



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 09:32 PM EST

PDB ID : 8FWG  
EMDB ID : EMD-29504  
Title : Structure of neck and portal vertex of Agrobacterium phage Milano, C5 symmetry  
Authors : Sonani, R.R.; Wang, F.; Esteves, N.C.; Kelly, R.J.; Sebastian, A.; Kreutzberger, M.A.B.; Leiman, P.G.; Scharf, B.E.; Egelman, E.H.  
Deposited on : 2023-01-22  
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

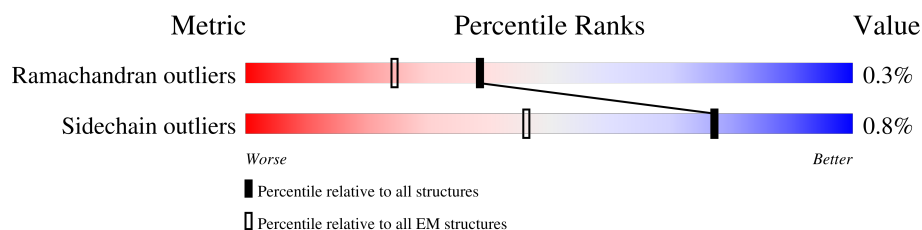
EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 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 3.45 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) |
|-----------------------|-----------------------------|-----------------------------|
| 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | a1    | 38     |                  |
| 1   | a2    | 38     |                  |
| 1   | a5    | 38     |                  |
| 1   | a6    | 38     |                  |
| 1   | a7    | 38     |                  |
| 1   | b1    | 38     |                  |
| 1   | b2    | 38     |                  |
| 1   | b5    | 38     |                  |
| 1   | b6    | 38     |                  |



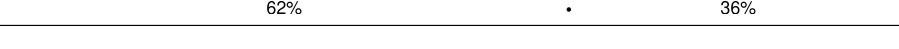
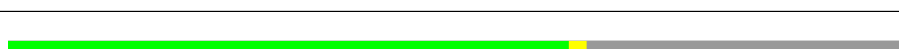



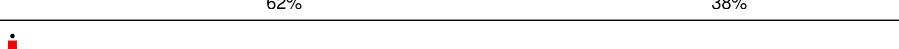



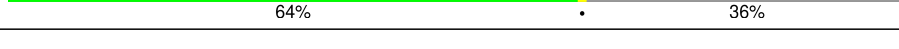

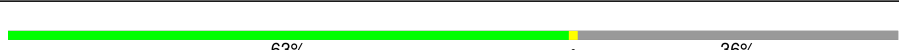


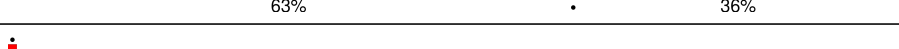







*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | b7    | 38     |    |
| 1   | c     | 38     |    |
| 1   | d     | 38     |    |
| 1   | d1    | 38     |    |
| 1   | d2    | 38     |    |
| 1   | d5    | 38     |    |
| 1   | d6    | 38     |    |
| 1   | d7    | 38     |    |
| 1   | e     | 38     |    |
| 1   | e1    | 38     |    |
| 1   | e2    | 38     |    |
| 1   | e5    | 38     |   |
| 1   | e6    | 38     |  |
| 1   | e7    | 38     |  |
| 1   | f     | 38     |  |
| 1   | g     | 38     |  |
| 2   | f1    | 217    |  |
| 2   | f2    | 217    |  |
| 2   | f5    | 217    |  |
| 2   | f6    | 217    |  |
| 2   | f7    | 217    |  |
| 3   | g1    | 465    |  |
| 3   | g2    | 465    |  |
| 3   | g5    | 465    |  |
| 3   | g6    | 465    |  |


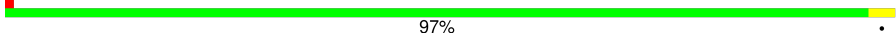
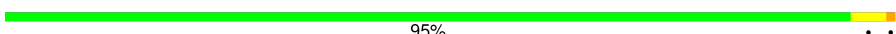
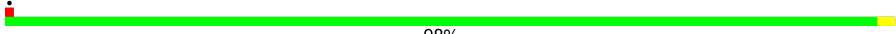


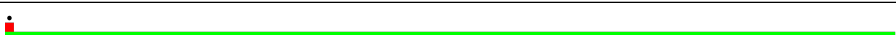
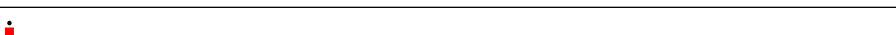
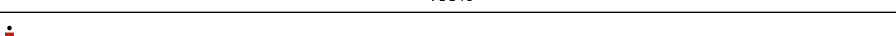
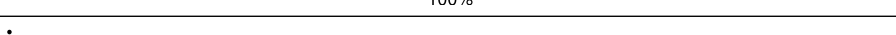
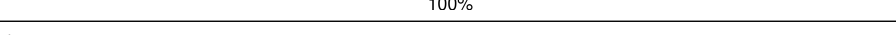
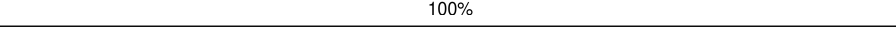
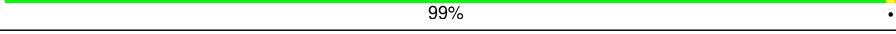
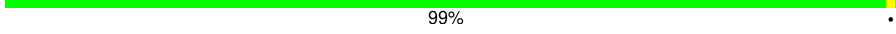
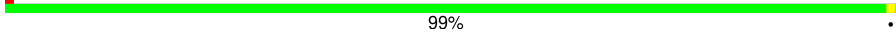
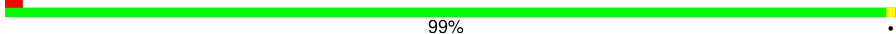
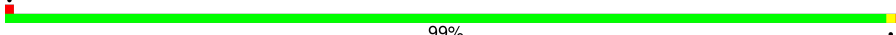
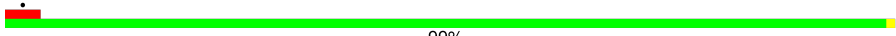





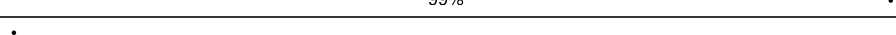
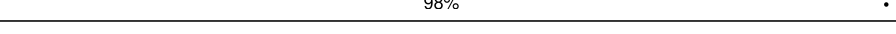
Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | g7    | 465    |    |
| 3   | h1    | 465    |    |
| 3   | h2    | 465    |    |
| 3   | h5    | 465    |    |
| 3   | h6    | 465    |    |
| 3   | h7    | 465    |    |
| 3   | k1    | 465    |    |
| 3   | k2    | 465    |    |
| 3   | k5    | 465    |    |
| 3   | k6    | 465    |   |
| 3   | k7    | 465    |  |
| 3   | n1    | 465    |  |
| 3   | n2    | 465    |  |
| 3   | n5    | 465    |  |
| 3   | n6    | 465    |  |
| 3   | n7    | 465    |  |
| 3   | o1    | 465    |  |
| 3   | o2    | 465    |  |
| 3   | o5    | 465    |  |
| 3   | o6    | 465    |  |
| 3   | o7    | 465    |  |
| 3   | r1    | 465    |  |
| 3   | r2    | 465    |  |
| 3   | r5    | 465    |  |
| 3   | r6    | 465    |  |

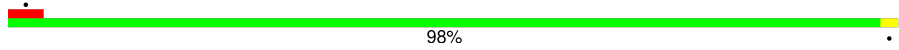
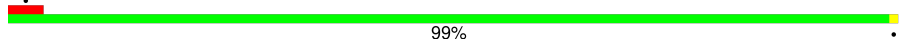
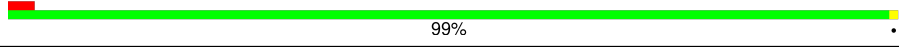
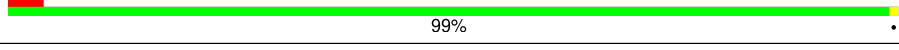
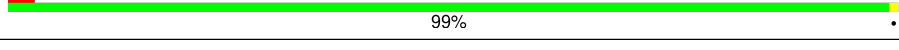
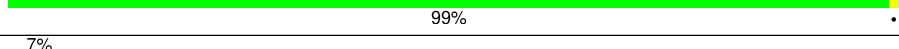
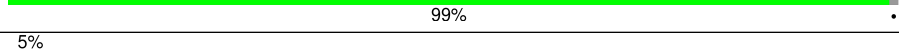
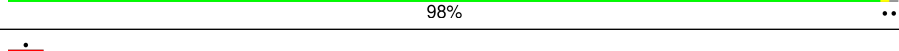
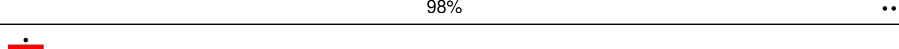
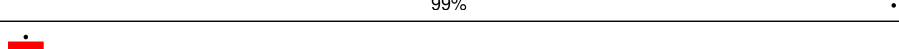
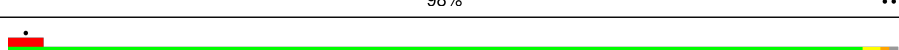
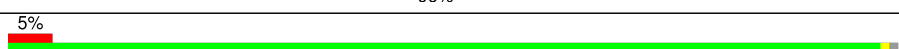
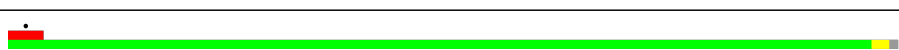
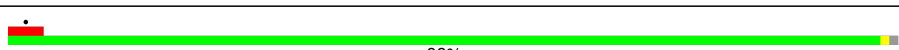
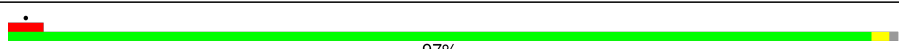
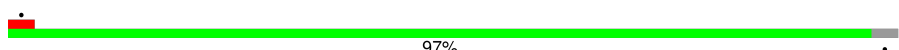

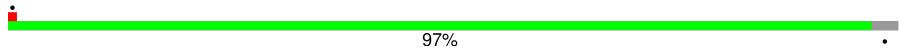
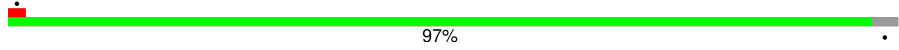
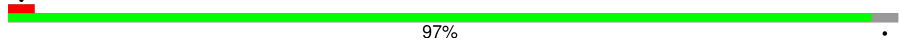
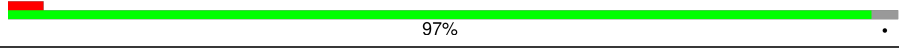
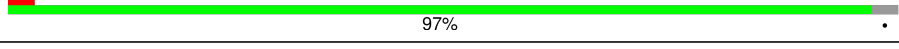
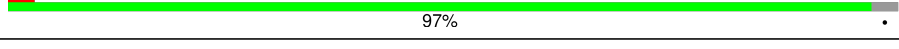
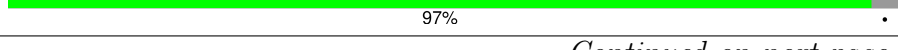

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | r7    | 465    |    |
| 4   | l1    | 137    |    |
| 4   | l2    | 137    |    |
| 4   | l5    | 137    |    |
| 4   | l6    | 137    |    |
| 4   | l7    | 137    |    |
| 4   | m1    | 137    |    |
| 4   | m2    | 137    |    |
| 4   | m5    | 137    |    |
| 4   | m6    | 137    |    |
| 4   | m7    | 137    |    |
| 4   | p1    | 137    |    |
| 4   | p2    | 137    |   |
| 4   | p5    | 137    |  |
| 4   | p6    | 137    |  |
| 4   | p7    | 137    |  |
| 4   | q1    | 137    |  |
| 4   | q2    | 137    |  |
| 4   | q5    | 137    |  |
| 4   | q6    | 137    |  |
| 4   | q7    | 137    |  |
| 4   | s1    | 137    |  |
| 4   | s2    | 137    |  |
| 4   | s5    | 137    |  |
| 4   | s6    | 137    |  |

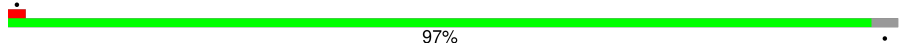
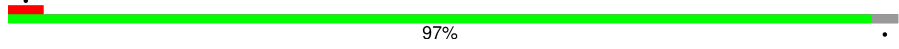
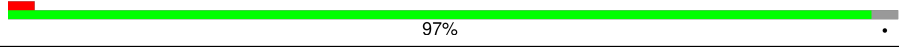
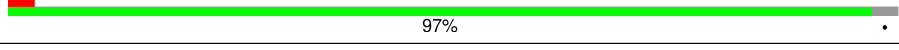
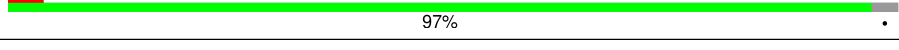
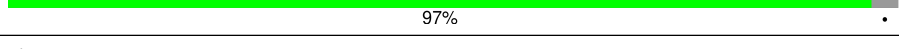
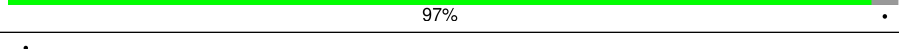
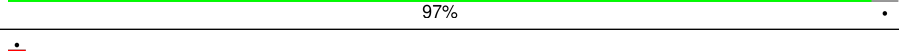
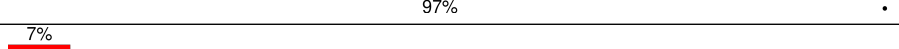
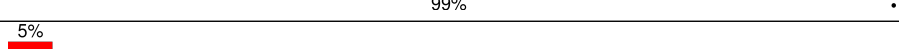
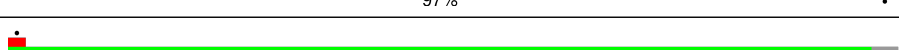
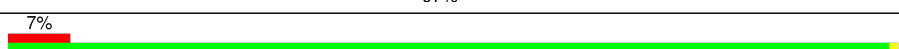
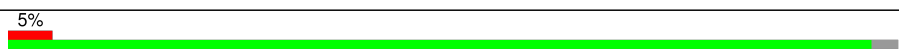
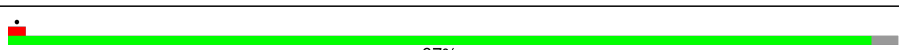
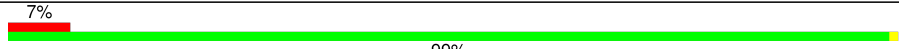
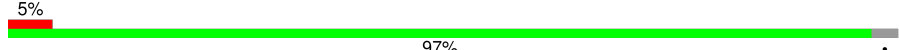

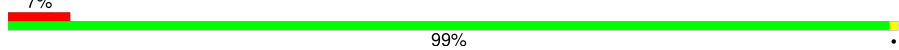
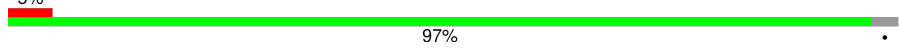
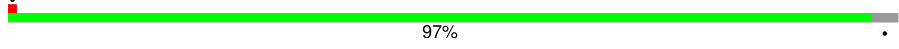
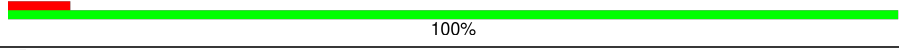
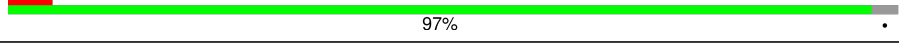
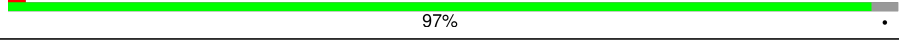
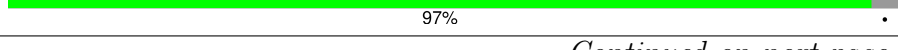

*Continued on next page...*

Continued from previous page...

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 4   | s7    | 137    |  98%     |
| 4   | t1    | 137    |  99%     |
| 4   | t2    | 137    |  99%     |
| 4   | t5    | 137    |  99%     |
| 4   | t6    | 137    |  99%     |
| 4   | t7    | 137    |  99%     |
| 4   | u1    | 137    |  7%99%   |
| 4   | u2    | 137    |  5%98%   |
| 4   | u5    | 137    |  98%     |
| 4   | u6    | 137    |  99%     |
| 4   | u7    | 137    |  98%     |
| 4   | v1    | 137    |  96%   |
| 4   | v2    | 137    |  5%98% |
| 4   | v5    | 137    |  97%   |
| 4   | v6    | 137    |  98%   |
| 4   | v7    | 137    |  97%   |
| 5   | 03    | 230    |  97%   |
| 5   | 13    | 230    |  97%   |
| 5   | 23    | 230    |  97%   |
| 5   | 33    | 230    |  97%   |
| 5   | 43    | 230    |  97%   |
| 5   | 53    | 230    |  97%   |
| 5   | 63    | 230    |  97%   |
| 5   | 73    | 230    |  97%   |
| 5   | 83    | 230    |  97%   |

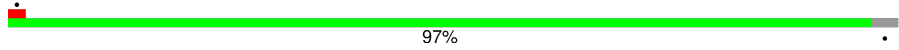
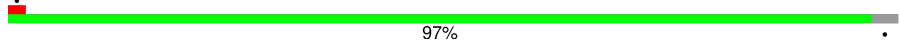
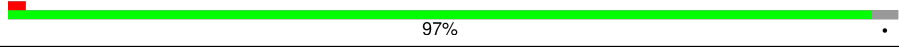
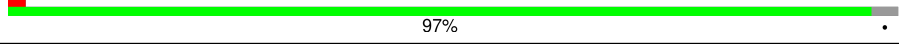
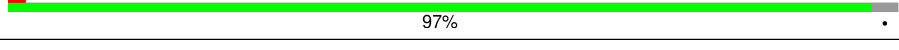
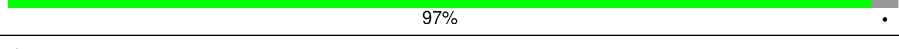
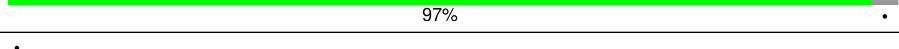
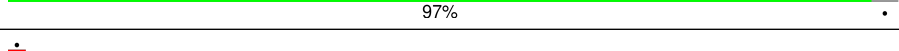
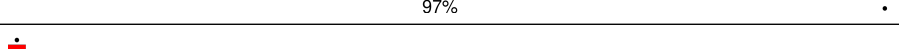
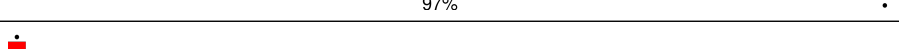
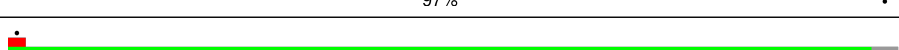
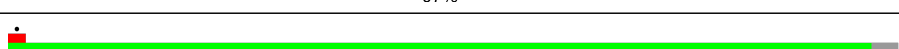
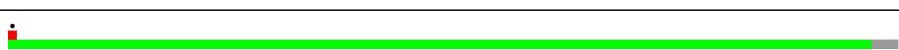
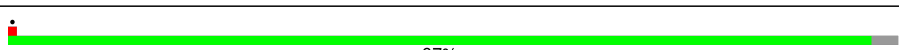
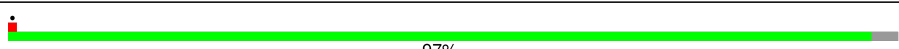
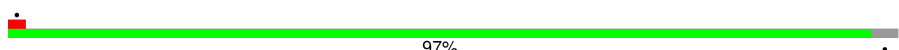

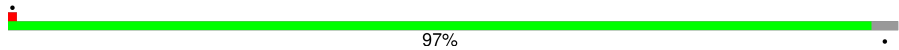
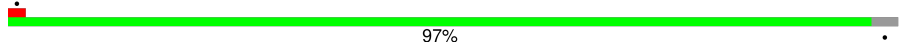
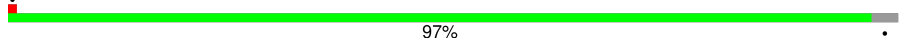
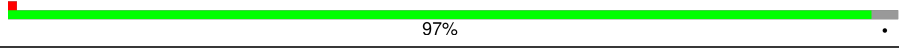
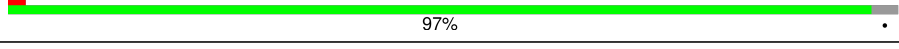
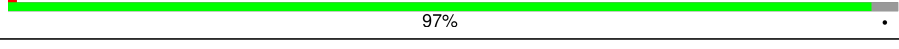
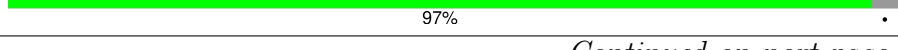

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 5   | 93    | 230    |  97%    |
| 5   | A3    | 230    |  97%    |
| 5   | B3    | 230    |  97%    |
| 5   | C3    | 230    |  97%    |
| 5   | D3    | 230    |  97%    |
| 5   | E3    | 230    |  97%    |
| 5   | F3    | 230    |  97%    |
| 5   | G3    | 230    |  97%    |
| 5   | J3    | 230    |  97%    |
| 5   | K3    | 230    |  99%    |
| 5   | L3    | 230    |  97%    |
| 5   | M3    | 230    |  97%  |
| 5   | N3    | 230    |  99%  |
| 5   | O3    | 230    |  97%  |
| 5   | P3    | 230    |  97%  |
| 5   | Q3    | 230    |  99%  |
| 5   | R3    | 230    |  97%  |
| 5   | S3    | 230    |  97%  |
| 5   | T3    | 230    |  99%  |
| 5   | U3    | 230    |  97%  |
| 5   | V3    | 230    |  97%  |
| 5   | W3    | 230    |  100% |
| 5   | X3    | 230    |  97%  |
| 5   | Y3    | 230    |  97%  |
| 5   | Z3    | 230    |  97%  |



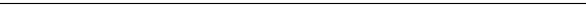

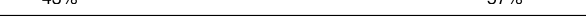

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 5   | a3    | 230    |    |
| 5   | b3    | 230    |    |
| 5   | c3    | 230    |    |
| 5   | d3    | 230    |    |
| 5   | e3    | 230    |    |
| 5   | f3    | 230    |    |
| 5   | g3    | 230    |    |
| 5   | h3    | 230    |    |
| 5   | i3    | 230    |    |
| 5   | j3    | 230    |    |
| 5   | k3    | 230    |    |
| 5   | l3    | 230    |  |
| 5   | m3    | 230    |  |
| 5   | n3    | 230    |  |
| 5   | o3    | 230    |  |
| 5   | p3    | 230    |  |
| 5   | q3    | 230    |  |
| 5   | r3    | 230    |  |
| 5   | s3    | 230    |  |
| 5   | t3    | 230    |  |
| 5   | u3    | 230    |  |
| 5   | v3    | 230    |  |
| 5   | w3    | 230    |  |
| 5   | x3    | 230    |  |
| 5   | y3    | 230    |  |

*Continued on next page...*



| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 5   | z3    | 230    |  <div>97%</div>    |
| 6   | A4    | 202    |  <div>43%57%</div> |
| 6   | B4    | 202    |  <div>42%57%</div> |
| 6   | C4    | 202    |  <div>42%57%</div> |
| 6   | D4    | 202    |  <div>40%57%</div> |
| 6   | E4    | 202    |  <div>42%57%</div> |

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 221120 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 Linking protein 2, gp128.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | a1    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | b1    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | d1    | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 246   | 155 | 46 | 40 | 5 |         |       |
| 1   | e1    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | a2    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | b2    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | d2    | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 246   | 155 | 46 | 40 | 5 |         |       |
| 1   | e2    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | a5    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | b5    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | d5    | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 246   | 155 | 46 | 40 | 5 |         |       |
| 1   | e5    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | a6    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | b6    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | d6    | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 246   | 155 | 46 | 40 | 5 |         |       |
| 1   | e6    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | a7    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | b7    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | d7    | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 246   | 155 | 46 | 40 | 5 |         |       |
| 1   | e7    | 28       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 209   | 131 | 40 | 33 | 5 |         |       |
| 1   | c     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 246   | 155 | 46 | 40 | 5 |         |       |
| 1   | d     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 246   | 155 | 46 | 40 | 5 |         |       |
| 1   | e     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 246   | 155 | 46 | 40 | 5 |         |       |
| 1   | f     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 246   | 155 | 46 | 40 | 5 |         |       |
| 1   | g     | 34       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 246   | 155 | 46 | 40 | 5 |         |       |

- Molecule 2 is a protein called Linking protein 1, gp16.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 2   | f1    | 20       | Total | C  | N  | O  | S | 0       | 0     |
|     |       |          | 140   | 88 | 27 | 23 | 2 |         |       |
| 2   | f2    | 20       | Total | C  | N  | O  | S | 0       | 0     |
|     |       |          | 140   | 88 | 27 | 23 | 2 |         |       |
| 2   | f5    | 20       | Total | C  | N  | O  | S | 0       | 0     |
|     |       |          | 140   | 88 | 27 | 23 | 2 |         |       |
| 2   | f6    | 20       | Total | C  | N  | O  | S | 0       | 0     |
|     |       |          | 140   | 88 | 27 | 23 | 2 |         |       |
| 2   | f7    | 20       | Total | C  | N  | O  | S | 0       | 0     |
|     |       |          | 140   | 88 | 27 | 23 | 2 |         |       |

- Molecule 3 is a protein called Major capsid protein, gp9.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | g1    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | h1    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | k1    | 288      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2257  | 1430 | 386 | 425 | 16 |         |       |
| 3   | n1    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | o1    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | r1    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | g2    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | h2    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | k2    | 288      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2257  | 1430 | 386 | 425 | 16 |         |       |
| 3   | n2    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | o2    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | r2    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | g5    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | h5    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | k5    | 288      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2257  | 1430 | 386 | 425 | 16 |         |       |
| 3   | n5    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | o5    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | r5    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | g6    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | h6    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | k6    | 288      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2257  | 1430 | 386 | 425 | 16 |         |       |
| 3   | n6    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | o6    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | r6    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | g7    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | h7    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | k7    | 288      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2257  | 1430 | 386 | 425 | 16 |         |       |
| 3   | n7    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | o7    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |
| 3   | r7    | 299      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2337  | 1483 | 397 | 441 | 16 |         |       |

- Molecule 4 is a protein called Minor capsid protein, gp10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | l1    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | m1    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | p1    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | q1    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | s1    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | t1    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | u1    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 649 | 156 | 199 | 7 |         |       |
| 4   | v1    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 649 | 156 | 199 | 7 |         |       |
| 4   | l2    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | m2    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | p2    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | q2    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | s2    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | t2    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | u2    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 649 | 156 | 199 | 7 |         |       |
| 4   | v2    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 649 | 156 | 199 | 7 |         |       |
| 4   | l5    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | m5    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | p5    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | q5    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | s5    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | t5    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | u5    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 649 | 156 | 199 | 7 |         |       |
| 4   | v5    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 649 | 156 | 199 | 7 |         |       |
| 4   | l6    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | m6    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | p6    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | q6    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | s6    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | t6    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | u6    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 649 | 156 | 199 | 7 |         |       |
| 4   | v6    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 649 | 156 | 199 | 7 |         |       |
| 4   | l7    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | m7    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | p7    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | q7    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | s7    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | t7    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 655 | 160 | 201 | 7 |         |       |
| 4   | u7    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 649 | 156 | 199 | 7 |         |       |
| 4   | v7    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 649 | 156 | 199 | 7 |         |       |

- Molecule 5 is a protein called Collar sheath protein, gp13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | J3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | K3    | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1723  | 1090 | 287 | 337 | 9 |         |       |
| 5   | L3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | M3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | N3    | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1723  | 1090 | 287 | 337 | 9 |         |       |
| 5   | O3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | P3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | Q3    | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1723  | 1090 | 287 | 337 | 9 |         |       |
| 5   | R3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | S3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | T3    | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1723  | 1090 | 287 | 337 | 9 |         |       |
| 5   | U3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | V3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | W3    | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1723  | 1090 | 287 | 337 | 9 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms         |           |          |          |        | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 5   | X3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | Y3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | Z3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | a3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | b3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | c3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | d3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | e3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | f3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | g3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | h3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | i3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | j3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | k3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | l3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | m3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | n3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | o3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | p3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | q3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |
| 5   | r3    | 223      | Total<br>1679 | C<br>1065 | N<br>279 | O<br>327 | S<br>8 | 0       | 0     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | s3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | t3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | u3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | v3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | w3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | x3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | y3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | z3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | 13    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | 23    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | 33    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | 43    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | 53    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | 63    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | 73    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | 83    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | 93    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | 03    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | A3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | B3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | C3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | D3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | E3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | F3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |
| 5   | G3    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1679  | 1065 | 279 | 327 | 8 |         |       |

- Molecule 6 is a protein called Neck 1 protein, gp14.

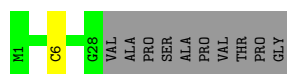
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | A4    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 671   | 429 | 120 | 118 | 4 |         |       |
| 6   | B4    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 671   | 429 | 120 | 118 | 4 |         |       |
| 6   | C4    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 671   | 429 | 120 | 118 | 4 |         |       |
| 6   | D4    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 671   | 429 | 120 | 118 | 4 |         |       |
| 6   | E4    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 671   | 429 | 120 | 118 | 4 |         |       |

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


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

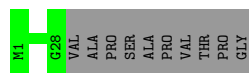
- Molecule 1: Linking protein 2, gp128

Chain a1: 



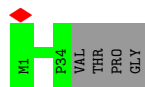
- Molecule 1: Linking protein 2, gp128

Chain b1: 



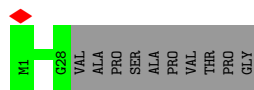
- Molecule 1: Linking protein 2, gp128

Chain d1: 



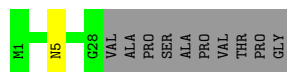
- Molecule 1: Linking protein 2, gp128

Chain e1: 

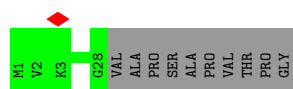
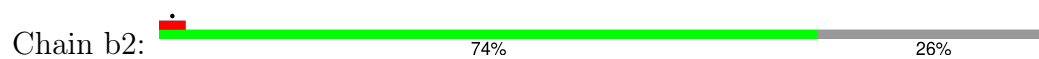


- Molecule 1: Linking protein 2, gp128

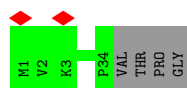
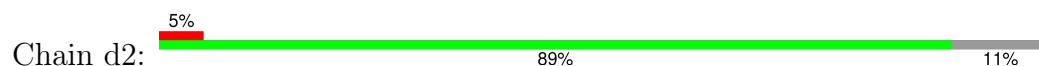
Chain a2: 



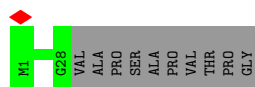
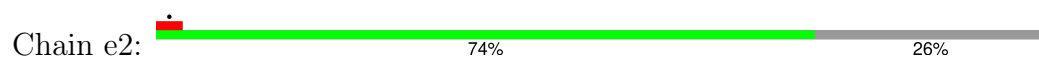
- Molecule 1: Linking protein 2, gp128



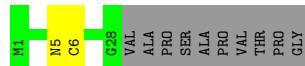
- Molecule 1: Linking protein 2, gp128



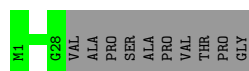
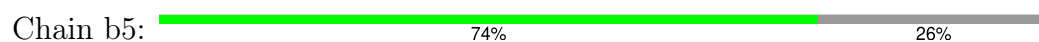
- Molecule 1: Linking protein 2, gp128



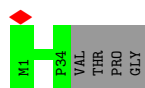
- Molecule 1: Linking protein 2, gp128



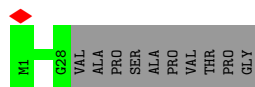
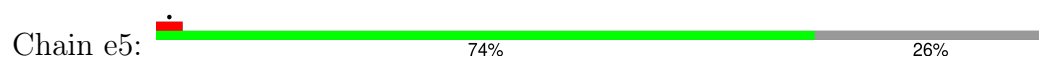
- Molecule 1: Linking protein 2, gp128



- Molecule 1: Linking protein 2, gp128

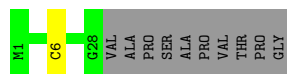


- Molecule 1: Linking protein 2, gp128



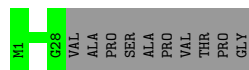
- Molecule 1: Linking protein 2, gp128

Chain a6:  71% 26%



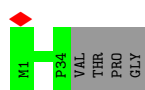
- Molecule 1: Linking protein 2, gp128

Chain b6:  74% 26%



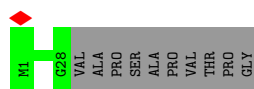
- Molecule 1: Linking protein 2, gp128

Chain d6:  89% 11%



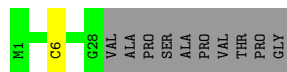
- Molecule 1: Linking protein 2, gp128

Chain e6:  74% 26%



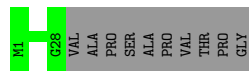
- Molecule 1: Linking protein 2, gp128

Chain a7:  71% 26%



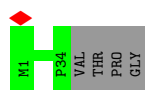
- Molecule 1: Linking protein 2, gp128

Chain b7:  74% 26%

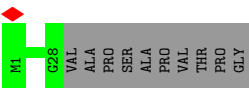


- Molecule 1: Linking protein 2, gp128

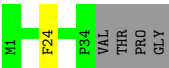
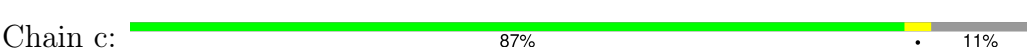
Chain d7:  89% 11%



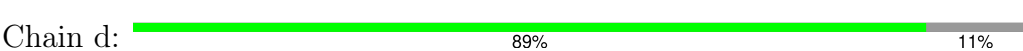
- Molecule 1: Linking protein 2, gp128



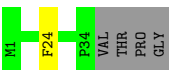
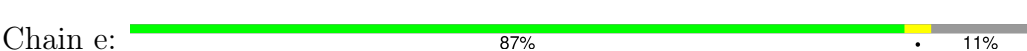
- Molecule 1: Linking protein 2, gp128



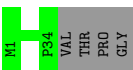
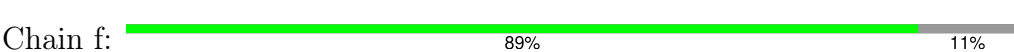
- Molecule 1: Linking protein 2, gp128



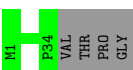
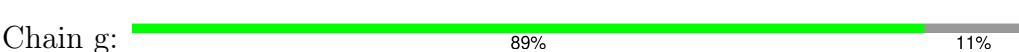
- Molecule 1: Linking protein 2, gp128



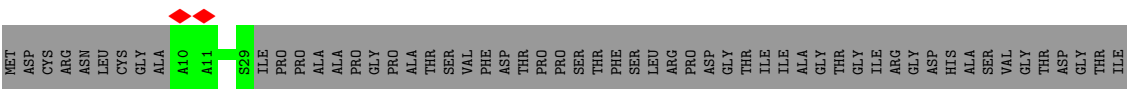
- Molecule 1: Linking protein 2, gp128



- Molecule 1: Linking protein 2, gp128

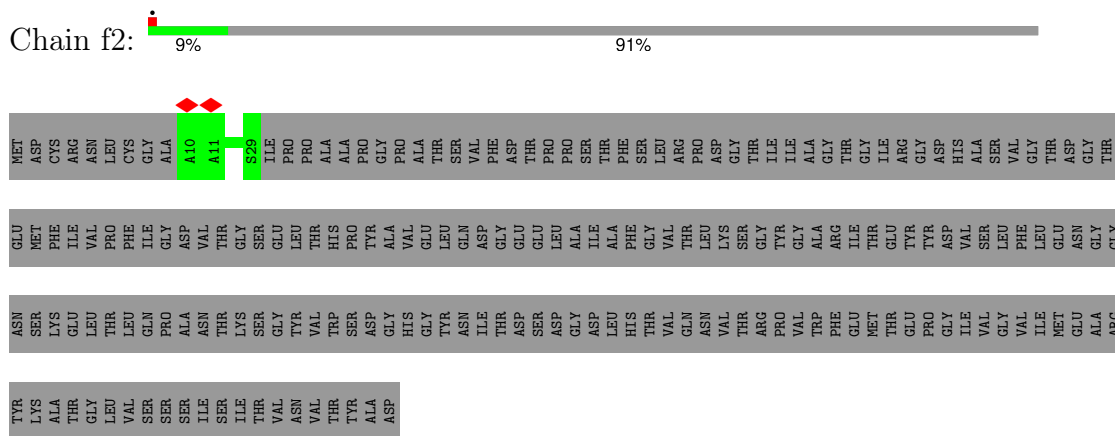


- Molecule 2: Linking protein 1, gp16

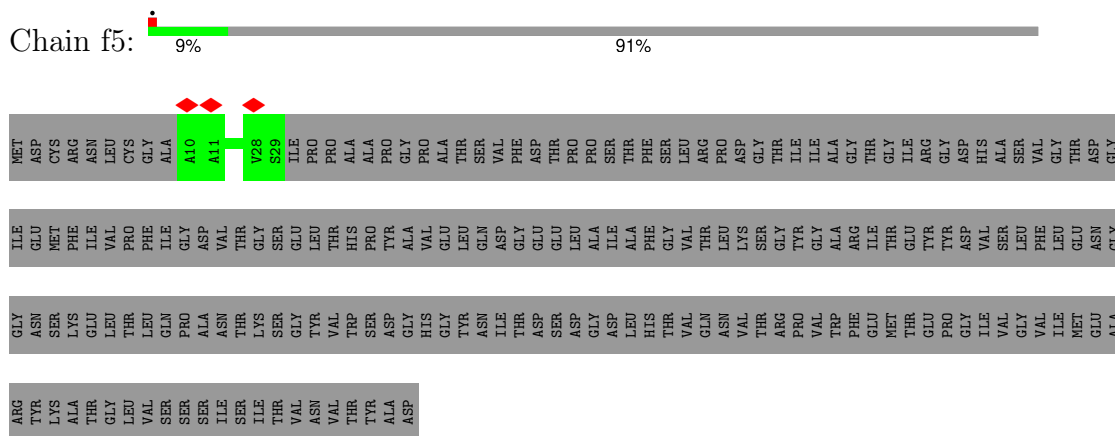


[illegible]

- Molecule 2: Linking protein 1, gp16



- Molecule 2: Linking protein 1, gp16



- Molecule 2: Linking protein 1, gp16



TYR  
LYS  
ALA  
THR  
GLY  
LEU  
VAL  
SER  
SER  
ILE  
SER  
ILE  
THR  
VAL  
ASN  
THR  
THR  
TYR  
ALA  
ASP

- Molecule 2: Linking protein 1, gp16

Chain f7:  9% 91%

MET  
ASP  
CYS  
ARG  
ASN  
LEU  
CYS  
GLY  
ALA  
A10  
A11  
V28  
S29  
ILE  
PRO  
PRO  
ALA  
ALA  
PRO  
GLY  
GLY  
ALA  
GLY  
THR  
SER  
VAL  
PHE  
GLY  
ASP  
THR  
PRO  
LEU  
ARG  
THR  
PRO  
ASP  
GLY  
THR  
THR  
ILE  
ILE  
ALA  
GLY  
THR  
THR  
ILE  
ILE  
ARG  
GLY  
TYR  
TYR  
ASP  
HIS  
ALA  
SER  
VAL  
SER  
VAL  
PHE  
LEU  
GLY  
THR  
ASP  
GLY  
THR

ILE  
GLU  
MET  
PHE  
ILE  
GLU  
VAL  
PRO  
PHE  
ILE  
GLY  
PRO  
GLN  
ASP  
THR  
HIS  
THR  
PRO  
TYR  
ASP  
GLY  
VAL  
HIS  
VAL  
GLY  
THR  
GLN  
SER  
ASN  
ILE  
THR  
GLY  
SER  
TYR  
VAL  
THR  
TRP  
SER  
ASP  
GLY  
HIS  
PHE  
THR  
VAL  
GLN  
THR  
ASN  
VAL  
VAL  
THR  
PHE  
GLU  
ILE  
THR  
THR  
GLY  
TYR  
PRO  
GLY  
ASP  
HIS  
ILE  
VAL  
MET  
GLU  
ASN  
GLY  
THR

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

ARG  
TYR  
LYS  
ALA  
THR  
GLY  
LEU  
VAL  
SER  
SER  
ILE  
SER  
ILE  
THR  
VAL  
ASN  
VAL  
THR  
TYR  
ALA  
ASP

- Molecule 3: Major capsid protein, gp9

Chain g1:  64% 36%

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

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

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

R393  
F403  
I464  
GLY

- Molecule 3: Major capsid protein, gp9

Chain h1:  63% 36%

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

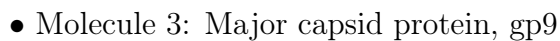
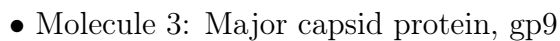
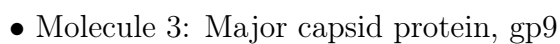
THR  
LYS  
GLU  
TYR  
ALA  
ASP  
GLU  
SER  
LEU  
ASN  
GLY  
LEU  
ASP  
ASP  
ILE  
HIS  
SER  
ASP  
ILE  
GLU  
HIS  
ASP  
VAL  
GLU  
THR  
LYS  
PHE  
GLY  
MET  
ASP  
MET  
ASP  
GLN  
ASP  
GLU  
LYS  
ALA  
THR  
THR  
ARG  
PHE  
GLY  
VAL  
GLY  
ASN  
ASP  
ASP  
ALA  
ILE  
GLU  
PHE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

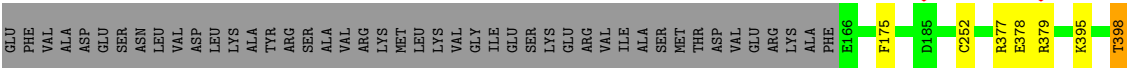
GLU  
PHE  
VAL  
ALA  
ASP  
GLU  
SER  
LEU  
ASN  
GLY  
LEU  
ASP  
ASP  
ILE  
HIS  
SER  
ASP  
ILE  
GLU  
HIS  
ASP  
VAL  
GLU  
THR  
LYS  
PHE  
GLY  
MET  
ASP  
MET  
ASP  
GLN  
ASP  
GLU  
LYS  
ALA  
THR  
THR  
ARG  
PHE  
GLY  
VAL  
GLY  
ASN  
ASP  
ASP  
ALA  
ILE  
GLU  
PHE  
ARG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

C455  
I464  
GLY

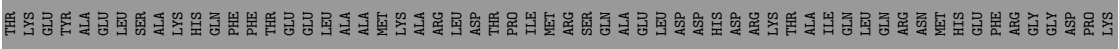
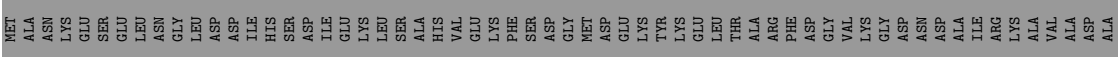
- Molecule 3: Major capsid protein, gp9



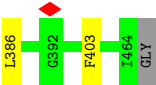
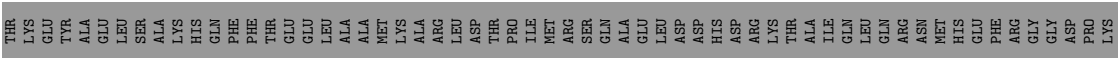
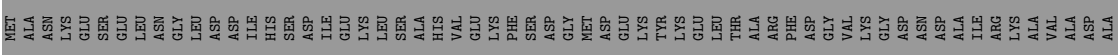




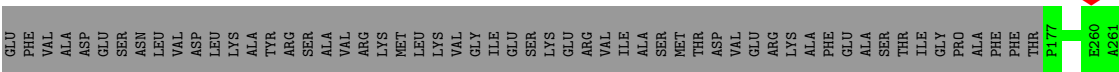
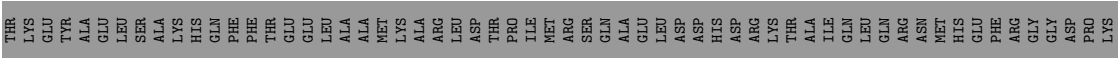
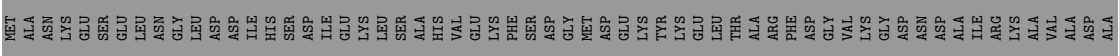
• Molecule 3: Major capsid protein, gp9



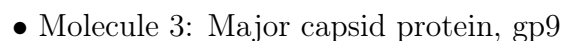
• Molecule 3: Major capsid protein, gp9

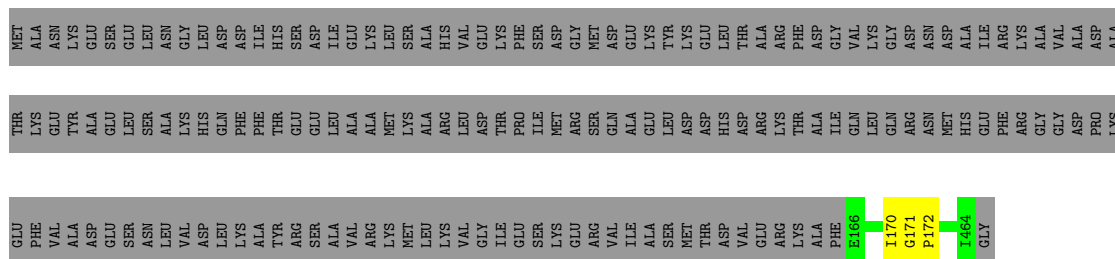


• Molecule 3: Major capsid protein, gp9

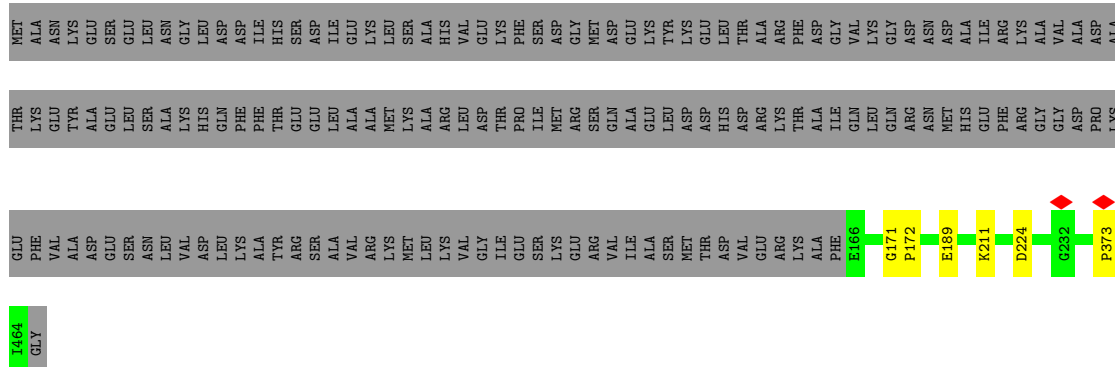




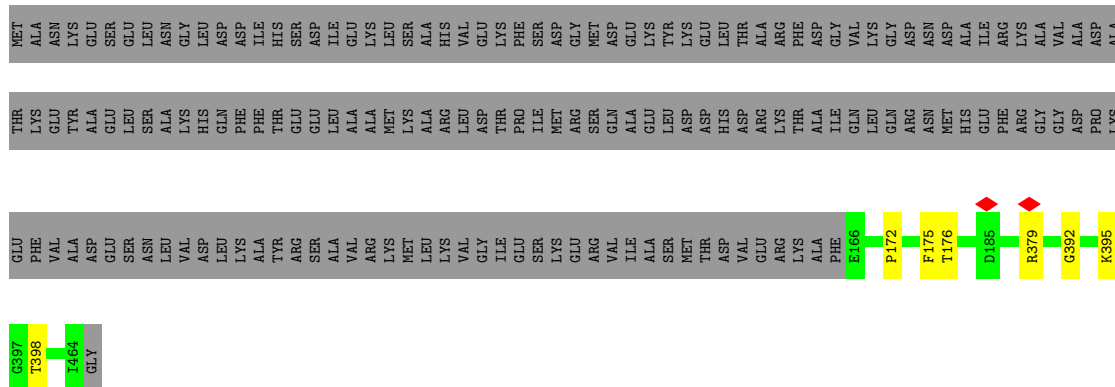




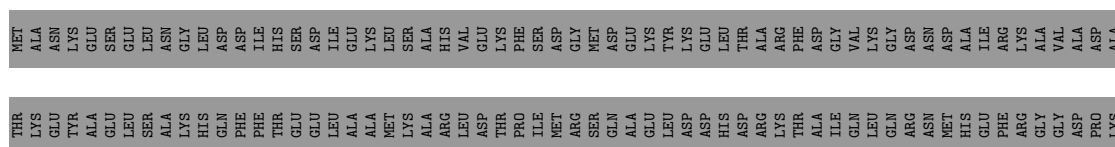
- Molecule 3: Major capsid protein, gp9

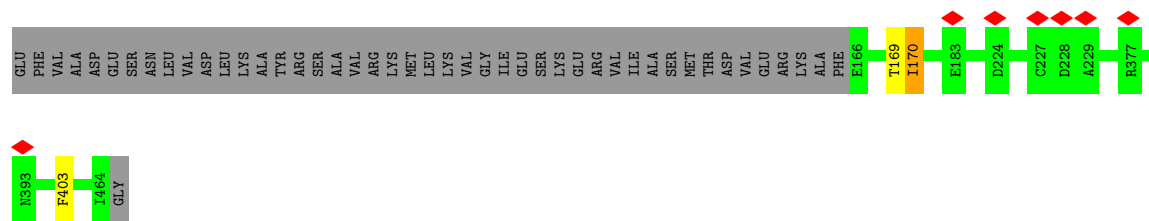


- Molecule 3: Major capsid protein, gp9

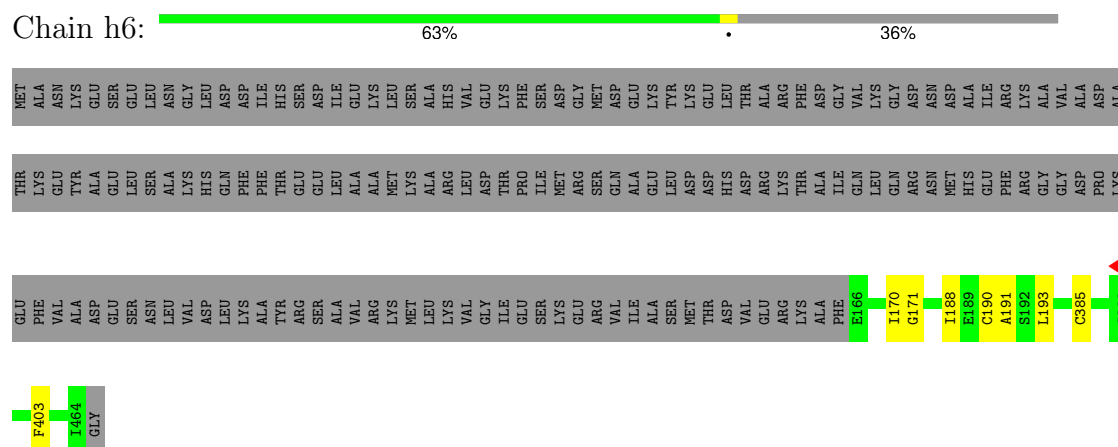


- Molecule 3: Major capsid protein, gp9

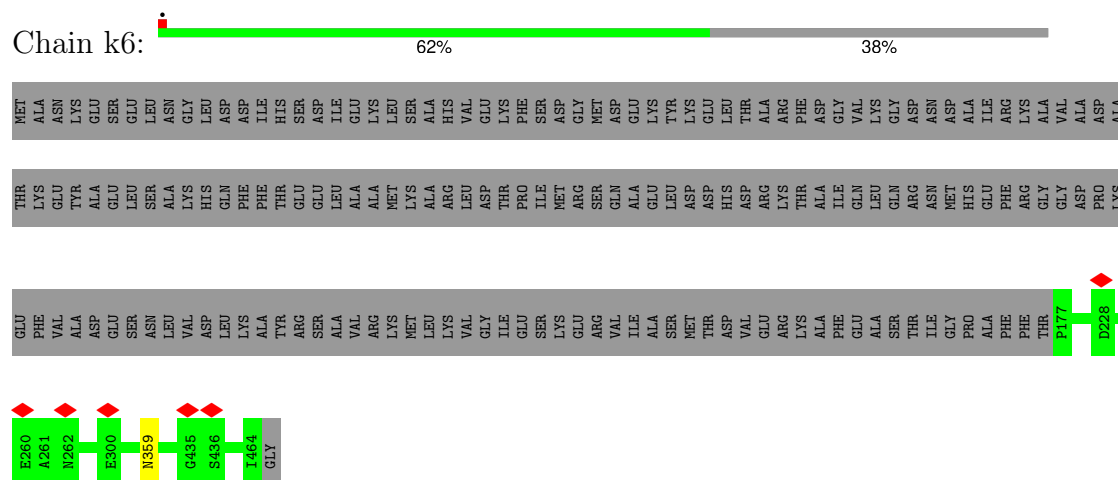




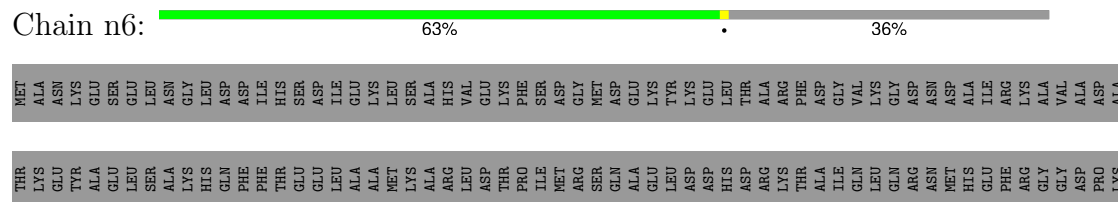
- Molecule 3: Major capsid protein, gp9

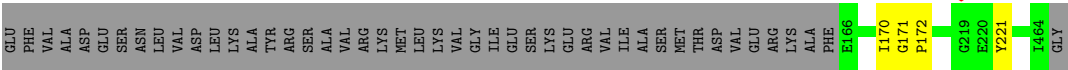


- Molecule 3: Major capsid protein, gp9

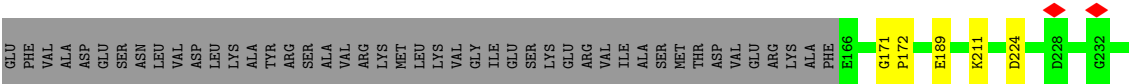
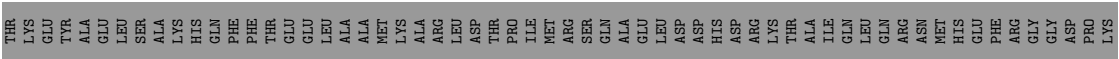
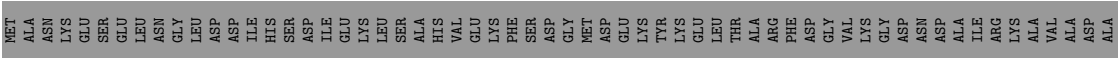


- Molecule 3: Major capsid protein, gp9

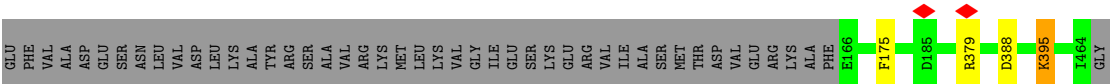
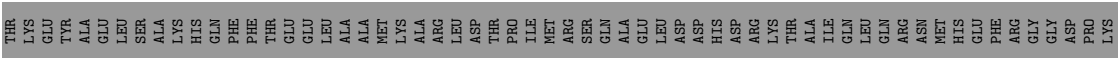
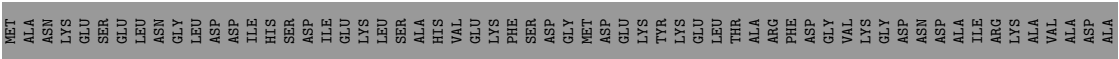




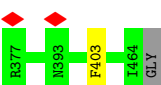
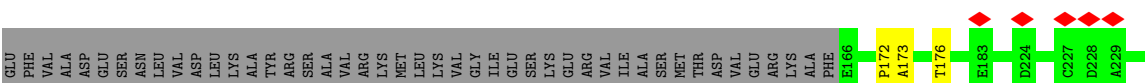
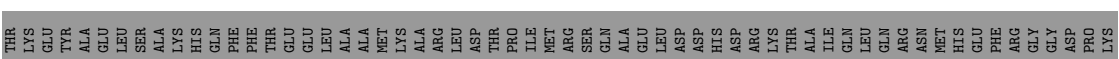
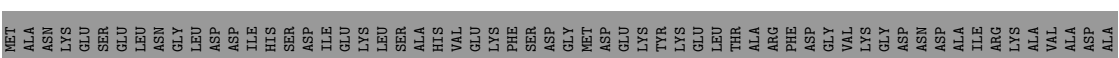
• Molecule 3: Major capsid protein, gp9



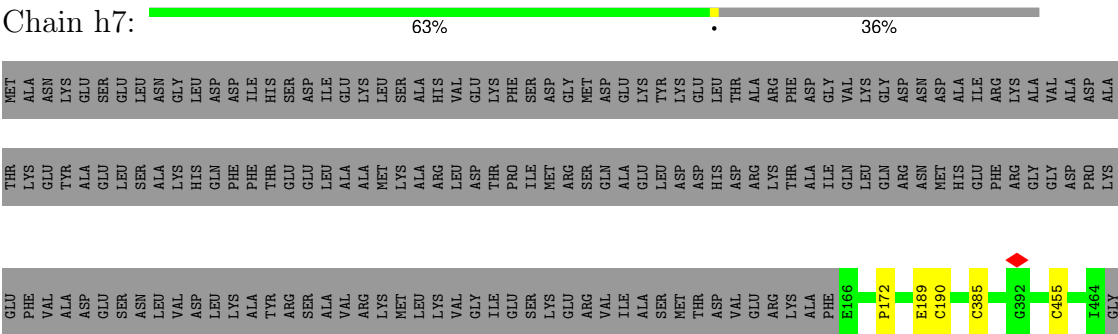
• Molecule 3: Major capsid protein, gp9



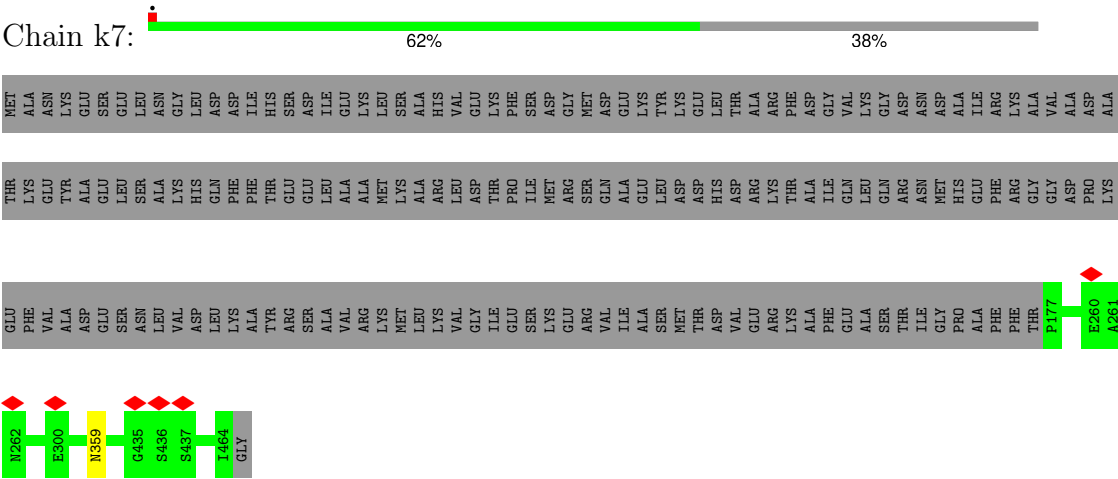
• Molecule 3: Major capsid protein, gp9



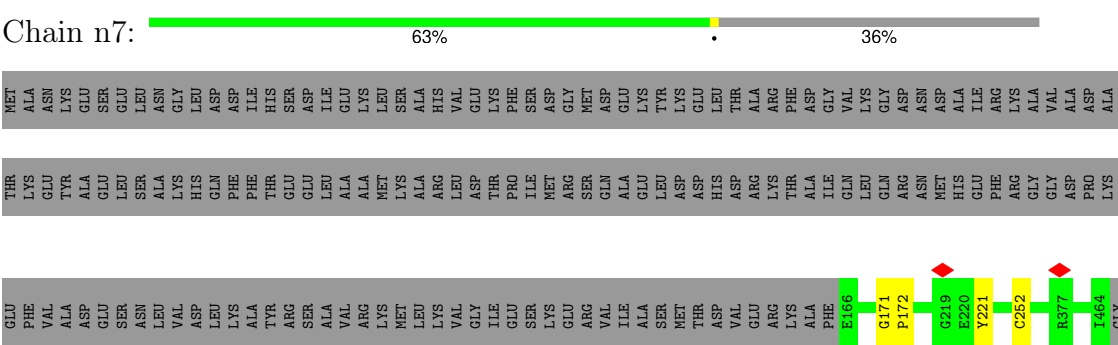
• Molecule 3: Major capsid protein, gp9



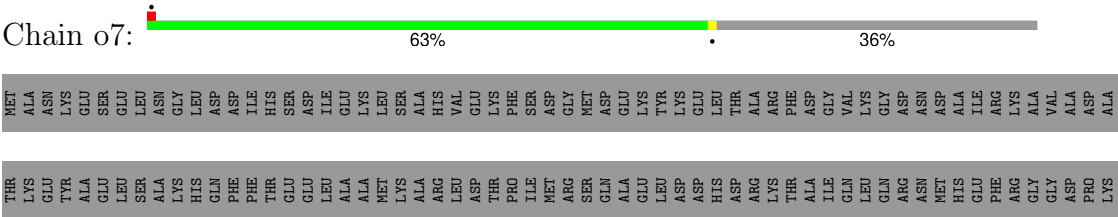
• Molecule 3: Major capsid protein, gp9



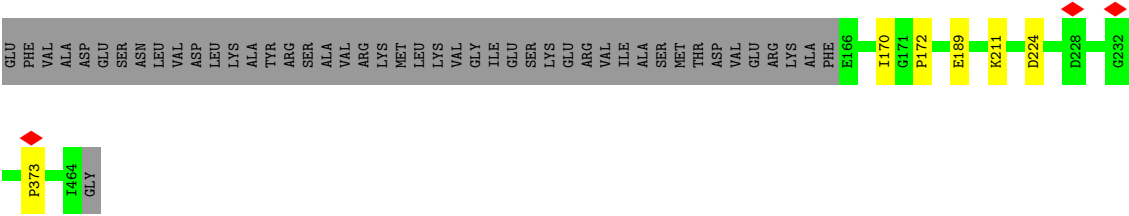
• Molecule 3: Major capsid protein, gp9



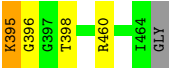
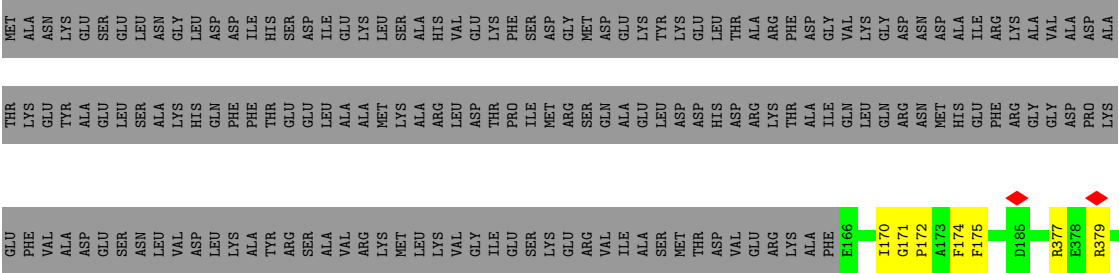
• Molecule 3: Major capsid protein, gp9



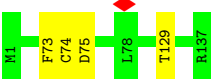




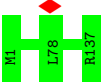
• Molecule 3: Major capsid protein, gp9



• Molecule 4: Minor capsid protein, gp10



• Molecule 4: Minor capsid protein, gp10

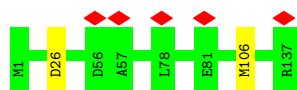


• Molecule 4: Minor capsid protein, gp10

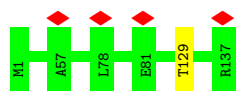


• Molecule 4: Minor capsid protein, gp10

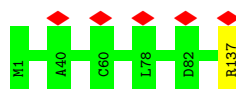




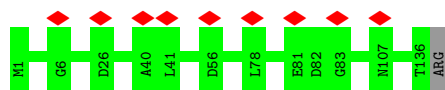
- Molecule 4: Minor capsid protein, gp10



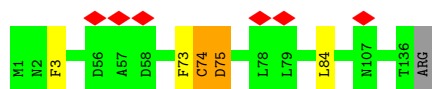
- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10

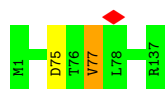


- Molecule 4: Minor capsid protein, gp10



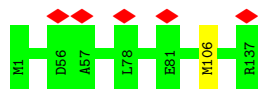
- Molecule 4: Minor capsid protein, gp10

Chain p2:  99%



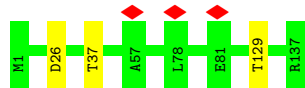
- Molecule 4: Minor capsid protein, gp10

Chain q2:  99%



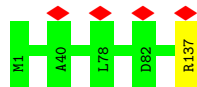
- Molecule 4: Minor capsid protein, gp10

Chain s2:  98%



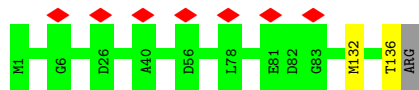
- Molecule 4: Minor capsid protein, gp10

Chain t2:  99%



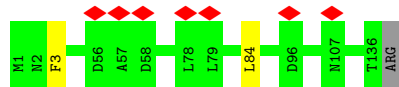
- Molecule 4: Minor capsid protein, gp10

Chain u2:  5% 98%



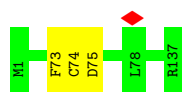
- Molecule 4: Minor capsid protein, gp10

Chain v2:  5% 98%



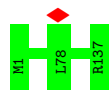
- Molecule 4: Minor capsid protein, gp10

Chain l5:  98%



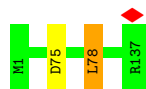
- Molecule 4: Minor capsid protein, gp10

Chain m5: 100%



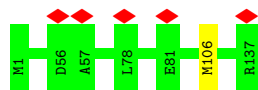
- Molecule 4: Minor capsid protein, gp10

Chain p5: 99%



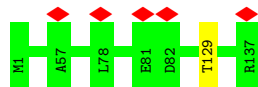
- Molecule 4: Minor capsid protein, gp10

Chain q5: 99%



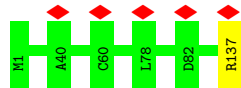
- Molecule 4: Minor capsid protein, gp10

Chain s5: 99%



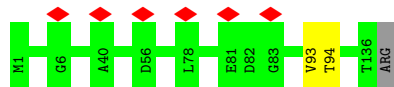
- Molecule 4: Minor capsid protein, gp10

Chain t5: 99%



- Molecule 4: Minor capsid protein, gp10

Chain u5: 98%



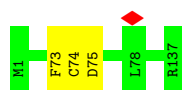
- Molecule 4: Minor capsid protein, gp10

Chain v5:  97%



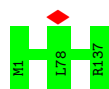
- Molecule 4: Minor capsid protein, gp10

Chain l6:  98%



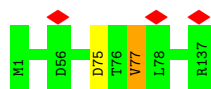
- Molecule 4: Minor capsid protein, gp10

Chain m6:  100%



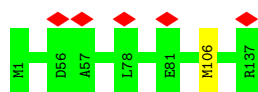
- Molecule 4: Minor capsid protein, gp10

Chain p6:  99%



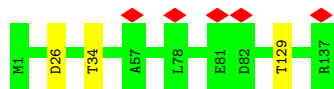
- Molecule 4: Minor capsid protein, gp10

Chain q6:  99%



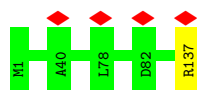
- Molecule 4: Minor capsid protein, gp10

Chain s6:  98%

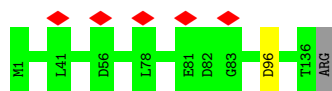
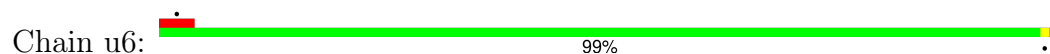


- Molecule 4: Minor capsid protein, gp10

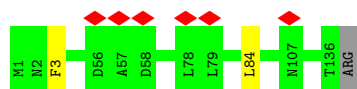
Chain t6:  99%



- Molecule 4: Minor capsid protein, gp10



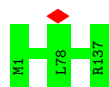
- Molecule 4: Minor capsid protein, gp10



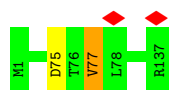
- Molecule 4: Minor capsid protein, gp10



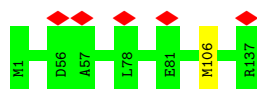
- Molecule 4: Minor capsid protein, gp10



- Molecule 4: Minor capsid protein, gp10

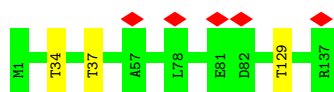


- Molecule 4: Minor capsid protein, gp10



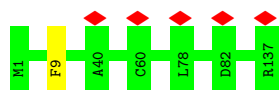
- Molecule 4: Minor capsid protein, gp10

Chain s7:  98%



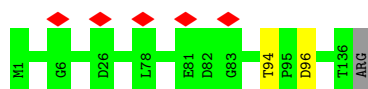
- Molecule 4: Minor capsid protein, gp10

Chain t7:  99%



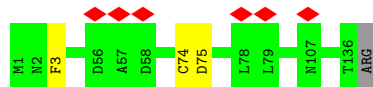
- Molecule 4: Minor capsid protein, gp10

Chain u7:  98%



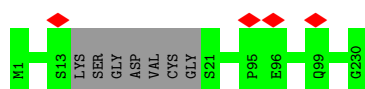
- Molecule 4: Minor capsid protein, gp10

Chain v7:  97%



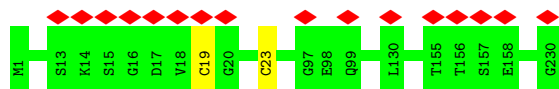
- Molecule 5: Collar sheath protein, gp13

Chain J3:  97%



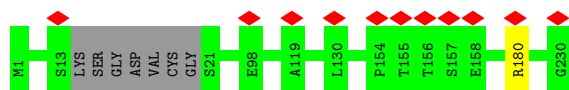
- Molecule 5: Collar sheath protein, gp13

Chain K3:  99%



- Molecule 5: Collar sheath protein, gp13

Chain L3:  97%



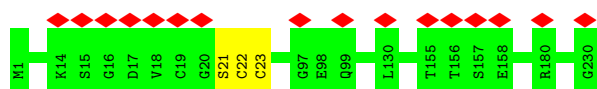
- Molecule 5: Collar sheath protein, gp13

Chain M3:  97%



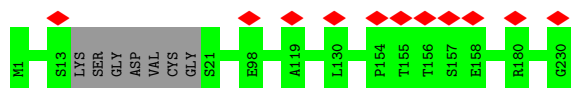
- Molecule 5: Collar sheath protein, gp13

Chain N3:  99%



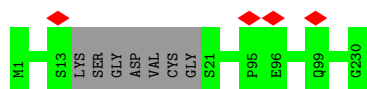
- Molecule 5: Collar sheath protein, gp13

Chain O3:  97%



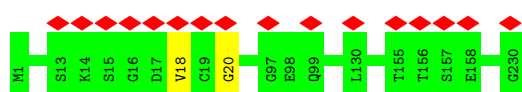
- Molecule 5: Collar sheath protein, gp13

Chain P3:  97%



- Molecule 5: Collar sheath protein, gp13

Chain Q3:  99%



- Molecule 5: Collar sheath protein, gp13

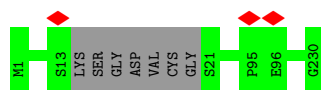
Chain R3:  97%



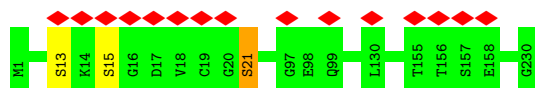
- Molecule 5: Collar sheath protein, gp13

Chain S3:  97%

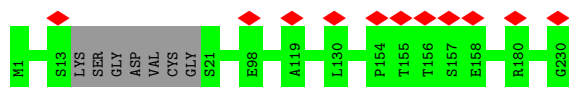




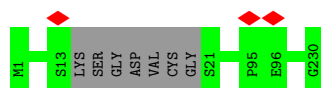
- Molecule 5: Collar sheath protein, gp13



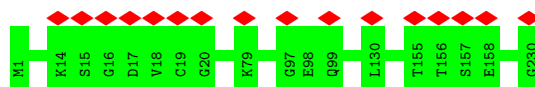
- Molecule 5: Collar sheath protein, gp13



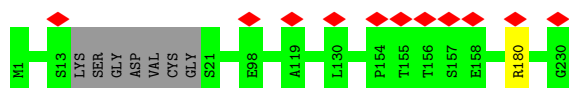
- Molecule 5: Collar sheath protein, gp13



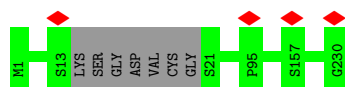
- Molecule 5: Collar sheath protein, gp13



- Molecule 5: Collar sheath protein, gp13

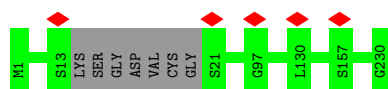


- Molecule 5: Collar sheath protein, gp13



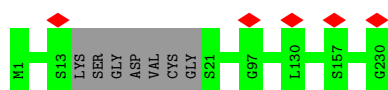
- Molecule 5: Collar sheath protein, gp13

Chain Z3:  97%



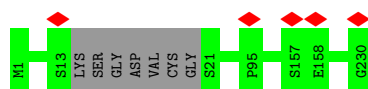
- Molecule 5: Collar sheath protein, gp13

Chain a3:  97%



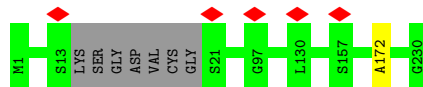
- Molecule 5: Collar sheath protein, gp13

Chain b3:  97%



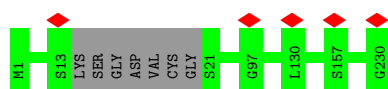
- Molecule 5: Collar sheath protein, gp13

Chain c3:  97%



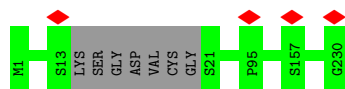
- Molecule 5: Collar sheath protein, gp13

Chain d3:  97%



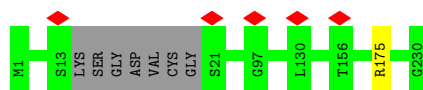
- Molecule 5: Collar sheath protein, gp13

Chain e3:  97%



- Molecule 5: Collar sheath protein, gp13

Chain f3:  97%



- Molecule 5: Collar sheath protein, gp13

Chain g3:  97%



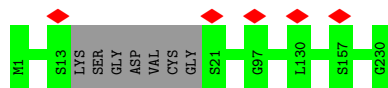
- Molecule 5: Collar sheath protein, gp13

Chain h3:  97%



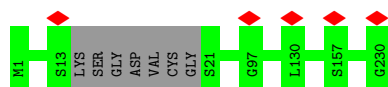
- Molecule 5: Collar sheath protein, gp13

Chain i3:  97%



- Molecule 5: Collar sheath protein, gp13

Chain j3:  97%



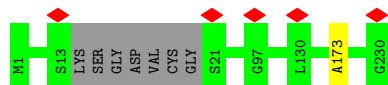
- Molecule 5: Collar sheath protein, gp13

Chain k3:  97%



- Molecule 5: Collar sheath protein, gp13

Chain l3:  97%

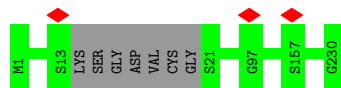


- Molecule 5: Collar sheath protein, gp13

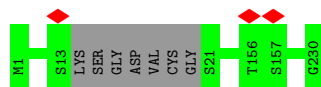
Chain m3:  97%



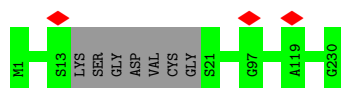
- Molecule 5: Collar sheath protein, gp13



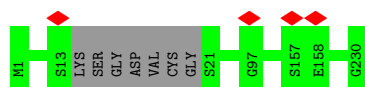
- Molecule 5: Collar sheath protein, gp13



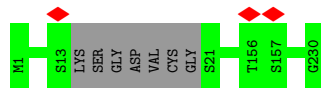
- Molecule 5: Collar sheath protein, gp13



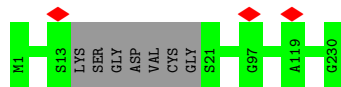
- Molecule 5: Collar sheath protein, gp13



- Molecule 5: Collar sheath protein, gp13

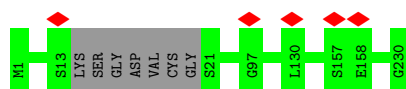


- Molecule 5: Collar sheath protein, gp13



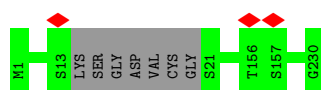
- Molecule 5: Collar sheath protein, gp13

Chain t3:  97%



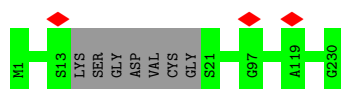
- Molecule 5: Collar sheath protein, gp13

Chain u3:  97%



- Molecule 5: Collar sheath protein, gp13

Chain v3:  97%



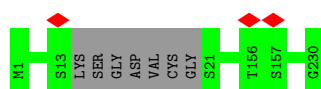
- Molecule 5: Collar sheath protein, gp13

Chain w3:  97%



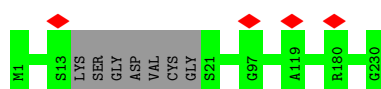
- Molecule 5: Collar sheath protein, gp13

Chain x3:  97%



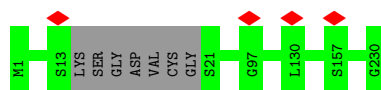
- Molecule 5: Collar sheath protein, gp13

Chain y3:  97%



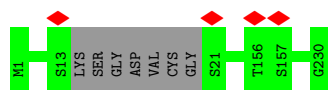
- Molecule 5: Collar sheath protein, gp13

Chain z3:  97%



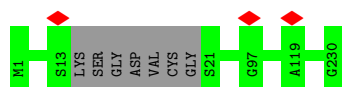
- Molecule 5: Collar sheath protein, gp13

Chain 13:  97%



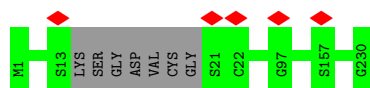
- Molecule 5: Collar sheath protein, gp13

Chain 23:  97%



- Molecule 5: Collar sheath protein, gp13

Chain 33:  97%



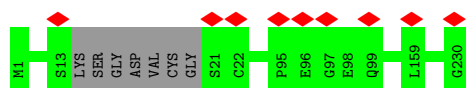
- Molecule 5: Collar sheath protein, gp13

Chain 43:  97%



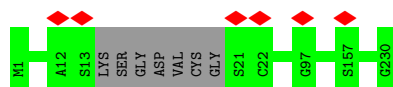
- Molecule 5: Collar sheath protein, gp13

Chain 53:  97%



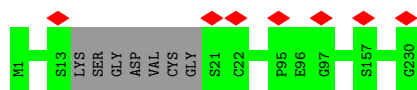
- Molecule 5: Collar sheath protein, gp13

Chain 63:  97%

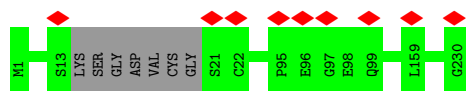


- Molecule 5: Collar sheath protein, gp13

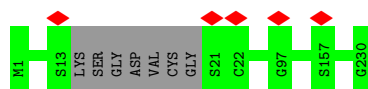
Chain 73:  97%



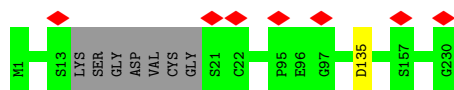
- Molecule 5: Collar sheath protein, gp13



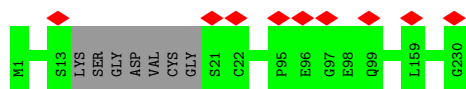
- Molecule 5: Collar sheath protein, gp13



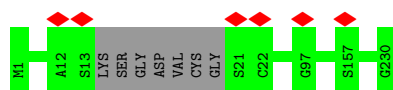
- Molecule 5: Collar sheath protein, gp13



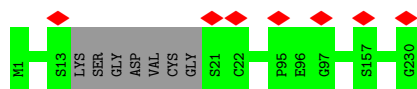
- Molecule 5: Collar sheath protein, gp13



- Molecule 5: Collar sheath protein, gp13

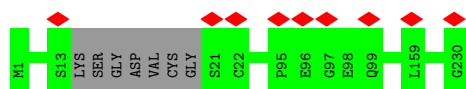


- Molecule 5: Collar sheath protein, gp13



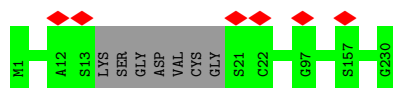
- Molecule 5: Collar sheath protein, gp13

Chain D3:  97%



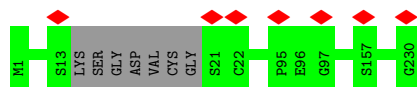
- Molecule 5: Collar sheath protein, gp13

Chain E3:  97%



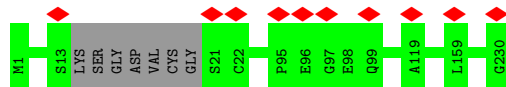
- Molecule 5: Collar sheath protein, gp13

Chain F3:  97%



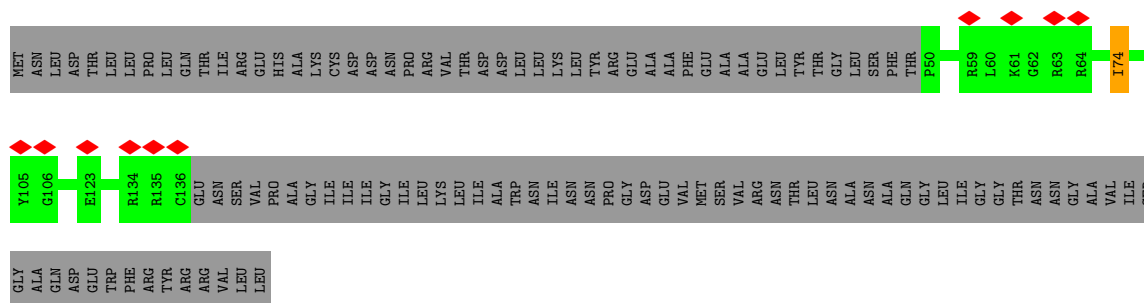
- Molecule 5: Collar sheath protein, gp13

Chain G3:  97%



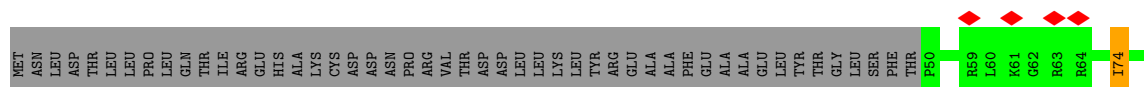
- Molecule 6: Neck 1 protein, gp14

Chain A4:  5% 43% 57%

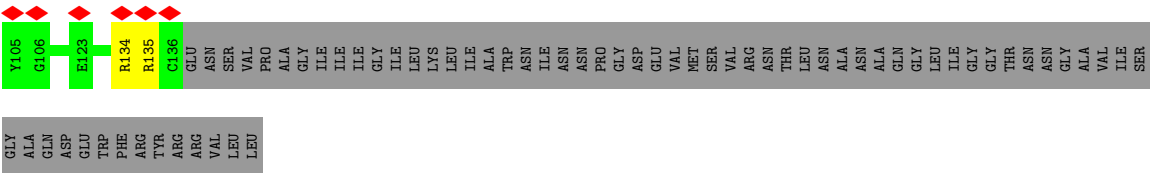


- Molecule 6: Neck 1 protein, gp14

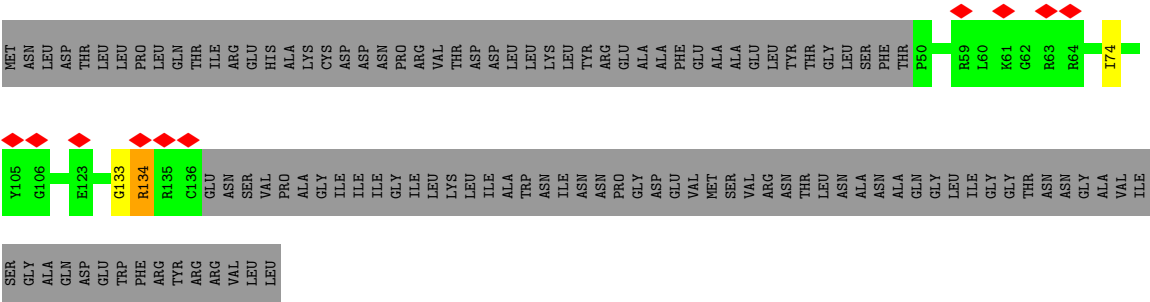
Chain B4:  5% 42% 57%



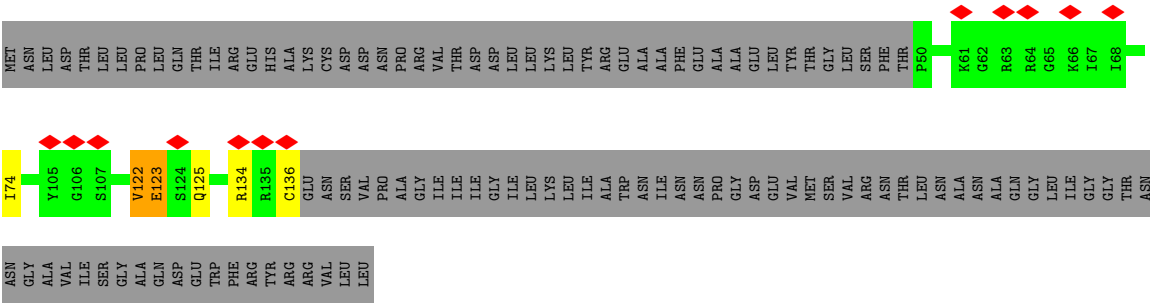




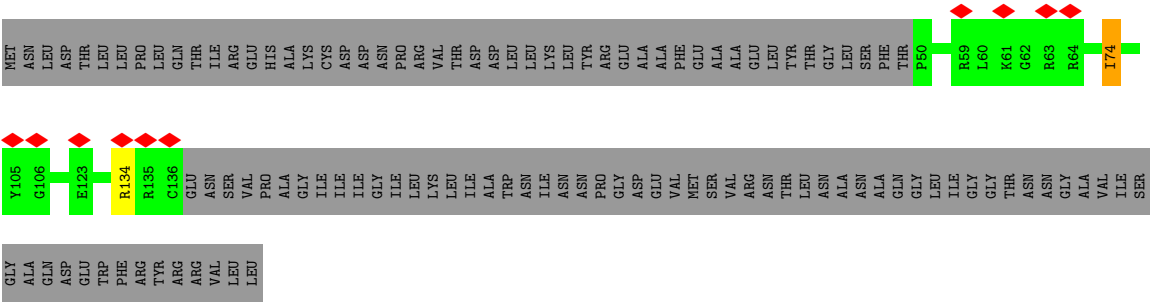
• Molecule 6: Neck 1 protein, gp14



• Molecule 6: Neck 1 protein, gp14



• Molecule 6: Neck 1 protein, gp14



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C5                               | Depositor |
| Number of particles used             | 10086                                   | 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 ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 1200                                    | Depositor |
| Maximum defocus (nm)                 | 2200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.857                                   | Depositor |
| Minimum map value                    | -0.549                                  | Depositor |
| Average map value                    | -0.001                                  | Depositor |
| Map value standard deviation         | 0.044                                   | Depositor |
| Recommended contour level            | 0.15                                    | Depositor |
| Map size (Å)                         | 648.0, 648.0, 648.0                     | wwPDB     |
| Map dimensions                       | 600, 600, 600                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.08, 1.08, 1.08                        | 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    | 0.36         | 0/213       | 0.54        | 0/288       |
| 1   | a2    | 0.30         | 0/213       | 0.53        | 0/288       |
| 1   | a5    | 0.37         | 0/213       | 0.54        | 0/288       |
| 1   | a6    | 0.35         | 0/213       | 0.53        | 0/288       |
| 1   | a7    | 0.34         | 0/213       | 0.53        | 0/288       |
| 1   | b1    | 0.31         | 0/213       | 0.52        | 0/288       |
| 1   | b2    | 0.31         | 0/213       | 0.49        | 0/288       |
| 1   | b5    | 0.30         | 0/213       | 0.50        | 0/288       |
| 1   | b6    | 0.30         | 0/213       | 0.50        | 0/288       |
| 1   | b7    | 0.33         | 0/213       | 0.46        | 0/288       |
| 1   | c     | 0.33         | 0/252       | 0.55        | 0/344       |
| 1   | d     | 0.37         | 0/252       | 0.54        | 0/344       |
| 1   | d1    | 0.31         | 0/252       | 0.58        | 0/344       |
| 1   | d2    | 0.31         | 0/252       | 0.59        | 0/344       |
| 1   | d5    | 0.31         | 0/252       | 0.60        | 0/344       |
| 1   | d6    | 0.30         | 0/252       | 0.57        | 0/344       |
| 1   | d7    | 0.31         | 0/252       | 0.59        | 0/344       |
| 1   | e     | 0.34         | 0/252       | 0.53        | 0/344       |
| 1   | e1    | 0.32         | 0/213       | 0.54        | 0/288       |
| 1   | e2    | 0.31         | 0/213       | 0.55        | 0/288       |
| 1   | e5    | 0.32         | 0/213       | 0.56        | 0/288       |
| 1   | e6    | 0.31         | 0/213       | 0.55        | 0/288       |
| 1   | e7    | 0.31         | 0/213       | 0.56        | 0/288       |
| 1   | f     | 0.42         | 0/252       | 0.57        | 0/344       |
| 1   | g     | 0.44         | 0/252       | 0.55        | 0/344       |
| 2   | f1    | 0.39         | 0/142       | 0.53        | 0/192       |
| 2   | f2    | 0.38         | 0/142       | 0.52        | 0/192       |
| 2   | f5    | 0.41         | 0/142       | 0.57        | 0/192       |
| 2   | f6    | 0.38         | 0/142       | 0.54        | 0/192       |
| 2   | f7    | 0.39         | 0/142       | 0.54        | 0/192       |
| 3   | g1    | 0.33         | 0/2396      | 0.49        | 0/3243      |
| 3   | g2    | 0.34         | 0/2396      | 0.49        | 0/3243      |
| 3   | g5    | 0.33         | 0/2396      | 0.48        | 0/3243      |
| 3   | g6    | 0.34         | 0/2396      | 0.49        | 0/3243      |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 3   | g7    | 0.33         | 0/2396  | 0.49        | 0/3243        |
| 3   | h1    | 0.38         | 0/2396  | 0.53        | 0/3243        |
| 3   | h2    | 0.38         | 0/2396  | 0.54        | 0/3243        |
| 3   | h5    | 0.38         | 0/2396  | 0.52        | 0/3243        |
| 3   | h6    | 0.38         | 0/2396  | 0.52        | 0/3243        |
| 3   | h7    | 0.37         | 0/2396  | 0.54        | 2/3243 (0.1%) |
| 3   | k1    | 0.34         | 0/2313  | 0.48        | 0/3128        |
| 3   | k2    | 0.34         | 0/2313  | 0.49        | 0/3128        |
| 3   | k5    | 0.34         | 0/2313  | 0.49        | 0/3128        |
| 3   | k6    | 0.34         | 0/2313  | 0.49        | 0/3128        |
| 3   | k7    | 0.35         | 0/2313  | 0.51        | 0/3128        |
| 3   | n1    | 0.35         | 0/2396  | 0.52        | 0/3243        |
| 3   | n2    | 0.34         | 0/2396  | 0.52        | 0/3243        |
| 3   | n5    | 0.34         | 0/2396  | 0.52        | 0/3243        |
| 3   | n6    | 0.34         | 0/2396  | 0.51        | 0/3243        |
| 3   | n7    | 0.34         | 0/2396  | 0.51        | 0/3243        |
| 3   | o1    | 0.31         | 0/2396  | 0.49        | 0/3243        |
| 3   | o2    | 0.31         | 0/2396  | 0.48        | 0/3243        |
| 3   | o5    | 0.31         | 0/2396  | 0.49        | 0/3243        |
| 3   | o6    | 0.31         | 0/2396  | 0.49        | 0/3243        |
| 3   | o7    | 0.31         | 0/2396  | 0.48        | 0/3243        |
| 3   | r1    | 0.33         | 0/2396  | 0.51        | 0/3243        |
| 3   | r2    | 0.33         | 0/2396  | 0.52        | 1/3243 (0.0%) |
| 3   | r5    | 0.34         | 0/2396  | 0.51        | 0/3243        |
| 3   | r6    | 0.33         | 0/2396  | 0.52        | 1/3243 (0.0%) |
| 3   | r7    | 0.34         | 0/2396  | 0.52        | 0/3243        |
| 4   | l1    | 0.32         | 0/1052  | 0.52        | 0/1443        |
| 4   | l2    | 0.33         | 0/1052  | 0.51        | 0/1443        |
| 4   | l5    | 0.33         | 0/1052  | 0.51        | 0/1443        |
| 4   | l6    | 0.33         | 0/1052  | 0.51        | 0/1443        |
| 4   | l7    | 0.32         | 0/1052  | 0.52        | 0/1443        |
| 4   | m1    | 0.34         | 0/1052  | 0.50        | 0/1443        |
| 4   | m2    | 0.34         | 0/1052  | 0.48        | 0/1443        |
| 4   | m5    | 0.34         | 0/1052  | 0.49        | 0/1443        |
| 4   | m6    | 0.34         | 0/1052  | 0.50        | 0/1443        |
| 4   | m7    | 0.34         | 0/1052  | 0.51        | 0/1443        |
| 4   | p1    | 0.31         | 0/1052  | 0.50        | 0/1443        |
| 4   | p2    | 0.31         | 0/1052  | 0.51        | 0/1443        |
| 4   | p5    | 0.31         | 0/1052  | 0.51        | 0/1443        |
| 4   | p6    | 0.30         | 0/1052  | 0.51        | 0/1443        |
| 4   | p7    | 0.31         | 0/1052  | 0.52        | 0/1443        |
| 4   | q1    | 0.31         | 0/1052  | 0.50        | 0/1443        |
| 4   | q2    | 0.31         | 0/1052  | 0.50        | 0/1443        |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 4   | q5    | 0.31         | 0/1052  | 0.49        | 0/1443  |
| 4   | q6    | 0.31         | 0/1052  | 0.49        | 0/1443  |
| 4   | q7    | 0.31         | 0/1052  | 0.49        | 0/1443  |
| 4   | s1    | 0.31         | 0/1052  | 0.50        | 0/1443  |
| 4   | s2    | 0.32         | 0/1052  | 0.50        | 0/1443  |
| 4   | s5    | 0.31         | 0/1052  | 0.49        | 0/1443  |
| 4   | s6    | 0.31         | 0/1052  | 0.50        | 0/1443  |
| 4   | s7    | 0.30         | 0/1052  | 0.49        | 0/1443  |
| 4   | t1    | 0.29         | 0/1052  | 0.50        | 0/1443  |
| 4   | t2    | 0.29         | 0/1052  | 0.50        | 0/1443  |
| 4   | t5    | 0.29         | 0/1052  | 0.49        | 0/1443  |
| 4   | t6    | 0.30         | 0/1052  | 0.47        | 0/1443  |
| 4   | t7    | 0.32         | 0/1052  | 0.54        | 0/1443  |
| 4   | u1    | 0.28         | 0/1040  | 0.52        | 0/1429  |
| 4   | u2    | 0.30         | 0/1040  | 0.53        | 0/1429  |
| 4   | u5    | 0.28         | 0/1040  | 0.51        | 0/1429  |
| 4   | u6    | 0.29         | 0/1040  | 0.53        | 0/1429  |
| 4   | u7    | 0.28         | 0/1040  | 0.52        | 0/1429  |
| 4   | v1    | 0.29         | 0/1040  | 0.50        | 0/1429  |
| 4   | v2    | 0.31         | 0/1040  | 0.53        | 0/1429  |
| 4   | v5    | 0.30         | 0/1040  | 0.51        | 0/1429  |
| 4   | v6    | 0.30         | 0/1040  | 0.52        | 0/1429  |
| 4   | v7    | 0.29         | 0/1040  | 0.51        | 0/1429  |
| 5   | 03    | 0.30         | 0/1723  | 0.47        | 0/2353  |
| 5   | 13    | 0.33         | 0/1723  | 0.48        | 0/2353  |
| 5   | 23    | 0.32         | 0/1723  | 0.49        | 0/2353  |
| 5   | 33    | 0.30         | 0/1723  | 0.46        | 0/2353  |
| 5   | 43    | 0.30         | 0/1723  | 0.46        | 0/2353  |
| 5   | 53    | 0.31         | 0/1723  | 0.48        | 0/2353  |
| 5   | 63    | 0.30         | 0/1723  | 0.47        | 0/2353  |
| 5   | 73    | 0.30         | 0/1723  | 0.46        | 0/2353  |
| 5   | 83    | 0.30         | 0/1723  | 0.48        | 0/2353  |
| 5   | 93    | 0.30         | 0/1723  | 0.47        | 0/2353  |
| 5   | A3    | 0.31         | 0/1723  | 0.47        | 0/2353  |
| 5   | B3    | 0.30         | 0/1723  | 0.47        | 0/2353  |
| 5   | C3    | 0.30         | 0/1723  | 0.47        | 0/2353  |
| 5   | D3    | 0.31         | 0/1723  | 0.48        | 0/2353  |
| 5   | E3    | 0.30         | 0/1723  | 0.47        | 0/2353  |
| 5   | F3    | 0.30         | 0/1723  | 0.47        | 0/2353  |
| 5   | G3    | 0.32         | 0/1723  | 0.50        | 0/2353  |
| 5   | J3    | 0.35         | 0/1723  | 0.47        | 0/2353  |
| 5   | K3    | 0.33         | 0/1768  | 0.47        | 0/2414  |
| 5   | L3    | 0.32         | 0/1723  | 0.47        | 0/2353  |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 5   | M3    | 0.35         | 0/1723  | 0.48        | 0/2353        |
| 5   | N3    | 0.35         | 0/1768  | 0.49        | 0/2414        |
| 5   | O3    | 0.32         | 0/1723  | 0.47        | 0/2353        |
| 5   | P3    | 0.35         | 0/1723  | 0.47        | 0/2353        |
| 5   | Q3    | 0.33         | 0/1768  | 0.48        | 1/2414 (0.0%) |
| 5   | R3    | 0.32         | 0/1723  | 0.47        | 0/2353        |
| 5   | S3    | 0.35         | 0/1723  | 0.47        | 0/2353        |
| 5   | T3    | 0.34         | 0/1768  | 0.49        | 0/2414        |
| 5   | U3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 5   | V3    | 0.35         | 0/1723  | 0.48        | 0/2353        |
| 5   | W3    | 0.33         | 0/1768  | 0.50        | 0/2414        |
| 5   | X3    | 0.32         | 0/1723  | 0.47        | 0/2353        |
| 5   | Y3    | 0.33         | 0/1723  | 0.46        | 0/2353        |
| 5   | Z3    | 0.34         | 0/1723  | 0.47        | 0/2353        |
| 5   | a3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 5   | b3    | 0.34         | 0/1723  | 0.47        | 0/2353        |
| 5   | c3    | 0.34         | 0/1723  | 0.48        | 0/2353        |
| 5   | d3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 5   | e3    | 0.34         | 0/1723  | 0.47        | 0/2353        |
| 5   | f3    | 0.35         | 0/1723  | 0.48        | 0/2353        |
| 5   | g3    | 0.33         | 0/1723  | 0.48        | 0/2353        |
| 5   | h3    | 0.33         | 0/1723  | 0.46        | 0/2353        |
| 5   | i3    | 0.35         | 0/1723  | 0.49        | 0/2353        |
| 5   | j3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 5   | k3    | 0.34         | 0/1723  | 0.47        | 0/2353        |
| 5   | l3    | 0.35         | 0/1723  | 0.49        | 0/2353        |
| 5   | m3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 5   | n3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 5   | o3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 5   | p3    | 0.32         | 0/1723  | 0.48        | 0/2353        |
| 5   | q3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 5   | r3    | 0.33         | 0/1723  | 0.48        | 0/2353        |
| 5   | s3    | 0.33         | 0/1723  | 0.48        | 0/2353        |
| 5   | t3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 5   | u3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 5   | v3    | 0.32         | 0/1723  | 0.47        | 0/2353        |
| 5   | w3    | 0.33         | 0/1723  | 0.46        | 0/2353        |
| 5   | x3    | 0.32         | 0/1723  | 0.47        | 0/2353        |
| 5   | y3    | 0.32         | 0/1723  | 0.47        | 0/2353        |
| 5   | z3    | 0.33         | 0/1723  | 0.47        | 0/2353        |
| 6   | A4    | 0.31         | 0/689   | 0.50        | 0/934         |
| 6   | B4    | 0.31         | 0/689   | 0.53        | 0/934         |
| 6   | C4    | 0.31         | 0/689   | 0.51        | 0/934         |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 6   | D4    | 0.29         | 0/689    | 0.50        | 0/934           |
| 6   | E4    | 0.31         | 0/689    | 0.53        | 0/934           |
| All | All   | 0.33         | 0/226900 | 0.49        | 5/309170 (0.0%) |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3   | r6    | 388 | ASP  | CB-CG-OD1 | 5.26  | 123.04      | 118.30   |
| 3   | h7    | 189 | GLU  | N-CA-C    | -5.25 | 96.83       | 111.00   |
| 3   | h7    | 385 | CYS  | CB-CA-C   | -5.15 | 100.09      | 110.40   |
| 5   | Q3    | 20  | GLY  | N-CA-C    | 5.12  | 125.90      | 113.10   |
| 3   | r2    | 388 | ASP  | CB-CG-OD1 | 5.05  | 122.85      | 118.30   |

There are no chirality outliers.

There are no planarity outliers.

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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    | 26/38 (68%) | 24 (92%) | 2 (8%)  | 0        | 100         | 100 |
| 1   | a2    | 26/38 (68%) | 25 (96%) | 1 (4%)  | 0        | 100         | 100 |
| 1   | a5    | 26/38 (68%) | 24 (92%) | 2 (8%)  | 0        | 100         | 100 |
| 1   | a6    | 26/38 (68%) | 24 (92%) | 2 (8%)  | 0        | 100         | 100 |
| 1   | a7    | 26/38 (68%) | 24 (92%) | 2 (8%)  | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 1   | b1    | 26/38 (68%)   | 25 (96%)  | 1 (4%)   | 0        | 100         | 100 |
| 1   | b2    | 26/38 (68%)   | 25 (96%)  | 1 (4%)   | 0        | 100         | 100 |
| 1   | b5    | 26/38 (68%)   | 25 (96%)  | 1 (4%)   | 0        | 100         | 100 |
| 1   | b6    | 26/38 (68%)   | 25 (96%)  | 1 (4%)   | 0        | 100         | 100 |
| 1   | b7    | 26/38 (68%)   | 25 (96%)  | 1 (4%)   | 0        | 100         | 100 |
| 1   | c     | 32/38 (84%)   | 29 (91%)  | 3 (9%)   | 0        | 100         | 100 |
| 1   | d     | 32/38 (84%)   | 29 (91%)  | 3 (9%)   | 0        | 100         | 100 |
| 1   | d1    | 32/38 (84%)   | 24 (75%)  | 8 (25%)  | 0        | 100         | 100 |
| 1   | d2    | 32/38 (84%)   | 26 (81%)  | 6 (19%)  | 0        | 100         | 100 |
| 1   | d5    | 32/38 (84%)   | 25 (78%)  | 7 (22%)  | 0        | 100         | 100 |
| 1   | d6    | 32/38 (84%)   | 25 (78%)  | 7 (22%)  | 0        | 100         | 100 |
| 1   | d7    | 32/38 (84%)   | 24 (75%)  | 8 (25%)  | 0        | 100         | 100 |
| 1   | e     | 32/38 (84%)   | 31 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 1   | e1    | 26/38 (68%)   | 19 (73%)  | 7 (27%)  | 0        | 100         | 100 |
| 1   | e2    | 26/38 (68%)   | 22 (85%)  | 4 (15%)  | 0        | 100         | 100 |
| 1   | e5    | 26/38 (68%)   | 21 (81%)  | 5 (19%)  | 0        | 100         | 100 |
| 1   | e6    | 26/38 (68%)   | 19 (73%)  | 7 (27%)  | 0        | 100         | 100 |
| 1   | e7    | 26/38 (68%)   | 18 (69%)  | 8 (31%)  | 0        | 100         | 100 |
| 1   | f     | 32/38 (84%)   | 31 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 1   | g     | 32/38 (84%)   | 31 (97%)  | 1 (3%)   | 0        | 100         | 100 |
| 2   | f1    | 18/217 (8%)   | 15 (83%)  | 3 (17%)  | 0        | 100         | 100 |
| 2   | f2    | 18/217 (8%)   | 16 (89%)  | 2 (11%)  | 0        | 100         | 100 |
| 2   | f5    | 18/217 (8%)   | 12 (67%)  | 6 (33%)  | 0        | 100         | 100 |
| 2   | f6    | 18/217 (8%)   | 15 (83%)  | 3 (17%)  | 0        | 100         | 100 |
| 2   | f7    | 18/217 (8%)   | 16 (89%)  | 2 (11%)  | 0        | 100         | 100 |
| 3   | g1    | 297/465 (64%) | 253 (85%) | 43 (14%) | 1 (0%)   | 37          | 69  |
| 3   | g2    | 297/465 (64%) | 251 (84%) | 44 (15%) | 2 (1%)   | 19          | 53  |
| 3   | g5    | 297/465 (64%) | 250 (84%) | 46 (16%) | 1 (0%)   | 37          | 69  |
| 3   | g6    | 297/465 (64%) | 250 (84%) | 46 (16%) | 1 (0%)   | 37          | 69  |
| 3   | g7    | 297/465 (64%) | 252 (85%) | 43 (14%) | 2 (1%)   | 19          | 53  |
| 3   | h1    | 297/465 (64%) | 243 (82%) | 51 (17%) | 3 (1%)   | 13          | 46  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 3   | h2    | 297/465 (64%) | 242 (82%) | 50 (17%) | 5 (2%)   | 7           | 36  |
| 3   | h5    | 297/465 (64%) | 242 (82%) | 53 (18%) | 2 (1%)   | 19          | 53  |
| 3   | h6    | 297/465 (64%) | 241 (81%) | 54 (18%) | 2 (1%)   | 19          | 53  |
| 3   | h7    | 297/465 (64%) | 247 (83%) | 48 (16%) | 2 (1%)   | 19          | 53  |
| 3   | k1    | 286/465 (62%) | 251 (88%) | 35 (12%) | 0        | 100         | 100 |
| 3   | k2    | 286/465 (62%) | 248 (87%) | 37 (13%) | 1 (0%)   | 37          | 69  |
| 3   | k5    | 286/465 (62%) | 248 (87%) | 38 (13%) | 0        | 100         | 100 |
| 3   | k6    | 286/465 (62%) | 251 (88%) | 34 (12%) | 1 (0%)   | 37          | 69  |
| 3   | k7    | 286/465 (62%) | 249 (87%) | 36 (13%) | 1 (0%)   | 37          | 69  |
| 3   | n1    | 297/465 (64%) | 247 (83%) | 49 (16%) | 1 (0%)   | 37          | 69  |
| 3   | n2    | 297/465 (64%) | 243 (82%) | 52 (18%) | 2 (1%)   | 19          | 53  |
| 3   | n5    | 297/465 (64%) | 245 (82%) | 50 (17%) | 2 (1%)   | 19          | 53  |
| 3   | n6    | 297/465 (64%) | 246 (83%) | 49 (16%) | 2 (1%)   | 19          | 53  |
| 3   | n7    | 297/465 (64%) | 249 (84%) | 46 (16%) | 2 (1%)   | 19          | 53  |
| 3   | o1    | 297/465 (64%) | 248 (84%) | 45 (15%) | 4 (1%)   | 10          | 41  |
| 3   | o2    | 297/465 (64%) | 245 (82%) | 47 (16%) | 5 (2%)   | 7           | 36  |
| 3   | o5    | 297/465 (64%) | 245 (82%) | 47 (16%) | 5 (2%)   | 7           | 36  |
| 3   | o6    | 297/465 (64%) | 242 (82%) | 50 (17%) | 5 (2%)   | 7           | 36  |
| 3   | o7    | 297/465 (64%) | 248 (84%) | 45 (15%) | 4 (1%)   | 10          | 41  |
| 3   | r1    | 297/465 (64%) | 254 (86%) | 42 (14%) | 1 (0%)   | 37          | 69  |
| 3   | r2    | 297/465 (64%) | 251 (84%) | 45 (15%) | 1 (0%)   | 37          | 69  |
| 3   | r5    | 297/465 (64%) | 250 (84%) | 44 (15%) | 3 (1%)   | 13          | 46  |
| 3   | r6    | 297/465 (64%) | 252 (85%) | 44 (15%) | 1 (0%)   | 37          | 69  |
| 3   | r7    | 297/465 (64%) | 255 (86%) | 37 (12%) | 5 (2%)   | 7           | 36  |
| 4   | l1    | 135/137 (98%) | 119 (88%) | 16 (12%) | 0        | 100         | 100 |
| 4   | l2    | 135/137 (98%) | 117 (87%) | 15 (11%) | 3 (2%)   | 5           | 32  |
| 4   | l5    | 135/137 (98%) | 120 (89%) | 14 (10%) | 1 (1%)   | 19          | 53  |
| 4   | l6    | 135/137 (98%) | 119 (88%) | 15 (11%) | 1 (1%)   | 19          | 53  |
| 4   | l7    | 135/137 (98%) | 121 (90%) | 13 (10%) | 1 (1%)   | 19          | 53  |
| 4   | m1    | 135/137 (98%) | 117 (87%) | 18 (13%) | 0        | 100         | 100 |
| 4   | m2    | 135/137 (98%) | 119 (88%) | 16 (12%) | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4   | m5    | 135/137 (98%) | 118 (87%) | 17 (13%) | 0        | 100         | 100 |
| 4   | m6    | 135/137 (98%) | 119 (88%) | 16 (12%) | 0        | 100         | 100 |
| 4   | m7    | 135/137 (98%) | 117 (87%) | 18 (13%) | 0        | 100         | 100 |
| 4   | p1    | 135/137 (98%) | 112 (83%) | 22 (16%) | 1 (1%)   | 19          | 53  |
| 4   | p2    | 135/137 (98%) | 111 (82%) | 23 (17%) | 1 (1%)   | 19          | 53  |
| 4   | p5    | 135/137 (98%) | 110 (82%) | 24 (18%) | 1 (1%)   | 19          | 53  |
| 4   | p6    | 135/137 (98%) | 111 (82%) | 23 (17%) | 1 (1%)   | 19          | 53  |
| 4   | p7    | 135/137 (98%) | 112 (83%) | 22 (16%) | 1 (1%)   | 19          | 53  |
| 4   | q1    | 135/137 (98%) | 120 (89%) | 15 (11%) | 0        | 100         | 100 |
| 4   | q2    | 135/137 (98%) | 119 (88%) | 16 (12%) | 0        | 100         | 100 |
| 4   | q5    | 135/137 (98%) | 117 (87%) | 18 (13%) | 0        | 100         | 100 |
| 4   | q6    | 135/137 (98%) | 122 (90%) | 13 (10%) | 0        | 100         | 100 |
| 4   | q7    | 135/137 (98%) | 120 (89%) | 15 (11%) | 0        | 100         | 100 |
| 4   | s1    | 135/137 (98%) | 125 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 4   | s2    | 135/137 (98%) | 124 (92%) | 10 (7%)  | 1 (1%)   | 19          | 53  |
| 4   | s5    | 135/137 (98%) | 125 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 4   | s6    | 135/137 (98%) | 124 (92%) | 10 (7%)  | 1 (1%)   | 19          | 53  |
| 4   | s7    | 135/137 (98%) | 125 (93%) | 10 (7%)  | 0        | 100         | 100 |
| 4   | t1    | 135/137 (98%) | 121 (90%) | 14 (10%) | 0        | 100         | 100 |
| 4   | t2    | 135/137 (98%) | 123 (91%) | 12 (9%)  | 0        | 100         | 100 |
| 4   | t5    | 135/137 (98%) | 122 (90%) | 13 (10%) | 0        | 100         | 100 |
| 4   | t6    | 135/137 (98%) | 124 (92%) | 11 (8%)  | 0        | 100         | 100 |
| 4   | t7    | 135/137 (98%) | 119 (88%) | 16 (12%) | 0        | 100         | 100 |
| 4   | u1    | 134/137 (98%) | 119 (89%) | 15 (11%) | 0        | 100         | 100 |
| 4   | u2    | 134/137 (98%) | 118 (88%) | 16 (12%) | 0        | 100         | 100 |
| 4   | u5    | 134/137 (98%) | 118 (88%) | 16 (12%) | 0        | 100         | 100 |
| 4   | u6    | 134/137 (98%) | 119 (89%) | 15 (11%) | 0        | 100         | 100 |
| 4   | u7    | 134/137 (98%) | 119 (89%) | 15 (11%) | 0        | 100         | 100 |
| 4   | v1    | 134/137 (98%) | 113 (84%) | 19 (14%) | 2 (2%)   | 8           | 38  |
| 4   | v2    | 134/137 (98%) | 111 (83%) | 23 (17%) | 0        | 100         | 100 |
| 4   | v5    | 134/137 (98%) | 113 (84%) | 21 (16%) | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 4   | v6    | 134/137 (98%) | 114 (85%) | 20 (15%) | 0        | 100         | 100 |
| 4   | v7    | 134/137 (98%) | 113 (84%) | 20 (15%) | 1 (1%)   | 19          | 53  |
| 5   | 03    | 219/230 (95%) | 201 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 5   | 13    | 219/230 (95%) | 200 (91%) | 19 (9%)  | 0        | 100         | 100 |
| 5   | 23    | 219/230 (95%) | 192 (88%) | 27 (12%) | 0        | 100         | 100 |
| 5   | 33    | 219/230 (95%) | 197 (90%) | 22 (10%) | 0        | 100         | 100 |
| 5   | 43    | 219/230 (95%) | 198 (90%) | 21 (10%) | 0        | 100         | 100 |
| 5   | 53    | 219/230 (95%) | 206 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 5   | 63    | 219/230 (95%) | 198 (90%) | 21 (10%) | 0        | 100         | 100 |
| 5   | 73    | 219/230 (95%) | 199 (91%) | 20 (9%)  | 0        | 100         | 100 |
| 5   | 83    | 219/230 (95%) | 206 (94%) | 13 (6%)  | 0        | 100         | 100 |
| 5   | 93    | 219/230 (95%) | 198 (90%) | 21 (10%) | 0        | 100         | 100 |
| 5   | A3    | 219/230 (95%) | 202 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 5   | B3    | 219/230 (95%) | 199 (91%) | 20 (9%)  | 0        | 100         | 100 |
| 5   | C3    | 219/230 (95%) | 199 (91%) | 20 (9%)  | 0        | 100         | 100 |
| 5   | D3    | 219/230 (95%) | 204 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 5   | E3    | 219/230 (95%) | 201 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 5   | F3    | 219/230 (95%) | 200 (91%) | 19 (9%)  | 0        | 100         | 100 |
| 5   | G3    | 219/230 (95%) | 203 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 5   | J3    | 219/230 (95%) | 201 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 5   | K3    | 228/230 (99%) | 210 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 5   | L3    | 219/230 (95%) | 200 (91%) | 19 (9%)  | 0        | 100         | 100 |
| 5   | M3    | 219/230 (95%) | 200 (91%) | 19 (9%)  | 0        | 100         | 100 |
| 5   | N3    | 228/230 (99%) | 207 (91%) | 20 (9%)  | 1 (0%)   | 30          | 64  |
| 5   | O3    | 219/230 (95%) | 198 (90%) | 21 (10%) | 0        | 100         | 100 |
| 5   | P3    | 219/230 (95%) | 202 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 5   | Q3    | 228/230 (99%) | 206 (90%) | 21 (9%)  | 1 (0%)   | 30          | 64  |
| 5   | R3    | 219/230 (95%) | 203 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 5   | S3    | 219/230 (95%) | 202 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 5   | T3    | 228/230 (99%) | 206 (90%) | 20 (9%)  | 2 (1%)   | 14          | 48  |
| 5   | U3    | 219/230 (95%) | 199 (91%) | 20 (9%)  | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 5   | V3    | 219/230 (95%) | 202 (92%) | 17 (8%)  | 0        | 100         | 100 |
| 5   | W3    | 228/230 (99%) | 206 (90%) | 22 (10%) | 0        | 100         | 100 |
| 5   | X3    | 219/230 (95%) | 201 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 5   | Y3    | 219/230 (95%) | 196 (90%) | 23 (10%) | 0        | 100         | 100 |
| 5   | Z3    | 219/230 (95%) | 198 (90%) | 21 (10%) | 0        | 100         | 100 |
| 5   | a3    | 219/230 (95%) | 198 (90%) | 21 (10%) | 0        | 100         | 100 |
| 5   | b3    | 219/230 (95%) | 199 (91%) | 20 (9%)  | 0        | 100         | 100 |
| 5   | c3    | 219/230 (95%) | 196 (90%) | 22 (10%) | 1 (0%)   | 25          | 59  |
| 5   | d3    | 219/230 (95%) | 199 (91%) | 20 (9%)  | 0        | 100         | 100 |
| 5   | e3    | 219/230 (95%) | 199 (91%) | 20 (9%)  | 0        | 100         | 100 |
| 5   | f3    | 219/230 (95%) | 195 (89%) | 24 (11%) | 0        | 100         | 100 |
| 5   | g3    | 219/230 (95%) | 201 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 5   | h3    | 219/230 (95%) | 196 (90%) | 23 (10%) | 0        | 100         | 100 |
| 5   | i3    | 219/230 (95%) | 196 (90%) | 23 (10%) | 0        | 100         | 100 |
| 5   | j3    | 219/230 (95%) | 197 (90%) | 22 (10%) | 0        | 100         | 100 |
| 5   | k3    | 219/230 (95%) | 198 (90%) | 21 (10%) | 0        | 100         | 100 |
| 5   | l3    | 219/230 (95%) | 196 (90%) | 22 (10%) | 1 (0%)   | 25          | 59  |
| 5   | m3    | 219/230 (95%) | 199 (91%) | 20 (9%)  | 0        | 100         | 100 |
| 5   | n3    | 219/230 (95%) | 197 (90%) | 22 (10%) | 0        | 100         | 100 |
| 5   | o3    | 219/230 (95%) | 201 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 5   | p3    | 219/230 (95%) | 192 (88%) | 27 (12%) | 0        | 100         | 100 |
| 5   | q3    | 219/230 (95%) | 199 (91%) | 20 (9%)  | 0        | 100         | 100 |
| 5   | r3    | 219/230 (95%) | 201 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 5   | s3    | 219/230 (95%) | 192 (88%) | 27 (12%) | 0        | 100         | 100 |
| 5   | t3    | 219/230 (95%) | 197 (90%) | 22 (10%) | 0        | 100         | 100 |
| 5   | u3    | 219/230 (95%) | 201 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 5   | v3    | 219/230 (95%) | 191 (87%) | 28 (13%) | 0        | 100         | 100 |
| 5   | w3    | 219/230 (95%) | 200 (91%) | 19 (9%)  | 0        | 100         | 100 |
| 5   | x3    | 219/230 (95%) | 199 (91%) | 20 (9%)  | 0        | 100         | 100 |
| 5   | y3    | 219/230 (95%) | 192 (88%) | 27 (12%) | 0        | 100         | 100 |
| 5   | z3    | 219/230 (95%) | 197 (90%) | 22 (10%) | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed          | Favoured    | Allowed    | Outliers | Percentiles |    |
|-----|-------|-------------------|-------------|------------|----------|-------------|----|
| 6   | A4    | 85/202 (42%)      | 66 (78%)    | 18 (21%)   | 1 (1%)   | 11          | 43 |
| 6   | B4    | 85/202 (42%)      | 72 (85%)    | 12 (14%)   | 1 (1%)   | 11          | 43 |
| 6   | C4    | 85/202 (42%)      | 67 (79%)    | 15 (18%)   | 3 (4%)   | 3           | 24 |
| 6   | D4    | 85/202 (42%)      | 71 (84%)    | 11 (13%)   | 3 (4%)   | 3           | 24 |
| 6   | E4    | 85/202 (42%)      | 71 (84%)    | 13 (15%)   | 1 (1%)   | 11          | 43 |
| All | All   | 28655/36275 (79%) | 25176 (88%) | 3381 (12%) | 98 (0%)  | 38          | 69 |

All (98) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | h1    | 172 | PRO  |
| 4   | p1    | 78  | LEU  |
| 3   | g2    | 457 | GLU  |
| 3   | h2    | 191 | ALA  |
| 4   | l2    | 75  | ASP  |
| 3   | o2    | 172 | PRO  |
| 5   | T3    | 21  | SER  |
| 5   | c3    | 172 | ALA  |
| 6   | A4    | 74  | ILE  |
| 6   | B4    | 74  | ILE  |
| 6   | C4    | 74  | ILE  |
| 6   | E4    | 74  | ILE  |
| 3   | g5    | 172 | PRO  |
| 4   | l5    | 75  | ASP  |
| 4   | p5    | 78  | LEU  |
| 3   | r5    | 172 | PRO  |
| 3   | g6    | 170 | ILE  |
| 4   | l6    | 75  | ASP  |
| 3   | g7    | 172 | PRO  |
| 3   | h7    | 172 | PRO  |
| 3   | h7    | 190 | CYS  |
| 4   | l7    | 75  | ASP  |
| 3   | r7    | 172 | PRO  |
| 3   | r1    | 398 | THR  |
| 4   | v1    | 74  | CYS  |
| 4   | v1    | 75  | ASP  |
| 3   | g2    | 170 | ILE  |
| 3   | h2    | 384 | ASN  |
| 4   | p2    | 77  | VAL  |
| 4   | s2    | 26  | ASP  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | N3    | 21  | SER  |
| 6   | D4    | 74  | ILE  |
| 6   | D4    | 122 | VAL  |
| 6   | D4    | 123 | GLU  |
| 3   | o5    | 171 | GLY  |
| 3   | h6    | 191 | ALA  |
| 3   | o6    | 172 | PRO  |
| 3   | n7    | 171 | GLY  |
| 4   | v7    | 75  | ASP  |
| 3   | g1    | 172 | PRO  |
| 3   | o1    | 189 | GLU  |
| 3   | n2    | 172 | PRO  |
| 3   | o2    | 189 | GLU  |
| 3   | r2    | 395 | LYS  |
| 6   | C4    | 134 | ARG  |
| 3   | h5    | 190 | CYS  |
| 3   | o5    | 172 | PRO  |
| 3   | o5    | 189 | GLU  |
| 3   | r5    | 396 | GLY  |
| 3   | k6    | 359 | ASN  |
| 3   | n6    | 171 | GLY  |
| 3   | o6    | 171 | GLY  |
| 3   | r6    | 395 | LYS  |
| 3   | g7    | 173 | ALA  |
| 3   | k7    | 359 | ASN  |
| 3   | n7    | 172 | PRO  |
| 3   | o7    | 189 | GLU  |
| 4   | p7    | 77  | VAL  |
| 3   | r7    | 396 | GLY  |
| 3   | h1    | 189 | GLU  |
| 3   | h1    | 190 | CYS  |
| 3   | o1    | 373 | PRO  |
| 3   | h2    | 172 | PRO  |
| 3   | k2    | 359 | ASN  |
| 3   | n2    | 171 | GLY  |
| 3   | o2    | 373 | PRO  |
| 5   | Q3    | 18  | VAL  |
| 5   | T3    | 13  | SER  |
| 5   | l3    | 173 | ALA  |
| 3   | o5    | 373 | PRO  |
| 3   | o6    | 189 | GLU  |
| 3   | o6    | 373 | PRO  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | p6    | 77  | VAL  |
| 4   | s6    | 26  | ASP  |
| 3   | o7    | 224 | ASP  |
| 3   | o7    | 373 | PRO  |
| 3   | r7    | 395 | LYS  |
| 3   | n1    | 172 | PRO  |
| 3   | o1    | 172 | PRO  |
| 3   | h2    | 190 | CYS  |
| 3   | o2    | 171 | GLY  |
| 3   | o2    | 224 | ASP  |
| 3   | o6    | 224 | ASP  |
| 3   | o7    | 172 | PRO  |
| 3   | r7    | 171 | GLY  |
| 3   | r7    | 174 | PHE  |
| 3   | o1    | 224 | ASP  |
| 3   | h2    | 382 | ILE  |
| 4   | l2    | 77  | VAL  |
| 6   | C4    | 133 | GLY  |
| 3   | n5    | 172 | PRO  |
| 3   | o5    | 224 | ASP  |
| 3   | h6    | 171 | GLY  |
| 3   | h5    | 172 | PRO  |
| 3   | n5    | 171 | GLY  |
| 4   | l2    | 83  | GLY  |
| 3   | n6    | 172 | PRO  |
| 3   | r5    | 392 | GLY  |

### 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    | 25/32 (78%) | 24 (96%)  | 1 (4%)   | 27          | 57 |
| 1   | a2    | 25/32 (78%) | 24 (96%)  | 1 (4%)   | 27          | 57 |
| 1   | a5    | 25/32 (78%) | 23 (92%)  | 2 (8%)   | 10          | 34 |
| 1   | a6    | 25/32 (78%) | 24 (96%)  | 1 (4%)   | 27          | 57 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | a7    | 25/32 (78%)   | 24 (96%)   | 1 (4%)   | 27          | 57  |
| 1   | b1    | 25/32 (78%)   | 25 (100%)  | 0        | 100         | 100 |
| 1   | b2    | 25/32 (78%)   | 25 (100%)  | 0        | 100         | 100 |
| 1   | b5    | 25/32 (78%)   | 25 (100%)  | 0        | 100         | 100 |
| 1   | b6    | 25/32 (78%)   | 25 (100%)  | 0        | 100         | 100 |
| 1   | b7    | 25/32 (78%)   | 25 (100%)  | 0        | 100         | 100 |
| 1   | c     | 29/32 (91%)   | 28 (97%)   | 1 (3%)   | 32          | 61  |
| 1   | d     | 29/32 (91%)   | 29 (100%)  | 0        | 100         | 100 |
| 1   | d1    | 29/32 (91%)   | 29 (100%)  | 0        | 100         | 100 |
| 1   | d2    | 29/32 (91%)   | 29 (100%)  | 0        | 100         | 100 |
| 1   | d5    | 29/32 (91%)   | 29 (100%)  | 0        | 100         | 100 |
| 1   | d6    | 29/32 (91%)   | 29 (100%)  | 0        | 100         | 100 |
| 1   | d7    | 29/32 (91%)   | 29 (100%)  | 0        | 100         | 100 |
| 1   | e     | 29/32 (91%)   | 28 (97%)   | 1 (3%)   | 32          | 61  |
| 1   | e1    | 25/32 (78%)   | 25 (100%)  | 0        | 100         | 100 |
| 1   | e2    | 25/32 (78%)   | 25 (100%)  | 0        | 100         | 100 |
| 1   | e5    | 25/32 (78%)   | 25 (100%)  | 0        | 100         | 100 |
| 1   | e6    | 25/32 (78%)   | 25 (100%)  | 0        | 100         | 100 |
| 1   | e7    | 25/32 (78%)   | 25 (100%)  | 0        | 100         | 100 |
| 1   | f     | 29/32 (91%)   | 29 (100%)  | 0        | 100         | 100 |
| 1   | g     | 29/32 (91%)   | 29 (100%)  | 0        | 100         | 100 |
| 2   | f1    | 15/175 (9%)   | 15 (100%)  | 0        | 100         | 100 |
| 2   | f2    | 15/175 (9%)   | 15 (100%)  | 0        | 100         | 100 |
| 2   | f5    | 15/175 (9%)   | 15 (100%)  | 0        | 100         | 100 |
| 2   | f6    | 15/175 (9%)   | 15 (100%)  | 0        | 100         | 100 |
| 2   | f7    | 15/175 (9%)   | 15 (100%)  | 0        | 100         | 100 |
| 3   | g1    | 240/379 (63%) | 238 (99%)  | 2 (1%)   | 79          | 87  |
| 3   | g2    | 240/379 (63%) | 234 (98%)  | 6 (2%)   | 42          | 69  |
| 3   | g5    | 240/379 (63%) | 240 (100%) | 0        | 100         | 100 |
| 3   | g6    | 240/379 (63%) | 237 (99%)  | 3 (1%)   | 65          | 81  |
| 3   | g7    | 240/379 (63%) | 238 (99%)  | 2 (1%)   | 79          | 87  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | h1    | 240/379 (63%)  | 234 (98%)  | 6 (2%)   | 42          | 69  |
| 3   | h2    | 240/379 (63%)  | 234 (98%)  | 6 (2%)   | 42          | 69  |
| 3   | h5    | 240/379 (63%)  | 233 (97%)  | 7 (3%)   | 37          | 65  |
| 3   | h6    | 240/379 (63%)  | 234 (98%)  | 6 (2%)   | 42          | 69  |
| 3   | h7    | 240/379 (63%)  | 239 (100%) | 1 (0%)   | 89          | 94  |
| 3   | k1    | 232/379 (61%)  | 231 (100%) | 1 (0%)   | 89          | 94  |
| 3   | k2    | 232/379 (61%)  | 231 (100%) | 1 (0%)   | 89          | 94  |
| 3   | k5    | 232/379 (61%)  | 232 (100%) | 0        | 100         | 100 |
| 3   | k6    | 232/379 (61%)  | 232 (100%) | 0        | 100         | 100 |
| 3   | k7    | 232/379 (61%)  | 232 (100%) | 0        | 100         | 100 |
| 3   | n1    | 240/379 (63%)  | 238 (99%)  | 2 (1%)   | 79          | 87  |
| 3   | n2    | 240/379 (63%)  | 238 (99%)  | 2 (1%)   | 79          | 87  |
| 3   | n5    | 240/379 (63%)  | 239 (100%) | 1 (0%)   | 89          | 94  |
| 3   | n6    | 240/379 (63%)  | 238 (99%)  | 2 (1%)   | 79          | 87  |
| 3   | n7    | 240/379 (63%)  | 238 (99%)  | 2 (1%)   | 79          | 87  |
| 3   | o1    | 240/379 (63%)  | 238 (99%)  | 2 (1%)   | 79          | 87  |
| 3   | o2    | 240/379 (63%)  | 239 (100%) | 1 (0%)   | 89          | 94  |
| 3   | o5    | 240/379 (63%)  | 239 (100%) | 1 (0%)   | 89          | 94  |
| 3   | o6    | 240/379 (63%)  | 239 (100%) | 1 (0%)   | 89          | 94  |
| 3   | o7    | 240/379 (63%)  | 238 (99%)  | 2 (1%)   | 79          | 87  |
| 3   | r1    | 240/379 (63%)  | 233 (97%)  | 7 (3%)   | 37          | 65  |
| 3   | r2    | 240/379 (63%)  | 234 (98%)  | 6 (2%)   | 42          | 69  |
| 3   | r5    | 240/379 (63%)  | 235 (98%)  | 5 (2%)   | 48          | 72  |
| 3   | r6    | 240/379 (63%)  | 237 (99%)  | 3 (1%)   | 65          | 81  |
| 3   | r7    | 240/379 (63%)  | 233 (97%)  | 7 (3%)   | 37          | 65  |
| 4   | l1    | 112/112 (100%) | 108 (96%)  | 4 (4%)   | 30          | 60  |
| 4   | l2    | 112/112 (100%) | 107 (96%)  | 5 (4%)   | 23          | 54  |
| 4   | l5    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | l6    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | l7    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | m1    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | m2    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 4   | m5    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 4   | m6    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 4   | m7    | 112/112 (100%) | 112 (100%) | 0        | 100         | 100 |
| 4   | p1    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | p2    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | p5    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | p6    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | p7    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | q1    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | q2    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | q5    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | q6    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | q7    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | s1    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | s2    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | s5    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | s6    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | s7    | 112/112 (100%) | 109 (97%)  | 3 (3%)   | 40          | 67  |
| 4   | t1    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | t2    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | t5    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | t6    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | t7    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | u1    | 111/112 (99%)  | 111 (100%) | 0        | 100         | 100 |
| 4   | u2    | 111/112 (99%)  | 109 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | u5    | 111/112 (99%)  | 109 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | u6    | 111/112 (99%)  | 110 (99%)  | 1 (1%)   | 75          | 86  |
| 4   | u7    | 111/112 (99%)  | 109 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | v1    | 111/112 (99%)  | 106 (96%)  | 5 (4%)   | 23          | 54  |
| 4   | v2    | 111/112 (99%)  | 109 (98%)  | 2 (2%)   | 54          | 75  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 4   | v5    | 111/112 (99%)  | 108 (97%)  | 3 (3%)   | 40          | 67  |
| 4   | v6    | 111/112 (99%)  | 109 (98%)  | 2 (2%)   | 54          | 75  |
| 4   | v7    | 111/112 (99%)  | 109 (98%)  | 2 (2%)   | 54          | 75  |
| 5   | 03    | 186/191 (97%)  | 185 (100%) | 1 (0%)   | 86          | 92  |
| 5   | 13    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | 23    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | 33    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | 43    | 186/191 (97%)  | 185 (100%) | 1 (0%)   | 86          | 92  |
| 5   | 53    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | 63    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | 73    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | 83    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | 93    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | A3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | B3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | C3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | D3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | E3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | F3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | G3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | J3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | K3    | 191/191 (100%) | 189 (99%)  | 2 (1%)   | 73          | 84  |
| 5   | L3    | 186/191 (97%)  | 185 (100%) | 1 (0%)   | 86          | 92  |
| 5   | M3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | N3    | 191/191 (100%) | 189 (99%)  | 2 (1%)   | 73          | 84  |
| 5   | O3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | P3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | Q3    | 191/191 (100%) | 191 (100%) | 0        | 100         | 100 |
| 5   | R3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | S3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | T3    | 191/191 (100%) | 189 (99%)  | 2 (1%)   | 73          | 84  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 5   | U3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | V3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | W3    | 191/191 (100%) | 191 (100%) | 0        | 100         | 100 |
| 5   | X3    | 186/191 (97%)  | 185 (100%) | 1 (0%)   | 86          | 92  |
| 5   | Y3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | Z3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | a3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | b3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | c3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | d3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | e3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | f3    | 186/191 (97%)  | 185 (100%) | 1 (0%)   | 86          | 92  |
| 5   | g3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | h3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | i3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | j3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | k3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | l3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | m3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | n3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | o3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | p3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | q3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | r3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | s3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | t3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | u3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | v3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | w3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | x3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |
| 5   | y3    | 186/191 (97%)  | 186 (100%) | 0        | 100         | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 5   | z3    | 186/191 (97%)     | 186 (100%)  | 0        | 100         | 100 |
| 6   | A4    | 73/168 (44%)      | 72 (99%)    | 1 (1%)   | 62          | 79  |
| 6   | B4    | 73/168 (44%)      | 70 (96%)    | 3 (4%)   | 26          | 56  |
| 6   | C4    | 73/168 (44%)      | 72 (99%)    | 1 (1%)   | 62          | 79  |
| 6   | D4    | 73/168 (44%)      | 68 (93%)    | 5 (7%)   | 13          | 41  |
| 6   | E4    | 73/168 (44%)      | 71 (97%)    | 2 (3%)   | 40          | 67  |
| All | All   | 23920/29825 (80%) | 23738 (99%) | 182 (1%) | 77          | 87  |

All (182) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | a1    | 6   | CYS  |
| 3   | g1    | 170 | ILE  |
| 3   | g1    | 403 | PHE  |
| 3   | h1    | 170 | ILE  |
| 3   | h1    | 188 | ILE  |
| 3   | h1    | 190 | CYS  |
| 3   | h1    | 386 | LEU  |
| 3   | h1    | 403 | PHE  |
| 3   | h1    | 455 | CYS  |
| 3   | k1    | 370 | THR  |
| 4   | l1    | 73  | PHE  |
| 4   | l1    | 74  | CYS  |
| 4   | l1    | 75  | ASP  |
| 4   | l1    | 129 | THR  |
| 3   | n1    | 170 | ILE  |
| 3   | n1    | 252 | CYS  |
| 3   | o1    | 170 | ILE  |
| 3   | o1    | 211 | LYS  |
| 4   | p1    | 75  | ASP  |
| 4   | p1    | 78  | LEU  |
| 4   | q1    | 26  | ASP  |
| 4   | q1    | 106 | MET  |
| 3   | r1    | 175 | PHE  |
| 3   | r1    | 252 | CYS  |
| 3   | r1    | 377 | ARG  |
| 3   | r1    | 378 | GLU  |
| 3   | r1    | 379 | ARG  |
| 3   | r1    | 395 | LYS  |
| 3   | r1    | 398 | THR  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | s1    | 129 | THR  |
| 4   | t1    | 137 | ARG  |
| 4   | v1    | 3   | PHE  |
| 4   | v1    | 73  | PHE  |
| 4   | v1    | 74  | CYS  |
| 4   | v1    | 75  | ASP  |
| 4   | v1    | 84  | LEU  |
| 1   | a2    | 5   | ASN  |
| 3   | g2    | 169 | THR  |
| 3   | g2    | 170 | ILE  |
| 3   | g2    | 403 | PHE  |
| 3   | g2    | 455 | CYS  |
| 3   | g2    | 456 | CYS  |
| 3   | g2    | 457 | GLU  |
| 3   | h2    | 170 | ILE  |
| 3   | h2    | 188 | ILE  |
| 3   | h2    | 189 | GLU  |
| 3   | h2    | 384 | ASN  |
| 3   | h2    | 386 | LEU  |
| 3   | h2    | 403 | PHE  |
| 3   | k2    | 370 | THR  |
| 4   | l2    | 73  | PHE  |
| 4   | l2    | 74  | CYS  |
| 4   | l2    | 76  | THR  |
| 4   | l2    | 77  | VAL  |
| 4   | l2    | 129 | THR  |
| 3   | n2    | 170 | ILE  |
| 3   | n2    | 252 | CYS  |
| 3   | o2    | 211 | LYS  |
| 4   | p2    | 75  | ASP  |
| 4   | p2    | 77  | VAL  |
| 4   | q2    | 106 | MET  |
| 3   | r2    | 175 | PHE  |
| 3   | r2    | 176 | THR  |
| 3   | r2    | 377 | ARG  |
| 3   | r2    | 379 | ARG  |
| 3   | r2    | 395 | LYS  |
| 3   | r2    | 398 | THR  |
| 4   | s2    | 37  | THR  |
| 4   | s2    | 129 | THR  |
| 4   | t2    | 137 | ARG  |
| 4   | u2    | 132 | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | u2    | 136 | THR  |
| 4   | v2    | 3   | PHE  |
| 4   | v2    | 84  | LEU  |
| 5   | K3    | 19  | CYS  |
| 5   | K3    | 23  | CYS  |
| 5   | L3    | 180 | ARG  |
| 5   | N3    | 22  | CYS  |
| 5   | N3    | 23  | CYS  |
| 5   | T3    | 15  | SER  |
| 5   | T3    | 21  | SER  |
| 5   | X3    | 180 | ARG  |
| 5   | f3    | 175 | ARG  |
| 5   | 43    | 135 | ASP  |
| 5   | 03    | 135 | ASP  |
| 6   | A4    | 74  | ILE  |
| 6   | B4    | 74  | ILE  |
| 6   | B4    | 134 | ARG  |
| 6   | B4    | 135 | ARG  |
| 6   | C4    | 134 | ARG  |
| 6   | D4    | 122 | VAL  |
| 6   | D4    | 123 | GLU  |
| 6   | D4    | 125 | GLN  |
| 6   | D4    | 134 | ARG  |
| 6   | D4    | 136 | CYS  |
| 6   | E4    | 74  | ILE  |
| 6   | E4    | 134 | ARG  |
| 1   | a5    | 5   | ASN  |
| 1   | a5    | 6   | CYS  |
| 3   | h5    | 170 | ILE  |
| 3   | h5    | 190 | CYS  |
| 3   | h5    | 221 | TYR  |
| 3   | h5    | 384 | ASN  |
| 3   | h5    | 386 | LEU  |
| 3   | h5    | 403 | PHE  |
| 3   | h5    | 455 | CYS  |
| 4   | l5    | 73  | PHE  |
| 4   | l5    | 74  | CYS  |
| 3   | n5    | 170 | ILE  |
| 3   | o5    | 211 | LYS  |
| 4   | p5    | 75  | ASP  |
| 4   | p5    | 78  | LEU  |
| 4   | q5    | 106 | MET  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | r5    | 175 | PHE  |
| 3   | r5    | 176 | THR  |
| 3   | r5    | 379 | ARG  |
| 3   | r5    | 395 | LYS  |
| 3   | r5    | 398 | THR  |
| 4   | s5    | 129 | THR  |
| 4   | t5    | 137 | ARG  |
| 4   | u5    | 93  | VAL  |
| 4   | u5    | 94  | THR  |
| 4   | v5    | 3   | PHE  |
| 4   | v5    | 73  | PHE  |
| 4   | v5    | 74  | CYS  |
| 1   | a6    | 6   | CYS  |
| 3   | g6    | 169 | THR  |
| 3   | g6    | 170 | ILE  |
| 3   | g6    | 403 | PHE  |
| 3   | h6    | 170 | ILE  |
| 3   | h6    | 188 | ILE  |
| 3   | h6    | 190 | CYS  |
| 3   | h6    | 193 | LEU  |
| 3   | h6    | 385 | CYS  |
| 3   | h6    | 403 | PHE  |
| 4   | l6    | 73  | PHE  |
| 4   | l6    | 74  | CYS  |
| 3   | n6    | 170 | ILE  |
| 3   | n6    | 221 | TYR  |
| 3   | o6    | 211 | LYS  |
| 4   | p6    | 75  | ASP  |
| 4   | p6    | 77  | VAL  |
| 4   | q6    | 106 | MET  |
| 3   | r6    | 175 | PHE  |
| 3   | r6    | 379 | ARG  |
| 3   | r6    | 395 | LYS  |
| 4   | s6    | 34  | THR  |
| 4   | s6    | 129 | THR  |
| 4   | t6    | 137 | ARG  |
| 4   | u6    | 96  | ASP  |
| 4   | v6    | 3   | PHE  |
| 4   | v6    | 84  | LEU  |
| 1   | a7    | 6   | CYS  |
| 3   | g7    | 176 | THR  |
| 3   | g7    | 403 | PHE  |

*Continued on next page...*



*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | h7    | 455 | CYS  |
| 4   | l7    | 73  | PHE  |
| 4   | l7    | 129 | THR  |
| 3   | n7    | 221 | TYR  |
| 3   | n7    | 252 | CYS  |
| 3   | o7    | 170 | ILE  |
| 3   | o7    | 211 | LYS  |
| 4   | p7    | 75  | ASP  |
| 4   | p7    | 77  | VAL  |
| 4   | q7    | 106 | MET  |
| 3   | r7    | 170 | ILE  |
| 3   | r7    | 175 | PHE  |
| 3   | r7    | 377 | ARG  |
| 3   | r7    | 379 | ARG  |
| 3   | r7    | 395 | LYS  |
| 3   | r7    | 398 | THR  |
| 3   | r7    | 460 | ARG  |
| 4   | s7    | 34  | THR  |
| 4   | s7    | 37  | THR  |
| 4   | s7    | 129 | THR  |
| 4   | t7    | 9   | PHE  |
| 4   | u7    | 94  | THR  |
| 4   | u7    | 96  | ASP  |
| 4   | v7    | 3   | PHE  |
| 4   | v7    | 74  | CYS  |
| 1   | c     | 24  | PHE  |
| 1   | e     | 24  | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (260) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | g1    | 187 | ASN  |
| 3   | g1    | 239 | HIS  |
| 3   | g1    | 359 | ASN  |
| 3   | g1    | 384 | ASN  |
| 3   | h1    | 277 | HIS  |
| 3   | h1    | 280 | ASN  |
| 3   | h1    | 314 | ASN  |
| 3   | h1    | 346 | GLN  |
| 3   | h1    | 347 | ASN  |
| 3   | h1    | 359 | ASN  |
| 3   | k1    | 324 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | k1    | 359 | ASN  |
| 3   | k1    | 431 | GLN  |
| 3   | k1    | 458 | HIS  |
| 4   | l1    | 122 | ASN  |
| 4   | m1    | 127 | GLN  |
| 3   | n1    | 280 | ASN  |
| 3   | n1    | 283 | GLN  |
| 3   | o1    | 282 | ASN  |
| 3   | o1    | 314 | ASN  |
| 3   | o1    | 346 | GLN  |
| 3   | o1    | 384 | ASN  |
| 3   | o1    | 458 | HIS  |
| 4   | p1    | 2   | ASN  |
| 4   | p1    | 122 | ASN  |
| 4   | p1    | 127 | GLN  |
| 3   | r1    | 254 | ASN  |
| 3   | r1    | 282 | ASN  |
| 3   | r1    | 292 | ASN  |
| 3   | r1    | 359 | ASN  |
| 3   | r1    | 384 | ASN  |
| 3   | r1    | 444 | GLN  |
| 4   | t1    | 52  | HIS  |
| 4   | t1    | 127 | GLN  |
| 4   | u1    | 125 | ASN  |
| 4   | v1    | 127 | GLN  |
| 1   | d2    | 5   | ASN  |
| 3   | g2    | 239 | HIS  |
| 3   | g2    | 359 | ASN  |
| 3   | g2    | 384 | ASN  |
| 3   | h2    | 277 | HIS  |
| 3   | h2    | 280 | ASN  |
| 3   | h2    | 314 | ASN  |
| 3   | h2    | 346 | GLN  |
| 3   | h2    | 359 | ASN  |
| 3   | k2    | 324 | GLN  |
| 3   | k2    | 431 | GLN  |
| 3   | k2    | 458 | HIS  |
| 4   | l2    | 122 | ASN  |
| 4   | m2    | 4   | ASN  |
| 4   | m2    | 127 | GLN  |
| 3   | n2    | 239 | HIS  |
| 3   | n2    | 280 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | n2    | 359 | ASN  |
| 3   | o2    | 282 | ASN  |
| 3   | o2    | 346 | GLN  |
| 3   | o2    | 384 | ASN  |
| 3   | o2    | 458 | HIS  |
| 4   | p2    | 2   | ASN  |
| 4   | p2    | 4   | ASN  |
| 4   | p2    | 122 | ASN  |
| 4   | p2    | 127 | GLN  |
| 3   | r2    | 254 | ASN  |
| 3   | r2    | 292 | ASN  |
| 3   | r2    | 347 | ASN  |
| 3   | r2    | 384 | ASN  |
| 4   | t2    | 127 | GLN  |
| 4   | u2    | 122 | ASN  |
| 4   | u2    | 125 | ASN  |
| 4   | v2    | 107 | ASN  |
| 5   | J3    | 142 | ASN  |
| 5   | K3    | 218 | HIS  |
| 5   | L3    | 182 | HIS  |
| 5   | M3    | 142 | ASN  |
| 5   | N3    | 108 | ASN  |
| 5   | N3    | 218 | HIS  |
| 5   | O3    | 182 | HIS  |
| 5   | P3    | 142 | ASN  |
| 5   | R3    | 112 | ASN  |
| 5   | R3    | 182 | HIS  |
| 5   | S3    | 142 | ASN  |
| 5   | S3    | 182 | HIS  |
| 5   | U3    | 182 | HIS  |
| 5   | V3    | 142 | ASN  |
| 5   | V3    | 182 | HIS  |
| 5   | W3    | 182 | HIS  |
| 5   | X3    | 112 | ASN  |
| 5   | X3    | 182 | HIS  |
| 5   | Y3    | 10  | ASN  |
| 5   | Y3    | 55  | ASN  |
| 5   | a3    | 182 | HIS  |
| 5   | b3    | 55  | ASN  |
| 5   | e3    | 55  | ASN  |
| 5   | g3    | 182 | HIS  |
| 5   | h3    | 55  | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | j3    | 182 | HIS  |
| 5   | k3    | 55  | ASN  |
| 5   | m3    | 99  | GLN  |
| 5   | n3    | 112 | ASN  |
| 5   | o3    | 55  | ASN  |
| 5   | o3    | 108 | ASN  |
| 5   | o3    | 144 | ASN  |
| 5   | p3    | 55  | ASN  |
| 5   | p3    | 120 | ASN  |
| 5   | q3    | 10  | ASN  |
| 5   | q3    | 112 | ASN  |
| 5   | r3    | 108 | ASN  |
| 5   | s3    | 55  | ASN  |
| 5   | s3    | 120 | ASN  |
| 5   | s3    | 218 | HIS  |
| 5   | t3    | 112 | ASN  |
| 5   | u3    | 55  | ASN  |
| 5   | u3    | 108 | ASN  |
| 5   | v3    | 55  | ASN  |
| 5   | v3    | 218 | HIS  |
| 5   | w3    | 112 | ASN  |
| 5   | w3    | 142 | ASN  |
| 5   | x3    | 55  | ASN  |
| 5   | x3    | 108 | ASN  |
| 5   | y3    | 55  | ASN  |
| 5   | y3    | 218 | HIS  |
| 5   | z3    | 112 | ASN  |
| 5   | 13    | 55  | ASN  |
| 5   | 13    | 108 | ASN  |
| 5   | 23    | 55  | ASN  |
| 5   | 23    | 120 | ASN  |
| 5   | 43    | 142 | ASN  |
| 5   | 53    | 55  | ASN  |
| 5   | 53    | 112 | ASN  |
| 5   | 53    | 120 | ASN  |
| 5   | 83    | 55  | ASN  |
| 5   | 83    | 120 | ASN  |
| 5   | 83    | 182 | HIS  |
| 5   | A3    | 55  | ASN  |
| 5   | A3    | 144 | ASN  |
| 5   | A3    | 182 | HIS  |
| 5   | B3    | 182 | HIS  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | D3    | 55  | ASN  |
| 5   | D3    | 120 | ASN  |
| 5   | D3    | 144 | ASN  |
| 5   | F3    | 112 | ASN  |
| 5   | G3    | 55  | ASN  |
| 5   | G3    | 112 | ASN  |
| 5   | G3    | 120 | ASN  |
| 5   | G3    | 182 | HIS  |
| 6   | A4    | 112 | GLN  |
| 6   | B4    | 112 | GLN  |
| 6   | D4    | 112 | GLN  |
| 6   | D4    | 125 | GLN  |
| 1   | d5    | 5   | ASN  |
| 3   | g5    | 178 | GLN  |
| 3   | g5    | 187 | ASN  |
| 3   | g5    | 239 | HIS  |
| 3   | g5    | 359 | ASN  |
| 3   | g5    | 384 | ASN  |
| 3   | h5    | 277 | HIS  |
| 3   | h5    | 280 | ASN  |
| 3   | h5    | 314 | ASN  |
| 3   | h5    | 346 | GLN  |
| 3   | h5    | 347 | ASN  |
| 3   | h5    | 359 | ASN  |
| 3   | k5    | 324 | GLN  |
| 3   | k5    | 346 | GLN  |
| 3   | k5    | 359 | ASN  |
| 3   | k5    | 431 | GLN  |
| 3   | k5    | 458 | HIS  |
| 4   | l5    | 122 | ASN  |
| 4   | m5    | 127 | GLN  |
| 3   | n5    | 280 | ASN  |
| 3   | n5    | 282 | ASN  |
| 3   | n5    | 283 | GLN  |
| 3   | o5    | 259 | GLN  |
| 3   | o5    | 282 | ASN  |
| 3   | o5    | 346 | GLN  |
| 3   | o5    | 384 | ASN  |
| 3   | o5    | 458 | HIS  |
| 4   | p5    | 2   | ASN  |
| 4   | p5    | 122 | ASN  |
| 4   | p5    | 127 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | r5    | 282 | ASN  |
| 3   | r5    | 292 | ASN  |
| 3   | r5    | 347 | ASN  |
| 3   | r5    | 359 | ASN  |
| 3   | r5    | 384 | ASN  |
| 4   | s5    | 109 | GLN  |
| 4   | t5    | 127 | GLN  |
| 4   | u5    | 122 | ASN  |
| 4   | u5    | 125 | ASN  |
| 4   | v5    | 30  | GLN  |
| 4   | v5    | 127 | GLN  |
| 1   | d6    | 5   | ASN  |
| 3   | g6    | 187 | ASN  |
| 3   | g6    | 239 | HIS  |
| 3   | g6    | 346 | GLN  |
| 3   | g6    | 384 | ASN  |
| 3   | h6    | 277 | HIS  |
| 3   | h6    | 280 | ASN  |
| 3   | h6    | 282 | ASN  |
| 3   | h6    | 314 | ASN  |
| 3   | h6    | 346 | GLN  |
| 3   | h6    | 359 | ASN  |
| 3   | k6    | 324 | GLN  |
| 3   | k6    | 431 | GLN  |
| 3   | k6    | 458 | HIS  |
| 4   | l6    | 122 | ASN  |
| 4   | m6    | 127 | GLN  |
| 3   | n6    | 280 | ASN  |
| 3   | n6    | 359 | ASN  |
| 3   | o6    | 259 | GLN  |
| 3   | o6    | 346 | GLN  |
| 3   | o6    | 384 | ASN  |
| 3   | o6    | 458 | HIS  |
| 4   | p6    | 122 | ASN  |
| 4   | p6    | 127 | GLN  |
| 3   | r6    | 254 | ASN  |
| 3   | r6    | 292 | ASN  |
| 3   | r6    | 359 | ASN  |
| 3   | r6    | 384 | ASN  |
| 4   | s6    | 109 | GLN  |
| 4   | t6    | 127 | GLN  |
| 4   | u6    | 125 | ASN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | v6    | 107 | ASN  |
| 1   | a7    | 5   | ASN  |
| 1   | d7    | 5   | ASN  |
| 3   | g7    | 187 | ASN  |
| 3   | g7    | 239 | HIS  |
| 3   | g7    | 359 | ASN  |
| 3   | g7    | 384 | ASN  |
| 3   | h7    | 314 | ASN  |
| 3   | h7    | 346 | GLN  |
| 3   | h7    | 359 | ASN  |
| 3   | k7    | 324 | GLN  |
| 3   | k7    | 346 | GLN  |
| 3   | k7    | 431 | GLN  |
| 3   | k7    | 458 | HIS  |
| 4   | l7    | 122 | ASN  |
| 4   | m7    | 127 | GLN  |
| 3   | n7    | 280 | ASN  |
| 3   | n7    | 283 | GLN  |
| 3   | n7    | 359 | ASN  |
| 3   | o7    | 259 | GLN  |
| 3   | o7    | 314 | ASN  |
| 3   | o7    | 346 | GLN  |
| 3   | o7    | 384 | ASN  |
| 3   | o7    | 458 | HIS  |
| 4   | p7    | 2   | ASN  |
| 4   | p7    | 109 | GLN  |
| 4   | p7    | 122 | ASN  |
| 4   | p7    | 127 | GLN  |
| 3   | r7    | 277 | HIS  |
| 3   | r7    | 282 | ASN  |
| 3   | r7    | 347 | ASN  |
| 3   | r7    | 384 | ASN  |
| 4   | s7    | 122 | ASN  |
| 4   | t7    | 127 | GLN  |
| 4   | u7    | 122 | ASN  |
| 4   | u7    | 125 | ASN  |
| 4   | v7    | 48  | ASN  |
| 4   | v7    | 127 | GLN  |
| 1   | f     | 11  | 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.



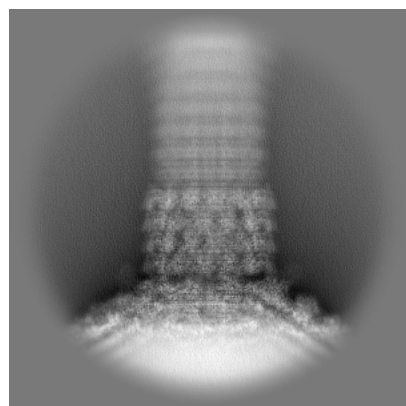
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29504. These allow visual inspection of the internal detail of the map and identification of artifacts.

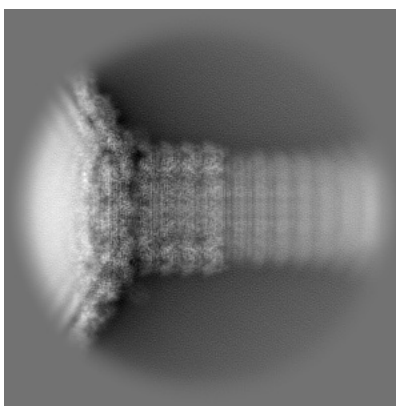
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

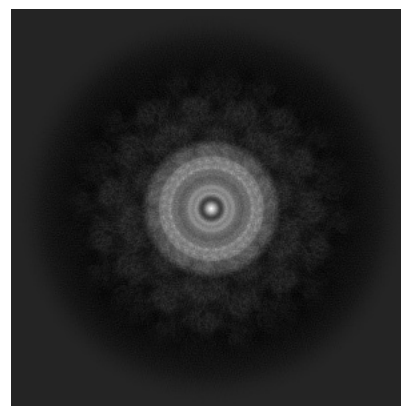
#### 6.1.1 Primary map



X

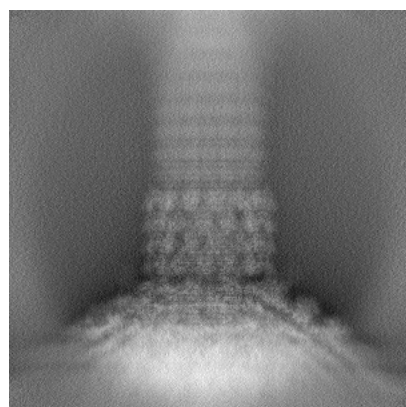


Y

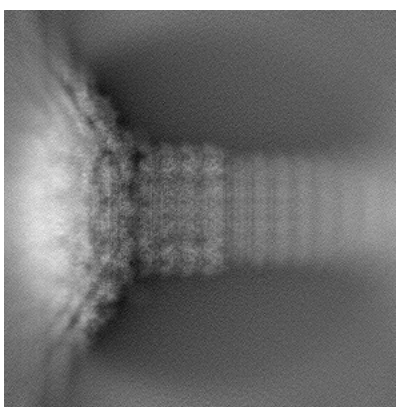


Z

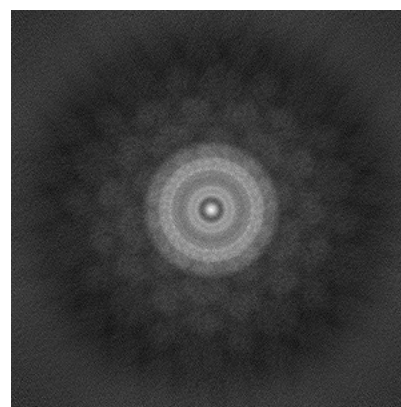
#### 6.1.2 Raw map



X



Y

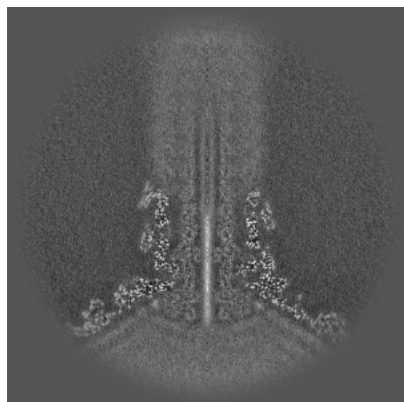


Z

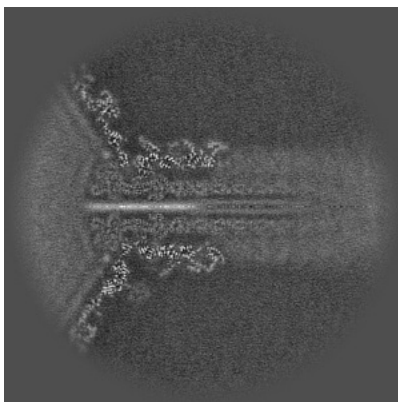
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

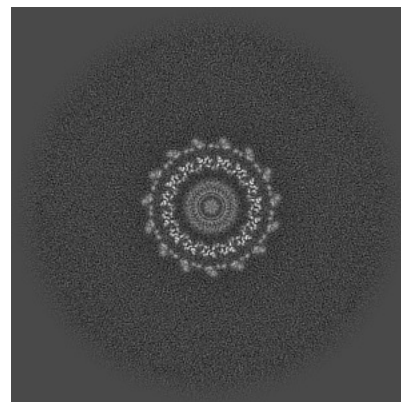
### 6.2.1 Primary map



X Index: 300

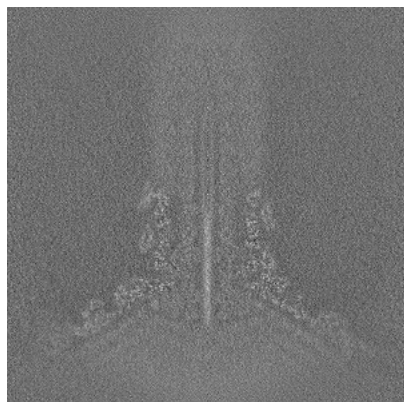


Y Index: 300

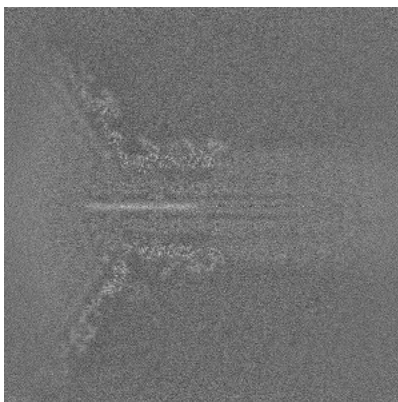


Z Index: 300

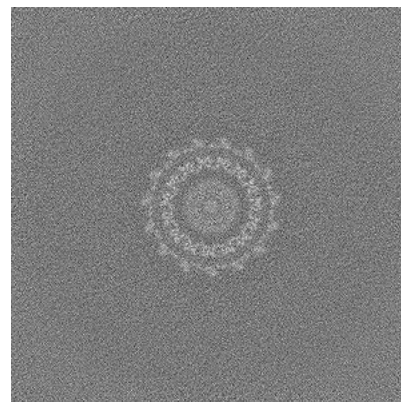
### 6.2.2 Raw map



X Index: 300



Y Index: 300

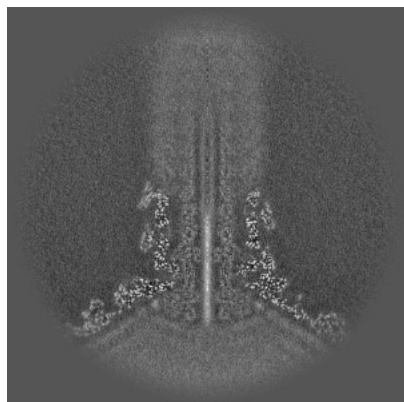


Z Index: 300

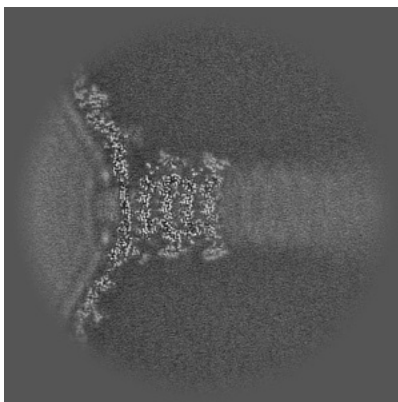
The images above show central slices of the map in three orthogonal directions.

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

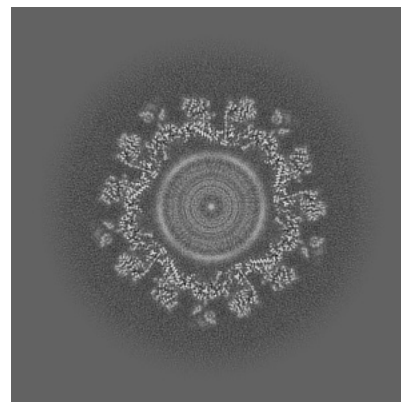
### 6.3.1 Primary map



X Index: 300

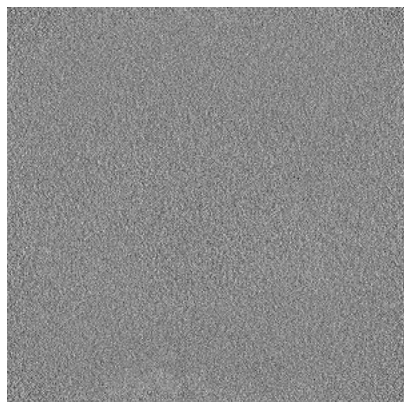


Y Index: 239

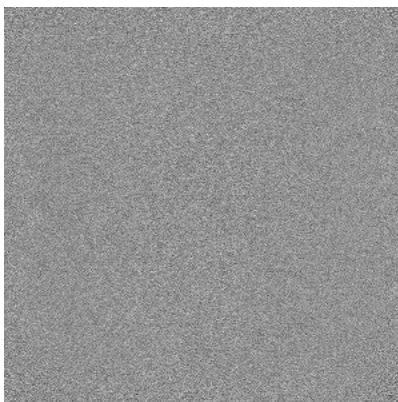


Z Index: 156

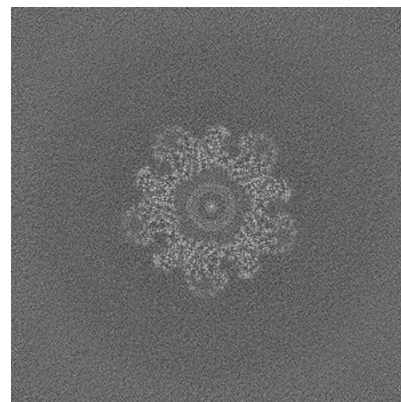
### 6.3.2 Raw map



X Index: 0



Y Index: 0



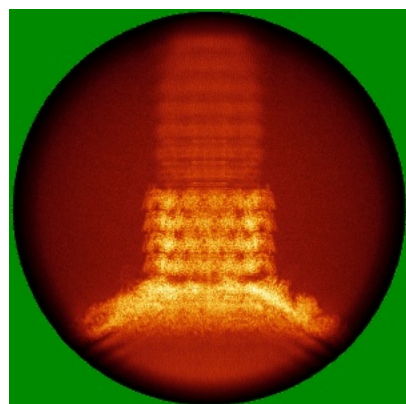
Z Index: 179

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

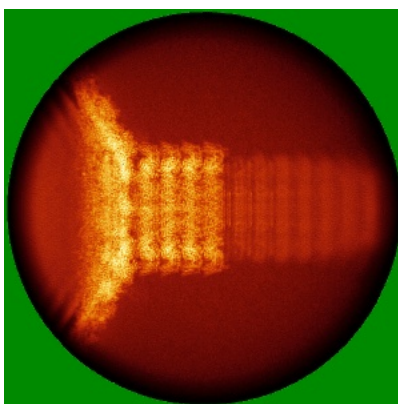


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

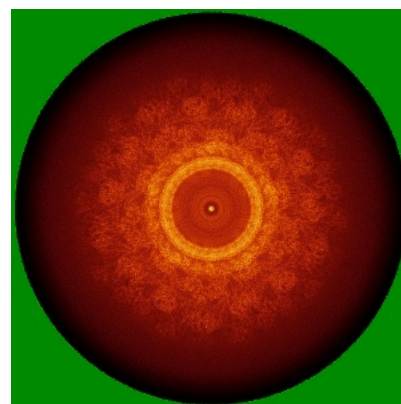
### 6.4.1 Primary map



X

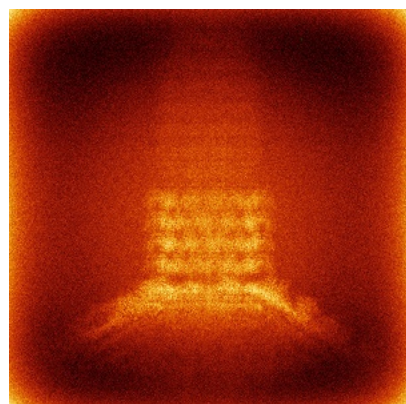


Y

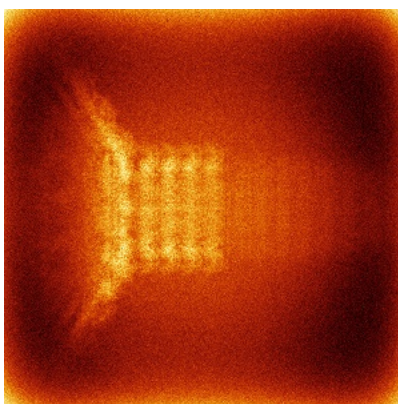


Z

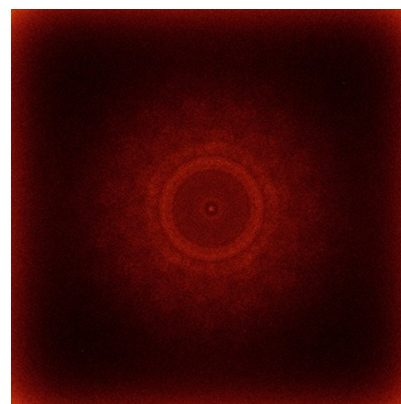
### 6.4.2 Raw map



X



Y

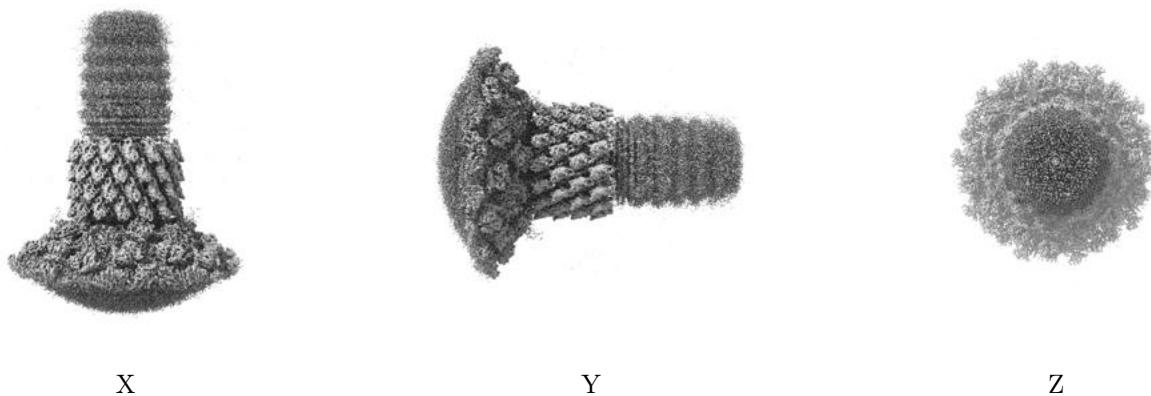


Z

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.

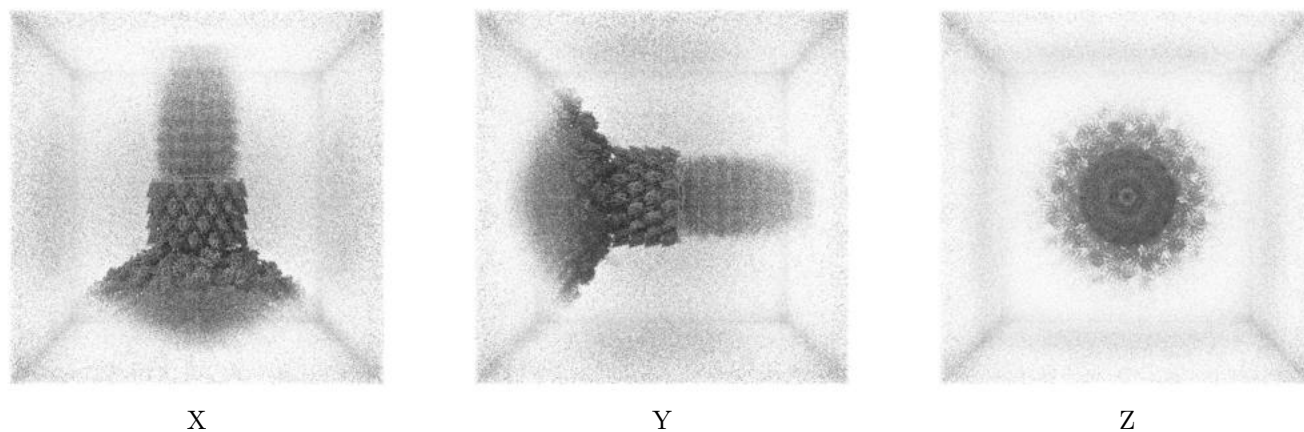
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

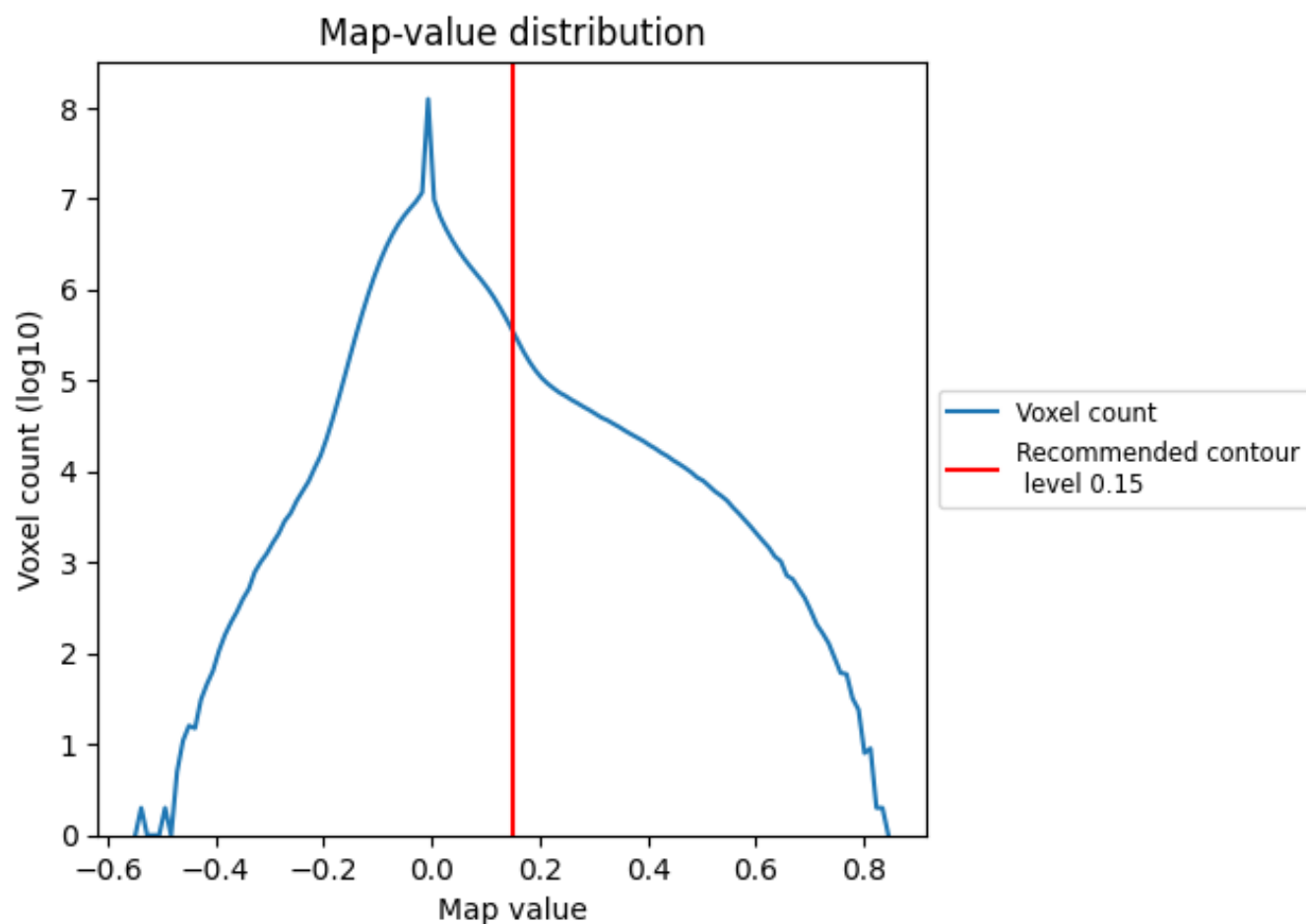
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

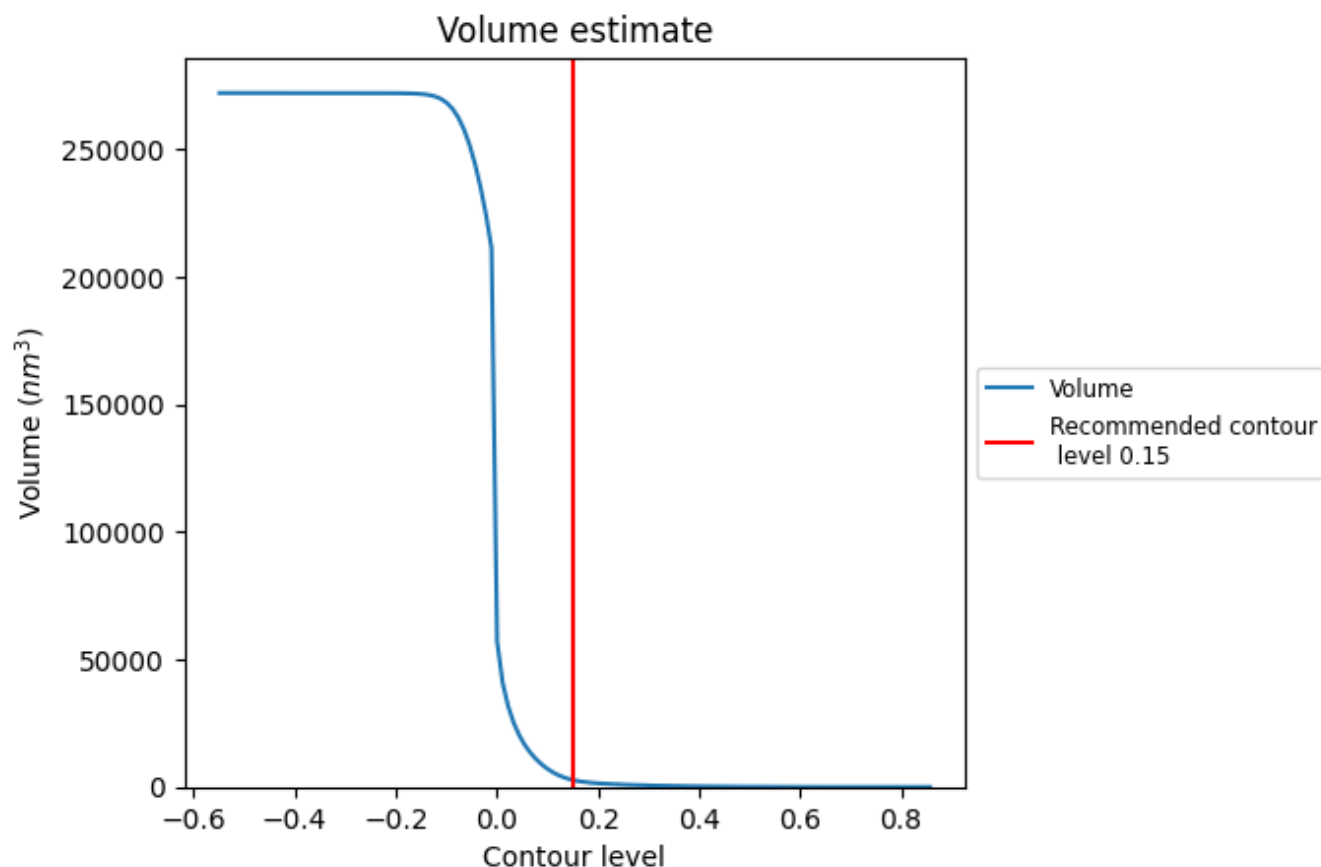
This section contains the results of statistical analysis of the map.

### 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.

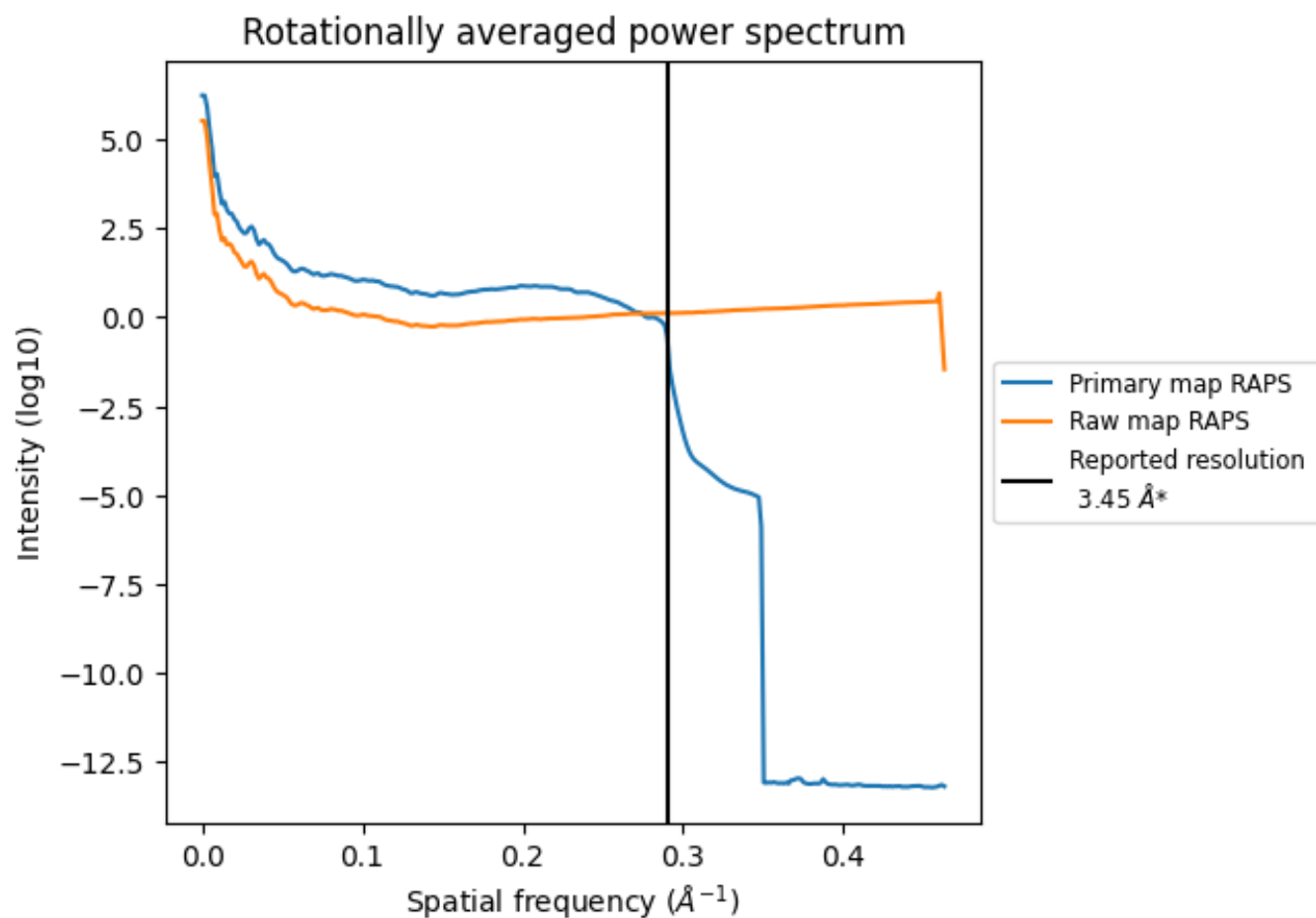
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2752 nm<sup>3</sup>; this corresponds to an approximate mass of 2486 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 ⓘ



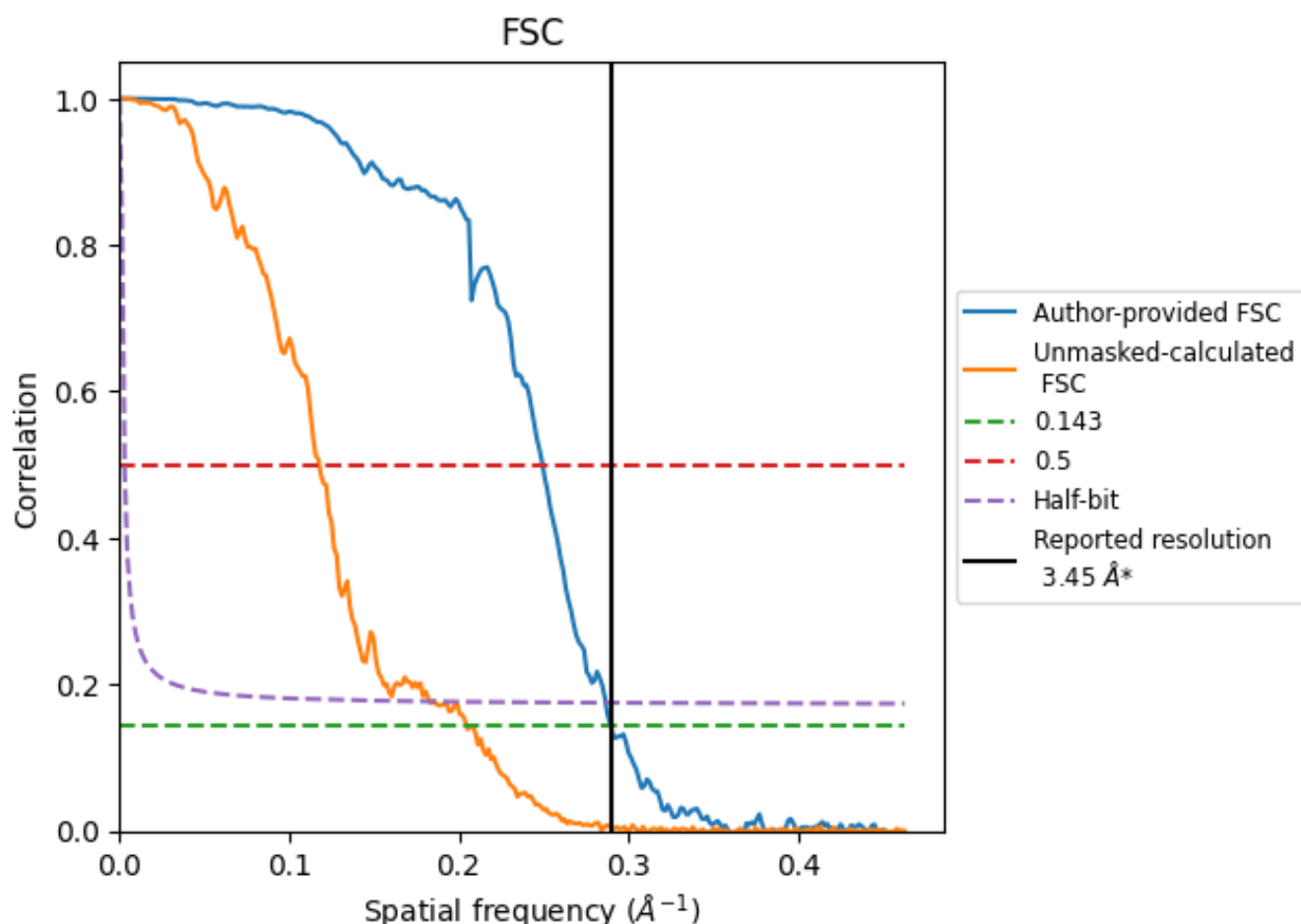
\*Reported resolution corresponds to spatial frequency of 0.290 Å<sup>-1</sup>



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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.290 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

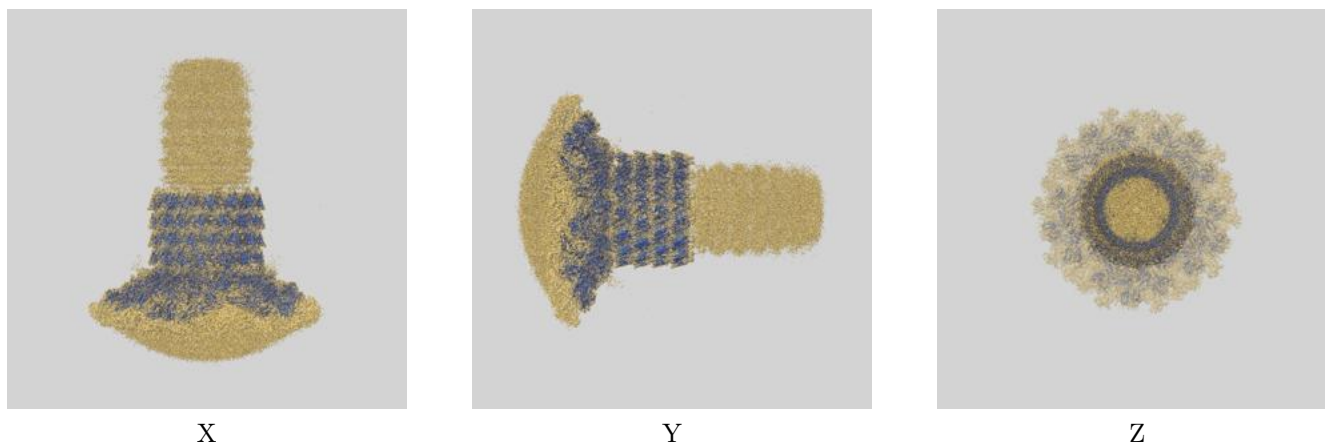
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.45                               | -    | -        |
| Author-provided FSC curve | 3.45                               | 4.01 | 3.49     |
| Unmasked-calculated*      | 4.89                               | 8.49 | 5.46     |

\*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 4.89 differs from the reported value 3.45 by more than 10 %

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

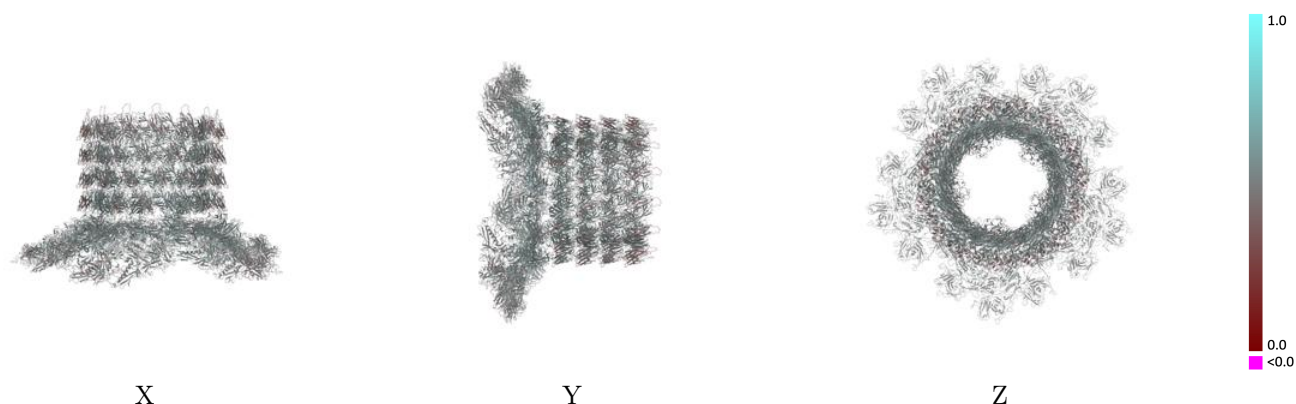
This section contains information regarding the fit between EMDB map EMD-29504 and PDB model 8FWG. Per-residue inclusion information can be found in section [3](#) on page [19](#).

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



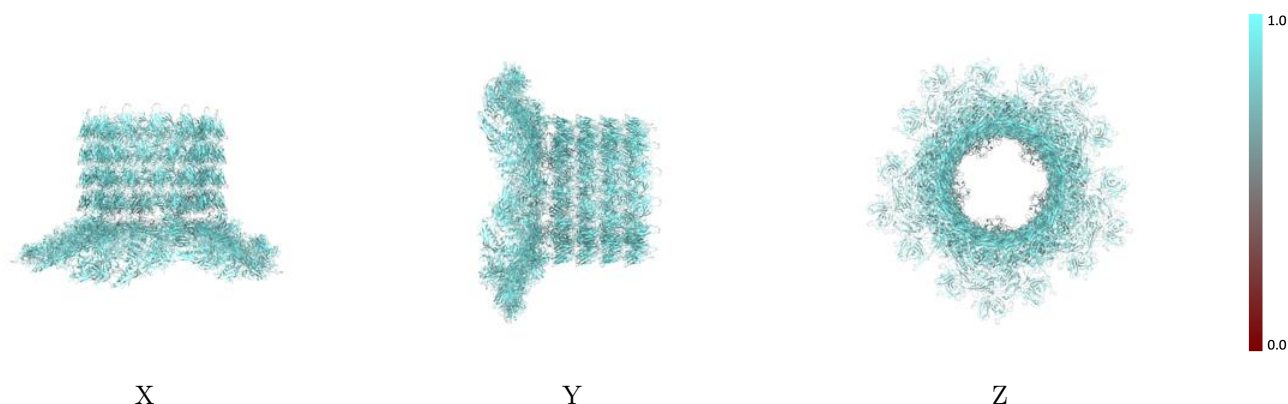
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



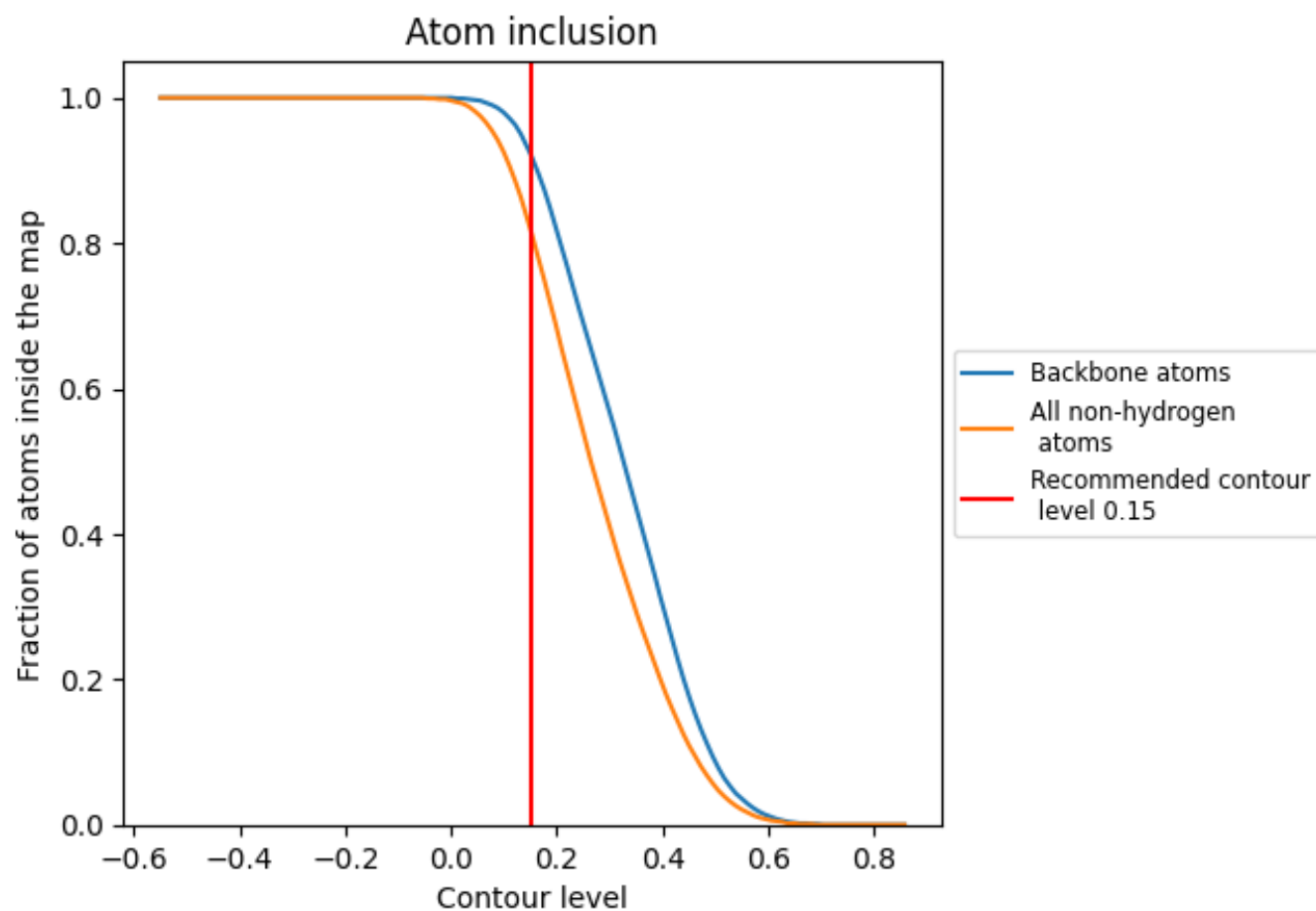
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 82% 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 (0.15) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8190   |  0.4910   |
| 03    |  0.8310   |  0.4670   |
| 13    |  0.8610   |  0.4970   |
| 23    |  0.8580   |  0.4900   |
| 33    |  0.8270   |  0.4600   |
| 43    |  0.8280   |  0.4650   |
| 53    |  0.8440   |  0.4610   |
| 63    |  0.8330   |  0.4570   |
| 73    |  0.8290   |  0.4680   |
| 83    |  0.8360   |  0.4610   |
| 93    |  0.8310   |  0.4590   |
| A3    |  0.8390   |  0.4630   |
| A4    |  0.6250   |  0.4810   |
| B3    |  0.8320   |  0.4590   |
| B4    |  0.6270  |  0.4770  |
| C3    |  0.8310 |  0.4670 |
| C4    |  0.6300 |  0.4730 |
| D3    |  0.8390 |  0.4630 |
| D4    |  0.6040 |  0.4550 |
| E3    |  0.8300 |  0.4630 |
| E4    |  0.6220 |  0.4700 |
| F3    |  0.8330 |  0.4670 |
| G3    |  0.8220 |  0.4520 |
| J3    |  0.8550 |  0.5110 |
| K3    |  0.8010 |  0.4930 |
| L3    |  0.8050 |  0.4920 |
| M3    |  0.8470 |  0.5120 |
| N3    |  0.7990 |  0.4960 |
| O3    |  0.8050 |  0.4920 |
| P3    |  0.8560 |  0.5130 |
| Q3    |  0.8060 |  0.4960 |
| R3    |  0.8100 |  0.4950 |
| S3    |  0.8590 |  0.5120 |
| T3    |  0.8070 |  0.4930 |
| U3    |  0.8020 |  0.4950 |























































































*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| V3    |  0.8560   |  0.5120   |
| W3    |  0.7950   |  0.4910   |
| X3    |  0.8100   |  0.4930   |
| Y3    |  0.8490   |  0.4960   |
| Z3    |  0.8550   |  0.4910   |
| a1    |  0.8330   |  0.5290   |
| a2    |  0.8370   |  0.5290   |
| a3    |  0.8420   |  0.4930   |
| a5    |  0.8330   |  0.5250   |
| a6    |  0.8180   |  0.5270   |
| a7    |  0.8470   |  0.5270   |
| b1    |  0.7680   |  0.5240   |
| b2    |  0.7540   |  0.5130   |
| b3    |  0.8500   |  0.4960   |
| b5    |  0.7830   |  0.5170   |
| b6    |  0.7680   |  0.5170   |
| b7    |  0.7730   |  0.5190   |
| c     |  0.8000  |  0.5160  |
| c3    |  0.8480 |  0.4890 |
| d     |  0.7920 |  0.4970 |
| d1    |  0.8000 |  0.5020 |
| d2    |  0.7790 |  0.4870 |
| d3    |  0.8500 |  0.4960 |
| d5    |  0.7920 |  0.5040 |
| d6    |  0.7870 |  0.5010 |
| d7    |  0.7920 |  0.4990 |
| e     |  0.7960 |  0.5000 |
| e1    |  0.7390 |  0.4810 |
| e2    |  0.7630 |  0.4870 |
| e3    |  0.8520 |  0.4960 |
| e5    |  0.7630 |  0.4830 |
| e6    |  0.7490 |  0.4860 |
| e7    |  0.7590 |  0.4840 |
| f     |  0.8000 |  0.5090 |
| f1    |  0.6990 |  0.5180 |
| f2    |  0.7130 |  0.5200 |
| f3    |  0.8480 |  0.4900 |
| f5    |  0.6990 |  0.5120 |
| f6    |  0.7130 |  0.5170 |
| f7    |  0.7060 |  0.5150 |
| g     |  0.7960 |  0.5010 |
| g1    |  0.8200 |  0.5060 |

*Continued on next page...*







*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| g2    |  0.8250   |  0.5060   |
| g3    |  0.8450   |  0.4950   |
| g5    |  0.8200   |  0.5040   |
| g6    |  0.8240   |  0.5040   |
| g7    |  0.8190   |  0.5030   |
| h1    |  0.8380   |  0.5170   |
| h2    |  0.8410   |  0.5190   |
| h3    |  0.8480   |  0.4970   |
| h5    |  0.8410   |  0.5180   |
| h6    |  0.8420   |  0.5170   |
| h7    |  0.8400   |  0.5160   |
| i3    |  0.8530   |  0.4920   |
| j3    |  0.8500   |  0.4930   |
| k1    |  0.8150   |  0.5140   |
| k2    |  0.8170   |  0.5160   |
| k3    |  0.8480   |  0.4960   |
| k5    |  0.8160   |  0.5150   |
| k6    |  0.8160   |  0.5170   |
| k7    |  0.8140  |  0.5100  |
| l1    |  0.8530 |  0.5170 |
| l2    |  0.8540 |  0.5160 |
| l3    |  0.8530 |  0.4890 |
| l5    |  0.8530 |  0.5170 |
| l6    |  0.8570 |  0.5170 |
| l7    |  0.8490 |  0.5140 |
| m1    |  0.8420 |  0.5130 |
| m2    |  0.8430 |  0.5140 |
| m3    |  0.8490 |  0.4950 |
| m5    |  0.8450 |  0.5170 |
| m6    |  0.8510 |  0.5140 |
| m7    |  0.8500 |  0.5150 |
| n1    |  0.8400 |  0.5090 |
| n2    |  0.8390 |  0.5090 |
| n3    |  0.8620 |  0.4890 |
| n5    |  0.8410 |  0.5100 |
| n6    |  0.8450 |  0.5120 |
| n7    |  0.8410 |  0.5100 |
| o1    |  0.8010 |  0.4790 |
| o2    |  0.8030 |  0.4790 |
| o3    |  0.8650 |  0.4960 |
| o5    |  0.8000 |  0.4800 |
| o6    |  0.8040 |  0.4790 |

*Continued on next page...*













*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| o7    |  0.7990   |  0.4820   |
| p1    |  0.8030   |  0.4890   |
| p2    |  0.8030   |  0.4860   |
| p3    |  0.8550   |  0.4890   |
| p5    |  0.8050   |  0.4860   |
| p6    |  0.8010   |  0.4870   |
| p7    |  0.8030   |  0.4840   |
| q1    |  0.7660   |  0.4690   |
| q2    |  0.7640   |  0.4680   |
| q3    |  0.8590   |  0.4890   |
| q5    |  0.7620   |  0.4660   |
| q6    |  0.7580   |  0.4690   |
| q7    |  0.7680   |  0.4690   |
| r1    |  0.8030   |  0.4940   |
| r2    |  0.8010   |  0.4920   |
| r3    |  0.8630   |  0.4960   |
| r5    |  0.8090   |  0.4930   |
| r6    |  0.8110   |  0.4920   |
| r7    |  0.8060  |  0.4870  |
| s1    |  0.7940 |  0.4890 |
| s2    |  0.7970 |  0.4890 |
| s3    |  0.8550 |  0.4910 |
| s5    |  0.7940 |  0.4900 |
| s6    |  0.7950 |  0.4900 |
| s7    |  0.7930 |  0.4890 |
| t1    |  0.7860 |  0.4690 |
| t2    |  0.7860 |  0.4710 |
| t3    |  0.8590 |  0.4890 |
| t5    |  0.7880 |  0.4700 |
| t6    |  0.7850 |  0.4720 |
| t7    |  0.7730 |  0.4670 |
| u1    |  0.7160 |  0.4480 |
| u2    |  0.7170 |  0.4490 |
| u3    |  0.8660 |  0.4960 |
| u5    |  0.7180 |  0.4520 |
| u6    |  0.7170 |  0.4490 |
| u7    |  0.7190 |  0.4490 |
| v1    |  0.7040 |  0.4500 |
| v2    |  0.7160 |  0.4490 |
| v3    |  0.8600 |  0.4890 |
| v5    |  0.7180 |  0.4540 |
| v6    |  0.7090 |  0.4530 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| v7    |  0.6980 |  0.4460 |
| w3    |  0.8670 |  0.4900 |
| x3    |  0.8640 |  0.4960 |
| y3    |  0.8530 |  0.4880 |
| z3    |  0.8630 |  0.4910 |