



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 10:32 pm GMT

PDB ID : 6HHT
EMDB ID : EMD-0217
Title : Echovirus 18 Open particle without two pentamers
Authors : Buchta, D.; Fuzik, T.; Hrebik, D.; Levdansky, Y.; Moravcova, J.; Plevka, P.
Deposited on : 2018-08-29
Resolution : 4.05 Å(reported)
Based on initial model : 6HBH

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

We welcome your comments at 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>.

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

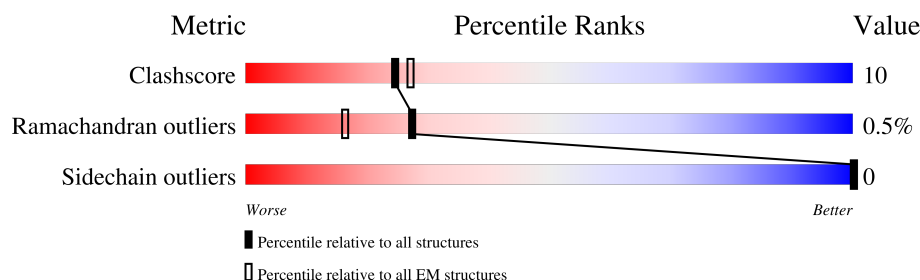
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.05 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.








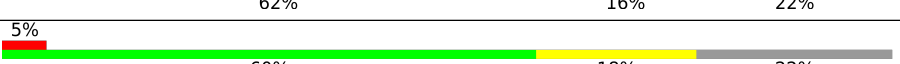

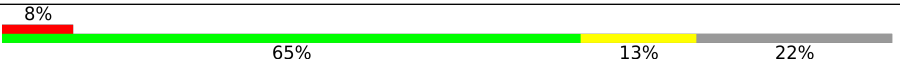


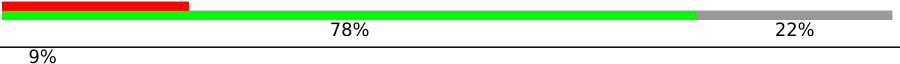
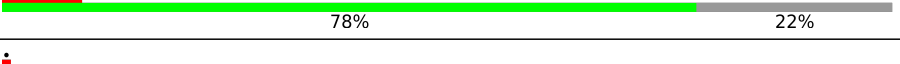

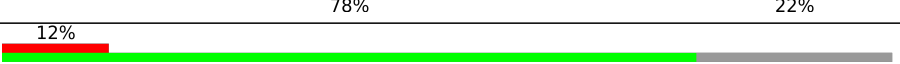
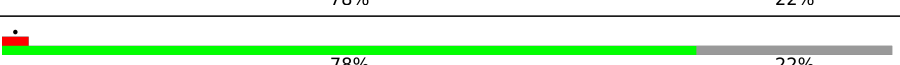










| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | A1 | 287 |  <p>21% 63% 15% 22%</p> |
| 1 | A2 | 287 |  <p>60% 60% 18% 22%</p> |
| 1 | D1 | 287 |  <p>60% 18% 22%</p> |
| 1 | D2 | 287 |  <p>66% 61% 17% 22%</p> |
| 1 | G1 | 287 |  <p>59% 19% 22%</p> |
| 1 | G2 | 287 |  <p>62% 16% 22%</p> |
| 1 | J1 | 287 |  <p>40% 61% 17% 22%</p> |
| 1 | J2 | 287 |  <p>41% 61% 17% 22%</p> |



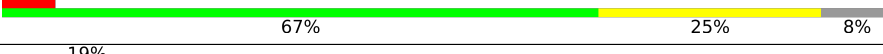

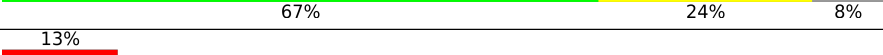
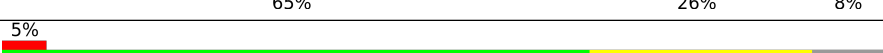

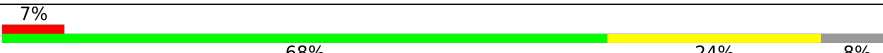
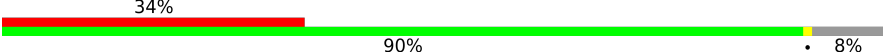
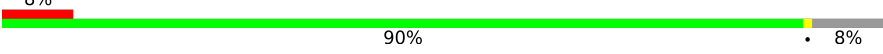
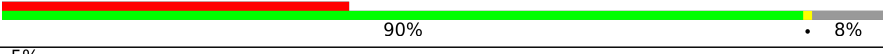
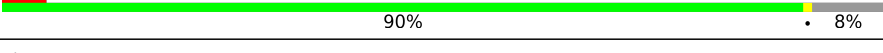

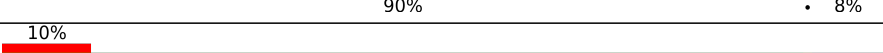
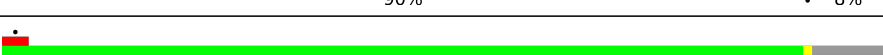
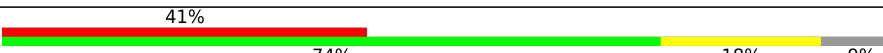


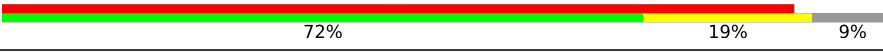


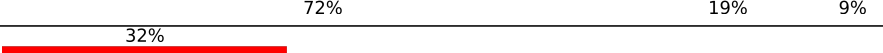



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | M1 | 287 |  |
| 1 | M2 | 287 |  |
| 1 | P1 | 287 |  |
| 1 | P2 | 287 |  |
| 1 | S1 | 287 |  |
| 1 | S2 | 287 |  |
| 1 | V1 | 287 |  |
| 1 | V2 | 287 |  |
| 1 | Y2 | 287 |  |
| 1 | b2 | 287 |  |
| 1 | e2 | 287 |  |
| 1 | h2 | 287 |  |
| 1 | k2 | 287 |  |
| 1 | n2 | 287 |  |
| 1 | q2 | 287 |  |
| 1 | t2 | 287 |  |
| 1 | w2 | 287 |  |
| 2 | B1 | 260 |  |
| 2 | B2 | 260 |  |
| 2 | E1 | 260 |  |
| 2 | E2 | 260 |  |
| 2 | H1 | 260 |  |
| 2 | H2 | 260 |  |
| 2 | K1 | 260 |  |
| 2 | K2 | 260 |  |



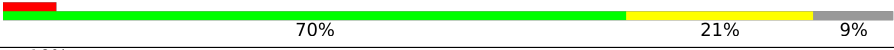



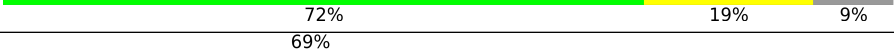
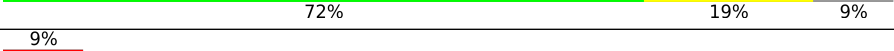
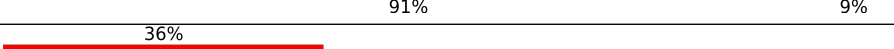
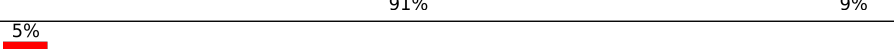
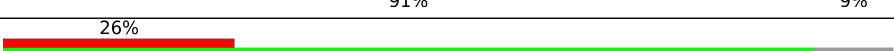
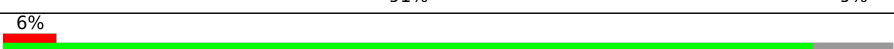





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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 2 | N1 | 260 |  |
| 2 | N2 | 260 |  |
| 2 | Q1 | 260 |  |
| 2 | Q2 | 260 |  |
| 2 | T1 | 260 |  |
| 2 | T2 | 260 |  |
| 2 | W1 | 260 |  |
| 2 | W2 | 260 |  |
| 2 | Z2 | 260 |  |
| 2 | c2 | 260 |  |
| 2 | f2 | 260 |  |
| 2 | i2 | 260 |  |
| 2 | l2 | 260 |  |
| 2 | o2 | 260 |  |
| 2 | r2 | 260 |  |
| 2 | u2 | 260 |  |
| 2 | x2 | 260 |  |
| 3 | C1 | 239 |  |
| 3 | C2 | 239 |  |
| 3 | F1 | 239 |  |
| 3 | F2 | 239 |  |
| 3 | I1 | 239 |  |
| 3 | I2 | 239 |  |
| 3 | L1 | 239 |  |
| 3 | L2 | 239 |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 3 | O1 | 239 |  |
| 3 | O2 | 239 |  |
| 3 | R1 | 239 |  |
| 3 | R2 | 239 |  |
| 3 | U1 | 239 |  |
| 3 | U2 | 239 |  |
| 3 | X1 | 239 |  |
| 3 | X2 | 239 |  |
| 3 | a2 | 239 |  |
| 3 | d2 | 239 |  |
| 3 | g2 | 239 |  |
| 3 | j2 | 239 |  |
| 3 | m2 | 239 |  |
| 3 | p2 | 239 |  |
| 3 | s2 | 239 |  |
| 3 | v2 | 239 |  |
| 3 | y2 | 239 |  |

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 129900 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 capsid protein 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A1 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | V1 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | S1 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | P1 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | M1 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | J1 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | G1 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | D1 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | A2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | w2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | t2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | q2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | n2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | k2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | h2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | e2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | b2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | Y2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | V2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | S2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | P2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | M2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | J2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | G2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |
| 1 | D2 | 224 | Total | C | N | O | S | 0 | 0 |
| | | | 1741 | 1117 | 305 | 305 | 14 | | |

- Molecule 2 is a protein called Echovirus 18 capsid protein 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | W1 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | T1 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | Q1 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | N1 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | K1 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | H1 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | E1 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | B1 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | x2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | u2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | r2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | o2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | l2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | i2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | f2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | c2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | Z2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | W2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | T2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | Q2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | N2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | K2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | H2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | E2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |
| 2 | B2 | 238 | Total | C | N | O | S | 0 | 0 |
| | | | 1821 | 1172 | 302 | 332 | 15 | | |

- Molecule 3 is a protein called Echovirus 18 capsid protein 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3 | X1 | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1634 | 1045 | 265 | 308 | 16 | | |
| 3 | U1 | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1634 | 1045 | 265 | 308 | 16 | | |
| 3 | R1 | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1634 | 1045 | 265 | 308 | 16 | | |
| 3 | O1 | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1634 | 1045 | 265 | 308 | 16 | | |
| 3 | L1 | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1634 | 1045 | 265 | 308 | 16 | | |

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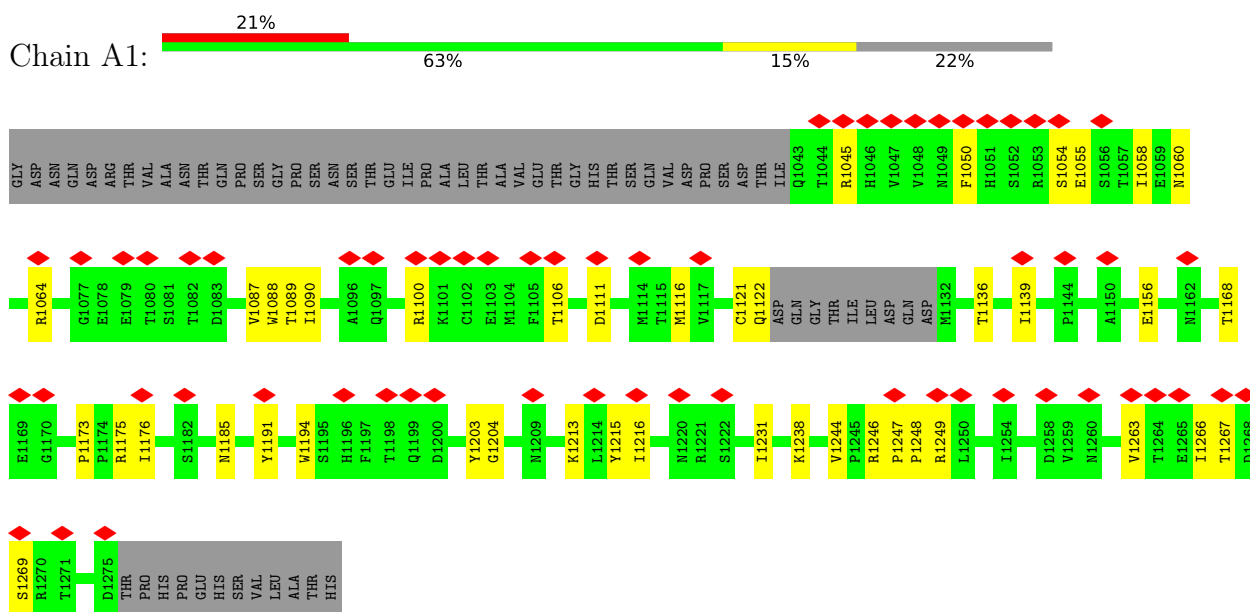
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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 3 | I1 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | F1 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | C1 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | y2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | v2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | s2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | p2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | m2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | j2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | g2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | d2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | a2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | X2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | U2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | R2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | O2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | L2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | I2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | F2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |
| 3 | C2 | 218 | Total 1634 | C 1045 | N 265 | O 308 | S 16 | 0 | 0 |

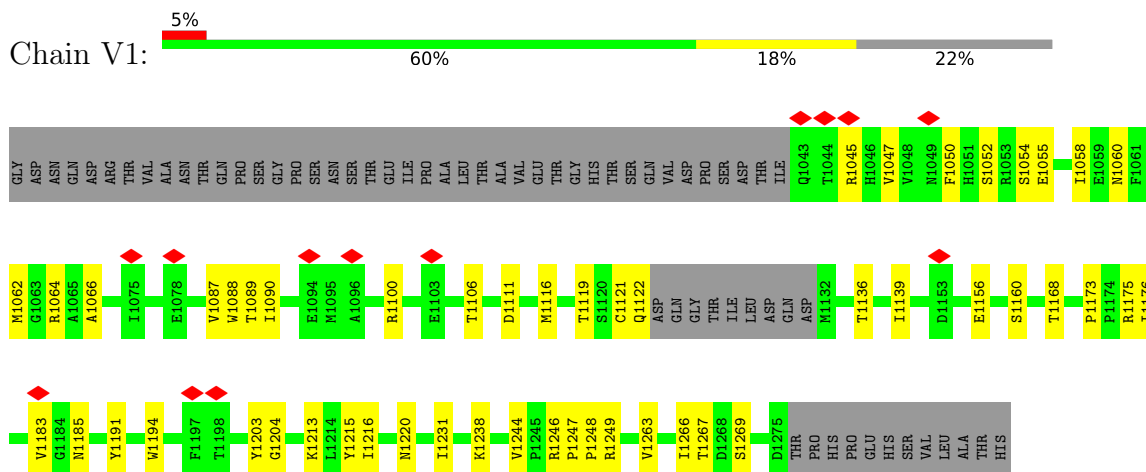
3 Residue-property plots

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.

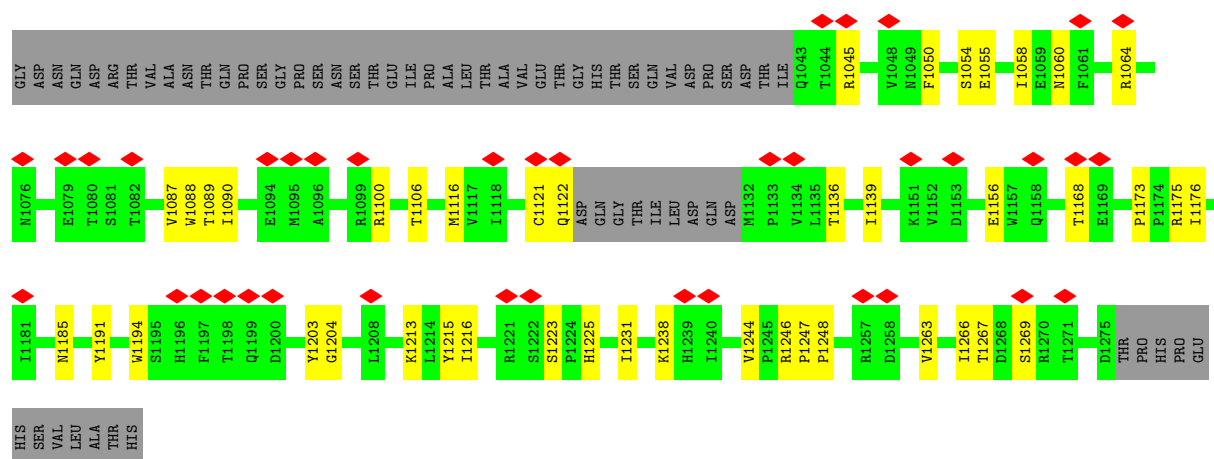
- Molecule 1: Echovirus 18 capsid protein 1



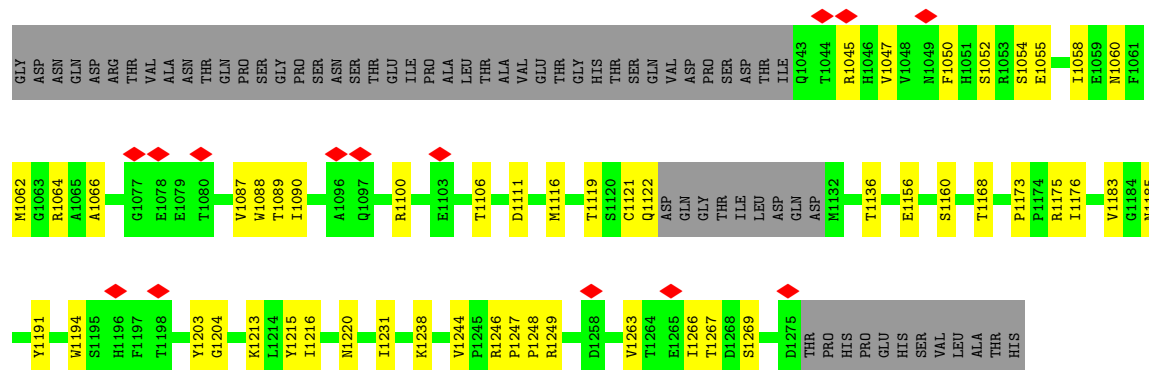
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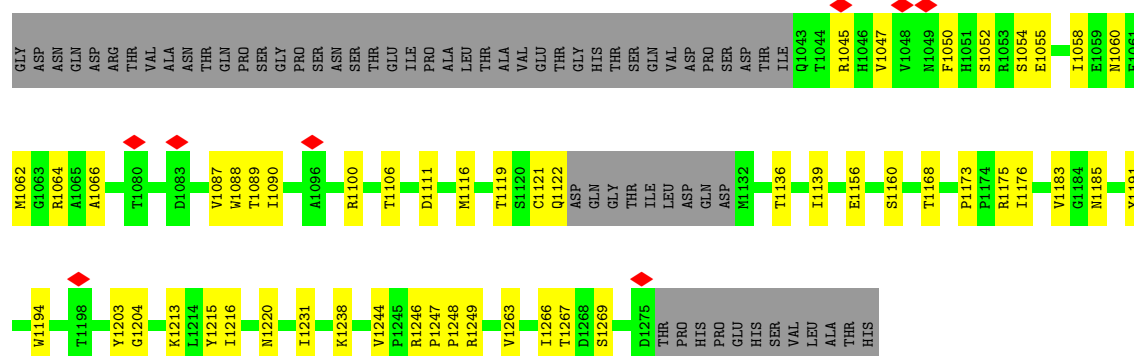
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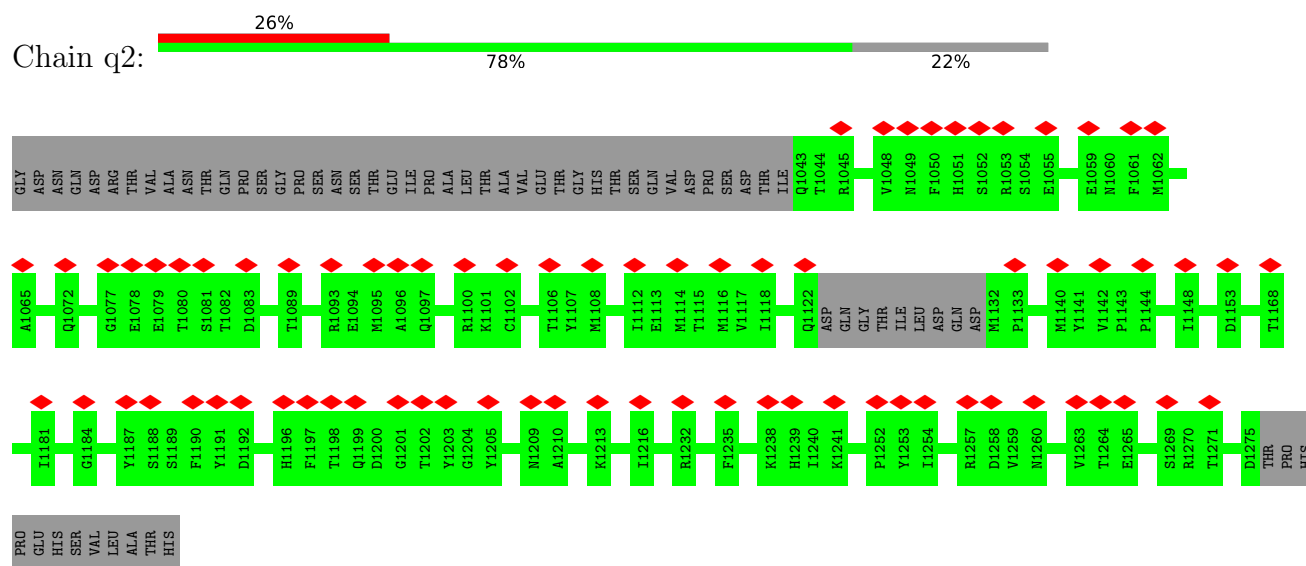


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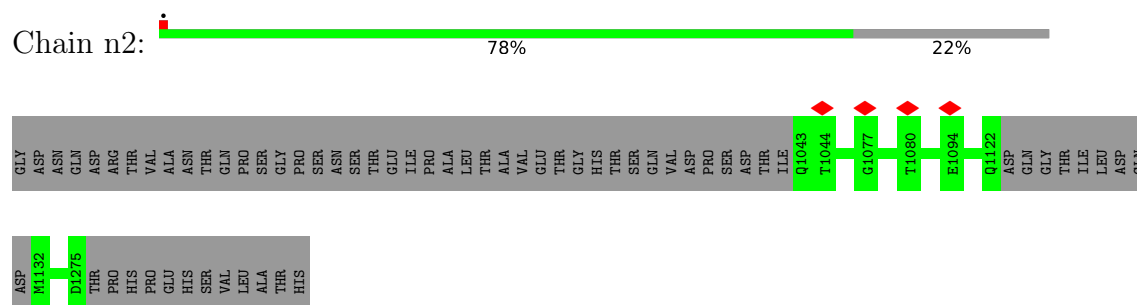


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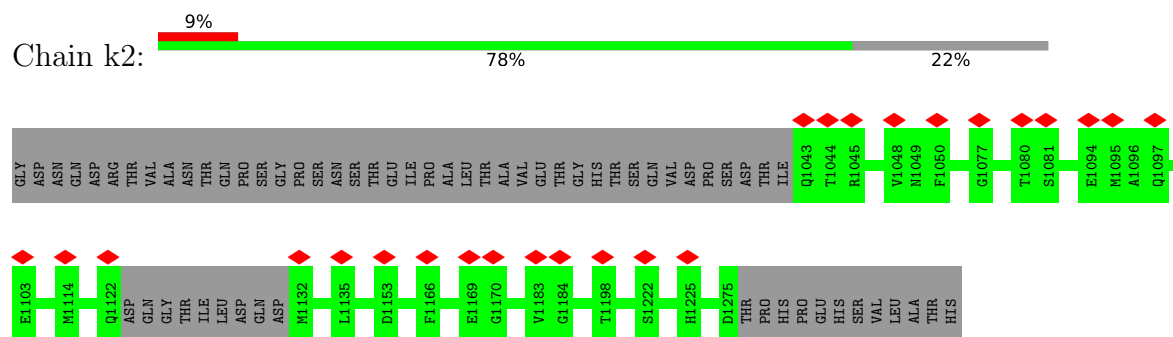




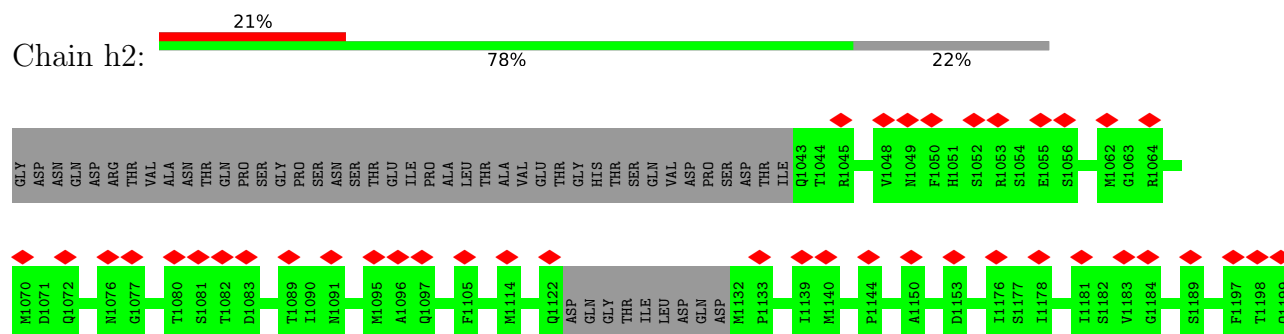
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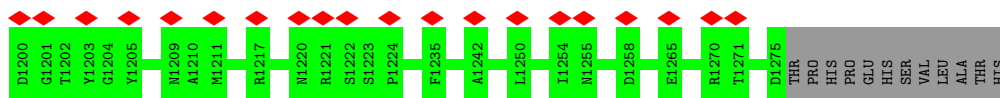


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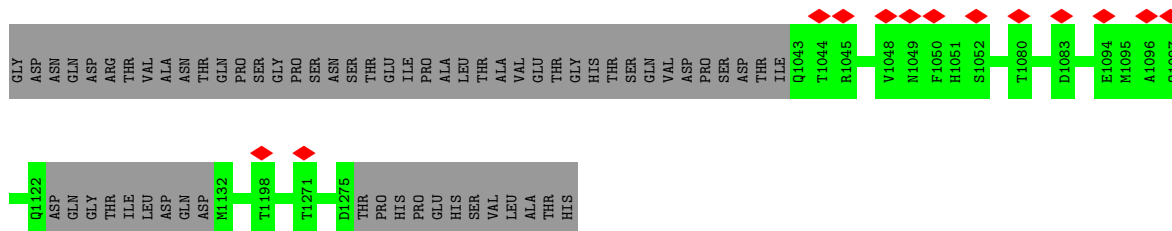
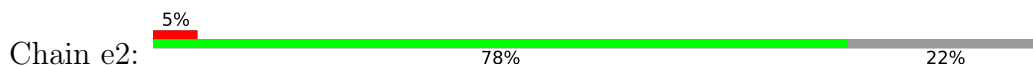


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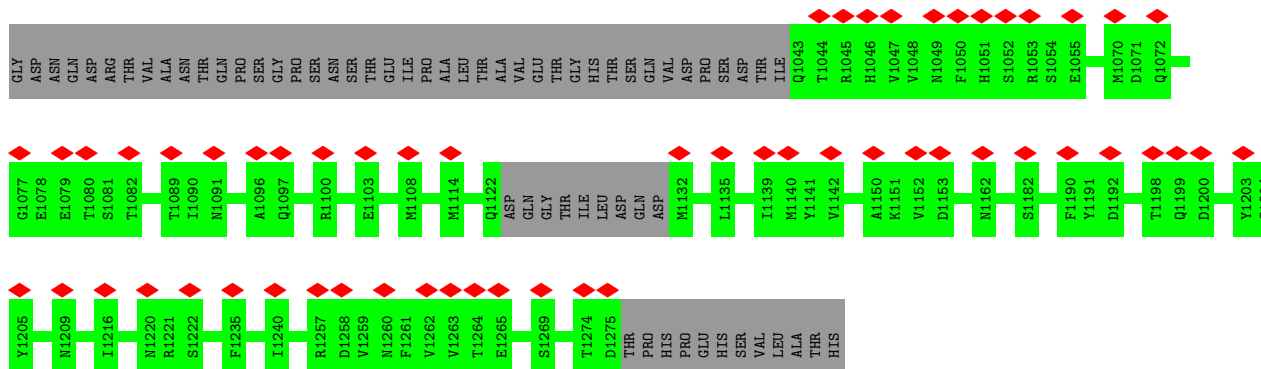
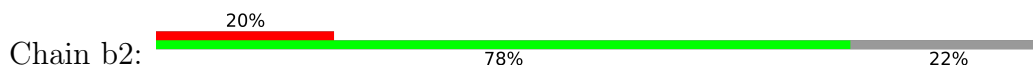




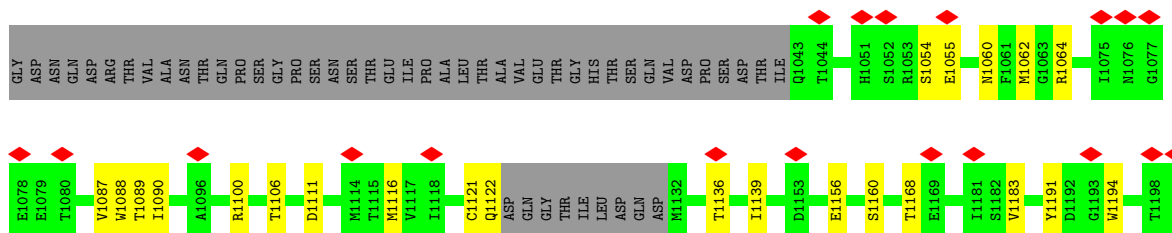
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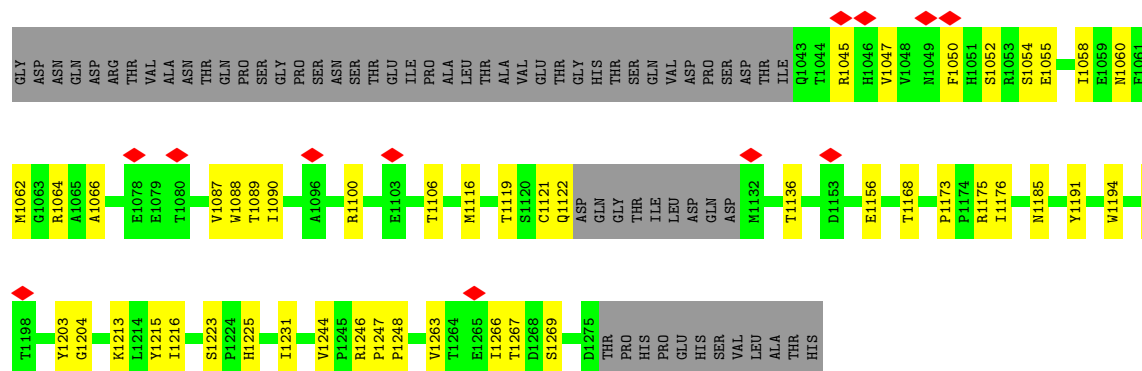


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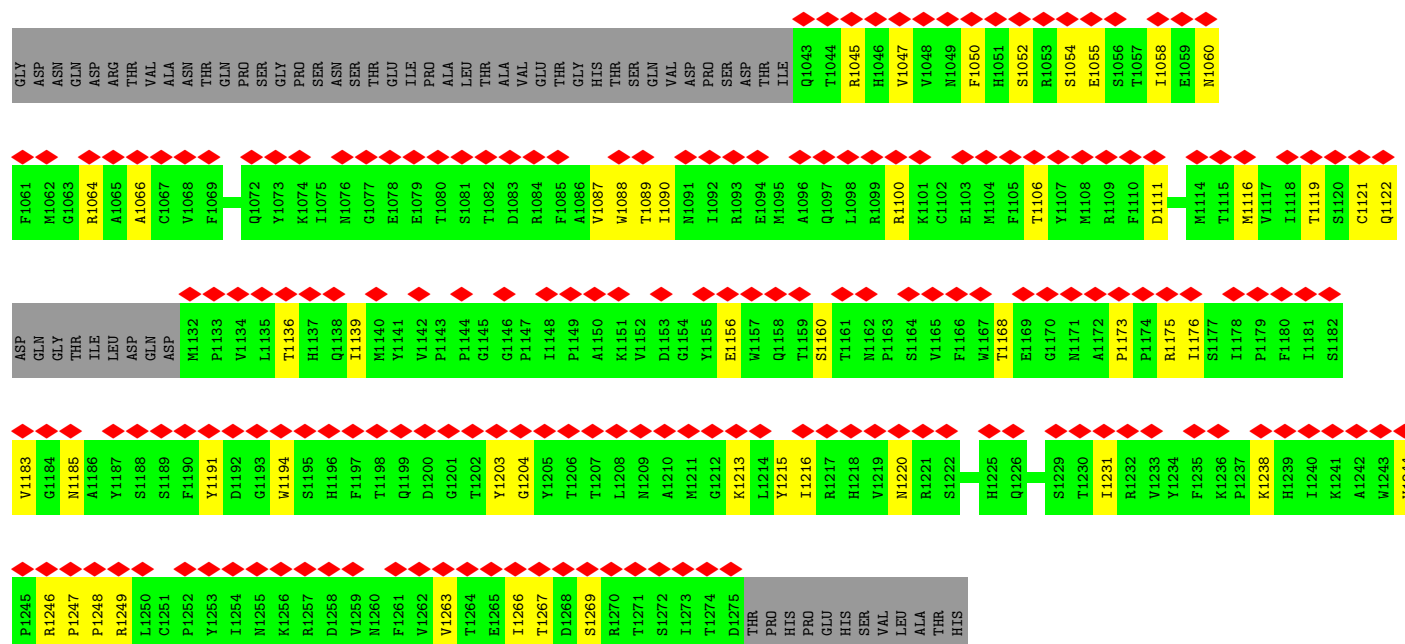


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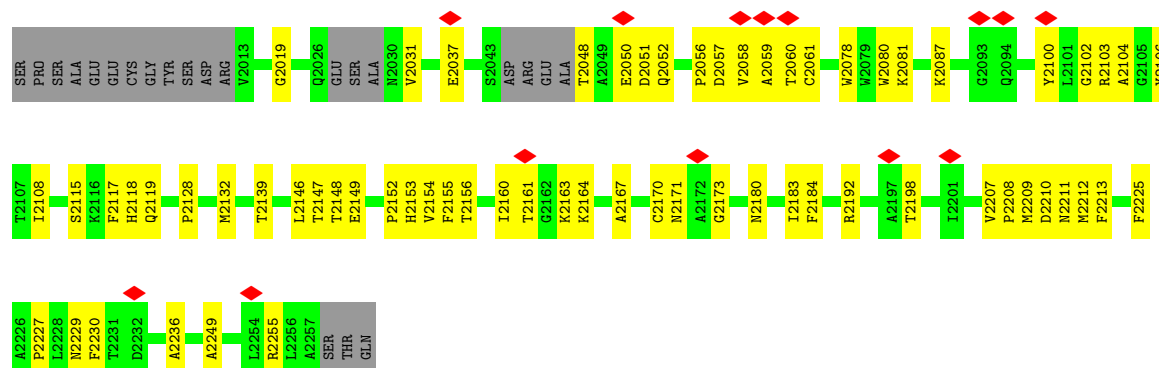




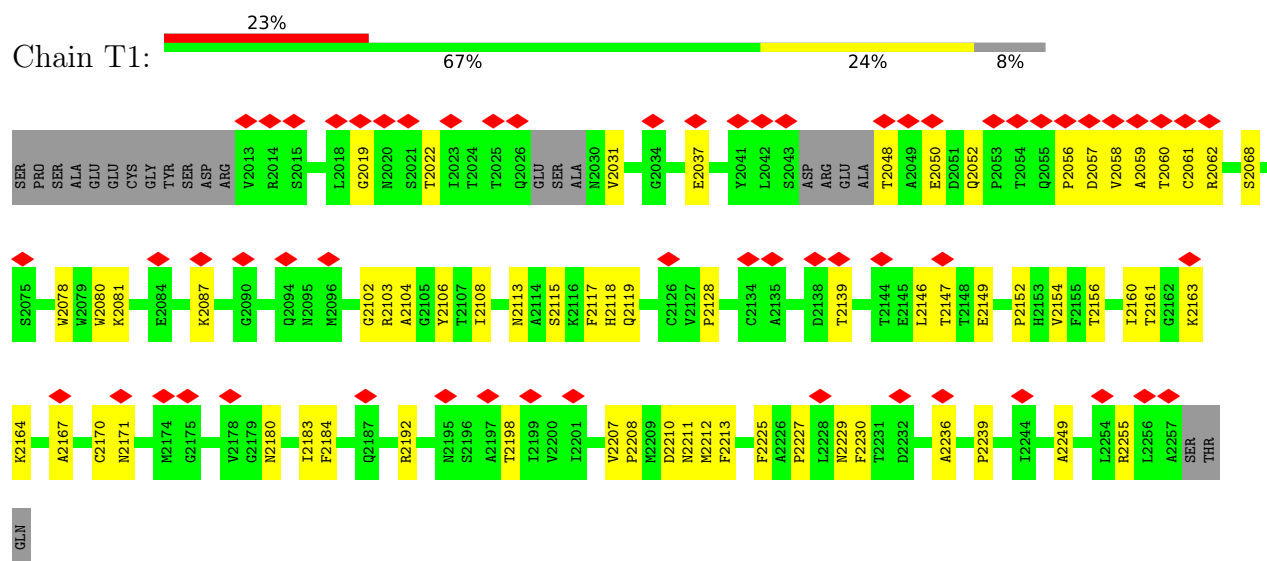
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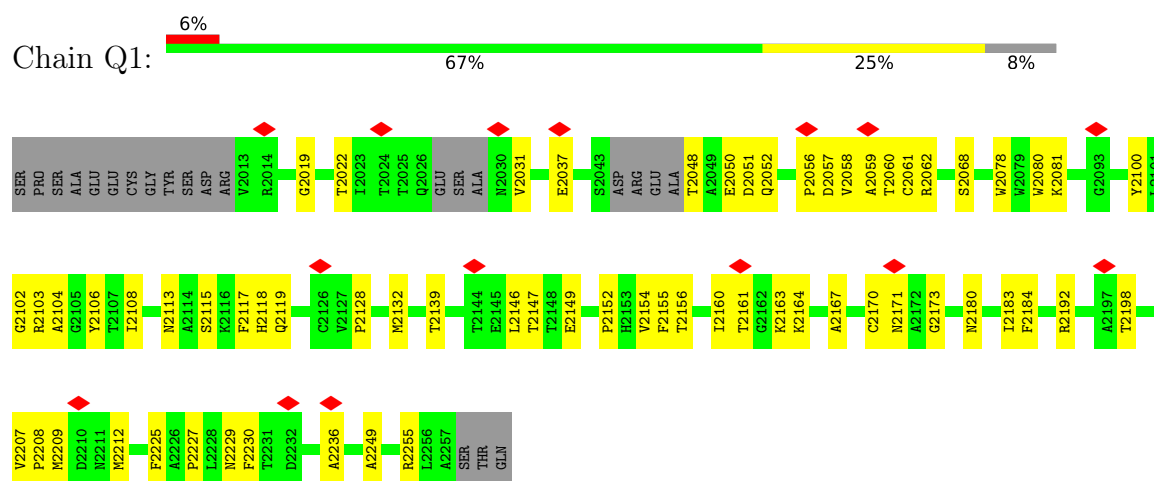
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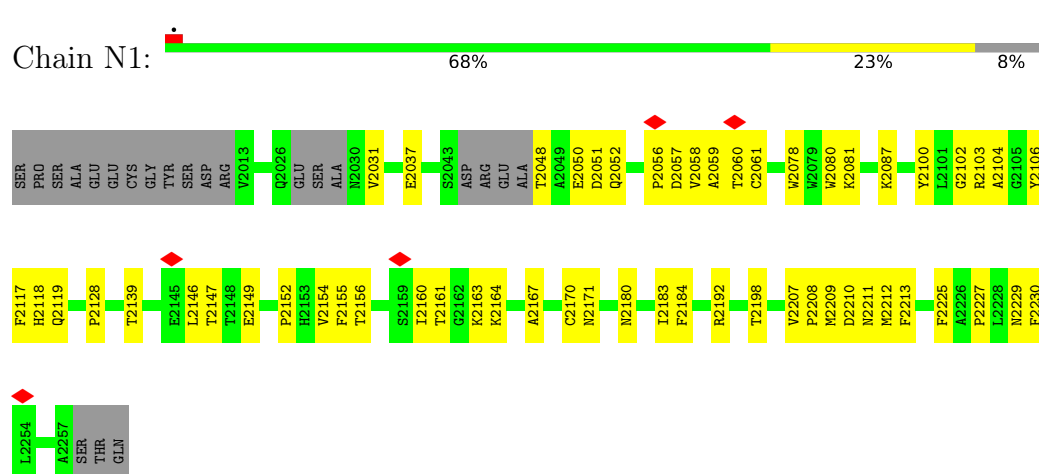
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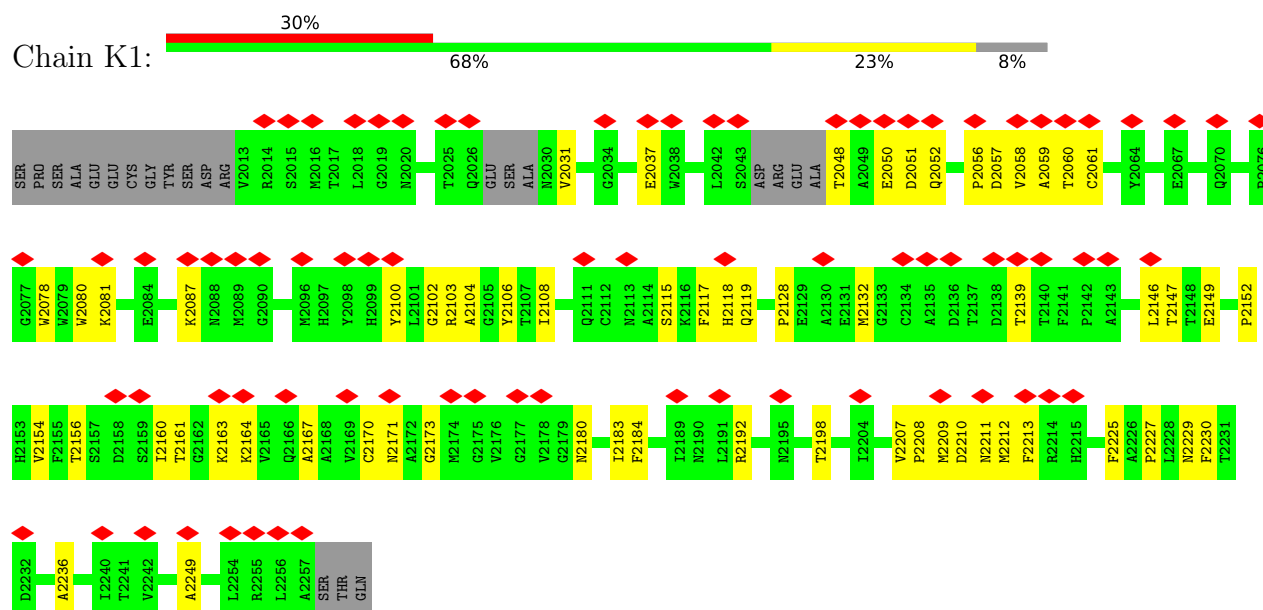
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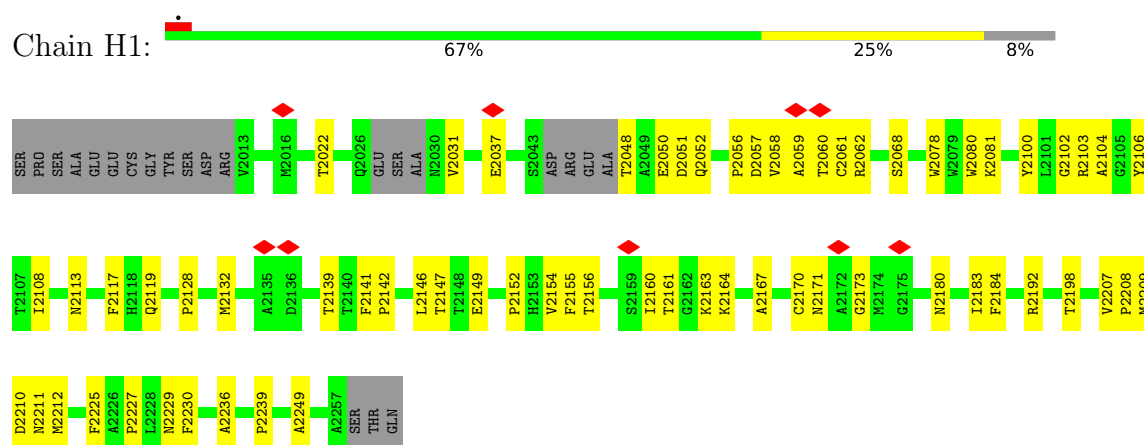
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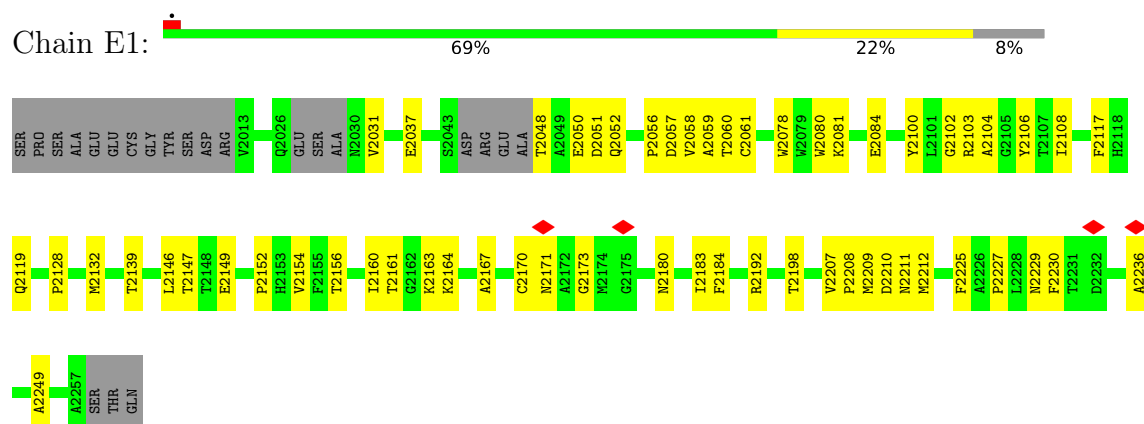
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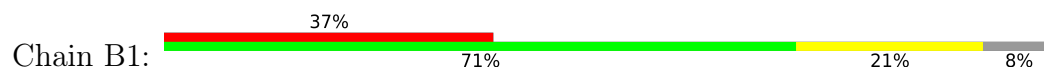
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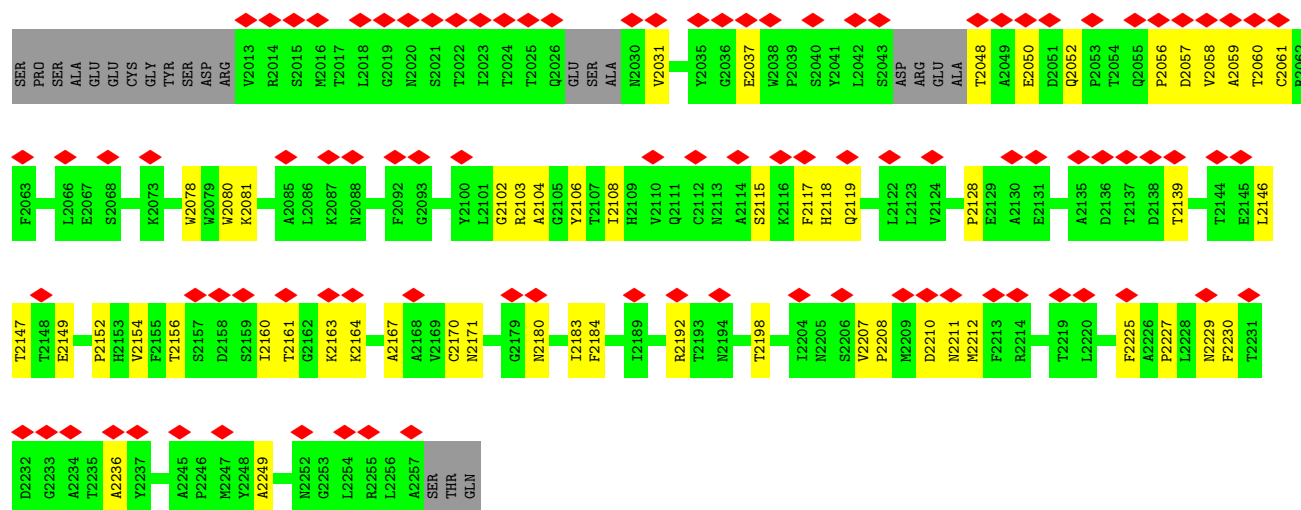


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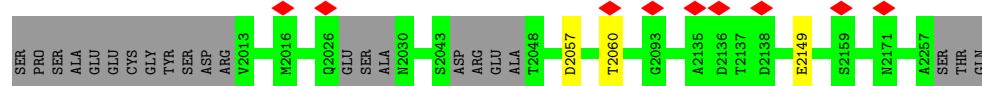


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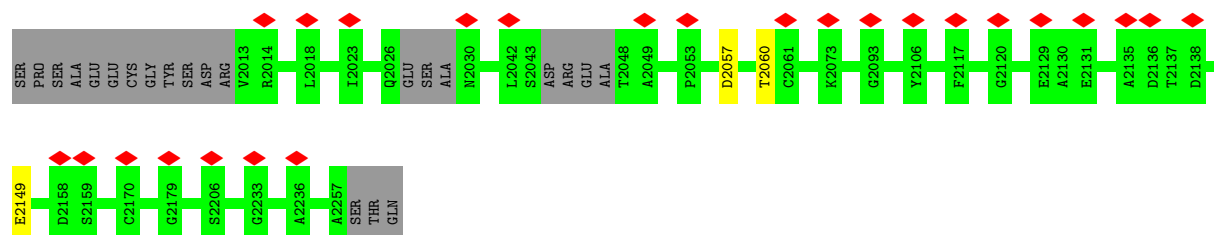
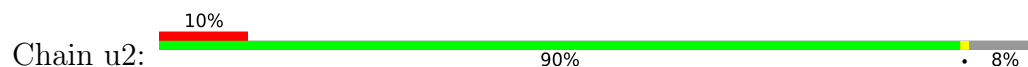




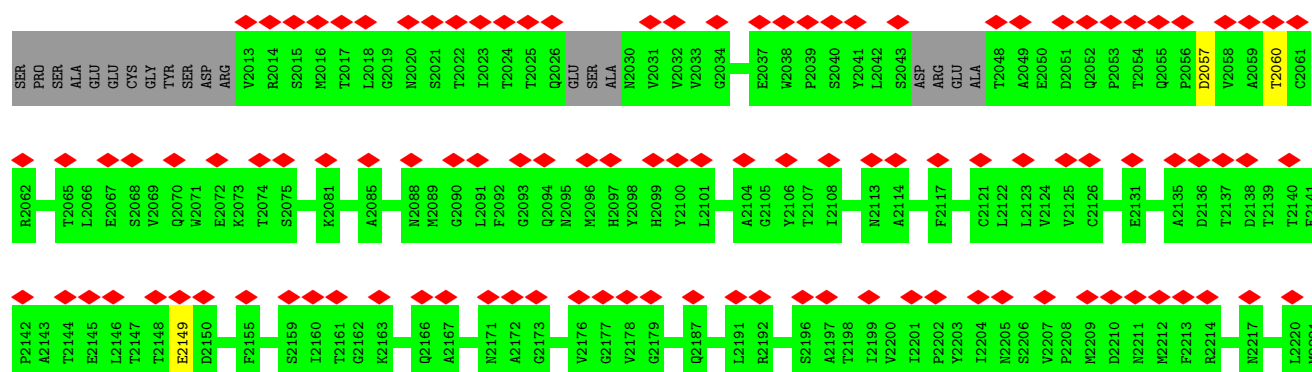
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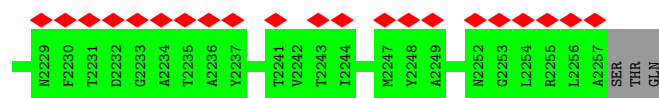


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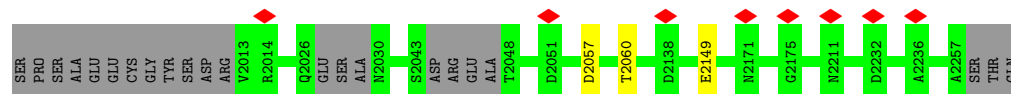


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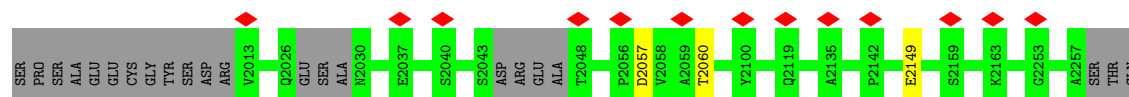
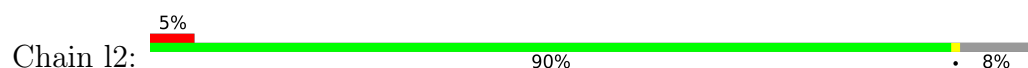




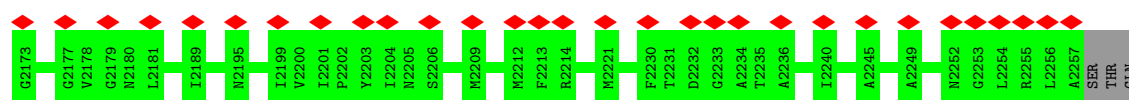
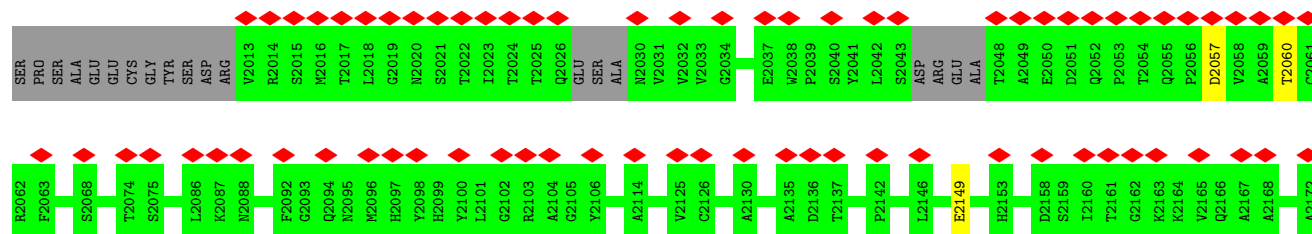
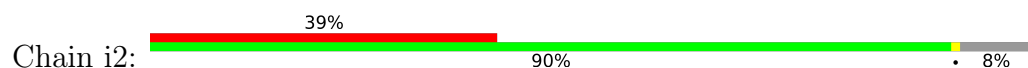
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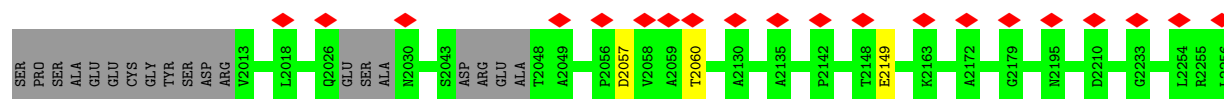
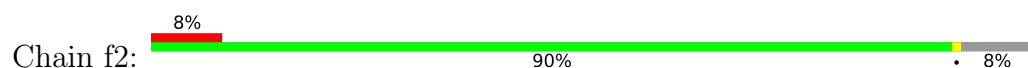
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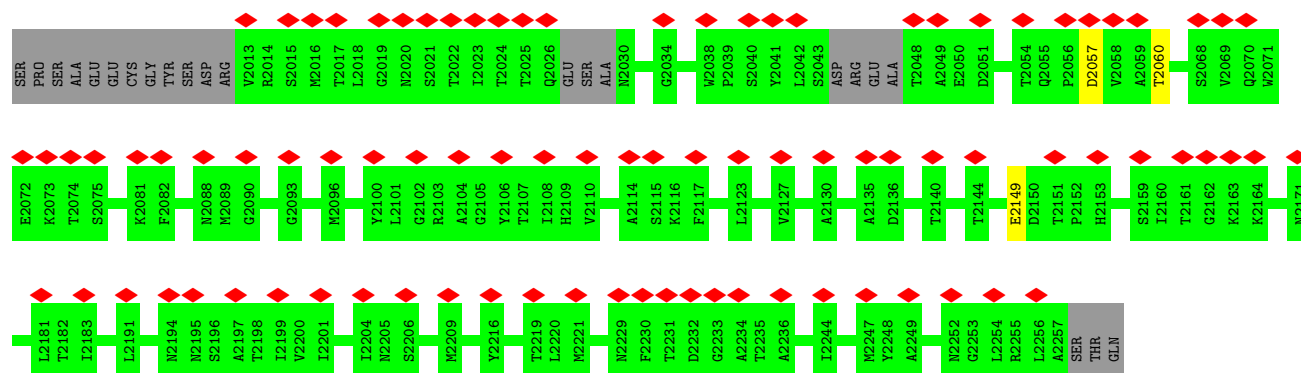


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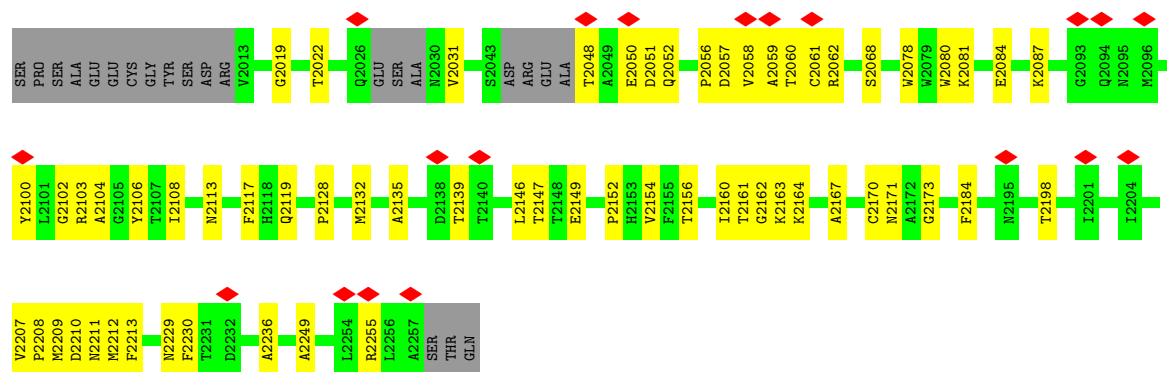


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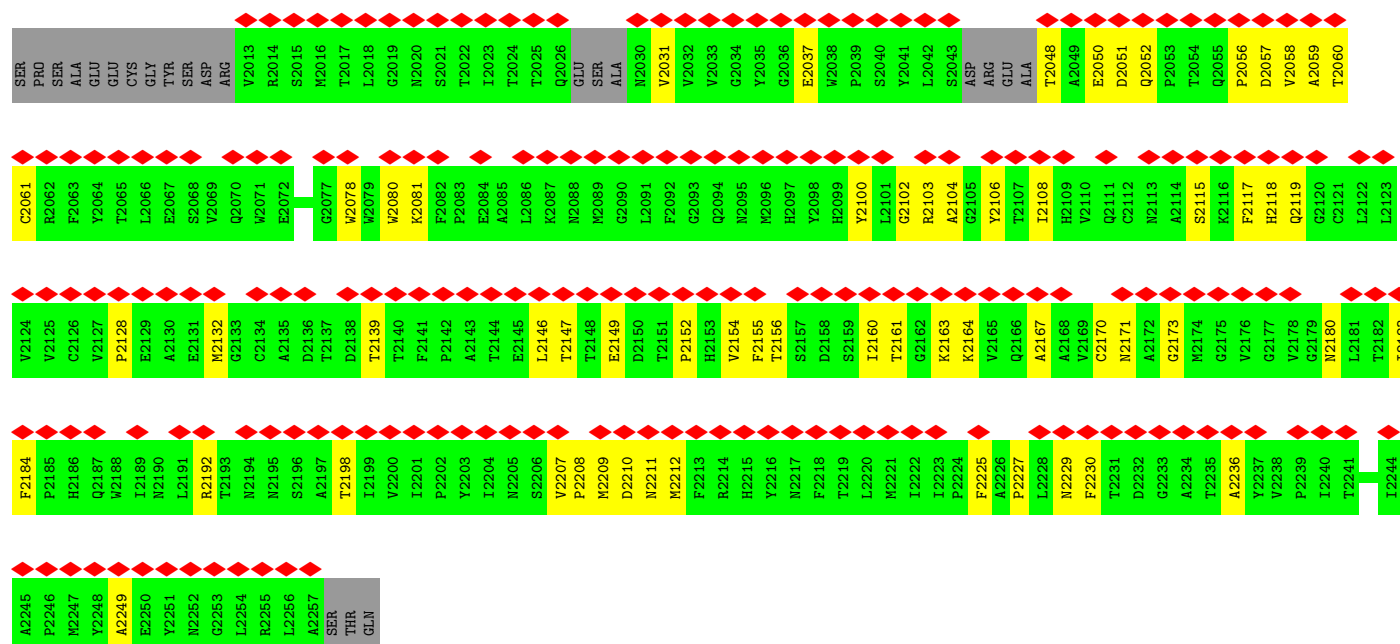
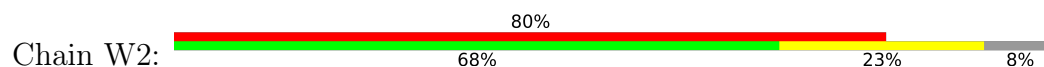




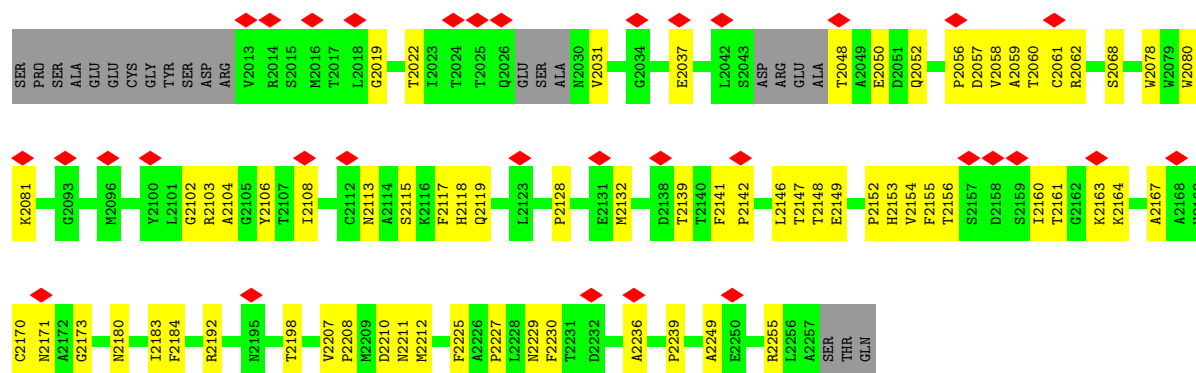
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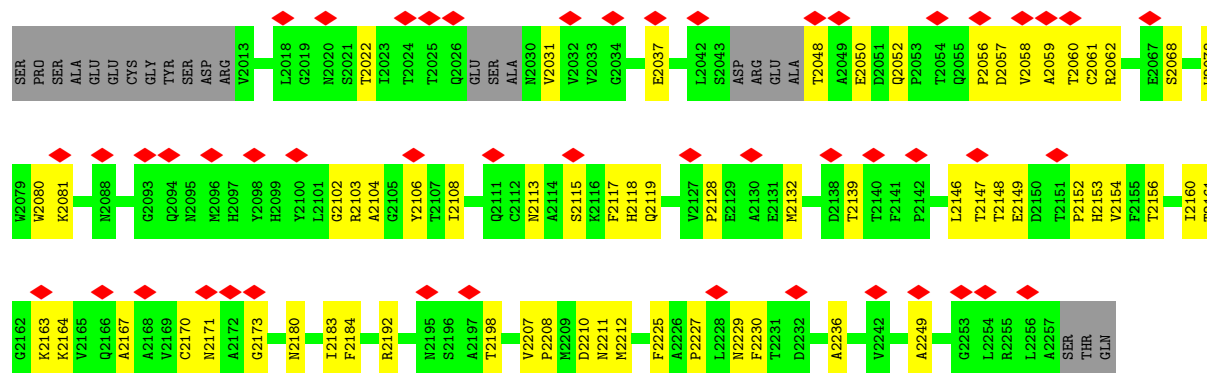
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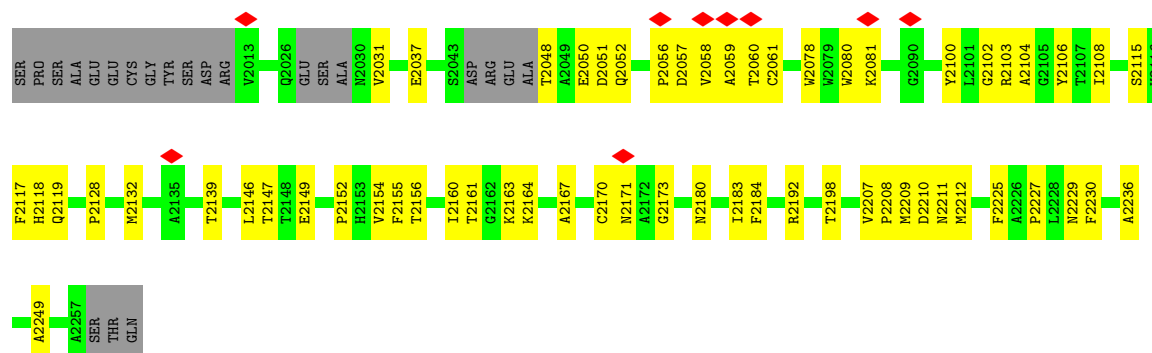
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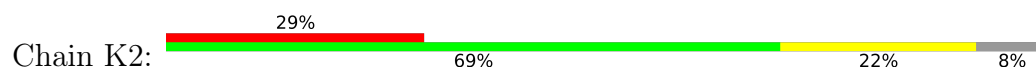
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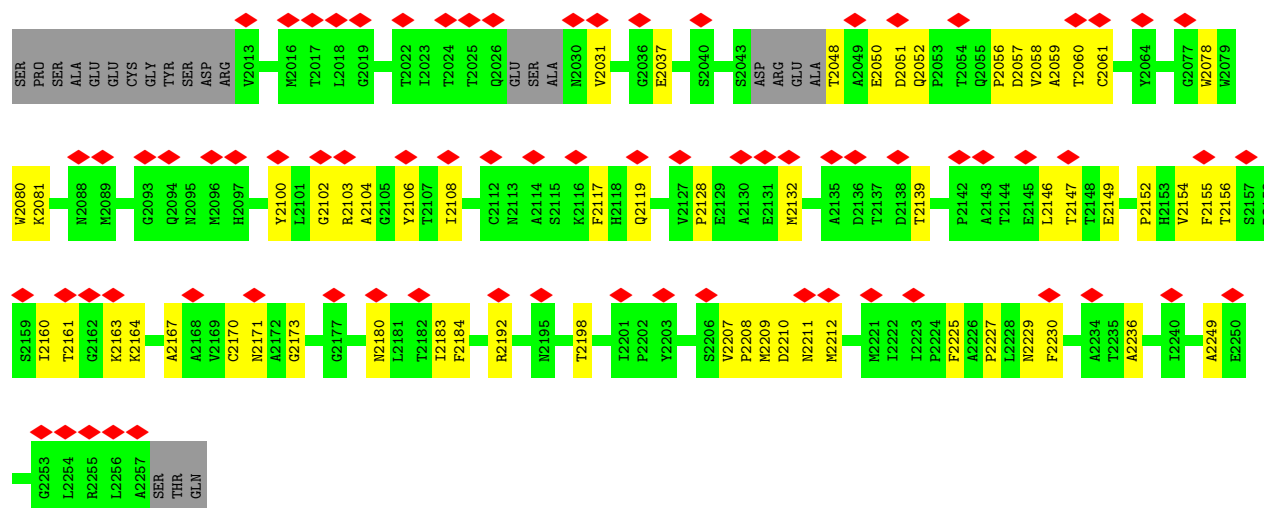


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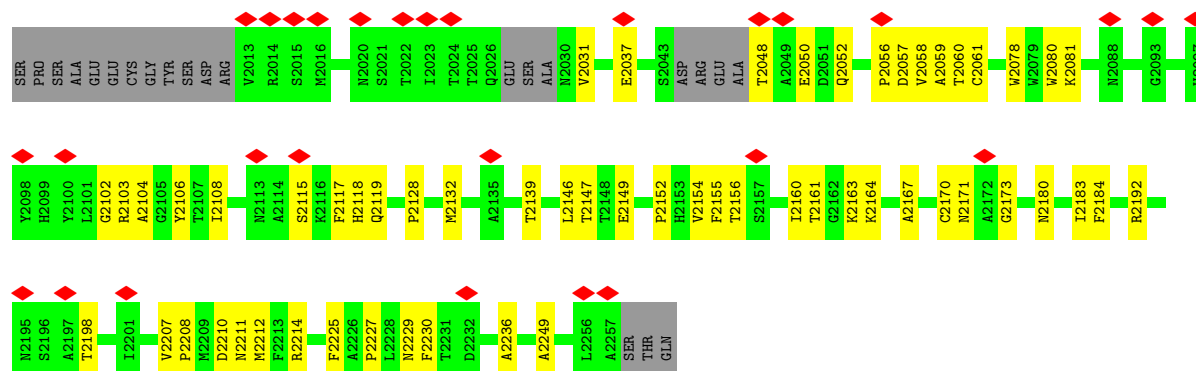
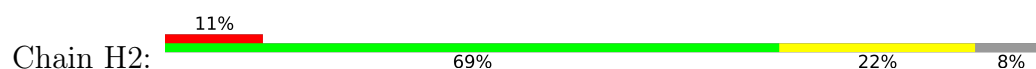


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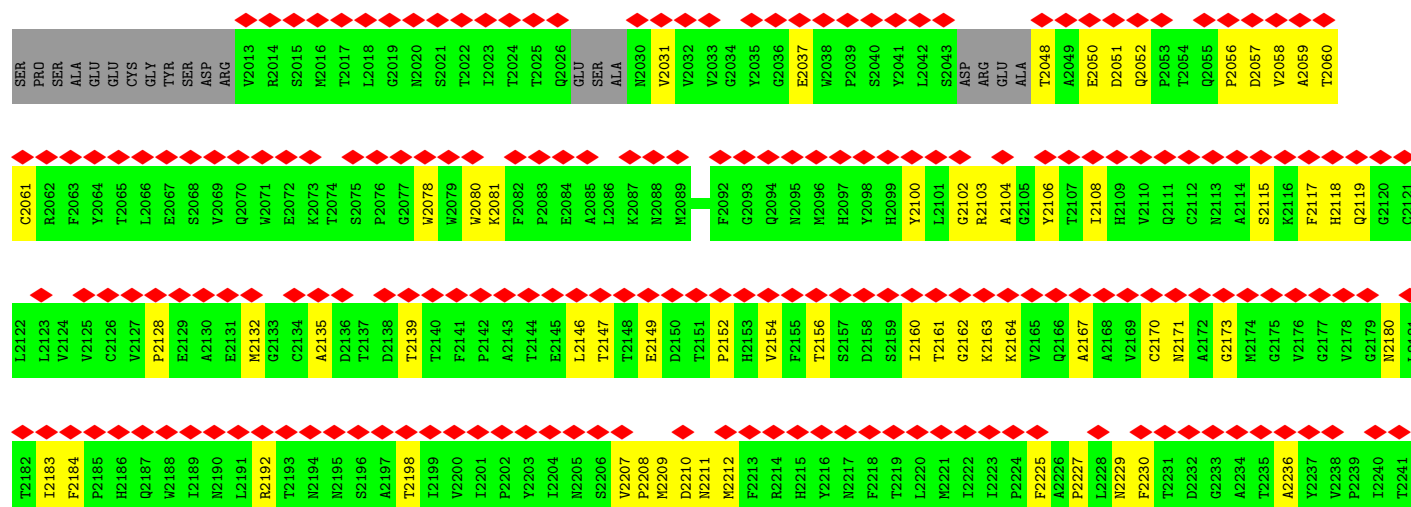
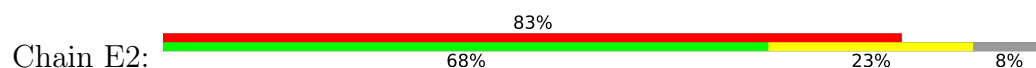




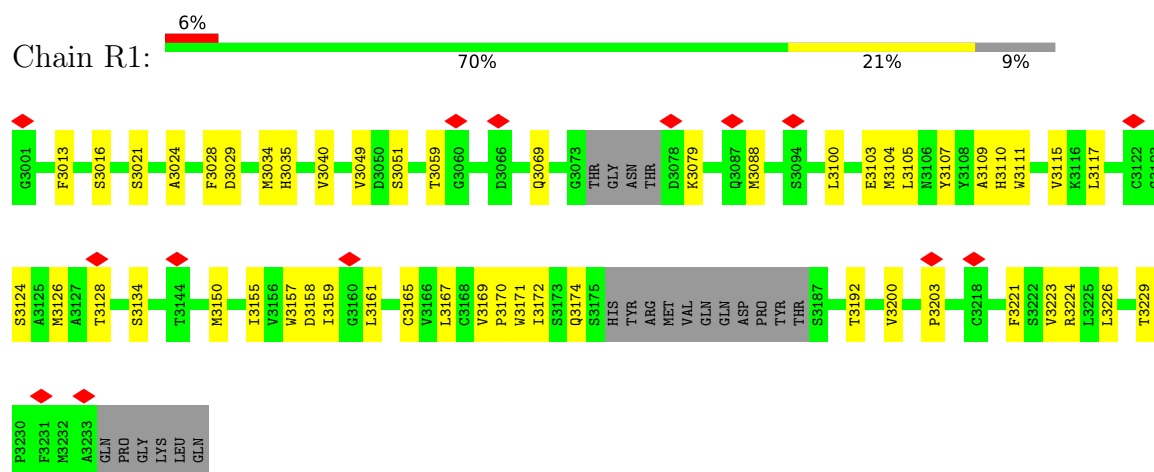
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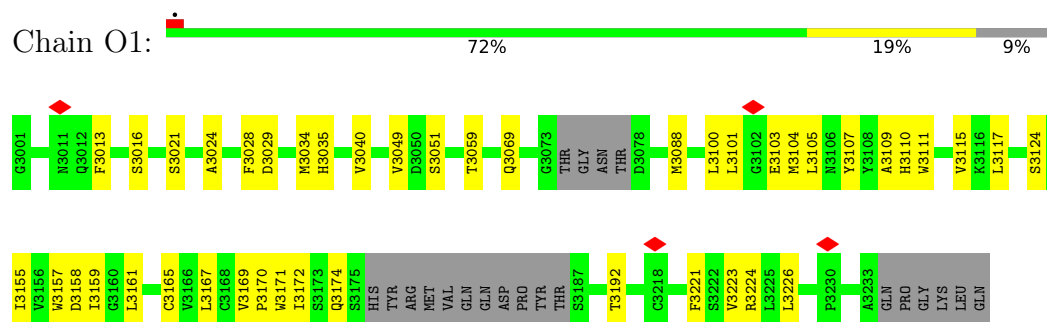
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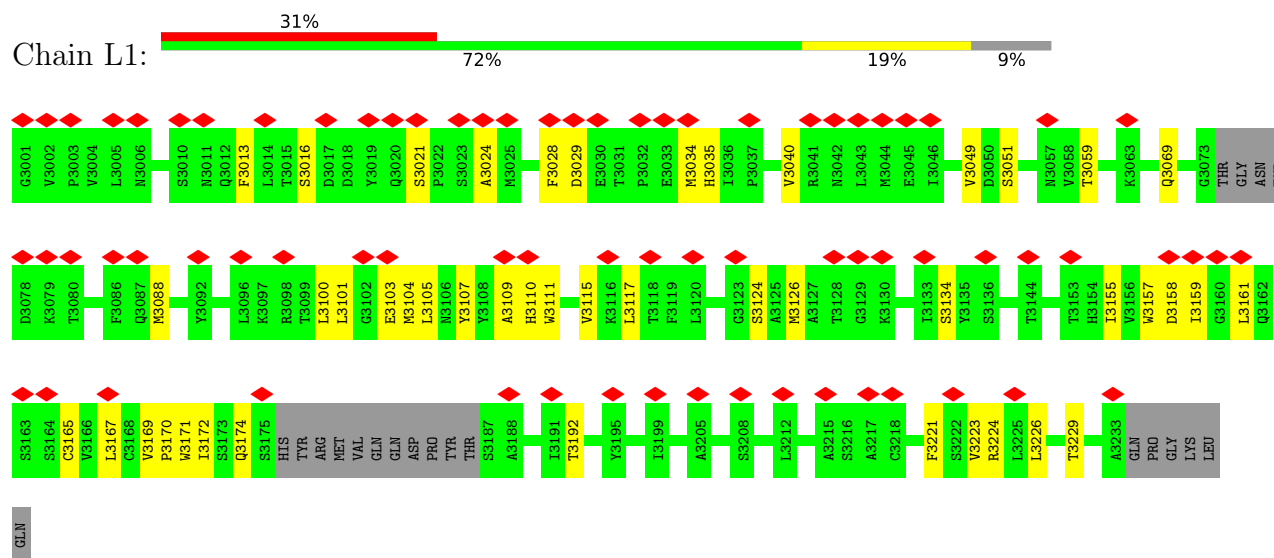
- Molecule 3: Echovirus 18 capsid protein 3



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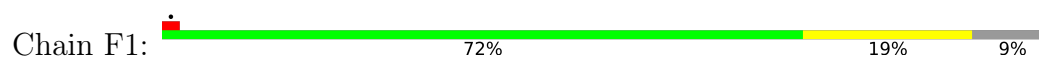
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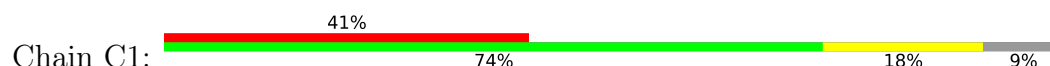
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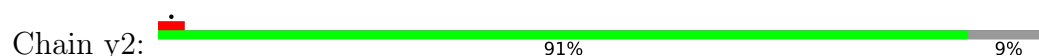
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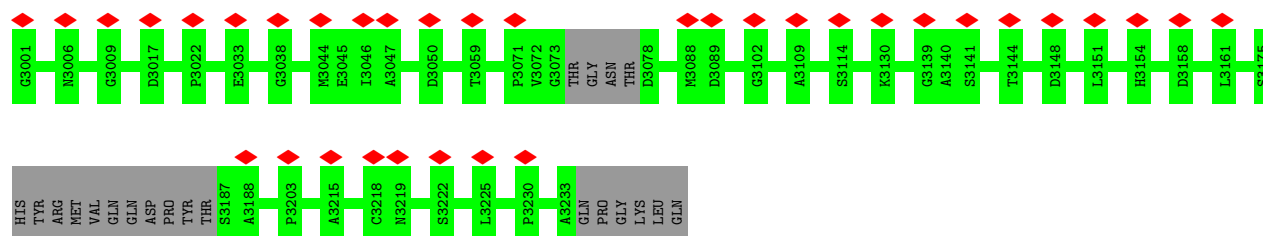


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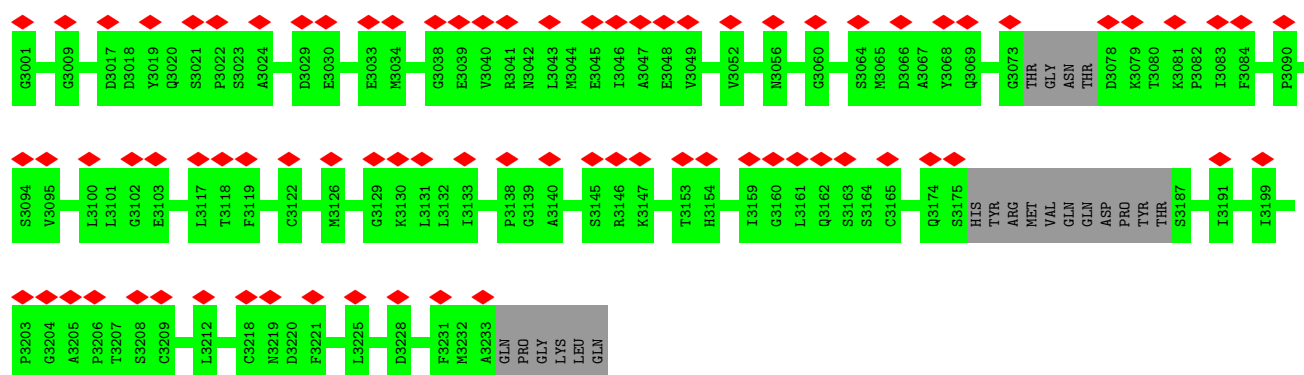


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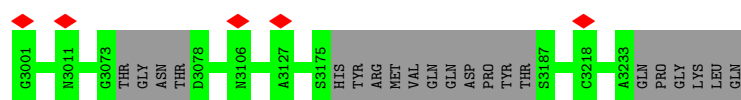




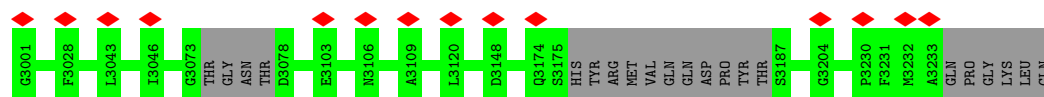
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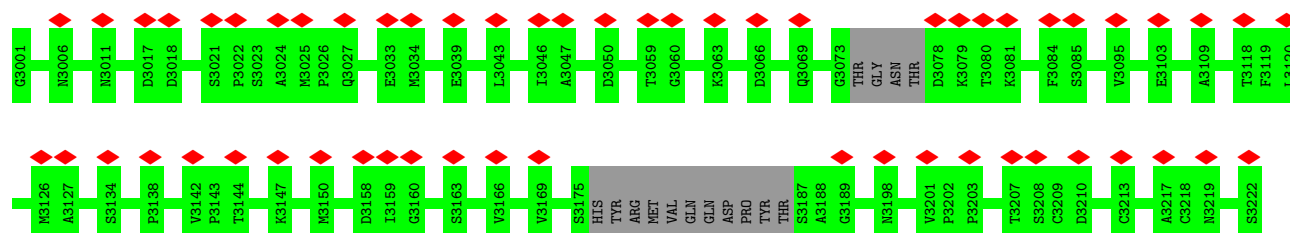
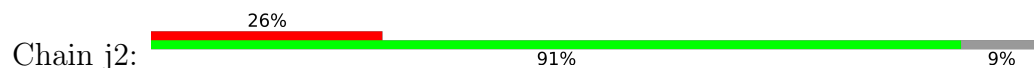
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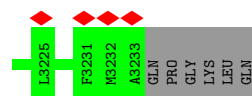


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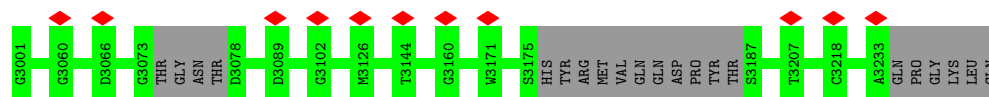


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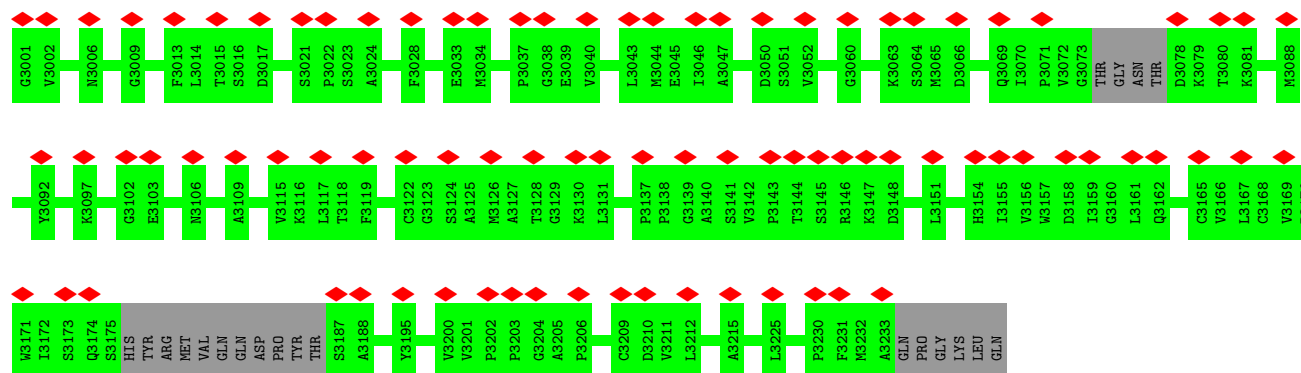




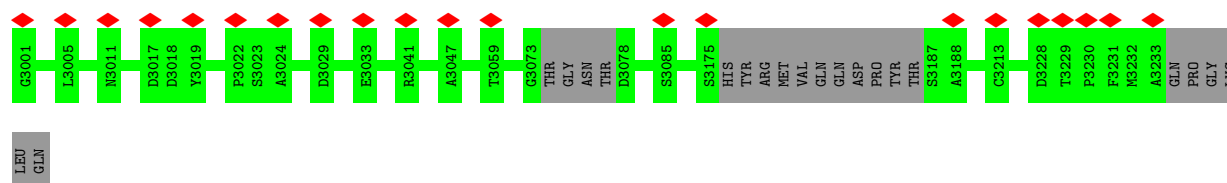
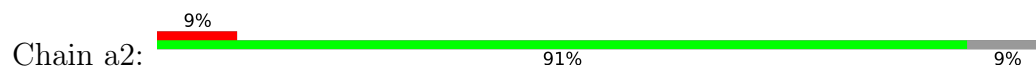
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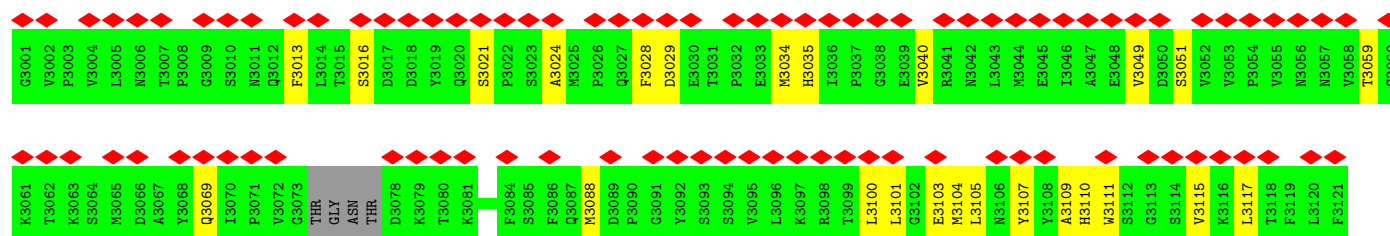
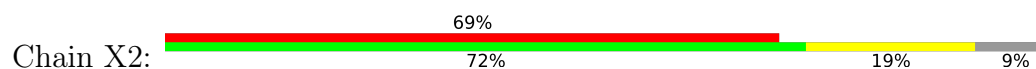
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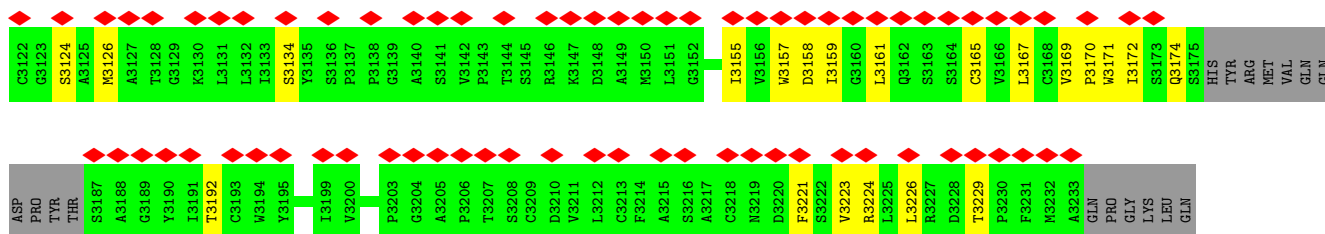


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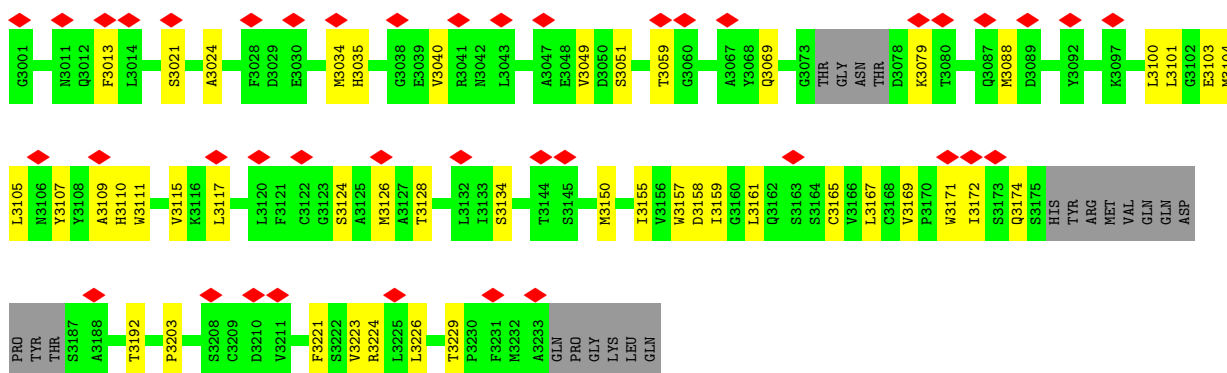
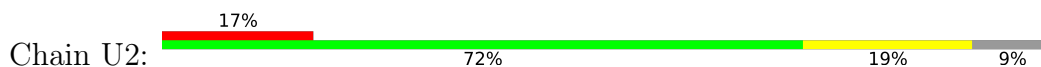


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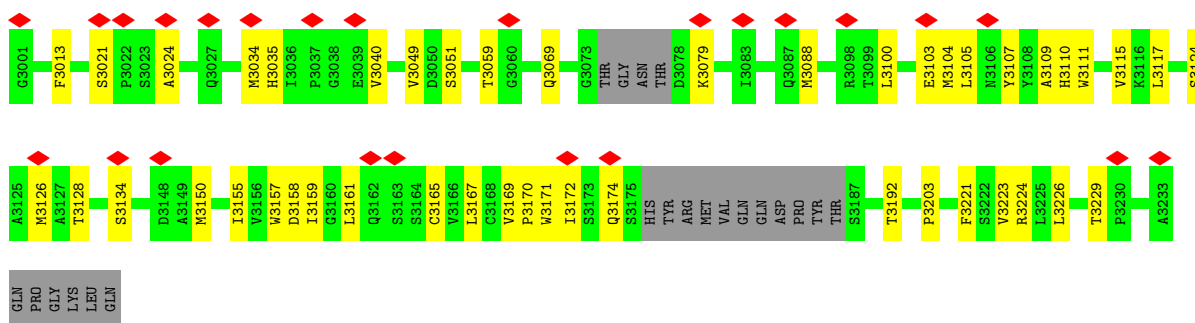
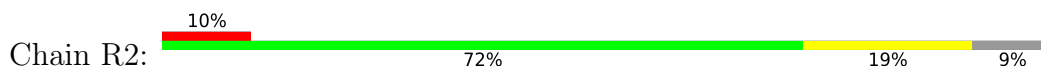




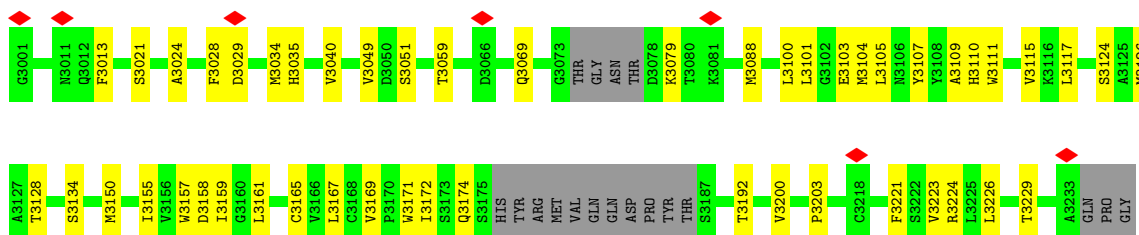
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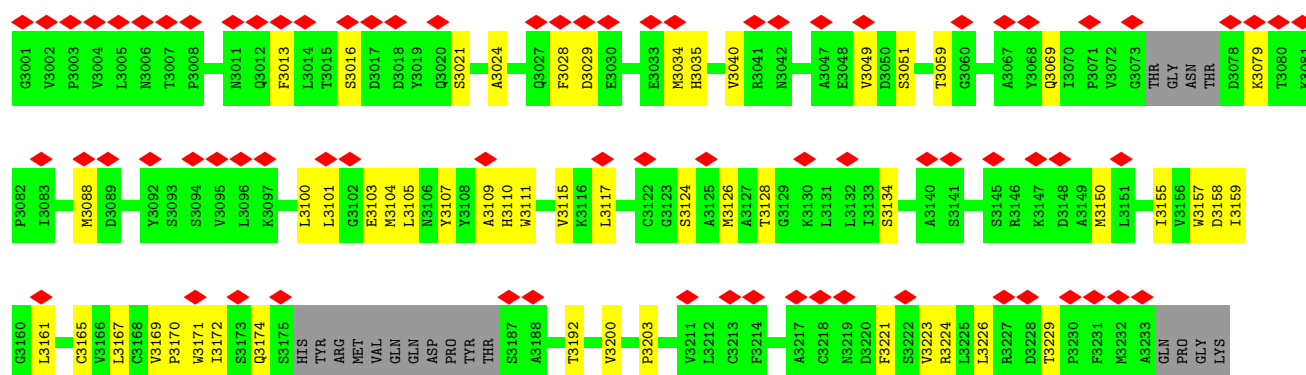
• Molecule 3: Echovirus 18 capsid protein 3



LYS
LEU
GLN

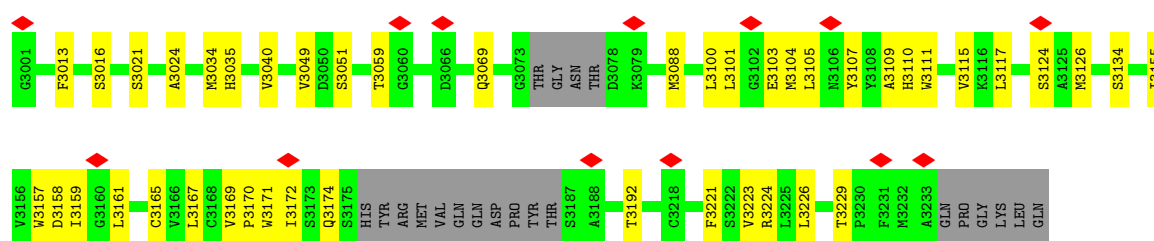
• Molecule 3: Echovirus 18 capsid protein 3

Chain L2: 32% 70% 21% 9%

LEU
GLN

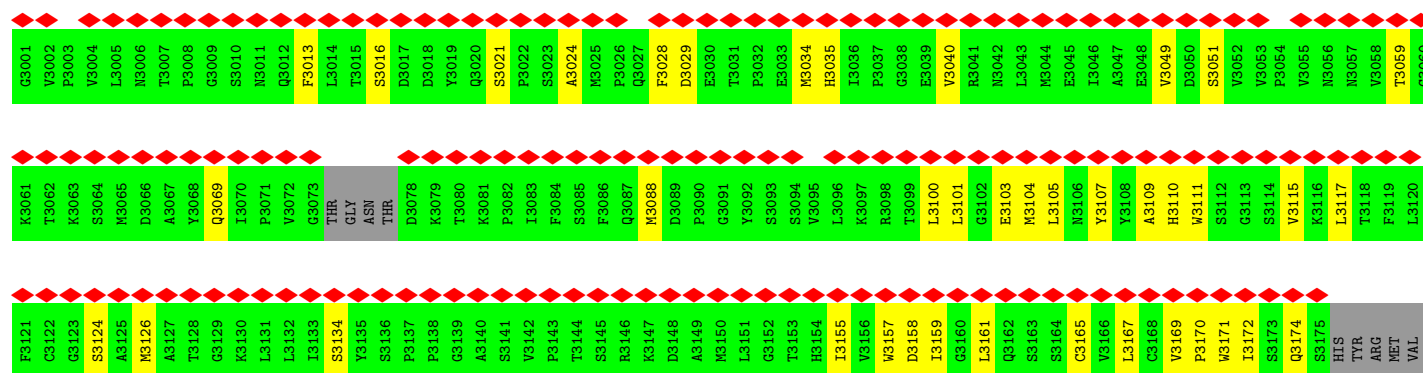
• Molecule 3: Echovirus 18 capsid protein 3

Chain I2: 5% 73% 18% 9%



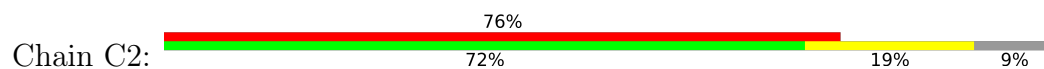
• Molecule 3: Echovirus 18 capsid protein 3

Chain F2: 89% 72% 19% 9%



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|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|
| GLN | GLN | ASP | PRO | TYR | THR | S3187 | A3188 | G3189 | Y3190 | I3191 | T3192 | C3193 | W3194 | Y3195 | Q3196 | T3197 | N3198 | I3199 | I3199 | V3200 | V3201 | P3202 | P3203 | G3204 | A3205 | P3206 | T3207 | S3208 | C3209 | D3210 | V3211 | L3212 | C3213 | F3214 | A3215 | S3216 | A3217 | C3218 | N3219 | D3220 | F3221 | S3222 | V3223 | R3224 | L3225 | L3226 | R3227 | D3228 | T3229 | P3230 | F3231 | W3232 | A3233 | GLN | PRO | GLY | LYS | LEU | GLN |
|-----|-----|-----|-----|-----|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|

● Molecule 3: Echovirus 18 capsid protein 3



| | | | | |
|--------------------------|---|--|---|---|
| ASP PRO TYR THR | S3187 A3188 G3189 Y3190 I3191 T3192 C3193 W3194 Y3195 Q3196 T3197 N3198 I3199 V3200 V3201 P3202 G3203 A3204 A3205 P3206 T3207 S3208 C3209 D3210 V3211 L3212 C3213 F3214 S3215 A3216 N3217 C3218 N3219 D3220 F3221 S3222 R3223 C3224 L3225 L3226 R3227 D3228 T3229 P3230 F3231 M3232 A3233 | G3123 S3124 A3125 M3126 A3127 T3128 G3129 K3130 L3131 L3132 I3133 S3134 Y3135 S3136 P3137 P3138 G3139 A3140 S3141 V3142 P3143 T3144 S3145 R3146 K3147 D3148 A3149 M3150 L3151 G3152 T3153 H3154 I3155 V3156 W3157 D3158 I3159 G3160 L3161 Q3162 S3163 S3164 C3165 V3166 L3167 C3168 V3169 P3170 W3171 I3172 S3173 Q3174 S3175 HIS TYR ARG MET VAL GLN GLN | T3062 K3063 S3064 M3065 D3066 A3067 Y3068 Q3069 I3070 P3071 V3072 G3073 THR GLY ASN THR D3078 K3079 T3080 K3081 P3082 T3083 F3084 S3085 F3086 Q3087 M3088 D3089 P3090 G3091 Y3092 V3095 L3096 K3097 R3098 T3099 L3100 L3101 G3102 E3103 M3104 L3105 N3106 Y3107 T3108 A3109 H3110 W3111 S3112 G3113 S3114 V3115 K3116 L3117 T3118 F3119 L3120 F3121 G3122 | G3001 V3002 P3003 V3004 L3005 N3006 T3007 P3008 G3009 S3010 N3011 Q3012 F3013 L3014 T3015 S3016 D3017 D3018 Y3019 Q3020 S3021 P3022 S3023 A3024 M3025 P3026 Q3027 F3028 D3029 E3030 E3033 M3034 H3035 I3036 P3037 G3038 E3039 V3040 R3041 N3042 L3043 M3044 E3045 I3046 A3047 E3048 V3049 D3050 S3051 V3052 V3053 P3054 V3055 N3056 N3057 V3058 T3059 G3060 K3061 |
|--------------------------|---|--|---|---|

4 Experimental information

| Property | Value | Source |
|--------------------------------------|--------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C2 | Depositor |
| Number of particles used | 7635 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 45.2 | Depositor |
| Minimum defocus (nm) | 651 | Depositor |
| Maximum defocus (nm) | 3282 | Depositor |
| Magnification | 79575 | Depositor |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 0.439 | Depositor |
| Minimum map value | -0.251 | Depositor |
| Average map value | 0.005 | Depositor |
| Map value standard deviation | 0.028 | Depositor |
| Recommended contour level | 0.07 | Depositor |
| Map size (\AA) | 371.35, 371.35, 371.35 | wwPDB |
| Map dimensions | 350, 350, 350 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.061, 1.061, 1.061 | Depositor |

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------|-------------|-------------|
| | | RMSZ | $\# Z > 5$ | RMSZ | $\# Z > 5$ |
| 1 | A1 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | A2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | D1 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | D2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | G1 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | G2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | J1 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | J2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | M1 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | M2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | P1 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | P2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | S1 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | S2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | V1 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | V2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | Y2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | b2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | e2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | h2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | k2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | n2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | q2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | t2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 1 | w2 | 0.27 | 0/1791 | 0.47 | 0/2442 |
| 2 | B1 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | B2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | E1 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | E2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | H1 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | H2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | K1 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | K2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | N1 | 0.27 | 0/1874 | 0.53 | 0/2567 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------|-------------|----------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | N2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | Q1 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | Q2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | T1 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | T2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | W1 | 0.26 | 0/1874 | 0.53 | 0/2567 |
| 2 | W2 | 0.26 | 0/1874 | 0.53 | 0/2567 |
| 2 | Z2 | 0.26 | 0/1874 | 0.53 | 0/2567 |
| 2 | c2 | 0.26 | 0/1874 | 0.53 | 0/2567 |
| 2 | f2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | i2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | l2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | o2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | r2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | u2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 2 | x2 | 0.27 | 0/1874 | 0.53 | 0/2567 |
| 3 | C1 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | C2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | F1 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | F2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | I1 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | I2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | L1 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | L2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | O1 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | O2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | R1 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | R2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | U1 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | U2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | X1 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | X2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | a2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | d2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | g2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | j2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | m2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | p2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | s2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | v2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| 3 | y2 | 0.26 | 0/1676 | 0.48 | 0/2287 |
| All | All | 0.27 | 0/133525 | 0.49 | 0/182400 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A1 | 1741 | 0 | 1659 | 36 | 0 |
| 1 | A2 | 1741 | 0 | 1659 | 46 | 0 |
| 1 | D1 | 1741 | 0 | 1659 | 45 | 0 |
| 1 | D2 | 1741 | 0 | 1659 | 45 | 0 |
| 1 | G1 | 1741 | 0 | 1659 | 46 | 0 |
| 1 | G2 | 1741 | 0 | 1659 | 41 | 0 |
| 1 | J1 | 1741 | 0 | 1659 | 43 | 0 |
| 1 | J2 | 1741 | 0 | 1659 | 44 | 0 |
| 1 | M1 | 1741 | 0 | 1659 | 45 | 0 |
| 1 | M2 | 1741 | 0 | 1659 | 40 | 0 |
| 1 | P1 | 1741 | 0 | 1659 | 44 | 0 |
| 1 | P2 | 1741 | 0 | 1659 | 42 | 0 |
| 1 | S1 | 1741 | 0 | 1659 | 36 | 0 |
| 1 | S2 | 1741 | 0 | 1659 | 38 | 0 |
| 1 | V1 | 1741 | 0 | 1659 | 45 | 0 |
| 1 | V2 | 1741 | 0 | 1659 | 45 | 0 |
| 1 | Y2 | 1741 | 0 | 1659 | 28 | 0 |
| 1 | b2 | 1741 | 0 | 1659 | 0 | 0 |
| 1 | e2 | 1741 | 0 | 1659 | 0 | 0 |
| 1 | h2 | 1741 | 0 | 1659 | 0 | 0 |
| 1 | k2 | 1741 | 0 | 1659 | 0 | 0 |
| 1 | n2 | 1741 | 0 | 1659 | 0 | 0 |
| 1 | q2 | 1741 | 0 | 1659 | 0 | 0 |
| 1 | t2 | 1741 | 0 | 1659 | 0 | 0 |
| 1 | w2 | 1741 | 0 | 1659 | 0 | 0 |
| 2 | B1 | 1821 | 0 | 1739 | 38 | 0 |
| 2 | B2 | 1821 | 0 | 1739 | 45 | 0 |
| 2 | E1 | 1821 | 0 | 1739 | 43 | 0 |
| 2 | E2 | 1821 | 0 | 1739 | 44 | 0 |
| 2 | H1 | 1821 | 0 | 1739 | 51 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | H2 | 1821 | 0 | 1739 | 42 | 0 |
| 2 | K1 | 1821 | 0 | 1739 | 44 | 0 |
| 2 | K2 | 1821 | 0 | 1739 | 43 | 0 |
| 2 | N1 | 1821 | 0 | 1739 | 46 | 0 |
| 2 | N2 | 1821 | 0 | 1739 | 44 | 0 |
| 2 | Q1 | 1821 | 0 | 1739 | 50 | 0 |
| 2 | Q2 | 1821 | 0 | 1739 | 45 | 0 |
| 2 | T1 | 1821 | 0 | 1739 | 47 | 0 |
| 2 | T2 | 1821 | 0 | 1739 | 50 | 0 |
| 2 | W1 | 1821 | 0 | 1739 | 49 | 0 |
| 2 | W2 | 1821 | 0 | 1739 | 44 | 0 |
| 2 | Z2 | 1821 | 0 | 1739 | 42 | 0 |
| 2 | c2 | 1821 | 0 | 1739 | 0 | 0 |
| 2 | f2 | 1821 | 0 | 1739 | 0 | 0 |
| 2 | i2 | 1821 | 0 | 1739 | 0 | 0 |
| 2 | l2 | 1821 | 0 | 1739 | 0 | 0 |
| 2 | o2 | 1821 | 0 | 1739 | 0 | 0 |
| 2 | r2 | 1821 | 0 | 1739 | 0 | 0 |
| 2 | u2 | 1821 | 0 | 1739 | 0 | 0 |
| 2 | x2 | 1821 | 0 | 1739 | 0 | 0 |
| 3 | C1 | 1634 | 0 | 1596 | 40 | 0 |
| 3 | C2 | 1634 | 0 | 1596 | 48 | 0 |
| 3 | F1 | 1634 | 0 | 1596 | 49 | 0 |
| 3 | F2 | 1634 | 0 | 1596 | 49 | 0 |
| 3 | I1 | 1634 | 0 | 1596 | 54 | 0 |
| 3 | I2 | 1634 | 0 | 1596 | 45 | 0 |
| 3 | L1 | 1634 | 0 | 1596 | 49 | 0 |
| 3 | L2 | 1634 | 0 | 1596 | 55 | 0 |
| 3 | O1 | 1634 | 0 | 1596 | 47 | 0 |
| 3 | O2 | 1634 | 0 | 1596 | 49 | 0 |
| 3 | R1 | 1634 | 0 | 1596 | 54 | 0 |
| 3 | R2 | 1634 | 0 | 1596 | 48 | 0 |
| 3 | U1 | 1634 | 0 | 1596 | 41 | 0 |
| 3 | U2 | 1634 | 0 | 1596 | 46 | 0 |
| 3 | X1 | 1634 | 0 | 1596 | 50 | 0 |
| 3 | X2 | 1634 | 0 | 1596 | 48 | 0 |
| 3 | a2 | 1634 | 0 | 1596 | 0 | 0 |
| 3 | d2 | 1634 | 0 | 1596 | 0 | 0 |
| 3 | g2 | 1634 | 0 | 1596 | 0 | 0 |
| 3 | j2 | 1634 | 0 | 1596 | 0 | 0 |
| 3 | m2 | 1634 | 0 | 1596 | 0 | 0 |
| 3 | p2 | 1634 | 0 | 1596 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 3 | s2 | 1634 | 0 | 1596 | 0 | 0 |
| 3 | v2 | 1634 | 0 | 1596 | 0 | 0 |
| 3 | y2 | 1634 | 0 | 1596 | 0 | 0 |
| All | All | 129900 | 0 | 124850 | 1686 | 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 10.

The worst 5 of 1686 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:J1:1216:ILE:HD13 | 1:J1:1231:ILE:HD13 | 1.56 | 0.88 |
| 1:S1:1216:ILE:HD13 | 1:S1:1231:ILE:HD13 | 1.56 | 0.87 |
| 1:M1:1216:ILE:HD13 | 1:M1:1231:ILE:HD13 | 1.56 | 0.87 |
| 1:V1:1216:ILE:HD13 | 1:V1:1231:ILE:HD13 | 1.56 | 0.87 |
| 1:P2:1216:ILE:HD13 | 1:P2:1231:ILE:HD13 | 1.56 | 0.86 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | A1 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | A2 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | D1 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | D2 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | G1 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | G2 | 220/287 (77%) | 199 (90%) | 21 (10%) | 0 | 100 | 100 |
| 1 | J1 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1 | J2 | 220/287 (77%) | 199 (90%) | 21 (10%) | 0 | 100 | 100 |
| 1 | M1 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | M2 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | P1 | 220/287 (77%) | 199 (90%) | 21 (10%) | 0 | 100 | 100 |
| 1 | P2 | 220/287 (77%) | 199 (90%) | 21 (10%) | 0 | 100 | 100 |
| 1 | S1 | 220/287 (77%) | 199 (90%) | 21 (10%) | 0 | 100 | 100 |
| 1 | S2 | 220/287 (77%) | 199 (90%) | 21 (10%) | 0 | 100 | 100 |
| 1 | V1 | 220/287 (77%) | 199 (90%) | 21 (10%) | 0 | 100 | 100 |
| 1 | V2 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | Y2 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | b2 | 220/287 (77%) | 199 (90%) | 21 (10%) | 0 | 100 | 100 |
| 1 | e2 | 220/287 (77%) | 199 (90%) | 21 (10%) | 0 | 100 | 100 |
| 1 | h2 | 220/287 (77%) | 199 (90%) | 21 (10%) | 0 | 100 | 100 |
| 1 | k2 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | n2 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | q2 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | t2 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 1 | w2 | 220/287 (77%) | 200 (91%) | 20 (9%) | 0 | 100 | 100 |
| 2 | B1 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | B2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | E1 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | E2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | H1 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | H2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | K1 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | K2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | N1 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | N2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | Q1 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | Q2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | T1 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 2 | T2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | W1 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | W2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | Z2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | c2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | f2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | i2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | l2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | o2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | r2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | u2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 2 | x2 | 232/260 (89%) | 204 (88%) | 25 (11%) | 3 (1%) | 10 | 42 |
| 3 | C1 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | C2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | F1 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | F2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | I1 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | I2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | L1 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | L2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | O1 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | O2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | R1 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | R2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | U1 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | U2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | X1 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | X2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | a2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | d2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | g2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 3 | j2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | m2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | p2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | s2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | v2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| 3 | y2 | 212/239 (89%) | 197 (93%) | 15 (7%) | 0 | 100 | 100 |
| All | All | 16600/19650 (84%) | 15015 (90%) | 1510 (9%) | 75 (0%) | 27 | 62 |

5 of 75 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 2 | W1 | 2060 | THR |
| 2 | W1 | 2149 | GLU |
| 2 | T1 | 2060 | THR |
| 2 | T1 | 2149 | GLU |
| 2 | Q1 | 2060 | THR |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | A1 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | A2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | D1 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | D2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | G1 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | G2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | J1 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | J2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | M1 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | M2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1 | P1 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | P2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | S1 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | S2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | V1 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | V2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | Y2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | b2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | e2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | h2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | k2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | n2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | q2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | t2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 1 | w2 | 182/259 (70%) | 182 (100%) | 0 | 100 | 100 |
| 2 | B1 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | B2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | E1 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | E2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | H1 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | H2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | K1 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | K2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | N1 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | N2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | Q1 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | Q2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | T1 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | T2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | W1 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | W2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|------------|----------|-------------|-----|
| 2 | Z2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | c2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | f2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | i2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | l2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | o2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | r2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | u2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 2 | x2 | 193/221 (87%) | 193 (100%) | 0 | 100 | 100 |
| 3 | C1 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | C2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | F1 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | F2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | I1 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | I2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | L1 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | L2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | O1 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | O2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | R1 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | R2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | U1 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | U2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | X1 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | X2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | a2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | d2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | g2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | j2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | m2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | p2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 3 | s2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | v2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| 3 | y2 | 184/209 (88%) | 184 (100%) | 0 | 100 | 100 |
| All | All | 13975/17225 (81%) | 13975 (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. 5 of 91 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 3 | a2 | 3110 | HIS |
| 3 | R2 | 3198 | ASN |
| 3 | a2 | 3198 | ASN |
| 3 | U2 | 3154 | HIS |
| 3 | O2 | 3154 | HIS |

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 ⓘ

There are no chain breaks in this entry.

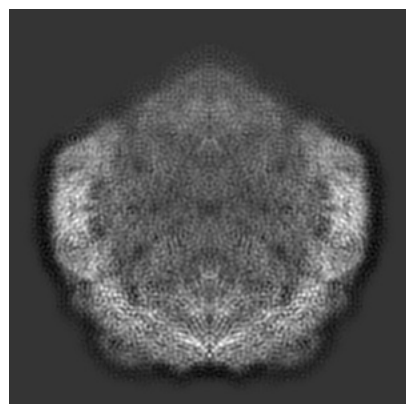
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0217. These allow visual inspection of the internal detail of the map and identification of artifacts.

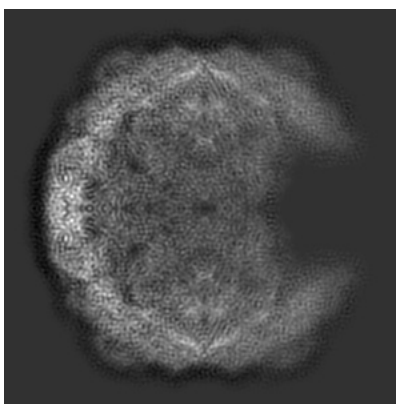
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

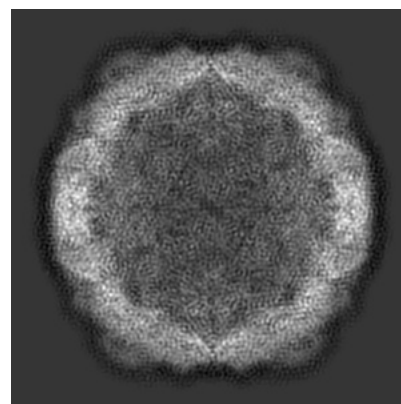
6.1.1 Primary map



X

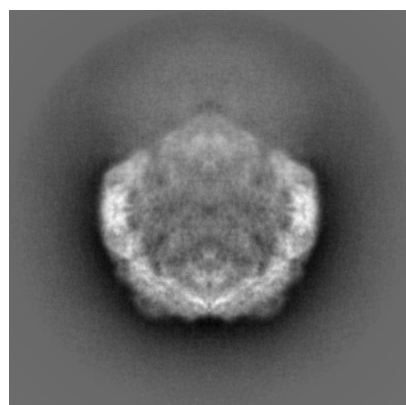


Y

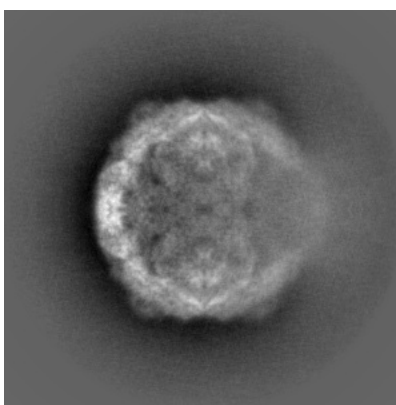


Z

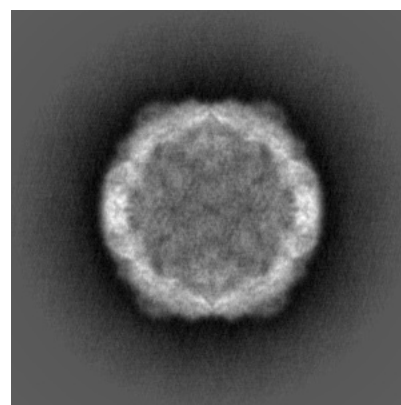
6.1.2 Raw map



X



Y



Z

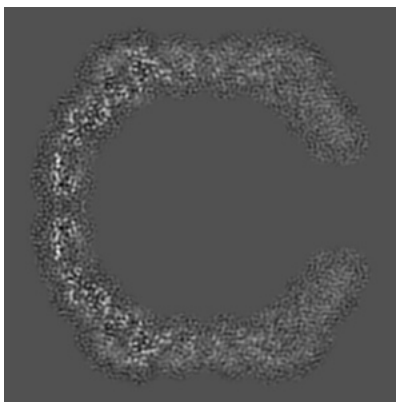
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

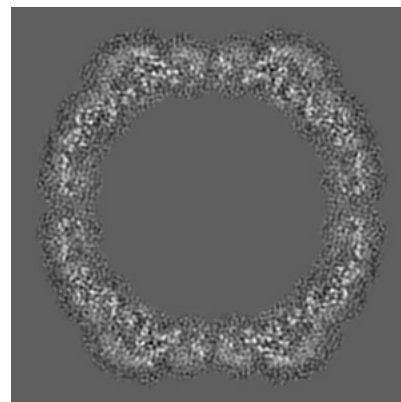
6.2.1 Primary map



X Index: 175

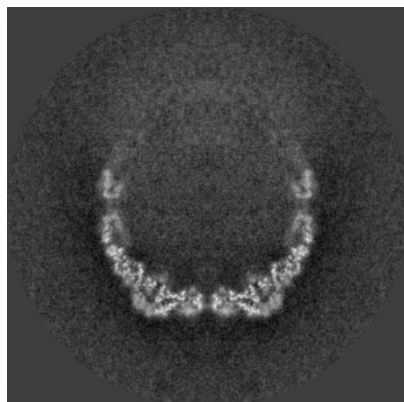


Y Index: 175

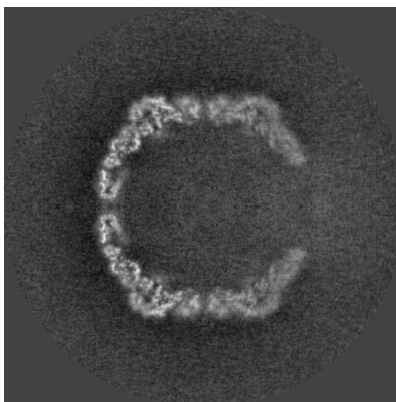


Z Index: 175

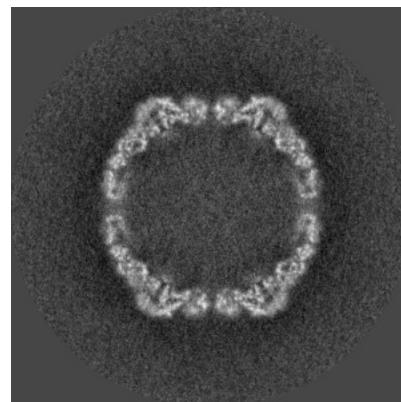
6.2.2 Raw map



X Index: 256



Y Index: 256

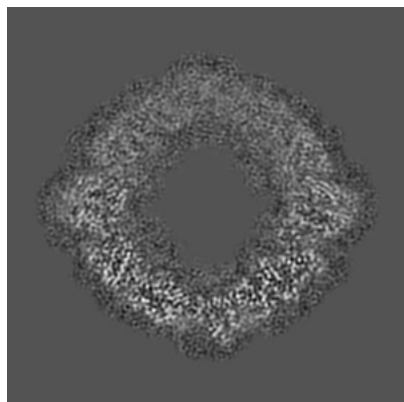


Z Index: 256

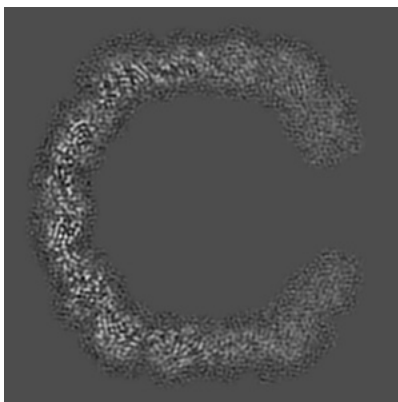
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

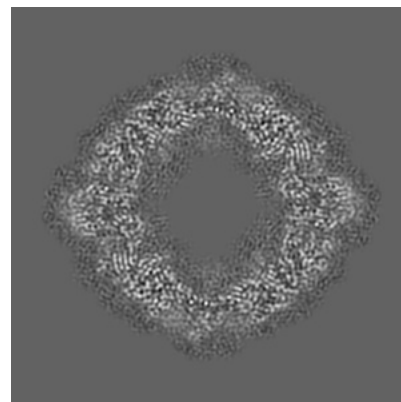
6.3.1 Primary map



X Index: 263

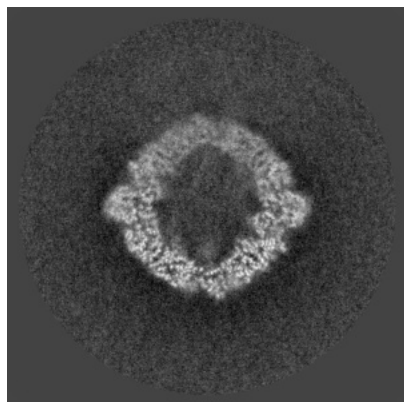


Y Index: 159

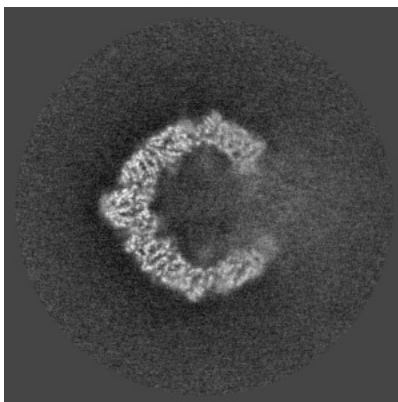


Z Index: 85

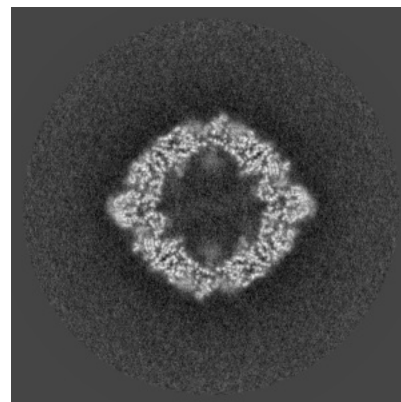
6.3.2 Raw map



X Index: 346



Y Index: 168

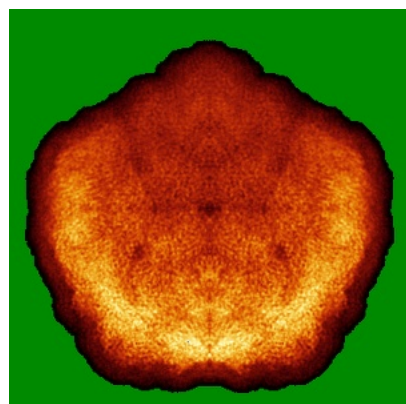


Z Index: 166

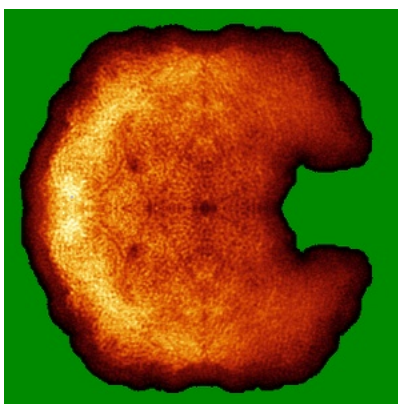
The images above show the largest variance slices of the map in three orthogonal directions.

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

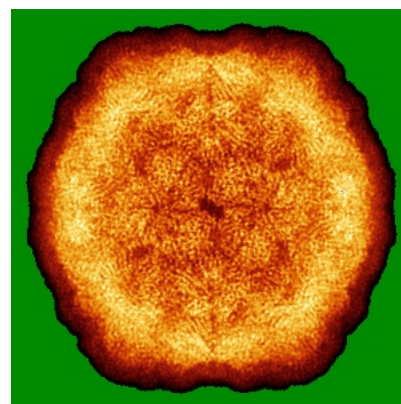
6.4.1 Primary map



X

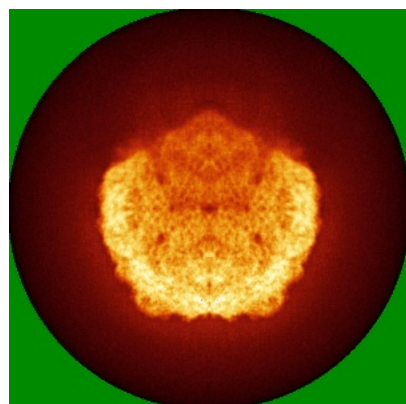


Y

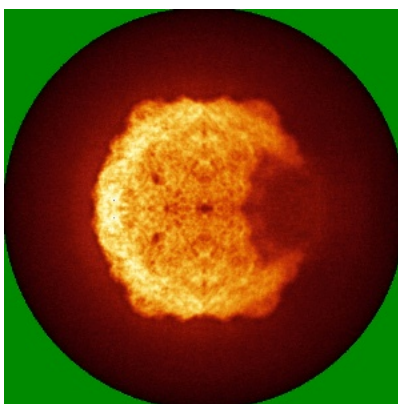


Z

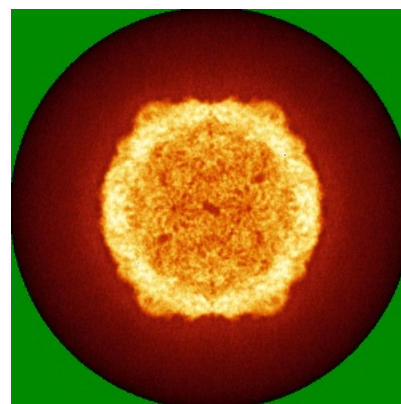
6.4.2 Raw map



X



Y

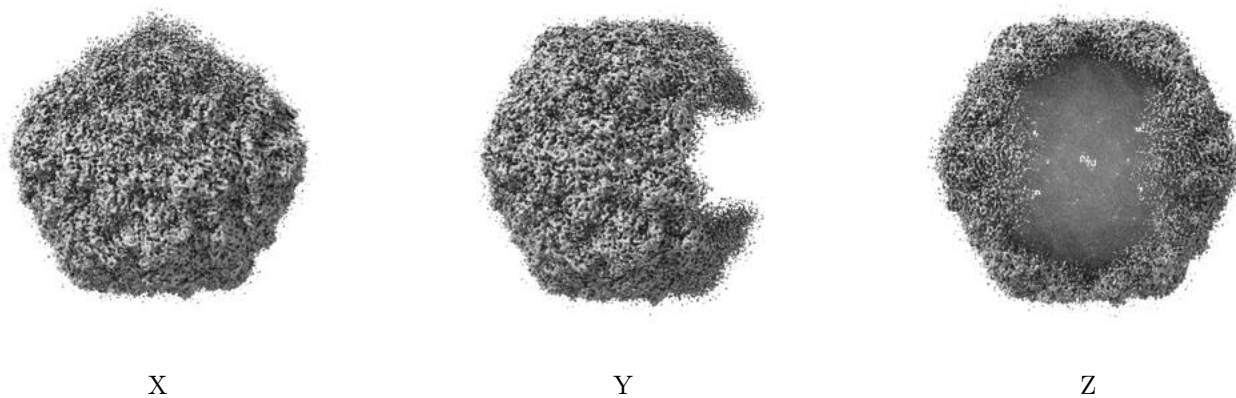


Z

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

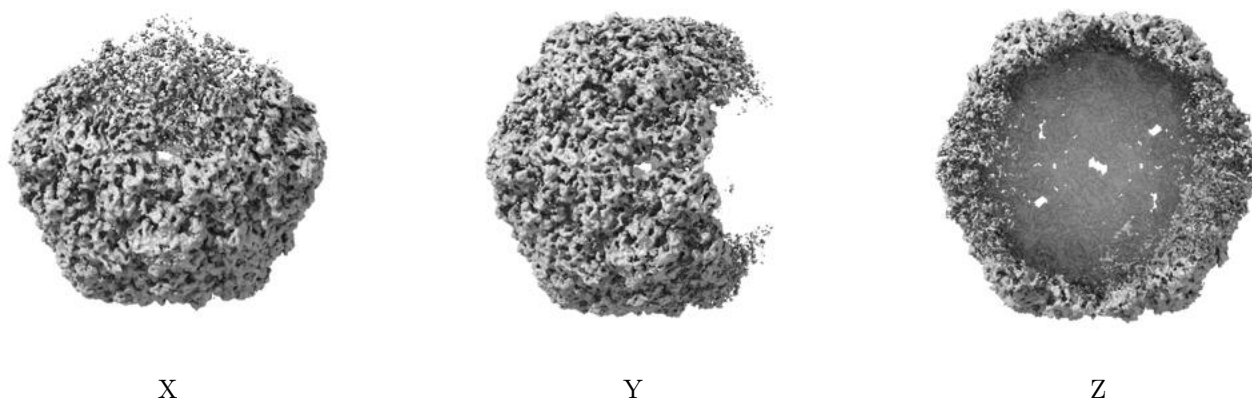
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

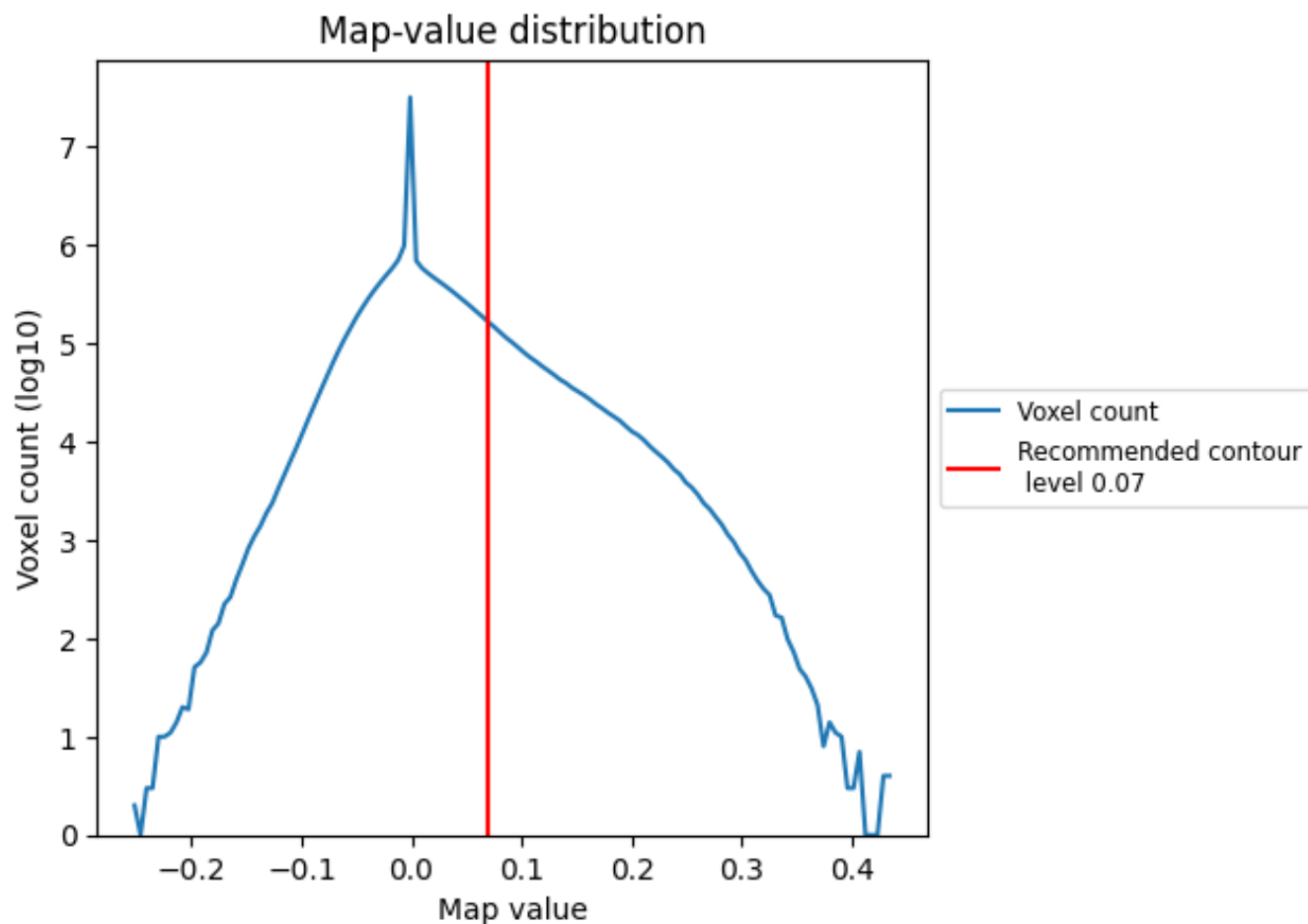
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

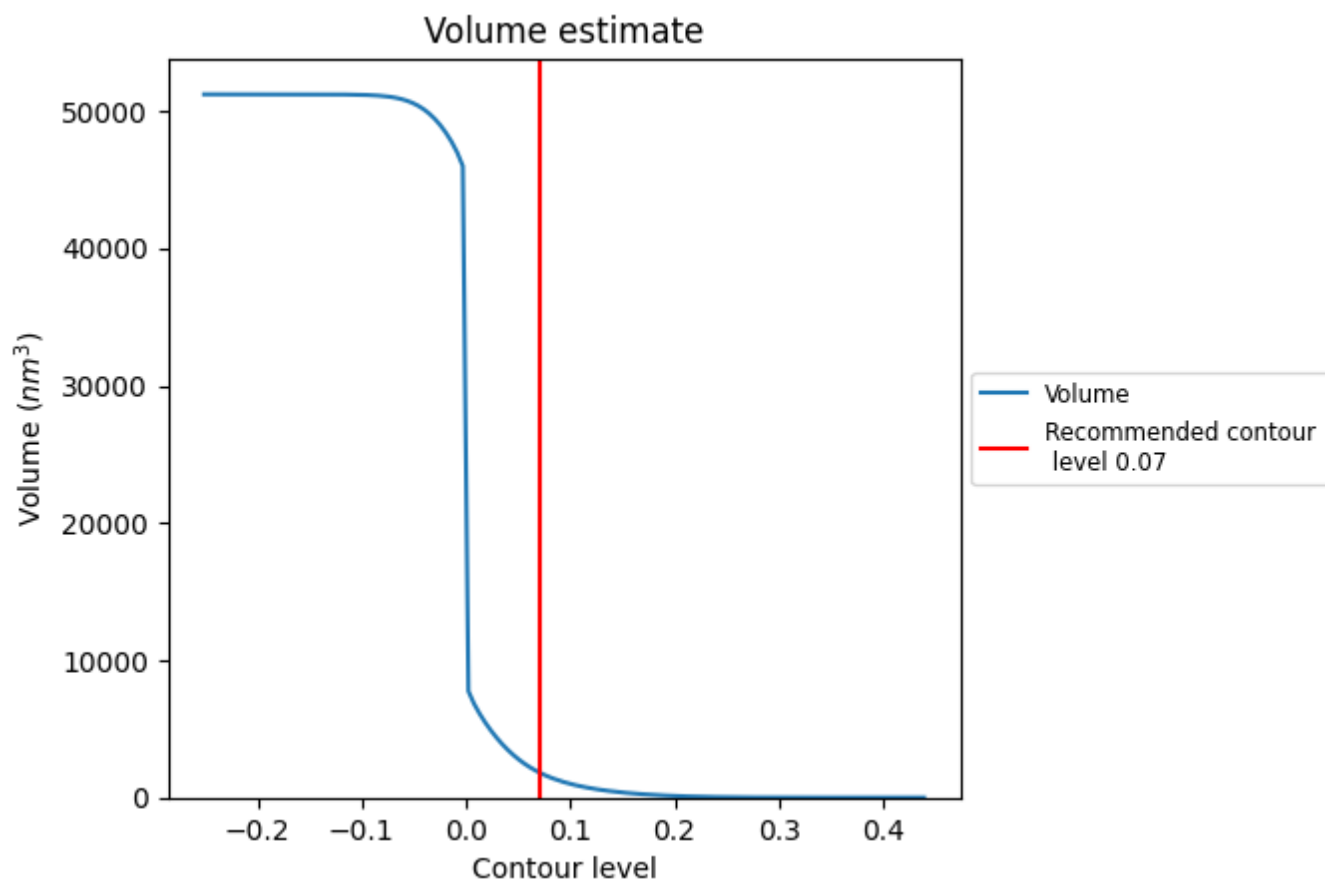
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

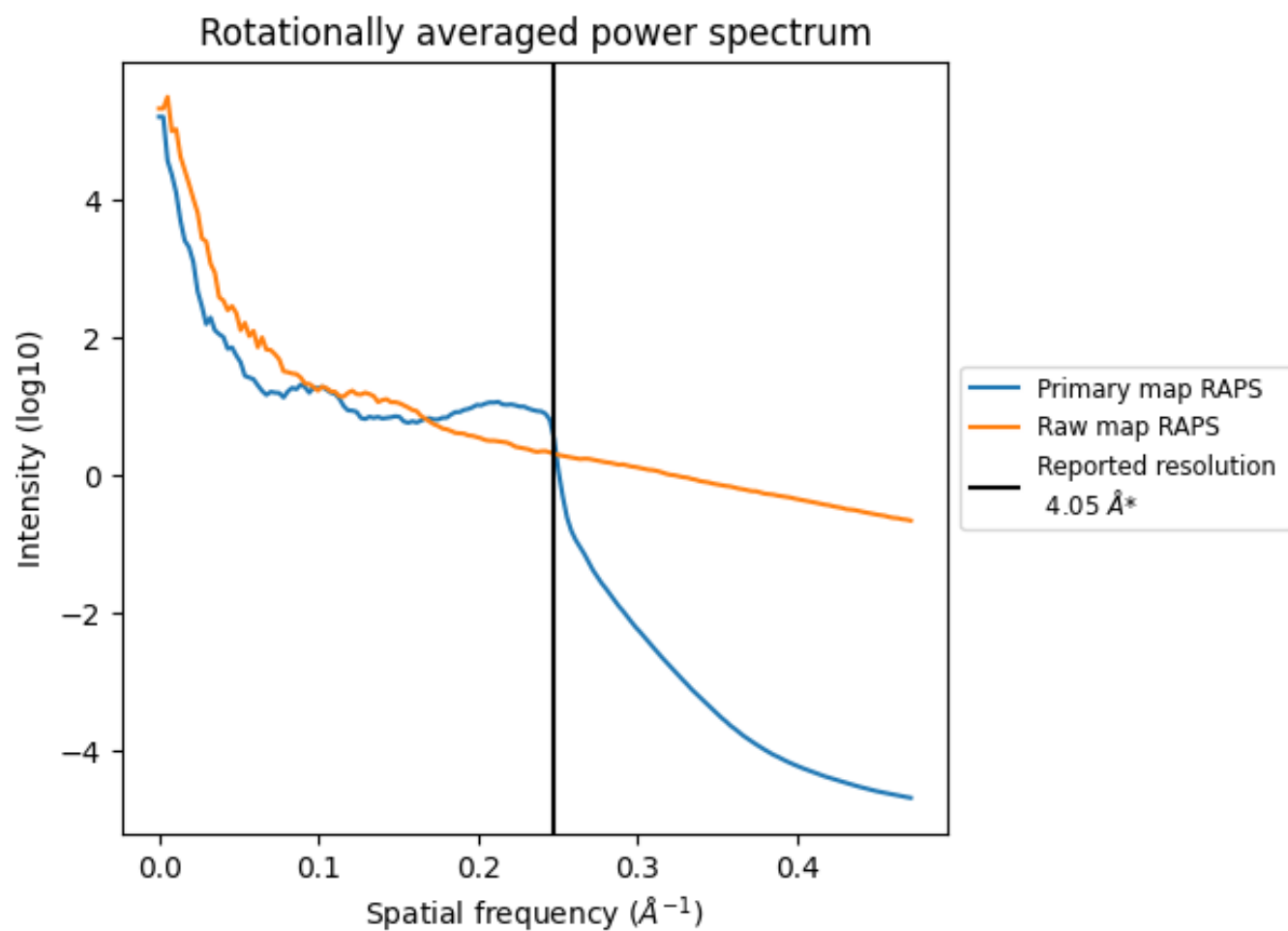
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1838 nm³; this corresponds to an approximate mass of 1661 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 ⓘ

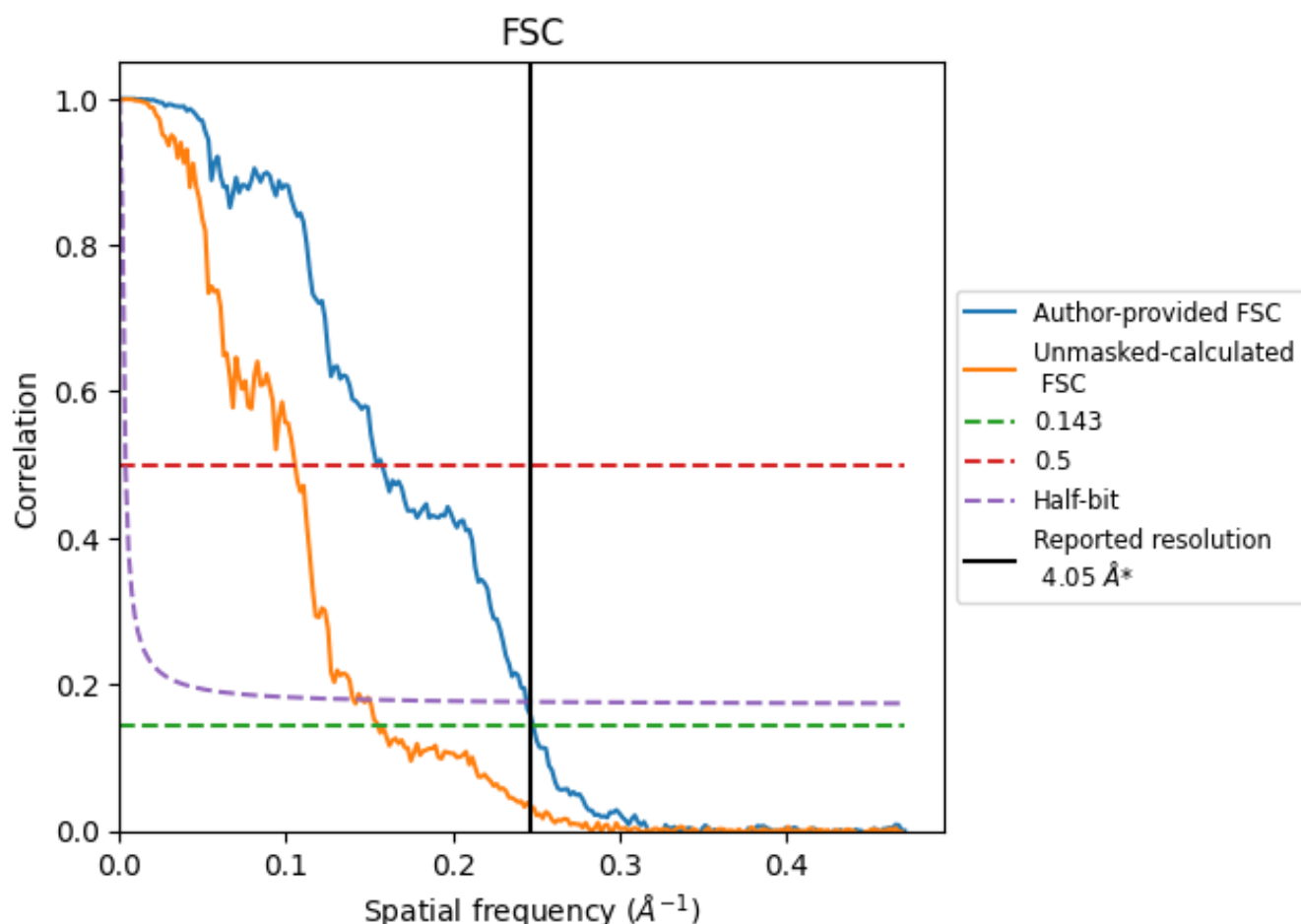


*Reported resolution corresponds to spatial frequency of 0.247 Å⁻¹

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 0.247 Å⁻¹

8.2 Resolution estimates [i](#)

| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.05 | - | - |
| Author-provided FSC curve | 4.03 | 6.48 | 4.10 |
| Unmasked-calculated* | 6.44 | 9.49 | 7.13 |

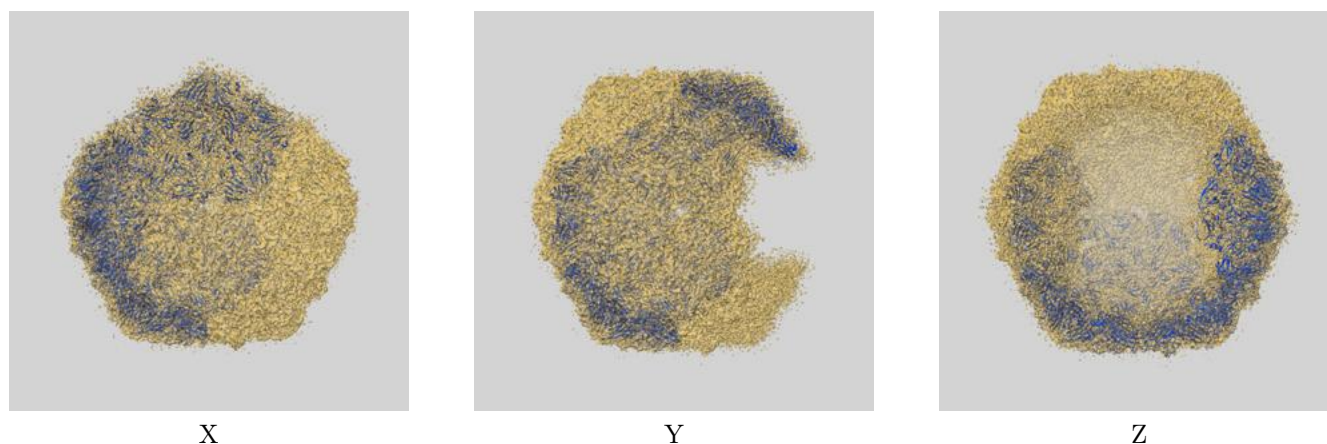
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.44 differs from the reported value 4.05 by more than 10 %

9 Map-model fit [i](#)

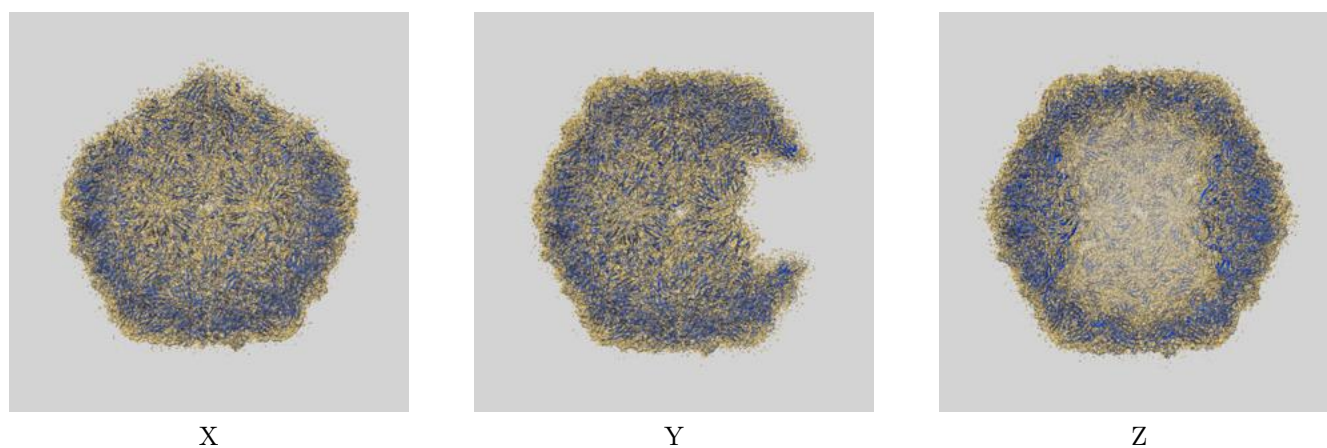
This section contains information regarding the fit between EMDB map EMD-0217 and PDB model 6HHT. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

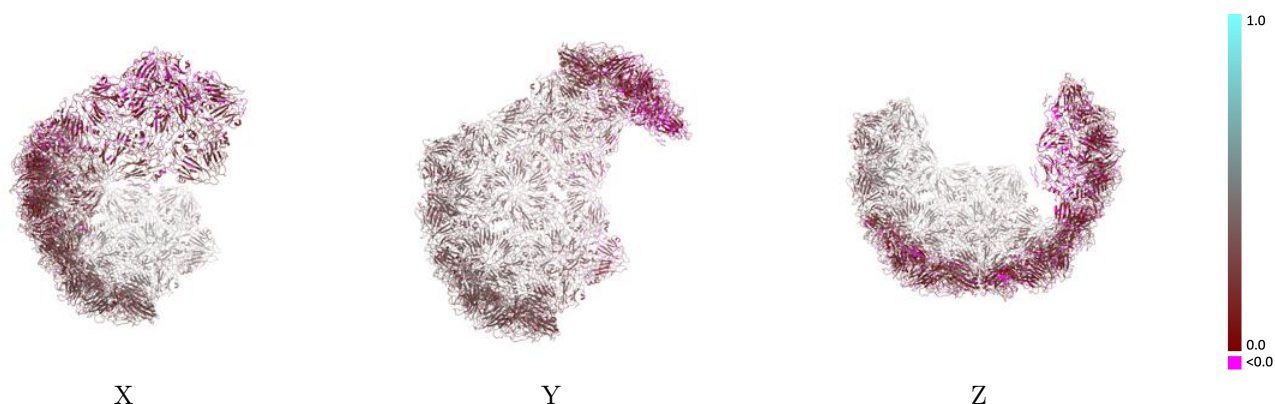


9.1.2 Map-model assembly overlay [i](#)



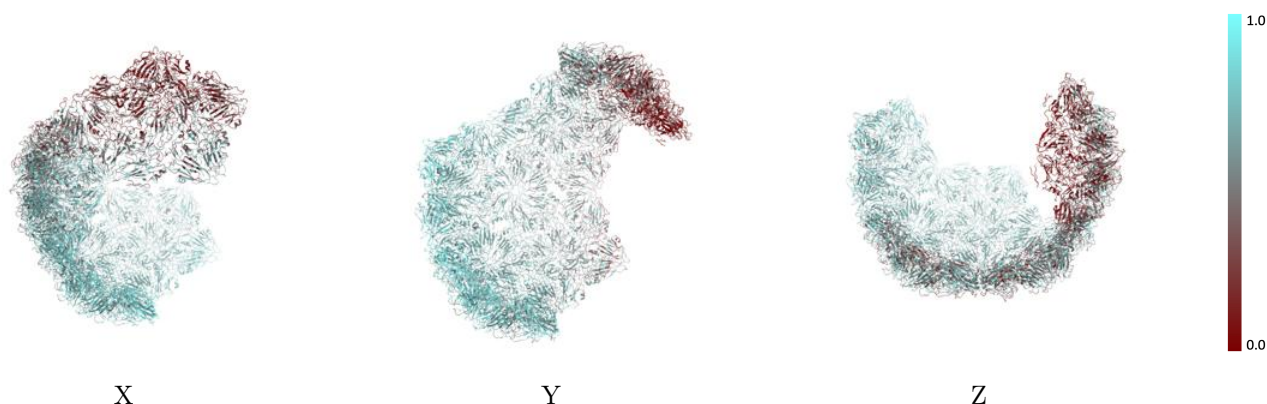
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



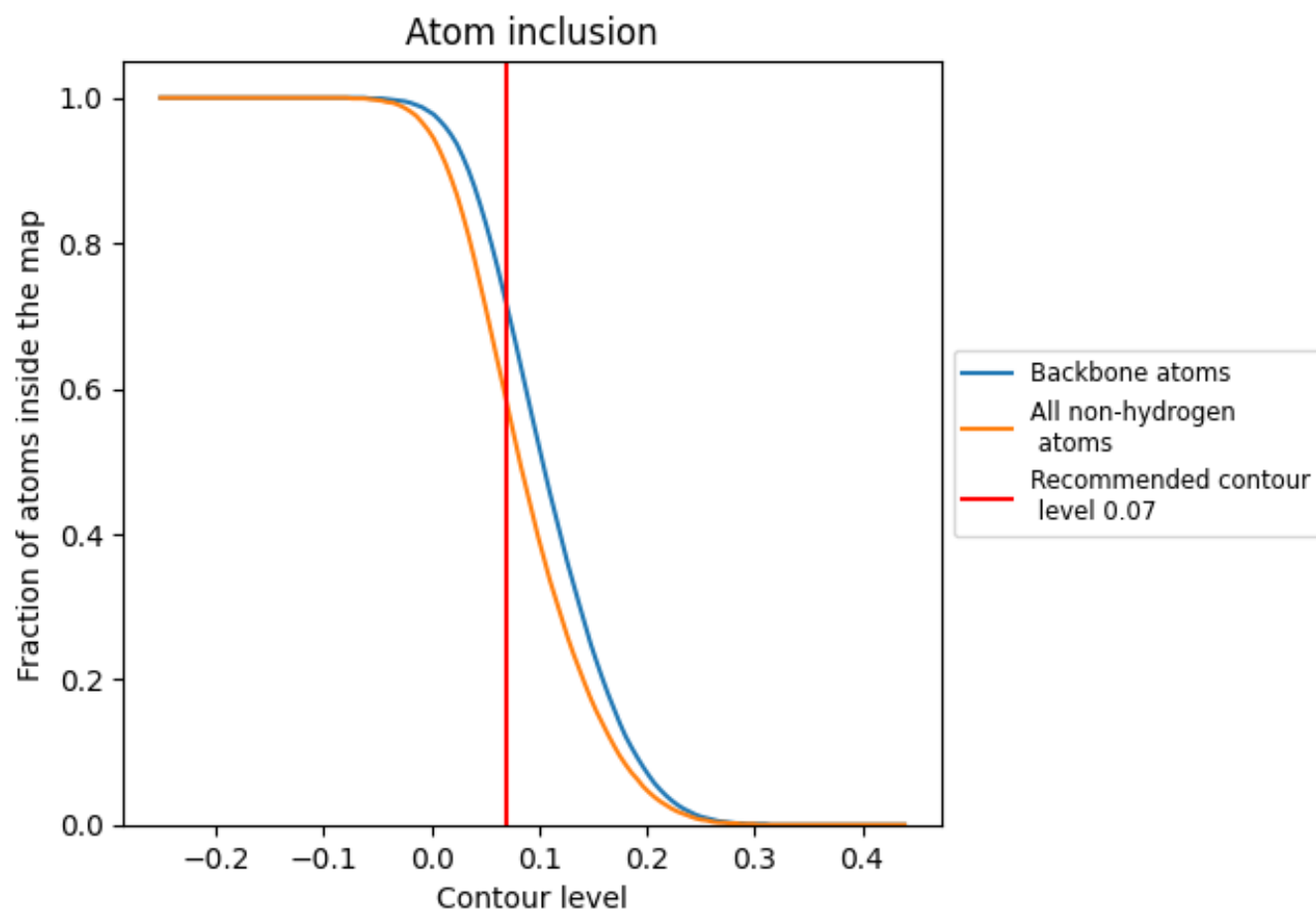
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



















































































The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.5810 |  0.2530 |
| A1 |  0.5440 |  0.2090 |
| A2 |  0.2680 |  0.1100 |
| B1 |  0.4540 |  0.1680 |
| B2 |  0.3070 |  0.1490 |
| C1 |  0.4330 |  0.1480 |
| C2 |  0.2250 |  0.1140 |
| D1 |  0.7300 |  0.3280 |
| D2 |  0.2160 |  0.0950 |
| E1 |  0.7430 |  0.3340 |
| E2 |  0.1210 |  0.0750 |
| F1 |  0.7400 |  0.3420 |
| F2 |  0.1110 |  0.0810 |
| G1 |  0.7340 |  0.3220 |
| G2 |  0.7010 |  0.3370 |
| H1 |  0.7250 |  0.3350 |
| H2 |  0.6630 |  0.3120 |
| I1 |  0.7280 |  0.3200 |
| I2 |  0.6930 |  0.3360 |
| J1 |  0.3970 |  0.1770 |
| J2 |  0.4010 |  0.1810 |
| K1 |  0.4980 |  0.2370 |
| K2 |  0.5070 |  0.2400 |
| L1 |  0.4790 |  0.2390 |
| L2 |  0.4780 |  0.2150 |
| M1 |  0.7410 |  0.3260 |
| M2 |  0.7280 |  0.3520 |
| N1 |  0.7340 |  0.3380 |
| N2 |  0.7200 |  0.3360 |
| O1 |  0.7540 |  0.3440 |
| O2 |  0.7200 |  0.3390 |
| P1 |  0.7170 |  0.3070 |
| P2 |  0.5980 |  0.2290 |
| Q1 |  0.6790 |  0.2690 |
| Q2 |  0.5950 |  0.2260 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| R1 |  0.6890 |  0.2900 |
| R2 |  0.6350 |  0.2440 |
| S1 |  0.6190 |  0.2430 |
| S2 |  0.6230 |  0.2380 |
| T1 |  0.5830 |  0.2580 |
| T2 |  0.6240 |  0.2460 |
| U1 |  0.6400 |  0.2730 |
| U2 |  0.5800 |  0.2150 |
| V1 |  0.7100 |  0.3080 |
| V2 |  0.2580 |  0.1220 |
| W1 |  0.6990 |  0.3020 |
| W2 |  0.1780 |  0.0930 |
| X1 |  0.7100 |  0.3290 |
| X2 |  0.2720 |  0.1550 |
| Y2 |  0.6610 |  0.2660 |
| Z2 |  0.6820 |  0.2930 |
| a2 |  0.6610 |  0.2980 |
| b2 |  0.5460 |  0.1820 |
| c2 |  0.4920 |  0.1700 |
| d2 |  0.4770 |  0.1500 |
| e2 |  0.7040 |  0.3350 |
| f2 |  0.6840 |  0.3200 |
| g2 |  0.6840 |  0.3170 |
| h2 |  0.5330 |  0.1960 |
| i2 |  0.4570 |  0.1890 |
| j2 |  0.5310 |  0.2020 |
| k2 |  0.6520 |  0.2670 |
| l2 |  0.6850 |  0.2950 |
| m2 |  0.6720 |  0.2870 |
| n2 |  0.7600 |  0.3590 |
| o2 |  0.7550 |  0.3540 |
| p2 |  0.7420 |  0.3560 |
| q2 |  0.5110 |  0.2000 |
| r2 |  0.3900 |  0.1630 |
| s2 |  0.4920 |  0.1970 |
| t2 |  0.6360 |  0.2640 |
| u2 |  0.6470 |  0.2650 |
| v2 |  0.6110 |  0.2450 |
| w2 |  0.7280 |  0.3520 |
| x2 |  0.7360 |  0.3410 |
| y2 |  0.7290 |  0.3440 |