



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:56 AM UTC

PDB ID : 6YFO / pdb\_00006yfo  
Title : Virus-like particle of bacteriophage GQ-907  
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.  
Deposited on : 2020-03-26  
Resolution : 3.48 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

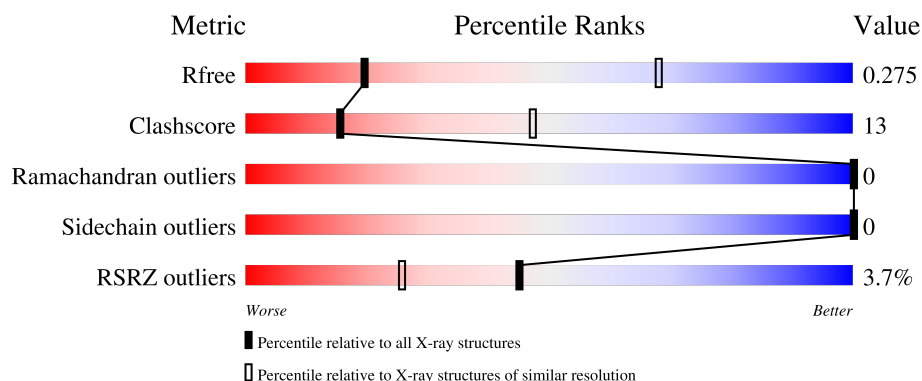
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.48 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1083 (3.52-3.44)                                      |
| Clashscore            | 190562                      | 1139 (3.52-3.44)                                      |
| Ramachandran outliers | 187476                      | 1111 (3.52-3.44)                                      |
| Sidechain outliers    | 187428                      | 1112 (3.52-3.44)                                      |
| RSRZ outliers         | 180081                      | 1082 (3.52-3.44)                                      |

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                         |
|-----|-------|--------|----------------------------------------------------------|
| 1   | AA    | 131    | <div> <div>5%</div> <div>79%</div> <div>21%</div> </div> |
| 1   | AB    | 131    | <div> <div>2%</div> <div>68%</div> <div>32%</div> </div> |
| 1   | AC    | 131    | <div> <div>5%</div> <div>73%</div> <div>27%</div> </div> |
| 1   | AD    | 131    | <div> <div>5%</div> <div>80%</div> <div>20%</div> </div> |
| 1   | AE    | 131    | <div> <div>2%</div> <div>68%</div> <div>32%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AF    | 131    |                  |
| 1   | AG    | 131    |                  |
| 1   | AH    | 131    |                  |
| 1   | AI    | 131    |                  |
| 1   | AJ    | 131    |                  |
| 1   | AK    | 131    |                  |
| 1   | AL    | 131    |                  |
| 1   | AM    | 131    |                  |
| 1   | AN    | 131    |                  |
| 1   | AO    | 131    |                  |
| 1   | AP    | 131    |                  |
| 1   | AQ    | 131    |                  |
| 1   | AR    | 131    |                  |
| 1   | AS    | 131    |                  |
| 1   | AT    | 131    |                  |
| 1   | AU    | 131    |                  |
| 1   | AV    | 131    |                  |
| 1   | AW    | 131    |                  |
| 1   | AX    | 131    |                  |
| 1   | AY    | 131    |                  |
| 1   | AZ    | 131    |                  |
| 1   | BA    | 131    |                  |
| 1   | BB    | 131    |                  |
| 1   | BC    | 131    |                  |
| 1   | BD    | 131    |                  |

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| Mol | Chain | Length | Quality of chain                                                      |
|-----|-------|--------|-----------------------------------------------------------------------|
| 1   | BE    | 131    | <div> <div></div> <div>4%</div> <div>79%</div> <div>21%</div> </div>  |
| 1   | BF    | 131    | <div> <div></div> <div>4%</div> <div>70%</div> <div>30%</div> </div>  |
| 1   | BG    | 131    | <div> <div></div> <div>4%</div> <div>74%</div> <div>26%</div> </div>  |
| 1   | BH    | 131    | <div> <div></div> <div>10%</div> <div>82%</div> <div>18%</div> </div> |
| 1   | BI    | 131    | <div> <div></div> <div>5%</div> <div>70%</div> <div>30%</div> </div>  |
| 1   | BJ    | 131    | <div> <div></div> <div>2%</div> <div>76%</div> <div>24%</div> </div>  |
| 1   | BK    | 131    | <div> <div></div> <div>6%</div> <div>80%</div> <div>20%</div> </div>  |
| 1   | BL    | 131    | <div> <div></div> <div></div> <div>69%</div> <div>31%</div> </div>    |
| 1   | BM    | 131    | <div> <div></div> <div>9%</div> <div>69%</div> <div>31%</div> </div>  |
| 1   | BN    | 131    | <div> <div></div> <div>5%</div> <div>83%</div> <div>17%</div> </div>  |
| 1   | BO    | 131    | <div> <div></div> <div>5%</div> <div>69%</div> <div>31%</div> </div>  |
| 1   | BP    | 131    | <div> <div></div> <div>5%</div> <div>73%</div> <div>27%</div> </div>  |
| 1   | BQ    | 131    | <div> <div></div> <div>5%</div> <div>83%</div> <div>17%</div> </div>  |
| 1   | BR    | 131    | <div> <div></div> <div>4%</div> <div>69%</div> <div>31%</div> </div>  |
| 1   | BS    | 131    | <div> <div></div> <div>2%</div> <div>78%</div> <div>22%</div> </div>  |
| 1   | BT    | 131    | <div> <div></div> <div></div> <div>81%</div> <div>19%</div> </div>    |
| 1   | BU    | 131    | <div> <div></div> <div>5%</div> <div>69%</div> <div>31%</div> </div>  |
| 1   | BV    | 131    | <div> <div></div> <div>5%</div> <div>73%</div> <div>27%</div> </div>  |
| 1   | BW    | 131    | <div> <div></div> <div>3%</div> <div>79%</div> <div>21%</div> </div>  |
| 1   | BX    | 131    | <div> <div></div> <div>2%</div> <div>67%</div> <div>33%</div> </div>  |
| 1   | BY    | 131    | <div> <div></div> <div>5%</div> <div>69%</div> <div>31%</div> </div>  |
| 1   | BZ    | 131    | <div> <div></div> <div>5%</div> <div>82%</div> <div>18%</div> </div>  |
| 1   | CA    | 131    | <div> <div></div> <div></div> <div>68%</div> <div>32%</div> </div>    |
| 1   | CB    | 131    | <div> <div></div> <div>2%</div> <div>76%</div> <div>24%</div> </div>  |
| 1   | CC    | 131    | <div> <div></div> <div>2%</div> <div>77%</div> <div>23%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |         |
|-----|-------|--------|------------------|---------|
| 1   | CD    | 131    | 5%               | 66% 34% |
| 1   | CE    | 131    | 5%               | 69% 31% |
| 1   | CF    | 131    | 6%               | 80% 20% |
| 1   | CG    | 131    | 2%               | 69% 31% |
| 1   | CH    | 131    | 8%               | 79% 21% |
| 1   | CI    | 131    | 2%               | 77% 23% |
| 1   | CJ    | 131    | 4%               | 69% 31% |
| 1   | CK    | 131    | 7%               | 74% 26% |
| 1   | CL    | 131    | 2%               | 80% 20% |
| 1   | CM    | 131    | 2%               | 69% 31% |
| 1   | CN    | 131    | 2%               | 75% 25% |
| 1   | CO    | 131    | 2%               | 82% 18% |
| 1   | CP    | 131    |                  | 70% 30% |
| 1   | CQ    | 131    | 2%               | 81% 19% |
| 1   | CR    | 131    | 5%               | 81% 19% |
| 1   | CS    | 131    | 4%               | 69% 31% |
| 1   | CT    | 131    | 8%               | 74% 26% |
| 1   | CU    | 131    | 2%               | 80% 20% |
| 1   | CV    | 131    | 2%               | 67% 33% |
| 1   | CW    | 131    | 2%               | 76% 24% |
| 1   | CX    | 131    | 4%               | 80% 20% |
| 1   | CY    | 131    | 2%               | 70% 30% |
| 1   | CZ    | 131    | %                | 76% 24% |
| 1   | DA    | 131    | 2%               | 79% 21% |
| 1   | DB    | 131    | 2%               | 69% 31% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | DC    | 131    |                  |
| 1   | DD    | 131    |                  |
| 1   | DE    | 131    |                  |
| 1   | DF    | 131    |                  |
| 1   | DG    | 131    |                  |
| 1   | DH    | 131    |                  |
| 1   | DI    | 131    |                  |
| 1   | DJ    | 131    |                  |
| 1   | DK    | 131    |                  |
| 1   | DL    | 131    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 87480 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   | AA    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AB    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AC    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AD    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AE    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AF    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AG    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AH    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AI    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AJ    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AK    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AL    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AM    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AN    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AO    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |
| 1   | AP    | 131      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 972   | 607 | 166 | 198 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 1   | AQ    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | AR    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | AS    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | AT    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | AU    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | AV    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | AW    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | AX    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | AY    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | AZ    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BA    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BB    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BC    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BD    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BE    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BF    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BG    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BH    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BI    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BJ    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BK    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 1   | BL    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BM    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BN    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BO    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BP    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BQ    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BR    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BS    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BT    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BU    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BV    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BW    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BX    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BY    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | BZ    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CA    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CB    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CC    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CD    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CE    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CF    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 1   | CG    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CH    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CI    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CJ    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CK    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CL    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CM    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CN    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CO    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CP    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CQ    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CR    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CS    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CT    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CU    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CV    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CW    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CX    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CY    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | CZ    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DA    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |

*Continued on next page...*

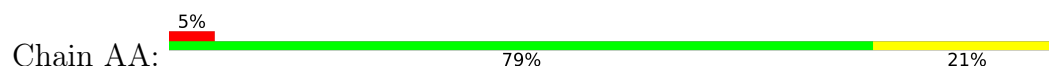
*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 1   | DB    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DC    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DD    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DE    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DF    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DG    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DH    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DI    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DJ    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DK    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |
| 1   | DL    | 131      | Total<br>972 | C<br>607 | N<br>166 | O<br>198 | S<br>1 | 0       | 0       | 0     |

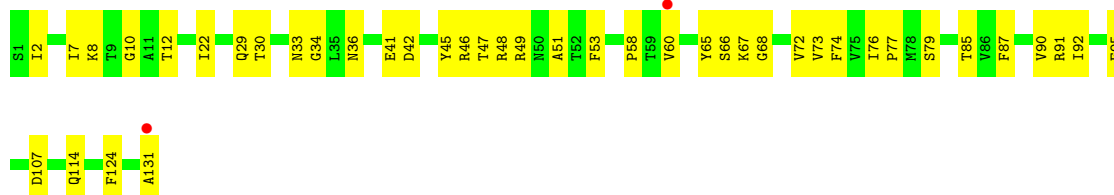
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

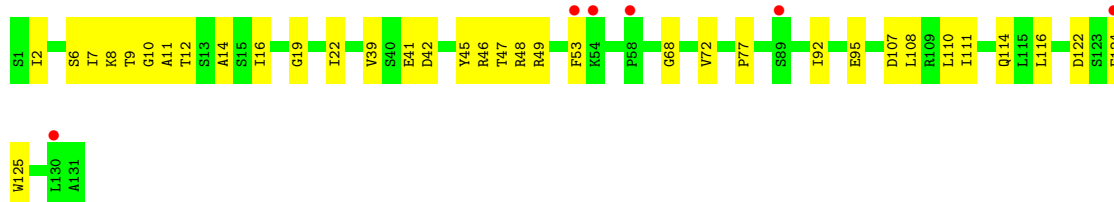
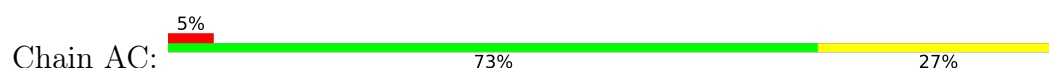
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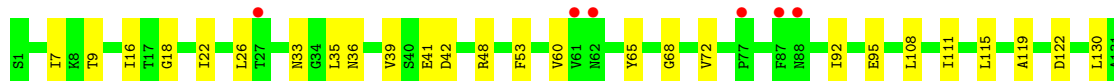
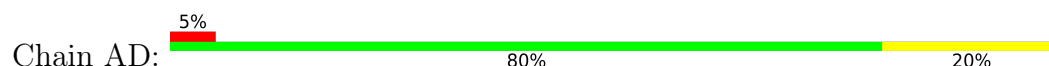
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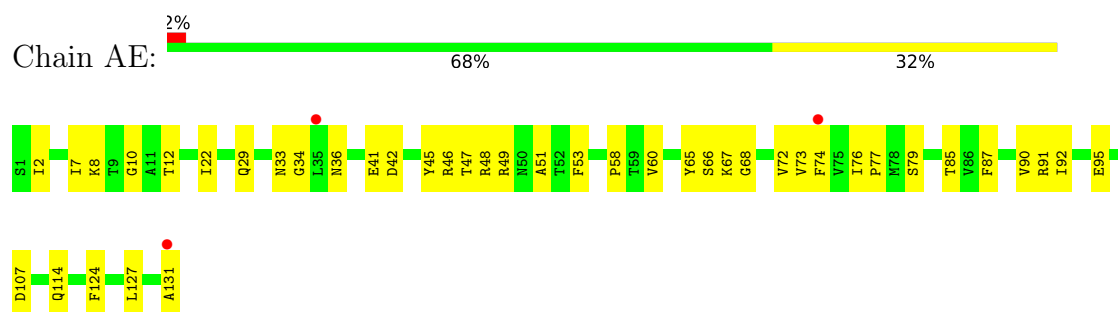
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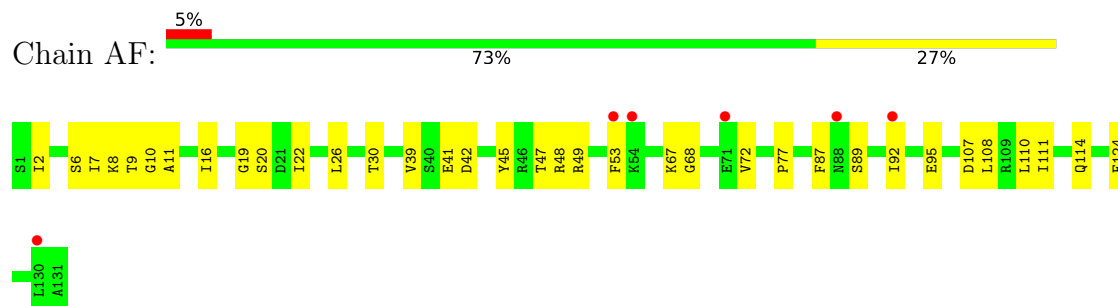
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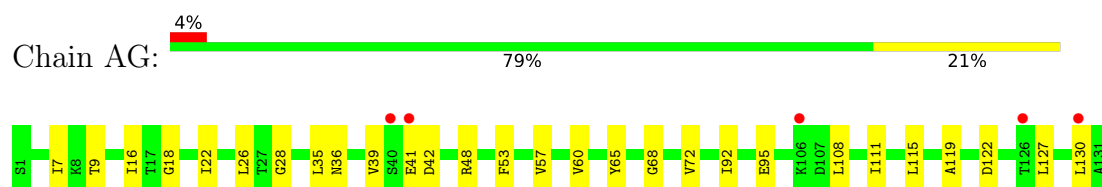
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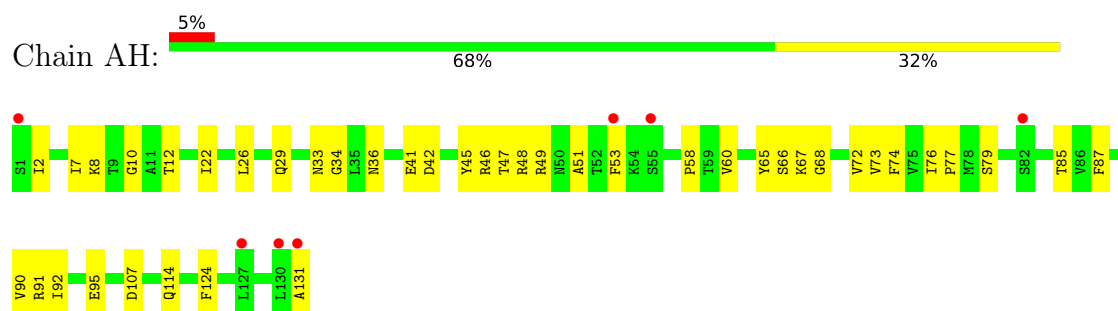
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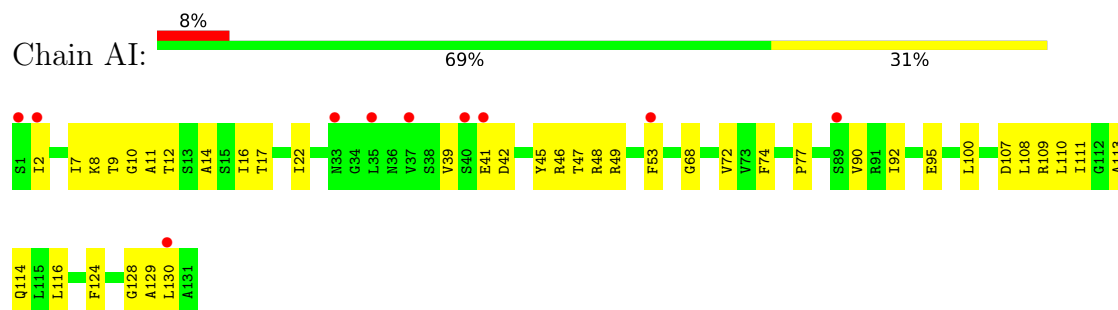
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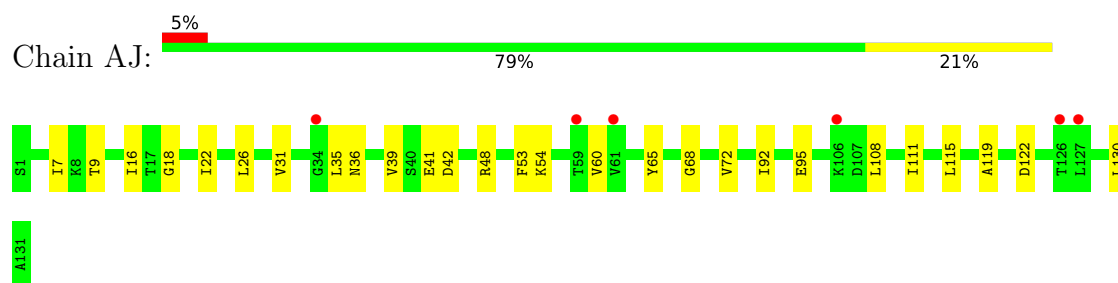
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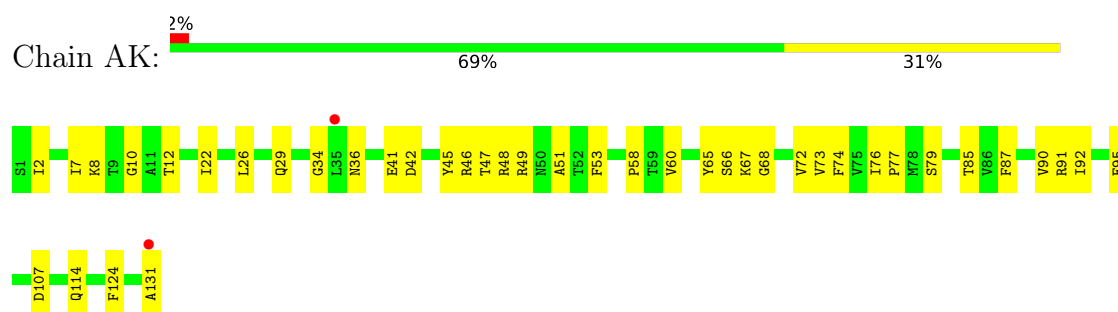
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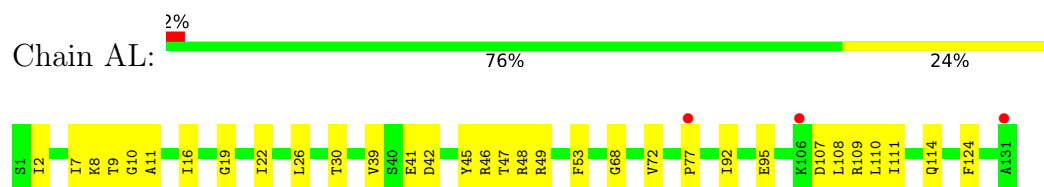
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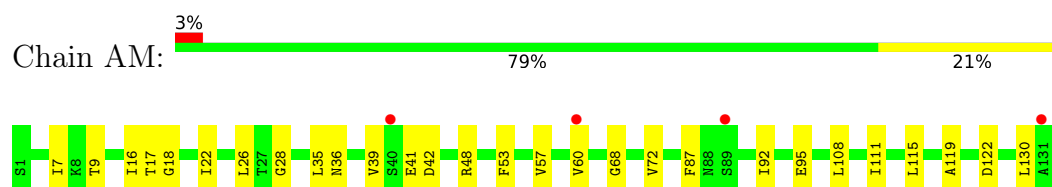
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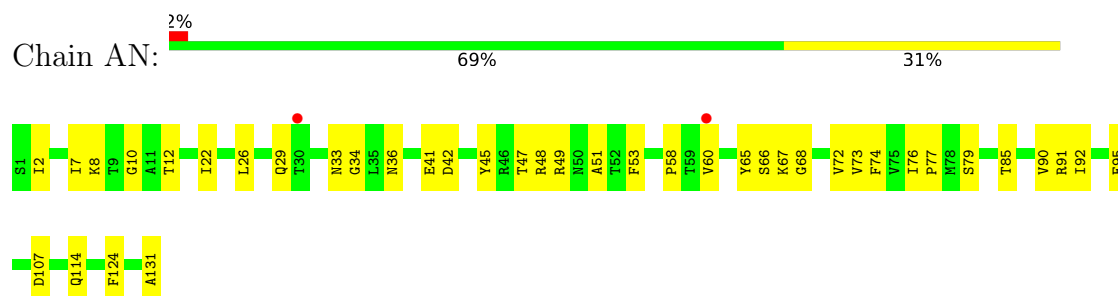
- Molecule 1: coat protein



- Molecule 1: coat protein

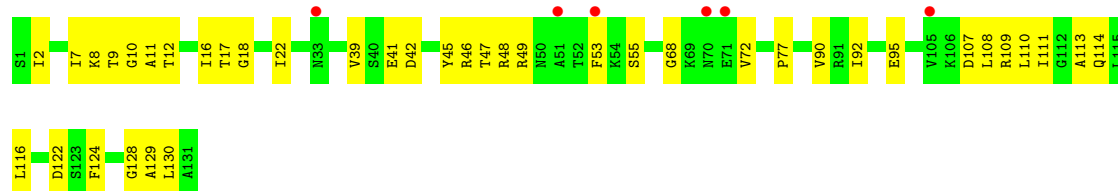


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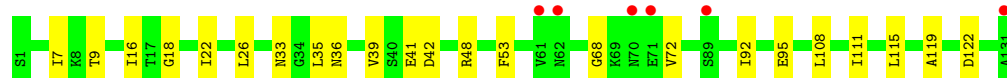
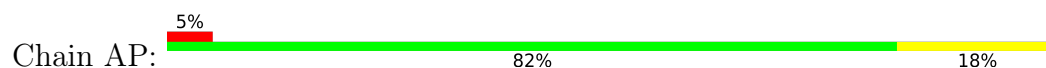


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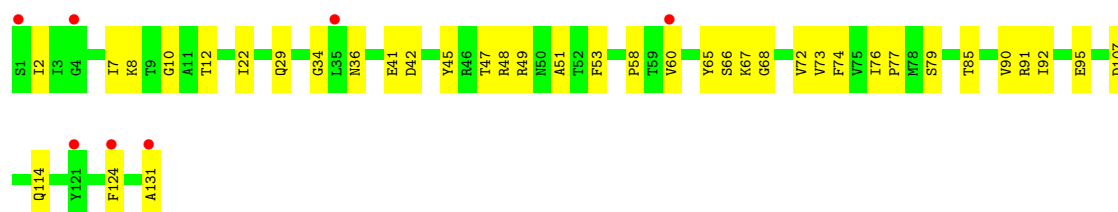
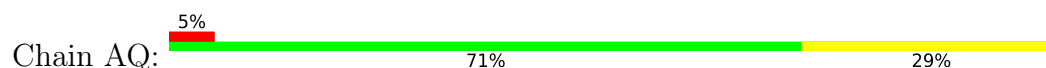




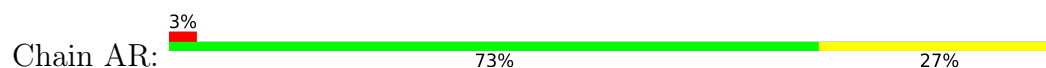
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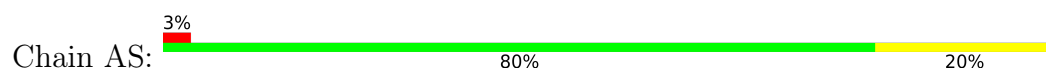
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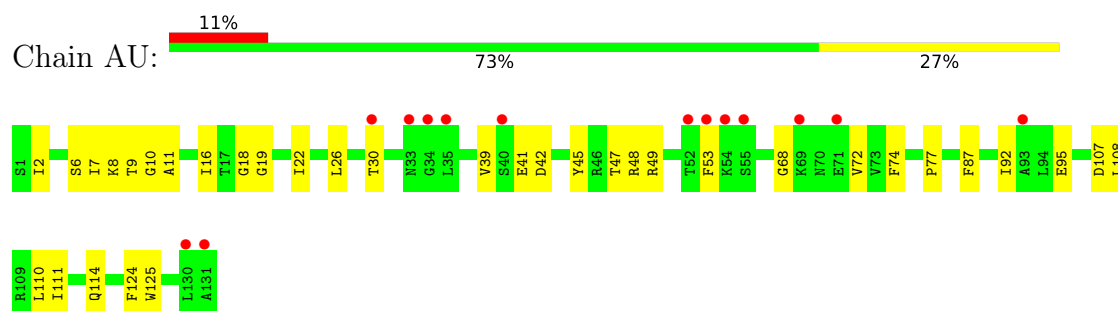
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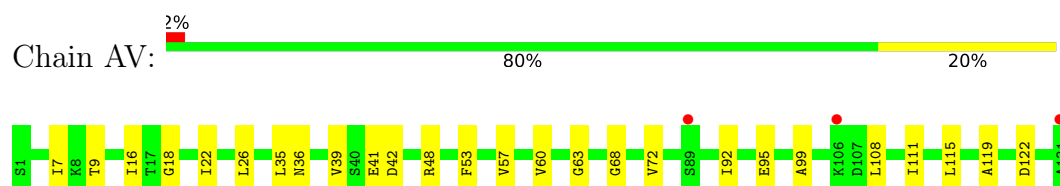
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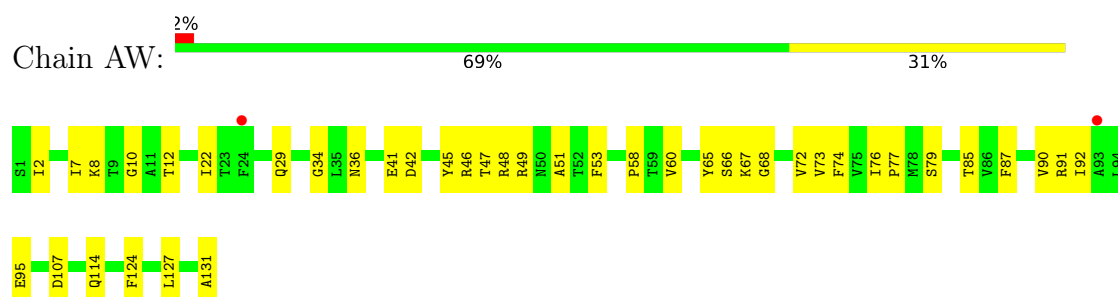
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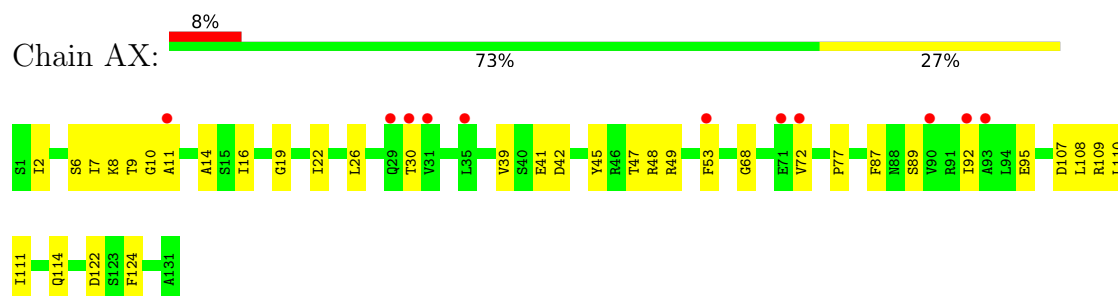
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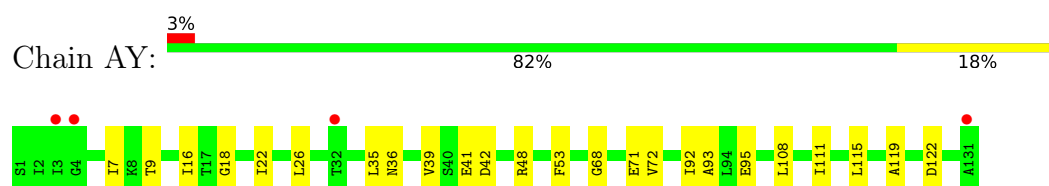
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- Molecule 1: coat protein

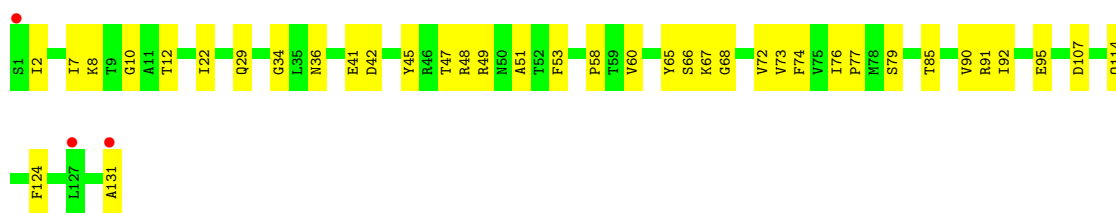


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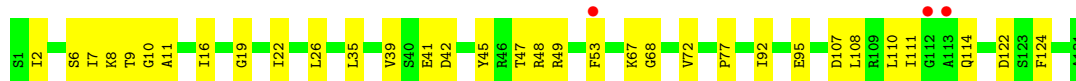
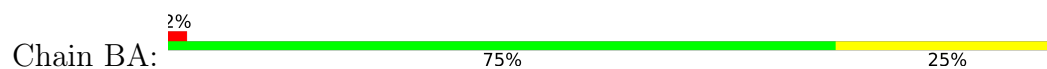


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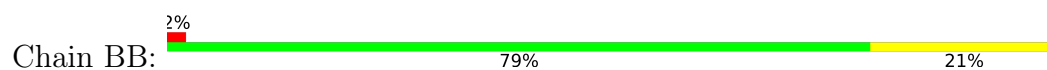




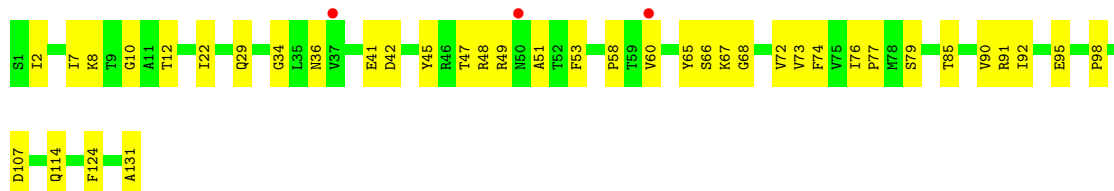
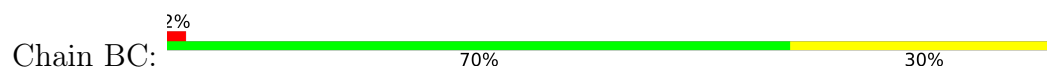
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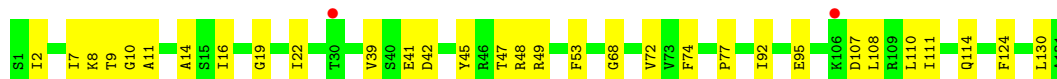
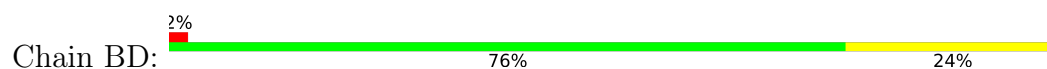
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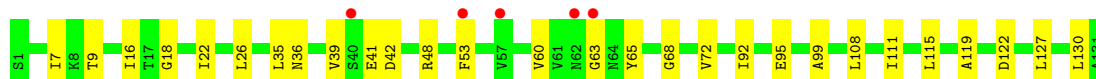
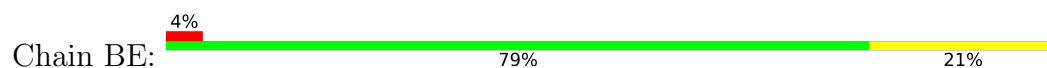
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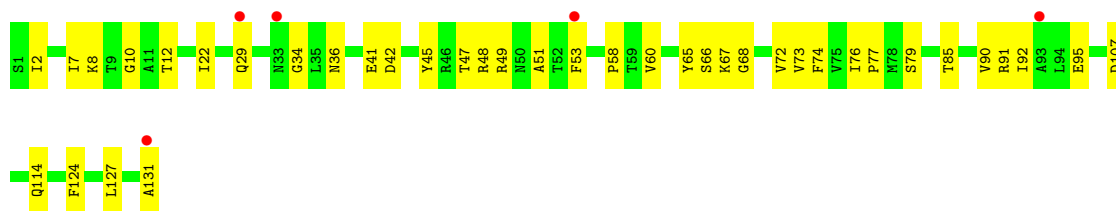


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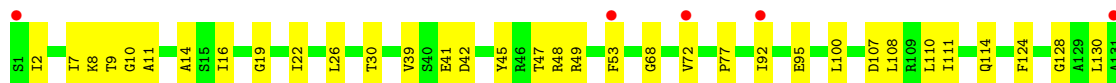
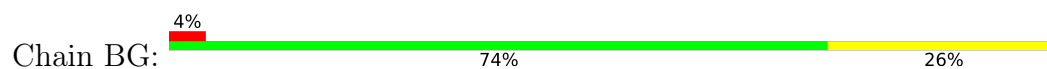


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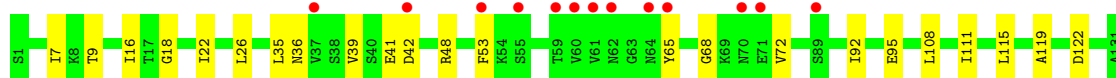
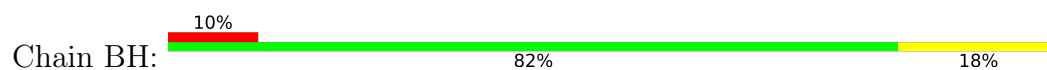




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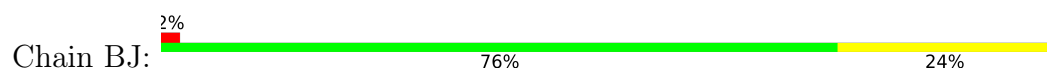
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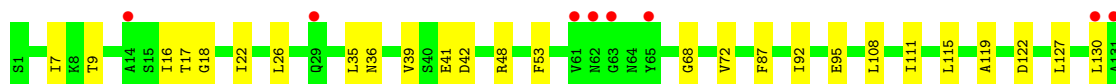
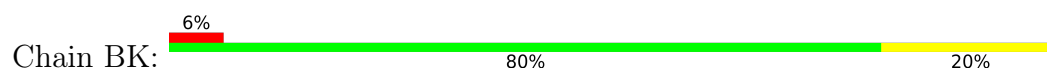
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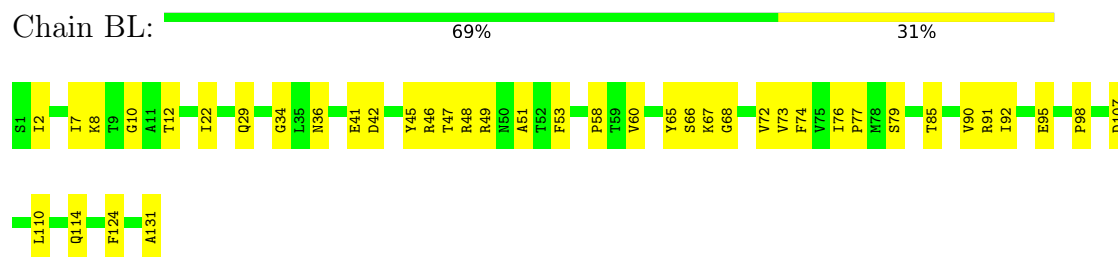
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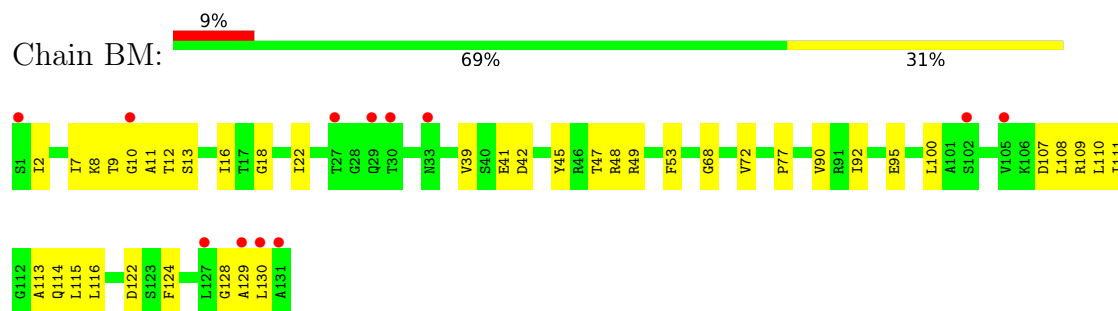
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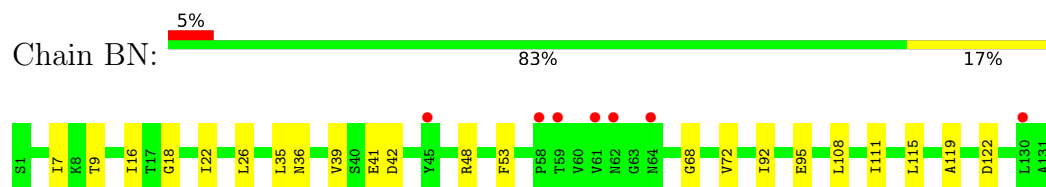
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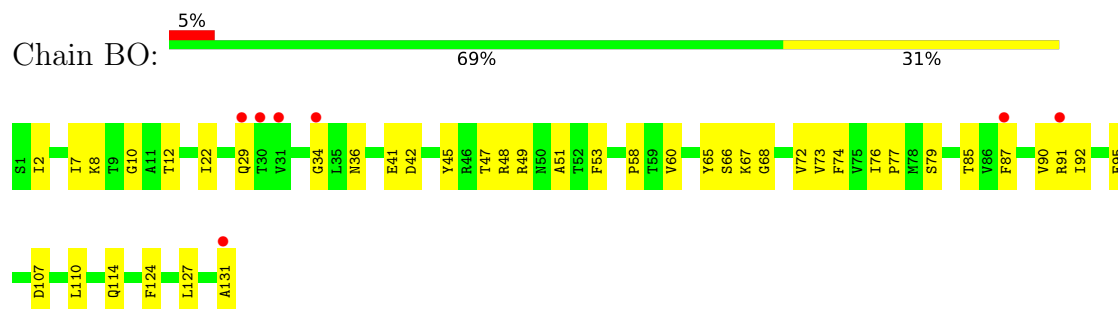
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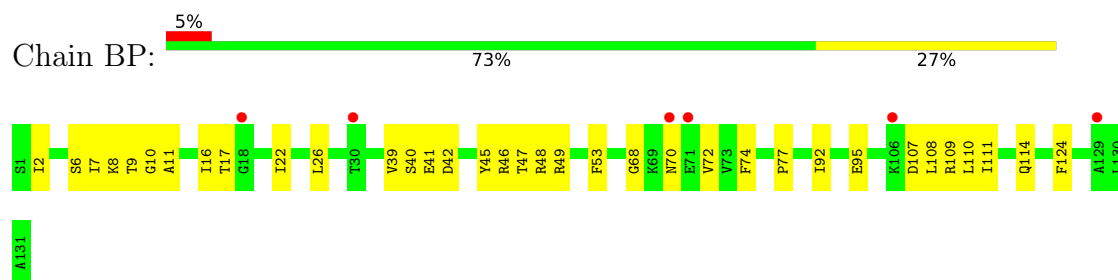
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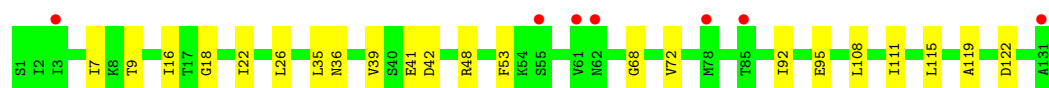
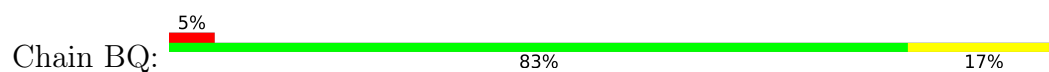
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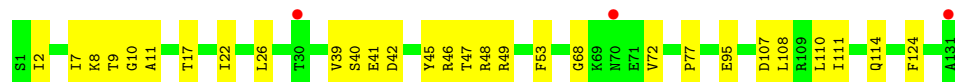
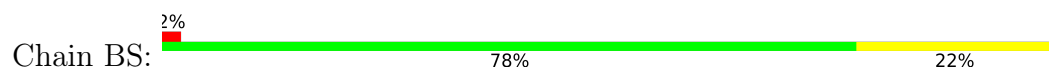
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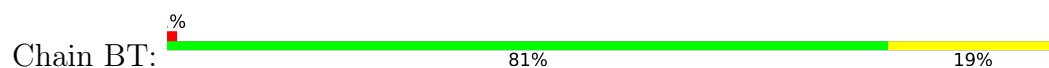
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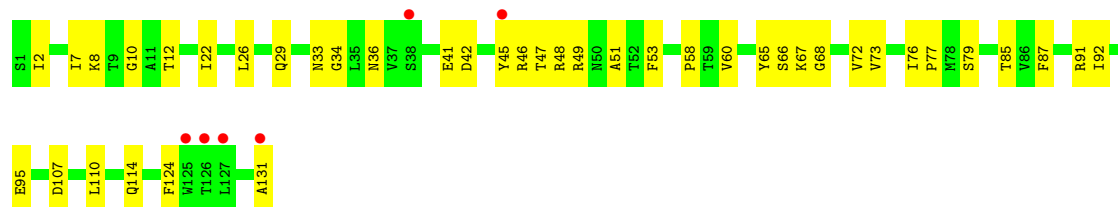
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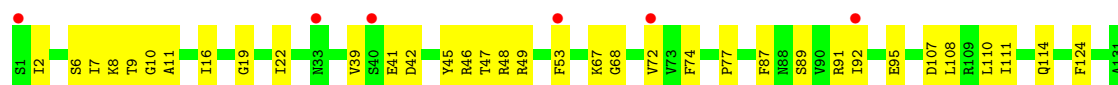
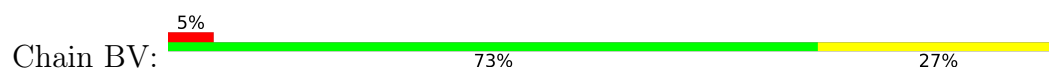
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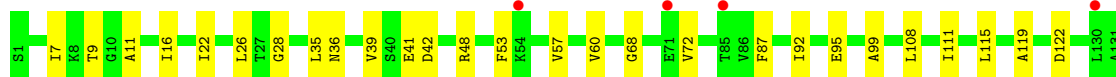
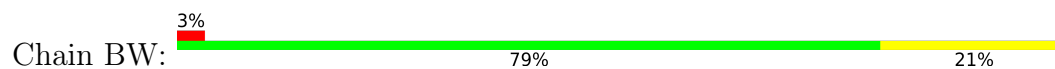
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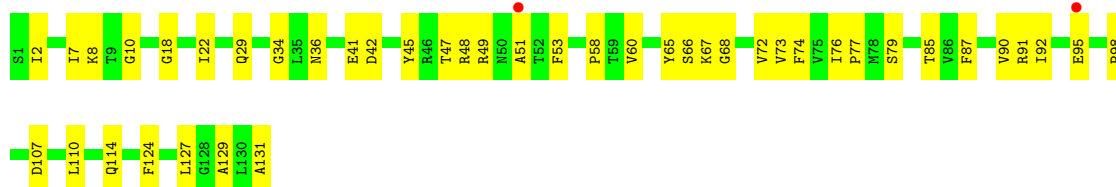
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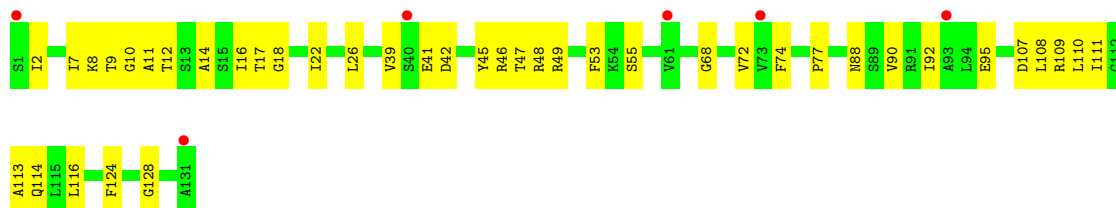
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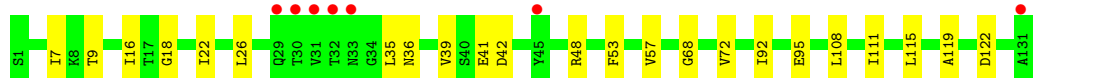
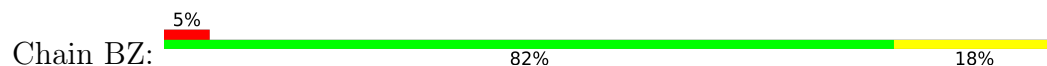
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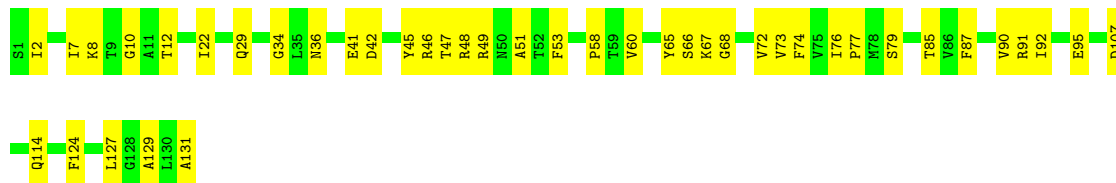
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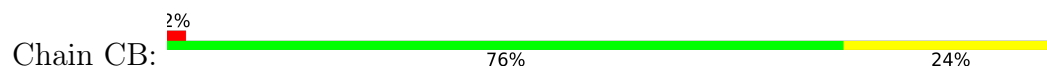
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- Molecule 1: coat protein

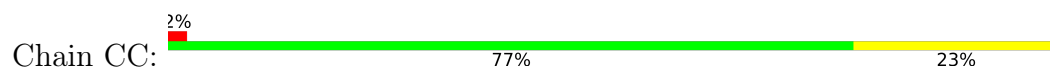


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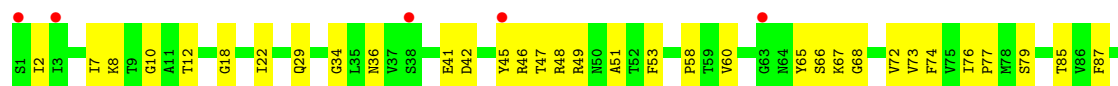




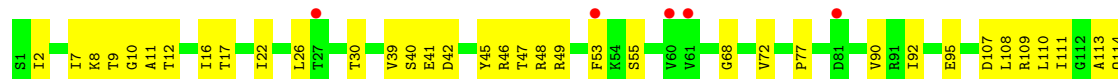
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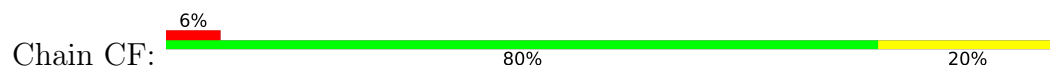
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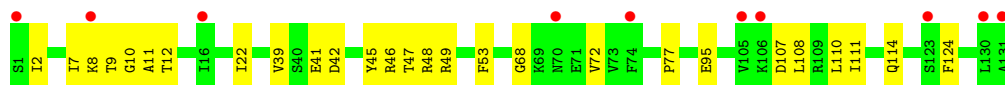
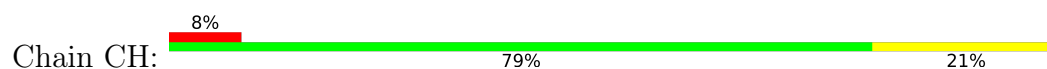


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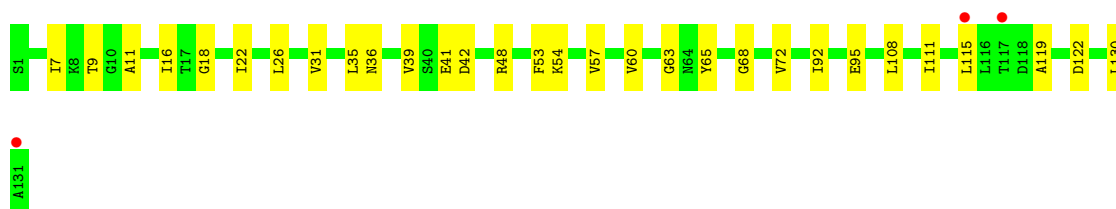
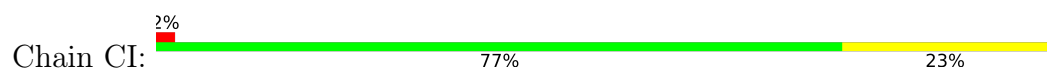




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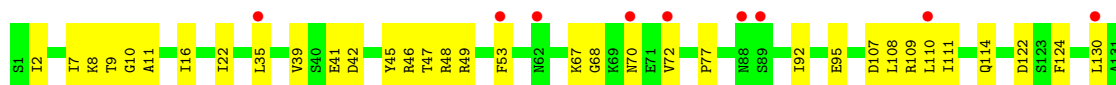
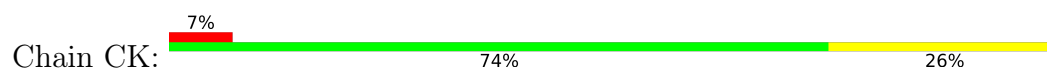
- Molecule 1: coat protein



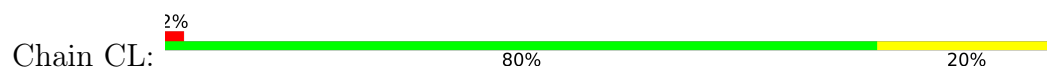
- Molecule 1: coat protein



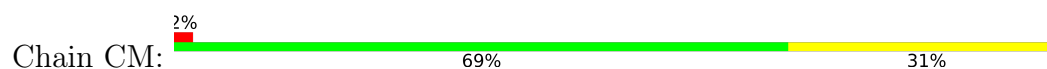
- Molecule 1: coat protein

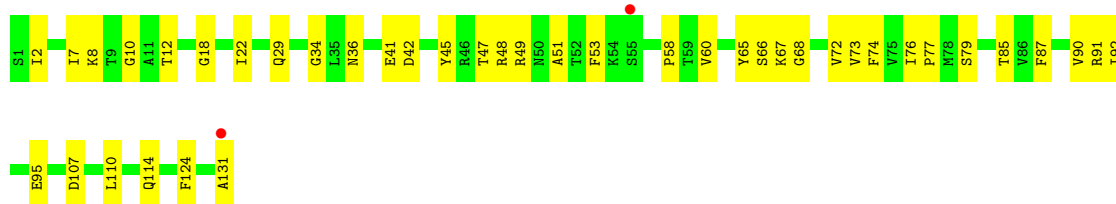


- Molecule 1: coat protein

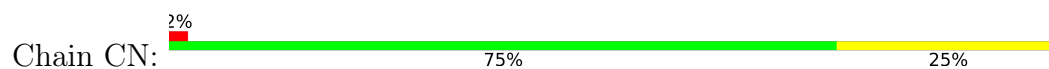


- Molecule 1: coat protein

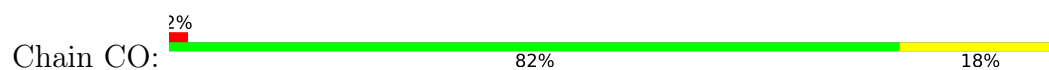




- Molecule 1: coat protein



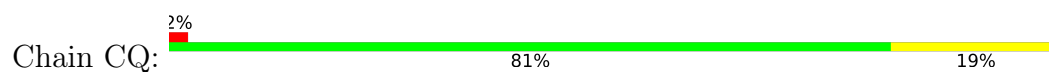
- Molecule 1: coat protein



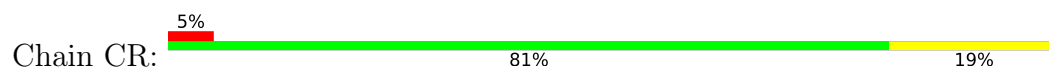
- Molecule 1: coat protein



- Molecule 1: coat protein

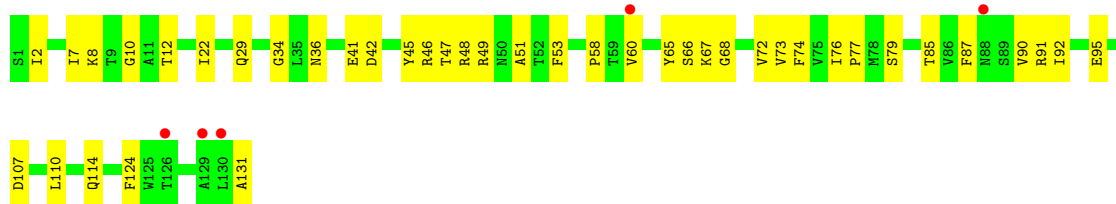


- Molecule 1: coat protein

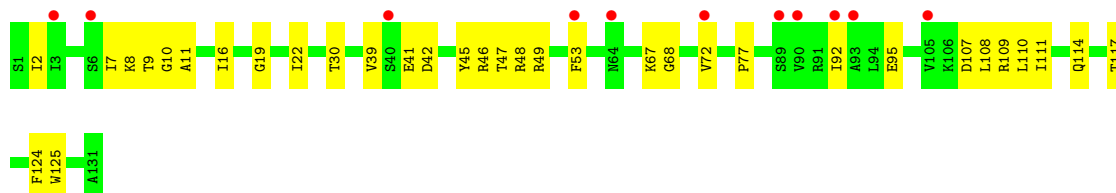
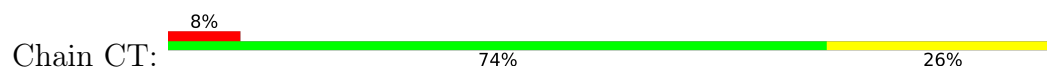


- Molecule 1: coat protein

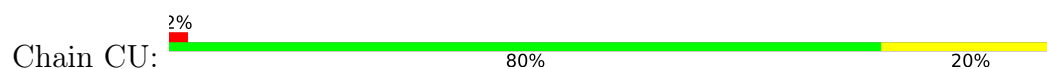




- Molecule 1: coat protein



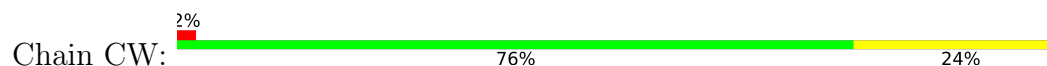
- Molecule 1: coat protein



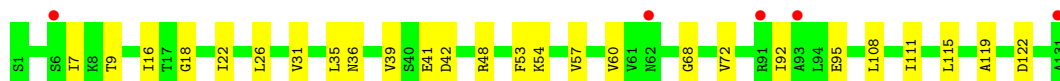
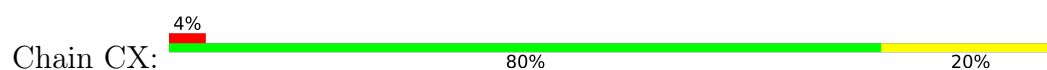
- Molecule 1: coat protein



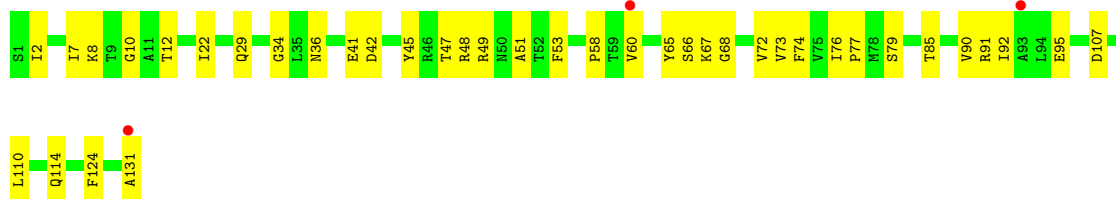
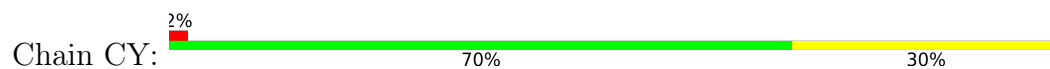
- Molecule 1: coat protein



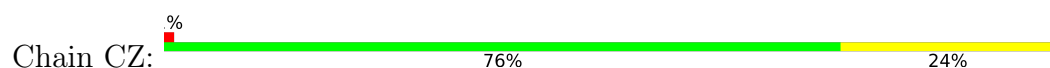
- Molecule 1: coat protein



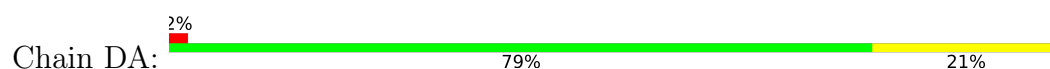
- Molecule 1: coat protein



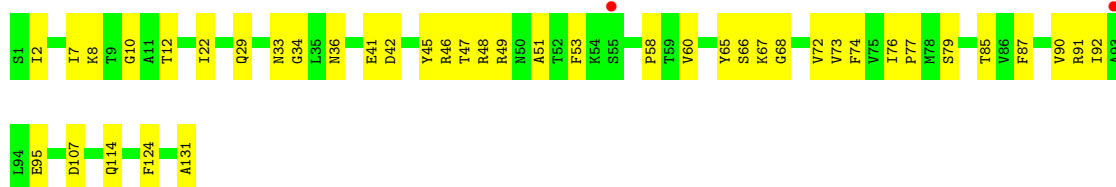
- Molecule 1: coat protein



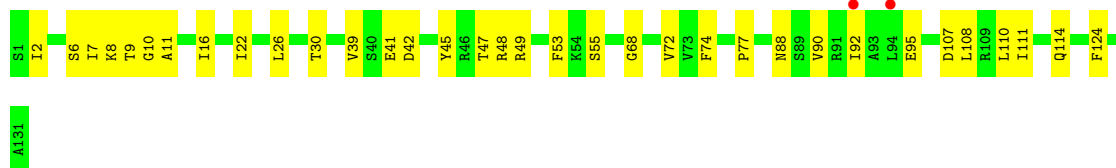
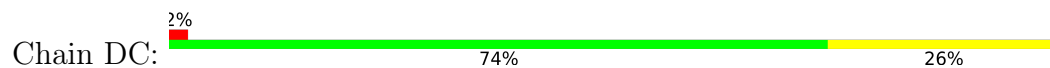
- Molecule 1: coat protein



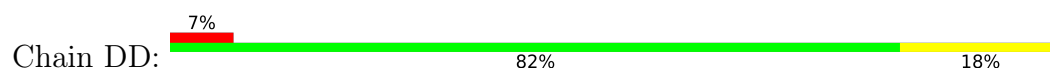
- Molecule 1: coat protein

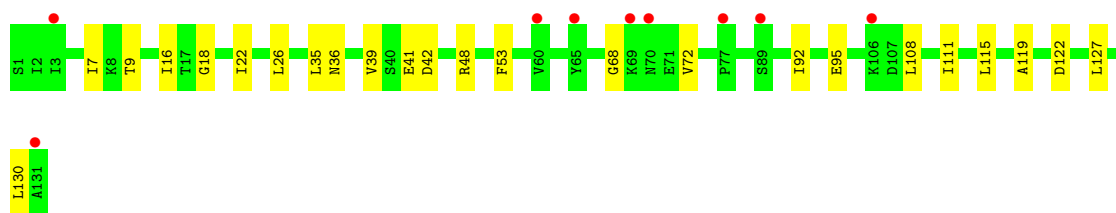


- Molecule 1: coat protein

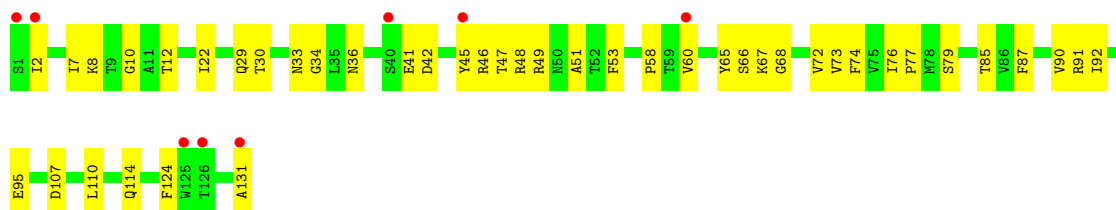


- Molecule 1: coat protein

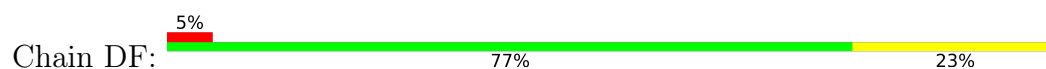




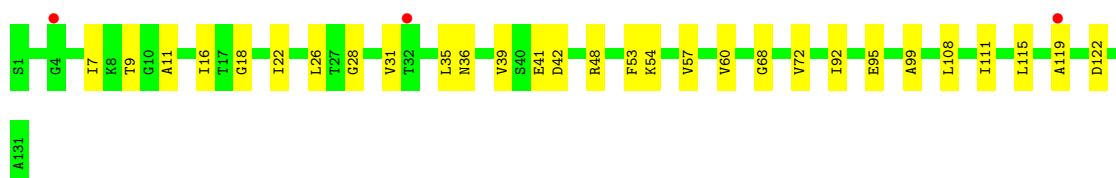
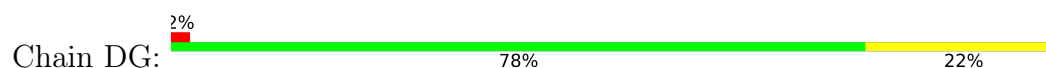
- Molecule 1: coat protein



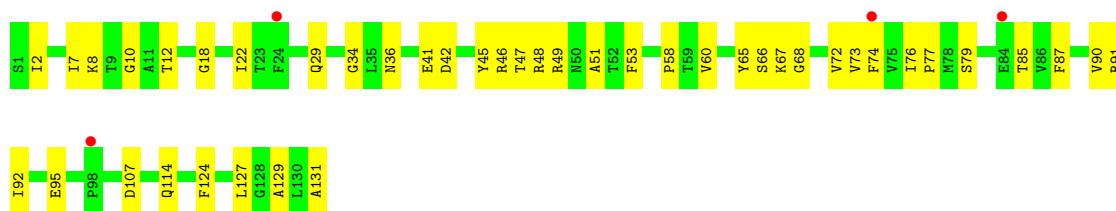
- Molecule 1: coat protein



- Molecule 1: coat protein

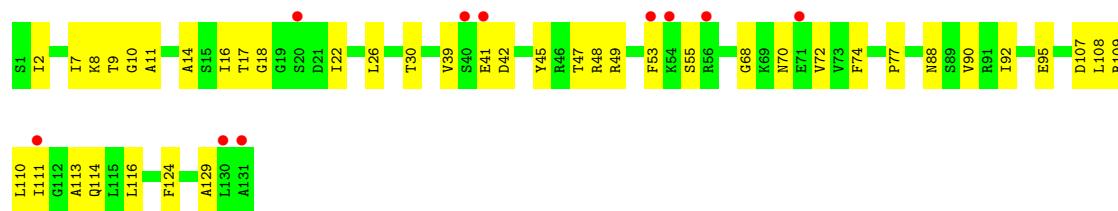


- Molecule 1: coat protein



- Molecule 1: coat protein





● Molecule 1: coat protein

Chain DJ: 82% 18%



● Molecule 1: coat protein

Chain DK: 4% 71% 29%



● Molecule 1: coat protein

Chain DL: 80% 20%



## 4 Data and refinement statistics

| Property                                                                | Value                                                                | Source           |
|-------------------------------------------------------------------------|----------------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                              | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 415.01Å 335.00Å 291.78Å<br>90.00° 134.66° 90.00°                     | Depositor        |
| Resolution (Å)                                                          | 49.14 – 3.48<br>49.14 – 3.48                                         | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 96.5 (49.14-3.48)<br>98.1 (49.14-3.48)                               | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.45                                                                 | Depositor        |
| $R_{sym}$                                                               | (Not available)                                                      | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.97 (at 3.48Å)                                                      | Xtriage          |
| Refinement program                                                      | PHENIX 1.14_3260                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.269 , 0.271<br>0.273 , 0.275                                       | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 10014 reflections (2.83%)                                            | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 121.7                                                                | Xtriage          |
| Anisotropy                                                              | 0.231                                                                | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 86.4                                                          | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$          | Xtriage          |
| Estimated twinning fraction                                             | 0.079 for h+2*k,-h-l<br>0.094 for h,-k,-h-l<br>0.095 for -h-2*k,-k,l | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                                 | EDS              |
| Total number of atoms                                                   | 87480                                                                | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 110.0                                                                | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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

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   | AA    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AB    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | AC    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | AD    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AE    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | AF    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | AG    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AH    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AI    | 0.23         | 0/985   | 0.54        | 0/1338  |
| 1   | AJ    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AK    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AL    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | AM    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AN    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | AO    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | AP    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AQ    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AR    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | AS    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AT    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AU    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | AV    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AW    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AX    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | AY    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | AZ    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BA    | 0.23         | 0/985   | 0.54        | 0/1338  |
| 1   | BB    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BC    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BD    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | BE    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BF    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BG    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | BH    | 0.24         | 0/985   | 0.52        | 0/1338  |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | BI    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | BJ    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | BK    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BL    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | BM    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | BN    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BO    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BP    | 0.23         | 0/985   | 0.54        | 0/1338  |
| 1   | BQ    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BR    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BS    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | BT    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BU    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BV    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | BW    | 0.24         | 0/985   | 0.52        | 0/1338  |
| 1   | BX    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | BY    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | BZ    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CA    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CB    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | CC    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CD    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CE    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | CF    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CG    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CH    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | CI    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CJ    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CK    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | CL    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CM    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CN    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | CO    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CP    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CQ    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | CR    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CS    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CT    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | CU    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CV    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CW    | 0.23         | 0/985   | 0.53        | 0/1338  |
| 1   | CX    | 0.24         | 0/985   | 0.53        | 0/1338  |
| 1   | CY    | 0.24         | 0/985   | 0.53        | 0/1338  |

| Mol | Chain | Bond lengths |         | Bond angles |          |
|-----|-------|--------------|---------|-------------|----------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5  |
| 1   | CZ    | 0.23         | 0/985   | 0.53        | 0/1338   |
| 1   | DA    | 0.24         | 0/985   | 0.53        | 0/1338   |
| 1   | DB    | 0.24         | 0/985   | 0.53        | 0/1338   |
| 1   | DC    | 0.23         | 0/985   | 0.53        | 0/1338   |
| 1   | DD    | 0.24         | 0/985   | 0.53        | 0/1338   |
| 1   | DE    | 0.24         | 0/985   | 0.53        | 0/1338   |
| 1   | DF    | 0.23         | 0/985   | 0.54        | 0/1338   |
| 1   | DG    | 0.24         | 0/985   | 0.53        | 0/1338   |
| 1   | DH    | 0.24         | 0/985   | 0.53        | 0/1338   |
| 1   | DI    | 0.23         | 0/985   | 0.53        | 0/1338   |
| 1   | DJ    | 0.24         | 0/985   | 0.53        | 0/1338   |
| 1   | DK    | 0.24         | 0/985   | 0.53        | 0/1338   |
| 1   | DL    | 0.23         | 0/985   | 0.53        | 0/1338   |
| All | All   | 0.23         | 0/88650 | 0.53        | 0/120420 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 972   | 0        | 977      | 26      | 0            |
| 1   | AB    | 972   | 0        | 977      | 39      | 0            |
| 1   | AC    | 972   | 0        | 977      | 41      | 0            |
| 1   | AD    | 972   | 0        | 977      | 25      | 0            |
| 1   | AE    | 972   | 0        | 977      | 42      | 0            |
| 1   | AF    | 972   | 0        | 977      | 41      | 0            |
| 1   | AG    | 972   | 0        | 977      | 27      | 0            |
| 1   | AH    | 972   | 0        | 977      | 38      | 0            |
| 1   | AI    | 972   | 0        | 977      | 52      | 0            |
| 1   | AJ    | 972   | 0        | 977      | 26      | 0            |
| 1   | AK    | 972   | 0        | 977      | 40      | 0            |
| 1   | AL    | 972   | 0        | 977      | 35      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AM    | 972   | 0        | 977      | 28      | 0            |
| 1   | AN    | 972   | 0        | 977      | 35      | 0            |
| 1   | AO    | 972   | 0        | 977      | 51      | 0            |
| 1   | AP    | 972   | 0        | 977      | 20      | 1            |
| 1   | AQ    | 972   | 0        | 977      | 29      | 0            |
| 1   | AR    | 972   | 0        | 977      | 37      | 1            |
| 1   | AS    | 972   | 0        | 977      | 28      | 0            |
| 1   | AT    | 972   | 0        | 977      | 39      | 0            |
| 1   | AU    | 972   | 0        | 977      | 39      | 0            |
| 1   | AV    | 972   | 0        | 977      | 25      | 0            |
| 1   | AW    | 972   | 0        | 977      | 38      | 0            |
| 1   | AX    | 972   | 0        | 977      | 37      | 0            |
| 1   | AY    | 972   | 0        | 977      | 21      | 0            |
| 1   | AZ    | 972   | 0        | 977      | 29      | 0            |
| 1   | BA    | 972   | 0        | 977      | 32      | 0            |
| 1   | BB    | 972   | 0        | 977      | 24      | 0            |
| 1   | BC    | 972   | 0        | 977      | 39      | 0            |
| 1   | BD    | 972   | 0        | 977      | 34      | 0            |
| 1   | BE    | 972   | 0        | 977      | 29      | 0            |
| 1   | BF    | 972   | 0        | 977      | 41      | 0            |
| 1   | BG    | 972   | 0        | 977      | 40      | 0            |
| 1   | BH    | 972   | 0        | 977      | 21      | 0            |
| 1   | BI    | 972   | 0        | 977      | 31      | 0            |
| 1   | BJ    | 972   | 0        | 977      | 43      | 0            |
| 1   | BK    | 972   | 0        | 977      | 25      | 0            |
| 1   | BL    | 972   | 0        | 977      | 43      | 0            |
| 1   | BM    | 972   | 0        | 977      | 56      | 0            |
| 1   | BN    | 972   | 0        | 977      | 20      | 0            |
| 1   | BO    | 972   | 0        | 977      | 36      | 0            |
| 1   | BP    | 972   | 0        | 977      | 46      | 0            |
| 1   | BQ    | 972   | 0        | 977      | 21      | 0            |
| 1   | BR    | 972   | 0        | 977      | 34      | 0            |
| 1   | BS    | 972   | 0        | 977      | 30      | 1            |
| 1   | BT    | 972   | 0        | 977      | 24      | 0            |
| 1   | BU    | 972   | 0        | 977      | 36      | 0            |
| 1   | BV    | 972   | 0        | 977      | 40      | 0            |
| 1   | BW    | 972   | 0        | 977      | 27      | 0            |
| 1   | BX    | 972   | 0        | 977      | 44      | 0            |
| 1   | BY    | 972   | 0        | 977      | 54      | 0            |
| 1   | BZ    | 972   | 0        | 977      | 21      | 0            |
| 1   | CA    | 972   | 0        | 977      | 44      | 0            |
| 1   | CB    | 972   | 0        | 977      | 32      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | CC    | 972   | 0        | 977      | 29      | 0            |
| 1   | CD    | 972   | 0        | 977      | 46      | 0            |
| 1   | CE    | 972   | 0        | 977      | 51      | 0            |
| 1   | CF    | 972   | 0        | 977      | 27      | 0            |
| 1   | CG    | 972   | 0        | 977      | 30      | 2            |
| 1   | CH    | 972   | 0        | 977      | 27      | 1            |
| 1   | CI    | 972   | 0        | 977      | 28      | 0            |
| 1   | CJ    | 972   | 0        | 977      | 34      | 0            |
| 1   | CK    | 972   | 0        | 977      | 46      | 0            |
| 1   | CL    | 972   | 0        | 977      | 25      | 0            |
| 1   | CM    | 972   | 0        | 977      | 35      | 0            |
| 1   | CN    | 972   | 0        | 977      | 44      | 0            |
| 1   | CO    | 972   | 0        | 977      | 21      | 0            |
| 1   | CP    | 972   | 0        | 977      | 37      | 0            |
| 1   | CQ    | 972   | 0        | 977      | 19      | 0            |
| 1   | CR    | 972   | 0        | 977      | 24      | 0            |
| 1   | CS    | 972   | 0        | 977      | 37      | 0            |
| 1   | CT    | 972   | 0        | 977      | 37      | 0            |
| 1   | CU    | 972   | 0        | 977      | 24      | 0            |
| 1   | CV    | 972   | 0        | 977      | 39      | 0            |
| 1   | CW    | 972   | 0        | 977      | 35      | 0            |
| 1   | CX    | 972   | 0        | 977      | 24      | 0            |
| 1   | CY    | 972   | 0        | 977      | 36      | 0            |
| 1   | CZ    | 972   | 0        | 977      | 35      | 0            |
| 1   | DA    | 972   | 0        | 977      | 26      | 0            |
| 1   | DB    | 972   | 0        | 977      | 36      | 0            |
| 1   | DC    | 972   | 0        | 977      | 39      | 0            |
| 1   | DD    | 972   | 0        | 977      | 24      | 0            |
| 1   | DE    | 972   | 0        | 977      | 38      | 0            |
| 1   | DF    | 972   | 0        | 977      | 33      | 0            |
| 1   | DG    | 972   | 0        | 977      | 29      | 0            |
| 1   | DH    | 972   | 0        | 977      | 40      | 0            |
| 1   | DI    | 972   | 0        | 977      | 55      | 0            |
| 1   | DJ    | 972   | 0        | 977      | 23      | 0            |
| 1   | DK    | 972   | 0        | 977      | 29      | 0            |
| 1   | DL    | 972   | 0        | 977      | 22      | 0            |
| All | All   | 87480 | 0        | 87930    | 2350    | 3            |

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 2350 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:BA:16:ILE:HD13  | 1:CW:114:GLN:HE21 | 1.10                     | 1.14              |
| 1:AX:16:ILE:HD13  | 1:CT:114:GLN:HE21 | 1.12                     | 1.12              |
| 1:BA:114:GLN:HE21 | 1:CW:16:ILE:HD13  | 1.11                     | 1.10              |
| 1:AX:114:GLN:HE21 | 1:CT:16:ILE:HD13  | 1.18                     | 1.08              |
| 1:AL:16:ILE:HD13  | 1:CB:114:GLN:HE21 | 1.19                     | 1.07              |

All (3) 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) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:BS:17:THR:O   | 1:CH:12:THR:OG1[2_555] | 2.03                     | 0.17              |
| 1:AR:30:THR:OG1 | 1:CG:33:ASN:OD1[2_555] | 2.04                     | 0.16              |
| 1:AP:33:ASN:OD1 | 1:CG:30:THR:OG1[2_555] | 2.13                     | 0.07              |

## 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   | AA    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | AB    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AC    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | AD    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | AE    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AF    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | AG    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | AH    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AI    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | AJ    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | AK    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | AL    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | AM    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | AN    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AO    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | AP    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | AQ    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AR    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | AS    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | AT    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AU    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | AV    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | AW    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AX    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | AY    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | AZ    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BA    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | BB    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | BC    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BD    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | BE    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | BF    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BG    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | BH    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | BI    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BJ    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | BK    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | BL    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BM    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | BN    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | BO    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BP    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | BQ    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | BR    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BS    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | BT    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | BU    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BV    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | BW    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | BX    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BY    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | BZ    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | CA    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CB    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | CC    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | CD    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CE    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | CF    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | CG    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CH    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | CI    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | CJ    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CK    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | CL    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | CM    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CN    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | CO    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | CP    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CQ    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | CR    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 1   | CS    | 129/131 (98%) | 128 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CT    | 129/131 (98%) | 129 (100%) | 0       | 0        | 100         | 100 |
| 1   | CU    | 129/131 (98%) | 127 (98%)  | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|---------|----------|-------------|-----|
| 1   | CV    | 129/131 (98%)     | 128 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | CW    | 129/131 (98%)     | 129 (100%)  | 0       | 0        | 100         | 100 |
| 1   | CX    | 129/131 (98%)     | 127 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 1   | CY    | 129/131 (98%)     | 128 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | CZ    | 129/131 (98%)     | 129 (100%)  | 0       | 0        | 100         | 100 |
| 1   | DA    | 129/131 (98%)     | 127 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 1   | DB    | 129/131 (98%)     | 128 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | DC    | 129/131 (98%)     | 129 (100%)  | 0       | 0        | 100         | 100 |
| 1   | DD    | 129/131 (98%)     | 127 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 1   | DE    | 129/131 (98%)     | 128 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | DF    | 129/131 (98%)     | 129 (100%)  | 0       | 0        | 100         | 100 |
| 1   | DG    | 129/131 (98%)     | 127 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 1   | DH    | 129/131 (98%)     | 128 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | DI    | 129/131 (98%)     | 129 (100%)  | 0       | 0        | 100         | 100 |
| 1   | DJ    | 129/131 (98%)     | 127 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 1   | DK    | 129/131 (98%)     | 128 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 1   | DL    | 129/131 (98%)     | 129 (100%)  | 0       | 0        | 100         | 100 |
| All | All   | 11610/11790 (98%) | 11520 (99%) | 90 (1%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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   | AA    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AB    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AC    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AD    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | AE    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AF    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AG    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AH    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AI    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AJ    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AK    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AL    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AM    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AN    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AO    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AP    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AQ    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AR    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AS    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AT    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AU    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AV    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AW    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AX    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AY    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | AZ    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BA    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BB    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BC    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BD    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BE    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BF    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BG    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BH    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BI    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | BJ    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BK    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BL    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BM    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BN    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BO    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BP    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BQ    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BR    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BS    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BT    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BU    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BV    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BW    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BX    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BY    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | BZ    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CA    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CB    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CC    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CD    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CE    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CF    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CG    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CH    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CI    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CJ    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CK    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CL    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CM    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |
| 1   | CN    | 108/108 (100%) | 108 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Rotameric   | Outliers | Percentiles |     |
|-----|-------|------------------|-------------|----------|-------------|-----|
| 1   | CO    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CP    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CQ    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CR    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CS    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CT    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CU    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CV    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CW    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CX    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CY    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | CZ    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DA    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DB    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DC    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DD    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DE    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DF    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DG    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DH    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DI    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DJ    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DK    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| 1   | DL    | 108/108 (100%)   | 108 (100%)  | 0        | 100         | 100 |
| All | All   | 9720/9720 (100%) | 9720 (100%) | 0        | 100         | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CT    | 70  | ASN  |
| 1   | DK    | 36  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CV    | 36  | ASN  |
| 1   | DE    | 29  | GLN  |
| 1   | BC    | 29  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 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   | AA    | 131/131 (100%) | 0.38   | 6 (4%) 37 21  | 64, 111, 139, 160     | 0     |
| 1   | AB    | 131/131 (100%) | 0.19   | 2 (1%) 72 48  | 64, 109, 138, 177     | 0     |
| 1   | AC    | 131/131 (100%) | 0.34   | 6 (4%) 37 21  | 64, 110, 142, 191     | 0     |
| 1   | AD    | 131/131 (100%) | 0.23   | 6 (4%) 37 21  | 64, 111, 139, 160     | 0     |
| 1   | AE    | 131/131 (100%) | 0.22   | 3 (2%) 61 37  | 64, 109, 138, 177     | 0     |
| 1   | AF    | 131/131 (100%) | 0.21   | 6 (4%) 37 21  | 64, 110, 142, 191     | 0     |
| 1   | AG    | 131/131 (100%) | 0.25   | 5 (3%) 44 25  | 64, 111, 139, 160     | 0     |
| 1   | AH    | 131/131 (100%) | 0.27   | 7 (5%) 32 19  | 64, 109, 138, 177     | 0     |
| 1   | AI    | 131/131 (100%) | 0.40   | 10 (7%) 20 13 | 64, 110, 142, 191     | 0     |
| 1   | AJ    | 131/131 (100%) | 0.13   | 6 (4%) 37 21  | 64, 111, 139, 160     | 0     |
| 1   | AK    | 131/131 (100%) | 0.00   | 2 (1%) 72 48  | 64, 109, 138, 177     | 0     |
| 1   | AL    | 131/131 (100%) | 0.03   | 3 (2%) 61 37  | 64, 110, 142, 191     | 0     |
| 1   | AM    | 131/131 (100%) | 0.24   | 4 (3%) 51 30  | 64, 111, 139, 160     | 0     |
| 1   | AN    | 131/131 (100%) | 0.09   | 2 (1%) 72 48  | 64, 109, 138, 177     | 0     |
| 1   | AO    | 131/131 (100%) | 0.41   | 6 (4%) 37 21  | 64, 110, 142, 191     | 0     |
| 1   | AP    | 131/131 (100%) | 0.04   | 6 (4%) 37 21  | 64, 111, 139, 160     | 0     |
| 1   | AQ    | 131/131 (100%) | 0.21   | 7 (5%) 32 19  | 64, 109, 138, 177     | 0     |
| 1   | AR    | 131/131 (100%) | 0.18   | 4 (3%) 51 30  | 64, 110, 142, 191     | 0     |
| 1   | AS    | 131/131 (100%) | 0.07   | 4 (3%) 51 30  | 64, 111, 139, 160     | 0     |
| 1   | AT    | 131/131 (100%) | 0.06   | 3 (2%) 61 37  | 64, 109, 138, 177     | 0     |
| 1   | AU    | 131/131 (100%) | 0.33   | 14 (10%) 11 8 | 64, 110, 142, 191     | 0     |
| 1   | AV    | 131/131 (100%) | 0.15   | 3 (2%) 61 37  | 64, 111, 139, 160     | 0     |
| 1   | AW    | 131/131 (100%) | 0.02   | 2 (1%) 72 48  | 64, 109, 138, 177     | 0     |
| 1   | AX    | 131/131 (100%) | 0.34   | 11 (8%) 17 12 | 64, 110, 142, 191     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2 |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------|-----|-----|-----------------------|-------|
| 1   | AY    | 131/131 (100%) | 0.10   | 4 (3%)  | 51  | 30  | 64, 111, 139, 160     | 0     |
| 1   | AZ    | 131/131 (100%) | 0.09   | 3 (2%)  | 61  | 37  | 64, 109, 138, 177     | 0     |
| 1   | BA    | 131/131 (100%) | 0.22   | 3 (2%)  | 61  | 37  | 64, 110, 142, 191     | 0     |
| 1   | BB    | 131/131 (100%) | 0.20   | 2 (1%)  | 72  | 48  | 64, 111, 139, 160     | 0     |
| 1   | BC    | 131/131 (100%) | 0.26   | 3 (2%)  | 61  | 37  | 64, 109, 138, 177     | 0     |
| 1   | BD    | 131/131 (100%) | 0.09   | 2 (1%)  | 72  | 48  | 64, 110, 142, 191     | 0     |
| 1   | BE    | 131/131 (100%) | 0.25   | 5 (3%)  | 44  | 25  | 64, 111, 139, 160     | 0     |
| 1   | BF    | 131/131 (100%) | 0.32   | 5 (3%)  | 44  | 25  | 64, 109, 138, 177     | 0     |
| 1   | BG    | 131/131 (100%) | 0.16   | 5 (3%)  | 44  | 25  | 64, 110, 142, 191     | 0     |
| 1   | BH    | 131/131 (100%) | 0.26   | 13 (9%) | 13  | 9   | 64, 111, 139, 160     | 0     |
| 1   | BI    | 131/131 (100%) | 0.18   | 7 (5%)  | 32  | 19  | 64, 109, 138, 177     | 0     |
| 1   | BJ    | 131/131 (100%) | 0.14   | 3 (2%)  | 61  | 37  | 64, 110, 142, 191     | 0     |
| 1   | BK    | 131/131 (100%) | 0.18   | 8 (6%)  | 27  | 17  | 64, 111, 139, 160     | 0     |
| 1   | BL    | 131/131 (100%) | 0.05   | 0       | 100 | 100 | 64, 109, 138, 177     | 0     |
| 1   | BM    | 131/131 (100%) | 0.50   | 12 (9%) | 14  | 10  | 64, 110, 142, 191     | 0     |
| 1   | BN    | 131/131 (100%) | 0.14   | 7 (5%)  | 32  | 19  | 64, 111, 139, 160     | 0     |
| 1   | BO    | 131/131 (100%) | 0.20   | 7 (5%)  | 32  | 19  | 64, 109, 138, 177     | 0     |
| 1   | BP    | 131/131 (100%) | 0.28   | 6 (4%)  | 37  | 21  | 64, 110, 142, 191     | 0     |
| 1   | BQ    | 131/131 (100%) | 0.25   | 7 (5%)  | 32  | 19  | 64, 111, 139, 160     | 0     |
| 1   | BR    | 131/131 (100%) | 0.15   | 5 (3%)  | 44  | 25  | 64, 109, 138, 177     | 0     |
| 1   | BS    | 131/131 (100%) | 0.21   | 3 (2%)  | 61  | 37  | 64, 110, 142, 191     | 0     |
| 1   | BT    | 131/131 (100%) | 0.11   | 1 (0%)  | 82  | 61  | 64, 111, 139, 160     | 0     |
| 1   | BU    | 131/131 (100%) | 0.14   | 6 (4%)  | 37  | 21  | 64, 109, 138, 177     | 0     |
| 1   | BV    | 131/131 (100%) | 0.19   | 6 (4%)  | 37  | 21  | 64, 110, 142, 191     | 0     |
| 1   | BW    | 131/131 (100%) | 0.22   | 4 (3%)  | 51  | 30  | 64, 111, 139, 160     | 0     |
| 1   | BX    | 131/131 (100%) | 0.05   | 2 (1%)  | 72  | 48  | 64, 109, 138, 177     | 0     |
| 1   | BY    | 131/131 (100%) | 0.34   | 6 (4%)  | 37  | 21  | 64, 110, 142, 191     | 0     |
| 1   | BZ    | 131/131 (100%) | 0.19   | 7 (5%)  | 32  | 19  | 64, 111, 139, 160     | 0     |
| 1   | CA    | 131/131 (100%) | 0.08   | 0       | 100 | 100 | 64, 109, 138, 177     | 0     |
| 1   | CB    | 131/131 (100%) | 0.06   | 3 (2%)  | 61  | 37  | 64, 110, 142, 191     | 0     |
| 1   | CC    | 131/131 (100%) | 0.14   | 3 (2%)  | 61  | 37  | 64, 111, 139, 160     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2 |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------|-----|-----|-----------------------|-------|
| 1   | CD    | 131/131 (100%) | 0.18   | 6 (4%)  | 37  | 21  | 64, 109, 138, 177     | 0     |
| 1   | CE    | 131/131 (100%) | 0.27   | 6 (4%)  | 37  | 21  | 64, 110, 142, 191     | 0     |
| 1   | CF    | 131/131 (100%) | 0.34   | 8 (6%)  | 27  | 17  | 64, 111, 139, 160     | 0     |
| 1   | CG    | 131/131 (100%) | 0.15   | 2 (1%)  | 72  | 48  | 64, 109, 138, 177     | 0     |
| 1   | CH    | 131/131 (100%) | 0.45   | 10 (7%) | 20  | 13  | 64, 110, 142, 191     | 0     |
| 1   | CI    | 131/131 (100%) | 0.24   | 3 (2%)  | 61  | 37  | 64, 111, 139, 160     | 0     |
| 1   | CJ    | 131/131 (100%) | 0.13   | 5 (3%)  | 44  | 25  | 64, 109, 138, 177     | 0     |
| 1   | CK    | 131/131 (100%) | 0.24   | 9 (6%)  | 23  | 15  | 64, 110, 142, 191     | 0     |
| 1   | CL    | 131/131 (100%) | 0.09   | 3 (2%)  | 61  | 37  | 64, 111, 139, 160     | 0     |
| 1   | CM    | 131/131 (100%) | -0.06  | 2 (1%)  | 72  | 48  | 64, 109, 138, 177     | 0     |
| 1   | CN    | 131/131 (100%) | 0.06   | 3 (2%)  | 61  | 37  | 64, 110, 142, 191     | 0     |
| 1   | CO    | 131/131 (100%) | 0.13   | 3 (2%)  | 61  | 37  | 64, 111, 139, 160     | 0     |
| 1   | CP    | 131/131 (100%) | -0.04  | 0       | 100 | 100 | 64, 109, 138, 177     | 0     |
| 1   | CQ    | 131/131 (100%) | 0.26   | 2 (1%)  | 72  | 48  | 64, 110, 142, 191     | 0     |
| 1   | CR    | 131/131 (100%) | 0.19   | 7 (5%)  | 32  | 19  | 64, 111, 139, 160     | 0     |
| 1   | CS    | 131/131 (100%) | 0.05   | 5 (3%)  | 44  | 25  | 64, 109, 138, 177     | 0     |
| 1   | CT    | 131/131 (100%) | 0.46   | 11 (8%) | 17  | 12  | 64, 110, 142, 191     | 0     |
| 1   | CU    | 131/131 (100%) | -0.15  | 3 (2%)  | 61  | 37  | 64, 111, 139, 160     | 0     |
| 1   | CV    | 131/131 (100%) | -0.00  | 3 (2%)  | 61  | 37  | 64, 109, 138, 177     | 0     |
| 1   | CW    | 131/131 (100%) | 0.26   | 3 (2%)  | 61  | 37  | 64, 110, 142, 191     | 0     |
| 1   | CX    | 131/131 (100%) | 0.04   | 5 (3%)  | 44  | 25  | 64, 111, 139, 160     | 0     |
| 1   | CY    | 131/131 (100%) | -0.11  | 3 (2%)  | 61  | 37  | 64, 109, 138, 177     | 0     |
| 1   | CZ    | 131/131 (100%) | -0.06  | 1 (0%)  | 82  | 61  | 64, 110, 142, 191     | 0     |
| 1   | DA    | 131/131 (100%) | 0.16   | 3 (2%)  | 61  | 37  | 64, 111, 139, 160     | 0     |
| 1   | DB    | 131/131 (100%) | 0.04   | 2 (1%)  | 72  | 48  | 64, 109, 138, 177     | 0     |
| 1   | DC    | 131/131 (100%) | 0.29   | 2 (1%)  | 72  | 48  | 64, 110, 142, 191     | 0     |
| 1   | DD    | 131/131 (100%) | 0.46   | 9 (6%)  | 23  | 15  | 64, 111, 139, 160     | 0     |
| 1   | DE    | 131/131 (100%) | 0.39   | 8 (6%)  | 27  | 17  | 64, 109, 138, 177     | 0     |
| 1   | DF    | 131/131 (100%) | 0.33   | 6 (4%)  | 37  | 21  | 64, 110, 142, 191     | 0     |
| 1   | DG    | 131/131 (100%) | 0.13   | 3 (2%)  | 61  | 37  | 64, 111, 139, 160     | 0     |
| 1   | DH    | 131/131 (100%) | 0.02   | 4 (3%)  | 51  | 30  | 64, 109, 138, 177     | 0     |

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| Mol | Chain | Analysed           | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|--------------------|--------|----------------|-----------------------|-------|
| 1   | DI    | 131/131 (100%)     | 0.46   | 10 (7%) 20 13  | 64, 110, 142, 191     | 0     |
| 1   | DJ    | 131/131 (100%)     | 0.02   | 0 100 100      | 64, 111, 139, 160     | 0     |
| 1   | DK    | 131/131 (100%)     | 0.14   | 5 (3%) 44 25   | 64, 109, 138, 177     | 0     |
| 1   | DL    | 131/131 (100%)     | 0.02   | 1 (0%) 82 61   | 64, 110, 142, 191     | 0     |
| All | All   | 11790/11790 (100%) | 0.18   | 432 (3%) 45 26 | 64, 110, 141, 191     | 0     |

The worst 5 of 432 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BH    | 61  | VAL  | 7.1  |
| 1   | AU    | 54  | LYS  | 6.5  |
| 1   | DE    | 131 | ALA  | 5.9  |
| 1   | BM    | 131 | ALA  | 5.7  |
| 1   | BH    | 62  | ASN  | 5.2  |

## 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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.