



## Full wwPDB EM Validation Report ⓘ

Jul 21, 2026 – 01:49 pm BST

PDB ID : 9SPU / pdb\_00009spu  
EMDB ID : EMD-55096  
Title : Echovirus 18 particle missing one pentamer in situ, symmetrized reconstruction (C5)  
Authors : Mukhamedova, L.; Plevka, P.  
Deposited on : 2025-09-18  
Resolution : 6.50 Å(reported)  
Based on initial model : 6hbk

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:

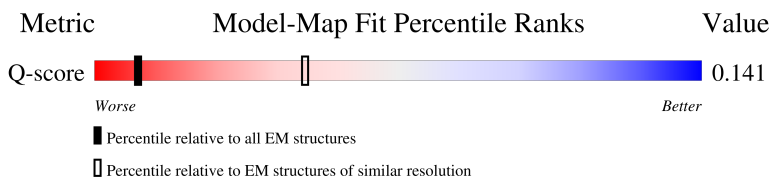
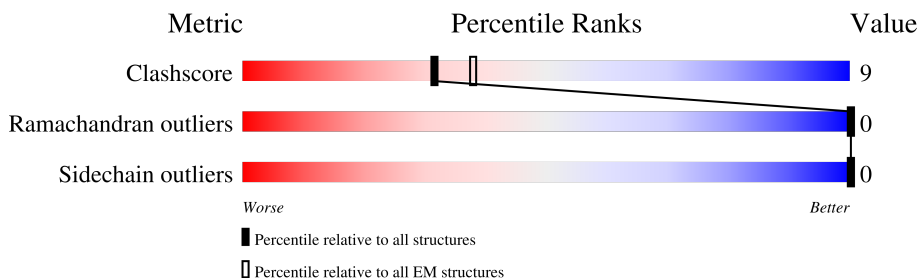
EMDB validation analysis : 0.0.1.dev133  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 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 6.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



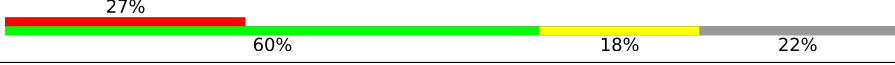
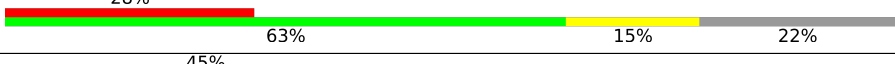
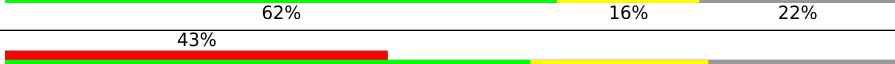
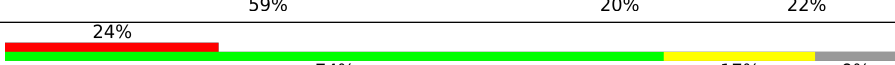
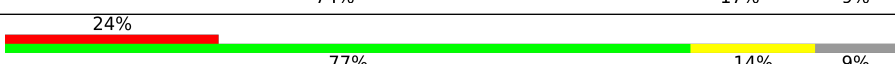
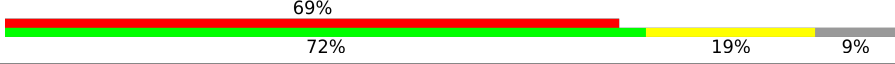
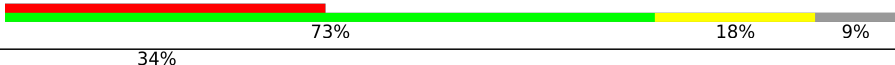
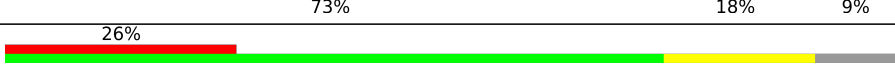
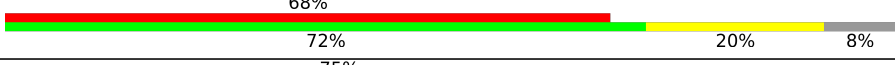
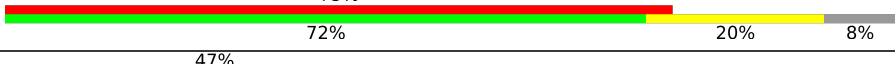
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 556 ( 6.00 - 7.00 )                                      |

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

| Mol | Chain | Length | Quality of chain                                                         |
|-----|-------|--------|--------------------------------------------------------------------------|
| 1   | A     | 287    | <div> <div>22%</div> <div>64%</div> <div>14%</div> <div>22%</div> </div> |
| 1   | D     | 287    | <div> <div>26%</div> <div>61%</div> <div>17%</div> <div>22%</div> </div> |
| 1   | G     | 287    | <div> <div>51%</div> <div>61%</div> <div>17%</div> <div>22%</div> </div> |
| 1   | J     | 287    | <div> <div>54%</div> <div>61%</div> <div>17%</div> <div>22%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | M     | 287    |    |
| 1   | P     | 287    |    |
| 1   | S     | 287    |    |
| 1   | V     | 287    |    |
| 1   | Y     | 287    |    |
| 1   | b     | 287    |    |
| 1   | e     | 287    |    |
| 2   | C     | 239    |    |
| 2   | F     | 239    |    |
| 2   | I     | 239    |    |
| 2   | L     | 239    |   |
| 2   | O     | 239    |  |
| 2   | R     | 239    |  |
| 2   | U     | 239    |  |
| 2   | X     | 239    |  |
| 2   | a     | 239    |  |
| 2   | d     | 239    |  |
| 2   | g     | 239    |  |
| 3   | B     | 260    |  |
| 3   | E     | 260    |  |
| 3   | H     | 260    |  |
| 3   | K     | 260    |  |
| 3   | N     | 260    |  |
| 3   | Q     | 260    |  |
| 3   | T     | 260    |  |

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| Mol | Chain | Length | Quality of chain                                                                                                          |
|-----|-------|--------|---------------------------------------------------------------------------------------------------------------------------|
| 3   | W     | 260    | <div><div>51%</div><div><div></div><div></div><div></div><div></div></div><div>71%</div><div>21%</div><div>8%</div></div> |
| 3   | Z     | 260    | <div><div>38%</div><div><div></div><div></div><div></div><div></div></div><div>72%</div><div>20%</div><div>8%</div></div> |
| 3   | c     | 260    | <div><div>35%</div><div><div></div><div></div><div></div><div></div></div><div>71%</div><div>21%</div><div>8%</div></div> |
| 3   | f     | 260    | <div><div>47%</div><div><div></div><div></div><div></div><div></div></div><div>72%</div><div>19%</div><div>8%</div></div> |

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 57156 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 Echovirus 18 viral protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |
| 1   | e     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |
| 1   | b     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |
| 1   | Y     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |
| 1   | V     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |
| 1   | S     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |
| 1   | P     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |
| 1   | M     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |
| 1   | J     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |
| 1   | G     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |
| 1   | D     | 224      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1741  | 1117 | 305 | 305 | 14 |         |       |

- Molecule 2 is a protein called Echovirus 18 viral protein 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | g     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |
| 2   | d     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |
| 2   | a     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |
| 2   | X     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | U     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |
| 2   | R     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |
| 2   | O     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |
| 2   | L     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |
| 2   | I     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |
| 2   | F     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |
| 2   | C     | 218      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1634  | 1045 | 265 | 308 | 16 |         |       |

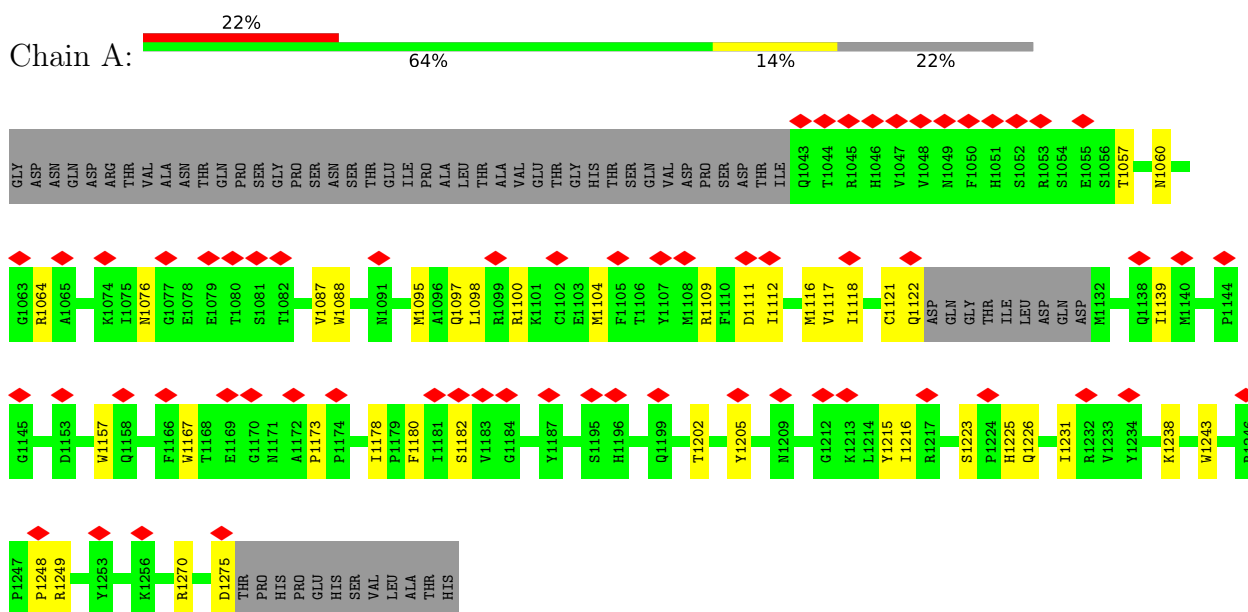
- Molecule 3 is a protein called Echovirus 18 viral protein 2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | f     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |
| 3   | c     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |
| 3   | Z     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |
| 3   | W     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |
| 3   | T     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |
| 3   | Q     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |
| 3   | N     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |
| 3   | K     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |
| 3   | H     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |
| 3   | E     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |
| 3   | B     | 238      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1821  | 1172 | 302 | 332 | 15 |         |       |

### 3 Residue-property plots

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

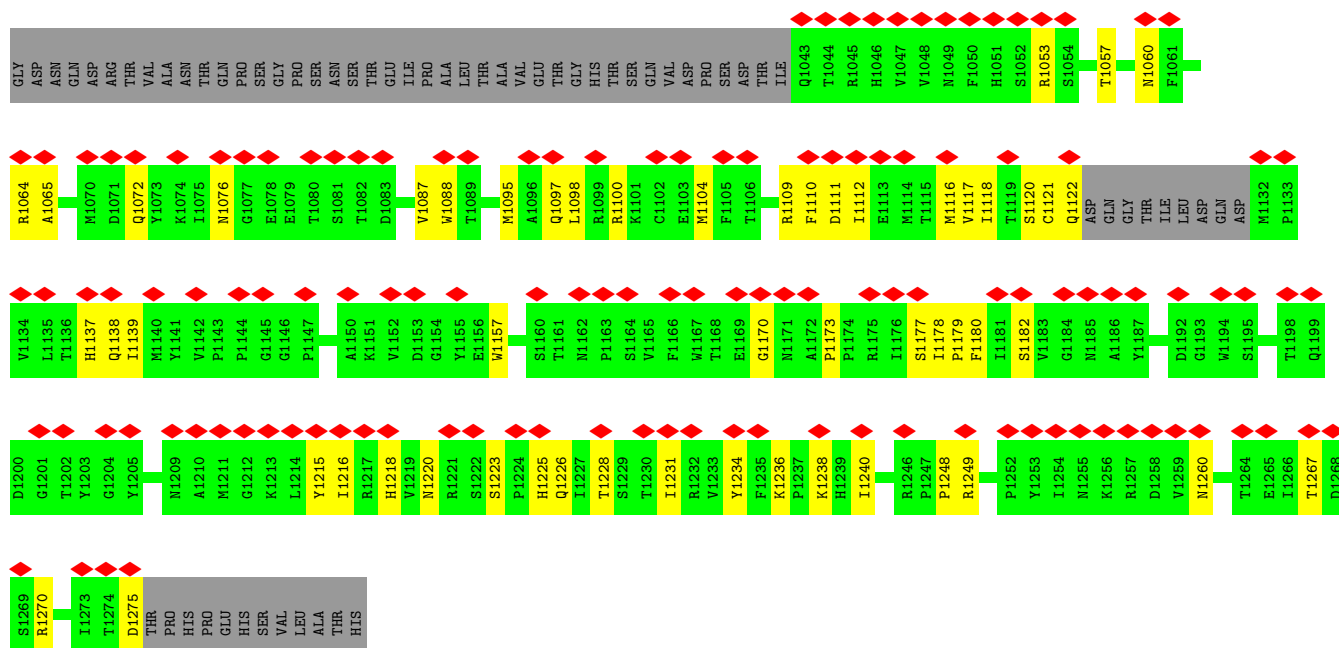
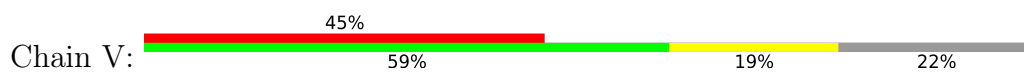
#### • Molecule 1: Echovirus 18 viral protein 1



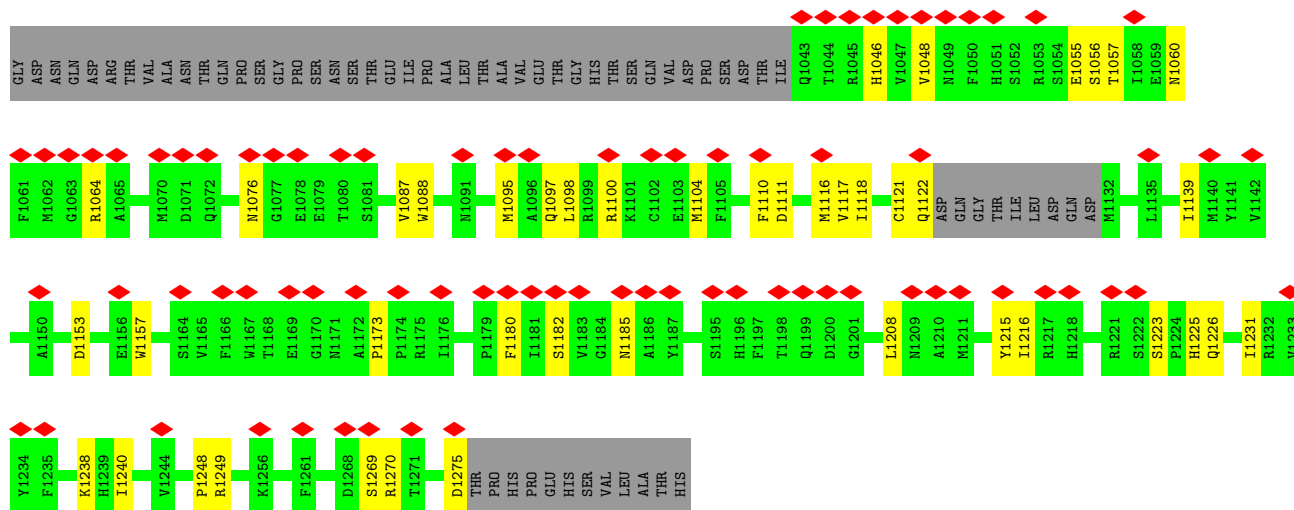
#### • Molecule 1: Echovirus 18 viral protein 1



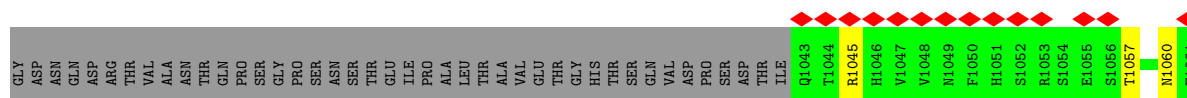


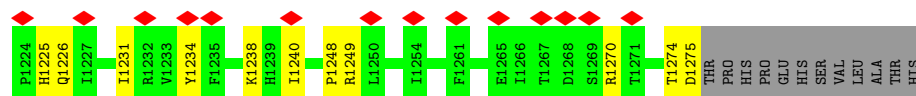
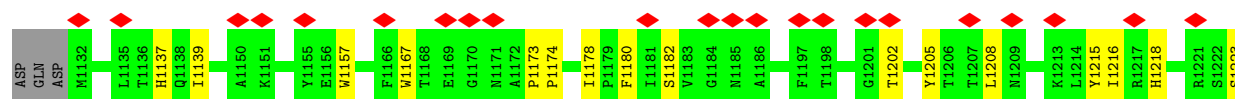
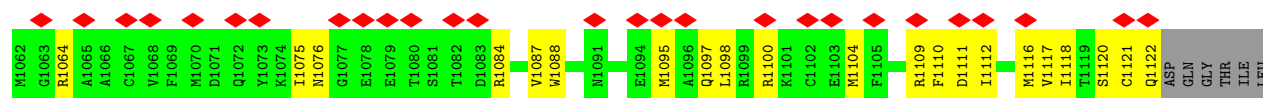


• Molecule 1: Echovirus 18 viral protein 1

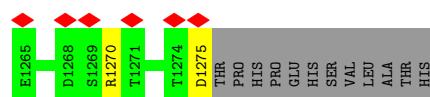
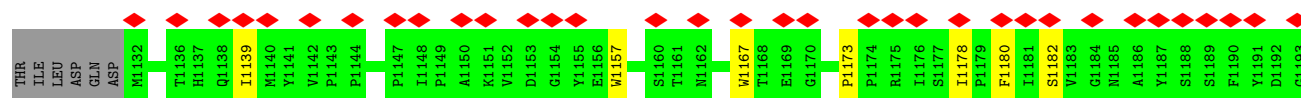
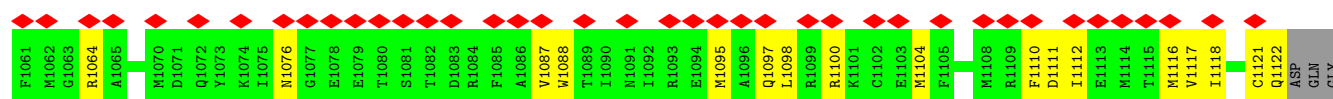
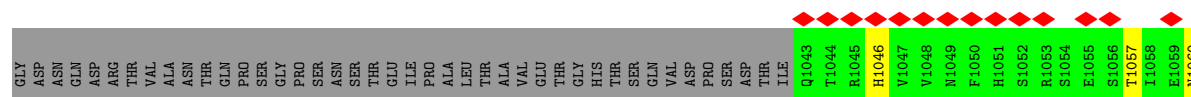


• Molecule 1: Echovirus 18 viral protein 1

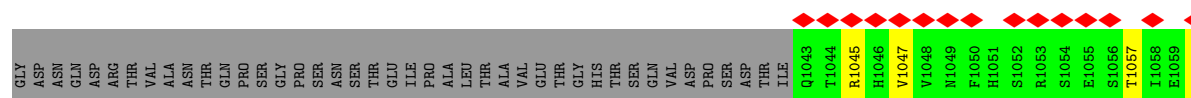


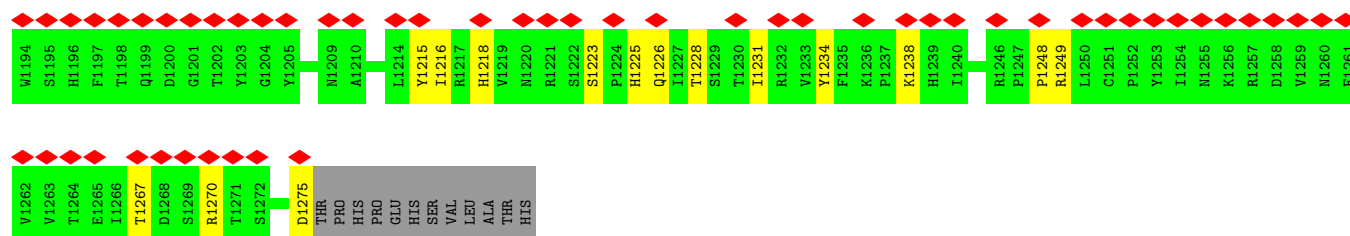


• Molecule 1: Echovirus 18 viral protein 1

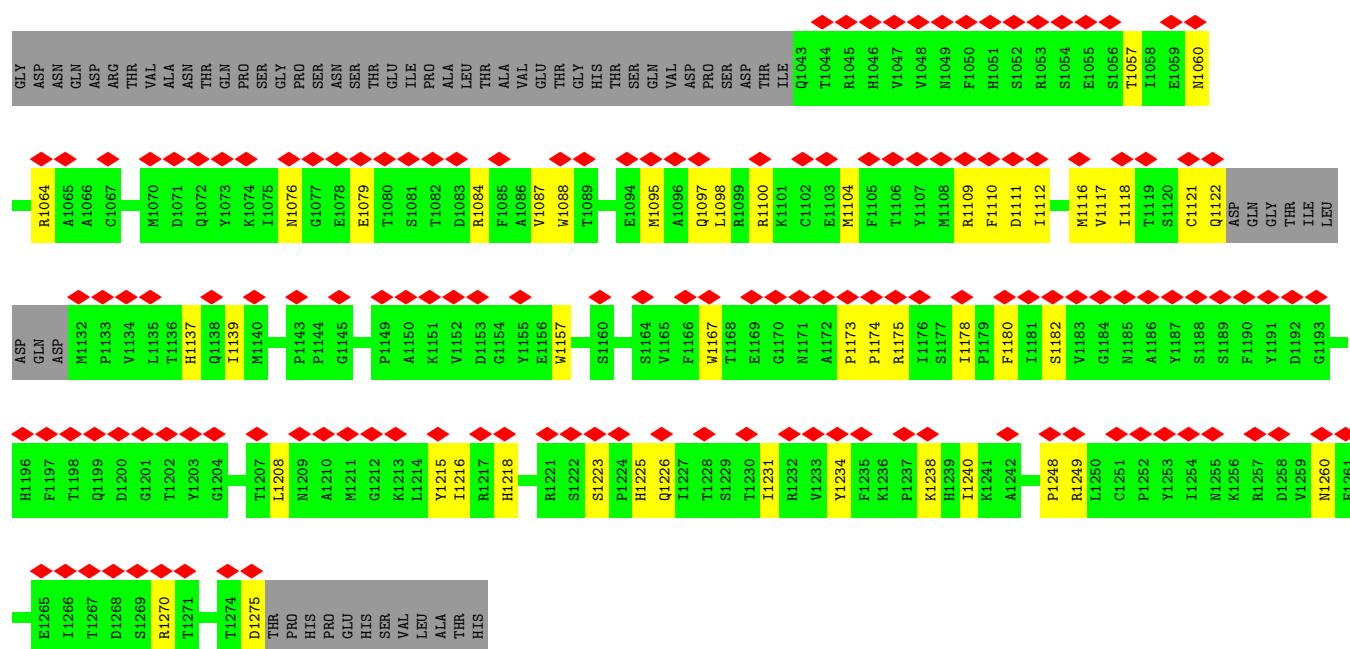


• Molecule 1: Echovirus 18 viral protein 1

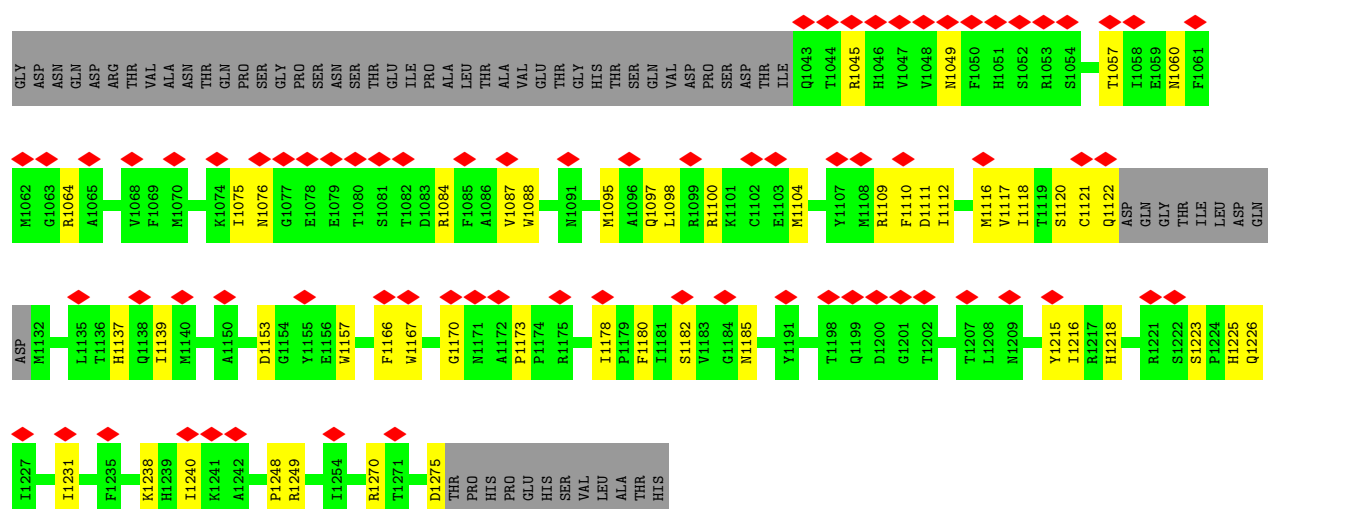




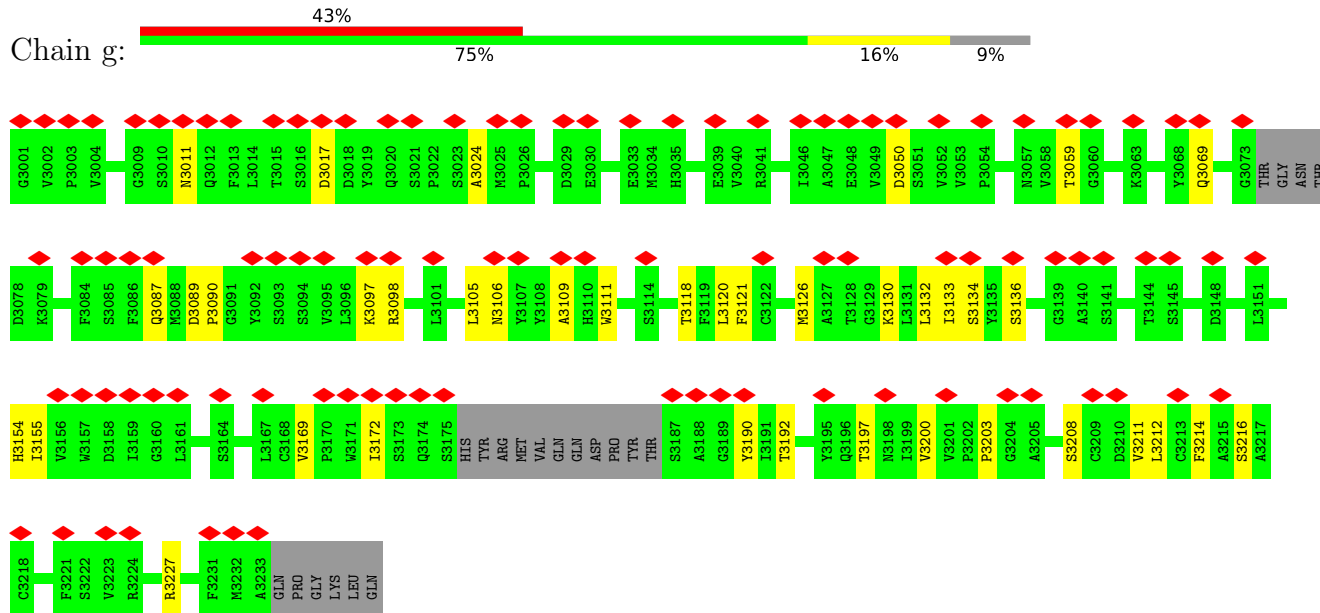
• Molecule 1: Echovirus 18 viral protein 1



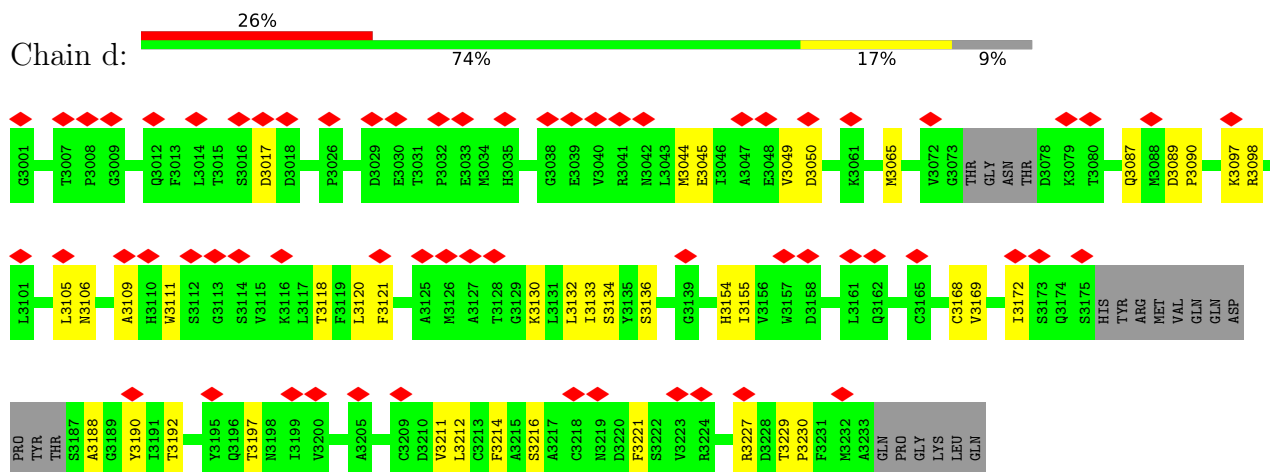
• Molecule 1: Echovirus 18 viral protein 1



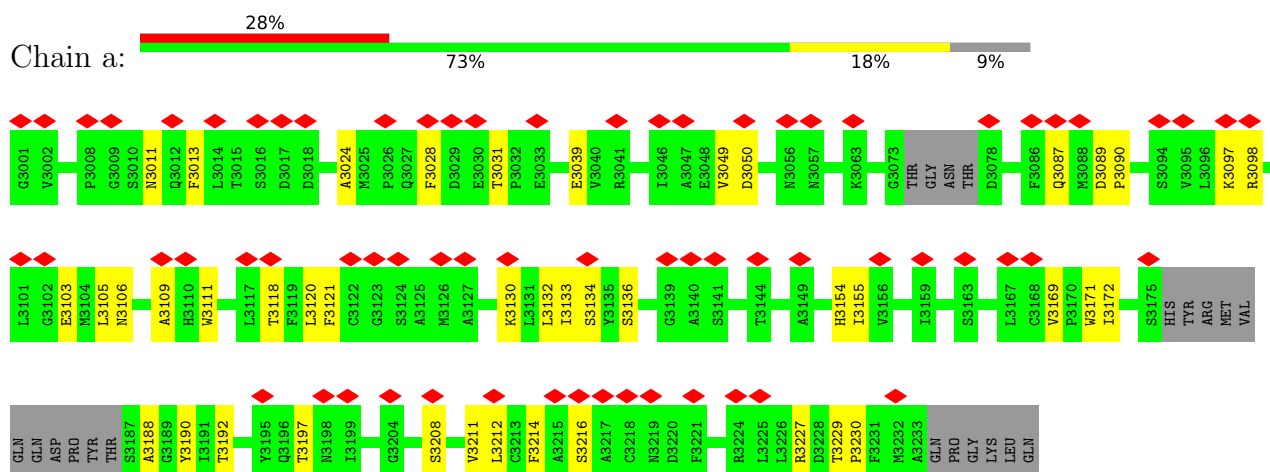
- Molecule 2: Echovirus 18 viral protein 3



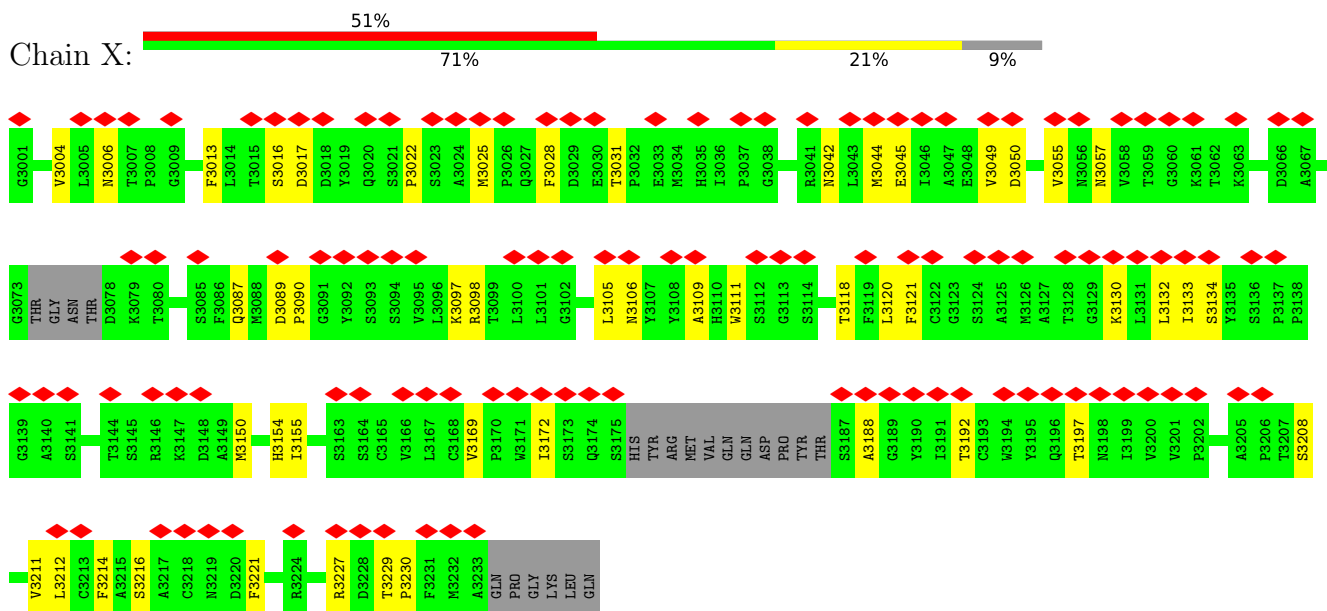
- Molecule 2: Echovirus 18 viral protein 3



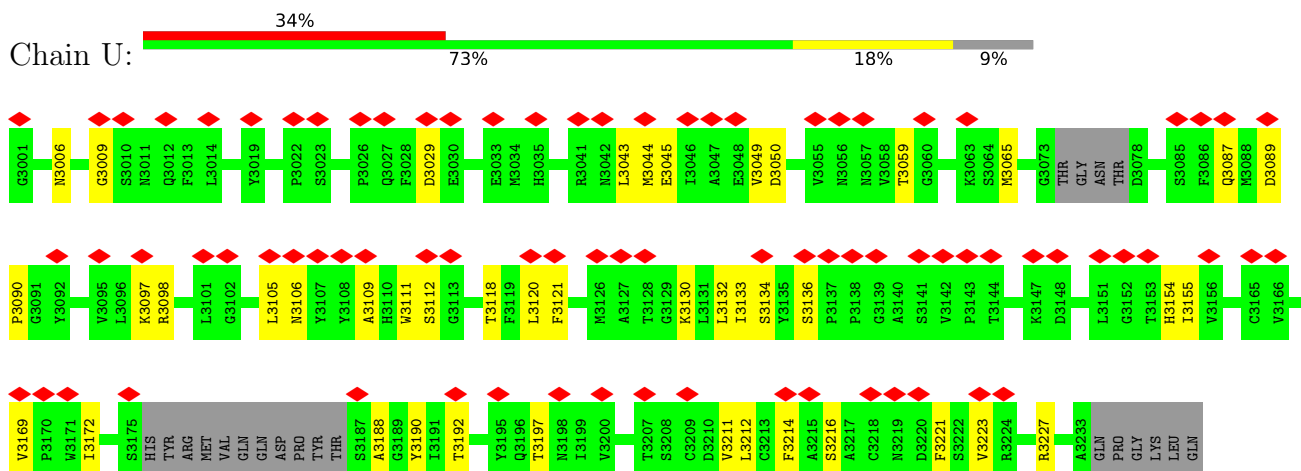
- Molecule 2: Echovirus 18 viral protein 3



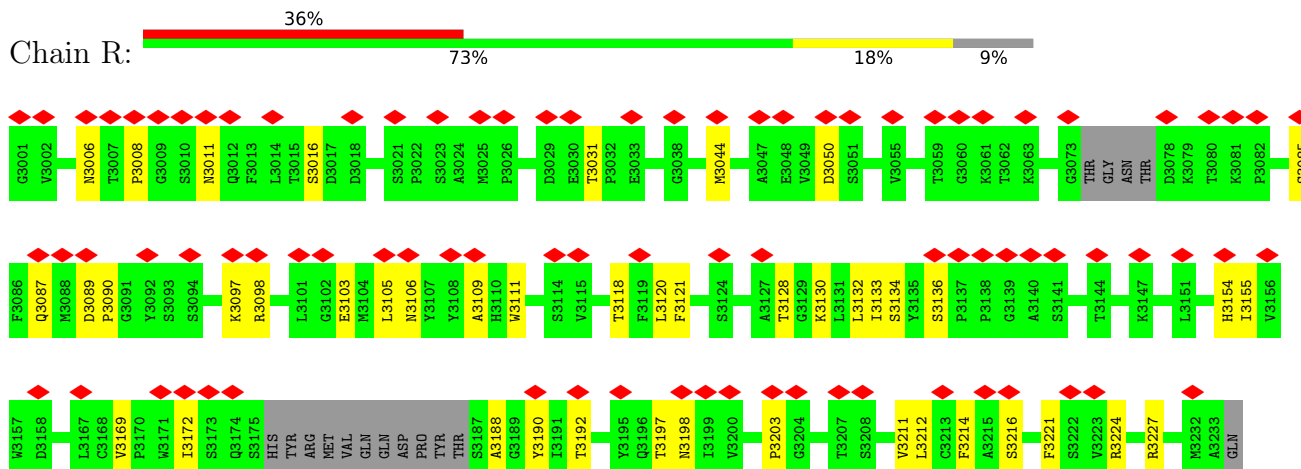
• Molecule 2: Echovirus 18 viral protein 3



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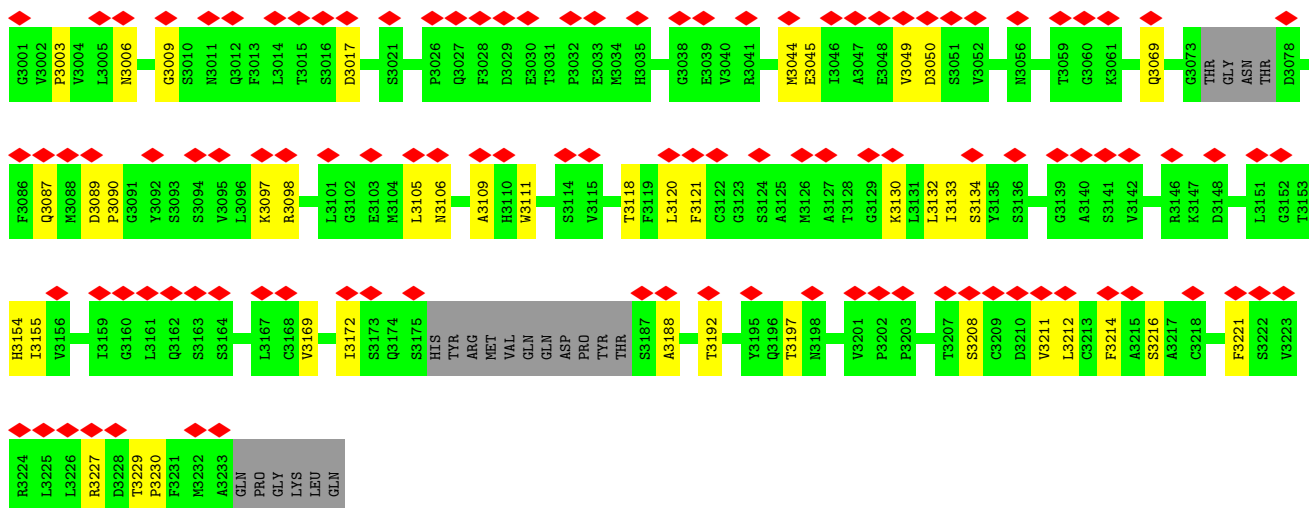
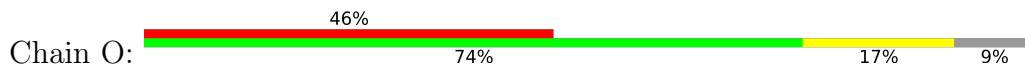


• Molecule 2: Echovirus 18 viral protein 3

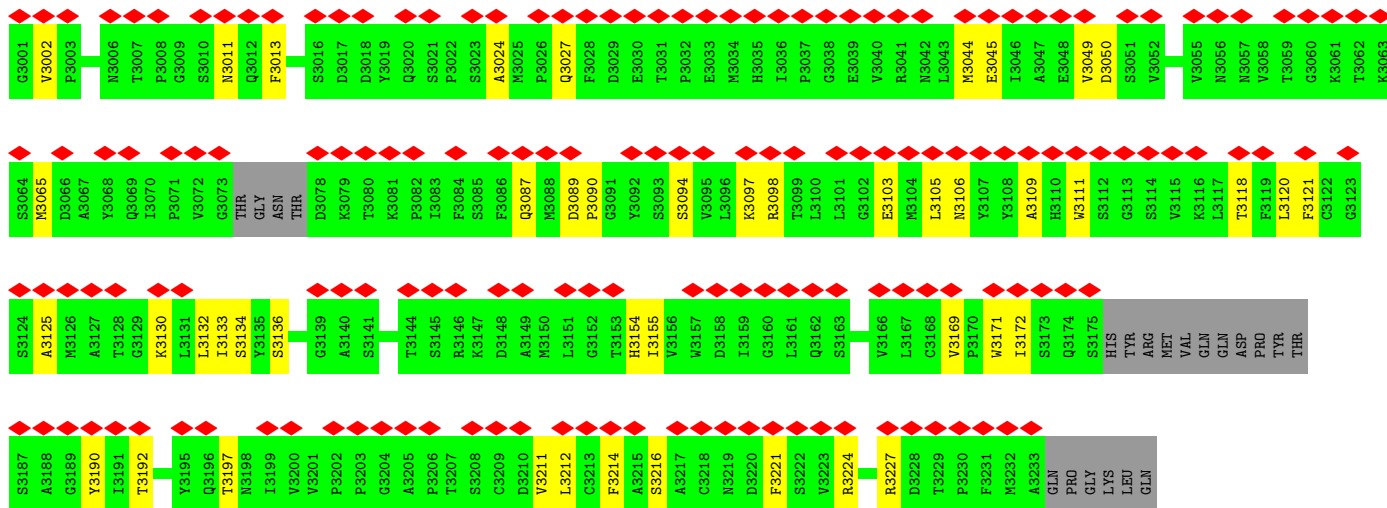


PRO  
GLY  
LYS  
LEU  
GLN

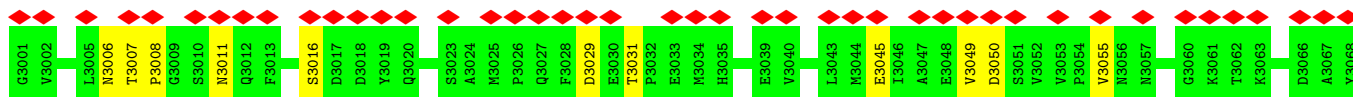
• Molecule 2: Echovirus 18 viral protein 3

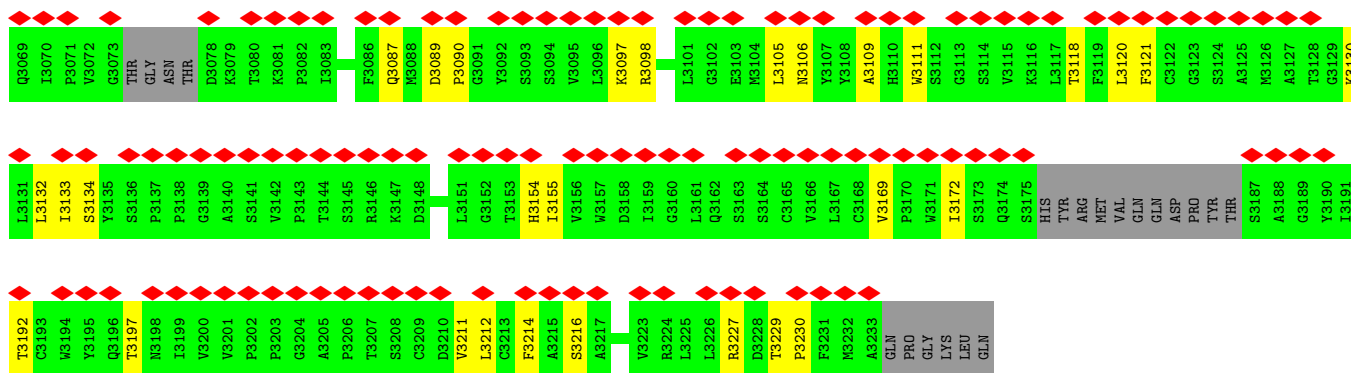


• Molecule 2: Echovirus 18 viral protein 3

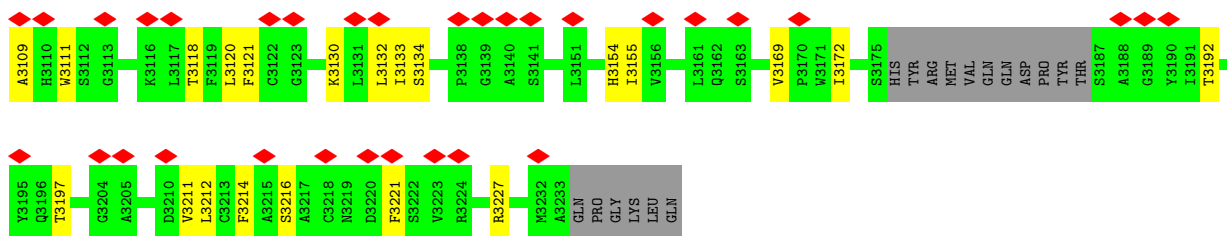


• Molecule 2: Echovirus 18 viral protein 3

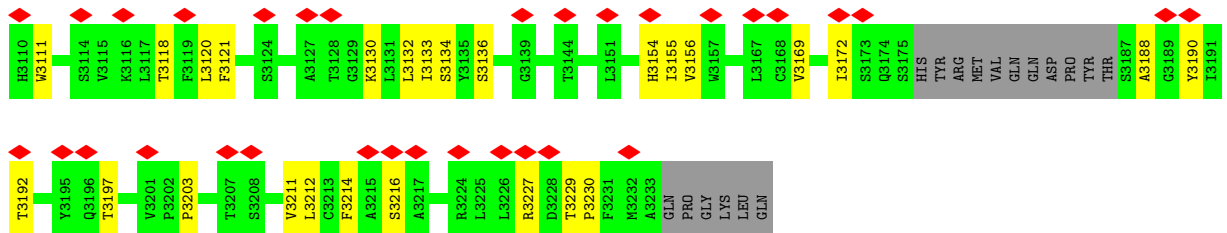
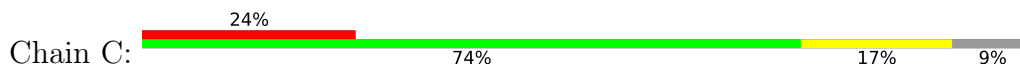




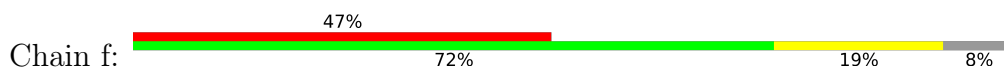
• Molecule 2: Echovirus 18 viral protein 3

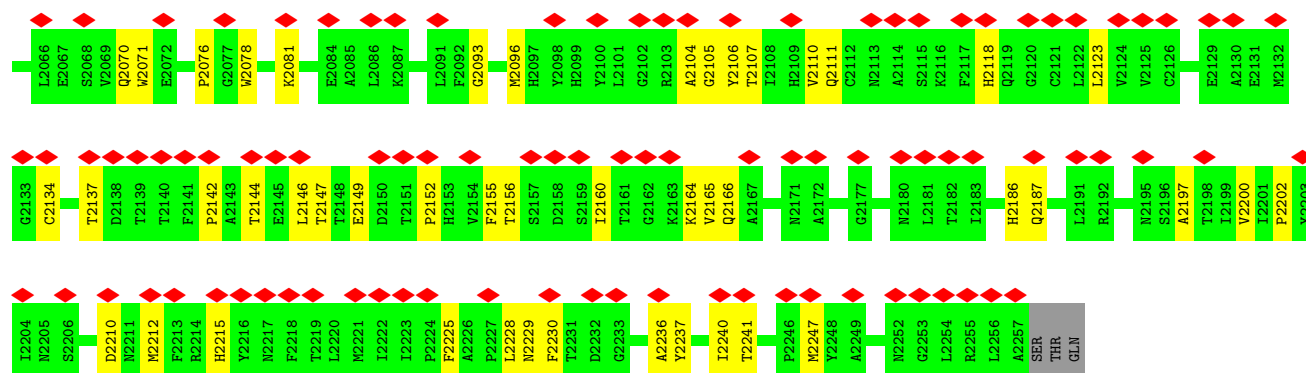


• Molecule 2: Echovirus 18 viral protein 3

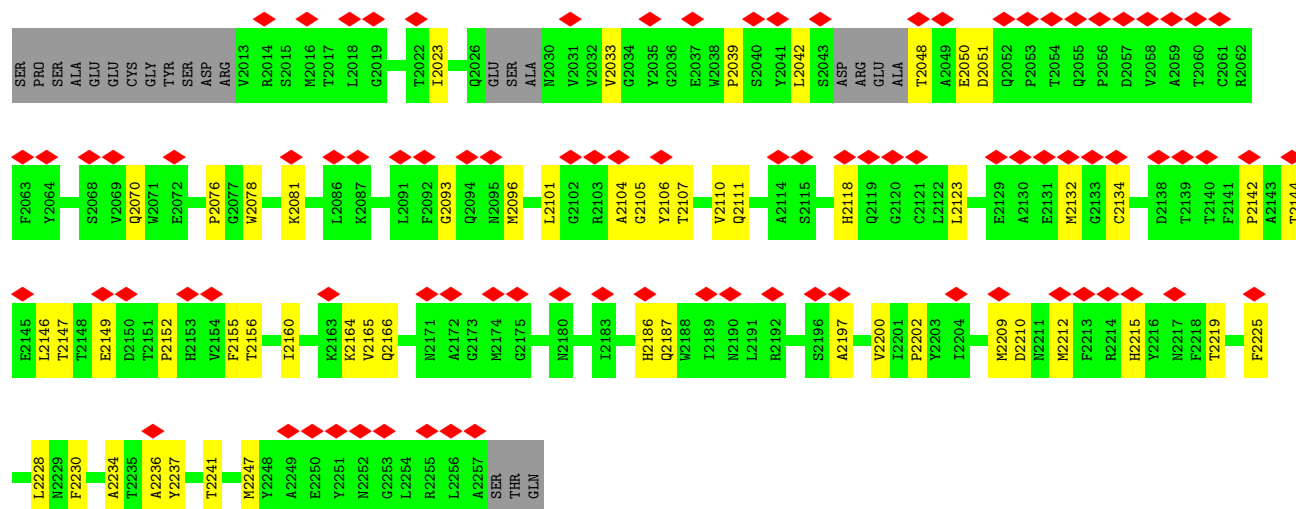


• Molecule 3: Echovirus 18 viral protein 2

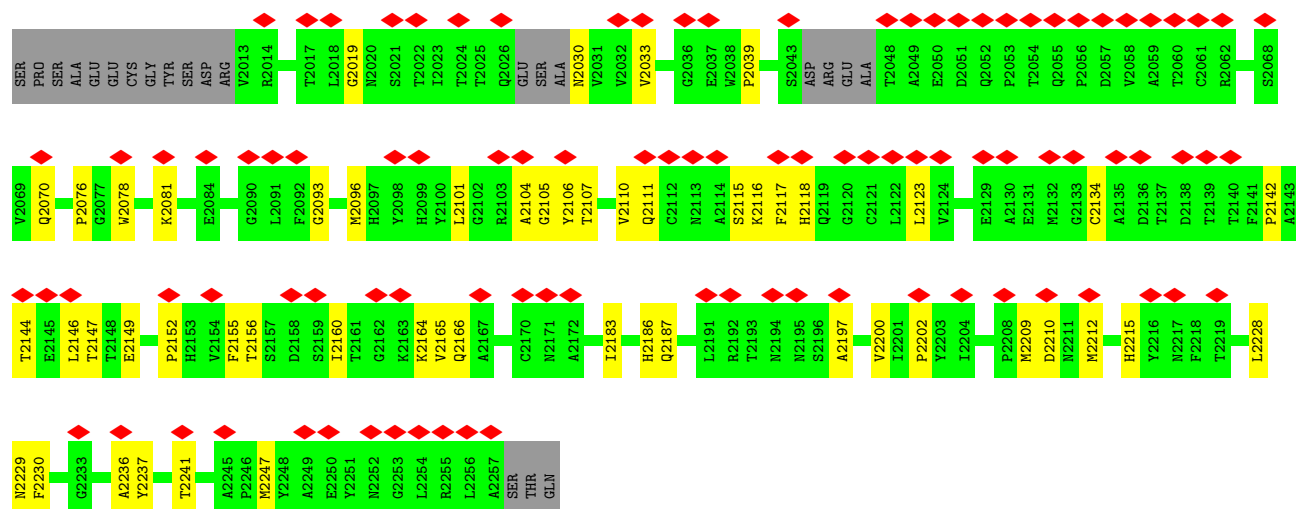
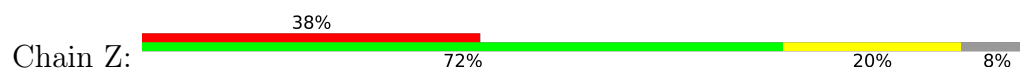




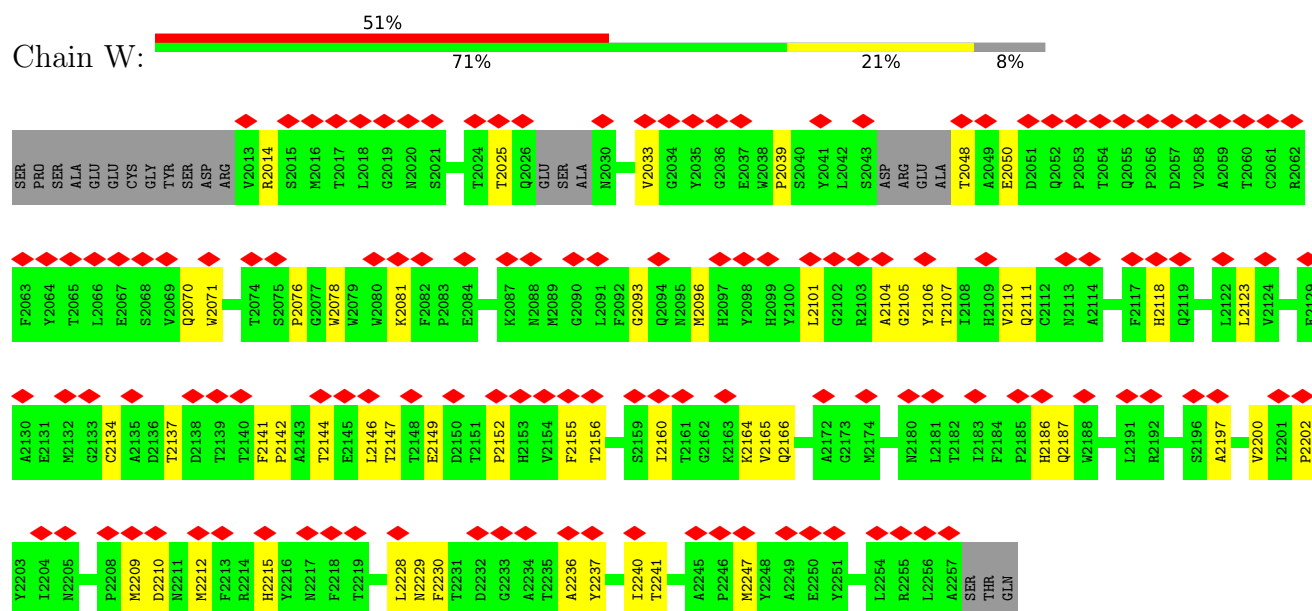
• Molecule 3: Echovirus 18 viral protein 2



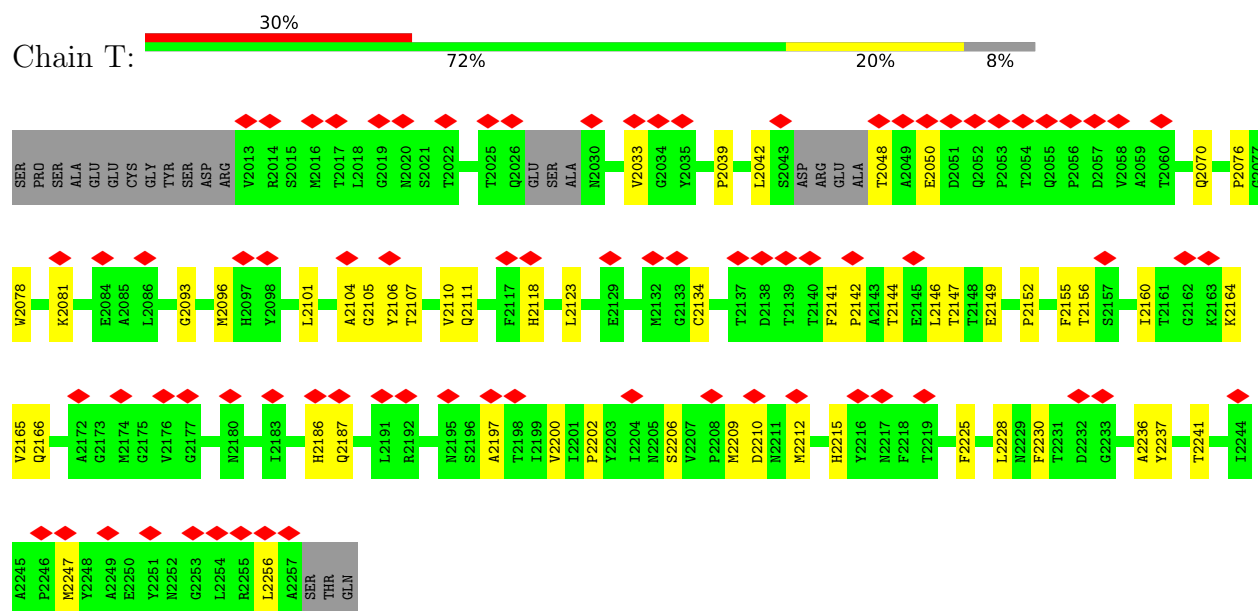
• Molecule 3: Echovirus 18 viral protein 2



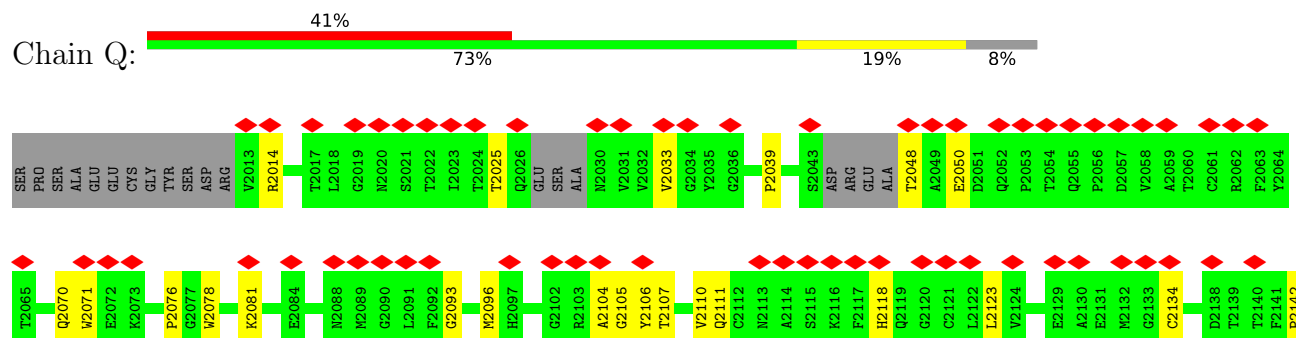
## Chain W:

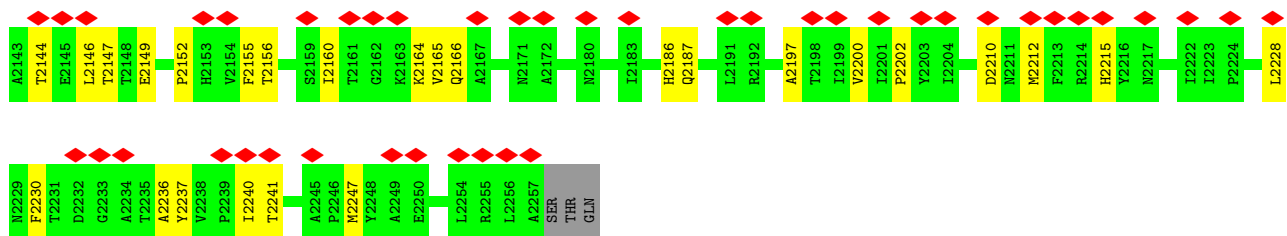


Chain T:

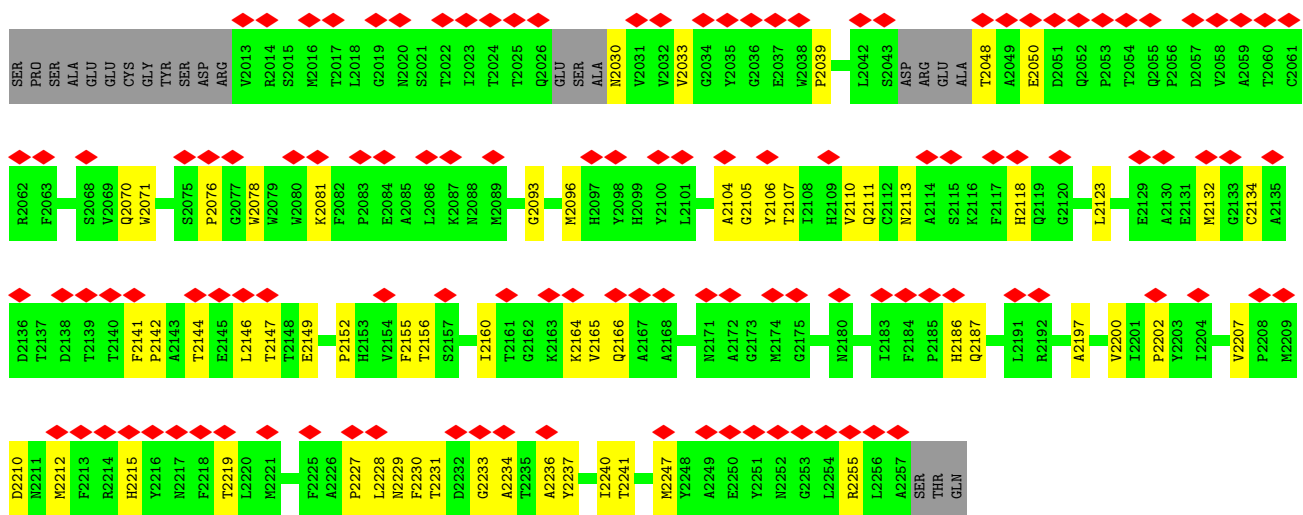


## Chain Q:

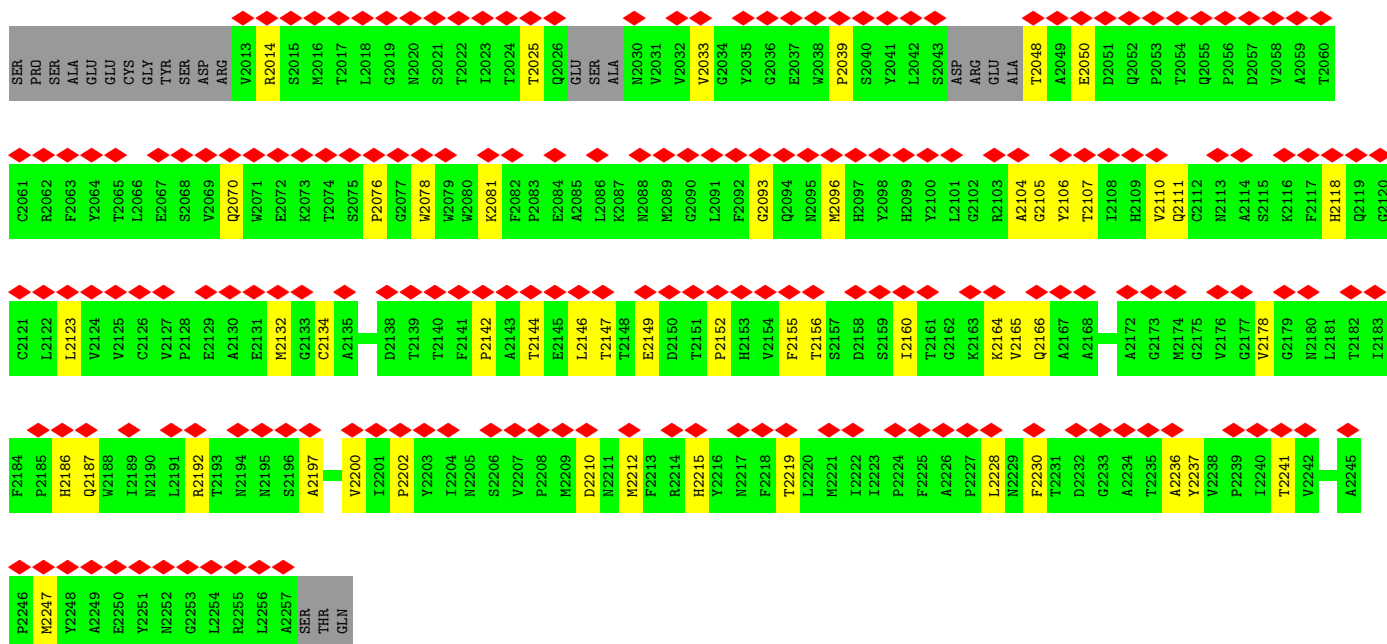
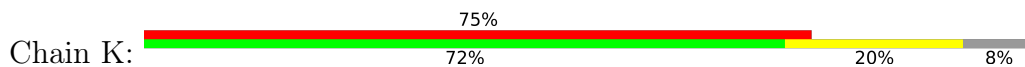




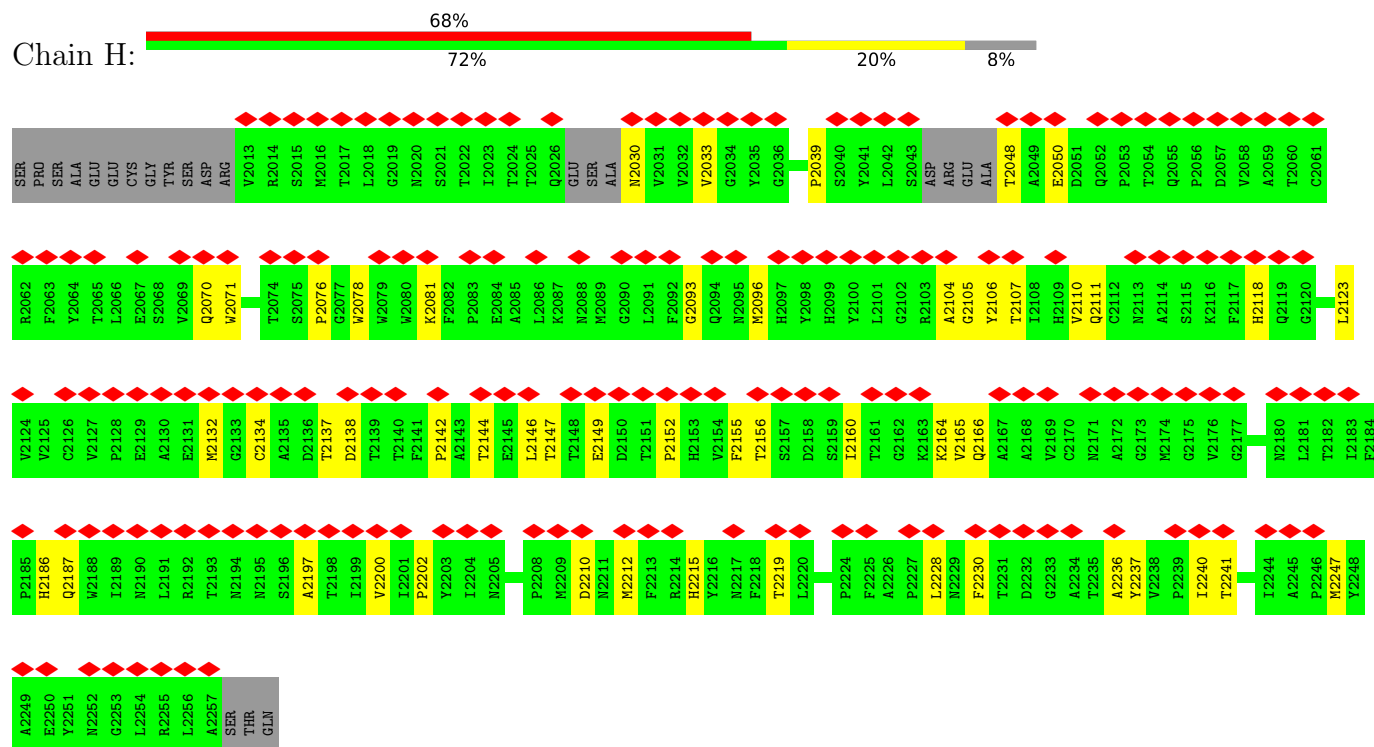
• Molecule 3: Echovirus 18 viral protein 2



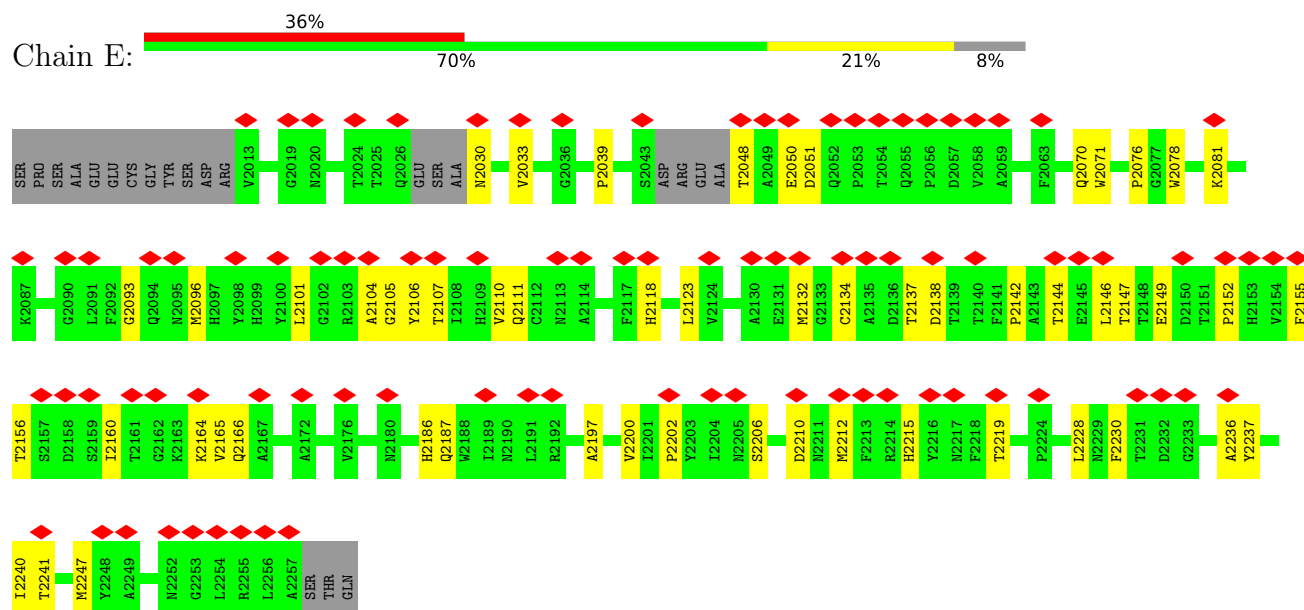
• Molecule 3: Echovirus 18 viral protein 2



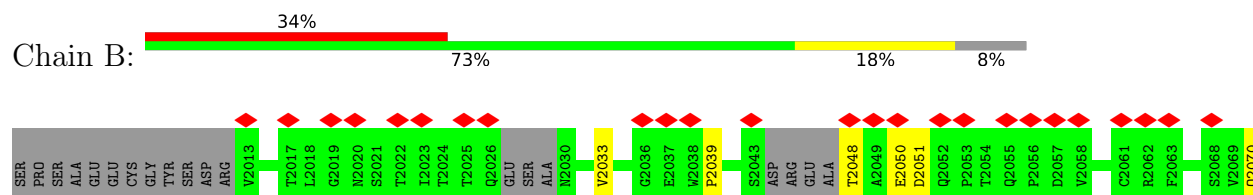
## Chain H:

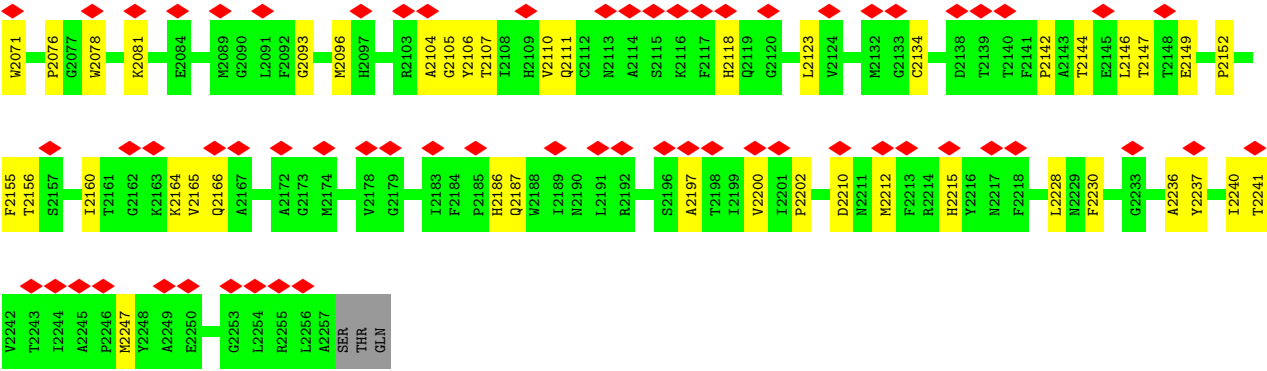


Chain E:



Chain B:





## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 3896                                    | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 34                                      | Depositor |
| Minimum defocus (nm)                 | 2500                                    | Depositor |
| Maximum defocus (nm)                 | 4500                                    | Depositor |
| Magnification                        | 42000                                   | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 10.368                                  | Depositor |
| Minimum map value                    | -7.422                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.827                                   | Depositor |
| Recommended contour level            | 3                                       | Depositor |
| Map size (Å)                         | 532.60034, 532.60034, 532.60034         | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 2.08047, 2.08047, 2.08047               | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 1   | D     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 1   | G     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 1   | J     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 1   | M     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 1   | P     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 1   | S     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 1   | V     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 1   | Y     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 1   | b     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 1   | e     | 0.08         | 0/1791      | 0.24        | 0/2442          |
| 2   | C     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 2   | F     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 2   | I     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 2   | L     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 2   | O     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 2   | R     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 2   | U     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 2   | X     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 2   | a     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 2   | d     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 2   | g     | 0.08         | 0/1676      | 0.23        | 0/2287          |
| 3   | B     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| 3   | E     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| 3   | H     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| 3   | K     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| 3   | N     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| 3   | Q     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| 3   | T     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| 3   | W     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| 3   | Z     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| 3   | c     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| 3   | f     | 0.09         | 0/1874      | 0.30        | 1/2567 (0.0%)   |
| All | All   | 0.09         | 0/58751     | 0.26        | 11/80256 (0.0%) |

There are no bond length outliers.

All (11) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 3   | Q     | 2149 | GLU  | CB-CA-C | -5.24 | 110.10      | 117.23   |
| 3   | H     | 2149 | GLU  | CB-CA-C | -5.23 | 110.11      | 117.23   |
| 3   | E     | 2149 | GLU  | CB-CA-C | -5.23 | 110.12      | 117.23   |
| 3   | Z     | 2149 | GLU  | CB-CA-C | -5.22 | 110.12      | 117.23   |
| 3   | T     | 2149 | GLU  | CB-CA-C | -5.22 | 110.13      | 117.23   |
| 3   | f     | 2149 | GLU  | CB-CA-C | -5.21 | 110.14      | 117.23   |
| 3   | B     | 2149 | GLU  | CB-CA-C | -5.21 | 110.14      | 117.23   |
| 3   | K     | 2149 | GLU  | CB-CA-C | -5.20 | 110.16      | 117.23   |
| 3   | c     | 2149 | GLU  | CB-CA-C | -5.19 | 110.17      | 117.23   |
| 3   | W     | 2149 | GLU  | CB-CA-C | -5.18 | 110.18      | 117.23   |
| 3   | N     | 2149 | GLU  | CB-CA-C | -5.17 | 110.20      | 117.23   |

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     | 1741  | 0        | 1659     | 26      | 0            |
| 1   | D     | 1741  | 0        | 1659     | 42      | 0            |
| 1   | G     | 1741  | 0        | 1659     | 36      | 0            |
| 1   | J     | 1741  | 0        | 1659     | 34      | 0            |
| 1   | M     | 1741  | 0        | 1659     | 31      | 0            |
| 1   | P     | 1741  | 0        | 1659     | 37      | 0            |
| 1   | S     | 1741  | 0        | 1659     | 29      | 0            |
| 1   | V     | 1741  | 0        | 1659     | 44      | 0            |
| 1   | Y     | 1741  | 0        | 1659     | 31      | 0            |
| 1   | b     | 1741  | 0        | 1659     | 34      | 0            |
| 1   | e     | 1741  | 0        | 1659     | 42      | 0            |
| 2   | C     | 1634  | 0        | 1596     | 28      | 0            |
| 2   | F     | 1634  | 0        | 1596     | 21      | 0            |
| 2   | I     | 1634  | 0        | 1596     | 30      | 0            |
| 2   | L     | 1634  | 0        | 1596     | 34      | 0            |
| 2   | O     | 1634  | 0        | 1596     | 32      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | R     | 1634  | 0        | 1596     | 36      | 0            |
| 2   | U     | 1634  | 0        | 1596     | 31      | 0            |
| 2   | X     | 1634  | 0        | 1596     | 39      | 0            |
| 2   | a     | 1634  | 0        | 1596     | 33      | 0            |
| 2   | d     | 1634  | 0        | 1596     | 27      | 0            |
| 2   | g     | 1634  | 0        | 1596     | 29      | 0            |
| 3   | B     | 1821  | 0        | 1739     | 30      | 0            |
| 3   | E     | 1821  | 0        | 1739     | 36      | 0            |
| 3   | H     | 1821  | 0        | 1739     | 34      | 0            |
| 3   | K     | 1821  | 0        | 1739     | 33      | 0            |
| 3   | N     | 1821  | 0        | 1739     | 43      | 0            |
| 3   | Q     | 1821  | 0        | 1739     | 30      | 0            |
| 3   | T     | 1821  | 0        | 1739     | 39      | 0            |
| 3   | W     | 1821  | 0        | 1739     | 36      | 0            |
| 3   | Z     | 1821  | 0        | 1739     | 38      | 0            |
| 3   | c     | 1821  | 0        | 1739     | 40      | 0            |
| 3   | f     | 1821  | 0        | 1739     | 33      | 0            |
| All | All   | 57156 | 0        | 54934    | 978     | 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 9.

All (978) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:a:3011:ASN:H    | 2:R:3006:ASN:HB2  | 1.29                     | 0.97              |
| 1:V:1053:ARG:HD2  | 2:X:3042:ASN:HD21 | 1.38                     | 0.88              |
| 3:c:2209:MET:O    | 1:D:1045:ARG:NH1  | 2.10                     | 0.85              |
| 2:O:3003:PRO:HB3  | 2:I:3007:THR:HG21 | 1.60                     | 0.84              |
| 1:e:1171:ASN:ND2  | 1:V:1170:GLY:O    | 2.14                     | 0.79              |
| 1:V:1270:ARG:NH2  | 2:X:3055:VAL:O    | 2.17                     | 0.77              |
| 2:L:3024:ALA:O    | 2:I:3016:SER:OG   | 2.02                     | 0.77              |
| 3:H:2123:LEU:HD11 | 3:H:2186:HIS:HB2  | 1.68                     | 0.76              |
| 3:E:2123:LEU:HD11 | 3:E:2186:HIS:HB2  | 1.68                     | 0.76              |
| 1:e:1138:GLN:NE2  | 1:V:1234:TYR:OH   | 2.17                     | 0.76              |
| 2:R:3203:PRO:HD3  | 3:N:2234:ALA:HB2  | 1.67                     | 0.76              |
| 3:T:2123:LEU:HD11 | 3:T:2186:HIS:HB2  | 1.68                     | 0.75              |
| 2:L:3011:ASN:H    | 2:I:3006:ASN:HB2  | 1.50                     | 0.75              |
| 3:B:2123:LEU:HD11 | 3:B:2186:HIS:HB2  | 1.68                     | 0.74              |
| 3:Q:2123:LEU:HD11 | 3:Q:2186:HIS:HB2  | 1.68                     | 0.74              |
| 3:f:2123:LEU:HD11 | 3:f:2186:HIS:HB2  | 1.68                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:W:2123:LEU:HD11 | 3:W:2186:HIS:HB2  | 1.68                     | 0.74              |
| 3:Z:2123:LEU:HD11 | 3:Z:2186:HIS:HB2  | 1.68                     | 0.74              |
| 3:c:2123:LEU:HD11 | 3:c:2186:HIS:HB2  | 1.68                     | 0.74              |
| 3:N:2123:LEU:HD11 | 3:N:2186:HIS:HB2  | 1.68                     | 0.74              |
| 3:K:2123:LEU:HD11 | 3:K:2186:HIS:HB2  | 1.68                     | 0.74              |
| 2:g:3024:ALA:O    | 2:X:3016:SER:OG   | 2.07                     | 0.73              |
| 2:O:3009:GLY:HA2  | 1:G:1174:PRO:HA   | 1.73                     | 0.70              |
| 2:g:3208:SER:OG   | 3:f:2229:ASN:ND2  | 2.23                     | 0.70              |
| 3:c:2225:PHE:CD1  | 2:d:3065:MET:HE1  | 2.27                     | 0.69              |
| 1:e:1043:GLN:N    | 1:M:1195:SER:O    | 2.25                     | 0.69              |
| 1:S:1269:SER:HB3  | 2:U:3059:THR:HG22 | 1.75                     | 0.68              |
| 1:S:1046:HIS:CE1  | 1:P:1208:LEU:HD21 | 2.28                     | 0.68              |
| 2:g:3011:ASN:H    | 2:X:3006:ASN:HB2  | 1.58                     | 0.67              |
| 2:a:3024:ALA:O    | 2:R:3016:SER:OG   | 2.12                     | 0.67              |
| 1:S:1185:ASN:ND2  | 3:T:2206:SER:O    | 2.28                     | 0.67              |
| 3:N:2229:ASN:ND2  | 2:O:3208:SER:OG   | 2.28                     | 0.67              |
| 1:D:1100:ARG:NH2  | 2:F:3103:GLU:OE2  | 2.30                     | 0.65              |
| 1:e:1046:HIS:CE1  | 1:M:1208:LEU:HD21 | 2.32                     | 0.65              |
| 2:g:3200:VAL:HG12 | 3:Z:2115:SER:HB3  | 1.79                     | 0.65              |
| 2:O:3006:ASN:HB2  | 2:I:3011:ASN:H    | 1.62                     | 0.64              |
| 2:O:3009:GLY:HA2  | 1:G:1175:ARG:H    | 1.61                     | 0.64              |
| 1:P:1109:ARG:HH22 | 2:R:3031:THR:HB   | 1.63                     | 0.64              |
| 1:V:1236:LYS:NZ   | 2:X:3017:ASP:OD1  | 2.31                     | 0.64              |
| 2:d:3118:THR:HB   | 2:d:3214:PHE:HB2  | 1.81                     | 0.62              |
| 2:O:3118:THR:HB   | 2:O:3214:PHE:HB2  | 1.81                     | 0.62              |
| 2:C:3118:THR:HB   | 2:C:3214:PHE:HB2  | 1.81                     | 0.62              |
| 1:D:1216:ILE:HD13 | 1:D:1231:ILE:HD13 | 1.82                     | 0.62              |
| 1:e:1216:ILE:HD13 | 1:e:1231:ILE:HD13 | 1.82                     | 0.62              |
| 1:P:1216:ILE:HD13 | 1:P:1231:ILE:HD13 | 1.82                     | 0.62              |
| 2:I:3118:THR:HB   | 2:I:3214:PHE:HB2  | 1.82                     | 0.62              |
| 2:F:3118:THR:HB   | 2:F:3214:PHE:HB2  | 1.82                     | 0.62              |
| 1:M:1216:ILE:HD13 | 1:M:1231:ILE:HD13 | 1.82                     | 0.62              |
| 2:L:3118:THR:HB   | 2:L:3214:PHE:HB2  | 1.82                     | 0.62              |
| 1:A:1216:ILE:HD13 | 1:A:1231:ILE:HD13 | 1.82                     | 0.62              |
| 1:G:1216:ILE:HD13 | 1:G:1231:ILE:HD13 | 1.82                     | 0.62              |
| 2:g:3118:THR:HB   | 2:g:3214:PHE:HB2  | 1.82                     | 0.62              |
| 2:U:3118:THR:HB   | 2:U:3214:PHE:HB2  | 1.82                     | 0.62              |
| 1:b:1216:ILE:HD13 | 1:b:1231:ILE:HD13 | 1.82                     | 0.62              |
| 2:R:3118:THR:HB   | 2:R:3214:PHE:HB2  | 1.82                     | 0.62              |
| 1:e:1220:ASN:ND2  | 1:V:1120:SER:O    | 2.32                     | 0.61              |
| 1:Y:1216:ILE:HD13 | 1:Y:1231:ILE:HD13 | 1.82                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:a:3118:THR:HB   | 2:a:3214:PHE:HB2  | 1.82                     | 0.61              |
| 2:X:3028:PHE:HE1  | 2:L:3224:ARG:HE   | 1.48                     | 0.61              |
| 1:J:1216:ILE:HD13 | 1:J:1231:ILE:HD13 | 1.82                     | 0.61              |
| 1:S:1216:ILE:HD13 | 1:S:1231:ILE:HD13 | 1.82                     | 0.61              |
| 2:X:3118:THR:HB   | 2:X:3214:PHE:HB2  | 1.81                     | 0.61              |
| 1:Y:1100:ARG:NH2  | 2:a:3103:GLU:OE2  | 2.33                     | 0.61              |
| 1:b:1049:ASN:HD21 | 3:T:2042:LEU:HD21 | 1.66                     | 0.60              |
| 1:V:1216:ILE:HD13 | 1:V:1231:ILE:HD13 | 1.82                     | 0.60              |
| 3:T:2225:PHE:CD1  | 2:U:3065:MET:HE1  | 2.36                     | 0.60              |
| 2:L:3090:PRO:HB2  | 2:L:3105:LEU:HD22 | 1.84                     | 0.60              |
| 2:d:3090:PRO:HB2  | 2:d:3105:LEU:HD22 | 1.84                     | 0.60              |
| 3:W:2146:LEU:HD21 | 3:W:2164:LYS:HB2  | 1.84                     | 0.60              |
| 3:K:2146:LEU:HD21 | 3:K:2164:LYS:HB2  | 1.84                     | 0.60              |
| 3:T:2146:LEU:HD21 | 3:T:2164:LYS:HB2  | 1.84                     | 0.59              |
| 3:E:2230:PHE:HZ   | 3:E:2236:ALA:HA   | 1.67                     | 0.59              |
| 3:W:2230:PHE:HZ   | 3:W:2236:ALA:HA   | 1.67                     | 0.59              |
| 2:U:3090:PRO:HB2  | 2:U:3105:LEU:HD22 | 1.84                     | 0.59              |
| 2:F:3090:PRO:HB2  | 2:F:3105:LEU:HD22 | 1.84                     | 0.59              |
| 2:g:3090:PRO:HB2  | 2:g:3105:LEU:HD22 | 1.84                     | 0.59              |
| 2:X:3090:PRO:HB2  | 2:X:3105:LEU:HD22 | 1.84                     | 0.59              |
| 3:K:2230:PHE:HZ   | 3:K:2236:ALA:HA   | 1.67                     | 0.59              |
| 2:I:3090:PRO:HB2  | 2:I:3105:LEU:HD22 | 1.84                     | 0.59              |
| 2:C:3090:PRO:HB2  | 2:C:3105:LEU:HD22 | 1.84                     | 0.59              |
| 3:B:2146:LEU:HD21 | 3:B:2164:LYS:HB2  | 1.84                     | 0.59              |
| 1:e:1104:MET:HE1  | 1:e:1248:PRO:HB3  | 1.85                     | 0.59              |
| 3:c:2210:ASP:OD2  | 3:c:2215:HIS:ND1  | 2.36                     | 0.59              |
| 3:c:2230:PHE:HZ   | 3:c:2236:ALA:HA   | 1.67                     | 0.59              |
| 3:Z:2229:ASN:ND2  | 2:a:3208:SER:OG   | 2.35                     | 0.59              |
| 1:V:1104:MET:HE1  | 1:V:1248:PRO:HB3  | 1.85                     | 0.59              |
| 3:H:2230:PHE:HZ   | 3:H:2236:ALA:HA   | 1.67                     | 0.59              |
| 1:Y:1104:MET:HE1  | 1:Y:1248:PRO:HB3  | 1.85                     | 0.59              |
| 1:A:1104:MET:HE1  | 1:A:1248:PRO:HB3  | 1.85                     | 0.59              |
| 3:f:2230:PHE:HZ   | 3:f:2236:ALA:HA   | 1.67                     | 0.59              |
| 1:M:1104:MET:HE1  | 1:M:1248:PRO:HB3  | 1.85                     | 0.59              |
| 2:O:3090:PRO:HB2  | 2:O:3105:LEU:HD22 | 1.84                     | 0.59              |
| 1:A:1109:ARG:HH22 | 2:C:3031:THR:HB   | 1.67                     | 0.59              |
| 3:f:2210:ASP:OD2  | 3:f:2215:HIS:ND1  | 2.36                     | 0.59              |
| 3:c:2225:PHE:HD1  | 2:d:3065:MET:HE1  | 1.68                     | 0.59              |
| 3:Z:2146:LEU:HD21 | 3:Z:2164:LYS:HB2  | 1.84                     | 0.59              |
| 1:P:1104:MET:HE1  | 1:P:1248:PRO:HB3  | 1.85                     | 0.59              |
| 3:N:2146:LEU:HD21 | 3:N:2164:LYS:HB2  | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:c:2146:LEU:HD21 | 3:c:2164:LYS:HB2  | 1.84                     | 0.58              |
| 1:S:1104:MET:HE1  | 1:S:1248:PRO:HB3  | 1.85                     | 0.58              |
| 3:N:2230:PHE:HZ   | 3:N:2236:ALA:HA   | 1.67                     | 0.58              |
| 3:E:2146:LEU:HD21 | 3:E:2164:LYS:HB2  | 1.84                     | 0.58              |
| 3:f:2146:LEU:HD21 | 3:f:2164:LYS:HB2  | 1.84                     | 0.58              |
| 3:Q:2210:ASP:OD2  | 3:Q:2215:HIS:ND1  | 2.36                     | 0.58              |
| 3:K:2192:ARG:NH1  | 2:L:3125:ALA:HA   | 2.18                     | 0.58              |
| 3:Z:2210:ASP:OD2  | 3:Z:2215:HIS:ND1  | 2.36                     | 0.58              |
| 3:Z:2230:PHE:HZ   | 3:Z:2236:ALA:HA   | 1.67                     | 0.58              |
| 2:R:3090:PRO:HB2  | 2:R:3105:LEU:HD22 | 1.84                     | 0.58              |
| 1:J:1138:GLN:NE2  | 1:G:1234:TYR:OH   | 2.32                     | 0.58              |
| 3:K:2210:ASP:OD2  | 3:K:2215:HIS:ND1  | 2.36                     | 0.58              |
| 3:B:2230:PHE:HZ   | 3:B:2236:ALA:HA   | 1.67                     | 0.58              |
| 1:b:1104:MET:HE1  | 1:b:1248:PRO:HB3  | 1.85                     | 0.58              |
| 2:a:3090:PRO:HB2  | 2:a:3105:LEU:HD22 | 1.84                     | 0.58              |
| 3:T:2210:ASP:OD2  | 3:T:2215:HIS:ND1  | 2.36                     | 0.58              |
| 3:Q:2146:LEU:HD21 | 3:Q:2164:LYS:HB2  | 1.84                     | 0.58              |
| 1:b:1236:LYS:NZ   | 2:d:3017:ASP:OD1  | 2.36                     | 0.58              |
| 1:V:1220:ASN:ND2  | 1:J:1120:SER:O    | 2.37                     | 0.58              |
| 3:T:2230:PHE:HZ   | 3:T:2236:ALA:HA   | 1.67                     | 0.58              |
| 3:H:2146:LEU:HD21 | 3:H:2164:LYS:HB2  | 1.84                     | 0.58              |
| 1:J:1104:MET:HE1  | 1:J:1248:PRO:HB3  | 1.85                     | 0.58              |
| 1:G:1104:MET:HE1  | 1:G:1248:PRO:HB3  | 1.85                     | 0.58              |
| 3:W:2210:ASP:OD2  | 3:W:2215:HIS:ND1  | 2.36                     | 0.58              |
| 3:E:2210:ASP:OD2  | 3:E:2215:HIS:ND1  | 2.36                     | 0.58              |
| 3:B:2210:ASP:OD2  | 3:B:2215:HIS:ND1  | 2.36                     | 0.58              |
| 3:N:2210:ASP:OD2  | 3:N:2215:HIS:ND1  | 2.36                     | 0.58              |
| 1:J:1100:ARG:NH2  | 2:L:3103:GLU:OE2  | 2.36                     | 0.58              |
| 3:c:2209:MET:CB   | 1:D:1045:ARG:HH22 | 2.17                     | 0.58              |
| 3:H:2210:ASP:OD2  | 3:H:2215:HIS:ND1  | 2.36                     | 0.58              |
| 1:D:1104:MET:HE1  | 1:D:1248:PRO:HB3  | 1.85                     | 0.58              |
| 3:Q:2230:PHE:HZ   | 3:Q:2236:ALA:HA   | 1.67                     | 0.57              |
| 1:J:1047:VAL:HG22 | 2:L:3171:TRP:CH2  | 2.39                     | 0.57              |
| 2:R:3203:PRO:HG2  | 3:N:2231:THR:OG1  | 2.04                     | 0.57              |
| 2:d:3168:CYS:H    | 3:T:2256:LEU:HD22 | 1.70                     | 0.56              |
| 2:a:3028:PHE:HE1  | 2:R:3224:ARG:HG3  | 1.70                     | 0.56              |
| 1:P:1100:ARG:NH2  | 2:R:3103:GLU:OE2  | 2.38                     | 0.56              |
| 1:M:1046:HIS:HE1  | 1:G:1208:LEU:HD11 | 1.70                     | 0.56              |
| 3:B:2110:VAL:O    | 3:B:2197:ALA:N    | 2.39                     | 0.56              |
| 3:c:2023:ILE:HG22 | 2:C:3156:VAL:HG21 | 1.88                     | 0.56              |
| 2:a:3013:PHE:HA   | 2:R:3008:PRO:HG3  | 1.88                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:3120:LEU:HD23 | 2:R:3212:LEU:HD12 | 1.88                     | 0.56              |
| 3:Z:2101:LEU:HA   | 1:P:1045:ARG:HH21 | 1.71                     | 0.56              |
| 2:d:3120:LEU:HD23 | 2:d:3212:LEU:HD12 | 1.88                     | 0.56              |
| 2:X:3120:LEU:HD23 | 2:X:3212:LEU:HD12 | 1.88                     | 0.56              |
| 1:S:1056:SER:O    | 2:U:3043:LEU:HB2  | 2.06                     | 0.56              |
| 1:e:1046:HIS:HE1  | 1:M:1208:LEU:HD11 | 1.71                     | 0.55              |
| 3:c:2110:VAL:O    | 3:c:2197:ALA:N    | 2.39                     | 0.55              |
| 3:Z:2110:VAL:O    | 3:Z:2197:ALA:N    | 2.39                     | 0.55              |
| 2:O:3120:LEU:HD23 | 2:O:3212:LEU:HD12 | 1.88                     | 0.55              |
| 1:b:1045:ARG:HH21 | 3:T:2101:LEU:HA   | 1.71                     | 0.55              |
| 3:T:2110:VAL:O    | 3:T:2197:ALA:N    | 2.39                     | 0.55              |
| 2:U:3120:LEU:HD23 | 2:U:3212:LEU:HD12 | 1.88                     | 0.55              |
| 2:g:3120:LEU:HD23 | 2:g:3212:LEU:HD12 | 1.88                     | 0.55              |
| 2:L:3120:LEU:HD23 | 2:L:3212:LEU:HD12 | 1.88                     | 0.55              |
| 3:N:2110:VAL:O    | 3:N:2197:ALA:N    | 2.39                     | 0.55              |
| 3:Z:2183:ILE:HD12 | 2:a:3049:VAL:HG21 | 1.89                     | 0.55              |
| 2:F:3120:LEU:HD23 | 2:F:3212:LEU:HD12 | 1.88                     | 0.55              |
| 2:C:3120:LEU:HD23 | 2:C:3212:LEU:HD12 | 1.88                     | 0.54              |
| 1:Y:1045:ARG:HE   | 3:E:2101:LEU:HD23 | 1.71                     | 0.54              |
| 2:a:3120:LEU:HD23 | 2:a:3212:LEU:HD12 | 1.88                     | 0.54              |
| 1:M:1046:HIS:CE1  | 1:G:1208:LEU:HD21 | 2.42                     | 0.54              |
| 3:W:2110:VAL:O    | 3:W:2197:ALA:N    | 2.39                     | 0.54              |
| 1:V:1260:ASN:HD21 | 3:W:2137:THR:HB   | 1.72                     | 0.54              |
| 2:I:3120:LEU:HD23 | 2:I:3212:LEU:HD12 | 1.88                     | 0.54              |
| 1:V:1053:ARG:HD2  | 2:X:3042:ASN:ND2  | 2.16                     | 0.54              |
| 1:V:1179:PRO:HG3  | 2:X:3025:MET:HB2  | 1.89                     | 0.54              |
| 3:K:2192:ARG:HH11 | 2:L:3125:ALA:HA   | 1.73                     | 0.53              |
| 1:Y:1220:ASN:ND2  | 1:P:1120:SER:O    | 2.42                     | 0.53              |
| 3:K:2110:VAL:O    | 3:K:2197:ALA:N    | 2.39                     | 0.53              |
| 3:H:2078:TRP:HB3  | 3:H:2152:PRO:HB2  | 1.91                     | 0.53              |
| 2:g:3059:THR:HG22 | 1:e:1269:SER:HB3  | 1.89                     | 0.53              |
| 1:V:1138:GLN:NE2  | 1:J:1234:TYR:OH   | 2.38                     | 0.53              |
| 2:U:3106:ASN:HA   | 2:U:3227:ARG:HH21 | 1.74                     | 0.53              |
| 3:E:2078:TRP:HB3  | 3:E:2152:PRO:HB2  | 1.91                     | 0.53              |
| 1:e:1046:HIS:CE1  | 1:M:1208:LEU:HD11 | 2.44                     | 0.53              |
| 3:Q:2110:VAL:O    | 3:Q:2197:ALA:N    | 2.39                     | 0.53              |
| 3:H:2110:VAL:O    | 3:H:2197:ALA:N    | 2.39                     | 0.53              |
| 2:d:3106:ASN:HA   | 2:d:3227:ARG:HH21 | 1.74                     | 0.53              |
| 2:X:3132:LEU:HD11 | 2:X:3154:HIS:HB2  | 1.91                     | 0.53              |
| 2:O:3003:PRO:HB3  | 2:I:3007:THR:CG2  | 2.37                     | 0.53              |
| 2:I:3106:ASN:HA   | 2:I:3227:ARG:HH21 | 1.74                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:L:3106:ASN:HA   | 2:L:3227:ARG:HH21 | 1.74                     | 0.53              |
| 3:f:2110:VAL:O    | 3:f:2197:ALA:N    | 2.39                     | 0.53              |
| 3:c:2209:MET:HB2  | 1:D:1045:ARG:HH22 | 1.74                     | 0.53              |
| 3:N:2078:TRP:HB3  | 3:N:2152:PRO:HB2  | 1.91                     | 0.53              |
| 3:f:2078:TRP:HB3  | 3:f:2152:PRO:HB2  | 1.91                     | 0.52              |
| 2:U:3132:LEU:HD11 | 2:U:3154:HIS:HB2  | 1.91                     | 0.52              |
| 2:R:3203:PRO:HG3  | 3:N:2233:GLY:CA   | 2.39                     | 0.52              |
| 2:F:3132:LEU:HD11 | 2:F:3154:HIS:HB2  | 1.91                     | 0.52              |
| 2:O:3106:ASN:HA   | 2:O:3227:ARG:HH21 | 1.74                     | 0.52              |
| 3:Z:2078:TRP:HB3  | 3:Z:2152:PRO:HB2  | 1.91                     | 0.52              |
| 2:X:3106:ASN:HA   | 2:X:3227:ARG:HH21 | 1.74                     | 0.52              |
| 3:E:2110:VAL:O    | 3:E:2197:ALA:N    | 2.39                     | 0.52              |
| 2:F:3106:ASN:HA   | 2:F:3227:ARG:HH21 | 1.74                     | 0.52              |
| 3:c:2078:TRP:HB3  | 3:c:2152:PRO:HB2  | 1.91                     | 0.52              |
| 3:T:2078:TRP:HB3  | 3:T:2152:PRO:HB2  | 1.91                     | 0.52              |
| 1:P:1223:SER:OG   | 1:P:1225:HIS:O    | 2.26                     | 0.52              |
| 2:C:3132:LEU:HD11 | 2:C:3154:HIS:HB2  | 1.91                     | 0.52              |
| 2:R:3106:ASN:HA   | 2:R:3227:ARG:HH21 | 1.74                     | 0.52              |
| 2:I:3132:LEU:HD11 | 2:I:3154:HIS:HB2  | 1.91                     | 0.52              |
| 2:g:3106:ASN:HA   | 2:g:3227:ARG:HH21 | 1.74                     | 0.52              |
| 3:Q:2118:HIS:HD2  | 3:Q:2228:LEU:HD11 | 1.75                     | 0.52              |
| 2:R:3132:LEU:HD11 | 2:R:3154:HIS:HB2  | 1.91                     | 0.52              |
| 2:O:3132:LEU:HD11 | 2:O:3154:HIS:HB2  | 1.91                     | 0.52              |
| 3:K:2078:TRP:HB3  | 3:K:2152:PRO:HB2  | 1.91                     | 0.52              |
| 1:G:1260:ASN:HD21 | 3:H:2137:THR:HB   | 1.74                     | 0.52              |
| 3:E:2118:HIS:HD2  | 3:E:2228:LEU:HD11 | 1.75                     | 0.52              |
| 3:B:2078:TRP:HB3  | 3:B:2152:PRO:HB2  | 1.91                     | 0.52              |
| 2:a:3106:ASN:HA   | 2:a:3227:ARG:HH21 | 1.74                     | 0.52              |
| 2:a:3132:LEU:HD11 | 2:a:3154:HIS:HB2  | 1.91                     | 0.52              |
| 3:K:2096:MET:HE3  | 3:K:2212:MET:HB3  | 1.92                     | 0.52              |
| 3:H:2118:HIS:HD2  | 3:H:2228:LEU:HD11 | 1.75                     | 0.52              |
| 3:c:2096:MET:HE3  | 3:c:2212:MET:HB3  | 1.92                     | 0.51              |
| 3:K:2118:HIS:HD2  | 3:K:2228:LEU:HD11 | 1.75                     | 0.51              |
| 2:a:3134:SER:OG   | 2:a:3192:THR:OG1  | 2.29                     | 0.51              |
| 3:W:2078:TRP:HB3  | 3:W:2152:PRO:HB2  | 1.91                     | 0.51              |
| 3:W:2118:HIS:HD2  | 3:W:2228:LEU:HD11 | 1.75                     | 0.51              |
| 2:X:3134:SER:OG   | 2:X:3192:THR:OG1  | 2.29                     | 0.51              |
| 2:R:3134:SER:OG   | 2:R:3192:THR:OG1  | 2.29                     | 0.51              |
| 2:g:3134:SER:OG   | 2:g:3192:THR:OG1  | 2.29                     | 0.51              |
| 3:c:2042:LEU:HD21 | 1:D:1049:ASN:ND2  | 2.24                     | 0.51              |
| 2:d:3132:LEU:HD11 | 2:d:3154:HIS:HB2  | 1.91                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:T:2118:HIS:HD2  | 3:T:2228:LEU:HD11 | 1.75                     | 0.51              |
| 3:N:2096:MET:HE3  | 3:N:2212:MET:HB3  | 1.92                     | 0.51              |
| 2:O:3134:SER:OG   | 2:O:3192:THR:OG1  | 2.29                     | 0.51              |
| 3:B:2070:GLN:HB3  | 3:B:2237:TYR:HB2  | 1.93                     | 0.51              |
| 3:Z:2070:GLN:HB3  | 3:Z:2237:TYR:HB2  | 1.93                     | 0.51              |
| 1:V:1223:SER:OG   | 1:V:1225:HIS:O    | 2.26                     | 0.51              |
| 3:T:2225:PHE:HD1  | 2:U:3065:MET:HE1  | 1.75                     | 0.51              |
| 3:Q:2078:TRP:HB3  | 3:Q:2152:PRO:HB2  | 1.91                     | 0.51              |
| 3:N:2070:GLN:HB3  | 3:N:2237:TYR:HB2  | 1.93                     | 0.51              |
| 2:g:3132:LEU:HD11 | 2:g:3154:HIS:HB2  | 1.91                     | 0.51              |
| 3:f:2096:MET:HE3  | 3:f:2212:MET:HB3  | 1.92                     | 0.51              |
| 1:P:1274:THR:O    | 2:R:3085:SER:HB3  | 2.11                     | 0.51              |
| 3:Q:2096:MET:HE3  | 3:Q:2212:MET:HB3  | 1.92                     | 0.51              |
| 1:J:1095:MET:HE3  | 1:J:1097:GLN:HB3  | 1.93                     | 0.51              |
| 3:B:2118:HIS:HD2  | 3:B:2228:LEU:HD11 | 1.75                     | 0.51              |
| 1:A:1095:MET:HE3  | 1:A:1097:GLN:HB3  | 1.93                     | 0.51              |
| 3:f:2118:HIS:HD2  | 3:f:2228:LEU:HD11 | 1.75                     | 0.51              |
| 3:c:2101:LEU:HD23 | 1:D:1045:ARG:NE   | 2.26                     | 0.51              |
| 3:c:2118:HIS:HD2  | 3:c:2228:LEU:HD11 | 1.75                     | 0.51              |
| 1:Y:1095:MET:HE3  | 1:Y:1097:GLN:HB3  | 1.93                     | 0.51              |
| 3:W:2101:LEU:HD23 | 1:J:1045:ARG:HE   | 1.76                     | 0.51              |
| 2:L:3132:LEU:HD11 | 2:L:3154:HIS:HB2  | 1.91                     | 0.51              |
| 2:U:3006:ASN:HB2  | 2:R:3011:ASN:H    | 1.76                     | 0.51              |
| 3:Z:2118:HIS:HD2  | 3:Z:2228:LEU:HD11 | 1.75                     | 0.51              |
| 2:a:3013:PHE:HD2  | 1:D:1166:PHE:CD1  | 2.28                     | 0.51              |
| 1:P:1095:MET:HE3  | 1:P:1097:GLN:HB3  | 1.93                     | 0.51              |
| 3:H:2070:GLN:HB3  | 3:H:2237:TYR:HB2  | 1.93                     | 0.51              |
| 2:C:3106:ASN:HA   | 2:C:3227:ARG:HH21 | 1.74                     | 0.51              |
| 1:e:1223:SER:OG   | 1:e:1225:HIS:O    | 2.26                     | 0.50              |
| 2:U:3134:SER:OG   | 2:U:3192:THR:OG1  | 2.29                     | 0.50              |
| 1:M:1111:ASP:O    | 1:M:1238:LYS:N    | 2.44                     | 0.50              |
| 2:d:3134:SER:OG   | 2:d:3192:THR:OG1  | 2.29                     | 0.50              |
| 3:Z:2096:MET:HE3  | 3:Z:2212:MET:HB3  | 1.92                     | 0.50              |
| 2:I:3134:SER:OG   | 2:I:3192:THR:OG1  | 2.29                     | 0.50              |
| 1:D:1095:MET:HE3  | 1:D:1097:GLN:HB3  | 1.93                     | 0.50              |
| 1:M:1270:ARG:NH1  | 1:M:1275:ASP:O    | 2.40                     | 0.50              |
| 2:C:3134:SER:OG   | 2:C:3192:THR:OG1  | 2.29                     | 0.50              |
| 3:c:2070:GLN:HB3  | 3:c:2237:TYR:HB2  | 1.93                     | 0.50              |
| 1:V:1111:ASP:O    | 1:V:1238:LYS:N    | 2.44                     | 0.50              |
| 3:W:2096:MET:HE3  | 3:W:2212:MET:HB3  | 1.92                     | 0.50              |
| 3:T:2096:MET:HE3  | 3:T:2212:MET:HB3  | 1.92                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:L:3013:PHE:HA  | 2:I:3008:PRO:HG3  | 1.94                     | 0.50              |
| 1:e:1095:MET:HE3 | 1:e:1097:GLN:HB3  | 1.93                     | 0.50              |
| 1:S:1223:SER:OG  | 1:S:1225:HIS:O    | 2.26                     | 0.50              |
| 1:P:1116:MET:HB3 | 1:P:1231:ILE:HD11 | 1.94                     | 0.50              |
| 2:L:3134:SER:OG  | 2:L:3192:THR:OG1  | 2.29                     | 0.50              |
| 1:e:1111:ASP:O   | 1:e:1238:LYS:N    | 2.45                     | 0.50              |
| 1:V:1260:ASN:ND2 | 3:W:2137:THR:HB   | 2.26                     | 0.50              |
| 3:W:2070:GLN:HB3 | 3:W:2237:TYR:HB2  | 1.93                     | 0.50              |
| 3:N:2118:HIS:HD2 | 3:N:2228:LEU:HD11 | 1.75                     | 0.50              |
| 3:H:2096:MET:HE3 | 3:H:2212:MET:HB3  | 1.92                     | 0.50              |
| 3:E:2070:GLN:HB3 | 3:E:2237:TYR:HB2  | 1.93                     | 0.50              |
| 1:b:1095:MET:HE3 | 1:b:1097:GLN:HB3  | 1.93                     | 0.50              |
| 3:T:2070:GLN:HB3 | 3:T:2237:TYR:HB2  | 1.93                     | 0.50              |
| 1:P:1111:ASP:O   | 1:P:1238:LYS:N    | 2.45                     | 0.50              |
| 3:N:2134:CYS:HA  | 3:N:2165:VAL:HA   | 1.94                     | 0.50              |
| 3:B:2096:MET:HE3 | 3:B:2212:MET:HB3  | 1.92                     | 0.50              |
| 1:Y:1111:ASP:O   | 1:Y:1238:LYS:N    | 2.44                     | 0.50              |
| 3:Z:2134:CYS:HA  | 3:Z:2165:VAL:HA   | 1.94                     | 0.50              |
| 3:E:2105:GLY:HA3 | 3:E:2247:MET:HB2  | 1.94                     | 0.50              |
| 3:B:2134:CYS:HA  | 3:B:2165:VAL:HA   | 1.94                     | 0.50              |
| 3:f:2105:GLY:HA3 | 3:f:2247:MET:HB2  | 1.94                     | 0.50              |
| 1:V:1095:MET:HE3 | 1:V:1097:GLN:HB3  | 1.93                     | 0.50              |
| 2:O:3109:ALA:HA  | 2:O:3227:ARG:HD3  | 1.94                     | 0.50              |
| 3:K:2070:GLN:HB3 | 3:K:2237:TYR:HB2  | 1.93                     | 0.50              |
| 1:G:1095:MET:HE3 | 1:G:1097:GLN:HB3  | 1.93                     | 0.50              |
| 1:A:1116:MET:HB3 | 1:A:1231:ILE:HD11 | 1.94                     | 0.49              |
| 2:d:3109:ALA:HA  | 2:d:3227:ARG:HD3  | 1.94                     | 0.49              |
| 1:S:1095:MET:HE3 | 1:S:1097:GLN:HB3  | 1.93                     | 0.49              |
| 1:M:1116:MET:HB3 | 1:M:1231:ILE:HD11 | 1.94                     | 0.49              |
| 3:N:2105:GLY:HA3 | 3:N:2247:MET:HB2  | 1.94                     | 0.49              |
| 3:E:2096:MET:HE3 | 3:E:2212:MET:HB3  | 1.92                     | 0.49              |
| 3:f:2070:GLN:HB3 | 3:f:2237:TYR:HB2  | 1.93                     | 0.49              |
| 3:W:2105:GLY:HA3 | 3:W:2247:MET:HB2  | 1.94                     | 0.49              |
| 2:X:3109:ALA:HA  | 2:X:3227:ARG:HD3  | 1.94                     | 0.49              |
| 1:D:1111:ASP:O   | 1:D:1238:LYS:N    | 2.45                     | 0.49              |
| 2:F:3109:ALA:HA  | 2:F:3227:ARG:HD3  | 1.94                     | 0.49              |
| 2:F:3134:SER:OG  | 2:F:3192:THR:OG1  | 2.29                     | 0.49              |
| 1:e:1116:MET:HB3 | 1:e:1231:ILE:HD11 | 1.94                     | 0.49              |
| 1:e:1166:PHE:CE2 | 1:V:1117:VAL:HG11 | 2.47                     | 0.49              |
| 3:Z:2105:GLY:HA3 | 3:Z:2247:MET:HB2  | 1.94                     | 0.49              |
| 3:Q:2070:GLN:HB3 | 3:Q:2237:TYR:HB2  | 1.93                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:L:3109:ALA:HA   | 2:L:3227:ARG:HD3  | 1.94                     | 0.49              |
| 1:G:1270:ARG:NH1  | 1:G:1275:ASP:O    | 2.40                     | 0.49              |
| 3:Q:2105:GLY:HA3  | 3:Q:2247:MET:HB2  | 1.94                     | 0.49              |
| 1:J:1111:ASP:O    | 1:J:1238:LYS:N    | 2.44                     | 0.49              |
| 2:I:3109:ALA:HA   | 2:I:3227:ARG:HD3  | 1.94                     | 0.49              |
| 3:B:2160:ILE:H    | 3:B:2166:GLN:HE22 | 1.61                     | 0.49              |
| 3:c:2105:GLY:HA3  | 3:c:2247:MET:HB2  | 1.94                     | 0.49              |
| 1:M:1095:MET:HE3  | 1:M:1097:GLN:HB3  | 1.93                     | 0.49              |
| 3:K:2134:CYS:HA   | 3:K:2165:VAL:HA   | 1.94                     | 0.49              |
| 1:e:1057:THR:OG1  | 1:e:1060:ASN:ND2  | 2.46                     | 0.49              |
| 1:V:1057:THR:OG1  | 1:V:1060:ASN:ND2  | 2.46                     | 0.49              |
| 1:V:1267:THR:HG22 | 2:X:3098:ARG:HG2  | 1.94                     | 0.49              |
| 3:T:2105:GLY:HA3  | 3:T:2247:MET:HB2  | 1.94                     | 0.49              |
| 1:J:1057:THR:OG1  | 1:J:1060:ASN:ND2  | 2.46                     | 0.49              |
| 3:K:2105:GLY:HA3  | 3:K:2247:MET:HB2  | 1.94                     | 0.49              |
| 1:D:1116:MET:HB3  | 1:D:1231:ILE:HD11 | 1.94                     | 0.49              |
| 1:V:1065:ALA:HB3  | 2:X:3013:PHE:HZ   | 1.77                     | 0.49              |
| 3:Q:2134:CYS:HA   | 3:Q:2165:VAL:HA   | 1.94                     | 0.49              |
| 1:Y:1057:THR:OG1  | 1:Y:1060:ASN:ND2  | 2.46                     | 0.49              |
| 1:Y:1138:GLN:NE2  | 1:P:1234:TYR:OH   | 2.43                     | 0.49              |
| 1:P:1057:THR:OG1  | 1:P:1060:ASN:ND2  | 2.46                     | 0.49              |
| 2:L:3130:LYS:N    | 2:L:3197:THR:OG1  | 2.46                     | 0.49              |
| 1:D:1057:THR:OG1  | 1:D:1060:ASN:ND2  | 2.46                     | 0.49              |
| 1:A:1057:THR:OG1  | 1:A:1060:ASN:ND2  | 2.46                     | 0.49              |
| 1:b:1220:ASN:ND2  | 1:D:1120:SER:O    | 2.45                     | 0.49              |
| 1:Y:1166:PHE:CE2  | 1:P:1117:VAL:HG11 | 2.48                     | 0.49              |
| 2:I:3130:LYS:N    | 2:I:3197:THR:OG1  | 2.46                     | 0.49              |
| 1:b:1100:ARG:NH1  | 1:b:1249:ARG:O    | 2.46                     | 0.49              |
| 1:S:1116:MET:HB3  | 1:S:1231:ILE:HD11 | 1.94                     | 0.49              |
| 1:M:1100:ARG:NH1  | 1:M:1249:ARG:O    | 2.46                     | 0.49              |
| 2:g:3109:ALA:HA   | 2:g:3227:ARG:HD3  | 1.94                     | 0.48              |
| 1:e:1138:GLN:NE2  | 1:V:1234:TYR:HH   | 2.10                     | 0.48              |
| 1:b:1046:HIS:CE1  | 1:S:1208:LEU:HD21 | 2.48                     | 0.48              |
| 3:W:2160:ILE:H    | 3:W:2166:GLN:HE22 | 1.61                     | 0.48              |
| 3:E:2134:CYS:HA   | 3:E:2165:VAL:HA   | 1.94                     | 0.48              |
| 2:C:3109:ALA:HA   | 2:C:3227:ARG:HD3  | 1.95                     | 0.48              |
| 1:e:1100:ARG:NH1  | 1:e:1249:ARG:O    | 2.46                     | 0.48              |
| 1:b:1045:ARG:NH1  | 3:T:2210:ASP:HA   | 2.28                     | 0.48              |
| 2:d:3130:LYS:N    | 2:d:3197:THR:OG1  | 2.46                     | 0.48              |
| 3:T:2160:ILE:H    | 3:T:2166:GLN:HE22 | 1.61                     | 0.48              |
| 2:L:3089:ASP:OD1  | 2:L:3089:ASP:N    | 2.47                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:H:2105:GLY:HA3  | 3:H:2247:MET:HB2  | 1.94                     | 0.48              |
| 3:E:2160:ILE:H    | 3:E:2166:GLN:HE22 | 1.61                     | 0.48              |
| 3:f:2134:CYS:HA   | 3:f:2165:VAL:HA   | 1.94                     | 0.48              |
| 1:b:1111:ASP:O    | 1:b:1238:LYS:N    | 2.44                     | 0.48              |
| 1:b:1116:MET:HB3  | 1:b:1231:ILE:HD11 | 1.94                     | 0.48              |
| 1:V:1116:MET:HB3  | 1:V:1231:ILE:HD11 | 1.94                     | 0.48              |
| 3:W:2134:CYS:HA   | 3:W:2165:VAL:HA   | 1.94                     | 0.48              |
| 1:S:1057:THR:OG1  | 1:S:1060:ASN:ND2  | 2.46                     | 0.48              |
| 2:U:3109:ALA:HA   | 2:U:3227:ARG:HD3  | 1.94                     | 0.48              |
| 1:P:1100:ARG:NH1  | 1:P:1249:ARG:O    | 2.46                     | 0.48              |
| 1:M:1057:THR:OG1  | 1:M:1060:ASN:ND2  | 2.46                     | 0.48              |
| 1:J:1116:MET:HB3  | 1:J:1231:ILE:HD11 | 1.94                     | 0.48              |
| 1:G:1057:THR:OG1  | 1:G:1060:ASN:ND2  | 2.46                     | 0.48              |
| 3:H:2134:CYS:HA   | 3:H:2165:VAL:HA   | 1.94                     | 0.48              |
| 1:D:1109:ARG:HH22 | 2:F:3031:THR:HB   | 1.78                     | 0.48              |
| 1:b:1057:THR:OG1  | 1:b:1060:ASN:ND2  | 2.46                     | 0.48              |
| 2:d:3089:ASP:OD1  | 2:d:3089:ASP:N    | 2.47                     | 0.48              |
| 1:S:1111:ASP:O    | 1:S:1238:LYS:N    | 2.45                     | 0.48              |
| 3:T:2134:CYS:HA   | 3:T:2165:VAL:HA   | 1.94                     | 0.48              |
| 3:H:2160:ILE:H    | 3:H:2166:GLN:HE22 | 1.61                     | 0.48              |
| 3:c:2134:CYS:HA   | 3:c:2165:VAL:HA   | 1.94                     | 0.48              |
| 1:Y:1116:MET:HB3  | 1:Y:1231:ILE:HD11 | 1.94                     | 0.48              |
| 1:V:1177:SER:HB3  | 2:X:3022:PRO:O    | 2.14                     | 0.48              |
| 1:J:1100:ARG:NH1  | 1:J:1249:ARG:O    | 2.46                     | 0.48              |
| 1:G:1100:ARG:NH1  | 1:G:1249:ARG:O    | 2.46                     | 0.48              |
| 2:C:3130:LYS:N    | 2:C:3197:THR:OG1  | 2.46                     | 0.48              |
| 3:Q:2160:ILE:H    | 3:Q:2166:GLN:HE22 | 1.61                     | 0.48              |
| 2:R:3109:ALA:HA   | 2:R:3227:ARG:HD3  | 1.94                     | 0.48              |
| 2:g:3203:PRO:HD2  | 3:Z:2117:PHE:HD2  | 1.79                     | 0.48              |
| 3:c:2160:ILE:H    | 3:c:2166:GLN:HE22 | 1.61                     | 0.48              |
| 1:Y:1100:ARG:NH1  | 1:Y:1249:ARG:O    | 2.46                     | 0.48              |
| 1:V:1180:PHE:CZ   | 1:V:1182:SER:HB3  | 2.49                     | 0.48              |
| 1:S:1180:PHE:CZ   | 1:S:1182:SER:HB3  | 2.49                     | 0.48              |
| 2:C:3089:ASP:OD1  | 2:C:3089:ASP:N    | 2.47                     | 0.48              |
| 1:A:1111:ASP:O    | 1:A:1238:LYS:N    | 2.44                     | 0.48              |
| 2:a:3109:ALA:HA   | 2:a:3227:ARG:HD3  | 1.94                     | 0.48              |
| 2:U:3029:ASP:OD1  | 2:U:3029:ASP:N    | 2.47                     | 0.48              |
| 2:U:3089:ASP:N    | 2:U:3089:ASP:OD1  | 2.47                     | 0.48              |
| 1:G:1111:ASP:O    | 1:G:1238:LYS:N    | 2.44                     | 0.48              |
| 1:G:1116:MET:HB3  | 1:G:1231:ILE:HD11 | 1.94                     | 0.48              |
| 3:H:2039:PRO:HB3  | 3:H:2202:PRO:HA   | 1.96                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:1180:PHE:CZ  | 1:D:1182:SER:HB3  | 2.49                     | 0.48              |
| 3:W:2039:PRO:HB3 | 3:W:2202:PRO:HA   | 1.96                     | 0.48              |
| 2:U:3130:LYS:N   | 2:U:3197:THR:OG1  | 2.46                     | 0.48              |
| 1:M:1180:PHE:CZ  | 1:M:1182:SER:HB3  | 2.49                     | 0.48              |
| 1:D:1270:ARG:NH1 | 1:D:1275:ASP:O    | 2.40                     | 0.48              |
| 1:b:1180:PHE:CZ  | 1:b:1182:SER:HB3  | 2.49                     | 0.48              |
| 2:X:3089:ASP:OD1 | 2:X:3089:ASP:N    | 2.47                     | 0.48              |
| 3:T:2039:PRO:HB3 | 3:T:2202:PRO:HA   | 1.96                     | 0.48              |
| 3:N:2039:PRO:HB3 | 3:N:2202:PRO:HA   | 1.96                     | 0.48              |
| 1:G:1180:PHE:CZ  | 1:G:1182:SER:HB3  | 2.49                     | 0.48              |
| 2:I:3029:ASP:OD1 | 2:I:3029:ASP:N    | 2.47                     | 0.48              |
| 1:A:1100:ARG:NH1 | 1:A:1249:ARG:O    | 2.46                     | 0.47              |
| 3:f:2160:ILE:H   | 3:f:2166:GLN:HE22 | 1.61                     | 0.47              |
| 3:Z:2039:PRO:HB3 | 3:Z:2202:PRO:HA   | 1.96                     | 0.47              |
| 1:V:1100:ARG:NH1 | 1:V:1249:ARG:O    | 2.46                     | 0.47              |
| 2:X:3130:LYS:N   | 2:X:3197:THR:OG1  | 2.46                     | 0.47              |
| 1:P:1180:PHE:CZ  | 1:P:1182:SER:HB3  | 2.49                     | 0.47              |
| 3:N:2160:ILE:H   | 3:N:2166:GLN:HE22 | 1.61                     | 0.47              |
| 3:E:2039:PRO:HB3 | 3:E:2202:PRO:HA   | 1.96                     | 0.47              |
| 3:f:2039:PRO:HB3 | 3:f:2202:PRO:HA   | 1.96                     | 0.47              |
| 2:X:3004:VAL:HA  | 2:L:3002:VAL:O    | 2.14                     | 0.47              |
| 1:S:1100:ARG:NH1 | 1:S:1249:ARG:O    | 2.46                     | 0.47              |
| 2:g:3089:ASP:OD1 | 2:g:3089:ASP:N    | 2.47                     | 0.47              |
| 3:Z:2160:ILE:H   | 3:Z:2166:GLN:HE22 | 1.61                     | 0.47              |
| 3:W:2187:GLN:HG2 | 3:W:2197:ALA:HB1  | 1.97                     | 0.47              |
| 2:g:3130:LYS:N   | 2:g:3197:THR:OG1  | 2.46                     | 0.47              |
| 3:Q:2039:PRO:HB3 | 3:Q:2202:PRO:HA   | 1.96                     | 0.47              |
| 3:Q:2076:PRO:HB2 | 3:Q:2155:PHE:HB2  | 1.97                     | 0.47              |
| 2:R:3130:LYS:N   | 2:R:3197:THR:OG1  | 2.46                     | 0.47              |
| 3:K:2104:ALA:HB3 | 3:K:2106:TYR:CZ   | 2.50                     | 0.47              |
| 3:K:2160:ILE:H   | 3:K:2166:GLN:HE22 | 1.61                     | 0.47              |
| 1:D:1100:ARG:NH1 | 1:D:1249:ARG:O    | 2.46                     | 0.47              |
| 3:E:2187:GLN:HG2 | 3:E:2197:ALA:HB1  | 1.97                     | 0.47              |
| 3:B:2105:GLY:HA3 | 3:B:2247:MET:HB2  | 1.94                     | 0.47              |
| 1:A:1180:PHE:CZ  | 1:A:1182:SER:HB3  | 2.49                     | 0.47              |
| 3:f:2107:THR:OG1 | 3:f:2247:MET:SD   | 2.73                     | 0.47              |
| 1:e:1180:PHE:CZ  | 1:e:1182:SER:HB3  | 2.49                     | 0.47              |
| 2:a:3089:ASP:N   | 2:a:3089:ASP:OD1  | 2.47                     | 0.47              |
| 3:W:2076:PRO:HB2 | 3:W:2155:PHE:HB2  | 1.97                     | 0.47              |
| 2:O:3006:ASN:HB2 | 2:I:3011:ASN:N    | 2.27                     | 0.47              |
| 3:K:2039:PRO:HB3 | 3:K:2202:PRO:HA   | 1.96                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:2039:PRO:HB3  | 3:B:2202:PRO:HA   | 1.96                     | 0.47              |
| 3:f:2076:PRO:HB2  | 3:f:2155:PHE:HB2  | 1.97                     | 0.47              |
| 3:Q:2104:ALA:HB3  | 3:Q:2106:TYR:CZ   | 2.50                     | 0.47              |
| 3:N:2081:LYS:HD2  | 3:N:2147:THR:HG21 | 1.97                     | 0.47              |
| 1:J:1223:SER:OG   | 1:J:1225:HIS:O    | 2.26                     | 0.47              |
| 3:K:2107:THR:OG1  | 3:K:2247:MET:SD   | 2.73                     | 0.47              |
| 3:H:2187:GLN:HG2  | 3:H:2197:ALA:HB1  | 1.97                     | 0.47              |
| 1:A:1270:ARG:NH1  | 1:A:1275:ASP:O    | 2.40                     | 0.47              |
| 3:f:2137:THR:HB   | 1:e:1260:ASN:ND2  | 2.30                     | 0.47              |
| 3:c:2187:GLN:HG2  | 3:c:2197:ALA:HB1  | 1.97                     | 0.47              |
| 1:Y:1180:PHE:CZ   | 1:Y:1182:SER:HB3  | 2.49                     | 0.47              |
| 3:Z:2081:LYS:HD2  | 3:Z:2147:THR:HG21 | 1.97                     | 0.47              |
| 3:W:2081:LYS:HD2  | 3:W:2147:THR:HG21 | 1.97                     | 0.47              |
| 3:W:2104:ALA:HB3  | 3:W:2106:TYR:CZ   | 2.50                     | 0.47              |
| 3:T:2076:PRO:HB2  | 3:T:2155:PHE:HB2  | 1.97                     | 0.47              |
| 3:T:2187:GLN:HG2  | 3:T:2197:ALA:HB1  | 1.97                     | 0.47              |
| 1:J:1180:PHE:CZ   | 1:J:1182:SER:HB3  | 2.49                     | 0.47              |
| 3:H:2104:ALA:HB3  | 3:H:2106:TYR:CZ   | 2.50                     | 0.47              |
| 3:B:2076:PRO:HB2  | 3:B:2155:PHE:HB2  | 1.97                     | 0.47              |
| 3:c:2039:PRO:HB3  | 3:c:2202:PRO:HA   | 1.96                     | 0.47              |
| 3:c:2076:PRO:HB2  | 3:c:2155:PHE:HB2  | 1.97                     | 0.47              |
| 3:c:2107:THR:OG1  | 3:c:2247:MET:SD   | 2.73                     | 0.47              |
| 3:K:2076:PRO:HB2  | 3:K:2155:PHE:HB2  | 1.97                     | 0.47              |
| 3:K:2081:LYS:HD2  | 3:K:2147:THR:HG21 | 1.97                     | 0.47              |
| 3:f:2081:LYS:HD2  | 3:f:2147:THR:HG21 | 1.97                     | 0.47              |
| 1:b:1223:SER:OG   | 1:b:1225:HIS:O    | 2.26                     | 0.47              |
| 3:Z:2076:PRO:HB2  | 3:Z:2155:PHE:HB2  | 1.97                     | 0.47              |
| 3:T:2104:ALA:HB3  | 3:T:2106:TYR:CZ   | 2.50                     | 0.47              |
| 3:N:2107:THR:OG1  | 3:N:2247:MET:SD   | 2.73                     | 0.47              |
| 3:K:2187:GLN:HG2  | 3:K:2197:ALA:HB1  | 1.97                     | 0.47              |
| 3:E:2104:ALA:HB3  | 3:E:2106:TYR:CZ   | 2.50                     | 0.47              |
| 2:g:3169:VAL:HG12 | 2:g:3172:ILE:HD11 | 1.97                     | 0.47              |
| 3:f:2187:GLN:HG2  | 3:f:2197:ALA:HB1  | 1.97                     | 0.47              |
| 3:c:2101:LEU:HD23 | 1:D:1045:ARG:HE   | 1.80                     | 0.47              |
| 1:V:1267:THR:HG22 | 2:X:3098:ARG:CG   | 2.44                     | 0.47              |
| 3:N:2187:GLN:HG2  | 3:N:2197:ALA:HB1  | 1.97                     | 0.47              |
| 2:F:3130:LYS:N    | 2:F:3197:THR:OG1  | 2.46                     | 0.47              |
| 2:g:3097:LYS:HG3  | 2:g:3098:ARG:HG2  | 1.97                     | 0.46              |
| 3:f:2137:THR:HB   | 1:e:1260:ASN:HD21 | 1.79                     | 0.46              |
| 3:c:2104:ALA:HB3  | 3:c:2106:TYR:CZ   | 2.50                     | 0.46              |
| 3:Z:2187:GLN:HG2  | 3:Z:2197:ALA:HB1  | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:2081:LYS:HD2  | 3:B:2147:THR:HG21 | 1.97                     | 0.46              |
| 3:f:2104:ALA:HB3  | 3:f:2106:TYR:CZ   | 2.50                     | 0.46              |
| 1:S:1270:ARG:NH1  | 1:S:1275:ASP:O    | 2.40                     | 0.46              |
| 2:U:3120:LEU:HB3  | 2:U:3212:LEU:HB2  | 1.98                     | 0.46              |
| 1:P:1270:ARG:NH1  | 1:P:1275:ASP:O    | 2.40                     | 0.46              |
| 2:R:3203:PRO:HG3  | 3:N:2234:ALA:N    | 2.30                     | 0.46              |
| 1:J:1047:VAL:HA   | 2:L:3171:TRP:HZ3  | 1.80                     | 0.46              |
| 2:I:3169:VAL:HG12 | 2:I:3172:ILE:HD11 | 1.97                     | 0.46              |
| 2:d:3169:VAL:HG12 | 2:d:3172:ILE:HD11 | 1.97                     | 0.46              |
| 2:U:3169:VAL:HG12 | 2:U:3172:ILE:HD11 | 1.97                     | 0.46              |
| 3:Q:2187:GLN:HG2  | 3:Q:2197:ALA:HB1  | 1.97                     | 0.46              |
| 2:L:3169:VAL:HG12 | 2:L:3172:ILE:HD11 | 1.98                     | 0.46              |
| 3:H:2107:THR:OG1  | 3:H:2247:MET:SD   | 2.73                     | 0.46              |
| 2:I:3089:ASP:OD1  | 2:I:3089:ASP:N    | 2.47                     | 0.46              |
| 3:E:2081:LYS:HD2  | 3:E:2147:THR:HG21 | 1.97                     | 0.46              |
| 3:c:2081:LYS:HD2  | 3:c:2147:THR:HG21 | 1.97                     | 0.46              |
| 1:P:1087:VAL:HG23 | 1:P:1088:TRP:H    | 1.81                     | 0.46              |
| 3:Q:2081:LYS:HD2  | 3:Q:2147:THR:HG21 | 1.97                     | 0.46              |
| 2:R:3169:VAL:HG12 | 2:R:3172:ILE:HD11 | 1.98                     | 0.46              |
| 3:N:2104:ALA:HB3  | 3:N:2106:TYR:CZ   | 2.50                     | 0.46              |
| 3:K:2178:VAL:HG11 | 2:L:3065:MET:HE3  | 1.98                     | 0.46              |
| 2:C:3120:LEU:HB3  | 2:C:3212:LEU:HB2  | 1.97                     | 0.46              |
| 3:B:2187:GLN:HG2  | 3:B:2197:ALA:HB1  | 1.97                     | 0.46              |
| 1:e:1087:VAL:HG23 | 1:e:1088:TRP:H    | 1.81                     | 0.46              |
| 2:d:3120:LEU:HB3  | 2:d:3212:LEU:HB2  | 1.97                     | 0.46              |
| 3:Z:2104:ALA:HB3  | 3:Z:2106:TYR:CZ   | 2.50                     | 0.46              |
| 3:Z:2142:PRO:HB2  | 3:Z:2144:THR:HG22 | 1.98                     | 0.46              |
| 2:a:3130:LYS:N    | 2:a:3197:THR:OG1  | 2.46                     | 0.46              |
| 1:S:1046:HIS:HE1  | 1:P:1208:LEU:HD21 | 1.78                     | 0.46              |
| 1:S:1116:MET:SD   | 1:S:1116:MET:N    | 2.89                     | 0.46              |
| 2:U:3097:LYS:HG3  | 2:U:3098:ARG:HG2  | 1.97                     | 0.46              |
| 2:L:3120:LEU:HB3  | 2:L:3212:LEU:HB2  | 1.97                     | 0.46              |
| 1:G:1116:MET:SD   | 1:G:1116:MET:N    | 2.89                     | 0.46              |
| 3:H:2081:LYS:HD2  | 3:H:2147:THR:HG21 | 1.97                     | 0.46              |
| 1:D:1087:VAL:HG23 | 1:D:1088:TRP:H    | 1.81                     | 0.46              |
| 2:C:3097:LYS:HG3  | 2:C:3098:ARG:HG2  | 1.97                     | 0.46              |
| 3:B:2104:ALA:HB3  | 3:B:2106:TYR:CZ   | 2.50                     | 0.46              |
| 1:e:1270:ARG:NH1  | 1:e:1275:ASP:O    | 2.40                     | 0.46              |
| 3:Z:2105:GLY:H    | 3:Z:2247:MET:H    | 1.64                     | 0.46              |
| 3:Q:2142:PRO:HB2  | 3:Q:2144:THR:HG22 | 1.98                     | 0.46              |
| 1:Y:1223:SER:OG   | 1:Y:1225:HIS:O    | 2.26                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:Z:2107:THR:OG1  | 3:Z:2247:MET:SD   | 2.73                     | 0.46              |
| 2:X:3111:TRP:HZ3  | 2:X:3172:ILE:HG22 | 1.81                     | 0.46              |
| 2:U:3111:TRP:HZ3  | 2:U:3172:ILE:HG22 | 1.81                     | 0.46              |
| 2:R:3089:ASP:N    | 2:R:3089:ASP:OD1  | 2.47                     | 0.46              |
| 1:J:1087:VAL:HG23 | 1:J:1088:TRP:H    | 1.81                     | 0.46              |
| 3:H:2076:PRO:HB2  | 3:H:2155:PHE:HB2  | 1.97                     | 0.46              |
| 3:B:2107:THR:OG1  | 3:B:2247:MET:SD   | 2.73                     | 0.46              |
| 1:A:1223:SER:OG   | 1:A:1225:HIS:O    | 2.26                     | 0.46              |
| 3:W:2142:PRO:HB2  | 3:W:2144:THR:HG22 | 1.98                     | 0.46              |
| 2:X:3097:LYS:HG3  | 2:X:3098:ARG:HG2  | 1.97                     | 0.46              |
| 3:Q:2107:THR:OG1  | 3:Q:2247:MET:SD   | 2.73                     | 0.46              |
| 1:M:1116:MET:SD   | 1:M:1116:MET:N    | 2.89                     | 0.46              |
| 3:N:2076:PRO:HB2  | 3:N:2155:PHE:HB2  | 1.97                     | 0.46              |
| 3:N:2105:GLY:H    | 3:N:2247:MET:H    | 1.64                     | 0.46              |
| 2:O:3089:ASP:OD1  | 2:O:3089:ASP:N    | 2.47                     | 0.46              |
| 2:O:3097:LYS:HG3  | 2:O:3098:ARG:HG2  | 1.97                     | 0.46              |
| 3:K:2105:GLY:H    | 3:K:2247:MET:H    | 1.64                     | 0.46              |
| 2:L:3111:TRP:HZ3  | 2:L:3172:ILE:HG22 | 1.81                     | 0.46              |
| 1:D:1116:MET:SD   | 1:D:1116:MET:N    | 2.89                     | 0.46              |
| 2:F:3120:LEU:HB3  | 2:F:3212:LEU:HB2  | 1.97                     | 0.46              |
| 1:Y:1116:MET:SD   | 1:Y:1116:MET:N    | 2.89                     | 0.46              |
| 2:a:3121:PHE:HD1  | 2:a:3211:VAL:HG22 | 1.81                     | 0.46              |
| 1:V:1087:VAL:HG23 | 1:V:1088:TRP:H    | 1.81                     | 0.46              |
| 3:W:2107:THR:OG1  | 3:W:2247:MET:SD   | 2.73                     | 0.46              |
| 1:J:1116:MET:SD   | 1:J:1116:MET:N    | 2.89                     | 0.46              |
| 2:C:3121:PHE:HD1  | 2:C:3211:VAL:HG22 | 1.81                     | 0.46              |
| 1:A:1087:VAL:HG23 | 1:A:1088:TRP:H    | 1.81                     | 0.46              |
| 1:Y:1087:VAL:HG23 | 1:Y:1088:TRP:H    | 1.81                     | 0.46              |
| 1:Y:1243:TRP:HD1  | 2:a:3039:GLU:HA   | 1.82                     | 0.46              |
| 2:a:3111:TRP:HZ3  | 2:a:3172:ILE:HG22 | 1.81                     | 0.46              |
| 2:X:3120:LEU:HB3  | 2:X:3212:LEU:HB2  | 1.97                     | 0.46              |
| 2:X:3169:VAL:HG12 | 2:X:3172:ILE:HD11 | 1.98                     | 0.46              |
| 1:S:1087:VAL:HG23 | 1:S:1088:TRP:H    | 1.81                     | 0.46              |
| 2:I:3111:TRP:HZ3  | 2:I:3172:ILE:HG22 | 1.81                     | 0.46              |
| 1:b:1116:MET:SD   | 1:b:1116:MET:N    | 2.89                     | 0.45              |
| 1:b:1157:TRP:CH2  | 1:b:1215:TYR:HB3  | 2.51                     | 0.45              |
| 2:d:3111:TRP:HZ3  | 2:d:3172:ILE:HG22 | 1.81                     | 0.45              |
| 2:a:3120:LEU:HB3  | 2:a:3212:LEU:HB2  | 1.98                     | 0.45              |
| 3:W:2105:GLY:H    | 3:W:2247:MET:H    | 1.64                     | 0.45              |
| 3:T:2142:PRO:HB2  | 3:T:2144:THR:HG22 | 1.98                     | 0.45              |
| 2:R:3097:LYS:HG3  | 2:R:3098:ARG:HG2  | 1.97                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:R:3120:LEU:HB3  | 2:R:3212:LEU:HB2  | 1.97                     | 0.45              |
| 3:K:2142:PRO:HB2  | 3:K:2144:THR:HG22 | 1.98                     | 0.45              |
| 2:I:3097:LYS:HG3  | 2:I:3098:ARG:HG2  | 1.97                     | 0.45              |
| 2:F:3111:TRP:HZ3  | 2:F:3172:ILE:HG22 | 1.81                     | 0.45              |
| 1:b:1270:ARG:NH1  | 1:b:1275:ASP:O    | 2.40                     | 0.45              |
| 1:P:1157:TRP:CH2  | 1:P:1215:TYR:HB3  | 2.52                     | 0.45              |
| 3:N:2142:PRO:HB2  | 3:N:2144:THR:HG22 | 1.98                     | 0.45              |
| 3:E:2076:PRO:HB2  | 3:E:2155:PHE:HB2  | 1.97                     | 0.45              |
| 2:R:3111:TRP:HZ3  | 2:R:3172:ILE:HG22 | 1.81                     | 0.45              |
| 3:E:2105:GLY:H    | 3:E:2247:MET:H    | 1.64                     | 0.45              |
| 3:E:2107:THR:OG1  | 3:E:2247:MET:SD   | 2.73                     | 0.45              |
| 3:B:2105:GLY:H    | 3:B:2247:MET:H    | 1.64                     | 0.45              |
| 1:A:1116:MET:SD   | 1:A:1116:MET:N    | 2.89                     | 0.45              |
| 2:g:3111:TRP:HZ3  | 2:g:3172:ILE:HG22 | 1.81                     | 0.45              |
| 2:a:3097:LYS:HG3  | 2:a:3098:ARG:HG2  | 1.97                     | 0.45              |
| 3:T:2105:GLY:H    | 3:T:2247:MET:H    | 1.64                     | 0.45              |
| 1:P:1116:MET:SD   | 1:P:1116:MET:N    | 2.89                     | 0.45              |
| 1:M:1087:VAL:HG23 | 1:M:1088:TRP:H    | 1.81                     | 0.45              |
| 2:O:3111:TRP:HZ3  | 2:O:3172:ILE:HG22 | 1.81                     | 0.45              |
| 2:O:3169:VAL:HG12 | 2:O:3172:ILE:HD11 | 1.97                     | 0.45              |
| 2:I:3120:LEU:HB3  | 2:I:3212:LEU:HB2  | 1.97                     | 0.45              |
| 1:D:1157:TRP:CH2  | 1:D:1215:TYR:HB3  | 2.52                     | 0.45              |
| 2:F:3097:LYS:HG3  | 2:F:3098:ARG:HG2  | 1.97                     | 0.45              |
| 2:C:3111:TRP:HZ3  | 2:C:3172:ILE:HG22 | 1.81                     | 0.45              |
| 2:a:3169:VAL:HG12 | 2:a:3172:ILE:HD11 | 1.98                     | 0.45              |
| 1:M:1157:TRP:CH2  | 1:M:1215:TYR:HB3  | 2.51                     | 0.45              |
| 2:O:3121:PHE:HD1  | 2:O:3211:VAL:HG22 | 1.81                     | 0.45              |
| 2:F:3089:ASP:N    | 2:F:3089:ASP:OD1  | 2.47                     | 0.45              |
| 1:e:1116:MET:SD   | 1:e:1116:MET:N    | 2.89                     | 0.45              |
| 2:X:3121:PHE:HD1  | 2:X:3211:VAL:HG22 | 1.81                     | 0.45              |
| 3:T:2081:LYS:HD2  | 3:T:2147:THR:HG21 | 1.97                     | 0.45              |
| 3:Q:2105:GLY:H    | 3:Q:2247:MET:H    | 1.64                     | 0.45              |
| 1:J:1157:TRP:CH2  | 1:J:1215:TYR:HB3  | 2.52                     | 0.45              |
| 2:L:3027:GLN:HG2  | 1:G:1060:ASN:OD1  | 2.16                     | 0.45              |
| 1:G:1157:TRP:CH2  | 1:G:1215:TYR:HB3  | 2.52                     | 0.45              |
| 2:I:3121:PHE:HD1  | 2:I:3211:VAL:HG22 | 1.81                     | 0.45              |
| 2:F:3121:PHE:HD1  | 2:F:3211:VAL:HG22 | 1.81                     | 0.45              |
| 2:g:3120:LEU:HB3  | 2:g:3212:LEU:HB2  | 1.97                     | 0.45              |
| 1:e:1157:TRP:CH2  | 1:e:1215:TYR:HB3  | 2.52                     | 0.45              |
| 2:d:3097:LYS:HG3  | 2:d:3098:ARG:HG2  | 1.97                     | 0.45              |
| 1:V:1109:ARG:HH12 | 2:X:3031:THR:HB   | 1.82                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:E:2142:PRO:HB2  | 3:E:2144:THR:HG22 | 1.98                     | 0.45              |
| 2:F:3169:VAL:HG12 | 2:F:3172:ILE:HD11 | 1.98                     | 0.45              |
| 3:f:2105:GLY:H    | 3:f:2247:MET:H    | 1.64                     | 0.45              |
| 1:V:1116:MET:SD   | 1:V:1116:MET:N    | 2.89                     | 0.45              |
| 1:G:1087:VAL:HG23 | 1:G:1088:TRP:H    | 1.81                     | 0.45              |
| 1:b:1087:VAL:HG23 | 1:b:1088:TRP:H    | 1.81                     | 0.45              |
| 3:Z:2076:PRO:HG2  | 3:Z:2155:PHE:H    | 1.82                     | 0.45              |
| 3:H:2105:GLY:H    | 3:H:2247:MET:H    | 1.64                     | 0.45              |
| 1:A:1157:TRP:CH2  | 1:A:1215:TYR:HB3  | 2.52                     | 0.45              |
| 3:c:2076:PRO:HG2  | 3:c:2155:PHE:H    | 1.82                     | 0.45              |
| 3:H:2142:PRO:HB2  | 3:H:2144:THR:HG22 | 1.98                     | 0.45              |
| 2:C:3169:VAL:HG12 | 2:C:3172:ILE:HD11 | 1.98                     | 0.45              |
| 3:c:2033:VAL:HA   | 3:c:2200:VAL:HB   | 1.99                     | 0.44              |
| 3:c:2105:GLY:H    | 3:c:2247:MET:H    | 1.64                     | 0.44              |
| 1:S:1157:TRP:CH2  | 1:S:1215:TYR:HB3  | 2.52                     | 0.44              |
| 3:N:2076:PRO:HG2  | 3:N:2155:PHE:H    | 1.82                     | 0.44              |
| 3:K:2033:VAL:HA   | 3:K:2200:VAL:HB   | 1.99                     | 0.44              |
| 2:L:3121:PHE:HD1  | 2:L:3211:VAL:HG22 | 1.81                     | 0.44              |
| 2:g:3203:PRO:HD2  | 3:Z:2117:PHE:CD2  | 2.52                     | 0.44              |
| 3:f:2142:PRO:HB2  | 3:f:2144:THR:HG22 | 1.98                     | 0.44              |
| 3:c:2142:PRO:HB2  | 3:c:2144:THR:HG22 | 1.98                     | 0.44              |
| 2:R:3121:PHE:HD1  | 2:R:3211:VAL:HG22 | 1.81                     | 0.44              |
| 3:B:2076:PRO:HG2  | 3:B:2155:PHE:H    | 1.82                     | 0.44              |
| 3:B:2142:PRO:HB2  | 3:B:2144:THR:HG22 | 1.98                     | 0.44              |
| 1:Y:1270:ARG:NH1  | 1:Y:1275:ASP:O    | 2.40                     | 0.44              |
| 3:Z:2033:VAL:HA   | 3:Z:2200:VAL:HB   | 1.99                     | 0.44              |
| 3:W:2209:MET:O    | 1:J:1045:ARG:NH1  | 2.50                     | 0.44              |
| 3:N:2033:VAL:HA   | 3:N:2200:VAL:HB   | 1.99                     | 0.44              |
| 2:L:3097:LYS:HG3  | 2:L:3098:ARG:HG2  | 1.97                     | 0.44              |
| 2:g:3121:PHE:HD1  | 2:g:3211:VAL:HG22 | 1.81                     | 0.44              |
| 1:e:1047:VAL:HB   | 3:N:2207:VAL:HG23 | 2.00                     | 0.44              |
| 2:d:3121:PHE:HD1  | 2:d:3211:VAL:HG22 | 1.81                     | 0.44              |
| 3:W:2033:VAL:HA   | 3:W:2200:VAL:HB   | 1.99                     | 0.44              |
| 2:O:3120:LEU:HB3  | 2:O:3212:LEU:HB2  | 1.98                     | 0.44              |
| 1:V:1157:TRP:CH2  | 1:V:1215:TYR:HB3  | 2.51                     | 0.44              |
| 3:Q:2076:PRO:HG2  | 3:Q:2155:PHE:H    | 1.82                     | 0.44              |
| 2:R:3198:ASN:OD1  | 3:N:2070:GLN:NE2  | 2.50                     | 0.44              |
| 2:O:3130:LYS:N    | 2:O:3197:THR:OG1  | 2.46                     | 0.44              |
| 3:f:2093:GLY:HA2  | 3:f:2096:MET:SD   | 2.58                     | 0.44              |
| 1:b:1171:ASN:ND2  | 1:D:1170:GLY:O    | 2.42                     | 0.44              |
| 1:M:1046:HIS:CE1  | 1:G:1208:LEU:HD11 | 2.51                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:Y:1157:TRP:CH2  | 1:Y:1215:TYR:HB3  | 2.52                     | 0.44              |
| 3:B:2033:VAL:HA   | 3:B:2200:VAL:HB   | 1.99                     | 0.44              |
| 3:Z:2093:GLY:HA2  | 3:Z:2096:MET:SD   | 2.58                     | 0.44              |
| 1:V:1270:ARG:NE   | 2:X:3057:ASN:OD1  | 2.50                     | 0.44              |
| 3:T:2033:VAL:HA   | 3:T:2200:VAL:HB   | 1.99                     | 0.44              |
| 3:T:2093:GLY:HA2  | 3:T:2096:MET:SD   | 2.58                     | 0.44              |
| 3:K:2076:PRO:HG2  | 3:K:2155:PHE:H    | 1.82                     | 0.44              |
| 3:H:2093:GLY:HA2  | 3:H:2096:MET:SD   | 2.58                     | 0.44              |
| 3:W:2076:PRO:HG2  | 3:W:2155:PHE:H    | 1.82                     | 0.44              |
| 3:f:2076:PRO:HG2  | 3:f:2155:PHE:H    | 1.83                     | 0.43              |
| 2:U:3121:PHE:HD1  | 2:U:3211:VAL:HG22 | 1.82                     | 0.43              |
| 1:P:1075:ILE:O    | 1:P:1084:ARG:NH2  | 2.45                     | 0.43              |
| 3:N:2093:GLY:HA2  | 3:N:2096:MET:SD   | 2.58                     | 0.43              |
| 3:H:2076:PRO:HG2  | 3:H:2155:PHE:H    | 1.83                     | 0.43              |
| 3:c:2093:GLY:HA2  | 3:c:2096:MET:SD   | 2.58                     | 0.43              |
| 3:T:2076:PRO:HG2  | 3:T:2155:PHE:H    | 1.82                     | 0.43              |
| 3:T:2107:THR:OG1  | 3:T:2247:MET:SD   | 2.73                     | 0.43              |
| 2:O:3009:GLY:CA   | 1:G:1175:ARG:H    | 2.29                     | 0.43              |
| 3:c:2101:LEU:HA   | 1:D:1045:ARG:HH21 | 1.83                     | 0.43              |
| 1:V:1270:ARG:NH1  | 1:V:1275:ASP:O    | 2.40                     | 0.43              |
| 2:R:3128:THR:CG2  | 3:N:2113:ASN:HB2  | 2.49                     | 0.43              |
| 2:O:3229:THR:HA   | 2:O:3230:PRO:HD3  | 1.88                     | 0.43              |
| 1:J:1267:THR:HB   | 2:L:3094:SER:O    | 2.18                     | 0.43              |
| 3:K:2014:ARG:O    | 3:K:2025:THR:OG1  | 2.33                     | 0.43              |
| 3:E:2033:VAL:HA   | 3:E:2200:VAL:HB   | 1.99                     | 0.43              |
| 3:B:2093:GLY:HA2  | 3:B:2096:MET:SD   | 2.58                     | 0.43              |
| 3:f:2033:VAL:HA   | 3:f:2200:VAL:HB   | 1.99                     | 0.43              |
| 3:E:2093:GLY:HA2  | 3:E:2096:MET:SD   | 2.58                     | 0.43              |
| 3:E:2156:THR:HG21 | 3:E:2160:ILE:HG21 | 2.01                     | 0.43              |
| 2:g:3126:MET:HE1  | 3:Z:2116:LYS:NZ   | 2.34                     | 0.43              |
| 2:d:3111:TRP:CZ3  | 2:d:3172:ILE:HG22 | 2.54                     | 0.43              |
| 2:a:3111:TRP:CZ3  | 2:a:3172:ILE:HG22 | 2.54                     | 0.43              |
| 2:X:3111:TRP:CZ3  | 2:X:3172:ILE:HG22 | 2.54                     | 0.43              |
| 3:T:2111:GLN:HB2  | 3:T:2241:THR:HB   | 2.01                     | 0.43              |
| 2:U:3111:TRP:CZ3  | 2:U:3172:ILE:HG22 | 2.54                     | 0.43              |
| 1:M:1223:SER:OG   | 1:M:1225:HIS:O    | 2.26                     | 0.43              |
| 1:e:1075:ILE:O    | 1:e:1084:ARG:NH2  | 2.45                     | 0.43              |
| 3:Z:2111:GLN:HB2  | 3:Z:2241:THR:HB   | 2.01                     | 0.43              |
| 3:W:2111:GLN:HB2  | 3:W:2241:THR:HB   | 2.01                     | 0.43              |
| 1:G:1260:ASN:ND2  | 3:H:2137:THR:HB   | 2.33                     | 0.43              |
| 1:D:1118:ILE:HD11 | 1:D:1139:ILE:HD11 | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:B:2111:GLN:HB2  | 3:B:2241:THR:HB   | 2.01                     | 0.43              |
| 1:V:1117:VAL:HG22 | 1:V:1173:PRO:HG2  | 2.01                     | 0.43              |
| 3:W:2093:GLY:HA2  | 3:W:2096:MET:SD   | 2.58                     | 0.43              |
| 3:T:2156:THR:HG21 | 3:T:2160:ILE:HG21 | 2.01                     | 0.43              |
| 1:G:1118:ILE:HD11 | 1:G:1139:ILE:HD11 | 2.01                     | 0.43              |
| 3:H:2033:VAL:HA   | 3:H:2200:VAL:HB   | 1.99                     | 0.43              |
| 2:I:3111:TRP:CZ3  | 2:I:3172:ILE:HG22 | 2.54                     | 0.43              |
| 3:E:2111:GLN:HB2  | 3:E:2241:THR:HB   | 2.01                     | 0.43              |
| 1:A:1117:VAL:HG22 | 1:A:1173:PRO:HG2  | 2.01                     | 0.43              |
| 3:f:2156:THR:HG21 | 3:f:2160:ILE:HG21 | 2.01                     | 0.43              |
| 3:c:2234:ALA:HB2  | 2:C:3203:PRO:HD3  | 2.00                     | 0.43              |
| 1:S:1117:VAL:HG22 | 1:S:1173:PRO:HG2  | 2.01                     | 0.43              |
| 1:P:1118:ILE:HD11 | 1:P:1139:ILE:HD11 | 2.01                     | 0.43              |
| 3:Q:2033:VAL:HA   | 3:Q:2200:VAL:HB   | 1.99                     | 0.43              |
| 3:Q:2156:THR:HG21 | 3:Q:2160:ILE:HG21 | 2.01                     | 0.43              |
| 3:N:2111:GLN:HB2  | 3:N:2241:THR:HB   | 2.01                     | 0.43              |
| 2:O:3111:TRP:CZ3  | 2:O:3172:ILE:HG22 | 2.54                     | 0.43              |
| 3:K:2093:GLY:HA2  | 3:K:2096:MET:SD   | 2.58                     | 0.43              |
| 3:E:2076:PRO:HG2  | 3:E:2155:PHE:H    | 1.82                     | 0.43              |
| 2:C:3111:TRP:CZ3  | 2:C:3172:ILE:HG22 | 2.54                     | 0.43              |
| 1:e:1118:ILE:HD11 | 1:e:1139:ILE:HD11 | 2.01                     | 0.43              |
| 3:Z:2156:THR:HG21 | 3:Z:2160:ILE:HG21 | 2.01                     | 0.43              |
| 1:J:1270:ARG:NH1  | 1:J:1275:ASP:O    | 2.40                     | 0.43              |
| 1:G:1109:ARG:HH22 | 2:I:3031:THR:HB   | 1.83                     | 0.43              |
| 2:d:3229:THR:HA   | 2:d:3230:PRO:HD3  | 1.88                     | 0.43              |
| 1:Y:1117:VAL:HG22 | 1:Y:1173:PRO:HG2  | 2.01                     | 0.43              |
| 2:a:3013:PHE:HD2  | 1:D:1166:PHE:HD1  | 1.65                     | 0.43              |
| 1:P:1117:VAL:HG22 | 1:P:1173:PRO:HG2  | 2.01                     | 0.43              |
| 3:Q:2111:GLN:HB2  | 3:Q:2241:THR:HB   | 2.01                     | 0.43              |
| 1:J:1117:VAL:HG22 | 1:J:1173:PRO:HG2  | 2.01                     | 0.43              |
| 3:H:2111:GLN:HB2  | 3:H:2241:THR:HB   | 2.01                     | 0.43              |
| 2:F:3111:TRP:CZ3  | 2:F:3172:ILE:HG22 | 2.54                     | 0.43              |
| 3:f:2111:GLN:HB2  | 3:f:2241:THR:HB   | 2.01                     | 0.42              |
| 3:c:2156:THR:HG21 | 3:c:2160:ILE:HG21 | 2.01                     | 0.42              |
| 2:a:3171:TRP:CZ2  | 3:E:2051:ASP:HA   | 2.54                     | 0.42              |
| 2:a:3229:THR:HA   | 2:a:3230:PRO:HD3  | 1.88                     | 0.42              |
| 1:V:1118:ILE:HD11 | 1:V:1139:ILE:HD11 | 2.01                     | 0.42              |
| 3:W:2156:THR:HG21 | 3:W:2160:ILE:HG21 | 2.01                     | 0.42              |
| 1:S:1153:ASP:OD1  | 1:S:1153:ASP:N    | 2.52                     | 0.42              |
| 1:G:1117:VAL:HG22 | 1:G:1173:PRO:HG2  | 2.01                     | 0.42              |
| 3:H:2156:THR:HG21 | 3:H:2160:ILE:HG21 | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:e:1047:VAL:HB   | 3:N:2207:VAL:CG2  | 2.48                     | 0.42              |
| 1:e:1060:ASN:O    | 1:e:1064:ARG:NH1  | 2.53                     | 0.42              |
| 1:b:1117:VAL:HG22 | 1:b:1173:PRO:HG2  | 2.01                     | 0.42              |
| 3:W:2229:ASN:ND2  | 2:X:3208:SER:OG   | 2.52                     | 0.42              |
| 3:Q:2093:GLY:HA2  | 3:Q:2096:MET:SD   | 2.58                     | 0.42              |
| 1:G:1270:ARG:NH2  | 2:I:3055:VAL:O    | 2.53                     | 0.42              |
| 1:A:1118:ILE:HD11 | 1:A:1139:ILE:HD11 | 2.01                     | 0.42              |
| 1:Y:1060:ASN:O    | 1:Y:1064:ARG:NH1  | 2.53                     | 0.42              |
| 1:M:1117:VAL:HG22 | 1:M:1173:PRO:HG2  | 2.01                     | 0.42              |
| 2:L:3050:ASP:HA   | 2:L:3216:SER:HB3  | 2.02                     | 0.42              |
| 1:D:1117:VAL:HG22 | 1:D:1173:PRO:HG2  | 2.01                     | 0.42              |
| 1:D:1153:ASP:OD1  | 1:D:1153:ASP:N    | 2.52                     | 0.42              |
| 1:A:1243:TRP:CD1  | 2:C:3039:GLU:HA   | 2.55                     | 0.42              |
| 2:g:3050:ASP:HA   | 2:g:3216:SER:HB3  | 2.02                     | 0.42              |
| 2:d:3050:ASP:HA   | 2:d:3216:SER:HB3  | 2.02                     | 0.42              |
| 2:X:3229:THR:HA   | 2:X:3230:PRO:HD3  | 1.88                     | 0.42              |
| 1:J:1076:ASN:OD1  | 1:J:1226:GLN:NE2  | 2.53                     | 0.42              |
| 1:G:1060:ASN:O    | 1:G:1064:ARG:NH1  | 2.53                     | 0.42              |
| 1:D:1185:ASN:ND2  | 3:E:2206:SER:O    | 2.53                     | 0.42              |
| 1:A:1060:ASN:O    | 1:A:1064:ARG:NH1  | 2.53                     | 0.42              |
| 1:A:1076:ASN:OD1  | 1:A:1226:GLN:NE2  | 2.53                     | 0.42              |
| 2:g:3111:TRP:CZ3  | 2:g:3172:ILE:HG22 | 2.54                     | 0.42              |
| 3:f:2110:VAL:HB   | 3:f:2197:ALA:HB3  | 2.02                     | 0.42              |
| 3:Q:2110:VAL:HB   | 3:Q:2197:ALA:HB3  | 2.02                     | 0.42              |
| 2:R:3111:TRP:CZ3  | 2:R:3172:ILE:HG22 | 2.54                     | 0.42              |
| 1:A:1095:MET:HE2  | 1:A:1098:LEU:HB2  | 2.02                     | 0.42              |
| 3:c:2110:VAL:HB   | 3:c:2197:ALA:HB3  | 2.02                     | 0.42              |
| 3:c:2111:GLN:HB2  | 3:c:2241:THR:HB   | 2.01                     | 0.42              |
| 1:Y:1075:ILE:O    | 1:Y:1084:ARG:NH2  | 2.45                     | 0.42              |
| 1:M:1118:ILE:HD11 | 1:M:1139:ILE:HD11 | 2.01                     | 0.42              |
| 2:O:3050:ASP:HA   | 2:O:3216:SER:HB3  | 2.02                     | 0.42              |
| 1:J:1153:ASP:OD1  | 1:J:1153:ASP:N    | 2.52                     | 0.42              |
| 3:K:2110:VAL:HB   | 3:K:2197:ALA:HB3  | 2.02                     | 0.42              |
| 3:K:2111:GLN:HB2  | 3:K:2241:THR:HB   | 2.01                     | 0.42              |
| 2:L:3111:TRP:CZ3  | 2:L:3172:ILE:HG22 | 2.54                     | 0.42              |
| 3:H:2048:THR:HG22 | 3:H:2050:GLU:H    | 1.85                     | 0.42              |
| 1:D:1060:ASN:O    | 1:D:1064:ARG:NH1  | 2.53                     | 0.42              |
| 2:C:3029:ASP:OD1  | 2:C:3029:ASP:N    | 2.47                     | 0.42              |
| 1:A:1243:TRP:HD1  | 2:C:3039:GLU:HA   | 1.85                     | 0.42              |
| 1:e:1076:ASN:OD1  | 1:e:1226:GLN:NE2  | 2.53                     | 0.42              |
| 1:Y:1076:ASN:OD1  | 1:Y:1226:GLN:NE2  | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:Z:2209:MET:O    | 1:P:1045:ARG:NH1  | 2.49                     | 0.42              |
| 1:J:1060:ASN:O    | 1:J:1064:ARG:NH1  | 2.53                     | 0.42              |
| 3:K:2048:THR:HG22 | 3:K:2050:GLU:H    | 1.85                     | 0.42              |
| 3:E:2048:THR:HG22 | 3:E:2050:GLU:H    | 1.85                     | 0.42              |
| 1:V:1076:ASN:OD1  | 1:V:1226:GLN:NE2  | 2.53                     | 0.42              |
| 1:S:1060:ASN:O    | 1:S:1064:ARG:NH1  | 2.53                     | 0.42              |
| 1:S:1118:ILE:HD11 | 1:S:1139:ILE:HD11 | 2.01                     | 0.42              |
| 2:U:3050:ASP:HA   | 2:U:3216:SER:HB3  | 2.02                     | 0.42              |
| 1:D:1075:ILE:O    | 1:D:1084:ARG:NH2  | 2.45                     | 0.42              |
| 1:D:1076:ASN:OD1  | 1:D:1226:GLN:NE2  | 2.53                     | 0.42              |
| 3:B:2156:THR:HG21 | 3:B:2160:ILE:HG21 | 2.01                     | 0.42              |
| 2:g:3069:GLN:NE2  | 3:f:2225:PHE:O    | 2.53                     | 0.42              |
| 1:b:1047:VAL:HG21 | 3:T:2209:MET:HB2  | 2.01                     | 0.42              |
| 1:b:1075:ILE:O    | 1:b:1084:ARG:NH2  | 2.45                     | 0.42              |
| 1:b:1095:MET:HE2  | 1:b:1098:LEU:HB2  | 2.02                     | 0.42              |
| 2:a:3031:THR:HG23 | 2:R:3224:ARG:NH2  | 2.34                     | 0.42              |
| 1:V:1095:MET:HE2  | 1:V:1098:LEU:HB2  | 2.02                     | 0.42              |
| 3:W:2014:ARG:O    | 3:W:2025:THR:OG1  | 2.33                     | 0.42              |
| 2:R:3050:ASP:HA   | 2:R:3216:SER:HB3  | 2.02                     | 0.42              |
| 1:M:1060:ASN:O    | 1:M:1064:ARG:NH1  | 2.53                     | 0.42              |
| 1:M:1076:ASN:OD1  | 1:M:1226:GLN:NE2  | 2.53                     | 0.42              |
| 1:M:1236:LYS:NZ   | 2:O:3017:ASP:OD1  | 2.52                     | 0.42              |
| 1:J:1118:ILE:HD11 | 1:J:1139:ILE:HD11 | 2.01                     | 0.42              |
| 3:K:2156:THR:HG21 | 3:K:2160:ILE:HG21 | 2.01                     | 0.42              |
| 1:G:1076:ASN:OD1  | 1:G:1226:GLN:NE2  | 2.53                     | 0.42              |
| 1:e:1117:VAL:HG22 | 1:e:1173:PRO:HG2  | 2.01                     | 0.42              |
| 2:X:3050:ASP:HA   | 2:X:3216:SER:HB3  | 2.01                     | 0.42              |
| 3:N:2156:THR:HG21 | 3:N:2160:ILE:HG21 | 2.01                     | 0.42              |
| 1:A:1112:ILE:HG12 | 1:A:1178:ILE:HB   | 2.02                     | 0.41              |
| 1:e:1095:MET:HE2  | 1:e:1098:LEU:HB2  | 2.02                     | 0.41              |
| 1:b:1060:ASN:O    | 1:b:1064:ARG:NH1  | 2.53                     | 0.41              |
| 3:Z:2146:LEU:HD11 | 3:Z:2165:VAL:H    | 1.85                     | 0.41              |
| 1:S:1076:ASN:OD1  | 1:S:1226:GLN:NE2  | 2.53                     | 0.41              |
| 3:T:2110:VAL:HB   | 3:T:2197:ALA:HB3  | 2.02                     | 0.41              |
| 3:N:2110:VAL:HB   | 3:N:2197:ALA:HB3  | 2.02                     | 0.41              |
| 2:F:3050:ASP:HA   | 2:F:3216:SER:HB3  | 2.02                     | 0.41              |
| 2:F:3133:ILE:HD12 | 2:F:3155:ILE:HD11 | 2.02                     | 0.41              |
| 2:C:3087:GLN:HE22 | 2:C:3188:ALA:H    | 1.68                     | 0.41              |
| 1:b:1076:ASN:OD1  | 1:b:1226:GLN:NE2  | 2.53                     | 0.41              |
| 3:Z:2110:VAL:HB   | 3:Z:2197:ALA:HB3  | 2.02                     | 0.41              |
| 2:a:3050:ASP:HA   | 2:a:3216:SER:HB3  | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:V:1060:ASN:O    | 1:V:1064:ARG:NH1  | 2.53                     | 0.41              |
| 2:X:3133:ILE:HD12 | 2:X:3155:ILE:HD11 | 2.02                     | 0.41              |
| 3:Q:2048:THR:HG22 | 3:Q:2050:GLU:H    | 1.85                     | 0.41              |
| 2:R:3133:ILE:HD12 | 2:R:3155:ILE:HD11 | 2.03                     | 0.41              |
| 1:D:1121:CYS:SG   | 1:D:1122:GLN:N    | 2.94                     | 0.41              |
| 1:b:1121:CYS:SG   | 1:b:1122:GLN:N    | 2.94                     | 0.41              |
| 3:c:2048:THR:HG22 | 3:c:2050:GLU:H    | 1.85                     | 0.41              |
| 1:Y:1112:ILE:HG12 | 1:Y:1178:ILE:HB   | 2.02                     | 0.41              |
| 3:W:2048:THR:HG22 | 3:W:2050:GLU:H    | 1.85                     | 0.41              |
| 3:T:2146:LEU:HD11 | 3:T:2165:VAL:H    | 1.85                     | 0.41              |
| 1:P:1060:ASN:O    | 1:P:1064:ARG:NH1  | 2.53                     | 0.41              |
| 1:G:1223:SER:OG   | 1:G:1225:HIS:O    | 2.26                     | 0.41              |
| 2:I:3050:ASP:HA   | 2:I:3216:SER:HB3  | 2.02                     | 0.41              |
| 2:C:3229:THR:HA   | 2:C:3230:PRO:HD3  | 1.88                     | 0.41              |
| 2:g:3087:GLN:HB3  | 2:g:3089:ASP:OD1  | 2.21                     | 0.41              |
| 2:g:3133:ILE:HD12 | 2:g:3155:ILE:HD11 | 2.02                     | 0.41              |
| 1:Y:1118:ILE:HD11 | 1:Y:1139:ILE:HD11 | 2.01                     | 0.41              |
| 3:Z:2019:GLY:CA   | 3:N:2255:ARG:HG2  | 2.51                     | 0.41              |
| 1:V:1121:CYS:SG   | 1:V:1122:GLN:N    | 2.94                     | 0.41              |
| 1:P:1076:ASN:OD1  | 1:P:1226:GLN:NE2  | 2.53                     | 0.41              |
| 1:P:1095:MET:HE2  | 1:P:1098:LEU:HB2  | 2.02                     | 0.41              |
| 1:M:1112:ILE:HG12 | 1:M:1178:ILE:HB   | 2.02                     | 0.41              |
| 3:N:2227:PRO:HD3  | 2:O:3069:GLN:HE22 | 1.86                     | 0.41              |
| 1:J:1075:ILE:O    | 1:J:1084:ARG:NH2  | 2.45                     | 0.41              |
| 1:G:1112:ILE:HG12 | 1:G:1178:ILE:HB   | 2.02                     | 0.41              |
| 3:H:2110:VAL:HB   | 3:H:2197:ALA:HB3  | 2.02                     | 0.41              |
| 2:I:3133:ILE:HD12 | 2:I:3155:ILE:HD11 | 2.02                     | 0.41              |
| 2:g:3136:SER:HB2  | 2:g:3190:TYR:HB2  | 2.03                     | 0.41              |
| 1:e:1121:CYS:SG   | 1:e:1122:GLN:N    | 2.94                     | 0.41              |
| 2:d:3136:SER:HB2  | 2:d:3190:TYR:HB2  | 2.03                     | 0.41              |
| 1:S:1121:CYS:SG   | 1:S:1122:GLN:N    | 2.94                     | 0.41              |
| 1:P:1121:CYS:SG   | 1:P:1122:GLN:N    | 2.94                     | 0.41              |
| 1:J:1121:CYS:SG   | 1:J:1122:GLN:N    | 2.94                     | 0.41              |
| 2:L:3087:GLN:HB3  | 2:L:3089:ASP:OD1  | 2.21                     | 0.41              |
| 2:L:3133:ILE:HD12 | 2:L:3155:ILE:HD11 | 2.02                     | 0.41              |
| 2:L:3136:SER:HB2  | 2:L:3190:TYR:HB2  | 2.03                     | 0.41              |
| 1:D:1095:MET:HE2  | 1:D:1098:LEU:HB2  | 2.02                     | 0.41              |
| 1:D:1112:ILE:HG12 | 1:D:1178:ILE:HB   | 2.02                     | 0.41              |
| 2:C:3133:ILE:HD12 | 2:C:3155:ILE:HD11 | 2.02                     | 0.41              |
| 1:b:1095:MET:HG3  | 1:b:1098:LEU:H    | 1.86                     | 0.41              |
| 2:d:3087:GLN:HB3  | 2:d:3089:ASP:OD1  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:a:3087:GLN:HB3  | 2:a:3089:ASP:OD1  | 2.21                     | 0.41              |
| 2:a:3136:SER:HB2  | 2:a:3190:TYR:HB2  | 2.03                     | 0.41              |
| 1:V:1095:MET:HG3  | 1:V:1098:LEU:H    | 1.86                     | 0.41              |
| 2:U:3009:GLY:HA2  | 1:P:1174:PRO:HA   | 2.02                     | 0.41              |
| 2:U:3133:ILE:HD12 | 2:U:3155:ILE:HD11 | 2.02                     | 0.41              |
| 3:Q:2014:ARG:O    | 3:Q:2025:THR:OG1  | 2.33                     | 0.41              |
| 3:N:2146:LEU:HD11 | 3:N:2165:VAL:H    | 1.85                     | 0.41              |
| 3:E:2146:LEU:HD11 | 3:E:2165:VAL:H    | 1.85                     | 0.41              |
| 2:C:3050:ASP:HA   | 2:C:3216:SER:HB3  | 2.02                     | 0.41              |
| 2:C:3136:SER:HB2  | 2:C:3190:TYR:HB2  | 2.03                     | 0.41              |
| 1:e:1110:PHE:HB3  | 1:e:1240:ILE:HG13 | 2.03                     | 0.41              |
| 1:b:1118:ILE:HD11 | 1:b:1139:ILE:HD11 | 2.01                     | 0.41              |
| 2:d:3133:ILE:HD12 | 2:d:3155:ILE:HD11 | 2.02                     | 0.41              |
| 1:Y:1153:ASP:OD1  | 1:Y:1153:ASP:N    | 2.52                     | 0.41              |
| 1:V:1110:PHE:HB3  | 1:V:1240:ILE:HG13 | 2.03                     | 0.41              |
| 3:W:2146:LEU:HD11 | 3:W:2165:VAL:H    | 1.85                     | 0.41              |
| 1:P:1095:MET:HG3  | 1:P:1098:LEU:H    | 1.86                     | 0.41              |
| 1:P:1110:PHE:HB3  | 1:P:1240:ILE:HG13 | 2.03                     | 0.41              |
| 2:R:3087:GLN:HB3  | 2:R:3089:ASP:OD1  | 2.21                     | 0.41              |
| 2:R:3087:GLN:HE22 | 2:R:3188:ALA:H    | 1.68                     | 0.41              |
| 1:M:1121:CYS:SG   | 1:M:1122:GLN:N    | 2.94                     | 0.41              |
| 2:O:3087:GLN:HE22 | 2:O:3188:ALA:H    | 1.68                     | 0.41              |
| 3:f:2048:THR:HG22 | 3:f:2050:GLU:H    | 1.85                     | 0.41              |
| 1:b:1049:ASN:ND2  | 3:T:2042:LEU:HD21 | 2.34                     | 0.41              |
| 1:Y:1167:TRP:HD1  | 1:Y:1173:PRO:HA   | 1.86                     | 0.41              |
| 2:a:3087:GLN:HE22 | 2:a:3188:ALA:H    | 1.68                     | 0.41              |
| 3:W:2071:TRP:HB2  | 3:W:2240:ILE:HD11 | 2.03                     | 0.41              |
| 3:W:2110:VAL:HB   | 3:W:2197:ALA:HB3  | 2.02                     | 0.41              |
| 3:T:2048:THR:HG22 | 3:T:2050:GLU:H    | 1.85                     | 0.41              |
| 2:R:3136:SER:HB2  | 2:R:3190:TYR:HB2  | 2.03                     | 0.41              |
| 1:J:1167:TRP:HD1  | 1:J:1173:PRO:HA   | 1.86                     | 0.41              |
| 1:G:1095:MET:HE2  | 1:G:1098:LEU:HB2  | 2.02                     | 0.41              |
| 3:H:2146:LEU:HD11 | 3:H:2165:VAL:H    | 1.85                     | 0.41              |
| 3:B:2048:THR:HG22 | 3:B:2050:GLU:H    | 1.85                     | 0.41              |
| 3:B:2146:LEU:HD11 | 3:B:2165:VAL:H    | 1.85                     | 0.41              |
| 1:A:1121:CYS:SG   | 1:A:1122:GLN:N    | 2.94                     | 0.41              |
| 1:A:1167:TRP:HD1  | 1:A:1173:PRO:HA   | 1.86                     | 0.41              |
| 2:g:3017:ASP:OD1  | 1:e:1236:LYS:NZ   | 2.54                     | 0.41              |
| 3:f:2146:LEU:HD11 | 3:f:2165:VAL:H    | 1.85                     | 0.41              |
| 1:e:1202:THR:HG22 | 1:e:1205:TYR:HB3  | 2.03                     | 0.41              |
| 1:b:1112:ILE:HG12 | 1:b:1178:ILE:HB   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:b:1167:TRP:HD1  | 1:b:1173:PRO:HA   | 1.86                     | 0.41              |
| 2:d:3087:GLN:HE22 | 2:d:3188:ALA:H    | 1.68                     | 0.41              |
| 1:Y:1137:HIS:CE1  | 1:Y:1218:HIS:HD2  | 2.39                     | 0.41              |
| 2:a:3133:ILE:HD12 | 2:a:3155:ILE:HD11 | 2.02                     | 0.41              |
| 1:V:1112:ILE:HG12 | 1:V:1178:ILE:HB   | 2.02                     | 0.41              |
| 1:S:1048:VAL:HG11 | 2:U:3112:SER:OG   | 2.21                     | 0.41              |
| 1:S:1055:GLU:HB3  | 2:U:3223:VAL:HG13 | 2.03                     | 0.41              |
| 2:U:3087:GLN:HE22 | 2:U:3188:ALA:H    | 1.69                     | 0.41              |
| 2:U:3136:SER:HB2  | 2:U:3190:TYR:HB2  | 2.03                     | 0.41              |
| 1:P:1137:HIS:CE1  | 1:P:1218:HIS:HD2  | 2.39                     | 0.41              |
| 1:M:1167:TRP:HD1  | 1:M:1173:PRO:HA   | 1.86                     | 0.41              |
| 1:J:1095:MET:HE2  | 1:J:1098:LEU:HB2  | 2.02                     | 0.41              |
| 1:J:1112:ILE:HG12 | 1:J:1178:ILE:HB   | 2.02                     | 0.41              |
| 3:K:2146:LEU:HD11 | 3:K:2165:VAL:H    | 1.85                     | 0.41              |
| 1:G:1121:CYS:SG   | 1:G:1122:GLN:N    | 2.94                     | 0.41              |
| 2:I:3087:GLN:HB3  | 2:I:3089:ASP:OD1  | 2.21                     | 0.41              |
| 3:E:2071:TRP:HB2  | 3:E:2240:ILE:HD11 | 2.03                     | 0.41              |
| 3:B:2071:TRP:HB2  | 3:B:2240:ILE:HD11 | 2.03                     | 0.41              |
| 3:B:2110:VAL:HB   | 3:B:2197:ALA:HB3  | 2.02                     | 0.41              |
| 3:f:2071:TRP:HB2  | 3:f:2240:ILE:HD11 | 2.03                     | 0.41              |
| 1:e:1137:HIS:CE1  | 1:e:1218:HIS:HD2  | 2.39                     | 0.41              |
| 1:b:1045:ARG:NH1  | 3:T:2209:MET:O    | 2.49                     | 0.41              |
| 2:d:3045:GLU:O    | 2:d:3049:VAL:HG23 | 2.21                     | 0.41              |
| 1:M:1095:MET:HG3  | 1:M:1098:LEU:H    | 1.86                     | 0.41              |
| 3:N:2030:ASN:OD1  | 3:N:2030:ASN:N    | 2.54                     | 0.41              |
| 1:J:1137:HIS:CE1  | 1:J:1218:HIS:HD2  | 2.39                     | 0.41              |
| 2:L:3044:MET:SD   | 2:L:3221:PHE:HB3  | 2.61                     | 0.41              |
| 2:L:3045:GLU:O    | 2:L:3049:VAL:HG23 | 2.21                     | 0.41              |
| 1:G:1167:TRP:HD1  | 1:G:1173:PRO:HA   | 1.86                     | 0.41              |
| 3:H:2030:ASN:OD1  | 3:H:2030:ASN:N    | 2.54                     | 0.41              |
| 2:I:3229:THR:HA   | 2:I:3230:PRO:HD3  | 1.88                     | 0.41              |
| 1:D:1095:MET:HG3  | 1:D:1098:LEU:H    | 1.86                     | 0.41              |
| 3:E:2110:VAL:HB   | 3:E:2197:ALA:HB3  | 2.02                     | 0.41              |
| 2:F:3045:GLU:O    | 2:F:3049:VAL:HG23 | 2.21                     | 0.41              |
| 1:A:1095:MET:HG3  | 1:A:1098:LEU:H    | 1.86                     | 0.40              |
| 1:e:1095:MET:HG3  | 1:e:1098:LEU:H    | 1.86                     | 0.40              |
| 1:Y:1110:PHE:HB3  | 1:Y:1240:ILE:HG13 | 2.03                     | 0.40              |
| 1:Y:1202:THR:HG22 | 1:Y:1205:TYR:HB3  | 2.03                     | 0.40              |
| 3:Z:2118:HIS:CD2  | 3:Z:2228:LEU:HD11 | 2.56                     | 0.40              |
| 2:X:3150:MET:HE3  | 2:X:3150:MET:HB3  | 2.01                     | 0.40              |
| 1:S:1110:PHE:HB3  | 1:S:1240:ILE:HG13 | 2.03                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:P:1112:ILE:HG12 | 1:P:1178:ILE:HB   | 2.02                     | 0.40              |
| 1:P:1167:TRP:HD1  | 1:P:1173:PRO:HA   | 1.86                     | 0.40              |
| 1:P:1202:THR:HG22 | 1:P:1205:TYR:HB3  | 2.03                     | 0.40              |
| 1:M:1110:PHE:HB3  | 1:M:1240:ILE:HG13 | 2.03                     | 0.40              |
| 3:N:2048:THR:HG22 | 3:N:2050:GLU:H    | 1.85                     | 0.40              |
| 3:N:2071:TRP:HB2  | 3:N:2240:ILE:HD11 | 2.03                     | 0.40              |
| 1:D:1137:HIS:CE1  | 1:D:1218:HIS:HD2  | 2.39                     | 0.40              |
| 1:D:1223:SER:OG   | 1:D:1225:HIS:O    | 2.26                     | 0.40              |
| 3:E:2030:ASN:OD1  | 3:E:2030:ASN:N    | 2.54                     | 0.40              |
| 1:e:1072:GLN:HB3  | 1:e:1228:THR:HG21 | 2.04                     | 0.40              |
| 1:e:1079:GLU:HA   | 1:e:1084:ARG:HH11 | 1.87                     | 0.40              |
| 1:b:1202:THR:HG22 | 1:b:1205:TYR:HB3  | 2.03                     | 0.40              |
| 3:c:2051:ASP:OD2  | 1:D:1049:ASN:HA   | 2.21                     | 0.40              |
| 3:Z:2030:ASN:OD1  | 3:Z:2030:ASN:N    | 2.54                     | 0.40              |
| 2:X:3044:MET:SD   | 2:X:3221:PHE:HB3  | 2.61                     | 0.40              |
| 2:U:3044:MET:SD   | 2:U:3221:PHE:HB3  | 2.62                     | 0.40              |
| 3:Q:2071:TRP:HB2  | 3:Q:2240:ILE:HD11 | 2.03                     | 0.40              |
| 3:Q:2146:LEU:HD11 | 3:Q:2165:VAL:H    | 1.85                     | 0.40              |
| 2:R:3044:MET:SD   | 2:R:3221:PHE:HB3  | 2.61                     | 0.40              |
| 2:O:3044:MET:SD   | 2:O:3221:PHE:HB3  | 2.61                     | 0.40              |
| 2:O:3087:GLN:HB3  | 2:O:3089:ASP:OD1  | 2.21                     | 0.40              |
| 2:O:3133:ILE:HD12 | 2:O:3155:ILE:HD11 | 2.02                     | 0.40              |
| 1:J:1072:GLN:HB3  | 1:J:1228:THR:HG21 | 2.04                     | 0.40              |
| 1:G:1137:HIS:CE1  | 1:G:1218:HIS:HD2  | 2.39                     | 0.40              |
| 3:H:2137:THR:OG1  | 3:H:2138:ASP:N    | 2.54                     | 0.40              |
| 2:C:3045:GLU:O    | 2:C:3049:VAL:HG23 | 2.22                     | 0.40              |
| 3:c:2132:MET:HE3  | 3:c:2219:THR:HG21 | 2.04                     | 0.40              |
| 3:W:2134:CYS:HB2  | 3:W:2141:PHE:HE2  | 1.87                     | 0.40              |
| 2:U:3087:GLN:HB3  | 2:U:3089:ASP:OD1  | 2.21                     | 0.40              |
| 1:M:1095:MET:HE2  | 1:M:1098:LEU:HB2  | 2.02                     | 0.40              |
| 2:O:3045:GLU:O    | 2:O:3049:VAL:HG23 | 2.21                     | 0.40              |
| 3:K:2132:MET:HE3  | 3:K:2219:THR:HG21 | 2.04                     | 0.40              |
| 1:G:1110:PHE:HB3  | 1:G:1240:ILE:HG13 | 2.03                     | 0.40              |
| 2:I:3045:GLU:O    | 2:I:3049:VAL:HG23 | 2.22                     | 0.40              |
| 1:D:1167:TRP:HD1  | 1:D:1173:PRO:HA   | 1.86                     | 0.40              |
| 3:E:2137:THR:OG1  | 3:E:2138:ASP:N    | 2.54                     | 0.40              |
| 2:C:3087:GLN:HB3  | 2:C:3089:ASP:OD1  | 2.21                     | 0.40              |
| 1:A:1202:THR:HG22 | 1:A:1205:TYR:HB3  | 2.03                     | 0.40              |
| 1:Y:1121:CYS:SG   | 1:Y:1122:GLN:N    | 2.94                     | 0.40              |
| 1:V:1072:GLN:HB3  | 1:V:1228:THR:HG21 | 2.04                     | 0.40              |
| 2:X:3087:GLN:HE22 | 2:X:3188:ALA:H    | 1.68                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:T:2134:CYS:HB2  | 3:T:2141:PHE:HE2  | 1.87                     | 0.40              |
| 2:U:3045:GLU:O    | 2:U:3049:VAL:HG23 | 2.22                     | 0.40              |
| 3:N:2134:CYS:HB2  | 3:N:2141:PHE:HE2  | 1.87                     | 0.40              |
| 1:G:1079:GLU:HA   | 1:G:1084:ARG:HH11 | 1.87                     | 0.40              |
| 3:H:2071:TRP:HB2  | 3:H:2240:ILE:HD11 | 2.03                     | 0.40              |
| 3:E:2118:HIS:CD2  | 3:E:2228:LEU:HD11 | 2.56                     | 0.40              |
| 3:B:2051:ASP:OD1  | 3:B:2051:ASP:N    | 2.53                     | 0.40              |
| 1:e:1112:ILE:HG12 | 1:e:1178:ILE:HB   | 2.02                     | 0.40              |
| 2:d:3044:MET:SD   | 2:d:3221:PHE:HB3  | 2.62                     | 0.40              |
| 1:V:1137:HIS:CE1  | 1:V:1218:HIS:HD2  | 2.39                     | 0.40              |
| 2:X:3045:GLU:O    | 2:X:3049:VAL:HG23 | 2.21                     | 0.40              |
| 2:X:3087:GLN:HB3  | 2:X:3089:ASP:OD1  | 2.21                     | 0.40              |
| 1:S:1095:MET:HE2  | 1:S:1098:LEU:HB2  | 2.02                     | 0.40              |
| 3:N:2132:MET:HE3  | 3:N:2219:THR:HG21 | 2.04                     | 0.40              |
| 3:H:2132:MET:HE3  | 3:H:2219:THR:HG21 | 2.04                     | 0.40              |
| 1:D:1076:ASN:O    | 1:D:1226:GLN:NE2  | 2.55                     | 0.40              |
| 1:D:1110:PHE:HB3  | 1:D:1240:ILE:HG13 | 2.03                     | 0.40              |
| 3:E:2132:MET:HE3  | 3:E:2219:THR:HG21 | 2.04                     | 0.40              |
| 2:F:3044:MET:SD   | 2:F:3221:PHE:HB3  | 2.61                     | 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     | 220/287 (77%) | 215 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | D     | 220/287 (77%) | 216 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | G     | 220/287 (77%) | 215 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | J     | 220/287 (77%) | 215 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 1   | M     | 220/287 (77%) | 215 (98%) | 5 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | P     | 220/287 (77%)   | 216 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 1   | S     | 220/287 (77%)   | 215 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | V     | 220/287 (77%)   | 215 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | Y     | 220/287 (77%)   | 215 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | b     | 220/287 (77%)   | 215 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 1   | e     | 220/287 (77%)   | 215 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 2   | C     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | F     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | I     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | L     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | O     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | R     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | U     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | X     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | a     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | d     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 2   | g     | 212/239 (89%)   | 208 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 3   | B     | 232/260 (89%)   | 217 (94%)  | 15 (6%)  | 0        | 100         | 100 |
| 3   | E     | 232/260 (89%)   | 218 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 3   | H     | 232/260 (89%)   | 218 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 3   | K     | 232/260 (89%)   | 217 (94%)  | 15 (6%)  | 0        | 100         | 100 |
| 3   | N     | 232/260 (89%)   | 217 (94%)  | 15 (6%)  | 0        | 100         | 100 |
| 3   | Q     | 232/260 (89%)   | 217 (94%)  | 15 (6%)  | 0        | 100         | 100 |
| 3   | T     | 232/260 (89%)   | 217 (94%)  | 15 (6%)  | 0        | 100         | 100 |
| 3   | W     | 232/260 (89%)   | 217 (94%)  | 15 (6%)  | 0        | 100         | 100 |
| 3   | Z     | 232/260 (89%)   | 219 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 3   | c     | 232/260 (89%)   | 218 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| 3   | f     | 232/260 (89%)   | 218 (94%)  | 14 (6%)  | 0        | 100         | 100 |
| All | All   | 7304/8646 (84%) | 7048 (96%) | 256 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 1   | D     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 1   | G     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 1   | J     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 1   | M     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 1   | P     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 1   | S     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 1   | V     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 1   | Y     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 1   | b     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 1   | e     | 182/259 (70%) | 182 (100%) | 0        | 100         | 100 |
| 2   | C     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 2   | F     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 2   | I     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 2   | L     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 2   | O     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 2   | R     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 2   | U     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 2   | X     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 2   | a     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 2   | d     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 2   | g     | 184/209 (88%) | 184 (100%) | 0        | 100         | 100 |
| 3   | B     | 193/221 (87%) | 193 (100%) | 0        | 100         | 100 |
| 3   | E     | 193/221 (87%) | 193 (100%) | 0        | 100         | 100 |
| 3   | H     | 193/221 (87%) | 193 (100%) | 0        | 100         | 100 |
| 3   | K     | 193/221 (87%) | 193 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 3   | N     | 193/221 (87%)   | 193 (100%)  | 0        | 100         | 100 |
| 3   | Q     | 193/221 (87%)   | 193 (100%)  | 0        | 100         | 100 |
| 3   | T     | 193/221 (87%)   | 193 (100%)  | 0        | 100         | 100 |
| 3   | W     | 193/221 (87%)   | 193 (100%)  | 0        | 100         | 100 |
| 3   | Z     | 193/221 (87%)   | 193 (100%)  | 0        | 100         | 100 |
| 3   | c     | 193/221 (87%)   | 193 (100%)  | 0        | 100         | 100 |
| 3   | f     | 193/221 (87%)   | 193 (100%)  | 0        | 100         | 100 |
| All | All   | 6149/7579 (81%) | 6149 (100%) | 0        | 100         | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1060 | ASN  |
| 1   | A     | 1226 | GLN  |
| 2   | g     | 3069 | GLN  |
| 2   | g     | 3087 | GLN  |
| 2   | g     | 3106 | ASN  |
| 2   | g     | 3198 | ASN  |
| 3   | f     | 2030 | ASN  |
| 3   | f     | 2094 | GLN  |
| 3   | f     | 2166 | GLN  |
| 3   | f     | 2187 | GLN  |
| 3   | f     | 2229 | ASN  |
| 1   | e     | 1046 | HIS  |
| 1   | e     | 1060 | ASN  |
| 1   | e     | 1072 | GLN  |
| 1   | e     | 1138 | GLN  |
| 1   | e     | 1218 | HIS  |
| 1   | e     | 1220 | ASN  |
| 1   | e     | 1226 | GLN  |
| 1   | b     | 1046 | HIS  |
| 1   | b     | 1049 | ASN  |
| 1   | b     | 1060 | ASN  |
| 1   | b     | 1072 | GLN  |
| 1   | b     | 1138 | GLN  |
| 1   | b     | 1220 | ASN  |
| 1   | b     | 1226 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | c     | 2030 | ASN  |
| 3   | c     | 2070 | GLN  |
| 3   | c     | 2088 | ASN  |
| 3   | c     | 2094 | GLN  |
| 3   | c     | 2109 | HIS  |
| 3   | c     | 2166 | GLN  |
| 3   | c     | 2187 | GLN  |
| 2   | d     | 3087 | GLN  |
| 2   | d     | 3106 | ASN  |
| 2   | d     | 3198 | ASN  |
| 1   | Y     | 1060 | ASN  |
| 1   | Y     | 1072 | GLN  |
| 1   | Y     | 1138 | GLN  |
| 1   | Y     | 1218 | HIS  |
| 1   | Y     | 1226 | GLN  |
| 3   | Z     | 2030 | ASN  |
| 3   | Z     | 2094 | GLN  |
| 3   | Z     | 2166 | GLN  |
| 3   | Z     | 2187 | GLN  |
| 2   | a     | 3012 | GLN  |
| 2   | a     | 3087 | GLN  |
| 2   | a     | 3106 | ASN  |
| 2   | a     | 3198 | ASN  |
| 1   | V     | 1046 | HIS  |
| 1   | V     | 1060 | ASN  |
| 1   | V     | 1072 | GLN  |
| 1   | V     | 1138 | GLN  |
| 1   | V     | 1220 | ASN  |
| 1   | V     | 1226 | GLN  |
| 1   | V     | 1260 | ASN  |
| 3   | W     | 2030 | ASN  |
| 3   | W     | 2088 | ASN  |
| 3   | W     | 2094 | GLN  |
| 3   | W     | 2166 | GLN  |
| 3   | W     | 2187 | GLN  |
| 3   | W     | 2229 | ASN  |
| 2   | X     | 3087 | GLN  |
| 2   | X     | 3106 | ASN  |
| 2   | X     | 3198 | ASN  |
| 1   | S     | 1046 | HIS  |
| 1   | S     | 1060 | ASN  |
| 1   | S     | 1072 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | S     | 1138 | GLN  |
| 1   | S     | 1226 | GLN  |
| 3   | T     | 2030 | ASN  |
| 3   | T     | 2094 | GLN  |
| 3   | T     | 2166 | GLN  |
| 3   | T     | 2187 | GLN  |
| 2   | U     | 3012 | GLN  |
| 2   | U     | 3087 | GLN  |
| 2   | U     | 3106 | ASN  |
| 2   | U     | 3198 | ASN  |
| 1   | P     | 1046 | HIS  |
| 1   | P     | 1072 | GLN  |
| 1   | P     | 1226 | GLN  |
| 3   | Q     | 2030 | ASN  |
| 3   | Q     | 2094 | GLN  |
| 3   | Q     | 2119 | GLN  |
| 3   | Q     | 2166 | GLN  |
| 3   | Q     | 2187 | GLN  |
| 2   | R     | 3087 | GLN  |
| 2   | R     | 3106 | ASN  |
| 2   | R     | 3198 | ASN  |
| 1   | M     | 1046 | HIS  |
| 1   | M     | 1060 | ASN  |
| 1   | M     | 1072 | GLN  |
| 1   | M     | 1138 | GLN  |
| 1   | M     | 1185 | ASN  |
| 1   | M     | 1226 | GLN  |
| 3   | N     | 2030 | ASN  |
| 3   | N     | 2070 | GLN  |
| 3   | N     | 2094 | GLN  |
| 3   | N     | 2119 | GLN  |
| 3   | N     | 2166 | GLN  |
| 3   | N     | 2187 | GLN  |
| 3   | N     | 2229 | ASN  |
| 2   | O     | 3069 | GLN  |
| 2   | O     | 3087 | GLN  |
| 2   | O     | 3106 | ASN  |
| 2   | O     | 3198 | ASN  |
| 1   | J     | 1046 | HIS  |
| 1   | J     | 1060 | ASN  |
| 1   | J     | 1072 | GLN  |
| 1   | J     | 1138 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | J     | 1218 | HIS  |
| 1   | J     | 1220 | ASN  |
| 1   | J     | 1226 | GLN  |
| 3   | K     | 2030 | ASN  |
| 3   | K     | 2094 | GLN  |
| 3   | K     | 2166 | GLN  |
| 3   | K     | 2187 | GLN  |
| 2   | L     | 3087 | GLN  |
| 2   | L     | 3106 | ASN  |
| 2   | L     | 3198 | ASN  |
| 1   | G     | 1072 | GLN  |
| 1   | G     | 1218 | HIS  |
| 1   | G     | 1226 | GLN  |
| 1   | G     | 1260 | ASN  |
| 3   | H     | 2030 | ASN  |
| 3   | H     | 2094 | GLN  |
| 3   | H     | 2166 | GLN  |
| 3   | H     | 2187 | GLN  |
| 2   | I     | 3011 | ASN  |
| 2   | I     | 3087 | GLN  |
| 2   | I     | 3106 | ASN  |
| 2   | I     | 3198 | ASN  |
| 1   | D     | 1049 | ASN  |
| 1   | D     | 1060 | ASN  |
| 1   | D     | 1072 | GLN  |
| 1   | D     | 1185 | ASN  |
| 1   | D     | 1218 | HIS  |
| 1   | D     | 1226 | GLN  |
| 3   | E     | 2030 | ASN  |
| 3   | E     | 2094 | GLN  |
| 3   | E     | 2166 | GLN  |
| 3   | E     | 2187 | GLN  |
| 2   | F     | 3012 | GLN  |
| 2   | F     | 3087 | GLN  |
| 2   | F     | 3106 | ASN  |
| 2   | F     | 3198 | ASN  |
| 2   | C     | 3087 | GLN  |
| 2   | C     | 3106 | ASN  |
| 2   | C     | 3154 | HIS  |
| 2   | C     | 3198 | ASN  |
| 3   | B     | 2030 | ASN  |
| 3   | B     | 2094 | GLN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 3   | B     | 2166 | GLN  |
| 3   | B     | 2187 | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

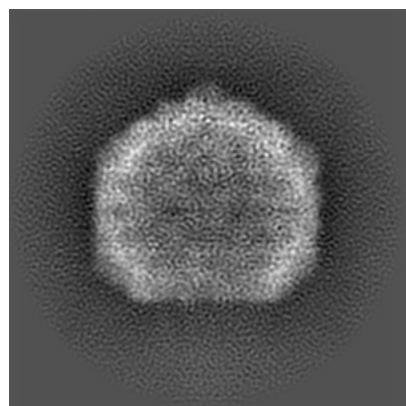
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55096. These allow visual inspection of the internal detail of the map and identification of artifacts.

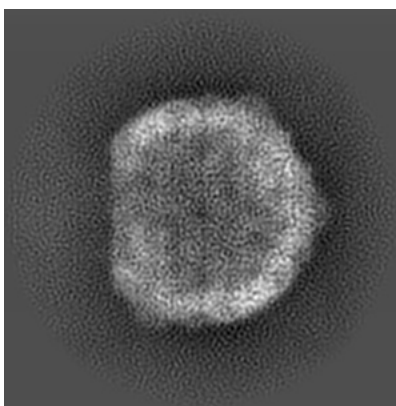
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

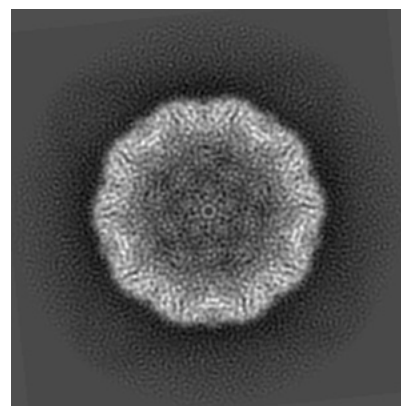
#### 6.1.1 Primary map



X

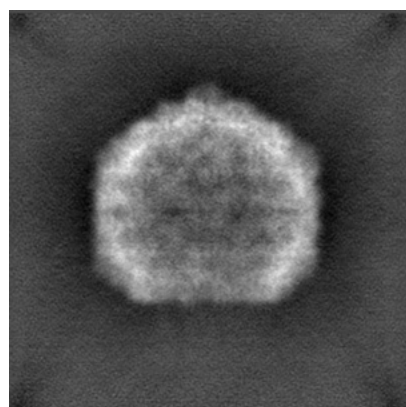


Y

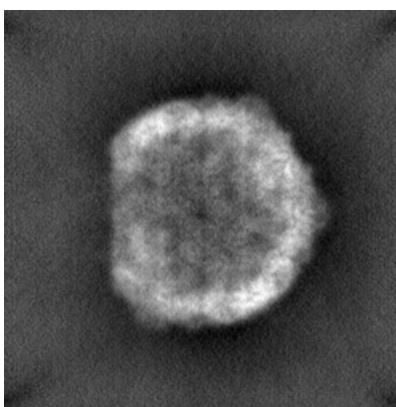


Z

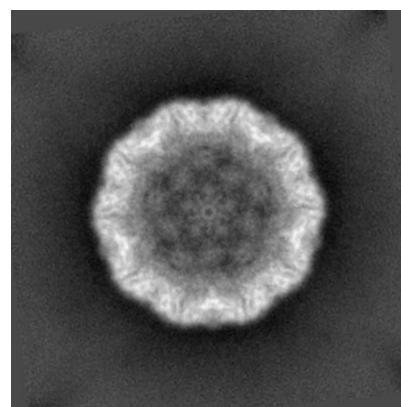
#### 6.1.2 Raw map



X



Y

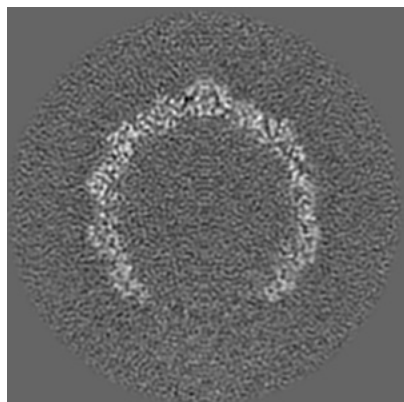


Z

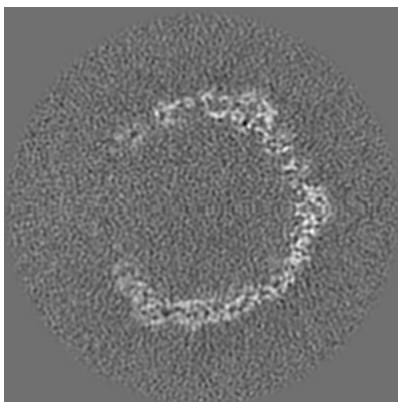
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

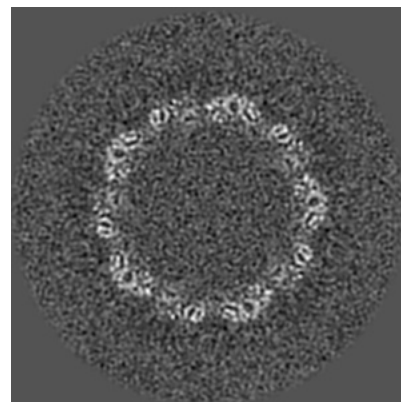
### 6.2.1 Primary map



X Index: 128

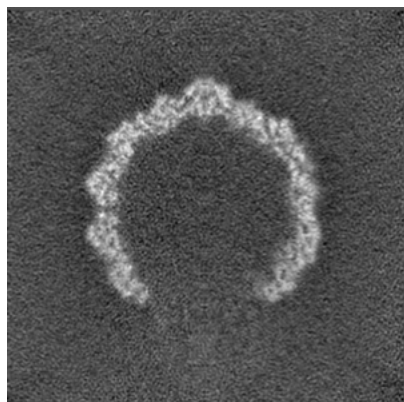


Y Index: 128

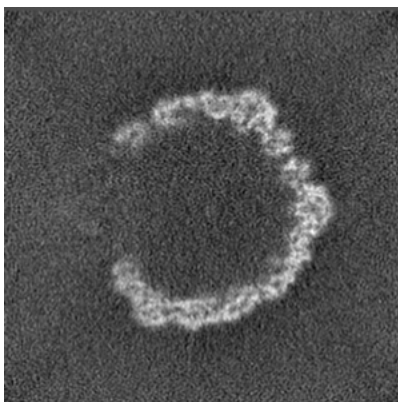


Z Index: 128

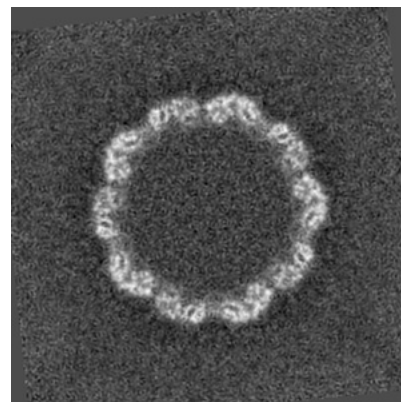
### 6.2.2 Raw map



X Index: 128



Y Index: 128

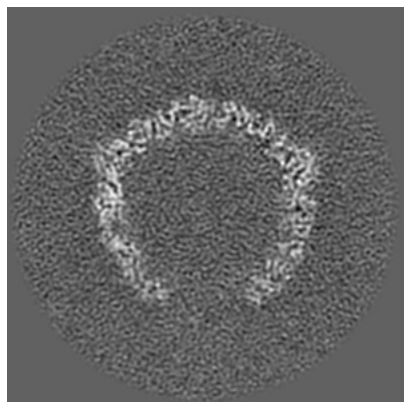


Z Index: 128

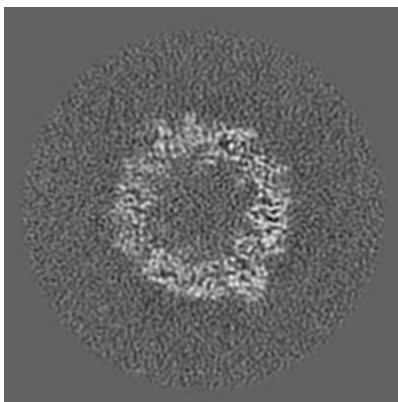
The images above show central slices of the map in three orthogonal directions.

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

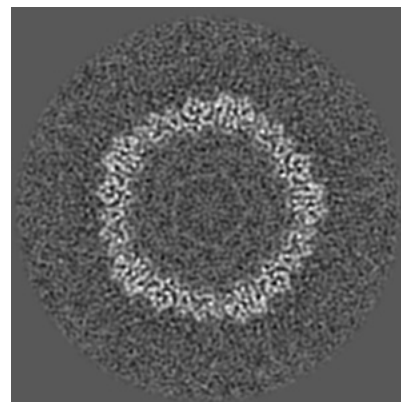
### 6.3.1 Primary map



X Index: 151

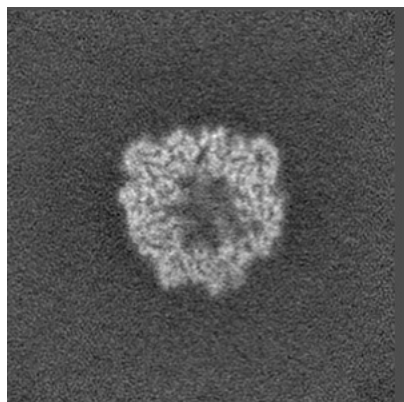


Y Index: 78

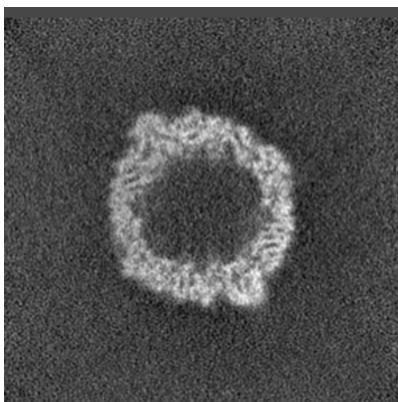


Z Index: 152

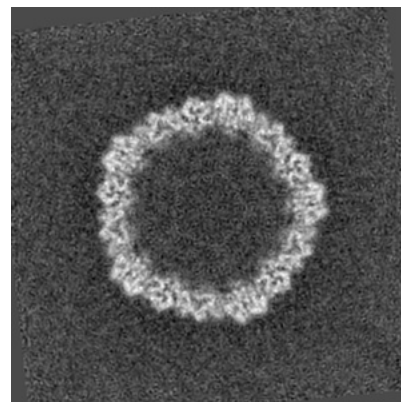
### 6.3.2 Raw map



X Index: 72



Y Index: 170

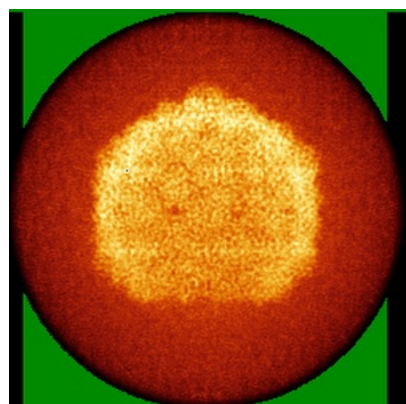


Z Index: 152

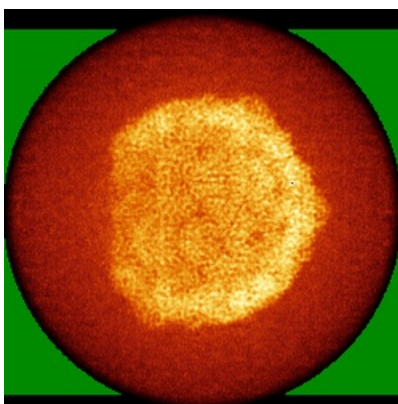
The images above show the largest variance slices of the map in three orthogonal directions.

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

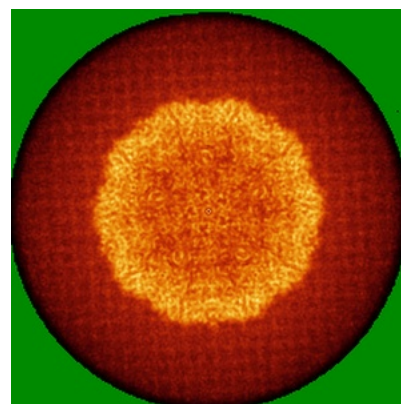
### 6.4.1 Primary map



X

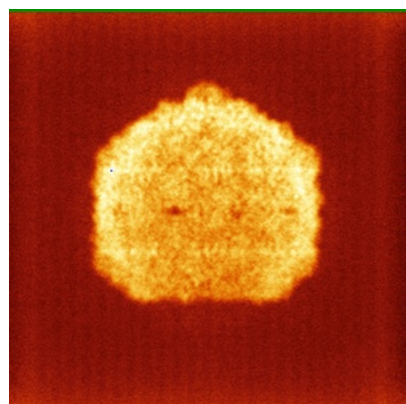


Y

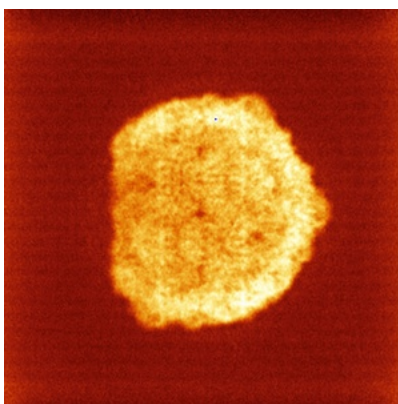


Z

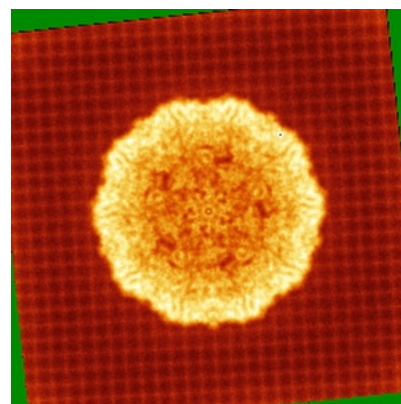
### 6.4.2 Raw map



X



Y

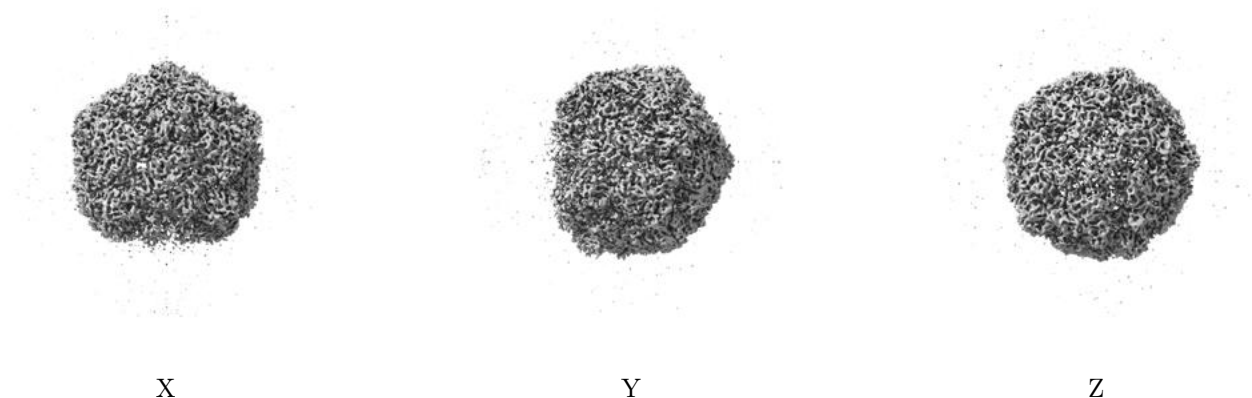


Z

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.

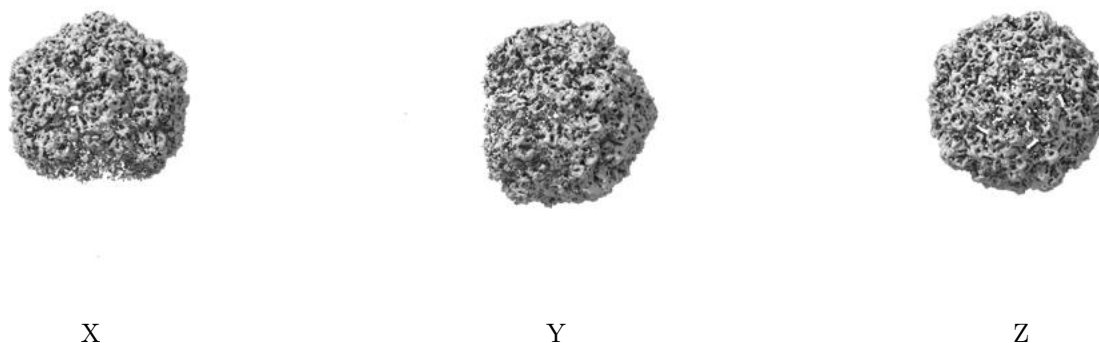
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.0. 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.

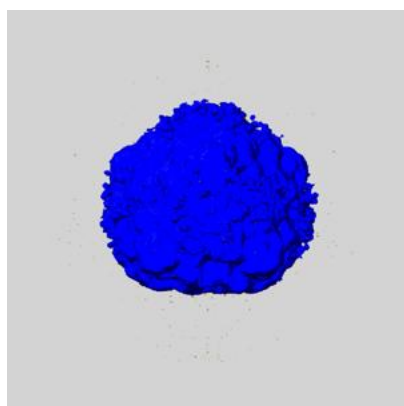
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

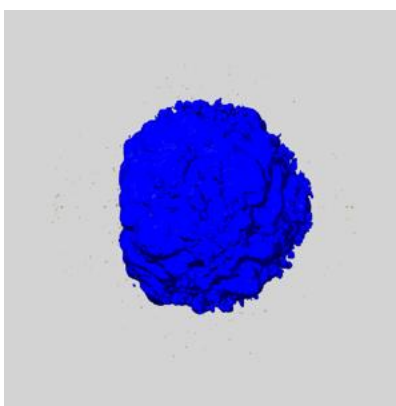
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

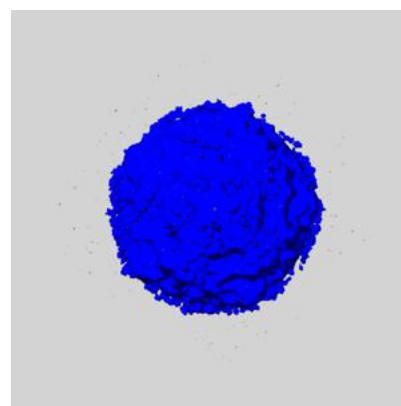
### 6.6.1 emd\_55096\_msk\_1.map [i](#)



X



Y

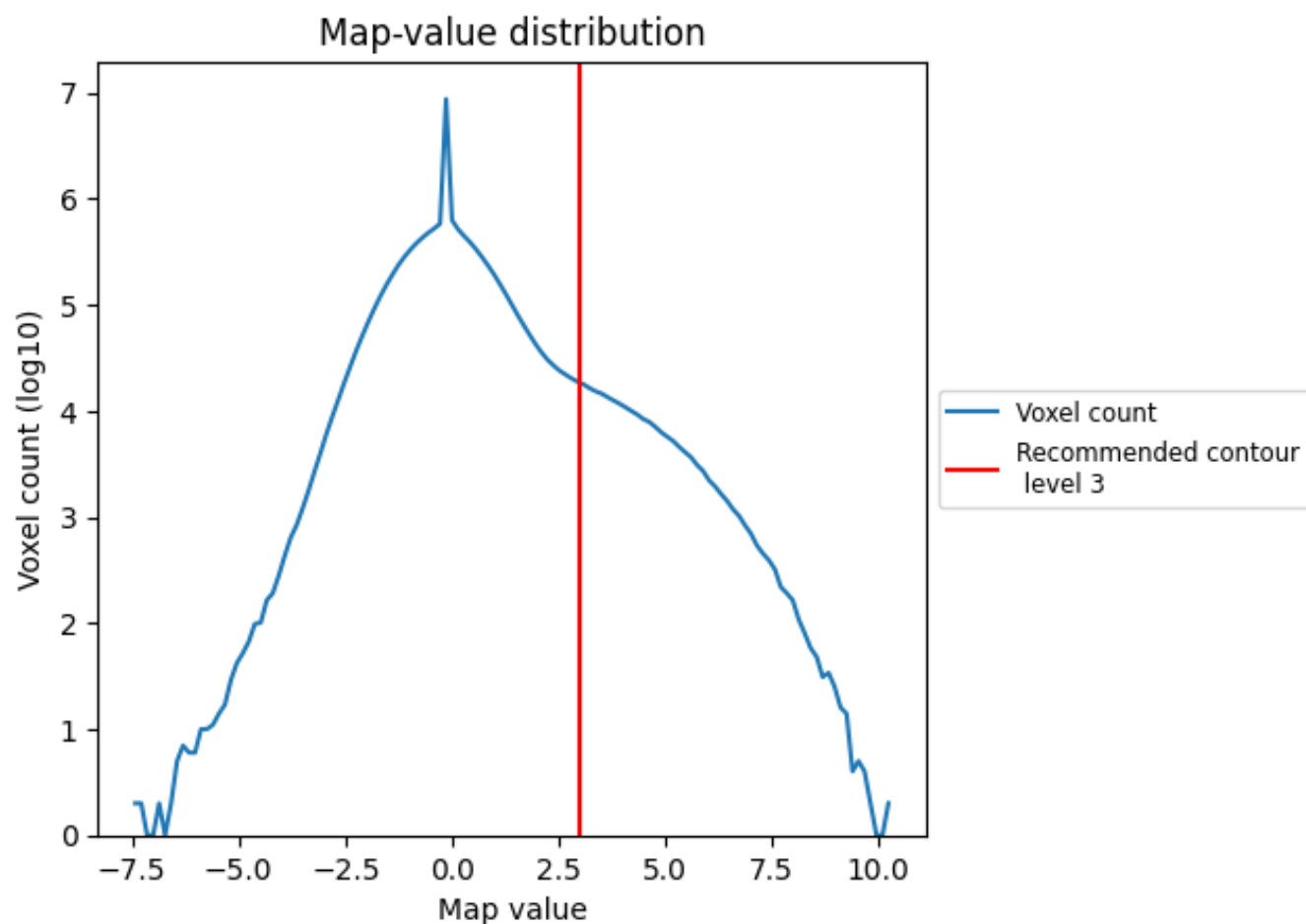


Z

## 7 Map analysis [i](#)

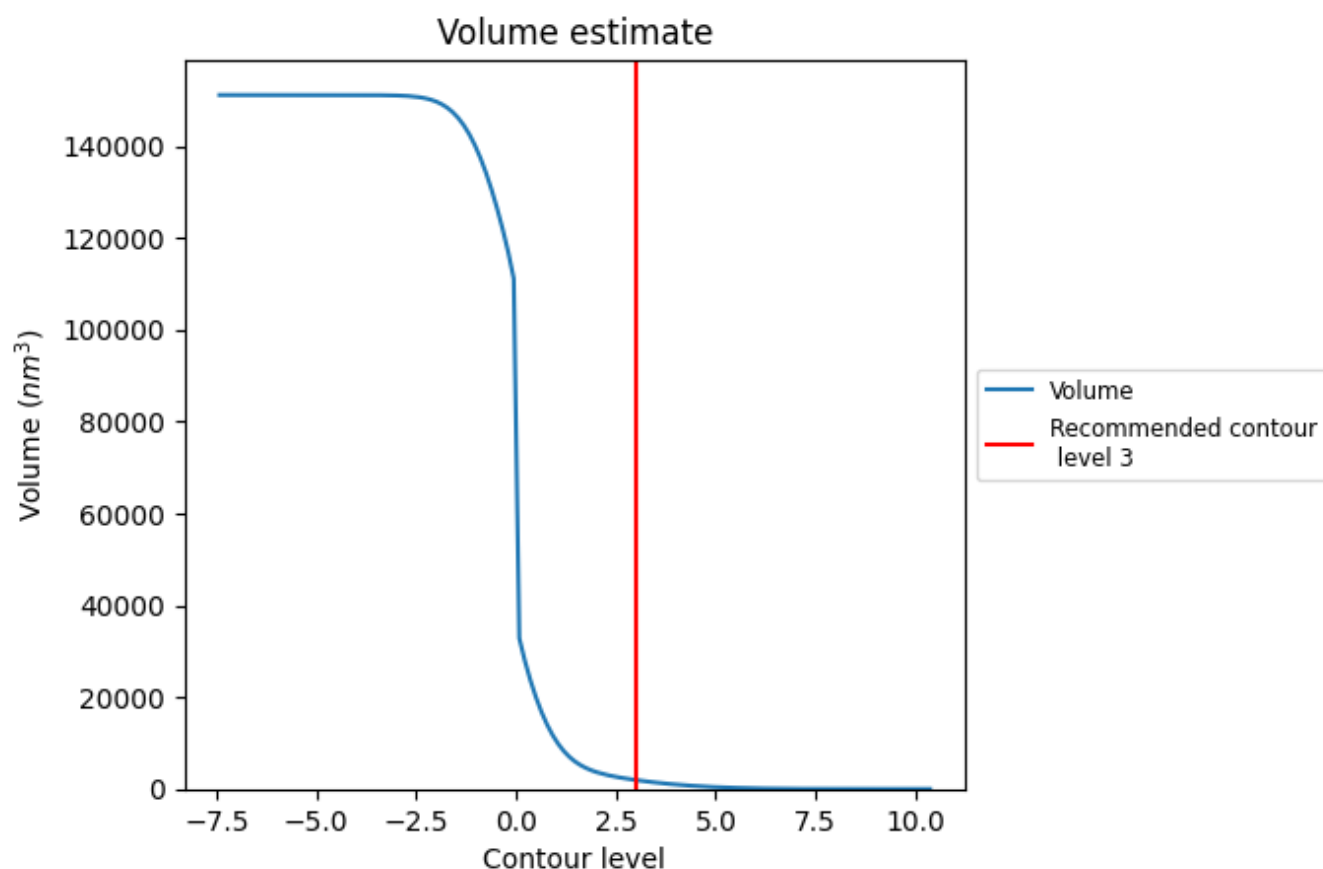
This section contains the results of statistical analysis of the map.

### 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.

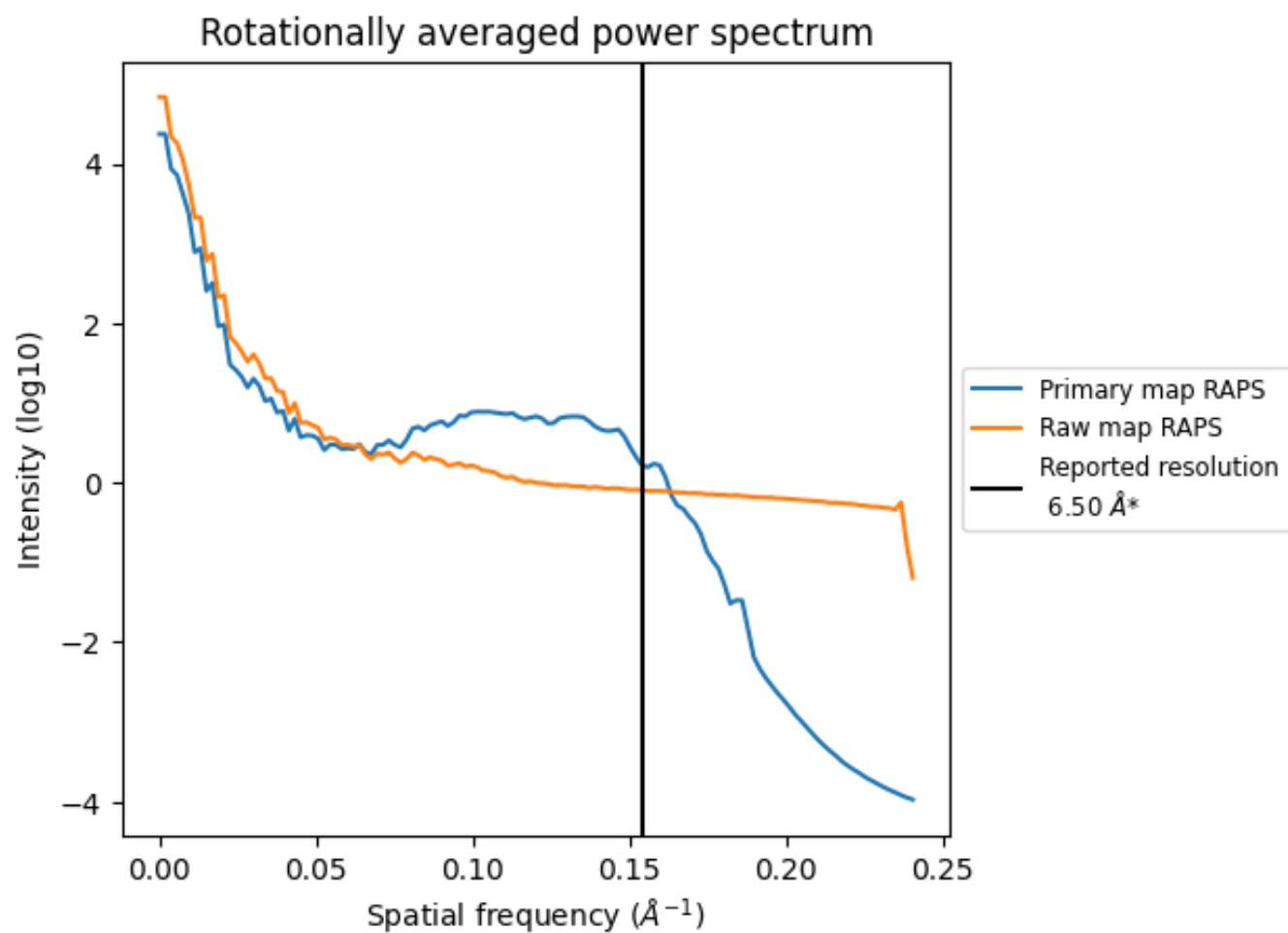
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1939 nm<sup>3</sup>; this corresponds to an approximate mass of 1751 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 ⓘ

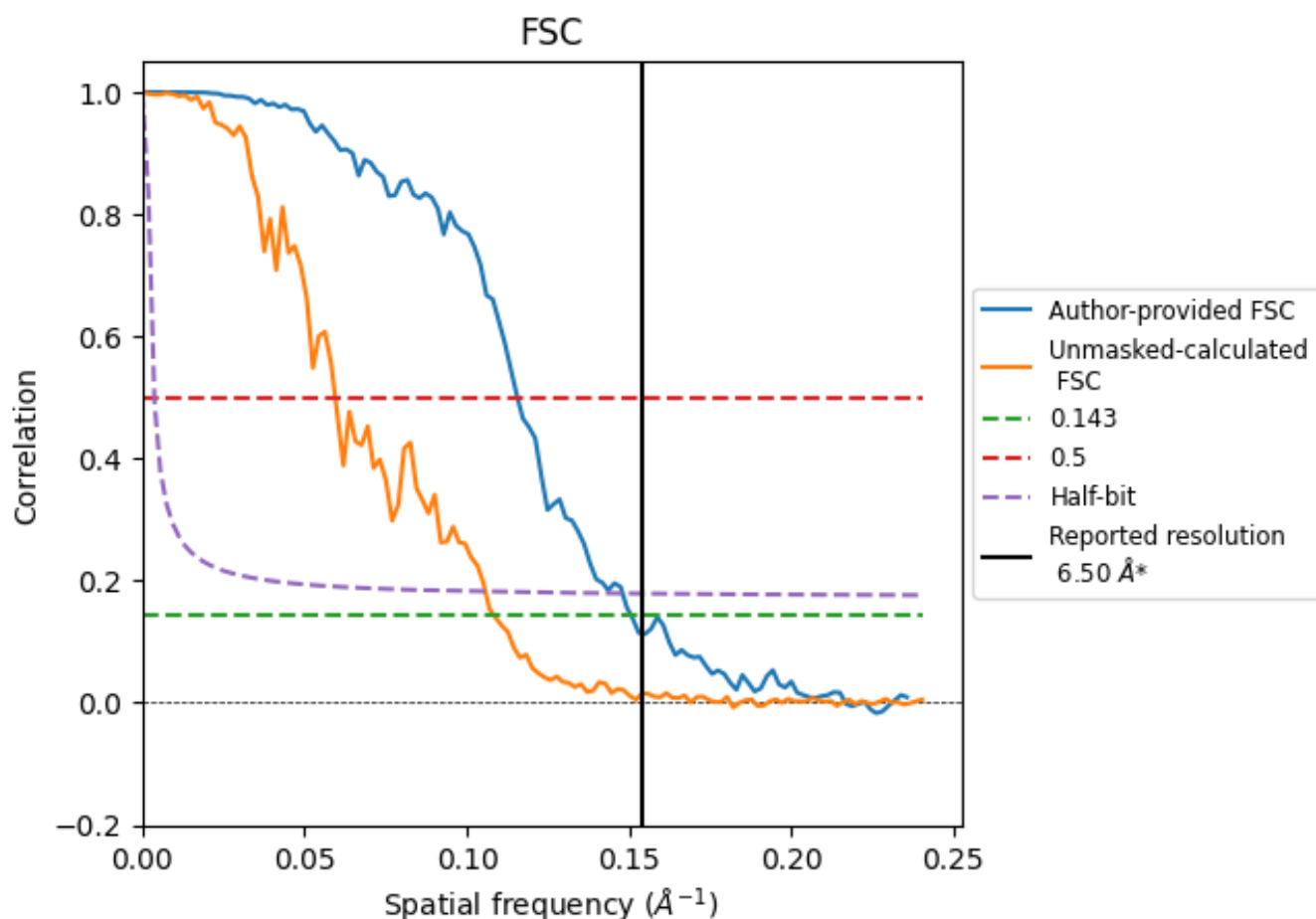


\*Reported resolution corresponds to spatial frequency of  $0.154 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.154  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 6.50                               | -     | -        |
| Author-provided FSC curve | 6.64                               | 8.65  | 6.76     |
| Unmasked-calculated*      | 9.23                               | 16.84 | 9.45     |

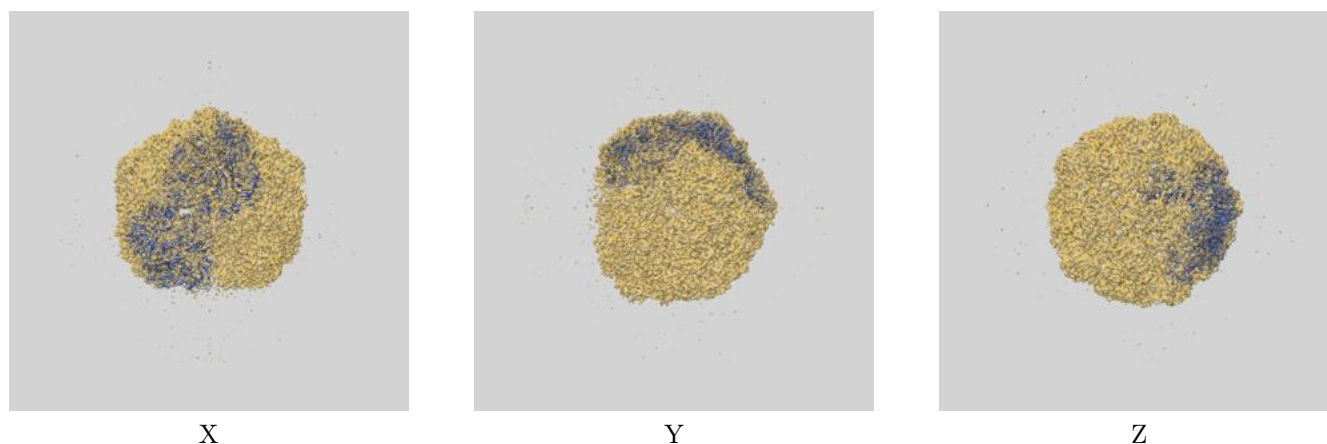
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.23 differs from the reported value 6.5 by more than 10 %

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

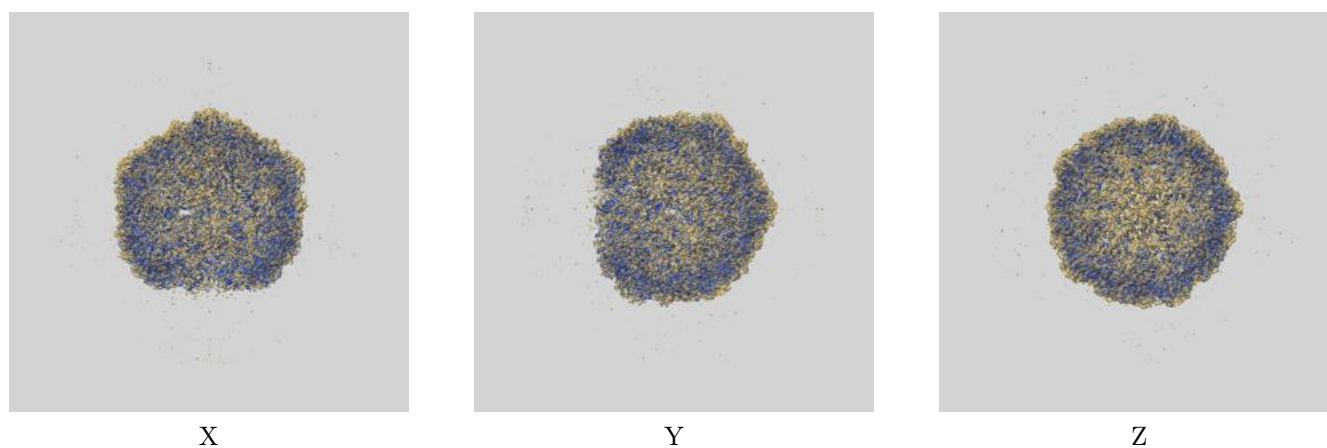
This section contains information regarding the fit between EMDB map EMD-55096 and PDB model 9SPU. Per-residue inclusion information can be found in section 3 on page 7.

### 9.1 Map-model overlays

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



#### 9.1.2 Map-model assembly overlay [i](#)



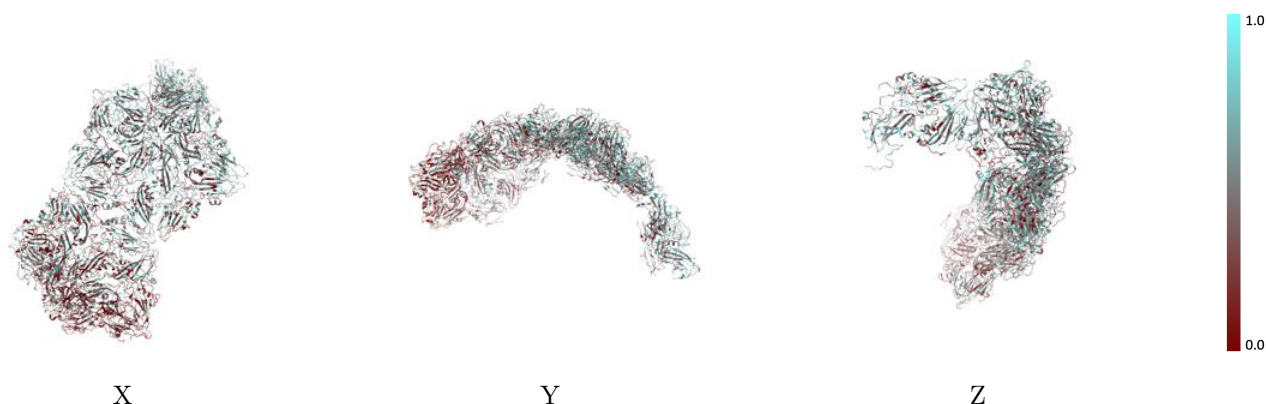
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



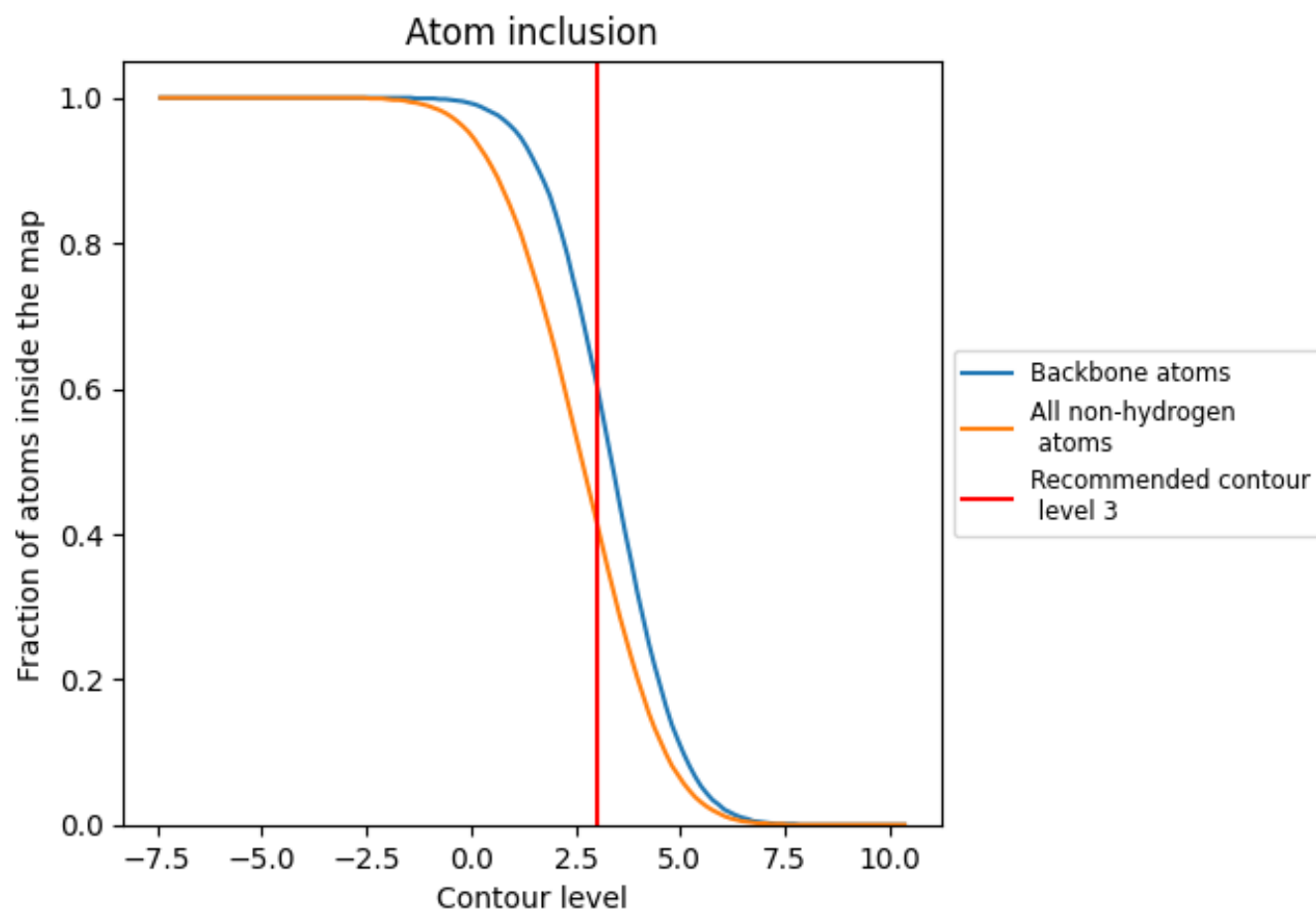
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 42% 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 (3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.4190   |  0.1410   |
| A     |  0.5410   |  0.1740   |
| B     |  0.4780   |  0.1460   |
| C     |  0.5450   |  0.1640   |
| D     |  0.5070   |  0.1590   |
| E     |  0.4680   |  0.1410   |
| F     |  0.5270   |  0.1730   |
| G     |  0.3150   |  0.1210   |
| H     |  0.2450   |  0.1160   |
| I     |  0.2400   |  0.1090   |
| J     |  0.2830   |  0.1130   |
| K     |  0.1740   |  0.1070   |
| L     |  0.2370   |  0.1230   |
| M     |  0.3730   |  0.1200   |
| N     |  0.3820  |  0.1370  |
| O     |  0.3950 |  0.1460 |
| P     |  0.5020 |  0.1460 |
| Q     |  0.4430 |  0.1480 |
| R     |  0.4800 |  0.1350 |
| S     |  0.5000 |  0.1510 |
| T     |  0.5060 |  0.1550 |
| U     |  0.4800 |  0.1420 |
| V     |  0.3730 |  0.1190 |
| W     |  0.3640 |  0.1600 |
| X     |  0.3610 |  0.1190 |
| Y     |  0.4690 |  0.1480 |
| Z     |  0.4610 |  0.1470 |
| a     |  0.5160 |  0.1760 |
| b     |  0.4970 |  0.1550 |
| c     |  0.4650 |  0.1580 |
| d     |  0.5210 |  0.1590 |
| e     |  0.3650 |  0.0990 |
| f     |  0.3960 |  0.1430 |
| g     |  0.4240 |  0.1480 |

