



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:55 am GMT

PDB ID : 4V4M  
Title : 1.45 Angstrom Structure of STNV coat protein  
Authors : Lane, S.W.; Dennis, C.A.; Lane, C.L.; Trinh, C.H.; Rizkallah, P.J.; Stockley, P.G.; Phillips, S.E.V.  
Deposited on : 2011-04-28  
Resolution : 1.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Xtriage (Phenix)               | : | 1.9-1692   |
| EDS                            | : | trunk28620   |
| Percentile statistics          | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac                         | : | 5.8.0135   |
| CCP4                           | : | 6.5.0  |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | recalc28972  |

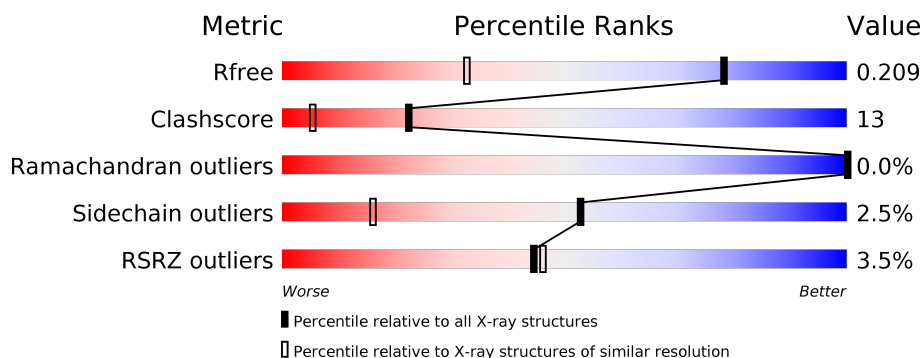
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 100719                      | 1510 (1.48-1.44)                                      |
| Clashscore            | 112137                      | 1573 (1.48-1.44)                                      |
| Ramachandran outliers | 110173                      | 1555 (1.48-1.44)                                      |
| Sidechain outliers    | 110143                      | 1555 (1.48-1.44)                                      |
| RSRZ outliers         | 101464                      | 1516 (1.48-1.44)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | 0     | 196    | <div> <div>4%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• 6%</div> </div> </div> |
| 1   | 1     | 196    | <div> <div>3%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• 6%</div> </div> </div> |
| 1   | 2     | 196    | <div> <div>3%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 6%</div> </div> </div> |
| 1   | 3     | 196    | <div> <div>4%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>• 6%</div> </div> </div> |
| 1   | 4     | 196    | <div> <div>4%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 6%</div> </div> </div> |
| 1   | 5     | 196    | <div> <div>5%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 6%</div> </div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 6     | 196    |                  |
| 1   | 7     | 196    |                  |
| 1   | A     | 196    |                  |
| 1   | B     | 196    |                  |
| 1   | C     | 196    |                  |
| 1   | D     | 196    |                  |
| 1   | E     | 196    |                  |
| 1   | F     | 196    |                  |
| 1   | G     | 196    |                  |
| 1   | H     | 196    |                  |
| 1   | I     | 196    |                  |
| 1   | J     | 196    |                  |
| 1   | K     | 196    |                  |
| 1   | L     | 196    |                  |
| 1   | M     | 196    |                  |
| 1   | N     | 196    |                  |
| 1   | O     | 196    |                  |
| 1   | P     | 196    |                  |
| 1   | Q     | 196    |                  |
| 1   | R     | 196    |                  |
| 1   | S     | 196    |                  |
| 1   | T     | 196    |                  |
| 1   | U     | 196    |                  |
| 1   | V     | 196    |                  |
| 1   | W     | 196    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | X     | 196    |                  |
| 1   | Y     | 196    |                  |
| 1   | Z     | 196    |                  |
| 1   | a     | 196    |                  |
| 1   | b     | 196    |                  |
| 1   | c     | 196    |                  |
| 1   | d     | 196    |                  |
| 1   | e     | 196    |                  |
| 1   | f     | 196    |                  |
| 1   | g     | 196    |                  |
| 1   | h     | 196    |                  |
| 1   | i     | 196    |                  |
| 1   | j     | 196    |                  |
| 1   | k     | 196    |                  |
| 1   | l     | 196    |                  |
| 1   | m     | 196    |                  |
| 1   | n     | 196    |                  |
| 1   | o     | 196    |                  |
| 1   | p     | 196    |                  |
| 1   | q     | 196    |                  |
| 1   | r     | 196    |                  |
| 1   | s     | 196    |                  |
| 1   | t     | 196    |                  |
| 1   | u     | 196    |                  |
| 1   | v     | 196    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | w     | 196    |                  |
| 1   | x     | 196    |                  |
| 1   | y     | 196    |                  |
| 1   | z     | 196    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | CA   | A     | 202 | -         | -        | -       | X                |
| 2   | CA   | B     | 203 | -         | -        | -       | X                |
| 2   | CA   | S     | 202 | -         | -        | -       | X                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 102135 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Coat protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | e     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1439  | 898 | 261 | 273 | 7 |         |         |       |
| 1   | f     | 184      | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1450  | 908 | 263 | 272 | 7 |         |         |       |
| 1   | g     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1437  | 898 | 260 | 272 | 7 |         |         |       |
| 1   | h     | 184      | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1451  | 906 | 265 | 274 | 6 |         |         |       |
| 1   | i     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1448  | 902 | 265 | 274 | 7 |         |         |       |
| 1   | j     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1441  | 898 | 264 | 273 | 6 |         |         |       |
| 1   | k     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1440  | 897 | 264 | 273 | 6 |         |         |       |
| 1   | l     | 184      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1432  | 893 | 260 | 272 | 7 |         |         |       |
| 1   | m     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1440  | 898 | 263 | 272 | 7 |         |         |       |
| 1   | n     | 184      | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1450  | 906 | 264 | 273 | 7 |         |         |       |
| 1   | o     | 184      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1433  | 893 | 261 | 273 | 6 |         |         |       |
| 1   | p     | 184      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1432  | 893 | 260 | 272 | 7 |         |         |       |
| 1   | q     | 184      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1432  | 893 | 260 | 272 | 7 |         |         |       |
| 1   | r     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1448  | 903 | 266 | 272 | 7 |         |         |       |
| 1   | s     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1436  | 897 | 260 | 272 | 7 |         |         |       |
| 1   | t     | 184      | Total | C   | N   | O   | S | 0       | 7       | 0     |
|     |       |          | 1472  | 919 | 272 | 274 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | u     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1440  | 898 | 263 | 272 | 7 |         |         |       |
| 1   | v     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1440  | 898 | 263 | 272 | 7 |         |         |       |
| 1   | w     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1444  | 902 | 263 | 272 | 7 |         |         |       |
| 1   | x     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1445  | 901 | 264 | 273 | 7 |         |         |       |
| 1   | y     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1436  | 897 | 260 | 272 | 7 |         |         |       |
| 1   | z     | 184      | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1451  | 907 | 264 | 273 | 7 |         |         |       |
| 1   | 0     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1440  | 898 | 263 | 272 | 7 |         |         |       |
| 1   | 1     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1446  | 902 | 264 | 273 | 7 |         |         |       |
| 1   | 2     | 184      | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1452  | 906 | 266 | 273 | 7 |         |         |       |
| 1   | 3     | 184      | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1454  | 907 | 267 | 273 | 7 |         |         |       |
| 1   | 4     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1443  | 900 | 262 | 274 | 7 |         |         |       |
| 1   | 5     | 184      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1432  | 892 | 261 | 273 | 6 |         |         |       |
| 1   | 6     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1448  | 903 | 266 | 272 | 7 |         |         |       |
| 1   | 7     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1438  | 897 | 261 | 273 | 7 |         |         |       |
| 1   | A     | 184      | Total | C   | N   | O   | S | 0       | 6       | 0     |
|     |       |          | 1460  | 913 | 265 | 275 | 7 |         |         |       |
| 1   | B     | 184      | Total | C   | N   | O   | S | 0       | 6       | 0     |
|     |       |          | 1464  | 917 | 267 | 273 | 7 |         |         |       |
| 1   | C     | 184      | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1454  | 906 | 265 | 276 | 7 |         |         |       |
| 1   | D     | 184      | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1445  | 905 | 260 | 273 | 7 |         |         |       |
| 1   | E     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1437  | 898 | 260 | 272 | 7 |         |         |       |
| 1   | F     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1438  | 897 | 261 | 273 | 7 |         |         |       |
| 1   | G     | 184      | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1450  | 906 | 264 | 273 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | H     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1440  | 898 | 263 | 272 | 7 |         |         |       |
| 1   | I     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1443  | 902 | 260 | 274 | 7 |         |         |       |
| 1   | J     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1440  | 898 | 263 | 272 | 7 |         |         |       |
| 1   | K     | 184      | Total | C   | N   | O   | S | 0       | 7       | 0     |
|     |       |          | 1470  | 919 | 269 | 275 | 7 |         |         |       |
| 1   | L     | 184      | Total | C   | N   | O   | S | 0       | 5       | 0     |
|     |       |          | 1458  | 913 | 266 | 272 | 7 |         |         |       |
| 1   | M     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1442  | 901 | 261 | 273 | 7 |         |         |       |
| 1   | N     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1445  | 901 | 264 | 273 | 7 |         |         |       |
| 1   | O     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1440  | 898 | 263 | 272 | 7 |         |         |       |
| 1   | P     | 184      | Total | C   | N   | O   | S | 0       | 6       | 0     |
|     |       |          | 1465  | 917 | 268 | 273 | 7 |         |         |       |
| 1   | Q     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1437  | 896 | 261 | 273 | 7 |         |         |       |
| 1   | R     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1442  | 903 | 260 | 272 | 7 |         |         |       |
| 1   | S     | 184      | Total | C   | N   | O   | S | 0       | 6       | 0     |
|     |       |          | 1465  | 916 | 268 | 274 | 7 |         |         |       |
| 1   | T     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1440  | 900 | 260 | 273 | 7 |         |         |       |
| 1   | U     | 184      | Total | C   | N   | O   | S | 0       | 4       | 0     |
|     |       |          | 1451  | 905 | 265 | 274 | 7 |         |         |       |
| 1   | V     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1443  | 902 | 260 | 274 | 7 |         |         |       |
| 1   | W     | 184      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1432  | 893 | 260 | 272 | 7 |         |         |       |
| 1   | X     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1437  | 898 | 260 | 272 | 7 |         |         |       |
| 1   | Y     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1445  | 901 | 264 | 273 | 7 |         |         |       |
| 1   | Z     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1448  | 903 | 266 | 272 | 7 |         |         |       |
| 1   | a     | 184      | Total | C   | N   | O   | S | 0       | 5       | 0     |
|     |       |          | 1456  | 910 | 265 | 274 | 7 |         |         |       |
| 1   | b     | 184      | Total | C   | N   | O   | S | 0       | 1       | 0     |
|     |       |          | 1432  | 893 | 260 | 272 | 7 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | c     | 184      | Total | C   | N   | O   | S | 0       | 3       | 0     |
|     |       |          | 1448  | 903 | 266 | 272 | 7 |         |         |       |
| 1   | d     | 184      | Total | C   | N   | O   | S | 0       | 2       | 0     |
|     |       |          | 1439  | 898 | 261 | 273 | 7 |         |         |       |

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | P     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | g     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | q     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | K     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | h     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | B     | 3        | Total | Ca | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 2   | c     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | 6     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | W     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | t     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | N     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | X     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | o     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | 2     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | y     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | S     | 2        | Total | Ca | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 2   | f     | 1        | Total | Ca | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | p     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | J     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | k     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | E     | 3        | Total<br>3 | Ca<br>3 | 0       | 0       |
| 2   | b     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | V     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | w     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | A     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | n     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | 5     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | x     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | R     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | s     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | M     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | j     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | 1     | 3        | Total<br>3 | Ca<br>3 | 0       | 0       |
| 2   | D     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | e     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | I     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | v     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Z     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | a     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | 4     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | U     | 3        | Total<br>3 | Ca<br>3 | 0       | 0       |
| 2   | r     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | L     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | m     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | 0     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | G     | 3        | Total<br>3 | Ca<br>3 | 0       | 0       |
| 2   | Q     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | d     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | H     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | i     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | C     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | 7     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | z     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | T     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |
| 2   | u     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | O     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Y     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | l     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | 3     | 2        | Total<br>2 | Ca<br>2 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | F     | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3   | e     | 258      | Total<br>258 | O<br>258 | 0       | 0       |
| 3   | f     | 231      | Total<br>231 | O<br>231 | 0       | 0       |
| 3   | g     | 260      | Total<br>260 | O<br>260 | 0       | 0       |
| 3   | h     | 281      | Total<br>281 | O<br>281 | 0       | 0       |
| 3   | i     | 282      | Total<br>282 | O<br>282 | 0       | 0       |
| 3   | j     | 267      | Total<br>267 | O<br>267 | 0       | 0       |
| 3   | k     | 256      | Total<br>256 | O<br>256 | 0       | 0       |
| 3   | l     | 257      | Total<br>257 | O<br>257 | 0       | 0       |
| 3   | m     | 252      | Total<br>252 | O<br>252 | 0       | 0       |
| 3   | n     | 251      | Total<br>251 | O<br>251 | 0       | 0       |
| 3   | o     | 262      | Total<br>262 | O<br>262 | 0       | 0       |
| 3   | p     | 238      | Total<br>238 | O<br>238 | 0       | 0       |
| 3   | q     | 258      | Total<br>258 | O<br>258 | 0       | 0       |
| 3   | r     | 287      | Total<br>287 | O<br>287 | 0       | 0       |
| 3   | s     | 226      | Total<br>226 | O<br>226 | 0       | 0       |
| 3   | t     | 236      | Total<br>236 | O<br>236 | 0       | 0       |
| 3   | u     | 240      | Total<br>240 | O<br>240 | 0       | 0       |
| 3   | v     | 249      | Total<br>249 | O<br>249 | 0       | 0       |

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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3   | w     | 279      | Total<br>279 | O<br>279 | 0       | 0       |
| 3   | x     | 260      | Total<br>260 | O<br>260 | 0       | 0       |
| 3   | y     | 294      | Total<br>294 | O<br>294 | 0       | 0       |
| 3   | z     | 264      | Total<br>264 | O<br>264 | 0       | 0       |
| 3   | 0     | 242      | Total<br>242 | O<br>242 | 0       | 0       |
| 3   | 1     | 256      | Total<br>256 | O<br>256 | 0       | 0       |
| 3   | 2     | 259      | Total<br>259 | O<br>259 | 0       | 0       |
| 3   | 3     | 245      | Total<br>245 | O<br>245 | 0       | 0       |
| 3   | 4     | 278      | Total<br>278 | O<br>278 | 0       | 0       |
| 3   | 5     | 247      | Total<br>247 | O<br>247 | 0       | 0       |
| 3   | 6     | 264      | Total<br>264 | O<br>264 | 0       | 0       |
| 3   | 7     | 249      | Total<br>249 | O<br>249 | 0       | 0       |
| 3   | A     | 246      | Total<br>246 | O<br>246 | 0       | 0       |
| 3   | B     | 235      | Total<br>235 | O<br>235 | 0       | 0       |
| 3   | C     | 250      | Total<br>250 | O<br>250 | 0       | 0       |
| 3   | D     | 255      | Total<br>255 | O<br>255 | 0       | 0       |
| 3   | E     | 229      | Total<br>229 | O<br>229 | 0       | 0       |
| 3   | F     | 217      | Total<br>217 | O<br>217 | 0       | 0       |
| 3   | G     | 253      | Total<br>253 | O<br>253 | 0       | 0       |
| 3   | H     | 248      | Total<br>248 | O<br>248 | 0       | 0       |
| 3   | I     | 240      | Total<br>240 | O<br>240 | 0       | 0       |

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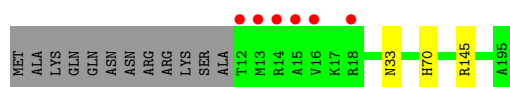
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| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3   | J     | 245      | Total<br>245 | O<br>245 | 0       | 0       |
| 3   | K     | 273      | Total<br>273 | O<br>273 | 0       | 0       |
| 3   | L     | 239      | Total<br>239 | O<br>239 | 0       | 0       |
| 3   | M     | 253      | Total<br>253 | O<br>253 | 0       | 0       |
| 3   | N     | 256      | Total<br>256 | O<br>256 | 0       | 0       |
| 3   | O     | 250      | Total<br>250 | O<br>250 | 0       | 0       |
| 3   | P     | 250      | Total<br>250 | O<br>250 | 0       | 0       |
| 3   | Q     | 255      | Total<br>255 | O<br>255 | 0       | 0       |
| 3   | R     | 286      | Total<br>286 | O<br>286 | 0       | 0       |
| 3   | S     | 237      | Total<br>237 | O<br>237 | 0       | 0       |
| 3   | T     | 295      | Total<br>295 | O<br>295 | 0       | 0       |
| 3   | U     | 266      | Total<br>266 | O<br>266 | 0       | 0       |
| 3   | V     | 258      | Total<br>258 | O<br>258 | 0       | 0       |
| 3   | W     | 256      | Total<br>256 | O<br>256 | 0       | 0       |
| 3   | X     | 256      | Total<br>256 | O<br>256 | 0       | 0       |
| 3   | Y     | 262      | Total<br>262 | O<br>262 | 0       | 0       |
| 3   | Z     | 285      | Total<br>285 | O<br>285 | 0       | 0       |
| 3   | a     | 257      | Total<br>257 | O<br>257 | 0       | 0       |
| 3   | b     | 254      | Total<br>254 | O<br>254 | 0       | 0       |
| 3   | c     | 269      | Total<br>269 | O<br>269 | 0       | 0       |
| 3   | d     | 244      | Total<br>244 | O<br>244 | 0       | 0       |

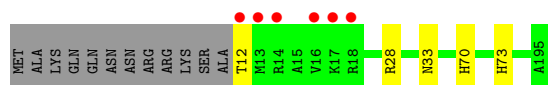
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

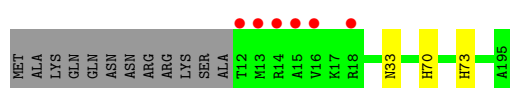
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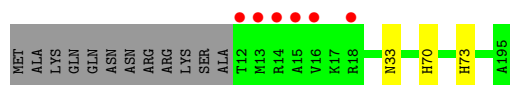
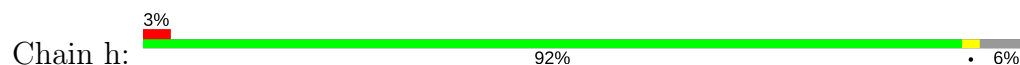
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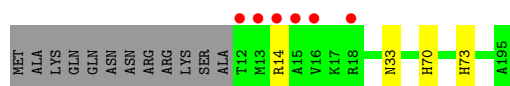
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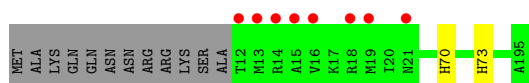
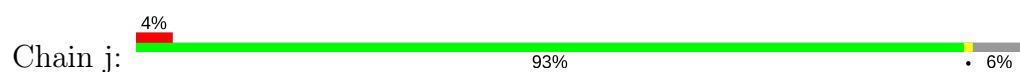
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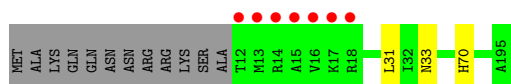
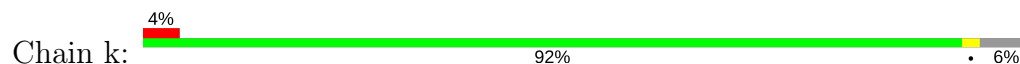
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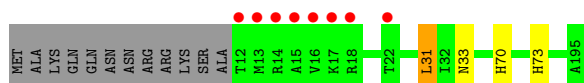
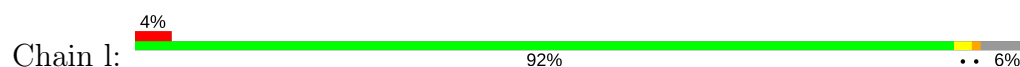
- Molecule 1: Coat protein



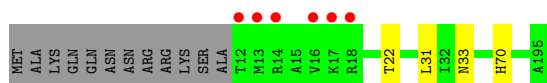
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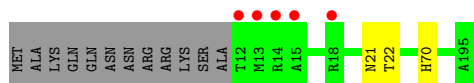
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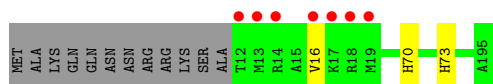
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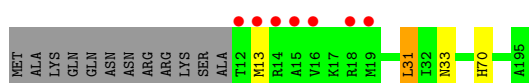
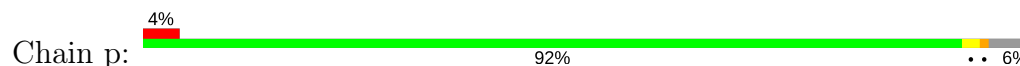
- Molecule 1: Coat protein



- Molecule 1: Coat protein

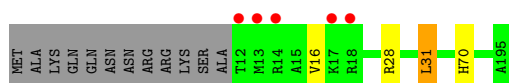
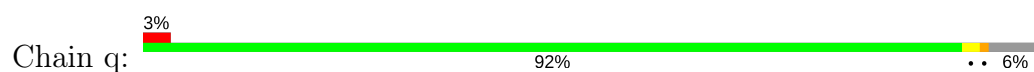


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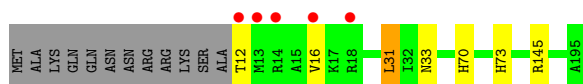
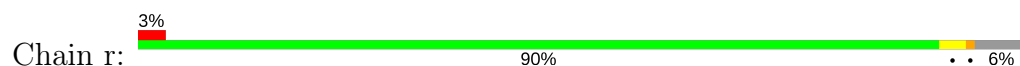


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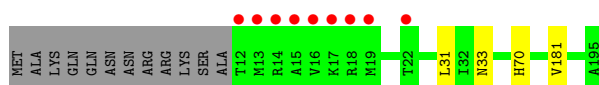




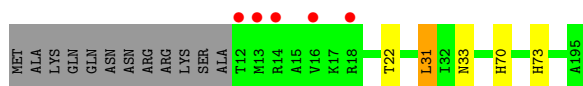
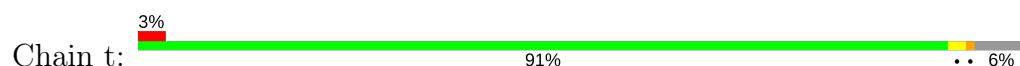
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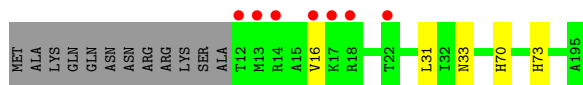
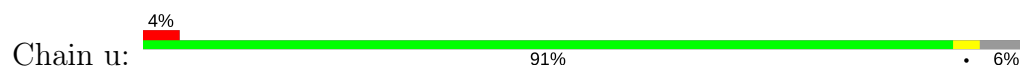
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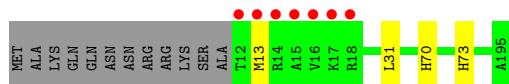
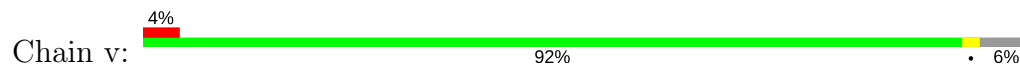
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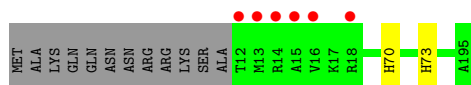
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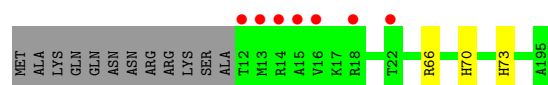
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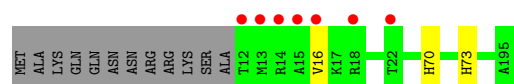
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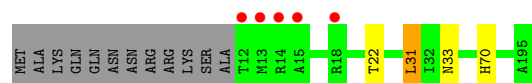
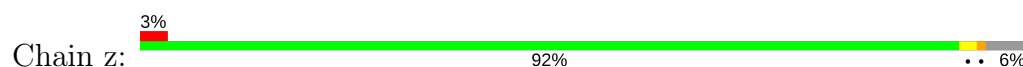
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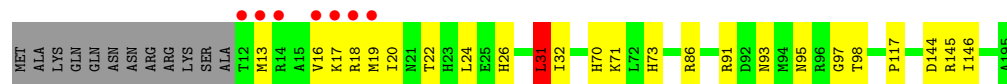
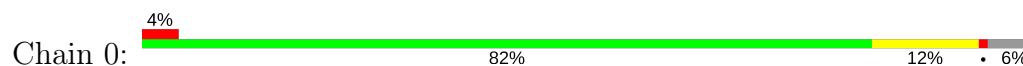
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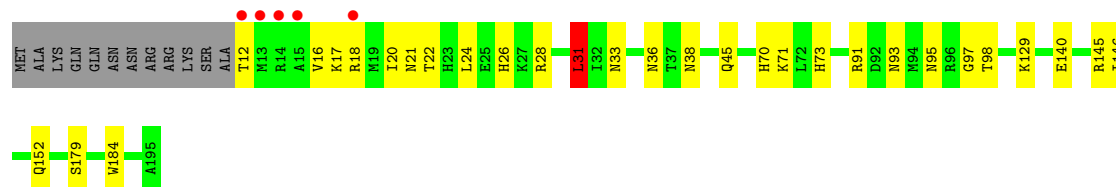
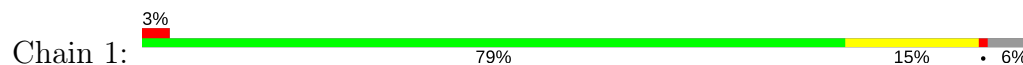
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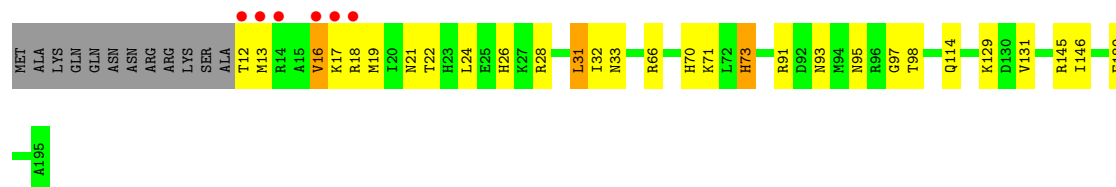
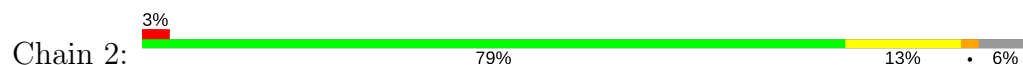
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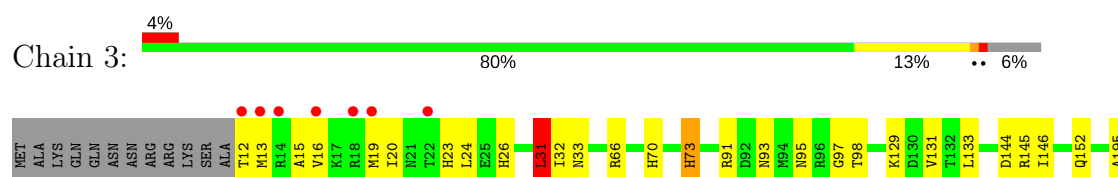
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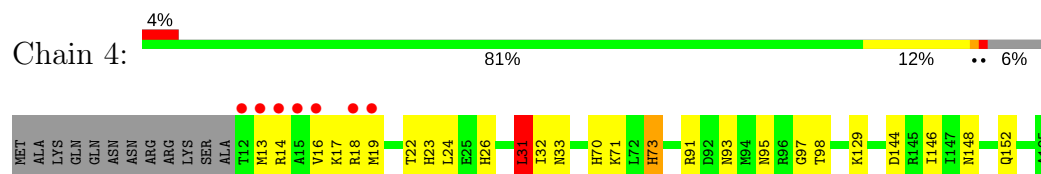
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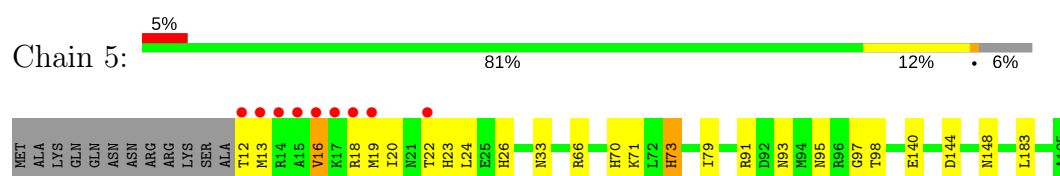
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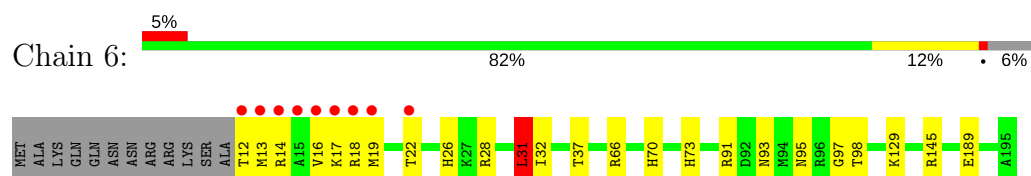
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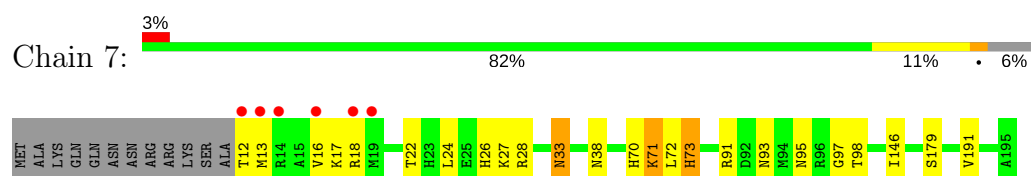
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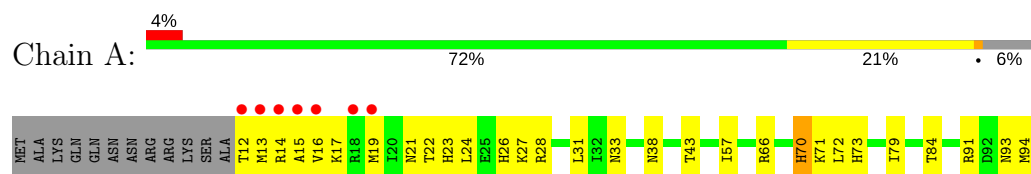
• Molecule 1: Coat protein



• Molecule 1: Coat protein



• Molecule 1: Coat protein

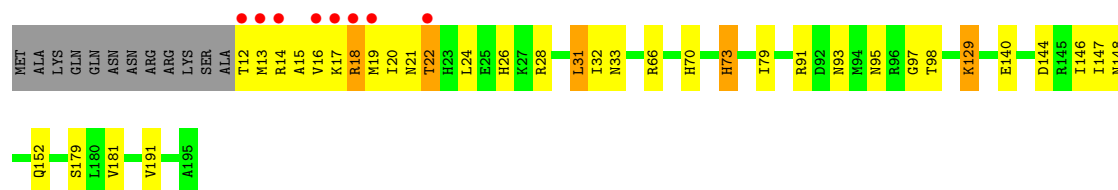


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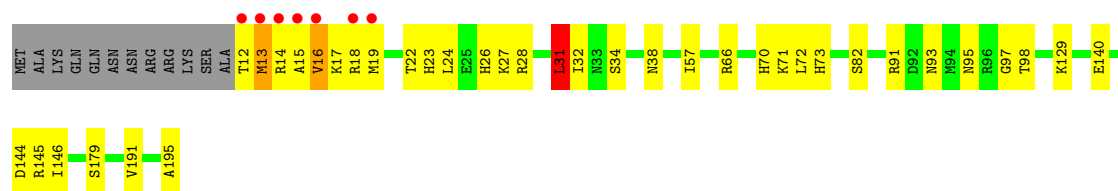




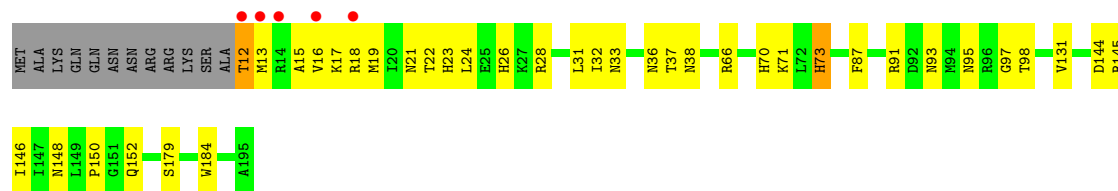
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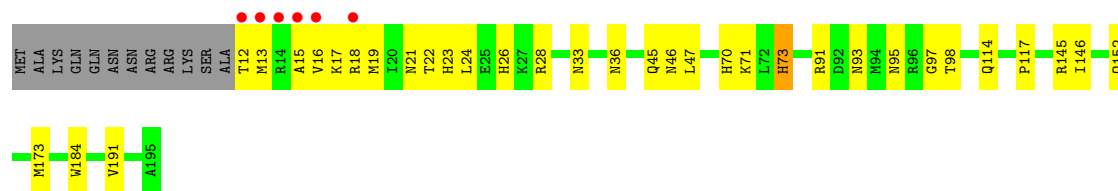
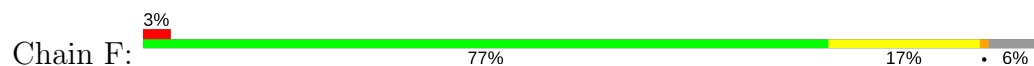
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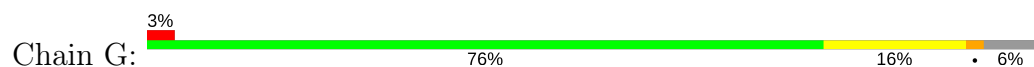
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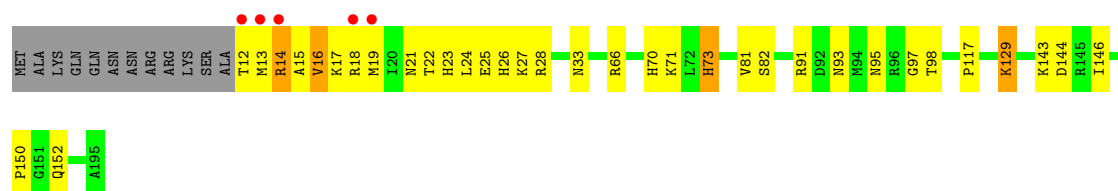


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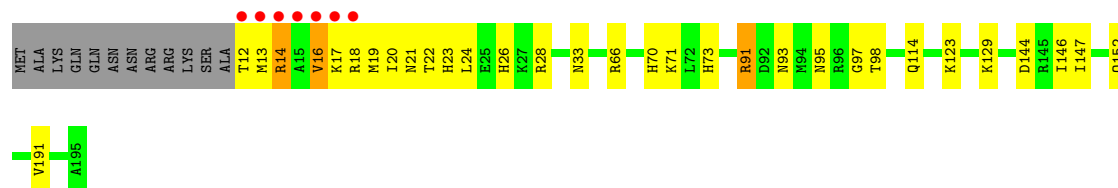
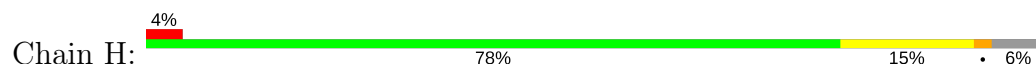


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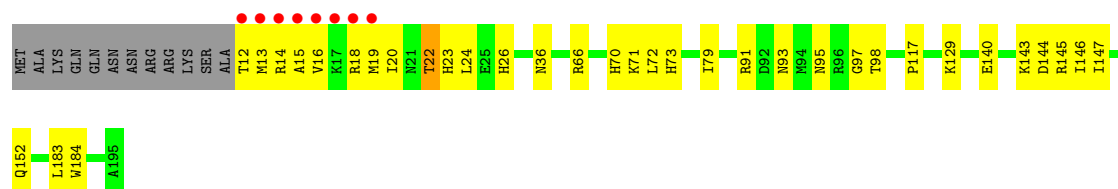
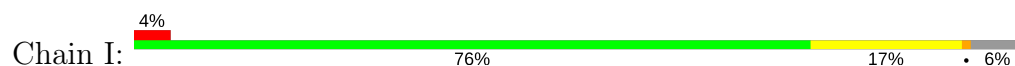




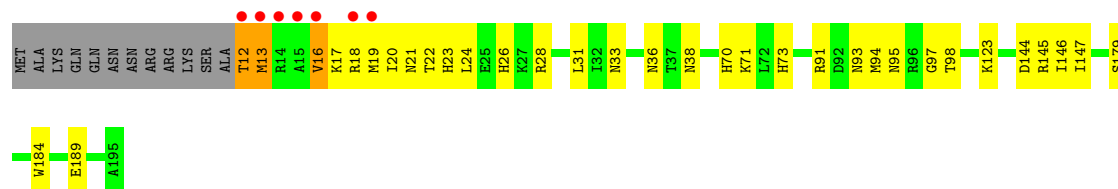
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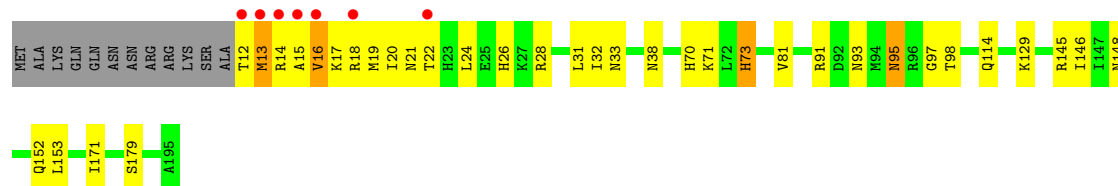
- Molecule 1: Coat protein



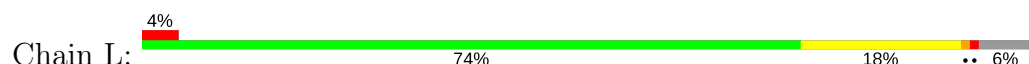
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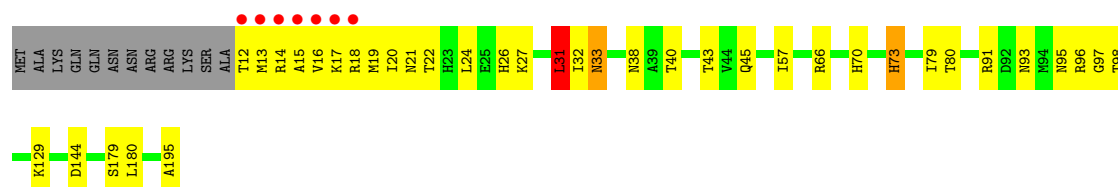


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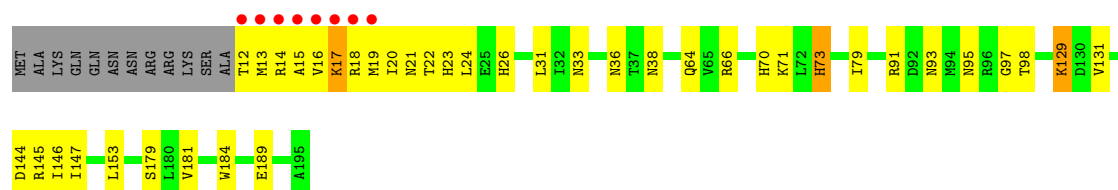


- Molecule 1: Coat protein

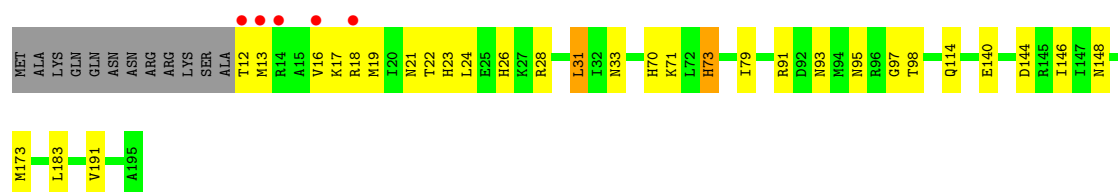
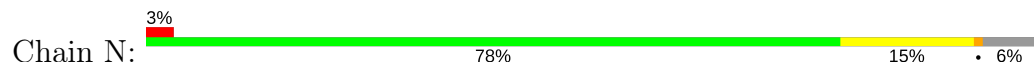




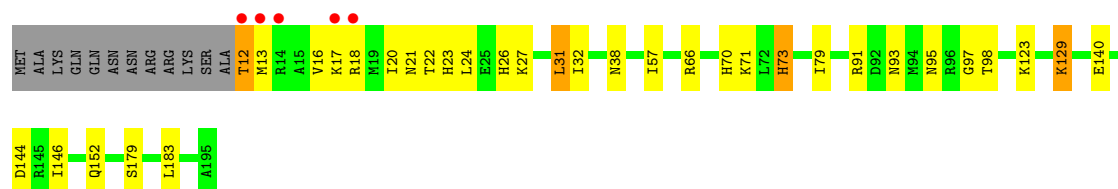
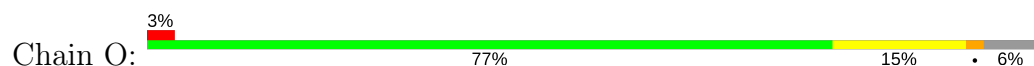
• Molecule 1: Coat protein



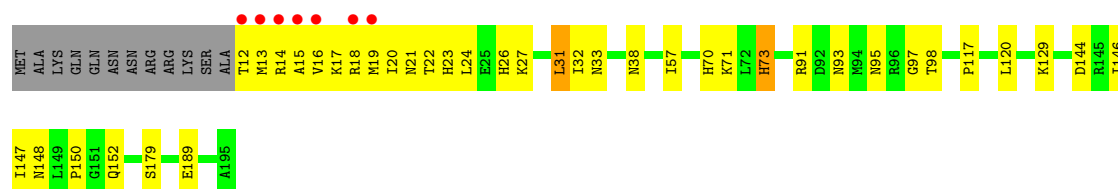
• Molecule 1: Coat protein



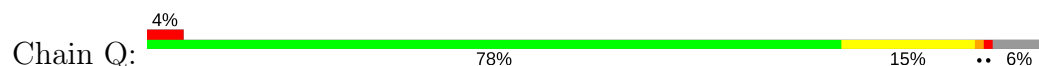
• Molecule 1: Coat protein

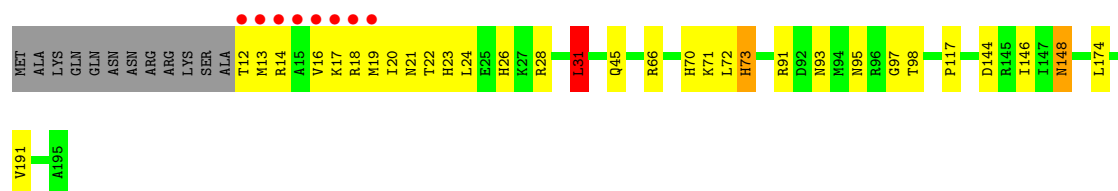


• Molecule 1: Coat protein

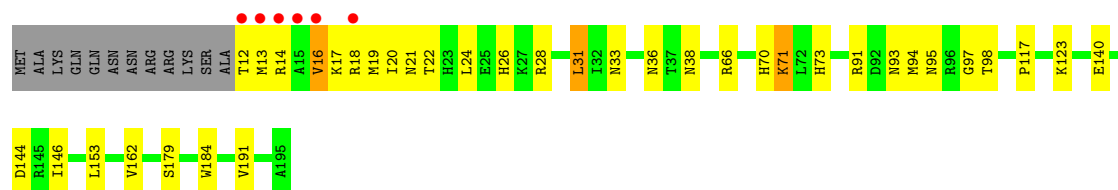


• Molecule 1: Coat protein





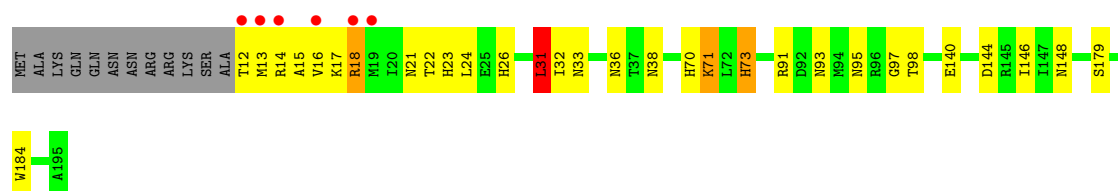
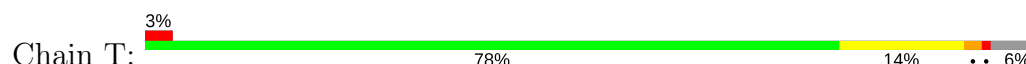
- Molecule 1: Coat protein



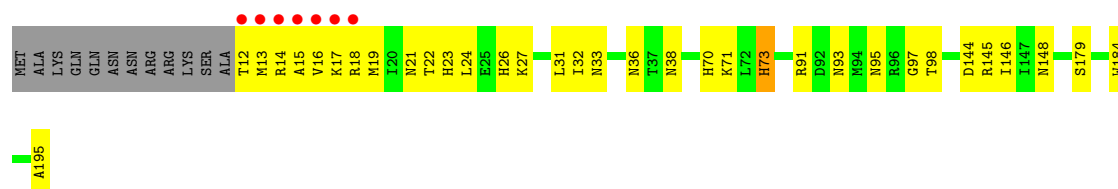
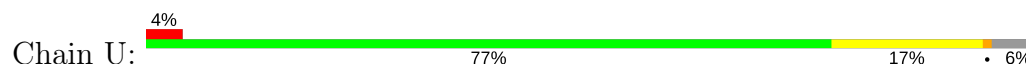
- Molecule 1: Coat protein



- Molecule 1: Coat protein

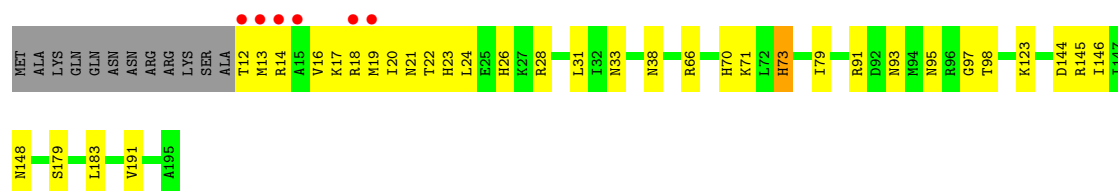


- Molecule 1: Coat protein

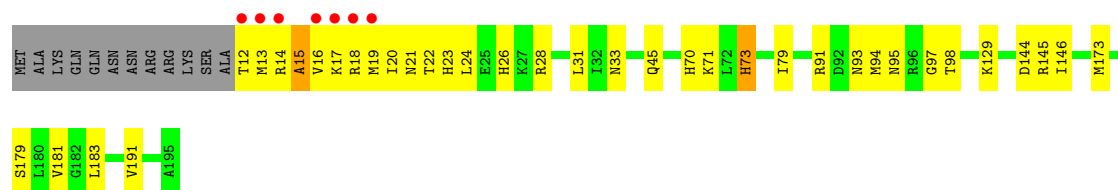
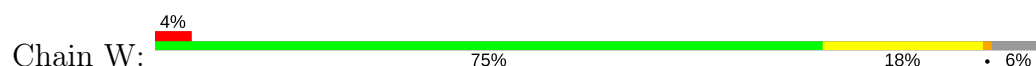


- Molecule 1: Coat protein

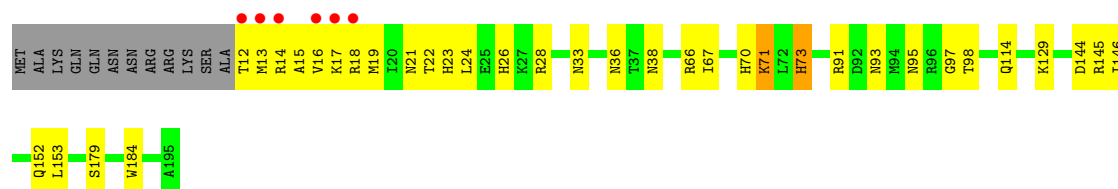
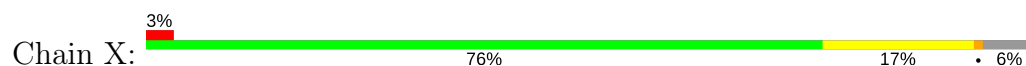




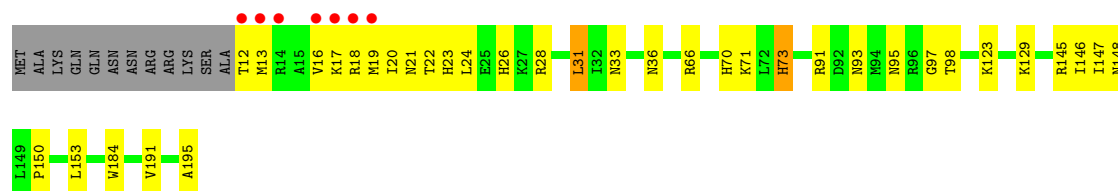
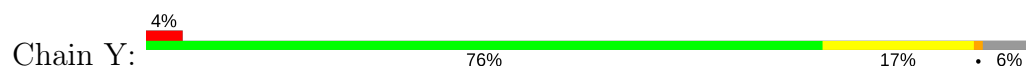
- Molecule 1: Coat protein



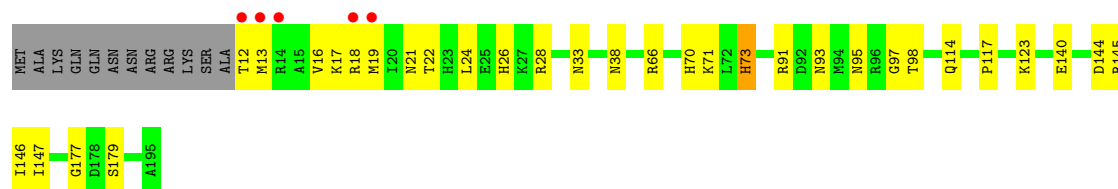
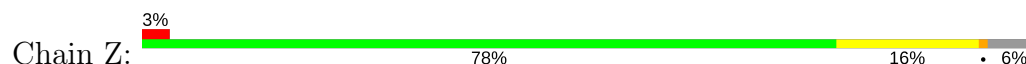
- Molecule 1: Coat protein



- Molecule 1: Coat protein



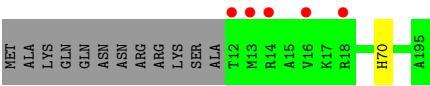
- Molecule 1: Coat protein



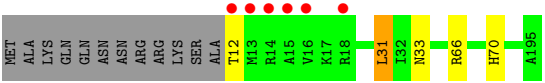
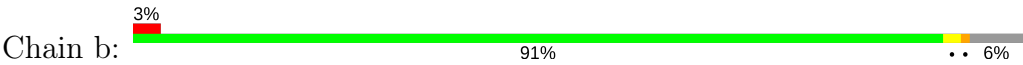
- Molecule 1: Coat protein



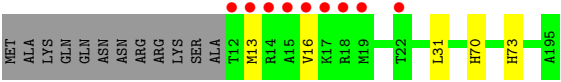
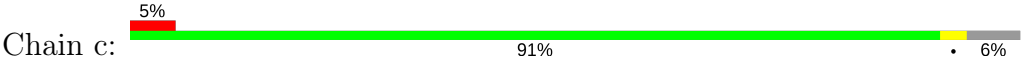




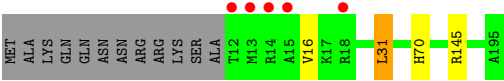
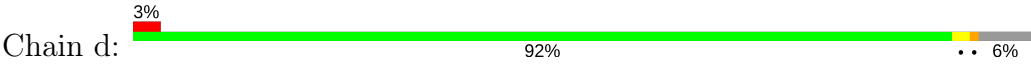
● Molecule 1: Coat protein



● Molecule 1: Coat protein



● Molecule 1: Coat protein



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | C 1 2 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 307.58Å 302.26Å 181.92Å<br>90.00° 92.77° 90.00°             | Depositor        |
| Resolution (Å)  | 12.00 – 1.45<br>12.00 – 1.45                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.9 (12.00-1.45)<br>76.2 (12.00-1.45)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.55 (at 1.45Å)   | Xtriage          |
| Refinement program  | REFMAC 5.5.0066   | Depositor        |
| R, $R_{free}$   | 0.175 , 0.208<br>0.185 , 0.209                              | Depositor<br>DCC |
| $R_{free}$ test set   | 111080 reflections (5.28%)                                  | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 10.1  | Xtriage          |
| Anisotropy  | 0.059   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.41 , 64.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction   | 0.007 for k,h,-l<br>0.009 for -k,-h,-l<br>0.013 for -h,-k,l | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 102135  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 15.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

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   | 0     | 0.47         | 0/1468  | 0.64        | 1/1988 (0.1%) |
| 1   | 1     | 0.45         | 0/1477  | 0.64        | 1/2000 (0.1%) |
| 1   | 2     | 0.45         | 0/1486  | 0.62        | 0/2012        |
| 1   | 3     | 0.45         | 0/1488  | 0.63        | 1/2014 (0.0%) |
| 1   | 4     | 0.46         | 0/1474  | 0.62        | 1/1997 (0.1%) |
| 1   | 5     | 0.46         | 0/1457  | 0.61        | 0/1975        |
| 1   | 6     | 0.44         | 0/1479  | 0.62        | 1/2002 (0.0%) |
| 1   | 7     | 0.44         | 0/1466  | 0.62        | 0/1986        |
| 1   | A     | 0.46         | 0/1500  | 0.65        | 0/2032        |
| 1   | B     | 0.46         | 0/1504  | 0.63        | 0/2036        |
| 1   | C     | 0.44         | 0/1485  | 0.61        | 0/2011        |
| 1   | D     | 0.44         | 0/1479  | 0.64        | 2/2004 (0.1%) |
| 1   | E     | 0.43         | 0/1465  | 0.62        | 0/1985        |
| 1   | F     | 0.44         | 0/1466  | 0.62        | 0/1986        |
| 1   | G     | 0.43         | 0/1484  | 0.62        | 0/2010        |
| 1   | H     | 0.45         | 0/1468  | 0.61        | 0/1988        |
| 1   | I     | 0.45         | 0/1474  | 0.62        | 0/1997        |
| 1   | J     | 0.46         | 0/1468  | 0.64        | 0/1988        |
| 1   | K     | 0.45         | 0/1513  | 0.67        | 0/2048        |
| 1   | L     | 0.44         | 0/1495  | 0.60        | 1/2024 (0.0%) |
| 1   | M     | 0.46         | 0/1473  | 0.61        | 0/1996        |
| 1   | N     | 0.43         | 0/1476  | 0.63        | 1/1999 (0.1%) |
| 1   | O     | 0.43         | 0/1468  | 0.61        | 0/1988        |
| 1   | P     | 0.46         | 0/1505  | 0.62        | 0/2036        |
| 1   | Q     | 0.45         | 0/1465  | 0.62        | 1/1985 (0.1%) |
| 1   | R     | 0.46         | 0/1473  | 0.63        | 0/1996        |
| 1   | S     | 0.47         | 0/1505  | 0.63        | 0/2037        |
| 1   | T     | 0.47         | 0/1471  | 0.67        | 2/1993 (0.1%) |
| 1   | U     | 0.46         | 0/1485  | 0.64        | 0/2011        |
| 1   | V     | 0.47         | 0/1474  | 0.64        | 0/1997        |
| 1   | W     | 0.44         | 0/1457  | 0.62        | 0/1974        |
| 1   | X     | 0.46         | 0/1465  | 0.61        | 0/1985        |

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | Y     | 0.47         | 0/1476  | 0.62        | 0/1999           |
| 1   | Z     | 0.47         | 0/1479  | 0.65        | 0/2002           |
| 1   | a     | 0.45         | 0/1493  | 0.64        | 0/2022           |
| 1   | b     | 0.47         | 0/1457  | 0.65        | 1/1974 (0.1%)    |
| 1   | c     | 0.48         | 0/1479  | 0.62        | 0/2002           |
| 1   | d     | 0.47         | 0/1464  | 0.64        | 1/1984 (0.1%)    |
| 1   | e     | 0.46         | 0/1464  | 0.64        | 0/1984           |
| 1   | f     | 0.44         | 0/1484  | 0.61        | 0/2010           |
| 1   | g     | 0.44         | 0/1465  | 0.62        | 0/1985           |
| 1   | h     | 0.47         | 0/1485  | 0.65        | 0/2012           |
| 1   | i     | 0.45         | 0/1476  | 0.61        | 0/1999           |
| 1   | j     | 0.45         | 0/1469  | 0.63        | 0/1990           |
| 1   | k     | 0.48         | 0/1468  | 0.64        | 0/1989           |
| 1   | l     | 0.46         | 0/1457  | 0.64        | 1/1974 (0.1%)    |
| 1   | m     | 0.43         | 0/1468  | 0.60        | 0/1988           |
| 1   | n     | 0.43         | 0/1484  | 0.62        | 0/2010           |
| 1   | o     | 0.45         | 0/1458  | 0.62        | 0/1976           |
| 1   | p     | 0.45         | 0/1457  | 0.64        | 1/1974 (0.1%)    |
| 1   | q     | 0.47         | 0/1457  | 0.64        | 1/1974 (0.1%)    |
| 1   | r     | 0.47         | 0/1479  | 0.65        | 1/2002 (0.0%)    |
| 1   | s     | 0.46         | 0/1464  | 0.63        | 0/1984           |
| 1   | t     | 0.44         | 0/1515  | 0.62        | 1/2050 (0.0%)    |
| 1   | u     | 0.46         | 0/1468  | 0.61        | 0/1988           |
| 1   | v     | 0.46         | 0/1468  | 0.64        | 0/1988           |
| 1   | w     | 0.47         | 0/1475  | 0.65        | 0/1998           |
| 1   | x     | 0.46         | 0/1476  | 0.63        | 0/1999           |
| 1   | y     | 0.46         | 0/1464  | 0.64        | 0/1984           |
| 1   | z     | 0.46         | 0/1485  | 0.64        | 2/2011 (0.1%)    |
| All | All   | 0.45         | 0/88547 | 0.63        | 21/119932 (0.0%) |

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 1   | l     | 31  | LEU  | CA-CB-CG | 6.64 | 130.58      | 115.30   |
| 1   | q     | 31  | LEU  | CA-CB-CG | 6.54 | 130.35      | 115.30   |
| 1   | p     | 31  | LEU  | CA-CB-CG | 6.10 | 129.32      | 115.30   |
| 1   | 4     | 31  | LEU  | CA-CB-CG | 5.94 | 128.96      | 115.30   |
| 1   | 3     | 31  | LEU  | CA-CB-CG | 5.89 | 128.85      | 115.30   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 1440  | 0        | 1449     | 31      | 0            |
| 1   | 1     | 1446  | 0        | 1457     | 43      | 0            |
| 1   | 2     | 1452  | 0        | 1469     | 68      | 0            |
| 1   | 3     | 1454  | 0        | 1470     | 57      | 0            |
| 1   | 4     | 1443  | 0        | 1450     | 54      | 0            |
| 1   | 5     | 1432  | 0        | 1433     | 46      | 0            |
| 1   | 6     | 1448  | 0        | 1462     | 48      | 0            |
| 1   | 7     | 1438  | 0        | 1444     | 37      | 0            |
| 1   | A     | 1460  | 0        | 1481     | 76      | 0            |
| 1   | B     | 1464  | 0        | 1492     | 93      | 0            |
| 1   | C     | 1454  | 0        | 1460     | 74      | 0            |
| 1   | D     | 1445  | 0        | 1463     | 57      | 0            |
| 1   | E     | 1437  | 0        | 1447     | 102     | 0            |
| 1   | F     | 1438  | 0        | 1444     | 70      | 0            |
| 1   | G     | 1450  | 0        | 1466     | 84      | 0            |
| 1   | H     | 1440  | 0        | 1449     | 77      | 0            |
| 1   | I     | 1443  | 0        | 1453     | 92      | 0            |
| 1   | J     | 1440  | 0        | 1449     | 67      | 0            |
| 1   | K     | 1470  | 0        | 1495     | 85      | 0            |
| 1   | L     | 1458  | 0        | 1484     | 73      | 0            |
| 1   | M     | 1442  | 0        | 1453     | 102     | 0            |
| 1   | N     | 1445  | 0        | 1455     | 95      | 0            |
| 1   | O     | 1440  | 0        | 1449     | 78      | 0            |
| 1   | P     | 1465  | 0        | 1494     | 123     | 0            |
| 1   | Q     | 1437  | 0        | 1442     | 73      | 0            |
| 1   | R     | 1442  | 0        | 1458     | 85      | 0            |
| 1   | S     | 1465  | 0        | 1487     | 74      | 0            |
| 1   | T     | 1440  | 0        | 1452     | 77      | 0            |
| 1   | U     | 1451  | 0        | 1463     | 84      | 0            |
| 1   | V     | 1443  | 0        | 1453     | 98      | 0            |
| 1   | W     | 1432  | 0        | 1436     | 83      | 0            |
| 1   | X     | 1437  | 0        | 1447     | 81      | 0            |
| 1   | Y     | 1445  | 0        | 1455     | 81      | 0            |
| 1   | Z     | 1448  | 0        | 1462     | 92      | 0            |
| 1   | a     | 1456  | 0        | 1474     | 0       | 0            |
| 1   | b     | 1432  | 0        | 1436     | 0       | 0            |
| 1   | c     | 1448  | 0        | 1462     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | d     | 1439  | 0        | 1444     | 0       | 0            |
| 1   | e     | 1439  | 0        | 1444     | 0       | 0            |
| 1   | f     | 1450  | 0        | 1471     | 0       | 0            |
| 1   | g     | 1437  | 0        | 1447     | 0       | 0            |
| 1   | h     | 1451  | 0        | 1465     | 0       | 0            |
| 1   | i     | 1448  | 0        | 1454     | 0       | 0            |
| 1   | j     | 1441  | 0        | 1448     | 0       | 0            |
| 1   | k     | 1440  | 0        | 1446     | 0       | 0            |
| 1   | l     | 1432  | 0        | 1436     | 0       | 0            |
| 1   | m     | 1440  | 0        | 1449     | 0       | 0            |
| 1   | n     | 1450  | 0        | 1466     | 0       | 0            |
| 1   | o     | 1433  | 0        | 1435     | 0       | 0            |
| 1   | p     | 1432  | 0        | 1436     | 0       | 0            |
| 1   | q     | 1432  | 0        | 1436     | 0       | 0            |
| 1   | r     | 1448  | 0        | 1462     | 0       | 0            |
| 1   | s     | 1436  | 0        | 1445     | 0       | 0            |
| 1   | t     | 1472  | 0        | 1502     | 0       | 0            |
| 1   | u     | 1440  | 0        | 1449     | 0       | 0            |
| 1   | v     | 1440  | 0        | 1449     | 0       | 0            |
| 1   | w     | 1444  | 0        | 1458     | 0       | 0            |
| 1   | x     | 1445  | 0        | 1455     | 0       | 0            |
| 1   | y     | 1436  | 0        | 1445     | 0       | 0            |
| 1   | z     | 1451  | 0        | 1468     | 0       | 0            |
| 2   | 0     | 2     | 0        | 0        | 0       | 0            |
| 2   | 1     | 3     | 0        | 0        | 0       | 0            |
| 2   | 2     | 2     | 0        | 0        | 0       | 0            |
| 2   | 3     | 2     | 0        | 0        | 0       | 0            |
| 2   | 4     | 2     | 0        | 0        | 0       | 0            |
| 2   | 5     | 2     | 0        | 0        | 0       | 0            |
| 2   | 6     | 2     | 0        | 0        | 0       | 0            |
| 2   | 7     | 1     | 0        | 0        | 0       | 0            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 3     | 0        | 0        | 0       | 0            |
| 2   | C     | 1     | 0        | 0        | 0       | 0            |
| 2   | D     | 1     | 0        | 0        | 0       | 0            |
| 2   | E     | 3     | 0        | 0        | 0       | 0            |
| 2   | F     | 1     | 0        | 0        | 0       | 0            |
| 2   | G     | 3     | 0        | 0        | 1       | 0            |
| 2   | H     | 1     | 0        | 0        | 0       | 0            |
| 2   | I     | 2     | 0        | 0        | 0       | 0            |
| 2   | J     | 1     | 0        | 0        | 0       | 0            |
| 2   | K     | 2     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | L     | 1     | 0        | 0        | 0       | 0            |
| 2   | M     | 1     | 0        | 0        | 0       | 0            |
| 2   | N     | 2     | 0        | 0        | 1       | 0            |
| 2   | O     | 1     | 0        | 0        | 0       | 0            |
| 2   | P     | 1     | 0        | 0        | 0       | 0            |
| 2   | Q     | 2     | 0        | 0        | 0       | 0            |
| 2   | R     | 2     | 0        | 0        | 0       | 0            |
| 2   | S     | 2     | 0        | 0        | 0       | 0            |
| 2   | T     | 2     | 0        | 0        | 0       | 0            |
| 2   | U     | 3     | 0        | 0        | 0       | 0            |
| 2   | V     | 2     | 0        | 0        | 0       | 0            |
| 2   | W     | 1     | 0        | 0        | 0       | 0            |
| 2   | X     | 1     | 0        | 0        | 0       | 0            |
| 2   | Y     | 1     | 0        | 0        | 0       | 0            |
| 2   | Z     | 1     | 0        | 0        | 0       | 0            |
| 2   | a     | 1     | 0        | 0        | 0       | 0            |
| 2   | b     | 2     | 0        | 0        | 0       | 0            |
| 2   | c     | 2     | 0        | 0        | 0       | 0            |
| 2   | d     | 1     | 0        | 0        | 0       | 0            |
| 2   | e     | 1     | 0        | 0        | 0       | 0            |
| 2   | f     | 1     | 0        | 0        | 0       | 0            |
| 2   | g     | 1     | 0        | 0        | 0       | 0            |
| 2   | h     | 1     | 0        | 0        | 0       | 0            |
| 2   | i     | 2     | 0        | 0        | 0       | 0            |
| 2   | j     | 2     | 0        | 0        | 0       | 0            |
| 2   | k     | 1     | 0        | 0        | 0       | 0            |
| 2   | l     | 1     | 0        | 0        | 0       | 0            |
| 2   | m     | 1     | 0        | 0        | 0       | 0            |
| 2   | n     | 2     | 0        | 0        | 0       | 0            |
| 2   | o     | 2     | 0        | 0        | 0       | 0            |
| 2   | p     | 1     | 0        | 0        | 0       | 0            |
| 2   | q     | 2     | 0        | 0        | 0       | 0            |
| 2   | r     | 1     | 0        | 0        | 0       | 0            |
| 2   | s     | 1     | 0        | 0        | 0       | 0            |
| 2   | t     | 1     | 0        | 0        | 0       | 0            |
| 2   | u     | 1     | 0        | 0        | 0       | 0            |
| 2   | v     | 1     | 0        | 0        | 0       | 0            |
| 2   | w     | 1     | 0        | 0        | 0       | 0            |
| 2   | x     | 1     | 0        | 0        | 0       | 0            |
| 2   | y     | 1     | 0        | 0        | 0       | 0            |
| 2   | z     | 1     | 0        | 0        | 0       | 0            |
| 3   | 0     | 242   | 0        | 0        | 6       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | 1     | 256   | 0        | 0        | 10      | 0            |
| 3   | 2     | 259   | 0        | 0        | 8       | 0            |
| 3   | 3     | 245   | 0        | 0        | 8       | 0            |
| 3   | 4     | 278   | 0        | 0        | 16      | 2            |
| 3   | 5     | 247   | 0        | 0        | 3       | 0            |
| 3   | 6     | 264   | 0        | 0        | 10      | 0            |
| 3   | 7     | 249   | 0        | 0        | 7       | 0            |
| 3   | A     | 246   | 0        | 0        | 18      | 0            |
| 3   | B     | 235   | 0        | 0        | 12      | 0            |
| 3   | C     | 250   | 0        | 0        | 10      | 0            |
| 3   | D     | 255   | 0        | 0        | 12      | 0            |
| 3   | E     | 229   | 0        | 0        | 18      | 0            |
| 3   | F     | 217   | 0        | 0        | 8       | 0            |
| 3   | G     | 253   | 0        | 0        | 16      | 0            |
| 3   | H     | 248   | 0        | 0        | 13      | 0            |
| 3   | I     | 240   | 0        | 0        | 16      | 0            |
| 3   | J     | 245   | 0        | 0        | 8       | 0            |
| 3   | K     | 273   | 0        | 0        | 18      | 0            |
| 3   | L     | 239   | 0        | 0        | 19      | 0            |
| 3   | M     | 253   | 0        | 0        | 13      | 0            |
| 3   | N     | 256   | 0        | 0        | 14      | 0            |
| 3   | O     | 250   | 0        | 0        | 23      | 0            |
| 3   | P     | 250   | 0        | 0        | 11      | 0            |
| 3   | Q     | 255   | 0        | 0        | 12      | 0            |
| 3   | R     | 286   | 0        | 0        | 12      | 0            |
| 3   | S     | 237   | 0        | 0        | 8       | 0            |
| 3   | T     | 295   | 0        | 0        | 14      | 1            |
| 3   | U     | 266   | 0        | 0        | 14      | 0            |
| 3   | V     | 258   | 0        | 0        | 15      | 0            |
| 3   | W     | 256   | 0        | 0        | 10      | 0            |
| 3   | X     | 256   | 0        | 0        | 12      | 0            |
| 3   | Y     | 262   | 0        | 0        | 17      | 0            |
| 3   | Z     | 285   | 0        | 0        | 18      | 0            |
| 3   | a     | 257   | 0        | 0        | 0       | 0            |
| 3   | b     | 254   | 0        | 0        | 0       | 0            |
| 3   | c     | 269   | 0        | 0        | 0       | 0            |
| 3   | d     | 244   | 0        | 0        | 0       | 0            |
| 3   | e     | 258   | 0        | 0        | 0       | 0            |
| 3   | f     | 231   | 0        | 0        | 0       | 0            |
| 3   | g     | 260   | 0        | 0        | 0       | 0            |
| 3   | h     | 281   | 0        | 0        | 0       | 2            |
| 3   | i     | 282   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 3   | j     | 267    | 0        | 0        | 0       | 0            |
| 3   | k     | 256    | 0        | 0        | 0       | 0            |
| 3   | l     | 257    | 0        | 0        | 0       | 0            |
| 3   | m     | 252    | 0        | 0        | 0       | 0            |
| 3   | n     | 251    | 0        | 0        | 0       | 0            |
| 3   | o     | 262    | 0        | 0        | 0       | 1            |
| 3   | p     | 238    | 0        | 0        | 0       | 0            |
| 3   | q     | 258    | 0        | 0        | 0       | 0            |
| 3   | r     | 287    | 0        | 0        | 0       | 4            |
| 3   | s     | 226    | 0        | 0        | 0       | 0            |
| 3   | t     | 236    | 0        | 0        | 0       | 0            |
| 3   | u     | 240    | 0        | 0        | 0       | 1            |
| 3   | v     | 249    | 0        | 0        | 0       | 0            |
| 3   | w     | 279    | 0        | 0        | 0       | 0            |
| 3   | x     | 260    | 0        | 0        | 0       | 0            |
| 3   | y     | 294    | 0        | 0        | 0       | 0            |
| 3   | z     | 264    | 0        | 0        | 0       | 0            |
| All | All   | 102135 | 0        | 87405    | 2109    | 6            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 2109 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1         | Atom-2         | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:I:19:MET:CE  | 1:Q:13:MET:CE  | 63.35                    | 1.59              |
| 1:G:19:MET:HE3 | 1:M:13:MET:CE  | 1.15                     | 1.55              |
| 1:Y:17:LYS:CB  | 1:Z:19:MET:HE1 | 61.89                    | 1.54              |
| 1:G:19:MET:CE  | 1:M:13:MET:HE3 | 1.10                     | 1.53              |
| 1:D:13:MET:CE  | 1:K:19:MET:HE3 | 45.00                    | 1.47              |

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|----------------------|--------------------------|-------------------|
| 3:r:405:HOH:O | 3:4:419:HOH:O[4_545] | 1.23                     | 0.97              |
| 3:h:501:HOH:O | 3:r:544:HOH:O[4_555] | 1.60                     | 0.60              |
| 3:h:442:HOH:O | 3:r:544:HOH:O[4_555] | 1.78                     | 0.42              |
| 3:T:434:HOH:O | 3:T:585:HOH:O[2_655] | 1.94                     | 0.26              |
| 3:o:317:HOH:O | 3:u:479:HOH:O[2_555] | 1.99                     | 0.21              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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   | 0     | 184/196 (94%) | 179 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | 1     | 185/196 (94%) | 178 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | 2     | 186/196 (95%) | 180 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | 3     | 186/196 (95%) | 181 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | 4     | 185/196 (94%) | 179 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | 5     | 183/196 (93%) | 179 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | 6     | 185/196 (94%) | 180 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | 7     | 184/196 (94%) | 179 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | A     | 188/196 (96%) | 183 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | B     | 188/196 (96%) | 183 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | C     | 186/196 (95%) | 181 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | D     | 186/196 (95%) | 181 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | E     | 184/196 (94%) | 176 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 1   | F     | 184/196 (94%) | 176 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 1   | G     | 186/196 (95%) | 178 (96%) | 7 (4%)  | 1 (0%)   | 32          | 8   |
| 1   | H     | 184/196 (94%) | 178 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | I     | 185/196 (94%) | 180 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | J     | 184/196 (94%) | 178 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | K     | 189/196 (96%) | 184 (97%) | 4 (2%)  | 1 (0%)   | 32          | 8   |
| 1   | L     | 187/196 (95%) | 182 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | M     | 185/196 (94%) | 178 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | N     | 185/196 (94%) | 180 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | O     | 184/196 (94%) | 180 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | P     | 188/196 (96%) | 182 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | Q     | 184/196 (94%) | 179 (97%) | 5 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | R     | 185/196 (94%) | 179 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | S     | 188/196 (96%) | 182 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | T     | 185/196 (94%) | 179 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | U     | 186/196 (95%) | 181 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | V     | 185/196 (94%) | 180 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | W     | 183/196 (93%) | 176 (96%) | 6 (3%)  | 1 (0%)   | 32          | 8   |
| 1   | X     | 184/196 (94%) | 180 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | Y     | 185/196 (94%) | 180 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | Z     | 185/196 (94%) | 179 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | a     | 187/196 (95%) | 182 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | b     | 183/196 (93%) | 179 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | c     | 185/196 (94%) | 179 (97%) | 5 (3%)  | 1 (0%)   | 32          | 8   |
| 1   | d     | 184/196 (94%) | 178 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | e     | 184/196 (94%) | 179 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | f     | 186/196 (95%) | 178 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 1   | g     | 184/196 (94%) | 178 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | h     | 186/196 (95%) | 181 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | i     | 185/196 (94%) | 179 (97%) | 5 (3%)  | 1 (0%)   | 32          | 8   |
| 1   | j     | 184/196 (94%) | 178 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | k     | 184/196 (94%) | 179 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | l     | 183/196 (93%) | 178 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | m     | 184/196 (94%) | 178 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | n     | 186/196 (95%) | 180 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | o     | 183/196 (93%) | 178 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | p     | 183/196 (93%) | 178 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | q     | 183/196 (93%) | 178 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | r     | 185/196 (94%) | 179 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | s     | 184/196 (94%) | 177 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | t     | 189/196 (96%) | 183 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 1   | u     | 184/196 (94%) | 180 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | v     | 184/196 (94%) | 179 (97%) | 5 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | w     | 185/196 (94%)     | 181 (98%)   | 4 (2%)   | 0        | 100         | 100 |
| 1   | x     | 185/196 (94%)     | 178 (96%)   | 7 (4%)   | 0        | 100         | 100 |
| 1   | y     | 184/196 (94%)     | 178 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 1   | z     | 186/196 (95%)     | 181 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| All | All   | 11101/11760 (94%) | 10766 (97%) | 330 (3%) | 5 (0%)   | 100         | 100 |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | W     | 15  | ALA  |
| 1   | G     | 14  | ARG  |
| 1   | K     | 13  | MET  |
| 1   | i     | 14  | ARG  |
| 1   | c     | 13  | MET  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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   | 0     | 159/167 (95%) | 157 (99%) | 2 (1%)   | 73          | 40 |
| 1   | 1     | 160/167 (96%) | 157 (98%) | 3 (2%)   | 62          | 25 |
| 1   | 2     | 161/167 (96%) | 156 (97%) | 5 (3%)   | 45          | 11 |
| 1   | 3     | 161/167 (96%) | 157 (98%) | 4 (2%)   | 53          | 16 |
| 1   | 4     | 160/167 (96%) | 156 (98%) | 4 (2%)   | 53          | 16 |
| 1   | 5     | 158/167 (95%) | 154 (98%) | 4 (2%)   | 53          | 16 |
| 1   | 6     | 160/167 (96%) | 158 (99%) | 2 (1%)   | 73          | 40 |
| 1   | 7     | 159/167 (95%) | 155 (98%) | 4 (2%)   | 53          | 16 |
| 1   | A     | 163/167 (98%) | 160 (98%) | 3 (2%)   | 64          | 27 |
| 1   | B     | 163/167 (98%) | 159 (98%) | 4 (2%)   | 53          | 16 |
| 1   | C     | 161/167 (96%) | 152 (94%) | 9 (6%)   | 25          | 2  |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | D     | 161/167 (96%) | 153 (95%) | 8 (5%)   | 28          | 3  |
| 1   | E     | 159/167 (95%) | 155 (98%) | 4 (2%)   | 53          | 16 |
| 1   | F     | 159/167 (95%) | 156 (98%) | 3 (2%)   | 62          | 25 |
| 1   | G     | 161/167 (96%) | 156 (97%) | 5 (3%)   | 45          | 11 |
| 1   | H     | 159/167 (95%) | 153 (96%) | 6 (4%)   | 38          | 6  |
| 1   | I     | 160/167 (96%) | 158 (99%) | 2 (1%)   | 73          | 40 |
| 1   | J     | 159/167 (95%) | 154 (97%) | 5 (3%)   | 45          | 11 |
| 1   | K     | 164/167 (98%) | 159 (97%) | 5 (3%)   | 46          | 11 |
| 1   | L     | 162/167 (97%) | 157 (97%) | 5 (3%)   | 45          | 11 |
| 1   | M     | 160/167 (96%) | 155 (97%) | 5 (3%)   | 45          | 11 |
| 1   | N     | 160/167 (96%) | 157 (98%) | 3 (2%)   | 62          | 25 |
| 1   | O     | 159/167 (95%) | 154 (97%) | 5 (3%)   | 45          | 11 |
| 1   | P     | 163/167 (98%) | 159 (98%) | 4 (2%)   | 53          | 16 |
| 1   | Q     | 159/167 (95%) | 154 (97%) | 5 (3%)   | 45          | 11 |
| 1   | R     | 160/167 (96%) | 154 (96%) | 6 (4%)   | 38          | 6  |
| 1   | S     | 163/167 (98%) | 159 (98%) | 4 (2%)   | 53          | 16 |
| 1   | T     | 160/167 (96%) | 153 (96%) | 7 (4%)   | 33          | 5  |
| 1   | U     | 161/167 (96%) | 158 (98%) | 3 (2%)   | 62          | 25 |
| 1   | V     | 160/167 (96%) | 157 (98%) | 3 (2%)   | 62          | 25 |
| 1   | W     | 158/167 (95%) | 155 (98%) | 3 (2%)   | 62          | 25 |
| 1   | X     | 159/167 (95%) | 155 (98%) | 4 (2%)   | 53          | 16 |
| 1   | Y     | 160/167 (96%) | 156 (98%) | 4 (2%)   | 53          | 16 |
| 1   | Z     | 160/167 (96%) | 157 (98%) | 3 (2%)   | 62          | 25 |
| 1   | a     | 162/167 (97%) | 161 (99%) | 1 (1%)   | 89          | 70 |
| 1   | b     | 158/167 (95%) | 153 (97%) | 5 (3%)   | 44          | 10 |
| 1   | c     | 160/167 (96%) | 156 (98%) | 4 (2%)   | 53          | 16 |
| 1   | d     | 159/167 (95%) | 155 (98%) | 4 (2%)   | 53          | 16 |
| 1   | e     | 159/167 (95%) | 156 (98%) | 3 (2%)   | 62          | 25 |
| 1   | f     | 161/167 (96%) | 156 (97%) | 5 (3%)   | 45          | 11 |
| 1   | g     | 159/167 (95%) | 156 (98%) | 3 (2%)   | 62          | 25 |
| 1   | h     | 161/167 (96%) | 158 (98%) | 3 (2%)   | 62          | 25 |

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| Mol | Chain | Analysed         | Rotameric  | Outliers | Percentiles |    |
|-----|-------|------------------|------------|----------|-------------|----|
| 1   | i     | 160/167 (96%)    | 157 (98%)  | 3 (2%)   | 62          | 25 |
| 1   | j     | 159/167 (95%)    | 157 (99%)  | 2 (1%)   | 73          | 40 |
| 1   | k     | 159/167 (95%)    | 156 (98%)  | 3 (2%)   | 62          | 25 |
| 1   | l     | 158/167 (95%)    | 154 (98%)  | 4 (2%)   | 53          | 16 |
| 1   | m     | 159/167 (95%)    | 155 (98%)  | 4 (2%)   | 53          | 16 |
| 1   | n     | 161/167 (96%)    | 158 (98%)  | 3 (2%)   | 62          | 25 |
| 1   | o     | 158/167 (95%)    | 155 (98%)  | 3 (2%)   | 62          | 25 |
| 1   | p     | 158/167 (95%)    | 154 (98%)  | 4 (2%)   | 53          | 16 |
| 1   | q     | 158/167 (95%)    | 154 (98%)  | 4 (2%)   | 53          | 16 |
| 1   | r     | 160/167 (96%)    | 152 (95%)  | 8 (5%)   | 28          | 3  |
| 1   | s     | 159/167 (95%)    | 154 (97%)  | 5 (3%)   | 45          | 11 |
| 1   | t     | 164/167 (98%)    | 159 (97%)  | 5 (3%)   | 46          | 11 |
| 1   | u     | 159/167 (95%)    | 154 (97%)  | 5 (3%)   | 45          | 11 |
| 1   | v     | 159/167 (95%)    | 155 (98%)  | 4 (2%)   | 53          | 16 |
| 1   | w     | 160/167 (96%)    | 158 (99%)  | 2 (1%)   | 73          | 40 |
| 1   | x     | 160/167 (96%)    | 157 (98%)  | 3 (2%)   | 62          | 25 |
| 1   | y     | 159/167 (95%)    | 156 (98%)  | 3 (2%)   | 62          | 25 |
| 1   | z     | 161/167 (96%)    | 156 (97%)  | 5 (3%)   | 45          | 11 |
| All | All   | 9601/10020 (96%) | 9357 (98%) | 244 (2%) | 53          | 16 |

5 of 244 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 7     | 71  | LYS  |
| 1   | E     | 12  | THR  |
| 1   | Y     | 70  | HIS  |
| 1   | A     | 33  | ASN  |
| 1   | C     | 70  | HIS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 487 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5     | 23  | HIS  |
| 1   | D     | 93  | ASN  |
| 1   | Z     | 95  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 5     | 95  | ASN  |
| 1   | A     | 73  | HIS  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 92 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1   | 0     | 184/196 (93%) | -0.50  | 7 (3%) 41 42 | 7, 10, 27, 62         | 0     |
| 1   | 1     | 184/196 (93%) | -0.44  | 5 (2%) 55 56 | 8, 10, 26, 63         | 0     |
| 1   | 2     | 184/196 (93%) | -0.51  | 6 (3%) 47 48 | 7, 10, 25, 61         | 0     |
| 1   | 3     | 184/196 (93%) | -0.45  | 7 (3%) 41 42 | 8, 11, 29, 61         | 0     |
| 1   | 4     | 184/196 (93%) | -0.52  | 7 (3%) 41 42 | 7, 10, 25, 58         | 0     |
| 1   | 5     | 184/196 (93%) | -0.43  | 9 (4%) 30 32 | 9, 11, 29, 64         | 0     |
| 1   | 6     | 184/196 (93%) | -0.44  | 9 (4%) 30 32 | 8, 11, 29, 64         | 0     |
| 1   | 7     | 184/196 (93%) | -0.46  | 6 (3%) 47 48 | 8, 11, 28, 61         | 0     |
| 1   | A     | 184/196 (93%) | -0.44  | 7 (3%) 41 42 | 8, 10, 29, 63         | 0     |
| 1   | B     | 184/196 (93%) | -0.47  | 7 (3%) 41 42 | 8, 11, 29, 62         | 0     |
| 1   | C     | 184/196 (93%) | -0.47  | 8 (4%) 36 37 | 9, 12, 28, 61         | 0     |
| 1   | D     | 184/196 (93%) | -0.50  | 7 (3%) 41 42 | 8, 10, 27, 64         | 0     |
| 1   | E     | 184/196 (93%) | -0.42  | 5 (2%) 55 56 | 9, 12, 27, 63         | 0     |
| 1   | F     | 184/196 (93%) | -0.43  | 6 (3%) 47 48 | 9, 12, 28, 63         | 0     |
| 1   | G     | 184/196 (93%) | -0.43  | 5 (2%) 55 56 | 9, 12, 29, 62         | 0     |
| 1   | H     | 184/196 (93%) | -0.47  | 7 (3%) 41 42 | 8, 11, 29, 64         | 0     |
| 1   | I     | 184/196 (93%) | -0.45  | 8 (4%) 36 37 | 9, 11, 29, 62         | 0     |
| 1   | J     | 184/196 (93%) | -0.47  | 7 (3%) 41 42 | 8, 11, 27, 60         | 0     |
| 1   | K     | 184/196 (93%) | -0.51  | 7 (3%) 41 42 | 7, 9, 27, 61          | 0     |
| 1   | L     | 184/196 (93%) | -0.45  | 7 (3%) 41 42 | 8, 11, 28, 62         | 0     |
| 1   | M     | 184/196 (93%) | -0.44  | 8 (4%) 36 37 | 7, 11, 28, 64         | 0     |
| 1   | N     | 184/196 (93%) | -0.40  | 5 (2%) 55 56 | 9, 12, 29, 63         | 0     |
| 1   | O     | 184/196 (93%) | -0.48  | 5 (2%) 55 56 | 9, 12, 29, 62         | 0     |
| 1   | P     | 184/196 (93%) | -0.46  | 7 (3%) 41 42 | 8, 11, 28, 62         | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1   | Q     | 184/196 (93%) | -0.43  | 8 (4%) 36 37 | 8, 11, 28, 62         | 0     |
| 1   | R     | 184/196 (93%) | -0.51  | 6 (3%) 47 48 | 7, 10, 27, 61         | 0     |
| 1   | S     | 184/196 (93%) | -0.44  | 5 (2%) 55 56 | 8, 11, 27, 62         | 0     |
| 1   | T     | 184/196 (93%) | -0.53  | 6 (3%) 47 48 | 7, 9, 27, 63          | 0     |
| 1   | U     | 184/196 (93%) | -0.48  | 7 (3%) 41 42 | 7, 9, 27, 64          | 0     |
| 1   | V     | 184/196 (93%) | -0.52  | 6 (3%) 47 48 | 7, 10, 26, 59         | 0     |
| 1   | W     | 184/196 (93%) | -0.45  | 7 (3%) 41 42 | 9, 11, 29, 65         | 0     |
| 1   | X     | 184/196 (93%) | -0.47  | 6 (3%) 47 48 | 8, 10, 28, 60         | 0     |
| 1   | Y     | 184/196 (93%) | -0.50  | 7 (3%) 41 42 | 7, 10, 28, 61         | 0     |
| 1   | Z     | 184/196 (93%) | -0.52  | 5 (2%) 55 56 | 6, 9, 28, 64          | 0     |
| 1   | a     | 184/196 (93%) | -0.48  | 5 (2%) 55 56 | 8, 11, 28, 59         | 0     |
| 1   | b     | 184/196 (93%) | -0.50  | 6 (3%) 47 48 | 7, 10, 27, 58         | 0     |
| 1   | c     | 184/196 (93%) | -0.49  | 9 (4%) 30 32 | 7, 10, 27, 64         | 0     |
| 1   | d     | 184/196 (93%) | -0.51  | 5 (2%) 55 56 | 7, 9, 27, 62          | 0     |
| 1   | e     | 184/196 (93%) | -0.46  | 6 (3%) 47 48 | 7, 10, 27, 63         | 0     |
| 1   | f     | 184/196 (93%) | -0.46  | 6 (3%) 47 48 | 9, 12, 29, 60         | 0     |
| 1   | g     | 184/196 (93%) | -0.45  | 6 (3%) 47 48 | 8, 11, 28, 63         | 0     |
| 1   | h     | 184/196 (93%) | -0.45  | 6 (3%) 47 48 | 7, 10, 25, 61         | 0     |
| 1   | i     | 184/196 (93%) | -0.46  | 6 (3%) 47 48 | 7, 10, 28, 60         | 0     |
| 1   | j     | 184/196 (93%) | -0.47  | 8 (4%) 36 37 | 7, 11, 26, 62         | 0     |
| 1   | k     | 184/196 (93%) | -0.47  | 7 (3%) 41 42 | 7, 10, 27, 61         | 0     |
| 1   | l     | 184/196 (93%) | -0.46  | 8 (4%) 36 37 | 7, 10, 27, 61         | 0     |
| 1   | m     | 184/196 (93%) | -0.43  | 6 (3%) 47 48 | 9, 12, 29, 64         | 0     |
| 1   | n     | 184/196 (93%) | -0.37  | 5 (2%) 55 56 | 9, 12, 30, 63         | 0     |
| 1   | o     | 184/196 (93%) | -0.51  | 7 (3%) 41 42 | 8, 11, 29, 64         | 0     |
| 1   | p     | 184/196 (93%) | -0.47  | 7 (3%) 41 42 | 8, 11, 26, 61         | 0     |
| 1   | q     | 184/196 (93%) | -0.50  | 5 (2%) 55 56 | 7, 10, 26, 61         | 0     |
| 1   | r     | 184/196 (93%) | -0.48  | 5 (2%) 55 56 | 7, 9, 27, 62          | 0     |
| 1   | s     | 184/196 (93%) | -0.47  | 9 (4%) 30 32 | 8, 11, 28, 61         | 0     |
| 1   | t     | 184/196 (93%) | -0.50  | 5 (2%) 55 56 | 8, 11, 29, 61         | 0     |
| 1   | u     | 184/196 (93%) | -0.48  | 7 (3%) 41 42 | 8, 11, 29, 60         | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 1   | v     | 184/196 (93%)     | -0.46  | 7 (3%) 41 42   | 7, 10, 27, 61         | 0     |
| 1   | w     | 184/196 (93%)     | -0.53  | 6 (3%) 47 48   | 7, 10, 25, 60         | 0     |
| 1   | x     | 184/196 (93%)     | -0.50  | 7 (3%) 41 42   | 7, 10, 27, 62         | 0     |
| 1   | y     | 184/196 (93%)     | -0.48  | 7 (3%) 41 42   | 7, 9, 26, 58          | 0     |
| 1   | z     | 184/196 (93%)     | -0.42  | 5 (2%) 55 56   | 8, 11, 27, 61         | 0     |
| All | All   | 11040/11760 (93%) | -0.47  | 391 (3%) 44 46 | 6, 11, 34, 65         | 0     |

The worst 5 of 391 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | x     | 12  | THR  | 9.1  |
| 1   | h     | 13  | MET  | 8.7  |
| 1   | k     | 12  | THR  | 8.7  |
| 1   | 3     | 12  | THR  | 8.4  |
| 1   | 1     | 13  | MET  | 8.3  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|------|----------------------------|-------|
| 2   | CA   | S     | 202 | 1/1   | 0.99 | 0.08 | 2.56 | 8,8,8,8                    | 0     |
| 2   | CA   | A     | 202 | 1/1   | 0.99 | 0.07 | 2.43 | 9,9,9,9                    | 0     |
| 2   | CA   | B     | 203 | 1/1   | 0.99 | 0.08 | 2.13 | 9,9,9,9                    | 0     |
| 2   | CA   | U     | 203 | 1/1   | 0.99 | 0.08 | 1.71 | 8,8,8,8                    | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 2   | CA   | 6     | 202 | 1/1   | 0.99 | 0.07 | 0.79  | 9,9,9,9                     | 0     |
| 2   | CA   | T     | 202 | 1/1   | 0.99 | 0.07 | 0.57  | 7,7,7,7                     | 0     |
| 2   | CA   | b     | 202 | 1/1   | 1.00 | 0.06 | 0.40  | 8,8,8,8                     | 0     |
| 2   | CA   | 0     | 201 | 1/1   | 0.99 | 0.06 | 0.36  | 8,8,8,8                     | 0     |
| 2   | CA   | j     | 202 | 1/1   | 1.00 | 0.06 | 0.30  | 8,8,8,8                     | 0     |
| 2   | CA   | Q     | 202 | 1/1   | 0.99 | 0.05 | 0.03  | 8,8,8,8                     | 0     |
| 2   | CA   | 5     | 202 | 1/1   | 0.99 | 0.06 | -0.03 | 9,9,9,9                     | 0     |
| 2   | CA   | 1     | 202 | 1/1   | 0.99 | 0.06 | -0.15 | 8,8,8,8                     | 0     |
| 2   | CA   | I     | 201 | 1/1   | 0.99 | 0.06 | -0.29 | 10,10,10,10                 | 0     |
| 2   | CA   | N     | 202 | 1/1   | 0.98 | 0.06 | -0.42 | 10,10,10,10                 | 0     |
| 2   | CA   | 3     | 202 | 1/1   | 0.99 | 0.05 | -0.53 | 9,9,9,9                     | 0     |
| 2   | CA   | V     | 201 | 1/1   | 0.99 | 0.05 | -0.60 | 6,6,6,6                     | 0     |
| 2   | CA   | 4     | 202 | 1/1   | 1.00 | 0.04 | -0.72 | 8,8,8,8                     | 0     |
| 2   | CA   | R     | 201 | 1/1   | 1.00 | 0.04 | -0.84 | 8,8,8,8                     | 0     |
| 2   | CA   | m     | 201 | 1/1   | 1.00 | 0.04 | -0.93 | 11,11,11,11                 | 0     |
| 2   | CA   | 1     | 201 | 1/1   | 1.00 | 0.04 | -0.96 | 9,9,9,9                     | 0     |
| 2   | CA   | b     | 201 | 1/1   | 1.00 | 0.03 | -1.01 | 9,9,9,9                     | 0     |
| 2   | CA   | E     | 202 | 1/1   | 0.99 | 0.04 | -1.05 | 9,9,9,9                     | 0     |
| 2   | CA   | P     | 201 | 1/1   | 0.99 | 0.04 | -1.11 | 10,10,10,10                 | 0     |
| 2   | CA   | 2     | 202 | 1/1   | 1.00 | 0.03 | -1.12 | 9,9,9,9                     | 0     |
| 2   | CA   | w     | 201 | 1/1   | 1.00 | 0.04 | -1.14 | 8,8,8,8                     | 0     |
| 2   | CA   | x     | 201 | 1/1   | 1.00 | 0.03 | -1.22 | 8,8,8,8                     | 0     |
| 2   | CA   | C     | 201 | 1/1   | 1.00 | 0.04 | -1.22 | 10,10,10,10                 | 0     |
| 2   | CA   | 7     | 201 | 1/1   | 1.00 | 0.03 | -1.24 | 9,9,9,9                     | 0     |
| 2   | CA   | N     | 201 | 1/1   | 0.99 | 0.04 | -1.30 | 11,11,11,11                 | 0     |
| 2   | CA   | K     | 201 | 1/1   | 1.00 | 0.04 | -1.32 | 9,9,9,9                     | 0     |
| 2   | CA   | M     | 201 | 1/1   | 1.00 | 0.03 | -1.35 | 9,9,9,9                     | 0     |
| 2   | CA   | h     | 201 | 1/1   | 1.00 | 0.03 | -1.39 | 8,8,8,8                     | 0     |
| 2   | CA   | g     | 201 | 1/1   | 1.00 | 0.03 | -1.41 | 8,8,8,8                     | 0     |
| 2   | CA   | f     | 201 | 1/1   | 1.00 | 0.02 | -1.44 | 10,10,10,10                 | 0     |
| 2   | CA   | Z     | 201 | 1/1   | 1.00 | 0.03 | -1.46 | 8,8,8,8                     | 0     |
| 2   | CA   | U     | 202 | 1/1   | 1.00 | 0.03 | -1.46 | 8,8,8,8                     | 0     |
| 2   | CA   | 6     | 201 | 1/1   | 1.00 | 0.03 | -1.47 | 9,9,9,9                     | 0     |
| 2   | CA   | y     | 201 | 1/1   | 1.00 | 0.02 | -1.48 | 8,8,8,8                     | 0     |
| 2   | CA   | c     | 201 | 1/1   | 1.00 | 0.03 | -1.51 | 7,7,7,7                     | 0     |
| 2   | CA   | v     | 201 | 1/1   | 1.00 | 0.03 | -1.53 | 8,8,8,8                     | 0     |
| 2   | CA   | W     | 201 | 1/1   | 0.99 | 0.03 | -1.57 | 10,10,10,10                 | 0     |
| 2   | CA   | G     | 203 | 1/1   | 0.99 | 0.05 | -1.59 | 9,9,9,9                     | 0     |
| 2   | CA   | p     | 201 | 1/1   | 1.00 | 0.02 | -1.59 | 9,9,9,9                     | 0     |
| 2   | CA   | i     | 201 | 1/1   | 1.00 | 0.03 | -1.65 | 8,8,8,8                     | 0     |
| 2   | CA   | 5     | 201 | 1/1   | 1.00 | 0.03 | -1.67 | 10,10,10,10                 | 0     |
| 2   | CA   | H     | 201 | 1/1   | 1.00 | 0.03 | -1.68 | 10,10,10,10                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 2   | CA   | X     | 201 | 1/1   | 1.00 | 0.03 | -1.70 | 9,9,9,9                     | 0     |
| 2   | CA   | D     | 201 | 1/1   | 1.00 | 0.03 | -1.70 | 9,9,9,9                     | 0     |
| 2   | CA   | 3     | 201 | 1/1   | 1.00 | 0.02 | -1.72 | 9,9,9,9                     | 0     |
| 2   | CA   | I     | 202 | 1/1   | 1.00 | 0.02 | -1.73 | 10,10,10,10                 | 0     |
| 2   | CA   | J     | 201 | 1/1   | 1.00 | 0.03 | -1.75 | 9,9,9,9                     | 0     |
| 2   | CA   | R     | 202 | 1/1   | 1.00 | 0.02 | -1.77 | 8,8,8,8                     | 0     |
| 2   | CA   | V     | 202 | 1/1   | 1.00 | 0.02 | -1.80 | 8,8,8,8                     | 0     |
| 2   | CA   | L     | 201 | 1/1   | 1.00 | 0.03 | -1.86 | 9,9,9,9                     | 0     |
| 2   | CA   | u     | 201 | 1/1   | 1.00 | 0.02 | -1.86 | 9,9,9,9                     | 0     |
| 2   | CA   | Y     | 201 | 1/1   | 1.00 | 0.03 | -1.89 | 9,9,9,9                     | 0     |
| 2   | CA   | z     | 201 | 1/1   | 1.00 | 0.02 | -1.89 | 9,9,9,9                     | 0     |
| 2   | CA   | E     | 201 | 1/1   | 1.00 | 0.02 | -1.92 | 9,9,9,9                     | 0     |
| 2   | CA   | d     | 201 | 1/1   | 1.00 | 0.03 | -1.92 | 8,8,8,8                     | 0     |
| 2   | CA   | 4     | 201 | 1/1   | 1.00 | 0.02 | -1.95 | 9,9,9,9                     | 0     |
| 2   | CA   | 0     | 202 | 1/1   | 1.00 | 0.02 | -1.96 | 8,8,8,8                     | 0     |
| 2   | CA   | o     | 201 | 1/1   | 1.00 | 0.03 | -1.98 | 9,9,9,9                     | 0     |
| 2   | CA   | F     | 201 | 1/1   | 1.00 | 0.02 | -2.09 | 9,9,9,9                     | 0     |
| 2   | CA   | Q     | 201 | 1/1   | 1.00 | 0.03 | -2.09 | 9,9,9,9                     | 0     |
| 2   | CA   | n     | 202 | 1/1   | 0.99 | 0.03 | -2.10 | 11,11,11,11                 | 0     |
| 2   | CA   | S     | 201 | 1/1   | 1.00 | 0.03 | -2.12 | 9,9,9,9                     | 0     |
| 2   | CA   | q     | 201 | 1/1   | 1.00 | 0.02 | -2.13 | 7,7,7,7                     | 0     |
| 2   | CA   | B     | 201 | 1/1   | 1.00 | 0.02 | -2.21 | 10,10,10,10                 | 0     |
| 2   | CA   | O     | 201 | 1/1   | 1.00 | 0.03 | -2.23 | 10,10,10,10                 | 0     |
| 2   | CA   | e     | 201 | 1/1   | 1.00 | 0.02 | -2.31 | 9,9,9,9                     | 0     |
| 2   | CA   | T     | 201 | 1/1   | 1.00 | 0.02 | -2.33 | 8,8,8,8                     | 0     |
| 2   | CA   | j     | 201 | 1/1   | 1.00 | 0.03 | -2.33 | 8,8,8,8                     | 0     |
| 2   | CA   | s     | 201 | 1/1   | 1.00 | 0.02 | -2.39 | 8,8,8,8                     | 0     |
| 2   | CA   | i     | 202 | 1/1   | 1.00 | 0.04 | -2.41 | 11,11,11,11                 | 0     |
| 2   | CA   | k     | 201 | 1/1   | 1.00 | 0.03 | -2.44 | 8,8,8,8                     | 0     |
| 2   | CA   | G     | 201 | 1/1   | 1.00 | 0.02 | -2.47 | 10,10,10,10                 | 0     |
| 2   | CA   | l     | 201 | 1/1   | 1.00 | 0.01 | -2.54 | 9,9,9,9                     | 0     |
| 2   | CA   | t     | 201 | 1/1   | 1.00 | 0.02 | -2.55 | 10,10,10,10                 | 0     |
| 2   | CA   | r     | 201 | 1/1   | 1.00 | 0.02 | -2.83 | 9,9,9,9                     | 0     |
| 2   | CA   | c     | 202 | 1/1   | 1.00 | 0.03 | -3.12 | 10,10,10,10                 | 0     |
| 2   | CA   | K     | 202 | 1/1   | 1.00 | 0.02 | -3.16 | 9,9,9,9                     | 0     |
| 2   | CA   | A     | 201 | 1/1   | 1.00 | 0.02 | -3.26 | 9,9,9,9                     | 0     |
| 2   | CA   | E     | 203 | 1/1   | 1.00 | 0.02 | -3.46 | 11,11,11,11                 | 0     |
| 2   | CA   | a     | 201 | 1/1   | 1.00 | 0.02 | -3.51 | 9,9,9,9                     | 0     |
| 2   | CA   | G     | 202 | 1/1   | 0.99 | 0.03 | -3.60 | 12,12,12,12                 | 0     |
| 2   | CA   | q     | 202 | 1/1   | 1.00 | 0.02 | -3.79 | 10,10,10,10                 | 0     |
| 2   | CA   | 2     | 201 | 1/1   | 1.00 | 0.02 | -3.97 | 10,10,10,10                 | 0     |
| 2   | CA   | n     | 201 | 1/1   | 1.00 | 0.02 | -4.17 | 11,11,11,11                 | 0     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|-----------------------------|-------|
| 2   | CA   | 1     | 203 | 1/1   | 1.00 | 0.03 | -4.28 | 10,10,10,10                 | 0     |
| 2   | CA   | U     | 201 | 1/1   | 1.00 | 0.02 | -4.36 | 9,9,9,9                     | 0     |
| 2   | CA   | o     | 202 | 1/1   | 1.00 | 0.02 | -5.01 | 12,12,12,12                 | 0     |
| 2   | CA   | B     | 202 | 1/1   | 1.00 | 0.02 | -6.11 | 10,10,10,10                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.