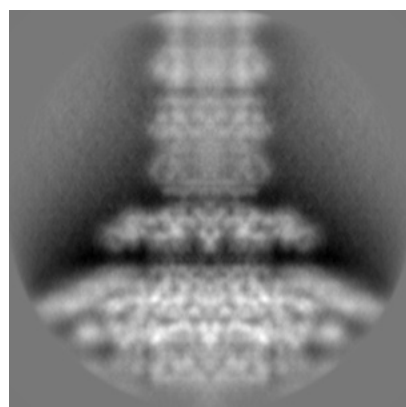


Y

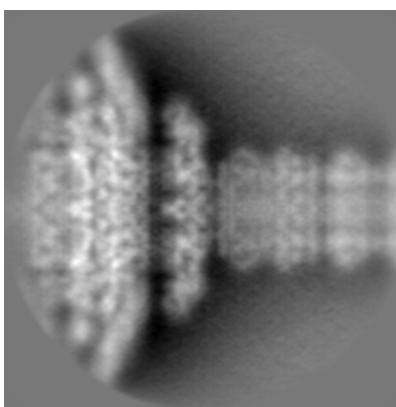


Z

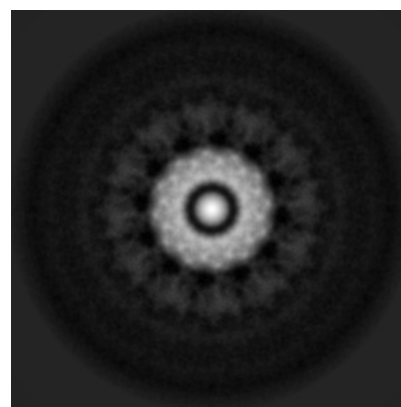
#### 6.1.2 Raw map



X



Y

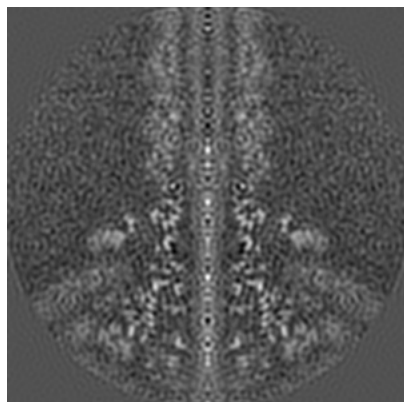


Z

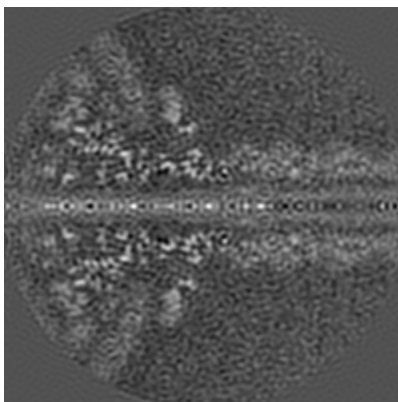
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

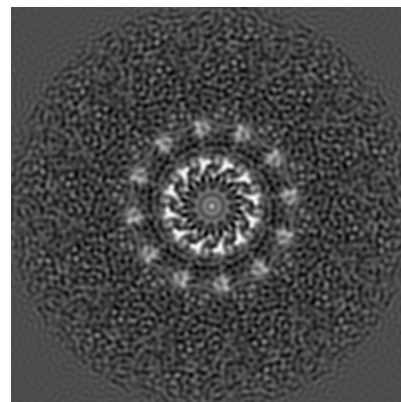
### 6.2.1 Primary map



X Index: 120

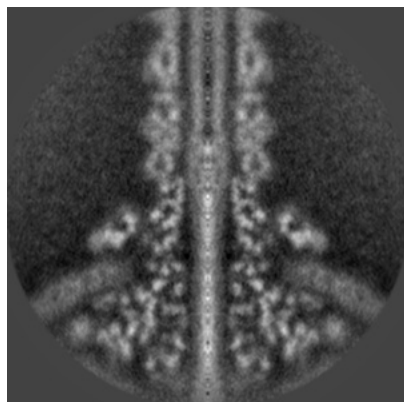


Y Index: 120

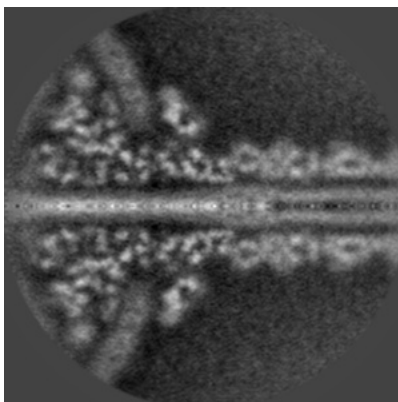


Z Index: 120

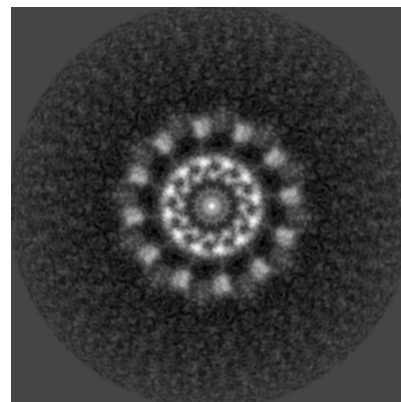
### 6.2.2 Raw map



X Index: 120



Y Index: 120

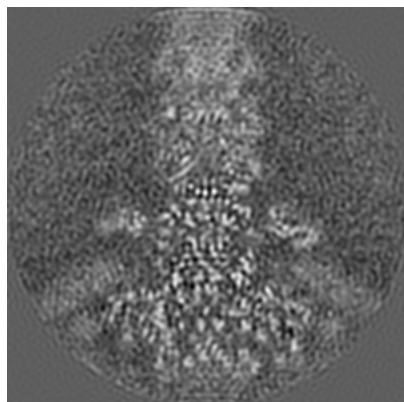


Z Index: 120

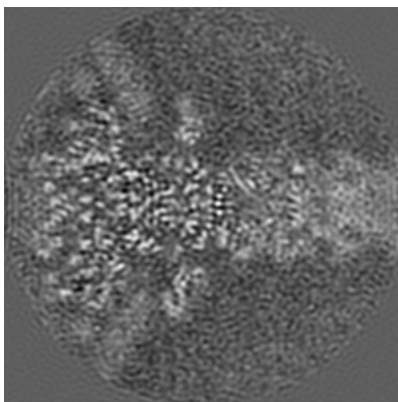
The images above show central slices of the map in three orthogonal directions.

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

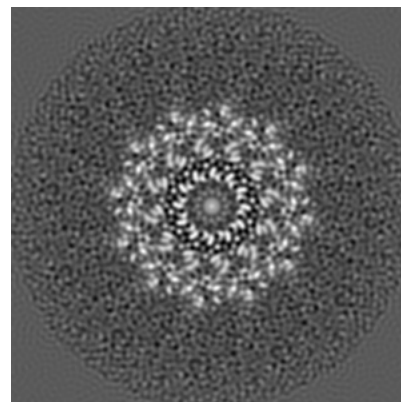
### 6.3.1 Primary map



X Index: 139

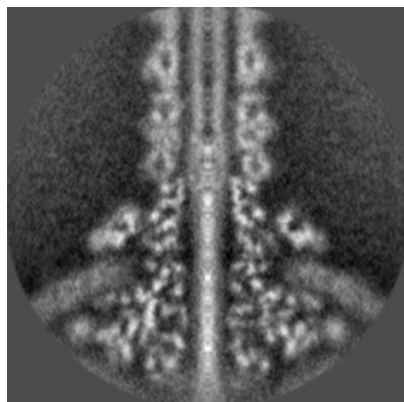


Y Index: 139

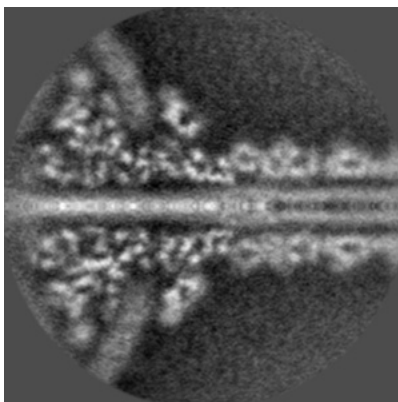


Z Index: 113

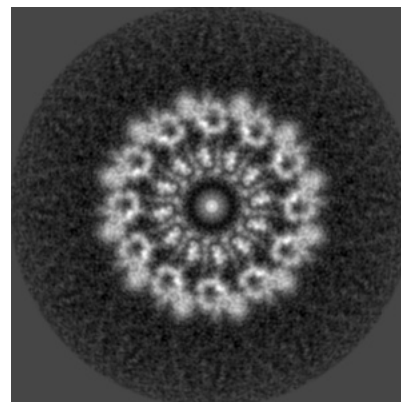
### 6.3.2 Raw map



X Index: 121



Y Index: 119



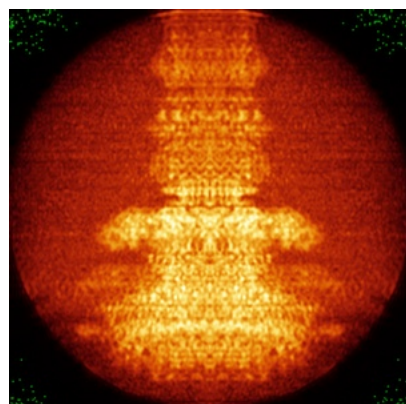
Z Index: 106

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

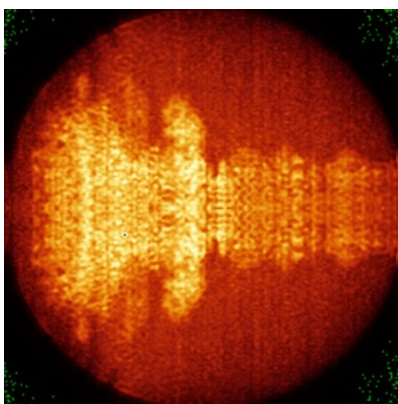


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

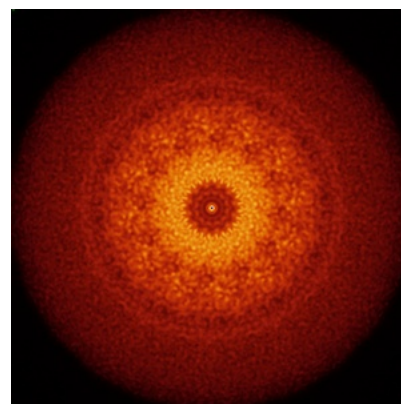
### 6.4.1 Primary map



X

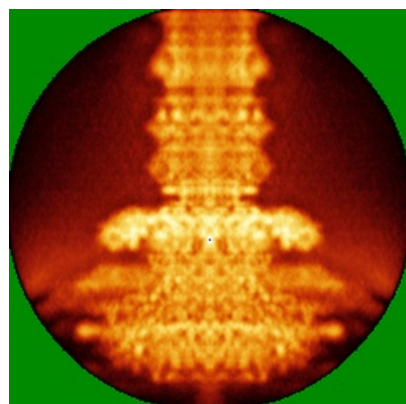


Y

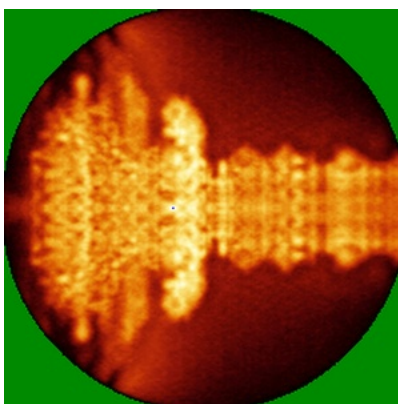


Z

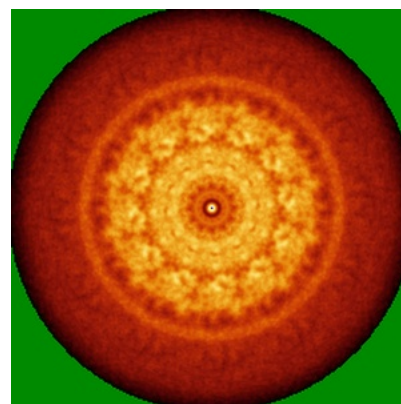
### 6.4.2 Raw map



X



Y



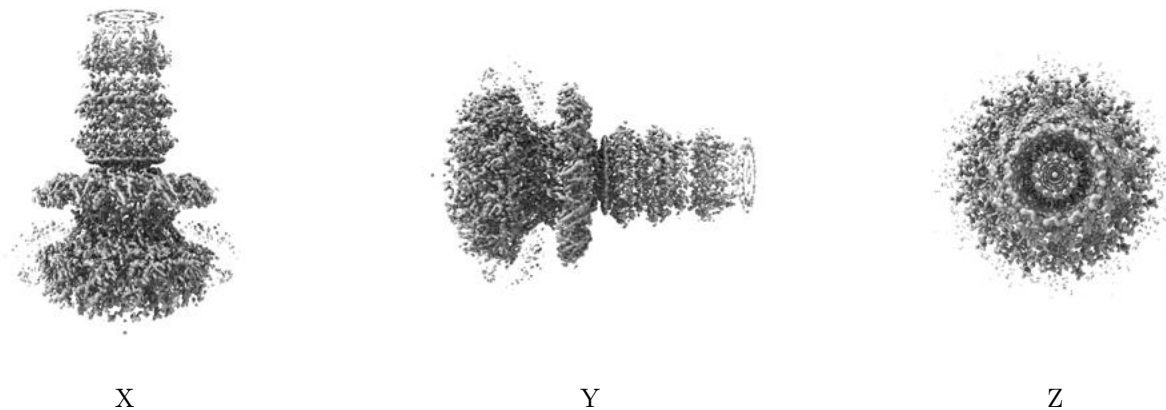
Z

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



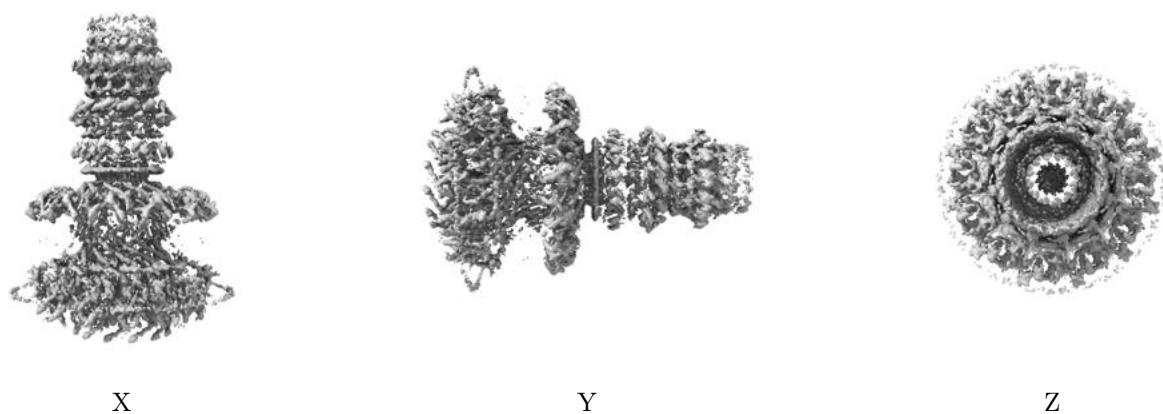
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0302. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

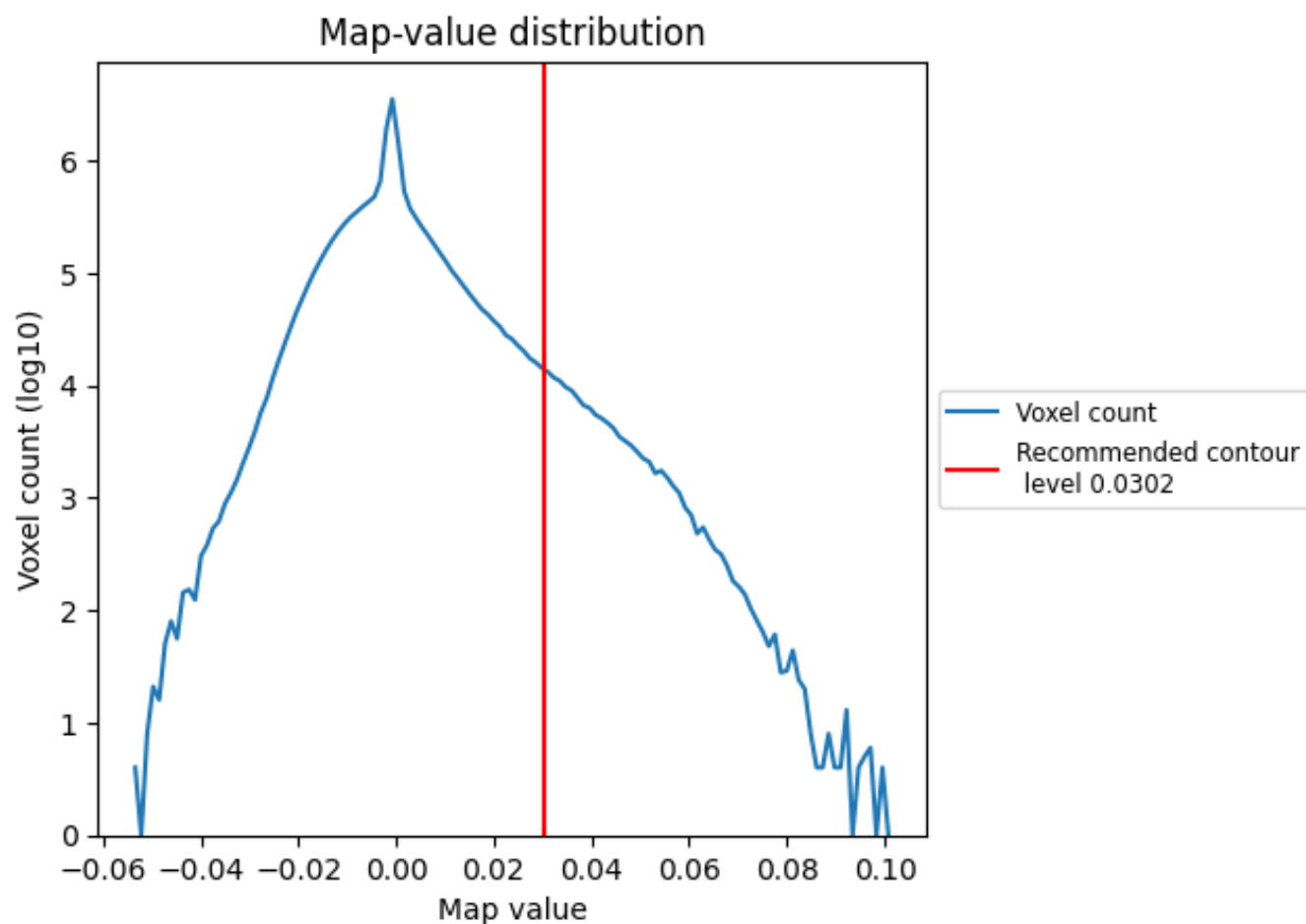
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

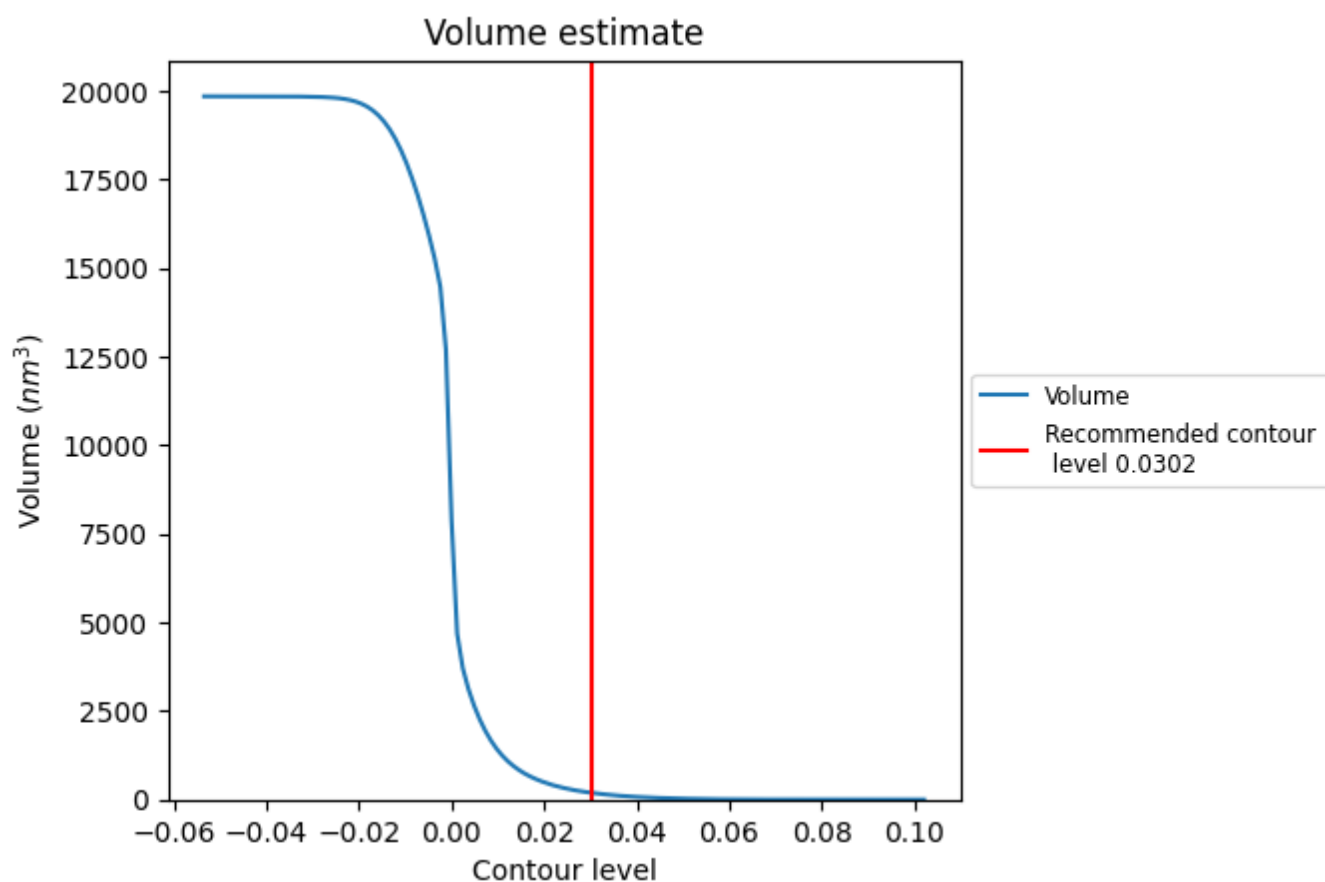
This section contains the results of statistical analysis of the map.

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



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

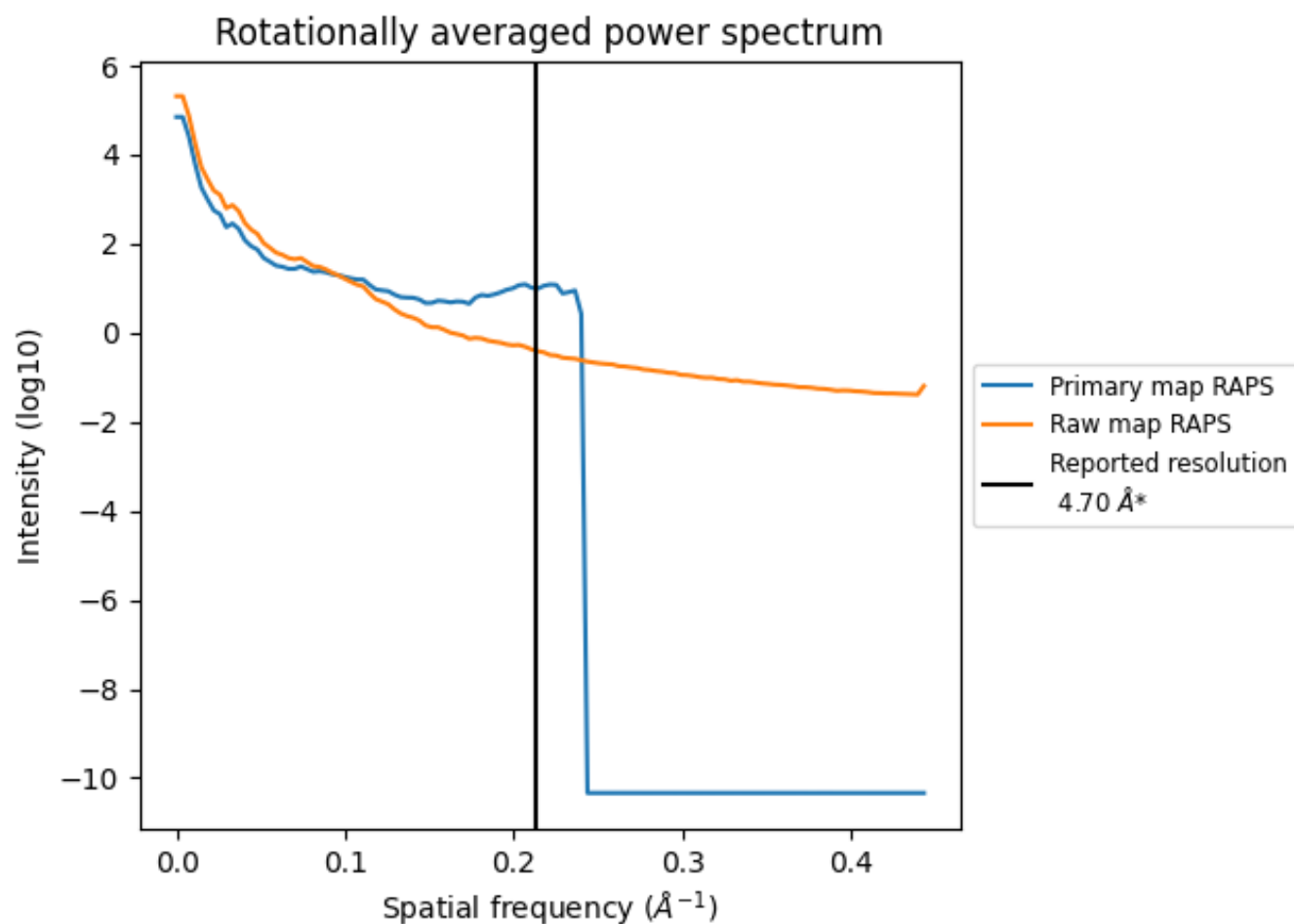
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm<sup>3</sup>; this corresponds to an approximate mass of 173 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 ⓘ

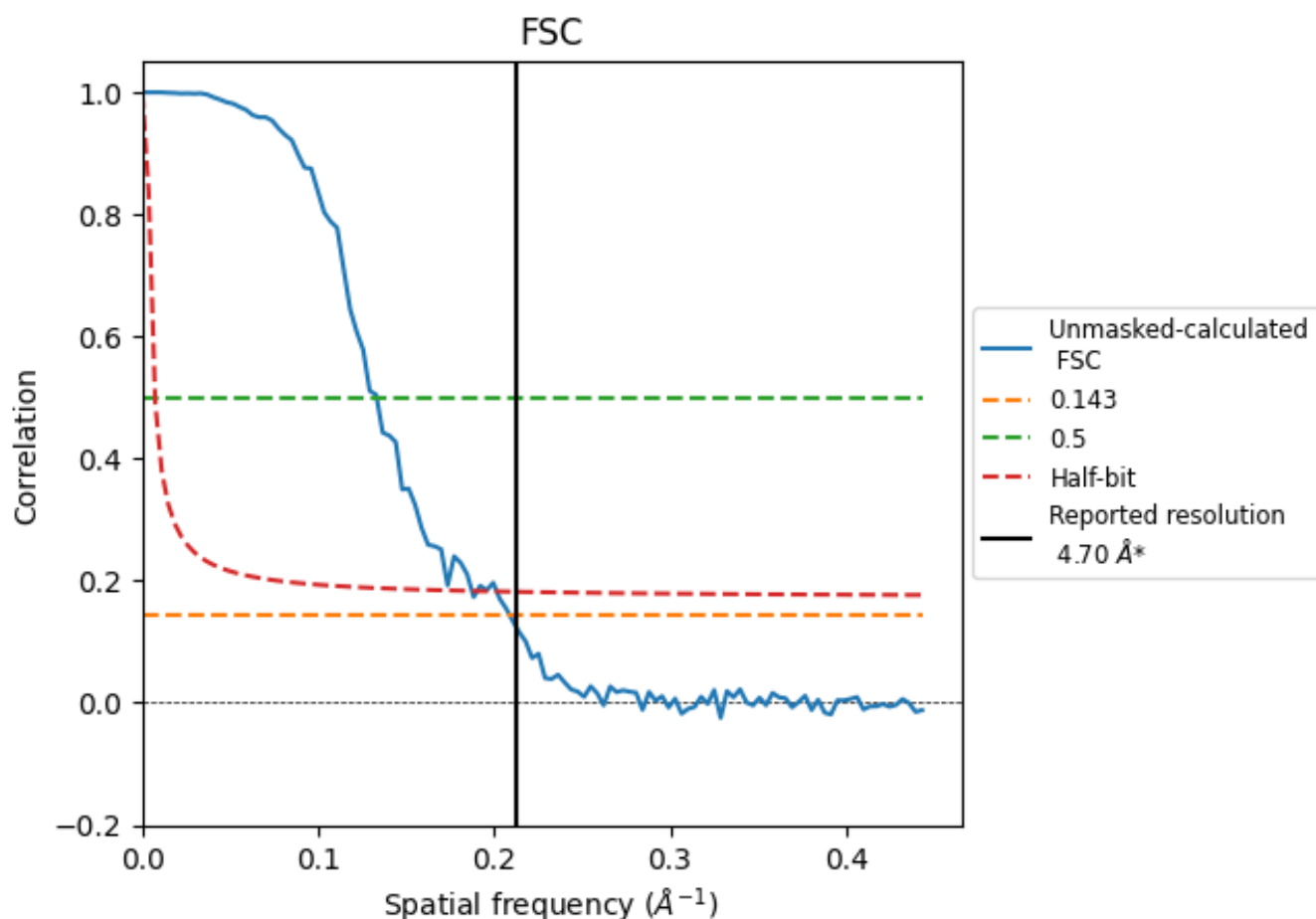


\*Reported resolution corresponds to spatial frequency of 0.213 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.213  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

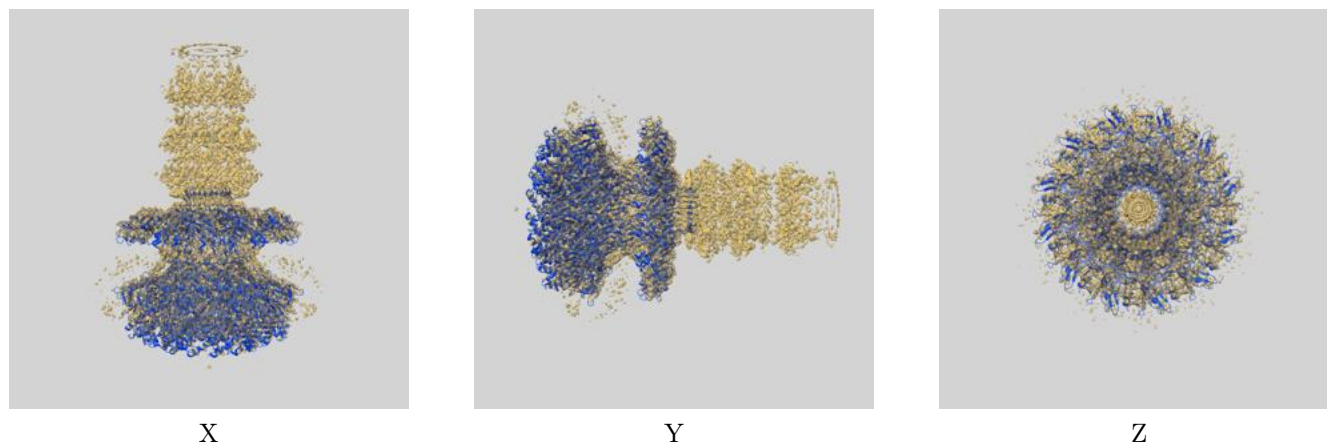
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.70                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 4.78                               | 7.51 | 5.34     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

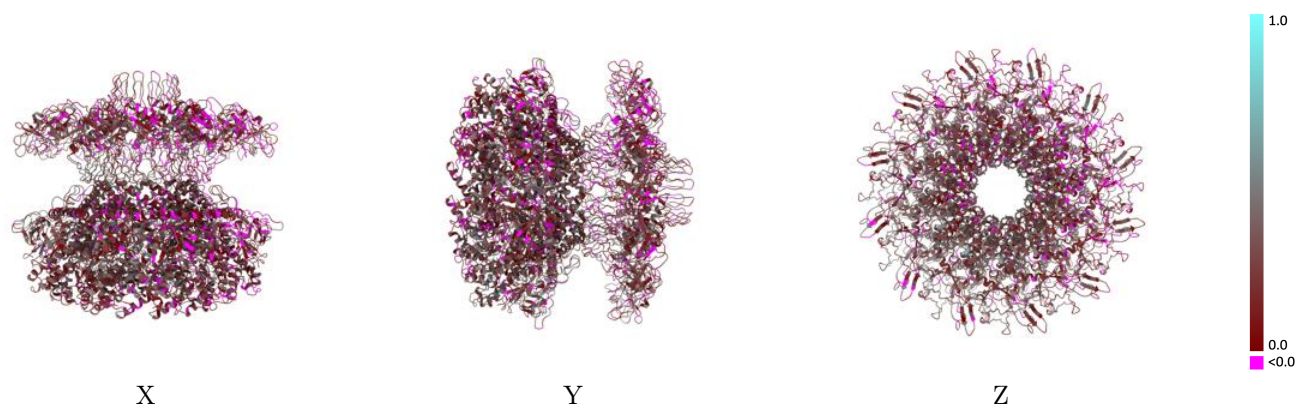
This section contains information regarding the fit between EMDB map EMD-34250 and PDB model 8GTD. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



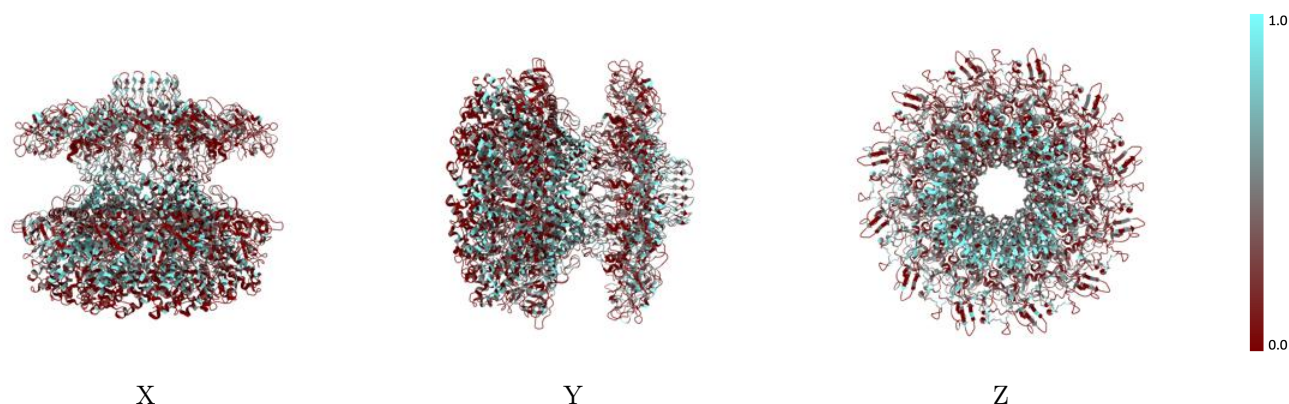
The images above show the 3D surface view of the map at the recommended contour level 0.0302 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

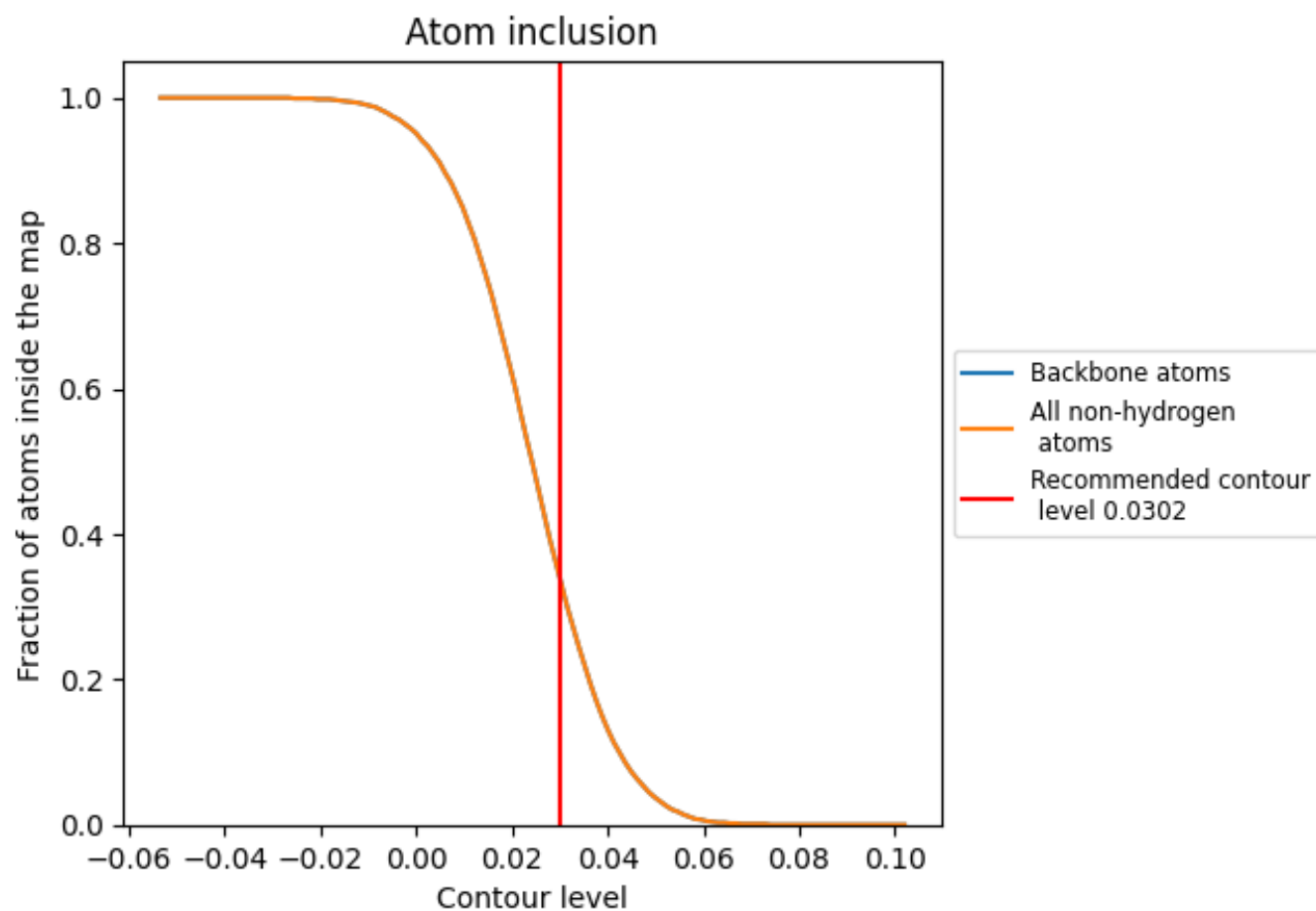
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0302).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 33% of all backbone atoms, 33% 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 (0.0302) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.3340   |  0.2380   |
| A     |  0.3310   |  0.2610   |
| B     |  0.3080   |  0.2390   |
| C     |  0.2740   |  0.2090   |
| D     |  0.2710   |  0.1910   |
| E     |  0.2740   |  0.1890   |
| F     |  0.2970   |  0.2020   |
| G     |  0.3070   |  0.2310   |
| H     |  0.3420   |  0.2570   |
| I     |  0.3850   |  0.2850   |
| J     |  0.3870   |  0.2900   |
| K     |  0.3820   |  0.2890   |
| L     |  0.3640   |  0.2830   |
| M     |  0.3170   |  0.2110   |
| N     |  0.3160  |  0.1880  |
| O     |  0.2870 |  0.1660 |
| P     |  0.2680 |  0.1600 |
| Q     |  0.2920 |  0.1740 |
| R     |  0.3390 |  0.2110 |
| S     |  0.3830 |  0.2550 |
| T     |  0.4150 |  0.2730 |
| U     |  0.4120 |  0.2730 |
| V     |  0.4240 |  0.2610 |
| W     |  0.4000 |  0.2500 |
| X     |  0.3550 |  0.2400 |

