



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 09:17 pm GMT

PDB ID : 4V6B  
Title : Crystal structure of human ferritin Phe167SerfsX26 mutant.  
Authors : Hurley, T.D.; Vidal, R.  
Deposited on : 2009-06-19  
Resolution : 2.85 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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

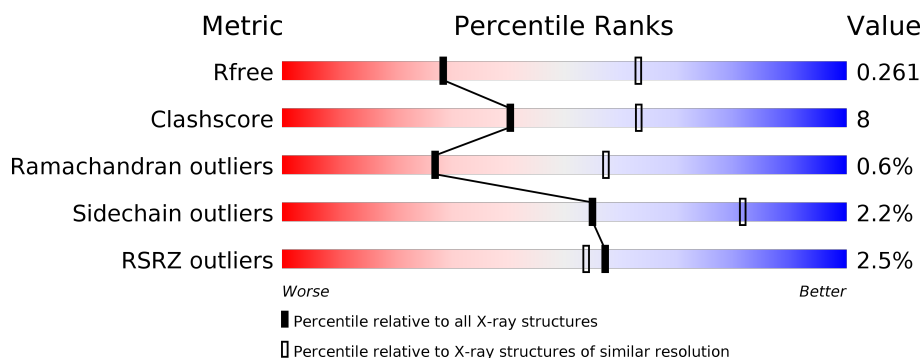
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 111664                      | 2715 (2.90-2.82)                                      |
| Clashscore            | 122126                      | 2976 (2.90-2.82)                                      |
| Ramachandran outliers | 120053                      | 2913 (2.90-2.82)                                      |
| Sidechain outliers    | 120020                      | 2916 (2.90-2.82)                                      |
| RSRZ outliers         | 108989                      | 2654 (2.90-2.82)                                      |

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

| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | AA    | 192    | <div> <div>3%</div> <div> <div></div> <div>56%</div> <div>26%</div> <div>•</div> <div>18%</div> </div> </div>  |
| 1   | AB    | 192    | <div> <div>4%</div> <div> <div></div> <div>57%</div> <div>27%</div> <div>•</div> <div>14%</div> </div> </div>  |
| 1   | AC    | 192    | <div> <div>2%</div> <div> <div></div> <div>63%</div> <div>20%</div> <div>•</div> <div>16%</div> </div> </div>  |
| 1   | AD    | 192    | <div> <div>2%</div> <div> <div></div> <div>53%</div> <div>29%</div> <div>•</div> <div>17%</div> </div> </div>  |
| 1   | AE    | 192    | <div> <div>5%</div> <div> <div></div> <div>49%</div> <div>34%</div> <div>••</div> <div>14%</div> </div> </div> |
| 1   | AF    | 192    | <div> <div>%</div> <div> <div></div> <div>54%</div> <div>27%</div> <div>•</div> <div>18%</div> </div> </div>   |





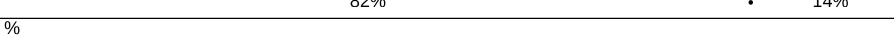
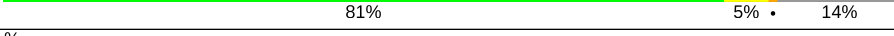



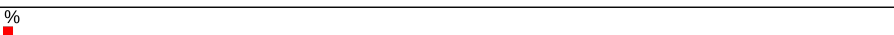
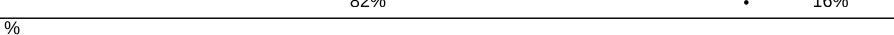










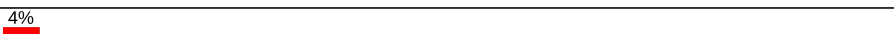
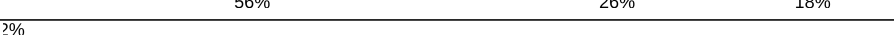


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | AG    | 192    |                  |
| 1   | AH    | 192    |                  |
| 1   | AI    | 192    |                  |
| 1   | AJ    | 192    |                  |
| 1   | AK    | 192    |                  |
| 1   | AL    | 192    |                  |
| 1   | AM    | 192    |                  |
| 1   | AN    | 192    |                  |
| 1   | AO    | 192    |                  |
| 1   | AP    | 192    |                  |
| 1   | AQ    | 192    |                  |
| 1   | AR    | 192    |                  |
| 1   | AS    | 192    |                  |
| 1   | AT    | 192    |                  |
| 1   | AU    | 192    |                  |
| 1   | AV    | 192    |                  |
| 1   | AW    | 192    |                  |
| 1   | AX    | 192    |                  |
| 1   | Aa    | 192    |                  |
| 1   | Ab    | 192    |                  |
| 1   | Ac    | 192    |                  |
| 1   | Ad    | 192    |                  |
| 1   | Ae    | 192    |                  |
| 1   | Af    | 192    |                  |
| 1   | Ag    | 192    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | Ah    | 192    |    |
| 1   | Ai    | 192    |    |
| 1   | Aj    | 192    |    |
| 1   | Ak    | 192    |    |
| 1   | Al    | 192    |    |
| 1   | Am    | 192    |    |
| 1   | An    | 192    |    |
| 1   | Ao    | 192    |    |
| 1   | Ap    | 192    |    |
| 1   | Aq    | 192    |    |
| 1   | Ar    | 192    |    |
| 1   | As    | 192    |    |
| 1   | At    | 192    |    |
| 1   | Au    | 192    |   |
| 1   | Av    | 192    |  |
| 1   | Aw    | 192    |  |
| 1   | Ax    | 192    |  |
| 1   | BA    | 192    |  |
| 1   | BB    | 192    |  |
| 1   | BC    | 192    |  |
| 1   | BD    | 192    |  |
| 1   | BE    | 192    |  |
| 1   | BF    | 192    |  |
| 1   | BG    | 192    |  |
| 1   | BH    | 192    |  |

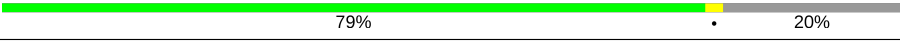















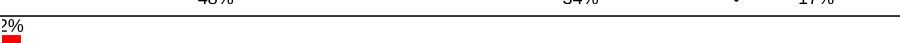
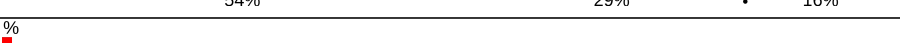
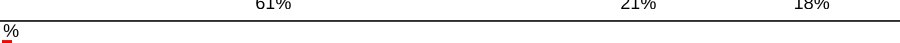

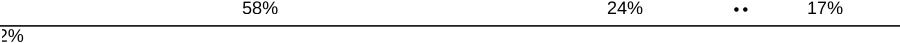
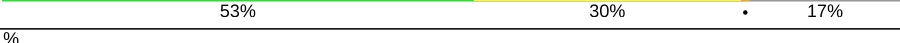



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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | BI    | 192    |                  |
| 1   | BJ    | 192    |                  |
| 1   | BK    | 192    |                  |
| 1   | BL    | 192    |                  |
| 1   | BM    | 192    |                  |
| 1   | BN    | 192    |                  |
| 1   | BO    | 192    |                  |
| 1   | BP    | 192    |                  |
| 1   | BQ    | 192    |                  |
| 1   | BR    | 192    |                  |
| 1   | BS    | 192    |                  |
| 1   | BT    | 192    |                  |
| 1   | BU    | 192    |                  |
| 1   | BV    | 192    |                  |
| 1   | BW    | 192    |                  |
| 1   | BX    | 192    |                  |
| 1   | Ba    | 192    |                  |
| 1   | Bb    | 192    |                  |
| 1   | Bc    | 192    |                  |
| 1   | Bd    | 192    |                  |
| 1   | Be    | 192    |                  |
| 1   | Bf    | 192    |                  |
| 1   | Bg    | 192    |                  |
| 1   | Bh    | 192    |                  |
| 1   | Bi    | 192    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | Bj    | 192    |    |
| 1   | Bk    | 192    |    |
| 1   | Bl    | 192    |    |
| 1   | Bm    | 192    |    |
| 1   | Bn    | 192    |    |
| 1   | Bo    | 192    |    |
| 1   | Bp    | 192    |    |
| 1   | Bq    | 192    |    |
| 1   | Br    | 192    |    |
| 1   | Bs    | 192    |    |
| 1   | Bt    | 192    |    |
| 1   | Bu    | 192    |    |
| 1   | Bv    | 192    |  |
| 1   | Bw    | 192    |  |
| 1   | Bx    | 192    |  |
| 1   | CA    | 192    |  |
| 1   | CB    | 192    |  |
| 1   | CC    | 192    |  |
| 1   | CD    | 192    |  |
| 1   | CE    | 192    |  |
| 1   | CF    | 192    |  |
| 1   | CG    | 192    |  |
| 1   | CH    | 192    |  |
| 1   | CI    | 192    |  |
| 1   | CJ    | 192    |  |

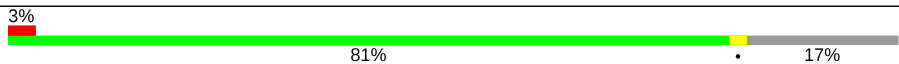

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | CK    | 192    |                  |
| 1   | CL    | 192    |                  |
| 1   | CM    | 192    |                  |
| 1   | CN    | 192    |                  |
| 1   | CO    | 192    |                  |
| 1   | CP    | 192    |                  |
| 1   | CQ    | 192    |                  |
| 1   | CR    | 192    |                  |
| 1   | CS    | 192    |                  |
| 1   | CT    | 192    |                  |
| 1   | CU    | 192    |                  |
| 1   | CV    | 192    |                  |
| 1   | CW    | 192    |                  |
| 1   | CX    | 192    |                  |
| 1   | Ca    | 192    |                  |
| 1   | Cb    | 192    |                  |
| 1   | Cc    | 192    |                  |
| 1   | Cd    | 192    |                  |
| 1   | Ce    | 192    |                  |
| 1   | Cf    | 192    |                  |
| 1   | Cg    | 192    |                  |
| 1   | Ch    | 192    |                  |
| 1   | Ci    | 192    |                  |
| 1   | Cj    | 192    |                  |
| 1   | Ck    | 192    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 1   | Cl    | 192    |    |
| 1   | Cm    | 192    |    |
| 1   | Cn    | 192    |    |
| 1   | Co    | 192    |    |
| 1   | Cp    | 192    |    |
| 1   | Cq    | 192    |    |
| 1   | Cr    | 192    |    |
| 1   | Cs    | 192    |    |
| 1   | Ct    | 192    |    |
| 1   | Cu    | 192    |    |
| 1   | Cv    | 192    |   |
| 1   | Cw    | 192    |  |
| 1   | Cx    | 192    |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 2   | CA   | Cl    | 201 | -         | -        | -       | X                |



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 187090 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 Ferritin.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | AA    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 800 | 222 | 243 | 5 |         |         |       |
| 1   | Aa    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | AB    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | Ab    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1287  | 810 | 225 | 246 | 6 |         |         |       |
| 1   | AC    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | Ac    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | AD    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |
| 1   | Ad    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | AE    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | Ae    | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 816 | 229 | 247 | 6 |         |         |       |
| 1   | AF    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 800 | 222 | 241 | 6 |         |         |       |
| 1   | Af    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | AG    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |
| 1   | Ag    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1254  | 791 | 219 | 238 | 6 |         |         |       |
| 1   | AH    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | Ah    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | AI    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 800 | 222 | 241 | 6 |         |         |       |
| 1   | Ai    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |
| 1   | AJ    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1262  | 795 | 221 | 240 | 6 |         |         |       |
| 1   | Aj    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | AK    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 799 | 224 | 240 | 6 |         |         |       |
| 1   | Ak    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | AL    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1261  | 795 | 221 | 240 | 5 |         |         |       |
| 1   | Al    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | AM    | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 816 | 229 | 247 | 6 |         |         |       |
| 1   | Am    | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 816 | 229 | 247 | 6 |         |         |       |
| 1   | AN    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | An    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1287  | 810 | 225 | 246 | 6 |         |         |       |
| 1   | AO    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | Ao    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | AP    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |
| 1   | Ap    | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 816 | 229 | 247 | 6 |         |         |       |
| 1   | AQ    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1319  | 829 | 232 | 252 | 6 |         |         |       |
| 1   | Aq    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | AR    | 164      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1308  | 823 | 228 | 251 | 6 |         |         |       |
| 1   | Ar    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | AS    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1279  | 805 | 224 | 245 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | As    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | AT    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 800 | 222 | 243 | 5 |         |         |       |
| 1   | At    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | AU    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | Au    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | AV    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1279  | 805 | 224 | 245 | 5 |         |         |       |
| 1   | Av    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1319  | 829 | 232 | 252 | 6 |         |         |       |
| 1   | AW    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 800 | 222 | 243 | 5 |         |         |       |
| 1   | Aw    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1287  | 810 | 225 | 246 | 6 |         |         |       |
| 1   | AX    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | Ax    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1254  | 791 | 219 | 238 | 6 |         |         |       |
| 1   | BA    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1331  | 838 | 233 | 254 | 6 |         |         |       |
| 1   | Ba    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 800 | 222 | 241 | 6 |         |         |       |
| 1   | BB    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 799 | 224 | 240 | 6 |         |         |       |
| 1   | Bb    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |
| 1   | BC    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1250  | 788 | 219 | 238 | 5 |         |         |       |
| 1   | Bc    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | BD    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1289  | 811 | 227 | 245 | 6 |         |         |       |
| 1   | Bd    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | BE    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |
| 1   | Be    | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1300  | 818 | 227 | 250 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | BF    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |
| 1   | Bf    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | BG    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1258  | 793 | 220 | 239 | 6 |         |         |       |
| 1   | Bg    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1258  | 793 | 220 | 239 | 6 |         |         |       |
| 1   | BH    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1246  | 786 | 218 | 237 | 5 |         |         |       |
| 1   | Bh    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |
| 1   | BI    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1254  | 791 | 219 | 238 | 6 |         |         |       |
| 1   | Bi    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 799 | 224 | 240 | 6 |         |         |       |
| 1   | BJ    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1261  | 795 | 221 | 240 | 5 |         |         |       |
| 1   | Bj    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1244  | 785 | 218 | 236 | 5 |         |         |       |
| 1   | BK    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1258  | 793 | 220 | 239 | 6 |         |         |       |
| 1   | Bk    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |
| 1   | BL    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1254  | 791 | 219 | 238 | 6 |         |         |       |
| 1   | Bl    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |
| 1   | BM    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 800 | 222 | 243 | 5 |         |         |       |
| 1   | Bm    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |
| 1   | BN    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |
| 1   | Bn    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1319  | 829 | 232 | 252 | 6 |         |         |       |
| 1   | BO    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | Bo    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1258  | 793 | 220 | 239 | 6 |         |         |       |
| 1   | BP    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | Bp    | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 816 | 229 | 247 | 6 |         |         |       |
| 1   | BQ    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | Bq    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1289  | 811 | 227 | 245 | 6 |         |         |       |
| 1   | BR    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | Br    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | BS    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1280  | 806 | 226 | 242 | 6 |         |         |       |
| 1   | Bs    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1254  | 791 | 219 | 238 | 6 |         |         |       |
| 1   | BT    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1261  | 795 | 221 | 240 | 5 |         |         |       |
| 1   | Bt    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 800 | 222 | 241 | 6 |         |         |       |
| 1   | BU    | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 816 | 229 | 247 | 6 |         |         |       |
| 1   | Bu    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1320  | 832 | 229 | 253 | 6 |         |         |       |
| 1   | BV    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1254  | 790 | 220 | 239 | 5 |         |         |       |
| 1   | Bv    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | BW    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1287  | 810 | 225 | 246 | 6 |         |         |       |
| 1   | Bw    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |
| 1   | BX    | 163      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1300  | 818 | 227 | 250 | 5 |         |         |       |
| 1   | Bx    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1261  | 795 | 221 | 240 | 5 |         |         |       |
| 1   | CA    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | Ca    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 800 | 222 | 242 | 5 |         |         |       |
| 1   | CB    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1287  | 810 | 225 | 246 | 6 |         |         |       |
| 1   | Cb    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | CC    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1261  | 795 | 221 | 240 | 5 |         |         |       |
| 1   | Cc    | 157      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1264  | 797 | 221 | 241 | 5 |         |         |       |
| 1   | CD    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | Cd    | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1240  | 783 | 217 | 235 | 5 |         |         |       |
| 1   | CE    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1289  | 811 | 227 | 245 | 6 |         |         |       |
| 1   | Ce    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1246  | 786 | 218 | 237 | 5 |         |         |       |
| 1   | CF    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1279  | 805 | 224 | 245 | 5 |         |         |       |
| 1   | Cf    | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1238  | 780 | 217 | 236 | 5 |         |         |       |
| 1   | CG    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1289  | 811 | 227 | 245 | 6 |         |         |       |
| 1   | Cg    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1279  | 805 | 224 | 245 | 5 |         |         |       |
| 1   | CH    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |
| 1   | Ch    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |
| 1   | CI    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | Ci    | 153      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1240  | 783 | 217 | 235 | 5 |         |         |       |
| 1   | CJ    | 165      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1319  | 829 | 232 | 252 | 6 |         |         |       |
| 1   | Cj    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1265  | 797 | 223 | 239 | 6 |         |         |       |
| 1   | CK    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1283  | 808 | 224 | 245 | 6 |         |         |       |
| 1   | Ck    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1246  | 786 | 218 | 237 | 5 |         |         |       |
| 1   | CL    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |
| 1   | Cl    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1250  | 788 | 219 | 238 | 5 |         |         |       |
| 1   | CM    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | Cm    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |
| 1   | CN    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1287  | 810 | 225 | 246 | 6 |         |         |       |
| 1   | Cn    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1254  | 791 | 219 | 238 | 6 |         |         |       |
| 1   | CO    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1280  | 806 | 226 | 242 | 6 |         |         |       |
| 1   | Co    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1250  | 788 | 219 | 238 | 5 |         |         |       |
| 1   | CP    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 800 | 222 | 241 | 6 |         |         |       |
| 1   | Cp    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 800 | 222 | 241 | 6 |         |         |       |
| 1   | CQ    | 162      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1298  | 816 | 229 | 247 | 6 |         |         |       |
| 1   | Cq    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1250  | 788 | 219 | 238 | 5 |         |         |       |
| 1   | CR    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1331  | 838 | 233 | 254 | 6 |         |         |       |
| 1   | Cr    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1246  | 786 | 218 | 237 | 5 |         |         |       |
| 1   | CS    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | Cs    | 154      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1244  | 785 | 218 | 236 | 5 |         |         |       |
| 1   | CT    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1269  | 800 | 222 | 241 | 6 |         |         |       |
| 1   | Ct    | 160      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1279  | 805 | 224 | 245 | 5 |         |         |       |
| 1   | CU    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1278  | 805 | 223 | 244 | 6 |         |         |       |
| 1   | Cu    | 159      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1275  | 803 | 223 | 244 | 5 |         |         |       |
| 1   | CV    | 158      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1270  | 800 | 222 | 243 | 5 |         |         |       |
| 1   | Cv    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1287  | 810 | 225 | 246 | 6 |         |         |       |
| 1   | CW    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1254  | 791 | 219 | 238 | 6 |         |         |       |
| 1   | Cw    | 155      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1250  | 788 | 219 | 238 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | CX    | 161      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1294  | 814 | 228 | 246 | 6 |         |         |       |
| 1   | Cx    | 156      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1265  | 797 | 223 | 239 | 6 |         |         |       |

There are 144 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| AA    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Aa    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AB    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ab    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AC    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ac    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AD    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ad    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AE    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ae    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AF    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Af    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AG    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ag    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AH    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ah    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AI    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ai    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AJ    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Aj    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AK    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ak    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AL    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Al    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AM    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Am    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AN    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| An    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AO    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ao    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AP    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ap    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AQ    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Aq    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| AR    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ar    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AS    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| As    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AT    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| At    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AU    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Au    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AV    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Av    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AW    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Aw    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| AX    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ax    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BA    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ba    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BB    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bb    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BC    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bc    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BD    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bd    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BE    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Be    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BF    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bf    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BG    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bg    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BH    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bh    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BI    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bi    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BJ    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bj    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BK    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bk    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BL    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bl    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BM    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bm    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BN    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bn    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| BO    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bo    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BP    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bp    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BQ    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bq    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BR    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Br    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BS    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bs    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BT    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bt    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BU    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bu    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BV    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bv    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BW    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bw    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| BX    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Bx    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CA    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ca    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CB    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cb    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CC    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cc    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CD    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cd    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CE    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ce    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CF    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cf    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CG    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cg    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CH    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ch    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CI    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ci    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CJ    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cj    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CK    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ck    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| CL    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cl    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CM    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cm    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CN    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cn    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CO    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Co    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CP    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cp    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CQ    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cq    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CR    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cr    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CS    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cs    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CT    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Ct    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CU    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cu    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CV    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cv    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CW    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cw    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| CX    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |
| Cx    | 0       | ARG      | -      | EXPRESSION TAG | UNP Q6S4P3 |

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

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 2   | Ag    | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | BA    | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | CA    | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | Ah    | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | AB    | 1        | Total Ca<br>1 1 | 0       | 0       |
| 2   | Ac    | 1        | Total Ca<br>1 1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | Bd    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CD    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Ce    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Cl    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BB    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Ba    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Ca    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CO    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Be    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Cb    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AA    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | An    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CH    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BC    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AM    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Bb    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Aj    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BN    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Ae    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BG    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

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| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2   | CC    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Bf    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BR    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Aa    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CE    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Cn    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Ck    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AL    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Bc    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Cg    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Bu    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Ad    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AH    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Bg    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AC    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | CB    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | Cp    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BD    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AO    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | AF    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |
| 2   | BH    | 1        | Total<br>1 | Ca<br>1 | 0       | 0       |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 3   | AA    | 10       | Total O<br>10 10 | 0       | 0       |
| 3   | Aa    | 47       | Total O<br>47 47 | 0       | 0       |
| 3   | AB    | 14       | Total O<br>14 14 | 0       | 0       |
| 3   | Ab    | 30       | Total O<br>30 30 | 0       | 0       |
| 3   | AC    | 15       | Total O<br>15 15 | 0       | 0       |
| 3   | Ac    | 32       | Total O<br>32 32 | 0       | 0       |
| 3   | AD    | 8        | Total O<br>8 8   | 0       | 0       |
| 3   | Ad    | 37       | Total O<br>37 37 | 0       | 0       |
| 3   | AE    | 27       | Total O<br>27 27 | 0       | 0       |
| 3   | Ae    | 26       | Total O<br>26 26 | 0       | 0       |
| 3   | AF    | 16       | Total O<br>16 16 | 0       | 0       |
| 3   | Af    | 48       | Total O<br>48 48 | 0       | 0       |
| 3   | AG    | 27       | Total O<br>27 27 | 0       | 0       |
| 3   | Ag    | 37       | Total O<br>37 37 | 0       | 0       |
| 3   | AH    | 28       | Total O<br>28 28 | 0       | 0       |
| 3   | Ah    | 28       | Total O<br>28 28 | 0       | 0       |
| 3   | AI    | 6        | Total O<br>6 6   | 0       | 0       |
| 3   | Ai    | 40       | Total O<br>40 40 | 0       | 0       |
| 3   | AJ    | 9        | Total O<br>9 9   | 0       | 0       |
| 3   | Aj    | 28       | Total O<br>28 28 | 0       | 0       |
| 3   | AK    | 15       | Total O<br>15 15 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | Ak    | 37       | Total<br>37 | O<br>37 | 0       | 0       |
| 3   | AL    | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 3   | Al    | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 3   | AM    | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 3   | Am    | 45       | Total<br>45 | O<br>45 | 0       | 0       |
| 3   | AN    | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 3   | An    | 41       | Total<br>41 | O<br>41 | 0       | 0       |
| 3   | AO    | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 3   | Ao    | 39       | Total<br>39 | O<br>39 | 0       | 0       |
| 3   | AP    | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 3   | Ap    | 32       | Total<br>32 | O<br>32 | 0       | 0       |
| 3   | AQ    | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 3   | Aq    | 33       | Total<br>33 | O<br>33 | 0       | 0       |
| 3   | AR    | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 3   | Ar    | 40       | Total<br>40 | O<br>40 | 0       | 0       |
| 3   | AS    | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 3   | As    | 44       | Total<br>44 | O<br>44 | 0       | 0       |
| 3   | AT    | 22       | Total<br>22 | O<br>22 | 0       | 0       |
| 3   | At    | 31       | Total<br>31 | O<br>31 | 0       | 0       |
| 3   | AU    | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 3   | Au    | 31       | Total<br>31 | O<br>31 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | AV    | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 3   | Av    | 19       | Total<br>19 | O<br>19 | 0       | 0       |
| 3   | AW    | 19       | Total<br>19 | O<br>19 | 0       | 0       |
| 3   | Aw    | 34       | Total<br>34 | O<br>34 | 0       | 0       |
| 3   | AX    | 33       | Total<br>33 | O<br>33 | 0       | 0       |
| 3   | Ax    | 31       | Total<br>31 | O<br>31 | 0       | 0       |
| 3   | BA    | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 3   | Ba    | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 3   | BB    | 5        | Total<br>5  | O<br>5  | 0       | 0       |
| 3   | Bb    | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 3   | BC    | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 3   | Bc    | 32       | Total<br>32 | O<br>32 | 0       | 0       |
| 3   | BD    | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 3   | Bd    | 27       | Total<br>27 | O<br>27 | 0       | 0       |
| 3   | BE    | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 3   | Be    | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 3   | BF    | 32       | Total<br>32 | O<br>32 | 0       | 0       |
| 3   | Bf    | 26       | Total<br>26 | O<br>26 | 0       | 0       |
| 3   | BG    | 7        | Total<br>7  | O<br>7  | 0       | 0       |
| 3   | Bg    | 7        | Total<br>7  | O<br>7  | 0       | 0       |
| 3   | BH    | 11       | Total<br>11 | O<br>11 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | Bh    | 19       | Total<br>19 | O<br>19 | 0       | 0       |
| 3   | BI    | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 3   | Bi    | 7        | Total<br>7  | O<br>7  | 0       | 0       |
| 3   | BJ    | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 3   | Bj    | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 3   | BK    | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 3   | Bk    | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 3   | BL    | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 3   | Bl    | 23       | Total<br>23 | O<br>23 | 0       | 0       |
| 3   | BM    | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 3   | Bm    | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 3   | BN    | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 3   | Bn    | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 3   | BO    | 13       | Total<br>13 | O<br>13 | 0       | 0       |
| 3   | Bo    | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 3   | BP    | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 3   | Bp    | 31       | Total<br>31 | O<br>31 | 0       | 0       |
| 3   | BQ    | 30       | Total<br>30 | O<br>30 | 0       | 0       |
| 3   | Bq    | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 3   | BR    | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 3   | Br    | 35       | Total<br>35 | O<br>35 | 0       | 0       |

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| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 3   | BS    | 37       | Total O<br>37 37 | 0       | 0       |
| 3   | Bs    | 15       | Total O<br>15 15 | 0       | 0       |
| 3   | BT    | 12       | Total O<br>12 12 | 0       | 0       |
| 3   | Bt    | 11       | Total O<br>11 11 | 0       | 0       |
| 3   | BU    | 5        | Total O<br>5 5   | 0       | 0       |
| 3   | Bu    | 28       | Total O<br>28 28 | 0       | 0       |
| 3   | BV    | 5        | Total O<br>5 5   | 0       | 0       |
| 3   | Bv    | 25       | Total O<br>25 25 | 0       | 0       |
| 3   | BW    | 25       | Total O<br>25 25 | 0       | 0       |
| 3   | Bw    | 39       | Total O<br>39 39 | 0       | 0       |
| 3   | BX    | 3        | Total O<br>3 3   | 0       | 0       |
| 3   | Bx    | 7        | Total O<br>7 7   | 0       | 0       |
| 3   | CA    | 29       | Total O<br>29 29 | 0       | 0       |
| 3   | Ca    | 11       | Total O<br>11 11 | 0       | 0       |
| 3   | CB    | 16       | Total O<br>16 16 | 0       | 0       |
| 3   | Cb    | 6        | Total O<br>6 6   | 0       | 0       |
| 3   | CC    | 7        | Total O<br>7 7   | 0       | 0       |
| 3   | Cc    | 7        | Total O<br>7 7   | 0       | 0       |
| 3   | CD    | 28       | Total O<br>28 28 | 0       | 0       |
| 3   | Cd    | 6        | Total O<br>6 6   | 0       | 0       |
| 3   | CE    | 15       | Total O<br>15 15 | 0       | 0       |

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| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | Ce    | 6        | Total<br>6  | O<br>6  | 0       | 0       |
| 3   | CF    | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 3   | Cf    | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 3   | CG    | 19       | Total<br>19 | O<br>19 | 0       | 0       |
| 3   | Cg    | 16       | Total<br>16 | O<br>16 | 0       | 0       |
| 3   | CH    | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 3   | Ch    | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 3   | CI    | 30       | Total<br>30 | O<br>30 | 0       | 0       |
| 3   | Ci    | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 3   | CJ    | 18       | Total<br>18 | O<br>18 | 0       | 0       |
| 3   | Cj    | 9        | Total<br>9  | O<br>9  | 0       | 0       |
| 3   | CK    | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 3   | Ck    | 11       | Total<br>11 | O<br>11 | 0       | 0       |
| 3   | CL    | 7        | Total<br>7  | O<br>7  | 0       | 0       |
| 3   | Cl    | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 3   | CM    | 23       | Total<br>23 | O<br>23 | 0       | 0       |
| 3   | Cm    | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 3   | CN    | 25       | Total<br>25 | O<br>25 | 0       | 0       |
| 3   | Cn    | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 3   | CO    | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 3   | Co    | 12       | Total<br>12 | O<br>12 | 0       | 0       |

*Continued on next page...*

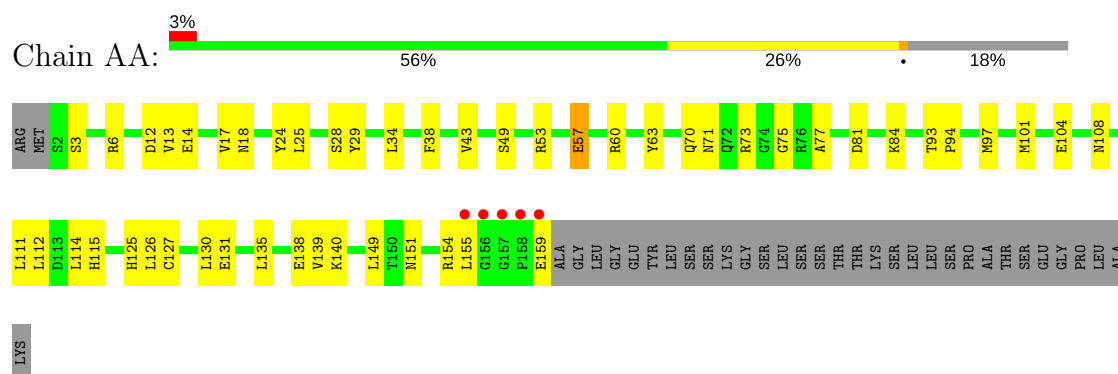
*Continued from previous page...*

| Mol | Chain | Residues | Atoms       |         | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 3   | CP    | 14       | Total<br>14 | O<br>14 | 0       | 0       |
| 3   | Cp    | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 3   | CQ    | 41       | Total<br>41 | O<br>41 | 0       | 0       |
| 3   | Cq    | 2        | Total<br>2  | O<br>2  | 0       | 0       |
| 3   | CR    | 20       | Total<br>20 | O<br>20 | 0       | 0       |
| 3   | Cr    | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 3   | CS    | 28       | Total<br>28 | O<br>28 | 0       | 0       |
| 3   | CT    | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 3   | Ct    | 17       | Total<br>17 | O<br>17 | 0       | 0       |
| 3   | CU    | 3        | Total<br>3  | O<br>3  | 0       | 0       |
| 3   | Cu    | 12       | Total<br>12 | O<br>12 | 0       | 0       |
| 3   | CV    | 8        | Total<br>8  | O<br>8  | 0       | 0       |
| 3   | Cv    | 4        | Total<br>4  | O<br>4  | 0       | 0       |
| 3   | CW    | 15       | Total<br>15 | O<br>15 | 0       | 0       |
| 3   | Cw    | 10       | Total<br>10 | O<br>10 | 0       | 0       |
| 3   | CX    | 21       | Total<br>21 | O<br>21 | 0       | 0       |
| 3   | Cx    | 12       | Total<br>12 | O<br>12 | 0       | 0       |

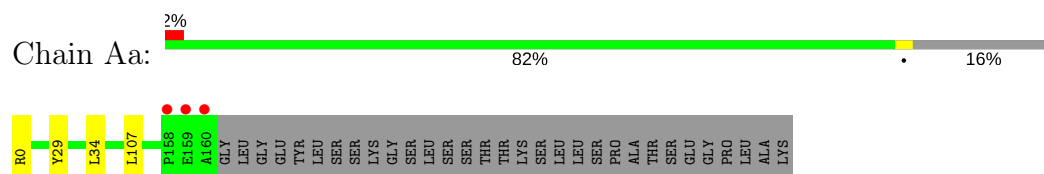
### 3 Residue-property plots [i](#)

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

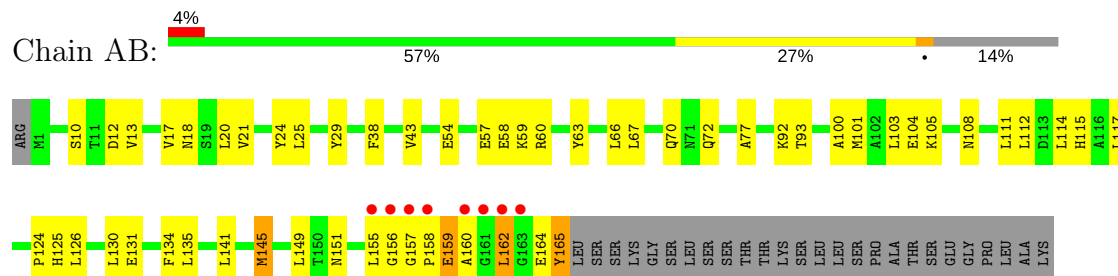
#### • Molecule 1: Ferritin



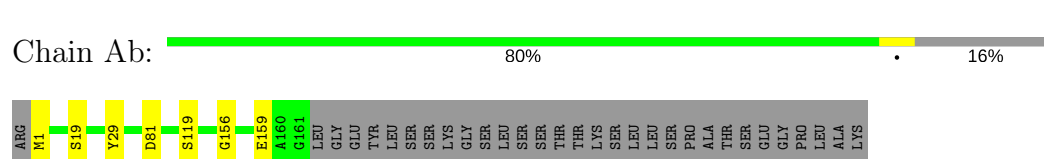
#### • Molecule 1: Ferritin



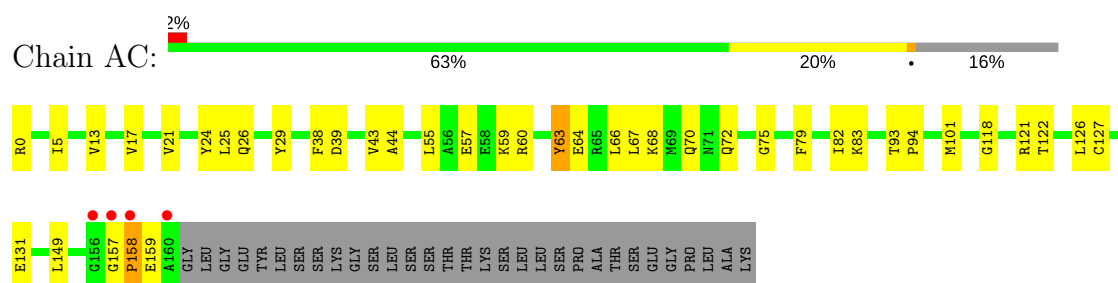
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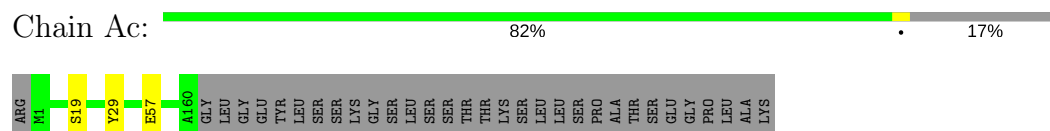
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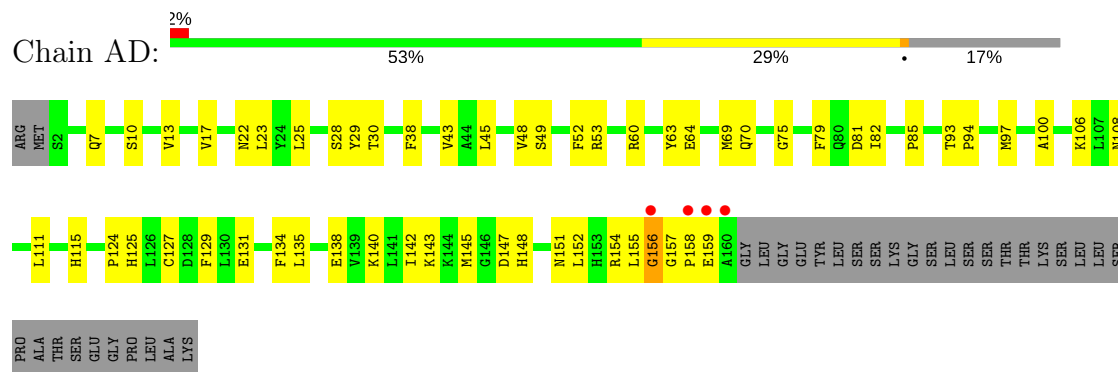
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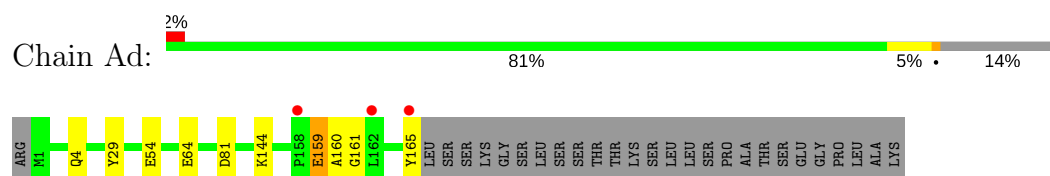
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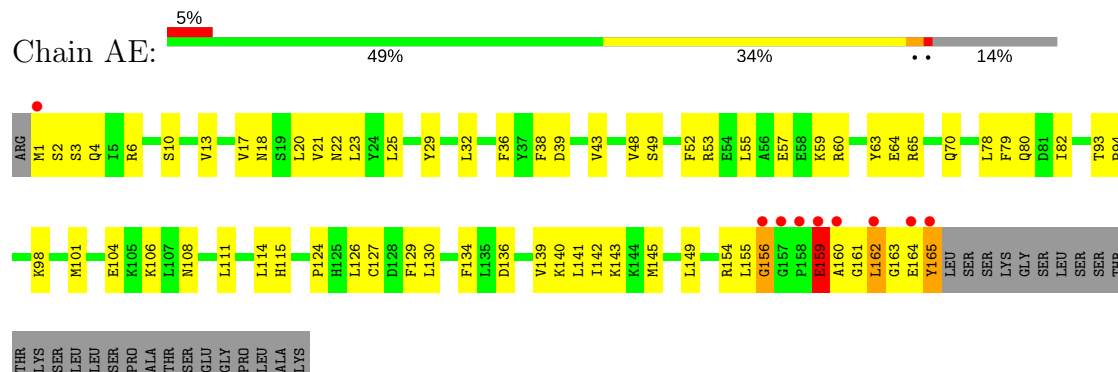
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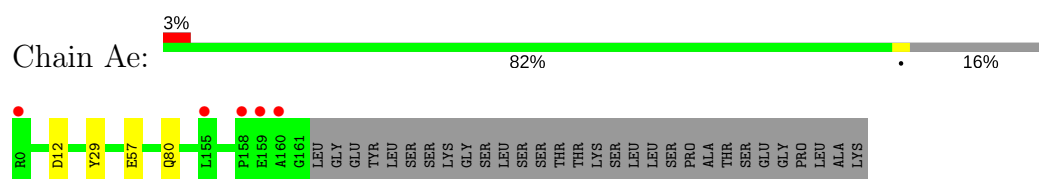
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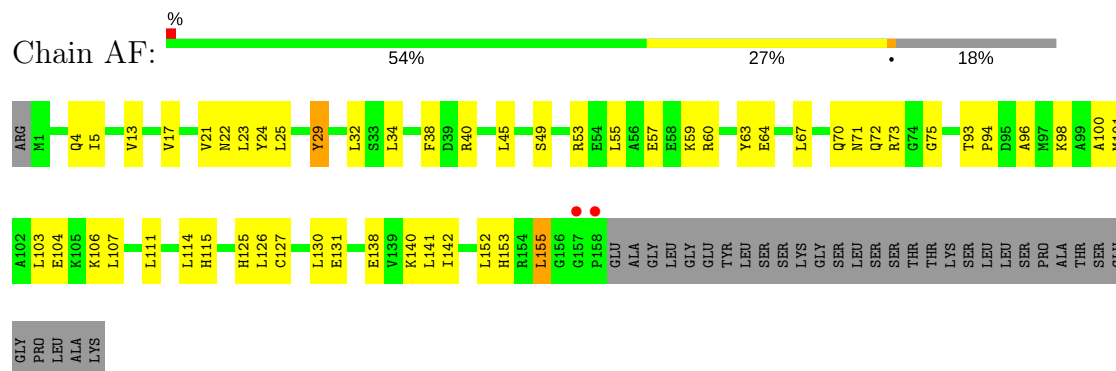
• Molecule 1: Ferritin



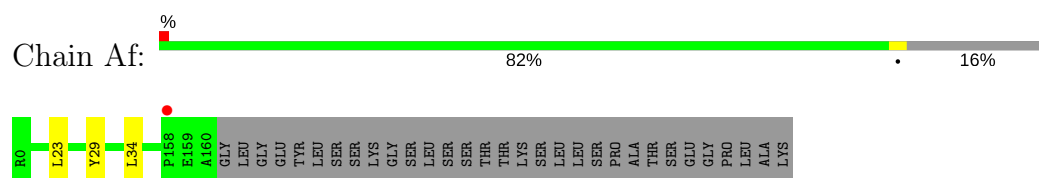
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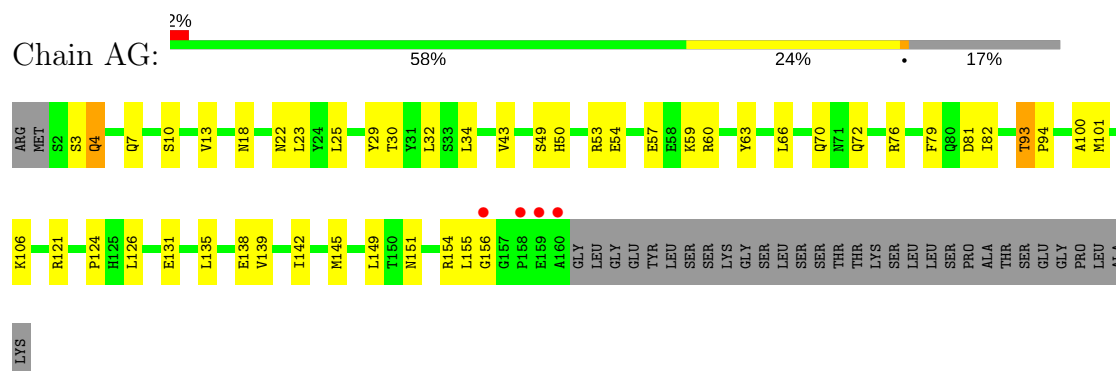
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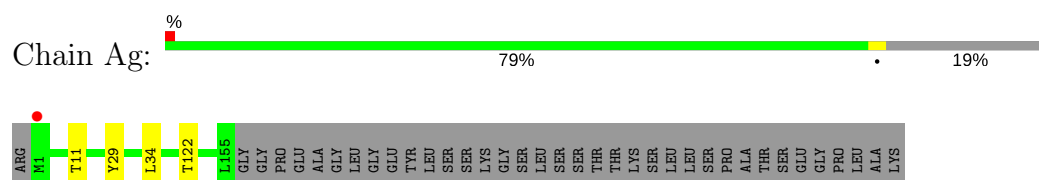
- Molecule 1: Ferritin



- Molecule 1: Ferritin

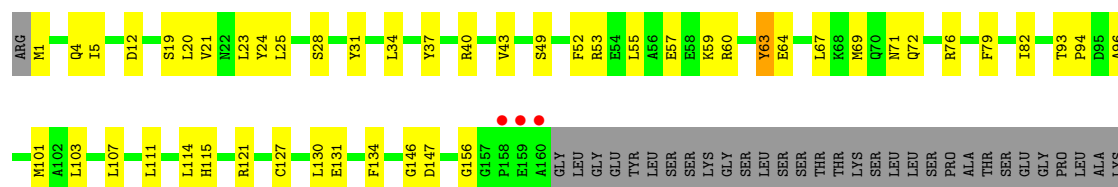


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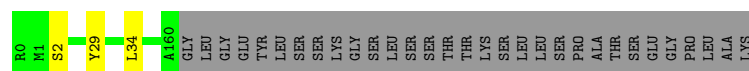
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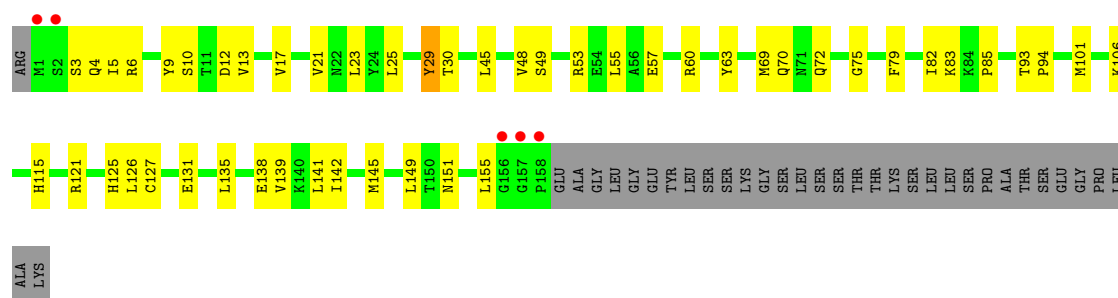
- Molecule 1: Ferritin

Chain Ah:   82% 16%



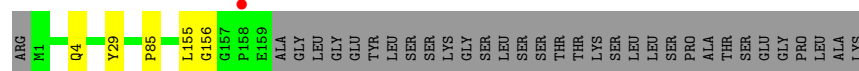
- Molecule 1: Ferritin

Chain Ai:    3% 57% 25% 18%



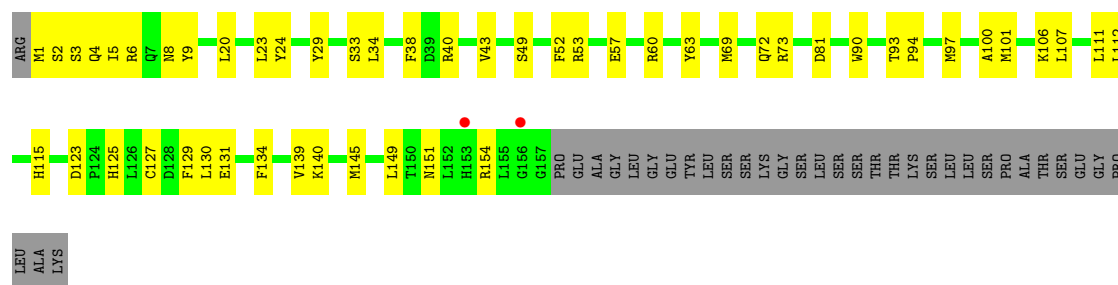
- Molecule 1: Ferritin

Chain Ai:   % 80% 17%



- Molecule 1: Ferritin

Chain Aj:    % 55% 27% 18%



- Molecule 1: Ferritin

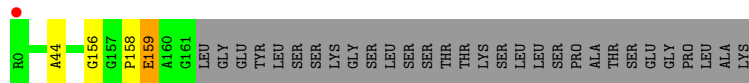
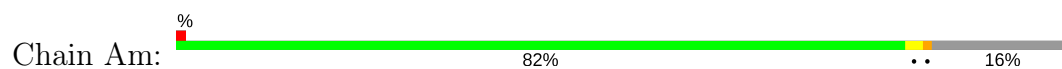
Chain Aj:    3% 81% 5% 14%





GLU  
GLY  
PRO  
LEU  
ALA  
LYS

## ● Molecule 1: Ferritin

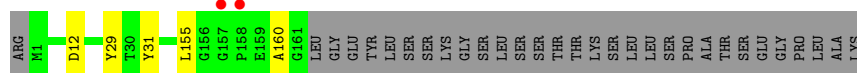
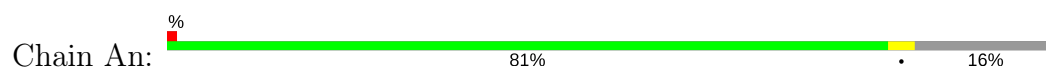


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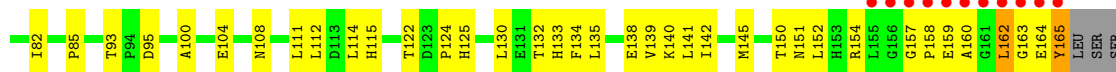
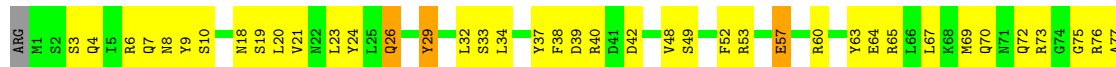


GLY  
PRO  
LEU  
ALA  
LYS

## ● Molecule 1: Ferritin

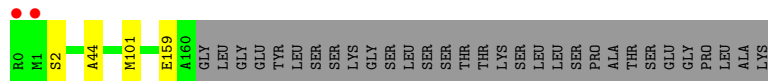
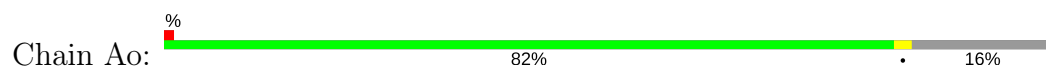


## ● Molecule 1: Ferritin

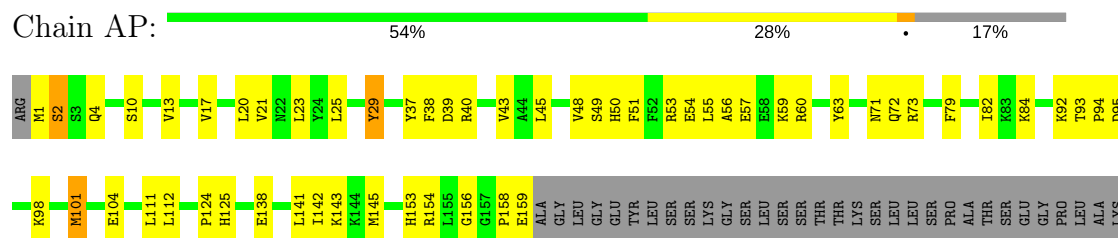


LYS  
GLY  
SER  
LEU  
SER  
THR  
LYS  
SER  
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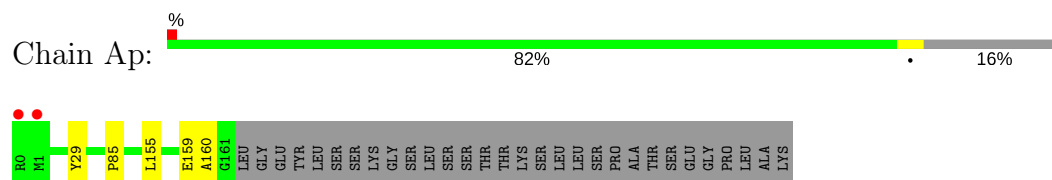
## ● Molecule 1: Ferritin



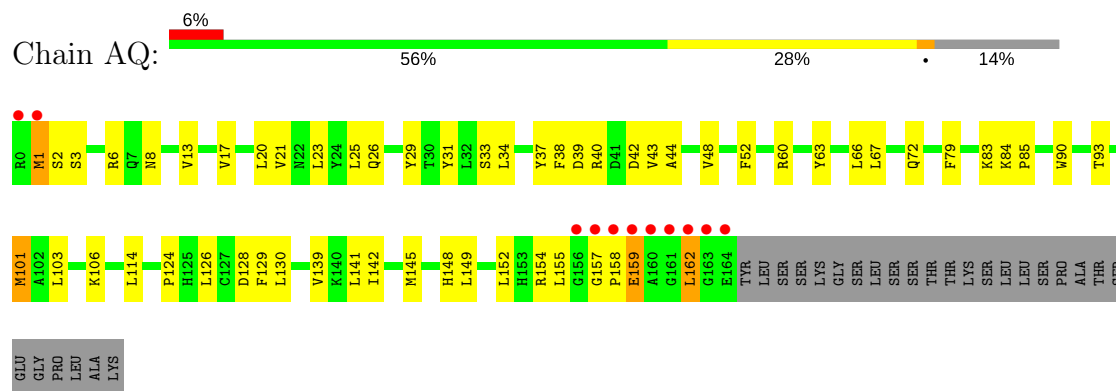
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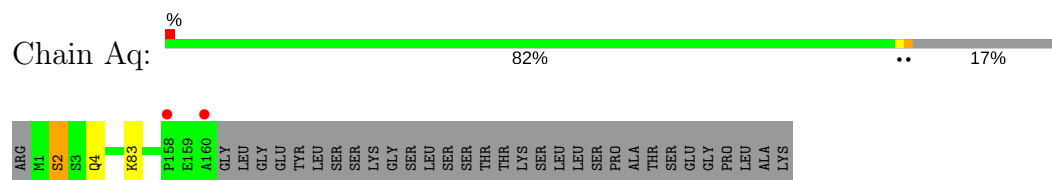
• Molecule 1: Ferritin



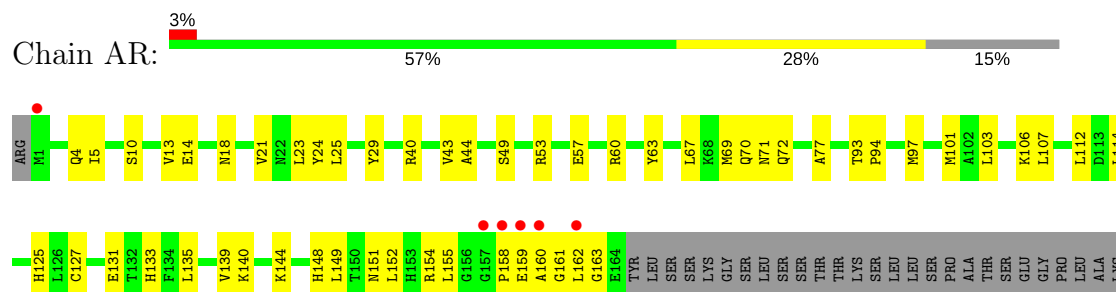
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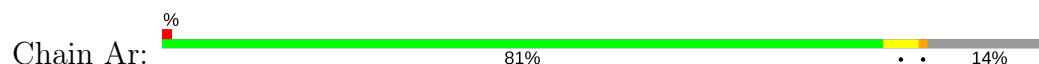
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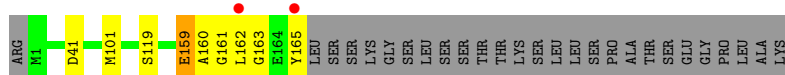


• Molecule 1: Ferritin



• Molecule 1: Ferritin

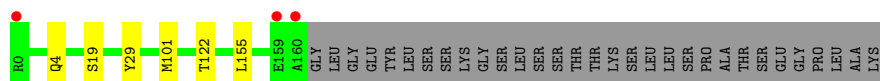
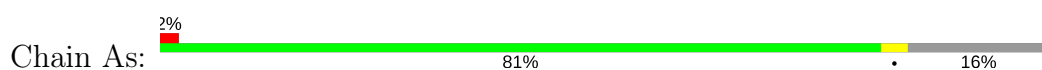




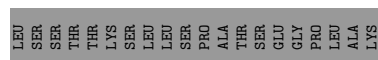
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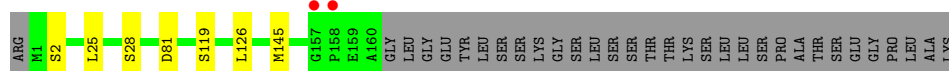
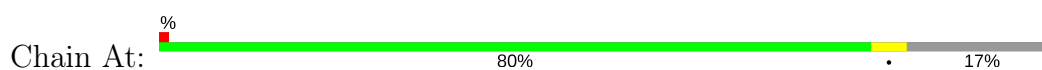
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• Molecule 1: Ferritin



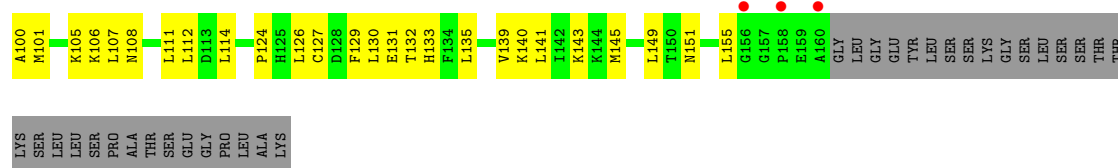
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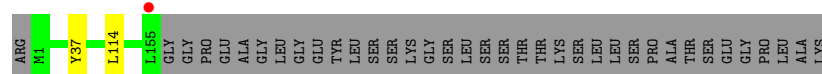
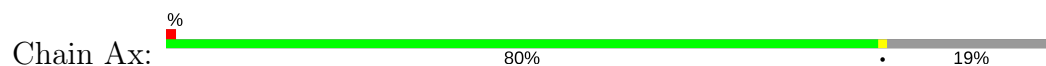
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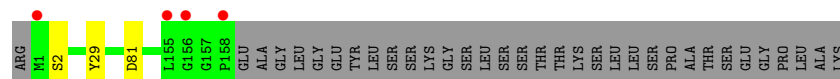
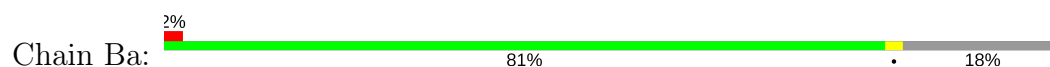
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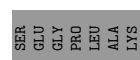
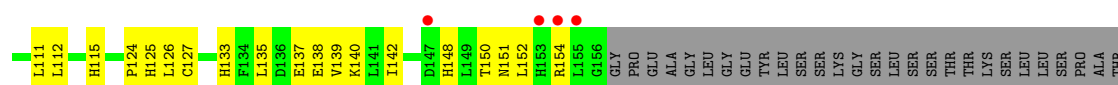
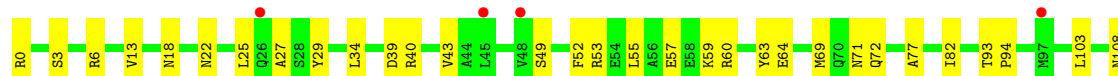
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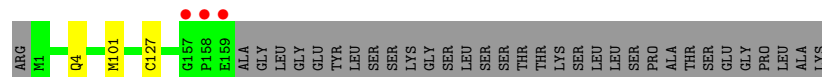
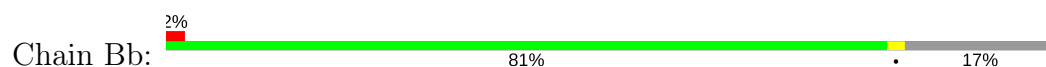
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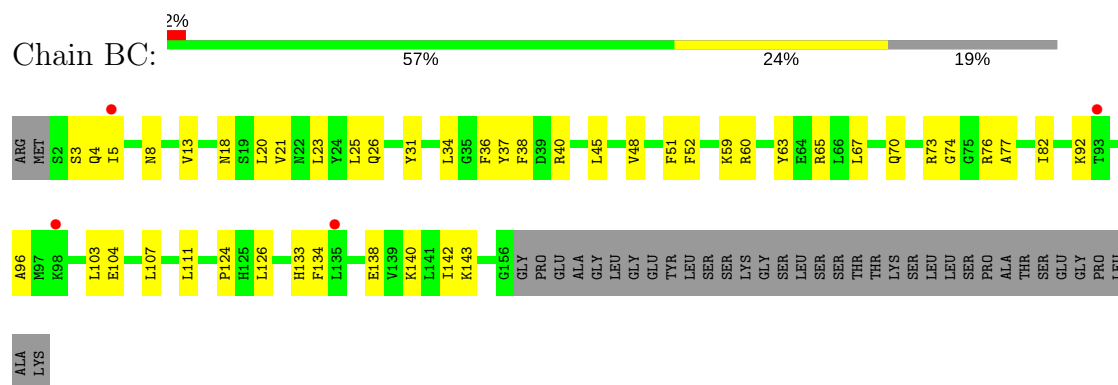
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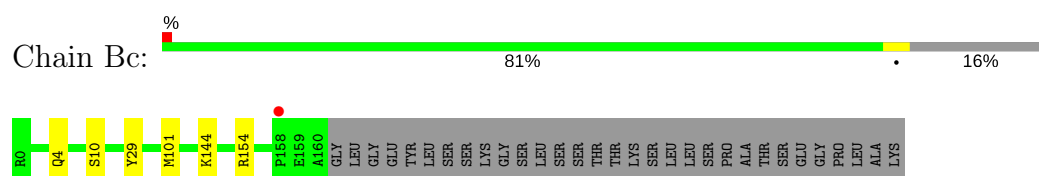
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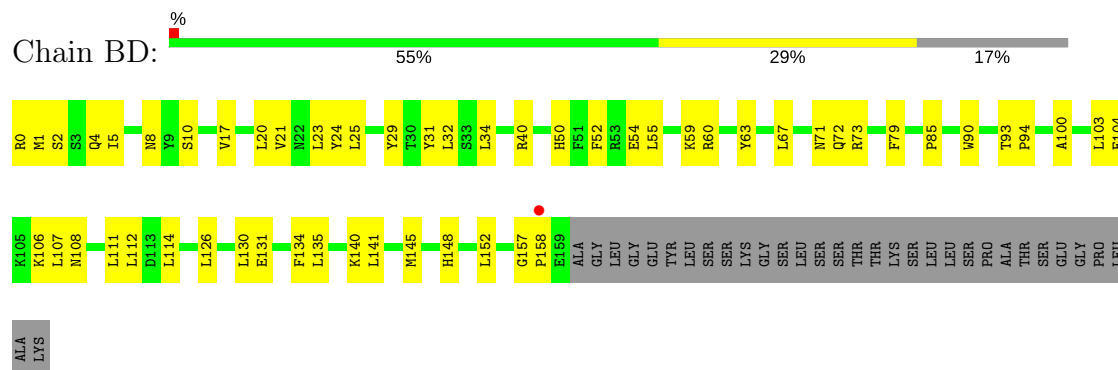
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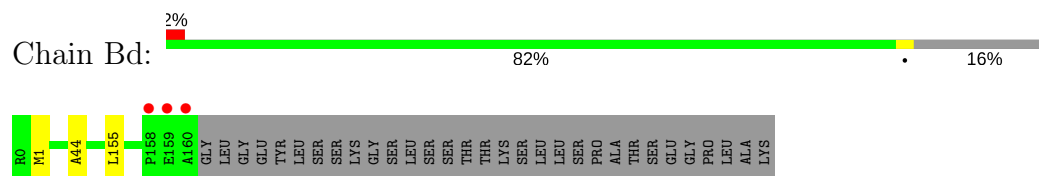
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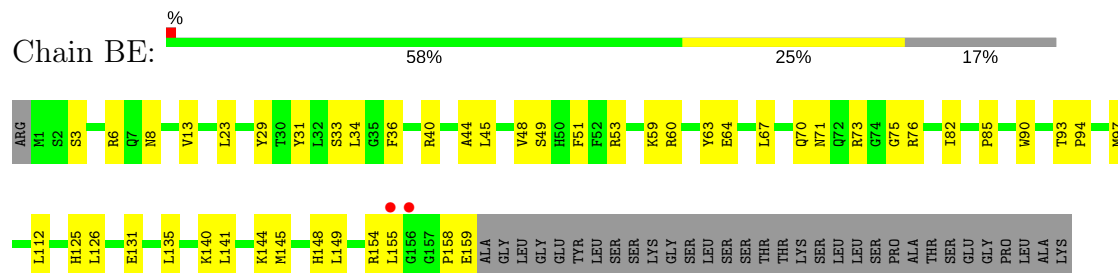
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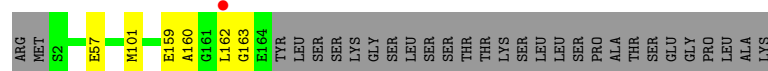
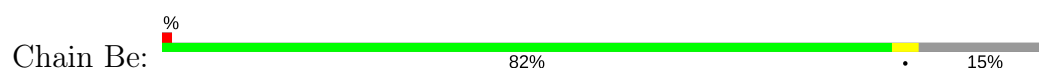
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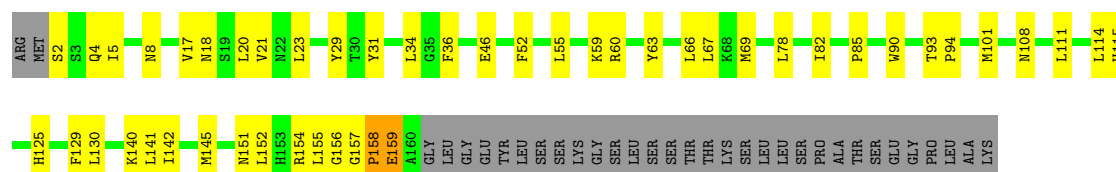
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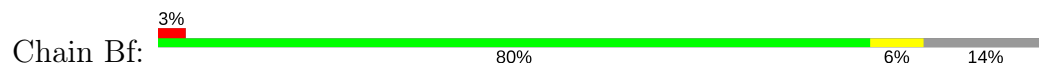
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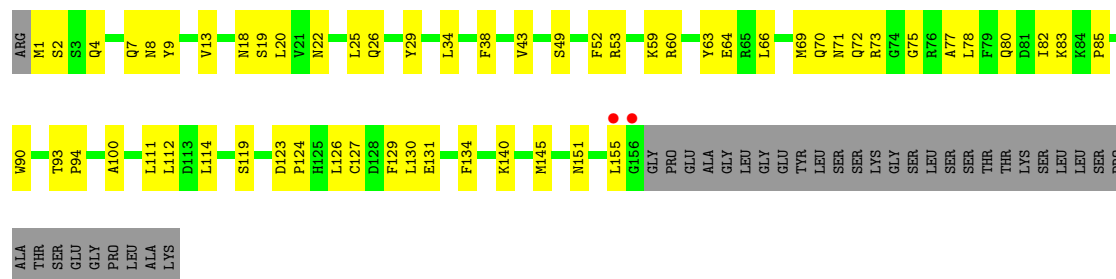
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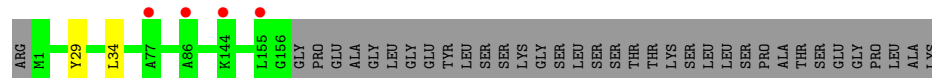
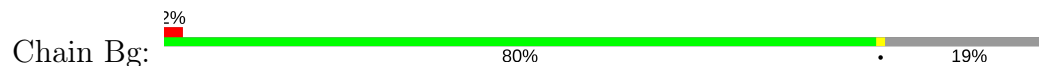
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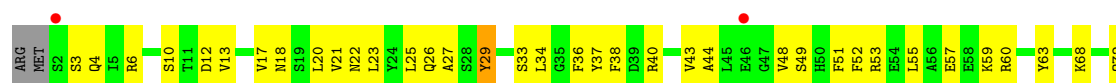
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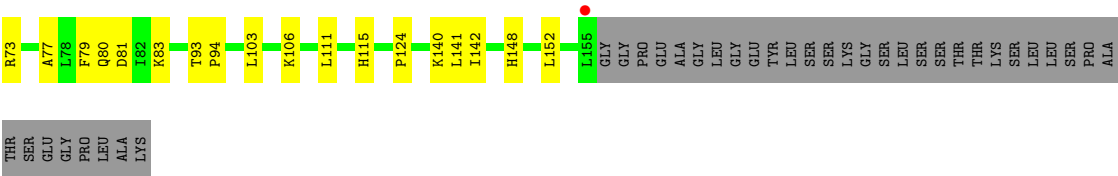
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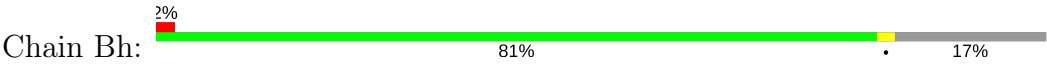
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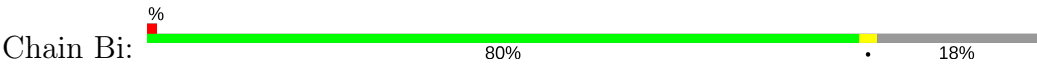
• Molecule 1: Ferritin



• Molecule 1: Ferritin



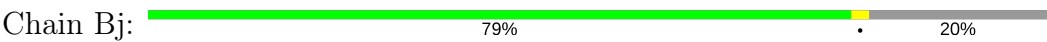
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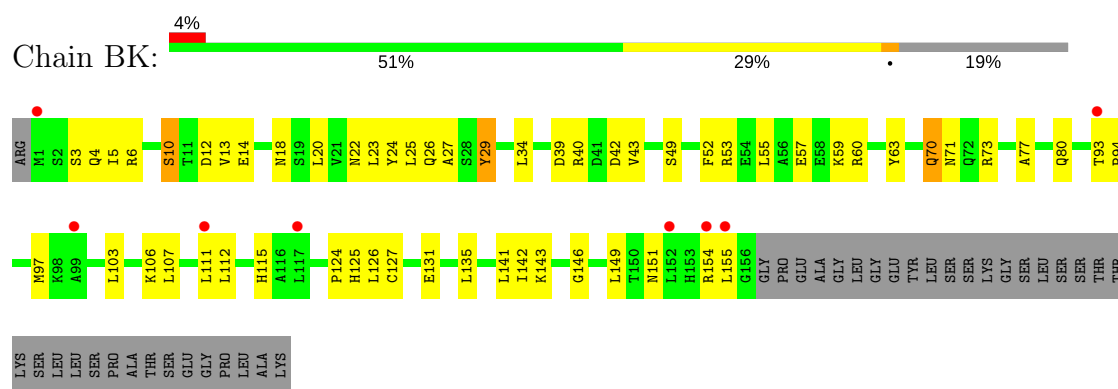
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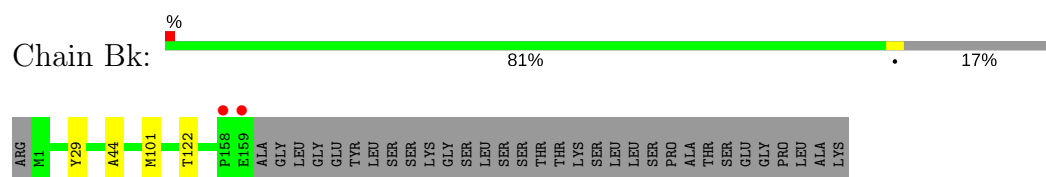
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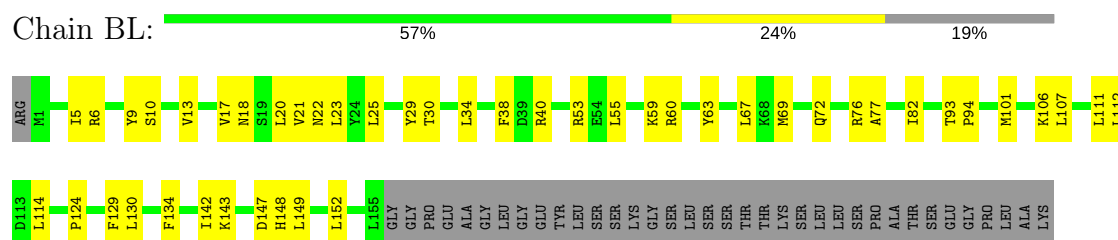
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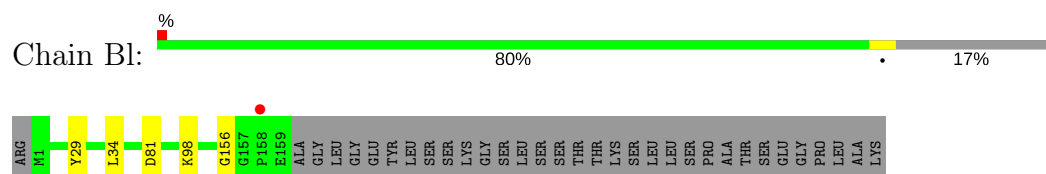
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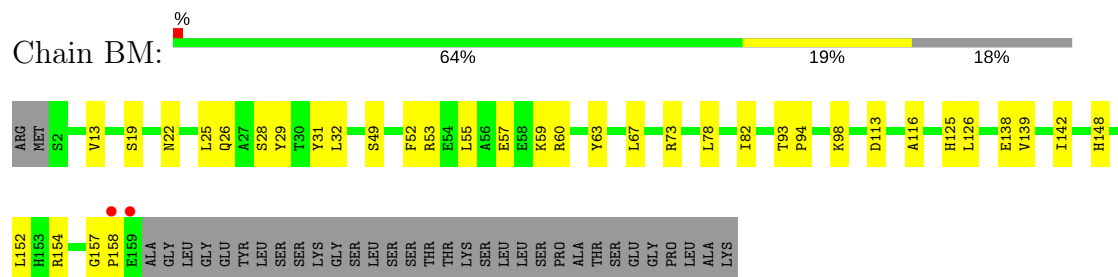
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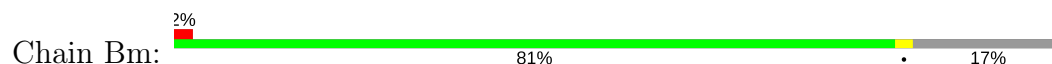
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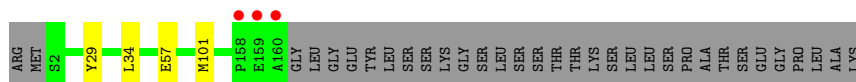


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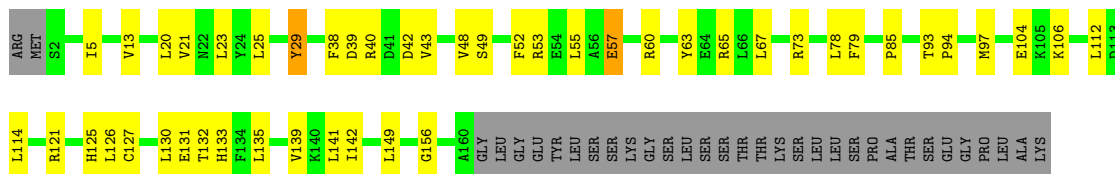


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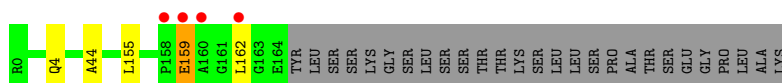
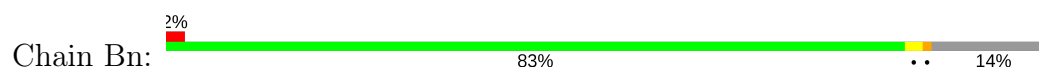




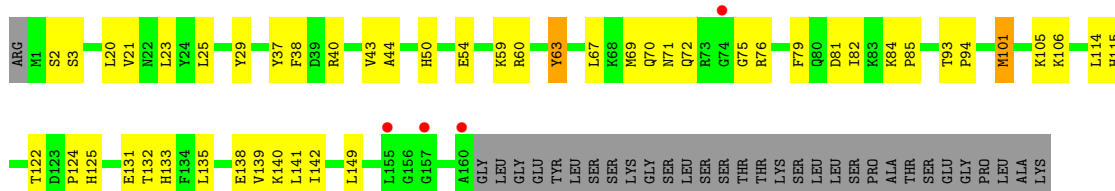
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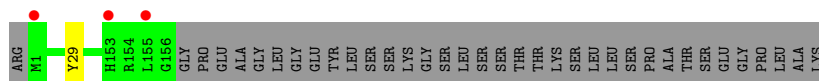
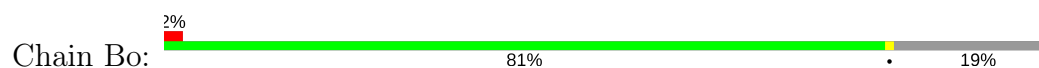
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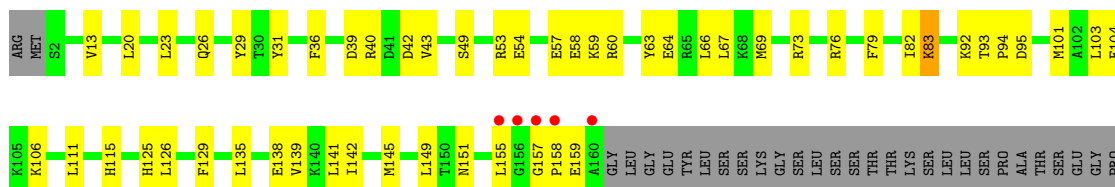
• Molecule 1: Ferritin



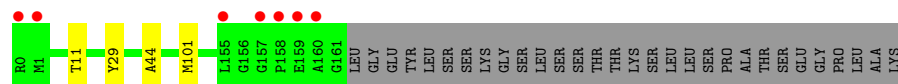
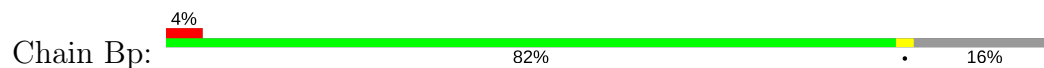
• Molecule 1: Ferritin



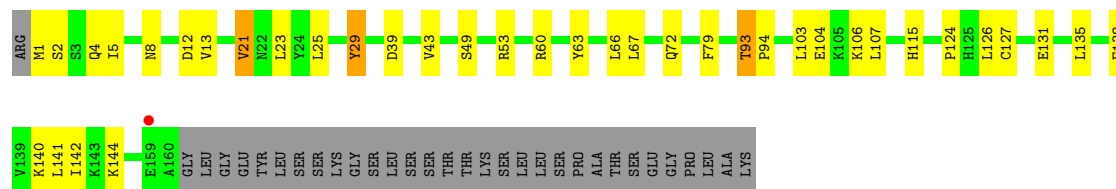
• Molecule 1: Ferritin



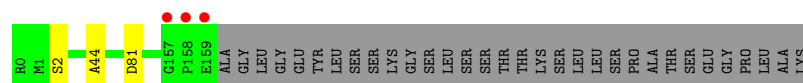
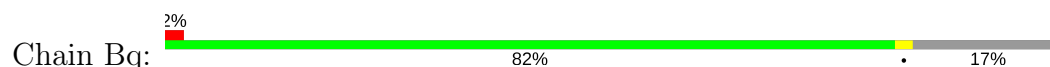
- Molecule 1: Ferritin



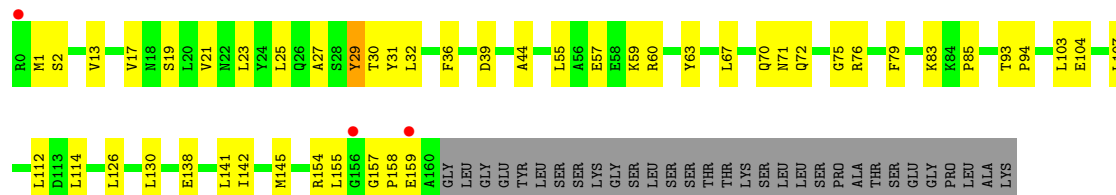
- Molecule 1: Ferritin



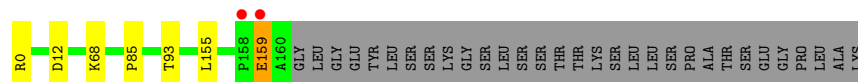
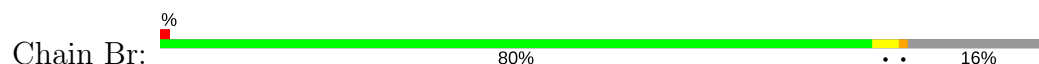
- Molecule 1: Ferritin



- Molecule 1: Ferritin



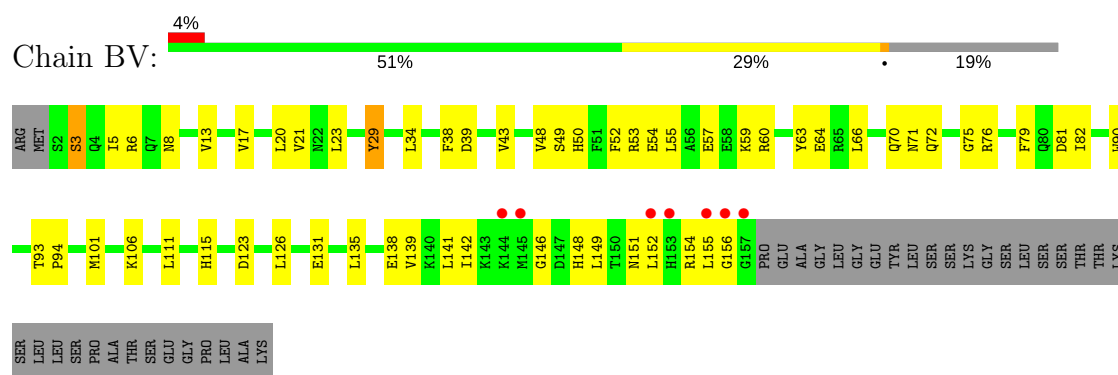
- Molecule 1: Ferritin



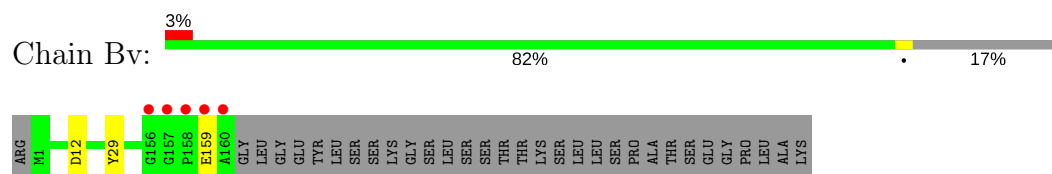
- Molecule 1: Ferritin



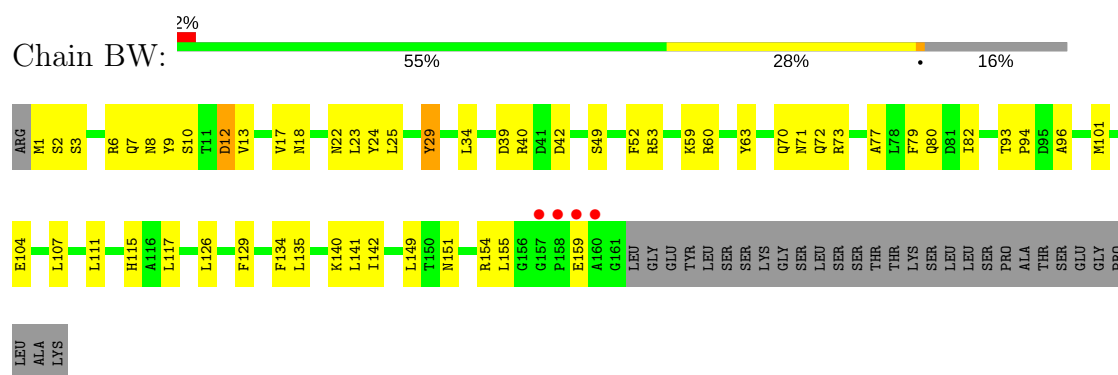




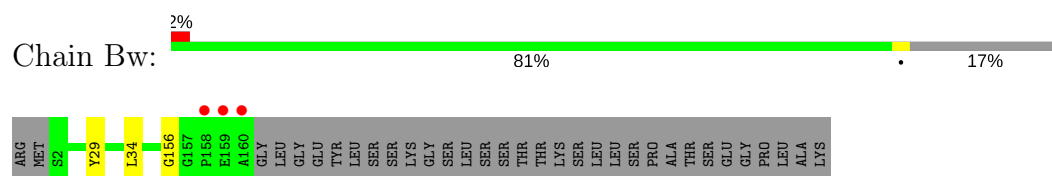
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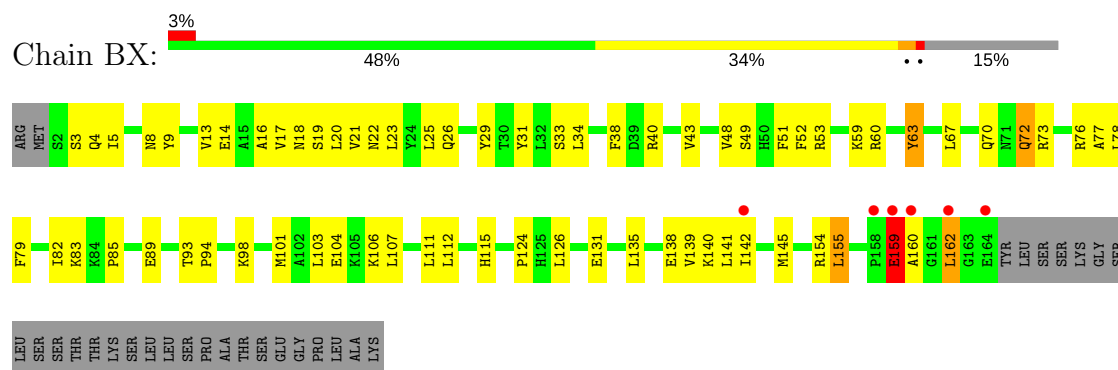
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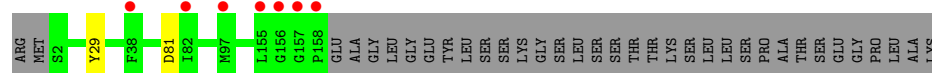
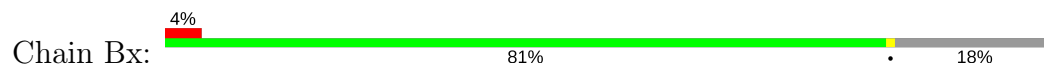
• Molecule 1: Ferritin



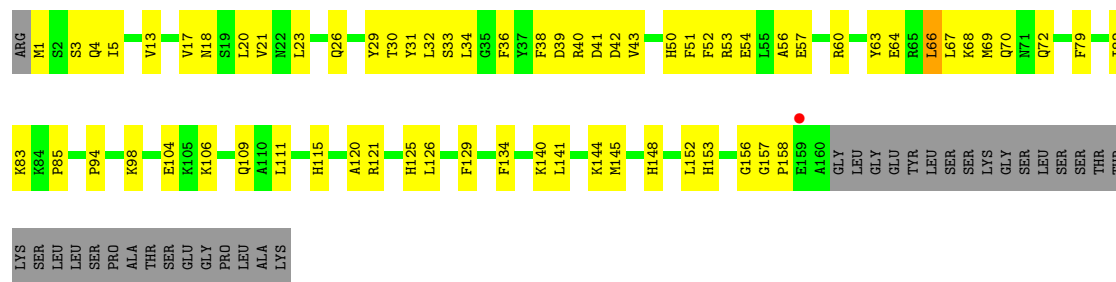
• Molecule 1: Ferritin



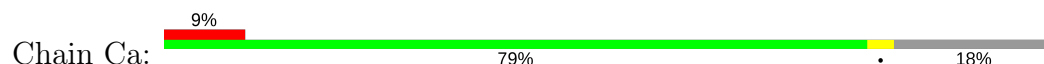
- Molecule 1: Ferritin



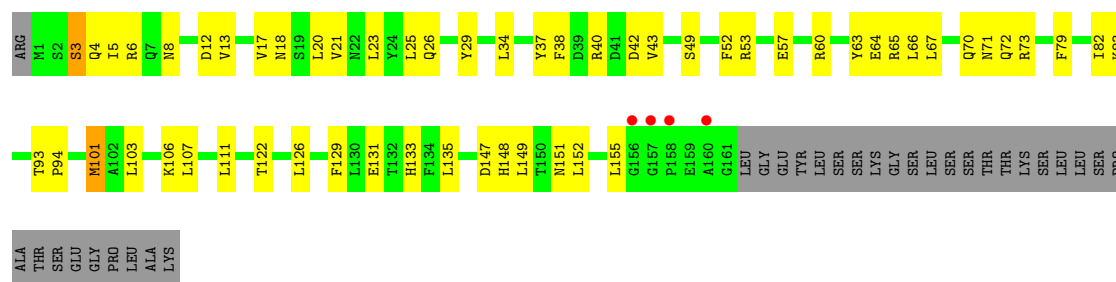
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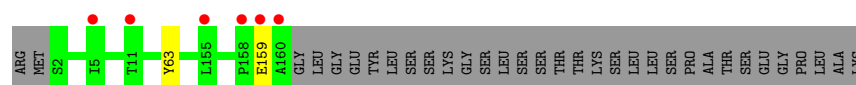
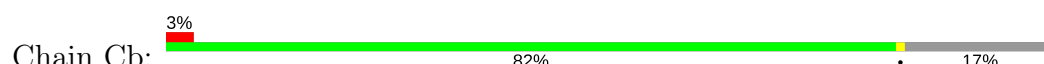
- Molecule 1: Ferritin



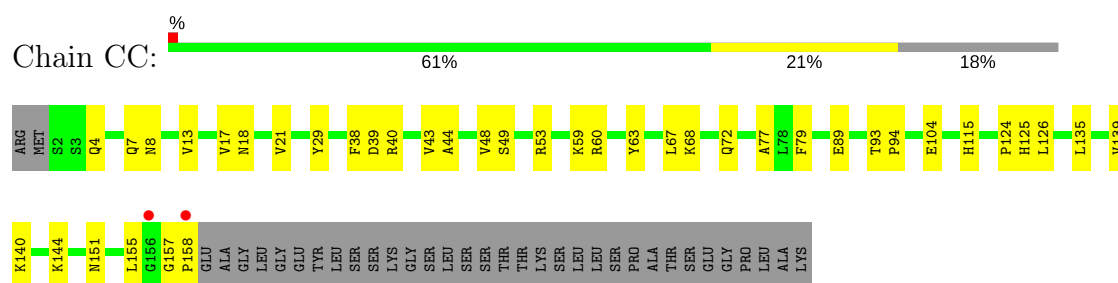
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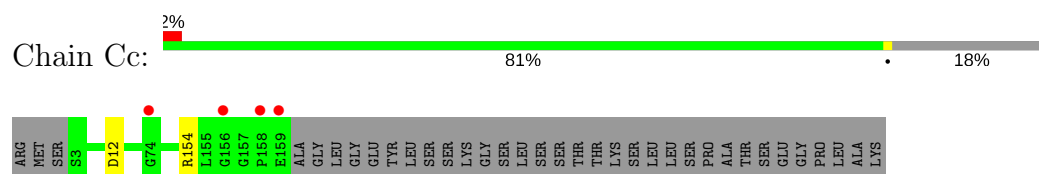
- Molecule 1: Ferritin



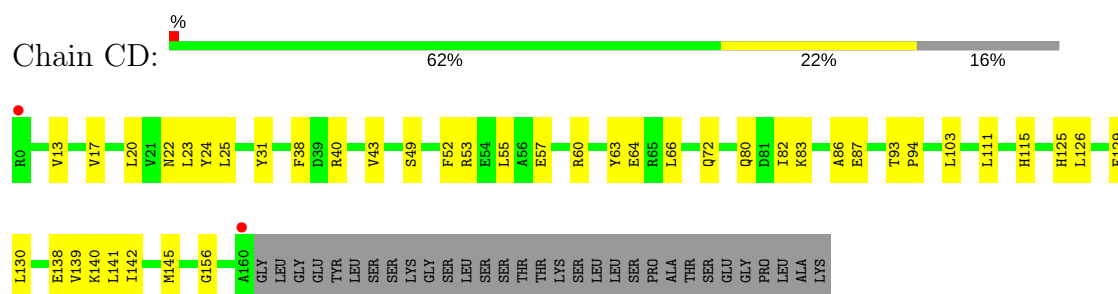
- Molecule 1: Ferritin



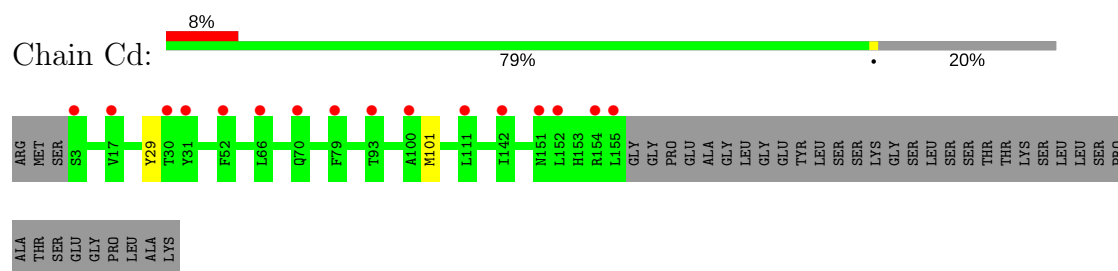
## • Molecule 1: Ferritin



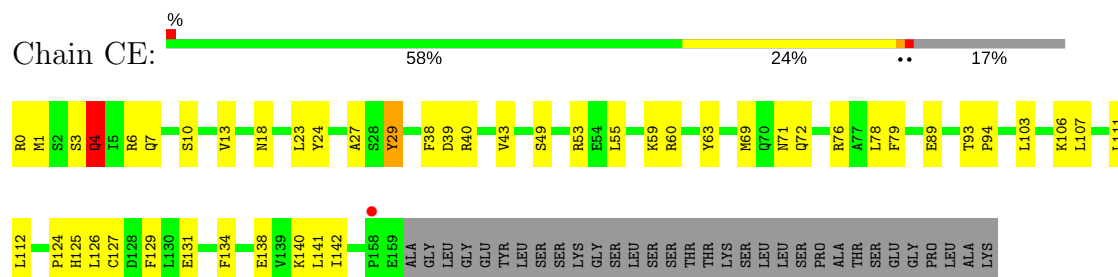
## • Molecule 1: Ferritin



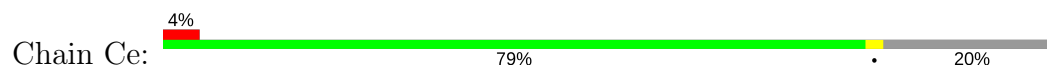
## • Molecule 1: Ferritin



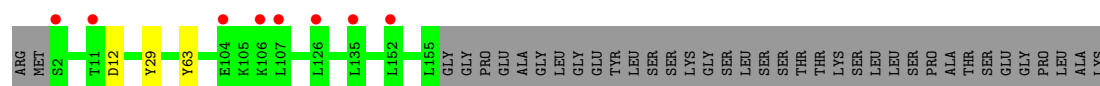
## • Molecule 1: Ferritin



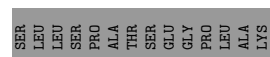
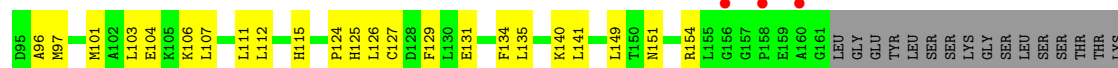
## • Molecule 1: Ferritin



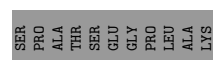
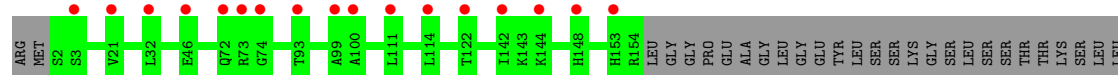
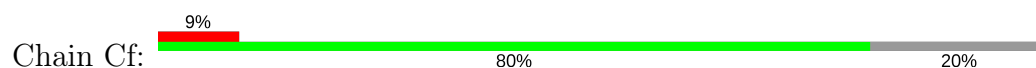




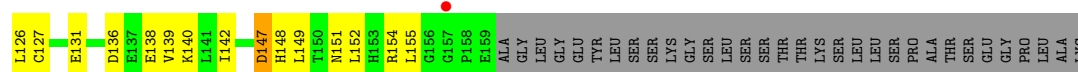
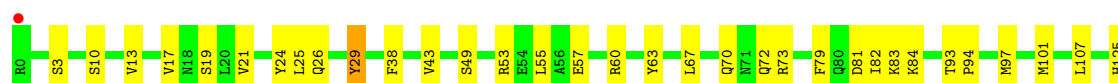
● Molecule 1: Ferritin



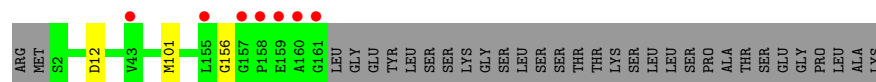
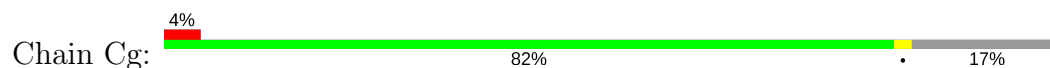
● Molecule 1: Ferritin



● Molecule 1: Ferritin



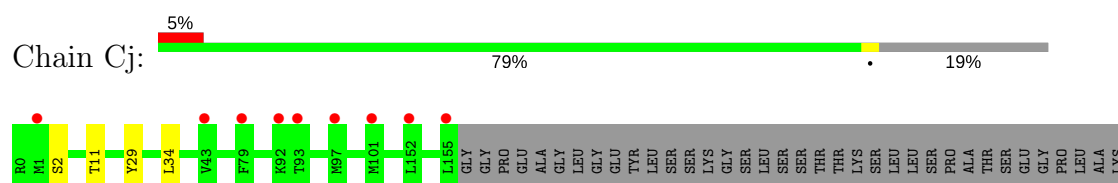
● Molecule 1: Ferritin



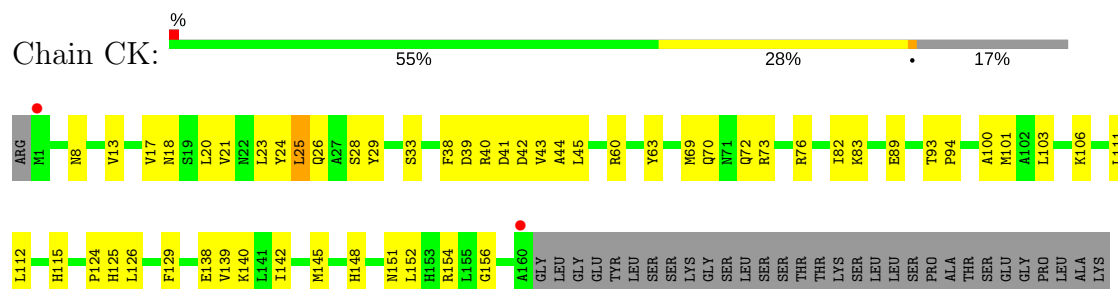
● Molecule 1: Ferritin



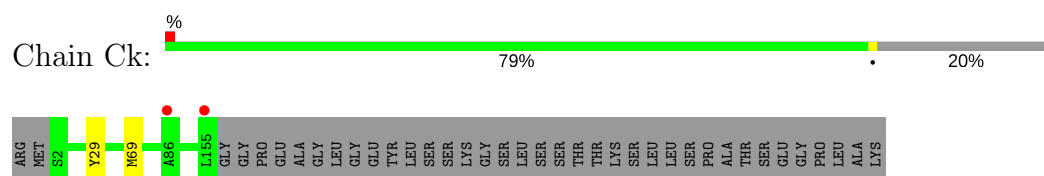




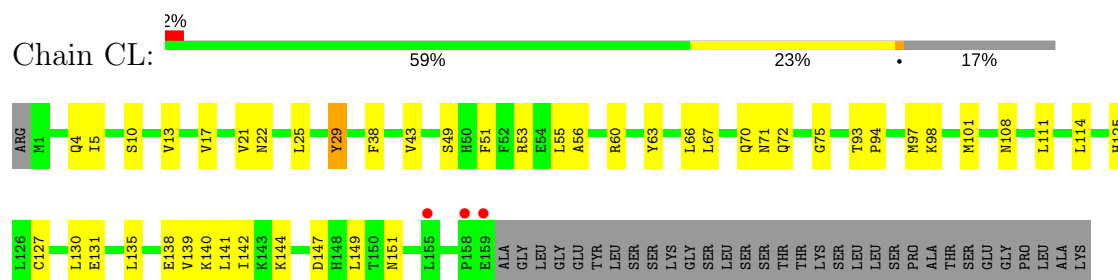
- Molecule 1: Ferritin



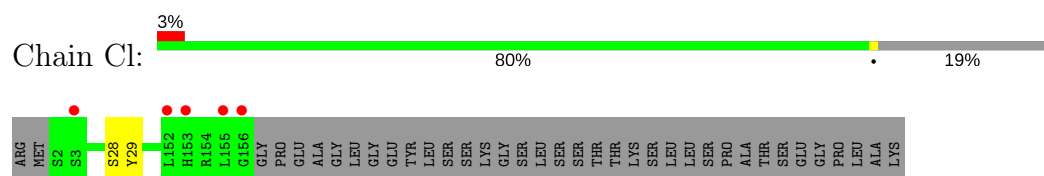
- Molecule 1: Ferritin



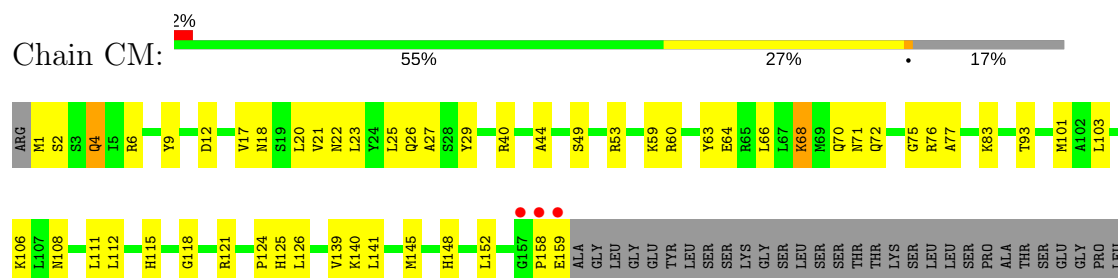
- Molecule 1: Ferritin



- Molecule 1: Ferritin

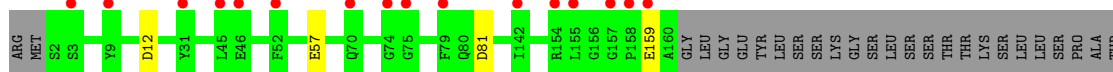
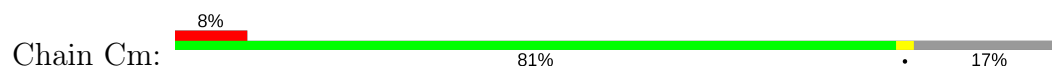


- Molecule 1: Ferritin

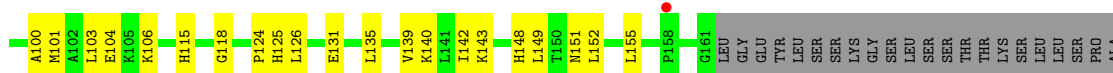


ALA  
LYS

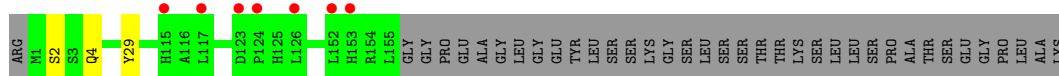
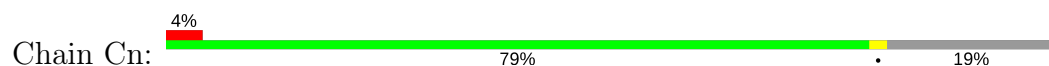
## • Molecule 1: Ferritin

SER  
GLU  
GLY  
PRO  
LEU  
ALA  
LYS

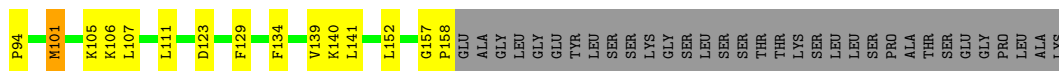
## • Molecule 1: Ferritin

THR  
SER  
GLU  
GLY  
PRO  
LEU  
ALA  
LYS

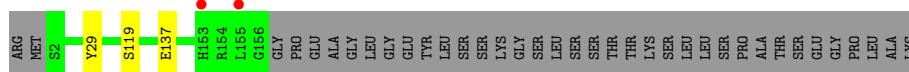
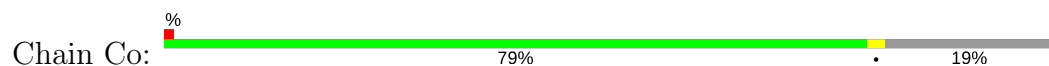
## • Molecule 1: Ferritin



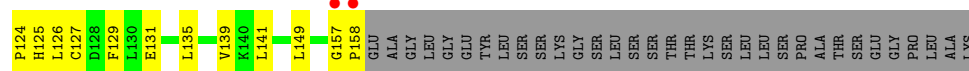
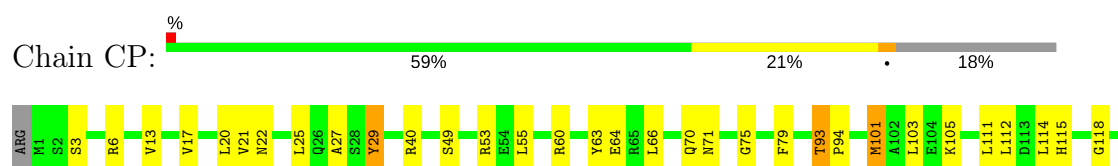
## • Molecule 1: Ferritin



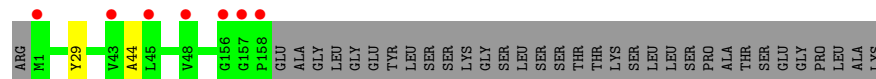
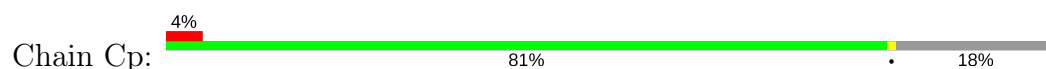
## • Molecule 1: Ferritin



## • Molecule 1: Ferritin



• Molecule 1: Ferritin

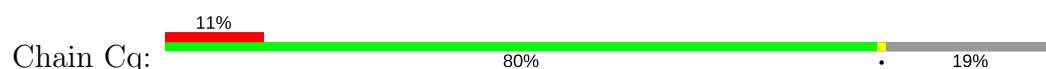


• Molecule 1: Ferritin



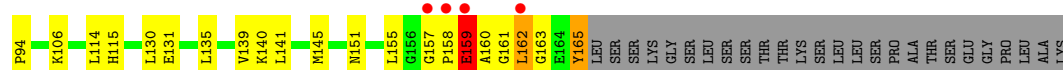
LYS

• Molecule 1: Ferritin

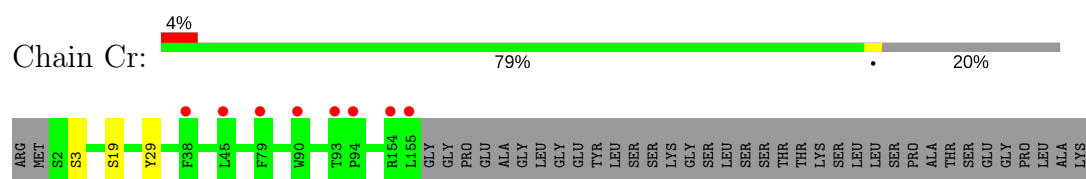


THR  
THR  
LYS  
SER  
LEU  
LEU  
SER  
PRO  
ALA  
THR  
SER  
GLY  
PRO  
LEU  
ALA  
LYS

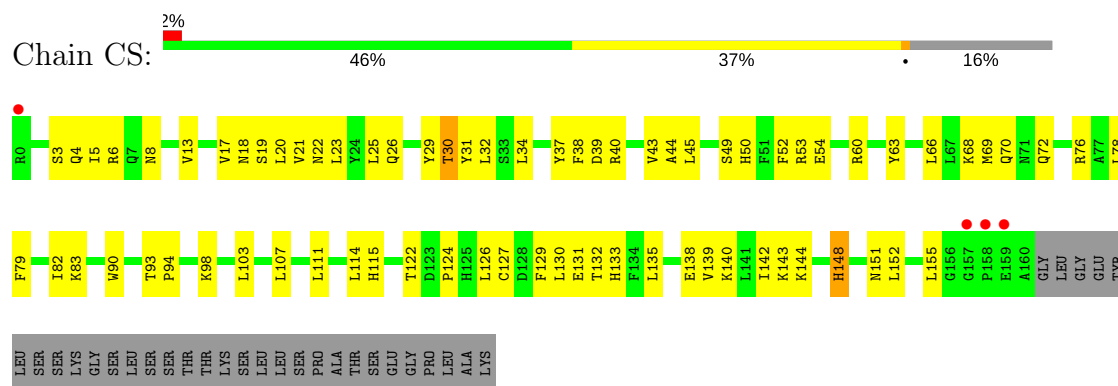
• Molecule 1: Ferritin



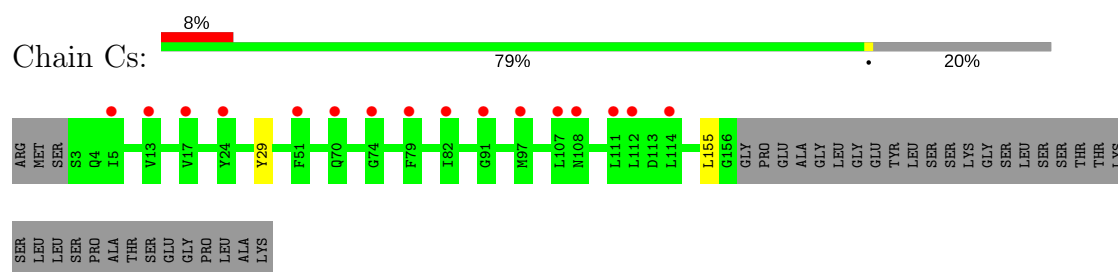
• Molecule 1: Ferritin



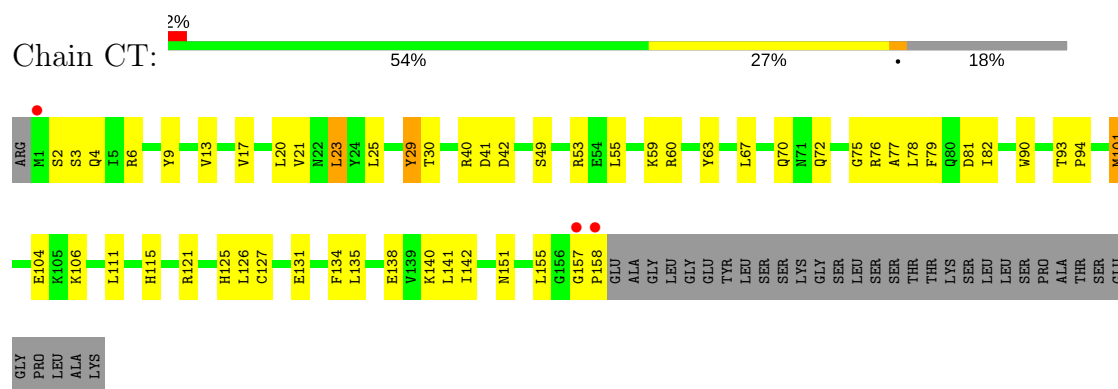
- Molecule 1: Ferritin



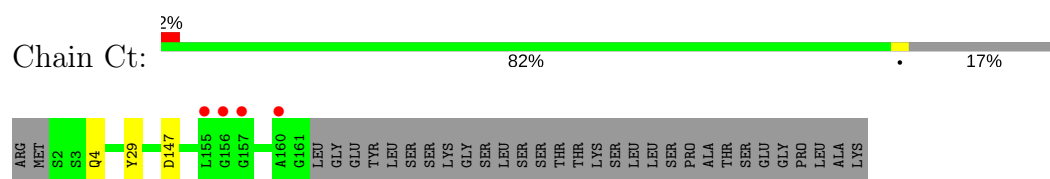
- Molecule 1: Ferritin



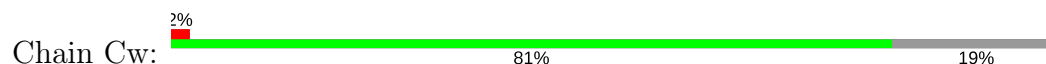
- Molecule 1: Ferritin

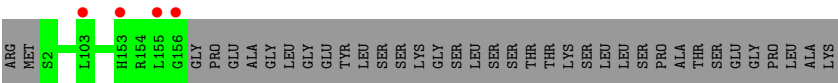


- Molecule 1: Ferritin

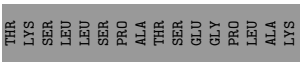
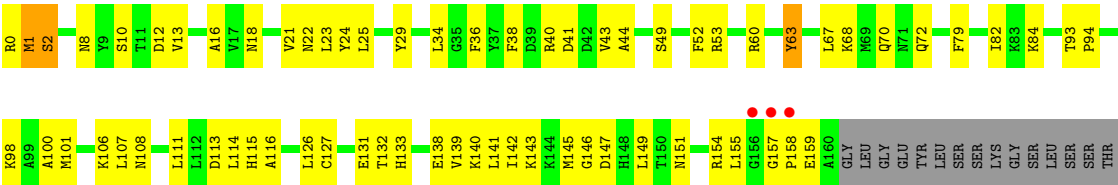


- Molecule 1: Ferritin

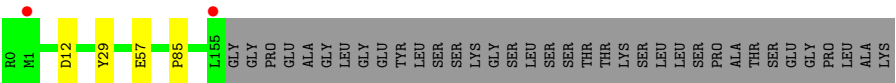
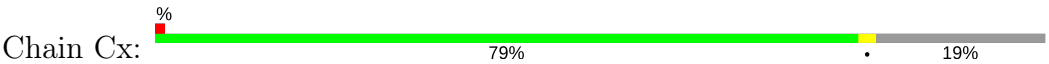




● Molecule 1: Ferritin



● Molecule 1: Ferritin





## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1   | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 212.34Å 236.94Å 249.71Å<br>94.69° 115.06° 114.96°           | Depositor        |
| Resolution (Å)  | 50.00 – 2.85<br>49.77 – 2.84                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.4 (50.00-2.85)<br>94.7 (49.77-2.84)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.08  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.80 (at 2.86Å)   | Xtriage          |
| Refinement program  | CNS   | Depositor        |
| R, $R_{free}$   | 0.249 , 0.291<br>0.224 , 0.261                              | Depositor<br>DCC |
| $R_{free}$ test set   | 42321 reflections (5.00%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 49.6  | Xtriage          |
| Anisotropy  | 0.321   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 49.4   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction   | 0.000 for h,-h-k,-h-l                                       | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 187090  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 54.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

| Mol | Chain | Bond lengths |             | Bond angles |               |
|-----|-------|--------------|-------------|-------------|---------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$   |
| 1   | AA    | 0.37         | 0/1294      | 0.54        | 0/1741        |
| 1   | AB    | 0.42         | 0/1345      | 0.63        | 0/1809        |
| 1   | AC    | 0.36         | 0/1318      | 0.56        | 0/1772        |
| 1   | AD    | 0.33         | 0/1299      | 0.52        | 0/1748        |
| 1   | AE    | 0.47         | 0/1345      | 0.64        | 0/1809        |
| 1   | AF    | 0.41         | 0/1293      | 0.56        | 0/1739        |
| 1   | AG    | 0.41         | 0/1299      | 0.61        | 0/1748        |
| 1   | AH    | 0.45         | 0/1307      | 0.60        | 0/1758        |
| 1   | AI    | 0.35         | 0/1293      | 0.55        | 0/1739        |
| 1   | AJ    | 0.38         | 0/1285      | 0.56        | 0/1727        |
| 1   | AK    | 0.39         | 0/1292      | 0.56        | 0/1736        |
| 1   | AL    | 0.32         | 0/1285      | 0.55        | 0/1729        |
| 1   | AM    | 0.44         | 0/1322      | 0.59        | 0/1777        |
| 1   | AN    | 0.43         | 0/1345      | 0.62        | 0/1809        |
| 1   | AO    | 0.43         | 0/1345      | 0.63        | 0/1809        |
| 1   | AP    | 0.51         | 0/1302      | 0.67        | 0/1751        |
| 1   | AQ    | 0.36         | 0/1343      | 0.57        | 0/1805        |
| 1   | AR    | 0.42         | 0/1332      | 0.58        | 0/1791        |
| 1   | AS    | 0.35         | 0/1303      | 0.54        | 0/1753        |
| 1   | AT    | 0.46         | 0/1294      | 0.62        | 0/1741        |
| 1   | AU    | 0.43         | 0/1307      | 0.59        | 0/1758        |
| 1   | AV    | 0.41         | 0/1303      | 0.58        | 0/1753        |
| 1   | AW    | 0.37         | 0/1294      | 0.55        | 0/1741        |
| 1   | AX    | 0.44         | 0/1307      | 0.61        | 0/1758        |
| 1   | Aa    | 0.47         | 0/1318      | 0.65        | 1/1772 (0.1%) |
| 1   | Ab    | 0.47         | 0/1311      | 0.60        | 0/1763        |
| 1   | Ac    | 0.45         | 0/1307      | 0.62        | 0/1758        |
| 1   | Ad    | 0.57         | 0/1345      | 0.70        | 1/1809 (0.1%) |
| 1   | Ae    | 0.51         | 0/1322      | 0.67        | 0/1777        |
| 1   | Af    | 0.47         | 0/1318      | 0.64        | 0/1772        |
| 1   | Ag    | 0.52         | 0/1277      | 0.63        | 0/1717        |
| 1   | Ah    | 0.51         | 0/1318      | 0.63        | 0/1772        |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 1   | Ai    | 0.54         | 0/1302        | 0.69        | 0/1751        |
| 1   | Aj    | 0.47         | 0/1345        | 0.66        | 0/1809        |
| 1   | Ak    | 0.44         | 0/1345        | 0.62        | 0/1809        |
| 1   | Al    | 0.48         | 0/1345        | 0.66        | 0/1809        |
| 1   | Am    | 0.49         | 0/1322        | 0.64        | 0/1777        |
| 1   | An    | 0.49         | 0/1311        | 0.63        | 0/1763        |
| 1   | Ao    | 0.48         | 0/1318        | 0.64        | 0/1772        |
| 1   | Ap    | 0.49         | 0/1322        | 0.65        | 0/1777        |
| 1   | Aq    | 0.49         | 0/1307        | 0.65        | 0/1758        |
| 1   | Ar    | 0.59         | 0/1345        | 0.69        | 1/1809 (0.1%) |
| 1   | As    | 0.47         | 0/1318        | 0.62        | 0/1772        |
| 1   | At    | 0.50         | 0/1307        | 0.62        | 0/1758        |
| 1   | Au    | 0.46         | 0/1307        | 0.61        | 0/1758        |
| 1   | Av    | 0.45         | 0/1343        | 0.61        | 0/1805        |
| 1   | Aw    | 0.57         | 2/1311 (0.2%) | 0.69        | 1/1763 (0.1%) |
| 1   | Ax    | 0.53         | 0/1277        | 0.63        | 0/1717        |
| 1   | BA    | 0.40         | 0/1356        | 0.60        | 0/1823        |
| 1   | BB    | 0.37         | 0/1292        | 0.60        | 1/1736 (0.1%) |
| 1   | BC    | 0.32         | 0/1273        | 0.53        | 0/1712        |
| 1   | BD    | 0.37         | 0/1313        | 0.58        | 0/1765        |
| 1   | BE    | 0.38         | 0/1302        | 0.59        | 0/1751        |
| 1   | BF    | 0.47         | 0/1299        | 0.62        | 0/1748        |
| 1   | BG    | 0.37         | 0/1281        | 0.57        | 0/1722        |
| 1   | BH    | 0.36         | 0/1269        | 0.54        | 0/1707        |
| 1   | BI    | 0.38         | 0/1277        | 0.56        | 0/1717        |
| 1   | BJ    | 0.37         | 0/1285        | 0.56        | 0/1729        |
| 1   | BK    | 0.35         | 0/1281        | 0.52        | 0/1722        |
| 1   | BL    | 0.34         | 0/1277        | 0.53        | 0/1717        |
| 1   | BM    | 0.45         | 0/1294        | 0.60        | 0/1741        |
| 1   | BN    | 0.42         | 0/1299        | 0.62        | 0/1748        |
| 1   | BO    | 0.35         | 0/1307        | 0.54        | 0/1758        |
| 1   | BP    | 0.38         | 0/1299        | 0.56        | 0/1748        |
| 1   | BQ    | 0.43         | 0/1307        | 0.59        | 0/1758        |
| 1   | BR    | 0.40         | 0/1318        | 0.57        | 0/1772        |
| 1   | BS    | 0.45         | 0/1304        | 0.59        | 0/1753        |
| 1   | BT    | 0.34         | 0/1285        | 0.57        | 0/1729        |
| 1   | BU    | 0.34         | 0/1322        | 0.53        | 0/1777        |
| 1   | BV    | 0.36         | 0/1277        | 0.57        | 0/1717        |
| 1   | BW    | 0.36         | 0/1311        | 0.55        | 0/1763        |
| 1   | BX    | 0.37         | 0/1324        | 0.59        | 0/1781        |
| 1   | Ba    | 0.33         | 0/1293        | 0.53        | 0/1739        |
| 1   | Bb    | 0.35         | 0/1302        | 0.52        | 0/1751        |
| 1   | Bc    | 0.43         | 0/1318        | 0.60        | 0/1772        |

| Mol | Chain | Bond lengths |               | Bond angles |               |
|-----|-------|--------------|---------------|-------------|---------------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5       |
| 1   | Bd    | 0.44         | 0/1318        | 0.59        | 0/1772        |
| 1   | Be    | 0.46         | 0/1324        | 0.62        | 0/1781        |
| 1   | Bf    | 0.43         | 0/1345        | 0.63        | 0/1809        |
| 1   | Bg    | 0.35         | 0/1281        | 0.53        | 0/1722        |
| 1   | Bh    | 0.39         | 0/1302        | 0.57        | 0/1751        |
| 1   | Bi    | 0.37         | 0/1292        | 0.57        | 0/1736        |
| 1   | Bj    | 0.34         | 0/1267        | 0.54        | 0/1704        |
| 1   | Bk    | 0.35         | 0/1302        | 0.54        | 0/1751        |
| 1   | Bl    | 0.43         | 0/1302        | 0.59        | 0/1751        |
| 1   | Bm    | 0.44         | 0/1299        | 0.61        | 0/1748        |
| 1   | Bn    | 0.41         | 0/1343        | 0.59        | 0/1805        |
| 1   | Bo    | 0.36         | 0/1281        | 0.57        | 0/1722        |
| 1   | Bp    | 0.42         | 0/1322        | 0.60        | 0/1777        |
| 1   | Bq    | 0.36         | 0/1313        | 0.55        | 0/1765        |
| 1   | Br    | 0.55         | 0/1318        | 0.69        | 0/1772        |
| 1   | Bs    | 0.37         | 0/1277        | 0.56        | 0/1717        |
| 1   | Bt    | 0.34         | 0/1293        | 0.55        | 0/1739        |
| 1   | Bu    | 0.48         | 0/1345        | 0.64        | 1/1809 (0.1%) |
| 1   | Bv    | 0.41         | 0/1307        | 0.56        | 0/1758        |
| 1   | Bw    | 0.51         | 0/1299        | 0.67        | 0/1748        |
| 1   | Bx    | 0.34         | 0/1285        | 0.55        | 0/1729        |
| 1   | CA    | 0.47         | 0/1307        | 0.61        | 0/1758        |
| 1   | CB    | 0.40         | 0/1311        | 0.58        | 0/1763        |
| 1   | CC    | 0.33         | 0/1285        | 0.53        | 0/1729        |
| 1   | CD    | 0.43         | 0/1318        | 0.60        | 0/1772        |
| 1   | CE    | 0.40         | 0/1313        | 0.56        | 0/1765        |
| 1   | CF    | 0.48         | 0/1303        | 0.61        | 0/1753        |
| 1   | CG    | 0.42         | 0/1313        | 0.58        | 0/1765        |
| 1   | CH    | 0.34         | 0/1302        | 0.53        | 0/1751        |
| 1   | CI    | 0.46         | 0/1307        | 0.63        | 0/1758        |
| 1   | CJ    | 0.52         | 1/1343 (0.1%) | 0.66        | 0/1805        |
| 1   | CK    | 0.36         | 0/1307        | 0.56        | 0/1758        |
| 1   | CL    | 0.35         | 0/1302        | 0.54        | 0/1751        |
| 1   | CM    | 0.46         | 0/1302        | 0.60        | 0/1751        |
| 1   | CN    | 0.45         | 0/1311        | 0.61        | 0/1763        |
| 1   | CO    | 0.36         | 0/1304        | 0.55        | 0/1753        |
| 1   | CP    | 0.38         | 0/1293        | 0.55        | 0/1739        |
| 1   | CQ    | 0.49         | 0/1322        | 0.61        | 0/1777        |
| 1   | CR    | 0.50         | 0/1356        | 0.65        | 0/1823        |
| 1   | CS    | 0.48         | 0/1318        | 0.61        | 0/1772        |
| 1   | CT    | 0.41         | 0/1293        | 0.55        | 0/1739        |
| 1   | CU    | 0.32         | 0/1302        | 0.52        | 0/1751        |
| 1   | CV    | 0.33         | 0/1294        | 0.55        | 0/1741        |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 1   | CW    | 0.37         | 0/1277          | 0.55        | 0/1717          |
| 1   | CX    | 0.43         | 0/1318          | 0.62        | 0/1772          |
| 1   | Ca    | 0.36         | 0/1293          | 0.59        | 0/1740          |
| 1   | Cb    | 0.34         | 0/1299          | 0.54        | 0/1748          |
| 1   | Cc    | 0.35         | 0/1288          | 0.55        | 0/1733          |
| 1   | Cd    | 0.34         | 0/1263          | 0.54        | 0/1699          |
| 1   | Ce    | 0.34         | 0/1269          | 0.53        | 0/1707          |
| 1   | Cf    | 0.34         | 0/1261          | 0.51        | 0/1696          |
| 1   | Cg    | 0.35         | 0/1303          | 0.53        | 0/1753          |
| 1   | Ch    | 0.39         | 0/1299          | 0.58        | 0/1748          |
| 1   | Ci    | 0.37         | 0/1263          | 0.54        | 0/1699          |
| 1   | Cj    | 0.35         | 0/1288          | 0.57        | 0/1731          |
| 1   | Ck    | 0.34         | 0/1269          | 0.54        | 0/1707          |
| 1   | Cl    | 0.35         | 0/1273          | 0.56        | 0/1712          |
| 1   | Cm    | 0.33         | 0/1299          | 0.53        | 0/1748          |
| 1   | Cn    | 0.33         | 0/1277          | 0.52        | 0/1717          |
| 1   | Co    | 0.41         | 0/1273          | 0.59        | 0/1712          |
| 1   | Cp    | 0.34         | 0/1293          | 0.55        | 0/1739          |
| 1   | Cq    | 0.36         | 0/1273          | 0.53        | 0/1712          |
| 1   | Cr    | 0.35         | 0/1269          | 0.52        | 0/1707          |
| 1   | Cs    | 0.34         | 0/1267          | 0.55        | 0/1704          |
| 1   | Ct    | 0.39         | 0/1303          | 0.58        | 0/1753          |
| 1   | Cu    | 0.36         | 0/1299          | 0.55        | 0/1748          |
| 1   | Cv    | 0.36         | 0/1311          | 0.54        | 0/1763          |
| 1   | Cw    | 0.35         | 0/1273          | 0.53        | 0/1712          |
| 1   | Cx    | 0.38         | 0/1288          | 0.58        | 0/1731          |
| All | All   | 0.41         | 3/187767 (0.0%) | 0.59        | 6/252515 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | AX    | 0                   | 1                   |
| 1   | An    | 0                   | 1                   |
| 1   | Ar    | 0                   | 1                   |
| 1   | Ax    | 0                   | 1                   |
| 1   | CR    | 0                   | 1                   |
| 1   | CX    | 0                   | 1                   |
| All | All   | 0                   | 6                   |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | Aw    | 1   | MET  | CG-SD | -8.22 | 1.59        | 1.81     |
| 1   | Aw    | 1   | MET  | SD-CE | -5.27 | 1.48        | 1.77     |
| 1   | CJ    | 159 | GLU  | CB-CG | 5.21  | 1.62        | 1.52     |

The worst 5 of 6 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | Aw    | 1   | MET  | CG-SD-CE | 7.72  | 112.55      | 100.20   |
| 1   | BB    | 0   | ARG  | N-CA-C   | 6.15  | 127.60      | 111.00   |
| 1   | Bu    | 161 | GLY  | N-CA-C   | -5.78 | 98.66       | 113.10   |
| 1   | Aa    | 107 | LEU  | CA-CB-CG | 5.20  | 127.26      | 115.30   |
| 1   | Ad    | 161 | GLY  | N-CA-C   | -5.16 | 100.19      | 113.10   |

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 1   | AX    | 63  | TYR  | Sidechain |
| 1   | An    | 31  | TYR  | Sidechain |
| 1   | Ar    | 163 | GLY  | Mainchain |
| 1   | Ax    | 37  | TYR  | Sidechain |
| 1   | CR    | 163 | GLY  | Mainchain |

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

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    | 1270  | 0        | 1243     | 31      | 0            |
| 1   | AB    | 1320  | 0        | 1292     | 48      | 0            |
| 1   | AC    | 1294  | 0        | 1273     | 34      | 0            |
| 1   | AD    | 1275  | 0        | 1248     | 50      | 0            |
| 1   | AE    | 1320  | 0        | 1292     | 70      | 0            |
| 1   | AF    | 1269  | 0        | 1249     | 56      | 0            |
| 1   | AG    | 1275  | 0        | 1248     | 46      | 0            |
| 1   | AH    | 1283  | 0        | 1260     | 48      | 0            |
| 1   | AI    | 1269  | 0        | 1249     | 39      | 0            |
| 1   | AJ    | 1262  | 0        | 1242     | 41      | 0            |
| 1   | AK    | 1269  | 0        | 1252     | 27      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AL    | 1261  | 0        | 1237     | 44      | 0            |
| 1   | AM    | 1298  | 0        | 1276     | 57      | 0            |
| 1   | AN    | 1320  | 0        | 1292     | 54      | 0            |
| 1   | AO    | 1320  | 0        | 1292     | 69      | 0            |
| 1   | AP    | 1278  | 0        | 1255     | 48      | 0            |
| 1   | AQ    | 1319  | 0        | 1296     | 52      | 0            |
| 1   | AR    | 1308  | 0        | 1283     | 48      | 0            |
| 1   | AS    | 1279  | 0        | 1251     | 34      | 0            |
| 1   | AT    | 1270  | 0        | 1243     | 65      | 0            |
| 1   | AU    | 1283  | 0        | 1260     | 44      | 0            |
| 1   | AV    | 1279  | 0        | 1251     | 36      | 0            |
| 1   | AW    | 1270  | 0        | 1243     | 49      | 0            |
| 1   | AX    | 1283  | 0        | 1260     | 56      | 0            |
| 1   | Aa    | 1294  | 0        | 1273     | 0       | 0            |
| 1   | Ab    | 1287  | 0        | 1263     | 0       | 0            |
| 1   | Ac    | 1283  | 0        | 1260     | 0       | 0            |
| 1   | Ad    | 1320  | 0        | 1292     | 0       | 0            |
| 1   | Ae    | 1298  | 0        | 1276     | 0       | 0            |
| 1   | Af    | 1294  | 0        | 1273     | 0       | 0            |
| 1   | Ag    | 1254  | 0        | 1236     | 0       | 0            |
| 1   | Ah    | 1294  | 0        | 1273     | 0       | 0            |
| 1   | Ai    | 1278  | 0        | 1255     | 0       | 0            |
| 1   | Aj    | 1320  | 0        | 1292     | 0       | 0            |
| 1   | Ak    | 1320  | 0        | 1292     | 0       | 0            |
| 1   | Al    | 1320  | 0        | 1292     | 0       | 0            |
| 1   | Am    | 1298  | 0        | 1276     | 0       | 0            |
| 1   | An    | 1287  | 0        | 1263     | 0       | 0            |
| 1   | Ao    | 1294  | 0        | 1273     | 0       | 0            |
| 1   | Ap    | 1298  | 0        | 1276     | 0       | 0            |
| 1   | Aq    | 1283  | 0        | 1260     | 0       | 0            |
| 1   | Ar    | 1320  | 0        | 1292     | 0       | 0            |
| 1   | As    | 1294  | 0        | 1273     | 0       | 0            |
| 1   | At    | 1283  | 0        | 1260     | 0       | 0            |
| 1   | Au    | 1283  | 0        | 1260     | 0       | 0            |
| 1   | Av    | 1319  | 0        | 1296     | 0       | 0            |
| 1   | Aw    | 1287  | 0        | 1263     | 0       | 0            |
| 1   | Ax    | 1254  | 0        | 1236     | 0       | 0            |
| 1   | BA    | 1331  | 0        | 1305     | 49      | 0            |
| 1   | BB    | 1269  | 0        | 1252     | 40      | 0            |
| 1   | BC    | 1250  | 0        | 1227     | 48      | 0            |
| 1   | BD    | 1289  | 0        | 1268     | 53      | 0            |
| 1   | BE    | 1278  | 0        | 1255     | 43      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | BF    | 1275  | 0        | 1248     | 39      | 0            |
| 1   | BG    | 1258  | 0        | 1239     | 49      | 0            |
| 1   | BH    | 1246  | 0        | 1224     | 47      | 0            |
| 1   | BI    | 1254  | 0        | 1236     | 45      | 0            |
| 1   | BJ    | 1261  | 0        | 1237     | 48      | 0            |
| 1   | BK    | 1258  | 0        | 1239     | 47      | 0            |
| 1   | BL    | 1254  | 0        | 1236     | 39      | 0            |
| 1   | BM    | 1270  | 0        | 1243     | 29      | 0            |
| 1   | BN    | 1275  | 0        | 1248     | 43      | 0            |
| 1   | BO    | 1283  | 0        | 1260     | 46      | 0            |
| 1   | BP    | 1275  | 0        | 1248     | 46      | 0            |
| 1   | BQ    | 1283  | 0        | 1260     | 30      | 0            |
| 1   | BR    | 1294  | 0        | 1273     | 41      | 0            |
| 1   | BS    | 1280  | 0        | 1262     | 40      | 0            |
| 1   | BT    | 1261  | 0        | 1237     | 49      | 0            |
| 1   | BU    | 1298  | 0        | 1276     | 45      | 0            |
| 1   | BV    | 1254  | 0        | 1230     | 49      | 0            |
| 1   | BW    | 1287  | 0        | 1263     | 50      | 0            |
| 1   | BX    | 1300  | 0        | 1271     | 65      | 0            |
| 1   | Ba    | 1269  | 0        | 1249     | 0       | 0            |
| 1   | Bb    | 1278  | 0        | 1255     | 0       | 0            |
| 1   | Bc    | 1294  | 0        | 1273     | 0       | 0            |
| 1   | Bd    | 1294  | 0        | 1273     | 0       | 0            |
| 1   | Be    | 1300  | 0        | 1271     | 0       | 0            |
| 1   | Bf    | 1320  | 0        | 1292     | 0       | 0            |
| 1   | Bg    | 1258  | 0        | 1239     | 0       | 0            |
| 1   | Bh    | 1278  | 0        | 1255     | 0       | 0            |
| 1   | Bi    | 1269  | 0        | 1252     | 0       | 0            |
| 1   | Bj    | 1244  | 0        | 1222     | 0       | 0            |
| 1   | Bk    | 1278  | 0        | 1255     | 0       | 0            |
| 1   | Bl    | 1278  | 0        | 1255     | 0       | 0            |
| 1   | Bm    | 1275  | 0        | 1248     | 0       | 0            |
| 1   | Bn    | 1319  | 0        | 1296     | 0       | 0            |
| 1   | Bo    | 1258  | 0        | 1239     | 0       | 0            |
| 1   | Bp    | 1298  | 0        | 1276     | 0       | 0            |
| 1   | Bq    | 1289  | 0        | 1268     | 0       | 0            |
| 1   | Br    | 1294  | 0        | 1273     | 0       | 0            |
| 1   | Bs    | 1254  | 0        | 1236     | 0       | 0            |
| 1   | Bt    | 1269  | 0        | 1249     | 0       | 0            |
| 1   | Bu    | 1320  | 0        | 1292     | 0       | 0            |
| 1   | Bv    | 1283  | 0        | 1260     | 0       | 0            |
| 1   | Bw    | 1275  | 0        | 1248     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | Bx    | 1261  | 0        | 1237     | 0       | 0            |
| 1   | CA    | 1283  | 0        | 1260     | 57      | 0            |
| 1   | CB    | 1287  | 0        | 1263     | 51      | 0            |
| 1   | CC    | 1261  | 0        | 1237     | 30      | 0            |
| 1   | CD    | 1294  | 0        | 1273     | 34      | 0            |
| 1   | CE    | 1289  | 0        | 1268     | 36      | 0            |
| 1   | CF    | 1279  | 0        | 1251     | 54      | 0            |
| 1   | CG    | 1289  | 0        | 1268     | 37      | 0            |
| 1   | CH    | 1278  | 0        | 1255     | 48      | 0            |
| 1   | CI    | 1283  | 0        | 1260     | 46      | 0            |
| 1   | CJ    | 1319  | 0        | 1296     | 77      | 0            |
| 1   | CK    | 1283  | 0        | 1260     | 40      | 0            |
| 1   | CL    | 1278  | 0        | 1255     | 41      | 0            |
| 1   | CM    | 1278  | 0        | 1255     | 41      | 0            |
| 1   | CN    | 1287  | 0        | 1263     | 45      | 0            |
| 1   | CO    | 1280  | 0        | 1262     | 40      | 0            |
| 1   | CP    | 1269  | 0        | 1249     | 32      | 0            |
| 1   | CQ    | 1298  | 0        | 1276     | 50      | 0            |
| 1   | CR    | 1331  | 0        | 1305     | 46      | 0            |
| 1   | CS    | 1294  | 0        | 1273     | 65      | 0            |
| 1   | CT    | 1269  | 0        | 1249     | 45      | 0            |
| 1   | CU    | 1278  | 0        | 1255     | 31      | 0            |
| 1   | CV    | 1270  | 0        | 1243     | 37      | 0            |
| 1   | CW    | 1254  | 0        | 1236     | 34      | 0            |
| 1   | CX    | 1294  | 0        | 1273     | 53      | 0            |
| 1   | Ca    | 1269  | 0        | 1243     | 0       | 0            |
| 1   | Cb    | 1275  | 0        | 1248     | 0       | 0            |
| 1   | Cc    | 1264  | 0        | 1238     | 0       | 0            |
| 1   | Cd    | 1240  | 0        | 1219     | 0       | 0            |
| 1   | Ce    | 1246  | 0        | 1224     | 0       | 0            |
| 1   | Cf    | 1238  | 0        | 1213     | 0       | 0            |
| 1   | Cg    | 1279  | 0        | 1251     | 0       | 0            |
| 1   | Ch    | 1275  | 0        | 1248     | 0       | 0            |
| 1   | Ci    | 1240  | 0        | 1219     | 0       | 0            |
| 1   | Cj    | 1265  | 0        | 1249     | 0       | 0            |
| 1   | Ck    | 1246  | 0        | 1224     | 0       | 0            |
| 1   | Cl    | 1250  | 0        | 1227     | 0       | 0            |
| 1   | Cm    | 1275  | 0        | 1248     | 0       | 0            |
| 1   | Cn    | 1254  | 0        | 1236     | 0       | 0            |
| 1   | Co    | 1250  | 0        | 1227     | 0       | 0            |
| 1   | Cp    | 1269  | 0        | 1249     | 0       | 0            |
| 1   | Cq    | 1250  | 0        | 1227     | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | Cr    | 1246  | 0        | 1224     | 0       | 0            |
| 1   | Cs    | 1244  | 0        | 1222     | 0       | 0            |
| 1   | Ct    | 1279  | 0        | 1251     | 0       | 0            |
| 1   | Cu    | 1275  | 0        | 1248     | 0       | 0            |
| 1   | Cv    | 1287  | 0        | 1263     | 0       | 0            |
| 1   | Cw    | 1250  | 0        | 1227     | 0       | 0            |
| 1   | Cx    | 1265  | 0        | 1249     | 0       | 0            |
| 2   | AA    | 1     | 0        | 0        | 0       | 0            |
| 2   | AB    | 1     | 0        | 0        | 0       | 0            |
| 2   | AC    | 1     | 0        | 0        | 0       | 0            |
| 2   | AF    | 1     | 0        | 0        | 0       | 0            |
| 2   | AH    | 1     | 0        | 0        | 0       | 0            |
| 2   | AL    | 1     | 0        | 0        | 0       | 0            |
| 2   | AM    | 1     | 0        | 0        | 0       | 0            |
| 2   | AO    | 1     | 0        | 0        | 0       | 0            |
| 2   | Aa    | 1     | 0        | 0        | 0       | 0            |
| 2   | Ac    | 1     | 0        | 0        | 0       | 0            |
| 2   | Ad    | 1     | 0        | 0        | 0       | 0            |
| 2   | Ae    | 1     | 0        | 0        | 0       | 0            |
| 2   | Ag    | 1     | 0        | 0        | 0       | 0            |
| 2   | Ah    | 1     | 0        | 0        | 0       | 0            |
| 2   | Aj    | 1     | 0        | 0        | 0       | 0            |
| 2   | An    | 1     | 0        | 0        | 0       | 0            |
| 2   | BA    | 1     | 0        | 0        | 0       | 0            |
| 2   | BB    | 1     | 0        | 0        | 0       | 0            |
| 2   | BC    | 1     | 0        | 0        | 0       | 0            |
| 2   | BD    | 1     | 0        | 0        | 0       | 0            |
| 2   | BG    | 1     | 0        | 0        | 0       | 0            |
| 2   | BH    | 1     | 0        | 0        | 0       | 0            |
| 2   | BN    | 1     | 0        | 0        | 0       | 0            |
| 2   | BR    | 1     | 0        | 0        | 0       | 0            |
| 2   | Ba    | 1     | 0        | 0        | 0       | 0            |
| 2   | Bb    | 1     | 0        | 0        | 0       | 0            |
| 2   | Bc    | 1     | 0        | 0        | 0       | 0            |
| 2   | Bd    | 1     | 0        | 0        | 0       | 0            |
| 2   | Be    | 1     | 0        | 0        | 0       | 0            |
| 2   | Bf    | 1     | 0        | 0        | 0       | 0            |
| 2   | Bg    | 1     | 0        | 0        | 0       | 0            |
| 2   | Bu    | 1     | 0        | 0        | 0       | 0            |
| 2   | CA    | 1     | 0        | 0        | 0       | 0            |
| 2   | CB    | 1     | 0        | 0        | 0       | 0            |
| 2   | CC    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | CD    | 1     | 0        | 0        | 0       | 0            |
| 2   | CE    | 1     | 0        | 0        | 0       | 0            |
| 2   | CF    | 1     | 0        | 0        | 0       | 0            |
| 2   | CH    | 1     | 0        | 0        | 0       | 0            |
| 2   | CO    | 1     | 0        | 0        | 0       | 0            |
| 2   | Ca    | 1     | 0        | 0        | 0       | 0            |
| 2   | Cb    | 1     | 0        | 0        | 0       | 0            |
| 2   | Ce    | 1     | 0        | 0        | 0       | 0            |
| 2   | Cg    | 1     | 0        | 0        | 0       | 0            |
| 2   | Ck    | 1     | 0        | 0        | 0       | 0            |
| 2   | Cl    | 1     | 0        | 0        | 0       | 0            |
| 2   | Cn    | 1     | 0        | 0        | 0       | 0            |
| 2   | Cp    | 1     | 0        | 0        | 0       | 0            |
| 3   | AA    | 10    | 0        | 0        | 0       | 0            |
| 3   | AB    | 14    | 0        | 0        | 0       | 0            |
| 3   | AC    | 15    | 0        | 0        | 1       | 0            |
| 3   | AD    | 8     | 0        | 0        | 1       | 0            |
| 3   | AE    | 27    | 0        | 0        | 0       | 0            |
| 3   | AF    | 16    | 0        | 0        | 0       | 0            |
| 3   | AG    | 27    | 0        | 0        | 0       | 0            |
| 3   | AH    | 28    | 0        | 0        | 1       | 0            |
| 3   | AI    | 6     | 0        | 0        | 0       | 0            |
| 3   | AJ    | 9     | 0        | 0        | 0       | 0            |
| 3   | AK    | 15    | 0        | 0        | 0       | 0            |
| 3   | AL    | 11    | 0        | 0        | 0       | 0            |
| 3   | AM    | 26    | 0        | 0        | 2       | 0            |
| 3   | AN    | 17    | 0        | 0        | 1       | 0            |
| 3   | AO    | 20    | 0        | 0        | 2       | 0            |
| 3   | AP    | 25    | 0        | 0        | 1       | 0            |
| 3   | AQ    | 21    | 0        | 0        | 0       | 0            |
| 3   | AR    | 18    | 0        | 0        | 0       | 0            |
| 3   | AS    | 20    | 0        | 0        | 1       | 0            |
| 3   | AT    | 22    | 0        | 0        | 2       | 0            |
| 3   | AU    | 20    | 0        | 0        | 1       | 0            |
| 3   | AV    | 17    | 0        | 0        | 0       | 0            |
| 3   | AW    | 19    | 0        | 0        | 2       | 0            |
| 3   | AX    | 33    | 0        | 0        | 1       | 0            |
| 3   | Aa    | 47    | 0        | 0        | 0       | 0            |
| 3   | Ab    | 30    | 0        | 0        | 0       | 0            |
| 3   | Ac    | 32    | 0        | 0        | 0       | 0            |
| 3   | Ad    | 37    | 0        | 0        | 0       | 0            |
| 3   | Ae    | 26    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | Af    | 48    | 0        | 0        | 0       | 0            |
| 3   | Ag    | 37    | 0        | 0        | 0       | 0            |
| 3   | Ah    | 28    | 0        | 0        | 0       | 0            |
| 3   | Ai    | 40    | 0        | 0        | 0       | 0            |
| 3   | Aj    | 28    | 0        | 0        | 0       | 0            |
| 3   | Ak    | 37    | 0        | 0        | 0       | 0            |
| 3   | Al    | 25    | 0        | 0        | 0       | 0            |
| 3   | Am    | 45    | 0        | 0        | 0       | 0            |
| 3   | An    | 41    | 0        | 0        | 0       | 0            |
| 3   | Ao    | 39    | 0        | 0        | 0       | 0            |
| 3   | Ap    | 32    | 0        | 0        | 0       | 0            |
| 3   | Aq    | 33    | 0        | 0        | 0       | 0            |
| 3   | Ar    | 40    | 0        | 0        | 0       | 0            |
| 3   | As    | 44    | 0        | 0        | 0       | 0            |
| 3   | At    | 31    | 0        | 0        | 0       | 0            |
| 3   | Au    | 31    | 0        | 0        | 0       | 0            |
| 3   | Av    | 19    | 0        | 0        | 0       | 0            |
| 3   | Aw    | 34    | 0        | 0        | 0       | 0            |
| 3   | Ax    | 31    | 0        | 0        | 0       | 0            |
| 3   | BA    | 15    | 0        | 0        | 0       | 0            |
| 3   | BB    | 5     | 0        | 0        | 0       | 0            |
| 3   | BC    | 2     | 0        | 0        | 0       | 0            |
| 3   | BD    | 10    | 0        | 0        | 2       | 0            |
| 3   | BE    | 15    | 0        | 0        | 0       | 0            |
| 3   | BF    | 32    | 0        | 0        | 0       | 0            |
| 3   | BG    | 7     | 0        | 0        | 0       | 0            |
| 3   | BH    | 11    | 0        | 0        | 0       | 0            |
| 3   | BI    | 20    | 0        | 0        | 0       | 0            |
| 3   | BJ    | 8     | 0        | 0        | 2       | 0            |
| 3   | BK    | 6     | 0        | 0        | 0       | 0            |
| 3   | BL    | 10    | 0        | 0        | 1       | 0            |
| 3   | BM    | 25    | 0        | 0        | 1       | 0            |
| 3   | BN    | 18    | 0        | 0        | 0       | 0            |
| 3   | BO    | 13    | 0        | 0        | 0       | 0            |
| 3   | BP    | 10    | 0        | 0        | 0       | 0            |
| 3   | BQ    | 30    | 0        | 0        | 0       | 0            |
| 3   | BR    | 21    | 0        | 0        | 0       | 0            |
| 3   | BS    | 37    | 0        | 0        | 0       | 0            |
| 3   | BT    | 12    | 0        | 0        | 2       | 0            |
| 3   | BU    | 5     | 0        | 0        | 0       | 0            |
| 3   | BV    | 5     | 0        | 0        | 0       | 0            |
| 3   | BW    | 25    | 0        | 0        | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | BX    | 3     | 0        | 0        | 0       | 0            |
| 3   | Ba    | 10    | 0        | 0        | 0       | 0            |
| 3   | Bb    | 4     | 0        | 0        | 0       | 0            |
| 3   | Bc    | 32    | 0        | 0        | 0       | 0            |
| 3   | Bd    | 27    | 0        | 0        | 0       | 0            |
| 3   | Be    | 26    | 0        | 0        | 0       | 0            |
| 3   | Bf    | 26    | 0        | 0        | 0       | 0            |
| 3   | Bg    | 7     | 0        | 0        | 0       | 0            |
| 3   | Bh    | 19    | 0        | 0        | 0       | 0            |
| 3   | Bi    | 7     | 0        | 0        | 0       | 0            |
| 3   | Bj    | 6     | 0        | 0        | 0       | 0            |
| 3   | Bk    | 6     | 0        | 0        | 0       | 0            |
| 3   | Bl    | 23    | 0        | 0        | 0       | 0            |
| 3   | Bm    | 25    | 0        | 0        | 0       | 0            |
| 3   | Bn    | 11    | 0        | 0        | 0       | 0            |
| 3   | Bo    | 9     | 0        | 0        | 0       | 0            |
| 3   | Bp    | 31    | 0        | 0        | 0       | 0            |
| 3   | Bq    | 18    | 0        | 0        | 0       | 0            |
| 3   | Br    | 35    | 0        | 0        | 0       | 0            |
| 3   | Bs    | 15    | 0        | 0        | 0       | 0            |
| 3   | Bt    | 11    | 0        | 0        | 0       | 0            |
| 3   | Bu    | 28    | 0        | 0        | 0       | 0            |
| 3   | Bv    | 25    | 0        | 0        | 0       | 0            |
| 3   | Bw    | 39    | 0        | 0        | 0       | 0            |
| 3   | Bx    | 7     | 0        | 0        | 0       | 0            |
| 3   | CA    | 29    | 0        | 0        | 0       | 0            |
| 3   | CB    | 16    | 0        | 0        | 0       | 0            |
| 3   | CC    | 7     | 0        | 0        | 0       | 0            |
| 3   | CD    | 28    | 0        | 0        | 1       | 0            |
| 3   | CE    | 15    | 0        | 0        | 0       | 0            |
| 3   | CF    | 25    | 0        | 0        | 1       | 0            |
| 3   | CG    | 19    | 0        | 0        | 0       | 0            |
| 3   | CH    | 10    | 0        | 0        | 0       | 0            |
| 3   | CI    | 30    | 0        | 0        | 1       | 0            |
| 3   | CJ    | 18    | 0        | 0        | 2       | 0            |
| 3   | CK    | 12    | 0        | 0        | 0       | 0            |
| 3   | CL    | 7     | 0        | 0        | 0       | 0            |
| 3   | CM    | 23    | 0        | 0        | 1       | 0            |
| 3   | CN    | 25    | 0        | 0        | 0       | 0            |
| 3   | CO    | 14    | 0        | 0        | 0       | 0            |
| 3   | CP    | 14    | 0        | 0        | 1       | 0            |
| 3   | CQ    | 41    | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 3   | CR    | 20     | 0        | 0        | 0       | 0            |
| 3   | CS    | 28     | 0        | 0        | 0       | 0            |
| 3   | CT    | 15     | 0        | 0        | 0       | 0            |
| 3   | CU    | 3      | 0        | 0        | 0       | 0            |
| 3   | CV    | 8      | 0        | 0        | 0       | 0            |
| 3   | CW    | 15     | 0        | 0        | 0       | 0            |
| 3   | CX    | 21     | 0        | 0        | 1       | 0            |
| 3   | Ca    | 11     | 0        | 0        | 0       | 0            |
| 3   | Cb    | 6      | 0        | 0        | 0       | 0            |
| 3   | Cc    | 7      | 0        | 0        | 0       | 0            |
| 3   | Cd    | 6      | 0        | 0        | 0       | 0            |
| 3   | Ce    | 6      | 0        | 0        | 0       | 0            |
| 3   | Cf    | 8      | 0        | 0        | 0       | 0            |
| 3   | Cg    | 16     | 0        | 0        | 0       | 0            |
| 3   | Ch    | 18     | 0        | 0        | 0       | 0            |
| 3   | Ci    | 9      | 0        | 0        | 0       | 0            |
| 3   | Cj    | 9      | 0        | 0        | 0       | 0            |
| 3   | Ck    | 11     | 0        | 0        | 0       | 0            |
| 3   | Cl    | 2      | 0        | 0        | 0       | 0            |
| 3   | Cm    | 2      | 0        | 0        | 0       | 0            |
| 3   | Cn    | 4      | 0        | 0        | 0       | 0            |
| 3   | Co    | 12     | 0        | 0        | 0       | 0            |
| 3   | Cp    | 10     | 0        | 0        | 0       | 0            |
| 3   | Cq    | 2      | 0        | 0        | 0       | 0            |
| 3   | Cr    | 4      | 0        | 0        | 0       | 0            |
| 3   | Ct    | 17     | 0        | 0        | 0       | 0            |
| 3   | Cu    | 12     | 0        | 0        | 0       | 0            |
| 3   | Cv    | 4      | 0        | 0        | 0       | 0            |
| 3   | Cw    | 10     | 0        | 0        | 0       | 0            |
| 3   | Cx    | 12     | 0        | 0        | 0       | 0            |
| All | All   | 187090 | 0        | 181001   | 2777    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2777 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:AJ:1:MET:HG3  | 1:AJ:2:SER:H      | 1.19                     | 1.02              |
| 1:AM:8:ASN:HD22 | 1:AR:112:LEU:HD13 | 2.24                     | 1.01              |
| 1:CB:8:ASN:HD22 | 1:CJ:112:LEU:HD13 | 2.31                     | 1.00              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:AE:23:LEU:HD11 | 1:AE:106:LYS:HE2 | 1.50                     | 0.94              |
| 1:BI:1:MET:HG3   | 1:BI:2:SER:H     | 1.32                     | 0.93              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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    | 156/192 (81%) | 151 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | AB    | 163/192 (85%) | 149 (91%) | 10 (6%) | 4 (2%)   | 6           | 20  |
| 1   | AC    | 159/192 (83%) | 146 (92%) | 10 (6%) | 3 (2%)   | 9           | 27  |
| 1   | AD    | 157/192 (82%) | 151 (96%) | 5 (3%)  | 1 (1%)   | 27          | 57  |
| 1   | AE    | 163/192 (85%) | 147 (90%) | 11 (7%) | 5 (3%)   | 4           | 16  |
| 1   | AF    | 156/192 (81%) | 151 (97%) | 4 (3%)  | 1 (1%)   | 27          | 57  |
| 1   | AG    | 157/192 (82%) | 150 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | AH    | 158/192 (82%) | 148 (94%) | 10 (6%) | 0        | 100         | 100 |
| 1   | AI    | 156/192 (81%) | 147 (94%) | 8 (5%)  | 1 (1%)   | 27          | 57  |
| 1   | AJ    | 155/192 (81%) | 149 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | AK    | 155/192 (81%) | 152 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | AL    | 155/192 (81%) | 147 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 1   | AM    | 160/192 (83%) | 151 (94%) | 7 (4%)  | 2 (1%)   | 13          | 37  |
| 1   | AN    | 163/192 (85%) | 154 (94%) | 7 (4%)  | 2 (1%)   | 14          | 39  |
| 1   | AO    | 163/192 (85%) | 148 (91%) | 11 (7%) | 4 (2%)   | 6           | 20  |
| 1   | AP    | 157/192 (82%) | 152 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | AQ    | 163/192 (85%) | 150 (92%) | 10 (6%) | 3 (2%)   | 9           | 29  |
| 1   | AR    | 162/192 (84%) | 152 (94%) | 8 (5%)  | 2 (1%)   | 14          | 39  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | AS    | 158/192 (82%) | 149 (94%) | 8 (5%)  | 1 (1%)   | 27          | 57  |
| 1   | AT    | 156/192 (81%) | 144 (92%) | 10 (6%) | 2 (1%)   | 13          | 37  |
| 1   | AU    | 158/192 (82%) | 152 (96%) | 5 (3%)  | 1 (1%)   | 27          | 57  |
| 1   | AV    | 158/192 (82%) | 148 (94%) | 8 (5%)  | 2 (1%)   | 13          | 37  |
| 1   | AW    | 156/192 (81%) | 150 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | AX    | 158/192 (82%) | 149 (94%) | 8 (5%)  | 1 (1%)   | 27          | 57  |
| 1   | Aa    | 159/192 (83%) | 153 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | Ab    | 159/192 (83%) | 151 (95%) | 6 (4%)  | 2 (1%)   | 13          | 37  |
| 1   | Ac    | 158/192 (82%) | 155 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | Ad    | 163/192 (85%) | 152 (93%) | 8 (5%)  | 3 (2%)   | 9           | 29  |
| 1   | Ae    | 160/192 (83%) | 157 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | Af    | 159/192 (83%) | 152 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | Ag    | 153/192 (80%) | 148 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | Ah    | 159/192 (83%) | 153 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | Ai    | 157/192 (82%) | 150 (96%) | 5 (3%)  | 2 (1%)   | 13          | 37  |
| 1   | Aj    | 163/192 (85%) | 147 (90%) | 11 (7%) | 5 (3%)   | 4           | 16  |
| 1   | Ak    | 163/192 (85%) | 153 (94%) | 8 (5%)  | 2 (1%)   | 14          | 39  |
| 1   | Al    | 163/192 (85%) | 149 (91%) | 10 (6%) | 4 (2%)   | 6           | 20  |
| 1   | Am    | 160/192 (83%) | 149 (93%) | 7 (4%)  | 4 (2%)   | 6           | 20  |
| 1   | An    | 159/192 (83%) | 149 (94%) | 8 (5%)  | 2 (1%)   | 13          | 37  |
| 1   | Ao    | 159/192 (83%) | 150 (94%) | 7 (4%)  | 2 (1%)   | 13          | 37  |
| 1   | Ap    | 160/192 (83%) | 150 (94%) | 7 (4%)  | 3 (2%)   | 9           | 27  |
| 1   | Aq    | 158/192 (82%) | 146 (92%) | 11 (7%) | 1 (1%)   | 27          | 57  |
| 1   | Ar    | 163/192 (85%) | 152 (93%) | 8 (5%)  | 3 (2%)   | 9           | 29  |
| 1   | As    | 159/192 (83%) | 153 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | At    | 158/192 (82%) | 151 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | Au    | 158/192 (82%) | 153 (97%) | 4 (2%)  | 1 (1%)   | 27          | 57  |
| 1   | Av    | 163/192 (85%) | 148 (91%) | 13 (8%) | 2 (1%)   | 14          | 39  |
| 1   | Aw    | 159/192 (83%) | 149 (94%) | 9 (6%)  | 1 (1%)   | 27          | 57  |
| 1   | Ax    | 153/192 (80%) | 150 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | BA    | 164/192 (85%) | 150 (92%) | 12 (7%) | 2 (1%)   | 14          | 39  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | BB    | 155/192 (81%) | 146 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | BC    | 153/192 (80%) | 148 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | BD    | 158/192 (82%) | 151 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | BE    | 157/192 (82%) | 150 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | BF    | 157/192 (82%) | 147 (94%) | 7 (4%)  | 3 (2%)   | 9           | 27  |
| 1   | BG    | 154/192 (80%) | 145 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | BH    | 152/192 (79%) | 146 (96%) | 5 (3%)  | 1 (1%)   | 24          | 54  |
| 1   | BI    | 153/192 (80%) | 150 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | BJ    | 155/192 (81%) | 147 (95%) | 7 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | BK    | 154/192 (80%) | 147 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | BL    | 153/192 (80%) | 149 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | BM    | 156/192 (81%) | 151 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | BN    | 157/192 (82%) | 150 (96%) | 6 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | BO    | 158/192 (82%) | 146 (92%) | 11 (7%) | 1 (1%)   | 27          | 57  |
| 1   | BP    | 157/192 (82%) | 150 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | BQ    | 158/192 (82%) | 152 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | BR    | 159/192 (83%) | 150 (94%) | 8 (5%)  | 1 (1%)   | 27          | 57  |
| 1   | BS    | 157/192 (82%) | 152 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | BT    | 155/192 (81%) | 150 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | BU    | 160/192 (83%) | 152 (95%) | 7 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | BV    | 154/192 (80%) | 149 (97%) | 3 (2%)  | 2 (1%)   | 13          | 37  |
| 1   | BW    | 159/192 (83%) | 154 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | BX    | 161/192 (84%) | 150 (93%) | 7 (4%)  | 4 (2%)   | 6           | 20  |
| 1   | Ba    | 156/192 (81%) | 149 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | Bb    | 157/192 (82%) | 148 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | Bc    | 159/192 (83%) | 147 (92%) | 12 (8%) | 0        | 100         | 100 |
| 1   | Bd    | 159/192 (83%) | 152 (96%) | 4 (2%)  | 3 (2%)   | 9           | 27  |
| 1   | Be    | 161/192 (84%) | 146 (91%) | 12 (8%) | 3 (2%)   | 9           | 27  |
| 1   | Bf    | 163/192 (85%) | 147 (90%) | 11 (7%) | 5 (3%)   | 4           | 16  |
| 1   | Bg    | 154/192 (80%) | 150 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | Bh    | 157/192 (82%) | 151 (96%) | 5 (3%)  | 1 (1%)   | 27          | 57  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | Bi    | 155/192 (81%) | 148 (96%) | 6 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | Bj    | 152/192 (79%) | 147 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | Bk    | 157/192 (82%) | 148 (94%) | 8 (5%)  | 1 (1%)   | 27          | 57  |
| 1   | Bl    | 157/192 (82%) | 150 (96%) | 6 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | Bm    | 157/192 (82%) | 151 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 1   | Bn    | 163/192 (85%) | 153 (94%) | 7 (4%)  | 3 (2%)   | 9           | 29  |
| 1   | Bo    | 154/192 (80%) | 149 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | Bp    | 160/192 (83%) | 148 (92%) | 11 (7%) | 1 (1%)   | 27          | 57  |
| 1   | Bq    | 158/192 (82%) | 150 (95%) | 6 (4%)  | 2 (1%)   | 13          | 37  |
| 1   | Br    | 159/192 (83%) | 148 (93%) | 9 (6%)  | 2 (1%)   | 13          | 37  |
| 1   | Bs    | 153/192 (80%) | 148 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | Bt    | 156/192 (81%) | 147 (94%) | 7 (4%)  | 2 (1%)   | 13          | 37  |
| 1   | Bu    | 163/192 (85%) | 152 (93%) | 9 (6%)  | 2 (1%)   | 14          | 39  |
| 1   | Bv    | 158/192 (82%) | 149 (94%) | 8 (5%)  | 1 (1%)   | 27          | 57  |
| 1   | Bw    | 157/192 (82%) | 150 (96%) | 6 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | Bx    | 155/192 (81%) | 147 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 1   | CA    | 158/192 (82%) | 153 (97%) | 4 (2%)  | 1 (1%)   | 27          | 57  |
| 1   | CB    | 159/192 (83%) | 154 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | CC    | 155/192 (81%) | 149 (96%) | 5 (3%)  | 1 (1%)   | 27          | 57  |
| 1   | CD    | 159/192 (83%) | 152 (96%) | 6 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | CE    | 158/192 (82%) | 149 (94%) | 7 (4%)  | 2 (1%)   | 13          | 37  |
| 1   | CF    | 158/192 (82%) | 150 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 1   | CG    | 158/192 (82%) | 153 (97%) | 4 (2%)  | 1 (1%)   | 27          | 57  |
| 1   | CH    | 157/192 (82%) | 146 (93%) | 10 (6%) | 1 (1%)   | 27          | 57  |
| 1   | CI    | 158/192 (82%) | 147 (93%) | 10 (6%) | 1 (1%)   | 27          | 57  |
| 1   | CJ    | 163/192 (85%) | 153 (94%) | 8 (5%)  | 2 (1%)   | 14          | 39  |
| 1   | CK    | 158/192 (82%) | 152 (96%) | 5 (3%)  | 1 (1%)   | 27          | 57  |
| 1   | CL    | 157/192 (82%) | 150 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | CM    | 157/192 (82%) | 148 (94%) | 7 (4%)  | 2 (1%)   | 13          | 37  |
| 1   | CN    | 159/192 (83%) | 152 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | CO    | 157/192 (82%) | 146 (93%) | 11 (7%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | CP    | 156/192 (81%) | 152 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | CQ    | 160/192 (83%) | 150 (94%) | 10 (6%) | 0        | 100         | 100 |
| 1   | CR    | 164/192 (85%) | 150 (92%) | 11 (7%) | 3 (2%)   | 9           | 29  |
| 1   | CS    | 159/192 (83%) | 150 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | CT    | 156/192 (81%) | 147 (94%) | 8 (5%)  | 1 (1%)   | 27          | 57  |
| 1   | CU    | 157/192 (82%) | 152 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | CV    | 156/192 (81%) | 149 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | CW    | 153/192 (80%) | 151 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | CX    | 159/192 (83%) | 147 (92%) | 10 (6%) | 2 (1%)   | 13          | 37  |
| 1   | Ca    | 156/192 (81%) | 148 (95%) | 5 (3%)  | 3 (2%)   | 9           | 27  |
| 1   | Cb    | 157/192 (82%) | 148 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | Cc    | 155/192 (81%) | 148 (96%) | 7 (4%)  | 0        | 100         | 100 |
| 1   | Cd    | 151/192 (79%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | Ce    | 152/192 (79%) | 148 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | Cf    | 151/192 (79%) | 146 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | Cg    | 158/192 (82%) | 150 (95%) | 7 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | Ch    | 157/192 (82%) | 149 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 1   | Ci    | 151/192 (79%) | 147 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | Cj    | 154/192 (80%) | 146 (95%) | 7 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | Ck    | 152/192 (79%) | 147 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 1   | Cl    | 153/192 (80%) | 150 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 1   | Cm    | 157/192 (82%) | 148 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 1   | Cn    | 153/192 (80%) | 149 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 1   | Co    | 153/192 (80%) | 151 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 1   | Cp    | 156/192 (81%) | 149 (96%) | 6 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | Cq    | 153/192 (80%) | 146 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 1   | Cr    | 152/192 (79%) | 147 (97%) | 4 (3%)  | 1 (1%)   | 24          | 54  |
| 1   | Cs    | 152/192 (79%) | 147 (97%) | 4 (3%)  | 1 (1%)   | 24          | 54  |
| 1   | Ct    | 158/192 (82%) | 154 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 1   | Cu    | 157/192 (82%) | 149 (95%) | 7 (4%)  | 1 (1%)   | 27          | 57  |
| 1   | Cv    | 159/192 (83%) | 151 (95%) | 8 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | Cw    | 153/192 (80%)     | 149 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 1   | Cx    | 154/192 (80%)     | 151 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| All | All   | 22658/27648 (82%) | 21530 (95%) | 982 (4%) | 146 (1%) | 27          | 57  |

5 of 146 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AE    | 162 | LEU  |
| 1   | AO    | 4   | GLN  |
| 1   | Aq    | 2   | SER  |
| 1   | Au    | 2   | SER  |
| 1   | Bi    | 2   | SER  |

### 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    | 134/161 (83%) | 128 (96%) | 6 (4%)   | 30          | 61 |
| 1   | AB    | 138/161 (86%) | 133 (96%) | 5 (4%)   | 38          | 70 |
| 1   | AC    | 136/161 (84%) | 132 (97%) | 4 (3%)   | 45          | 76 |
| 1   | AD    | 134/161 (83%) | 133 (99%) | 1 (1%)   | 85          | 95 |
| 1   | AE    | 138/161 (86%) | 136 (99%) | 2 (1%)   | 69          | 88 |
| 1   | AF    | 134/161 (83%) | 131 (98%) | 3 (2%)   | 55          | 81 |
| 1   | AG    | 134/161 (83%) | 131 (98%) | 3 (2%)   | 55          | 81 |
| 1   | AH    | 135/161 (84%) | 131 (97%) | 4 (3%)   | 44          | 75 |
| 1   | AI    | 134/161 (83%) | 131 (98%) | 3 (2%)   | 55          | 81 |
| 1   | AJ    | 133/161 (83%) | 132 (99%) | 1 (1%)   | 83          | 94 |
| 1   | AK    | 134/161 (83%) | 132 (98%) | 2 (2%)   | 67          | 87 |
| 1   | AL    | 133/161 (83%) | 130 (98%) | 3 (2%)   | 53          | 81 |
| 1   | AM    | 136/161 (84%) | 133 (98%) | 3 (2%)   | 55          | 81 |
| 1   | AN    | 138/161 (86%) | 135 (98%) | 3 (2%)   | 55          | 81 |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1   | AO    | 138/161 (86%) | 127 (92%) | 11 (8%)  | 13          | 34 |
| 1   | AP    | 135/161 (84%) | 128 (95%) | 7 (5%)   | 25          | 55 |
| 1   | AQ    | 138/161 (86%) | 136 (99%) | 2 (1%)   | 69          | 88 |
| 1   | AR    | 137/161 (85%) | 135 (98%) | 2 (2%)   | 67          | 87 |
| 1   | AS    | 134/161 (83%) | 130 (97%) | 4 (3%)   | 44          | 75 |
| 1   | AT    | 134/161 (83%) | 132 (98%) | 2 (2%)   | 67          | 87 |
| 1   | AU    | 135/161 (84%) | 131 (97%) | 4 (3%)   | 44          | 75 |
| 1   | AV    | 134/161 (83%) | 133 (99%) | 1 (1%)   | 85          | 95 |
| 1   | AW    | 134/161 (83%) | 133 (99%) | 1 (1%)   | 85          | 95 |
| 1   | AX    | 135/161 (84%) | 134 (99%) | 1 (1%)   | 85          | 95 |
| 1   | Aa    | 136/161 (84%) | 133 (98%) | 3 (2%)   | 55          | 81 |
| 1   | Ab    | 135/161 (84%) | 130 (96%) | 5 (4%)   | 37          | 69 |
| 1   | Ac    | 135/161 (84%) | 132 (98%) | 3 (2%)   | 55          | 81 |
| 1   | Ad    | 138/161 (86%) | 131 (95%) | 7 (5%)   | 26          | 56 |
| 1   | Ae    | 136/161 (84%) | 132 (97%) | 4 (3%)   | 45          | 76 |
| 1   | Af    | 136/161 (84%) | 133 (98%) | 3 (2%)   | 55          | 81 |
| 1   | Ag    | 133/161 (83%) | 129 (97%) | 4 (3%)   | 44          | 75 |
| 1   | Ah    | 136/161 (84%) | 133 (98%) | 3 (2%)   | 55          | 81 |
| 1   | Ai    | 135/161 (84%) | 132 (98%) | 3 (2%)   | 55          | 81 |
| 1   | Aj    | 138/161 (86%) | 132 (96%) | 6 (4%)   | 32          | 63 |
| 1   | Ak    | 138/161 (86%) | 133 (96%) | 5 (4%)   | 38          | 70 |
| 1   | Al    | 138/161 (86%) | 131 (95%) | 7 (5%)   | 26          | 56 |
| 1   | Am    | 136/161 (84%) | 135 (99%) | 1 (1%)   | 85          | 95 |
| 1   | An    | 135/161 (84%) | 133 (98%) | 2 (2%)   | 67          | 87 |
| 1   | Ao    | 136/161 (84%) | 134 (98%) | 2 (2%)   | 67          | 87 |
| 1   | Ap    | 136/161 (84%) | 134 (98%) | 2 (2%)   | 67          | 87 |
| 1   | Aq    | 135/161 (84%) | 132 (98%) | 3 (2%)   | 55          | 81 |
| 1   | Ar    | 138/161 (86%) | 133 (96%) | 5 (4%)   | 38          | 70 |
| 1   | As    | 136/161 (84%) | 130 (96%) | 6 (4%)   | 31          | 62 |
| 1   | At    | 135/161 (84%) | 128 (95%) | 7 (5%)   | 25          | 55 |
| 1   | Au    | 135/161 (84%) | 130 (96%) | 5 (4%)   | 37          | 69 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | Av    | 138/161 (86%) | 135 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Aw    | 135/161 (84%) | 128 (95%)  | 7 (5%)   | 25          | 55  |
| 1   | Ax    | 133/161 (83%) | 132 (99%)  | 1 (1%)   | 83          | 94  |
| 1   | BA    | 139/161 (86%) | 134 (96%)  | 5 (4%)   | 38          | 70  |
| 1   | BB    | 134/161 (83%) | 132 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | BC    | 132/161 (82%) | 130 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | BD    | 136/161 (84%) | 135 (99%)  | 1 (1%)   | 85          | 95  |
| 1   | BE    | 135/161 (84%) | 135 (100%) | 0        | 100         | 100 |
| 1   | BF    | 134/161 (83%) | 132 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | BG    | 133/161 (83%) | 131 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | BH    | 132/161 (82%) | 129 (98%)  | 3 (2%)   | 53          | 81  |
| 1   | BI    | 133/161 (83%) | 132 (99%)  | 1 (1%)   | 83          | 94  |
| 1   | BJ    | 133/161 (83%) | 130 (98%)  | 3 (2%)   | 53          | 81  |
| 1   | BK    | 133/161 (83%) | 128 (96%)  | 5 (4%)   | 36          | 68  |
| 1   | BL    | 133/161 (83%) | 132 (99%)  | 1 (1%)   | 83          | 94  |
| 1   | BM    | 134/161 (83%) | 132 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | BN    | 134/161 (83%) | 132 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | BO    | 135/161 (84%) | 132 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | BP    | 134/161 (83%) | 131 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | BQ    | 135/161 (84%) | 130 (96%)  | 5 (4%)   | 37          | 69  |
| 1   | BR    | 136/161 (84%) | 134 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | BS    | 135/161 (84%) | 134 (99%)  | 1 (1%)   | 85          | 95  |
| 1   | BT    | 133/161 (83%) | 131 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | BU    | 136/161 (84%) | 135 (99%)  | 1 (1%)   | 85          | 95  |
| 1   | BV    | 132/161 (82%) | 130 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | BW    | 135/161 (84%) | 133 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | BX    | 136/161 (84%) | 133 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Ba    | 134/161 (83%) | 131 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Bb    | 135/161 (84%) | 132 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Bc    | 136/161 (84%) | 130 (96%)  | 6 (4%)   | 31          | 62  |
| 1   | Bd    | 136/161 (84%) | 136 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | Be    | 136/161 (84%) | 133 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Bf    | 138/161 (86%) | 132 (96%)  | 6 (4%)   | 32          | 63  |
| 1   | Bg    | 133/161 (83%) | 131 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Bh    | 135/161 (84%) | 132 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Bi    | 134/161 (83%) | 132 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Bj    | 131/161 (81%) | 128 (98%)  | 3 (2%)   | 53          | 81  |
| 1   | Bk    | 135/161 (84%) | 132 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Bl    | 135/161 (84%) | 131 (97%)  | 4 (3%)   | 44          | 75  |
| 1   | Bm    | 134/161 (83%) | 130 (97%)  | 4 (3%)   | 44          | 75  |
| 1   | Bn    | 138/161 (86%) | 135 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Bo    | 133/161 (83%) | 132 (99%)  | 1 (1%)   | 83          | 94  |
| 1   | Bp    | 136/161 (84%) | 133 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Bq    | 136/161 (84%) | 135 (99%)  | 1 (1%)   | 85          | 95  |
| 1   | Br    | 136/161 (84%) | 130 (96%)  | 6 (4%)   | 31          | 62  |
| 1   | Bs    | 133/161 (83%) | 131 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Bt    | 134/161 (83%) | 130 (97%)  | 4 (3%)   | 44          | 75  |
| 1   | Bu    | 138/161 (86%) | 133 (96%)  | 5 (4%)   | 38          | 70  |
| 1   | Bv    | 135/161 (84%) | 133 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Bw    | 134/161 (83%) | 132 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Bx    | 133/161 (83%) | 131 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | CA    | 135/161 (84%) | 131 (97%)  | 4 (3%)   | 44          | 75  |
| 1   | CB    | 135/161 (84%) | 130 (96%)  | 5 (4%)   | 37          | 69  |
| 1   | CC    | 133/161 (83%) | 131 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | CD    | 136/161 (84%) | 136 (100%) | 0        | 100         | 100 |
| 1   | CE    | 136/161 (84%) | 134 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | CF    | 134/161 (83%) | 130 (97%)  | 4 (3%)   | 44          | 75  |
| 1   | CG    | 136/161 (84%) | 131 (96%)  | 5 (4%)   | 37          | 69  |
| 1   | CH    | 135/161 (84%) | 132 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | CI    | 135/161 (84%) | 130 (96%)  | 5 (4%)   | 37          | 69  |
| 1   | CJ    | 138/161 (86%) | 133 (96%)  | 5 (4%)   | 38          | 70  |
| 1   | CK    | 135/161 (84%) | 131 (97%)  | 4 (3%)   | 44          | 75  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | CL    | 135/161 (84%) | 133 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | CM    | 135/161 (84%) | 130 (96%)  | 5 (4%)   | 37          | 69  |
| 1   | CN    | 135/161 (84%) | 133 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | CO    | 135/161 (84%) | 133 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | CP    | 134/161 (83%) | 131 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | CQ    | 136/161 (84%) | 129 (95%)  | 7 (5%)   | 26          | 56  |
| 1   | CR    | 139/161 (86%) | 136 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | CS    | 136/161 (84%) | 131 (96%)  | 5 (4%)   | 37          | 69  |
| 1   | CT    | 134/161 (83%) | 130 (97%)  | 4 (3%)   | 44          | 75  |
| 1   | CU    | 135/161 (84%) | 135 (100%) | 0        | 100         | 100 |
| 1   | CV    | 134/161 (83%) | 132 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | CW    | 133/161 (83%) | 132 (99%)  | 1 (1%)   | 83          | 94  |
| 1   | CX    | 136/161 (84%) | 134 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Ca    | 133/161 (83%) | 130 (98%)  | 3 (2%)   | 53          | 81  |
| 1   | Cb    | 134/161 (83%) | 132 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Cc    | 133/161 (83%) | 131 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Cd    | 131/161 (81%) | 129 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Ce    | 132/161 (82%) | 129 (98%)  | 3 (2%)   | 53          | 81  |
| 1   | Cf    | 131/161 (81%) | 131 (100%) | 0        | 100         | 100 |
| 1   | Cg    | 134/161 (83%) | 132 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Ch    | 134/161 (83%) | 131 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Ci    | 131/161 (81%) | 131 (100%) | 0        | 100         | 100 |
| 1   | Cj    | 134/161 (83%) | 131 (98%)  | 3 (2%)   | 55          | 81  |
| 1   | Ck    | 132/161 (82%) | 130 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Cl    | 132/161 (82%) | 130 (98%)  | 2 (2%)   | 67          | 87  |
| 1   | Cm    | 134/161 (83%) | 130 (97%)  | 4 (3%)   | 44          | 75  |
| 1   | Cn    | 133/161 (83%) | 130 (98%)  | 3 (2%)   | 53          | 81  |
| 1   | Co    | 132/161 (82%) | 129 (98%)  | 3 (2%)   | 53          | 81  |
| 1   | Cp    | 134/161 (83%) | 133 (99%)  | 1 (1%)   | 85          | 95  |
| 1   | Cq    | 132/161 (82%) | 131 (99%)  | 1 (1%)   | 83          | 94  |
| 1   | Cr    | 132/161 (82%) | 130 (98%)  | 2 (2%)   | 67          | 87  |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 1   | Cs    | 131/161 (81%)     | 130 (99%)   | 1 (1%)   | 83          | 94  |
| 1   | Ct    | 134/161 (83%)     | 131 (98%)   | 3 (2%)   | 55          | 81  |
| 1   | Cu    | 134/161 (83%)     | 131 (98%)   | 3 (2%)   | 55          | 81  |
| 1   | Cv    | 135/161 (84%)     | 132 (98%)   | 3 (2%)   | 55          | 81  |
| 1   | Cw    | 132/161 (82%)     | 132 (100%)  | 0        | 100         | 100 |
| 1   | Cx    | 134/161 (83%)     | 130 (97%)   | 4 (3%)   | 44          | 75  |
| All | All   | 19400/23184 (84%) | 18968 (98%) | 432 (2%) | 55          | 81  |

5 of 432 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | Bc    | 154 | ARG  |
| 1   | BM    | 26  | GLN  |
| 1   | CR    | 63  | TYR  |
| 1   | BF    | 101 | MET  |
| 1   | Bi    | 29  | TYR  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 253 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | BM    | 8   | ASN  |
| 1   | Bv    | 72  | GLN  |
| 1   | Cs    | 72  | GLN  |
| 1   | Bo    | 50  | HIS  |
| 1   | Bs    | 26  | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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    | 158/192 (82%) | -0.35  | 5 (3%) 47 42  | 31, 61, 82, 117       | 0     |
| 1   | AB    | 165/192 (85%) | -0.24  | 8 (4%) 30 26  | 26, 54, 95, 109       | 0     |
| 1   | AC    | 161/192 (83%) | -0.32  | 4 (2%) 57 54  | 38, 58, 77, 111       | 0     |
| 1   | AD    | 159/192 (82%) | -0.24  | 4 (2%) 57 54  | 51, 68, 82, 118       | 0     |
| 1   | AE    | 165/192 (85%) | -0.40  | 9 (5%) 25 20  | 12, 34, 96, 112       | 0     |
| 1   | AF    | 158/192 (82%) | -0.49  | 2 (1%) 77 75  | 19, 47, 66, 104       | 0     |
| 1   | AG    | 159/192 (82%) | -0.45  | 4 (2%) 57 54  | 31, 47, 63, 123       | 0     |
| 1   | AH    | 160/192 (83%) | -0.25  | 3 (1%) 66 64  | 21, 42, 69, 112       | 0     |
| 1   | AI    | 158/192 (82%) | -0.21  | 5 (3%) 47 42  | 54, 70, 84, 114       | 0     |
| 1   | AJ    | 157/192 (81%) | -0.28  | 2 (1%) 77 75  | 25, 60, 79, 99        | 0     |
| 1   | AK    | 157/192 (81%) | -0.35  | 1 (0%) 89 88  | 33, 59, 75, 101       | 0     |
| 1   | AL    | 157/192 (81%) | -0.18  | 4 (2%) 57 54  | 52, 68, 82, 120       | 0     |
| 1   | AM    | 162/192 (84%) | -0.47  | 3 (1%) 66 64  | 17, 39, 69, 112       | 0     |
| 1   | AN    | 165/192 (85%) | -0.33  | 6 (3%) 42 36  | 31, 48, 89, 107       | 0     |
| 1   | AO    | 165/192 (85%) | -0.21  | 11 (6%) 18 13 | 17, 46, 87, 110       | 0     |
| 1   | AP    | 159/192 (82%) | -0.54  | 0 100 100     | 7, 30, 51, 102        | 0     |
| 1   | AQ    | 165/192 (85%) | -0.15  | 11 (6%) 18 13 | 33, 62, 90, 110       | 0     |
| 1   | AR    | 164/192 (85%) | -0.35  | 6 (3%) 41 35  | 20, 46, 89, 111       | 0     |
| 1   | AS    | 160/192 (83%) | -0.21  | 6 (3%) 40 34  | 32, 56, 87, 117       | 0     |
| 1   | AT    | 158/192 (82%) | -0.51  | 1 (0%) 89 88  | 15, 43, 62, 110       | 0     |
| 1   | AU    | 160/192 (83%) | -0.49  | 1 (0%) 89 88  | 24, 42, 68, 107       | 0     |
| 1   | AV    | 160/192 (83%) | -0.20  | 7 (4%) 34 29  | 30, 49, 82, 115       | 0     |
| 1   | AW    | 158/192 (82%) | -0.33  | 2 (1%) 77 75  | 26, 56, 76, 113       | 0     |
| 1   | AX    | 160/192 (83%) | -0.35  | 3 (1%) 66 64  | 23, 45, 78, 118       | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1   | Aa    | 161/192 (83%) | -0.51  | 3 (1%) 66 64 | 12, 30, 54, 109       | 0     |
| 1   | Ab    | 161/192 (83%) | -0.58  | 0 100 100    | 13, 35, 65, 110       | 0     |
| 1   | Ac    | 160/192 (83%) | -0.56  | 0 100 100    | 15, 35, 66, 103       | 0     |
| 1   | Ad    | 165/192 (85%) | -0.58  | 3 (1%) 68 66 | 7, 26, 87, 107        | 0     |
| 1   | Ae    | 162/192 (84%) | -0.33  | 5 (3%) 49 43 | 8, 29, 65, 113        | 0     |
| 1   | Af    | 161/192 (83%) | -0.45  | 1 (0%) 89 88 | 10, 28, 56, 106       | 0     |
| 1   | Ag    | 155/192 (80%) | -0.65  | 1 (0%) 89 88 | 8, 28, 45, 70         | 0     |
| 1   | Ah    | 161/192 (83%) | -0.42  | 0 100 100    | 12, 32, 55, 109       | 0     |
| 1   | Ai    | 159/192 (82%) | -0.54  | 1 (0%) 89 88 | 8, 23, 46, 96         | 0     |
| 1   | Aj    | 165/192 (85%) | -0.20  | 5 (3%) 50 45 | 12, 31, 85, 109       | 0     |
| 1   | Ak    | 165/192 (85%) | -0.34  | 7 (4%) 36 30 | 18, 37, 86, 107       | 0     |
| 1   | Al    | 165/192 (85%) | -0.39  | 1 (0%) 89 88 | 8, 33, 81, 108        | 0     |
| 1   | Am    | 162/192 (84%) | -0.49  | 1 (0%) 89 88 | 11, 31, 57, 102       | 0     |
| 1   | An    | 161/192 (83%) | -0.58  | 2 (1%) 79 77 | 13, 28, 56, 96        | 0     |
| 1   | Ao    | 161/192 (83%) | -0.50  | 2 (1%) 79 77 | 11, 32, 54, 105       | 0     |
| 1   | Ap    | 162/192 (84%) | -0.58  | 2 (1%) 79 77 | 11, 30, 63, 101       | 0     |
| 1   | Aq    | 160/192 (83%) | -0.51  | 2 (1%) 77 75 | 9, 30, 58, 110        | 0     |
| 1   | Ar    | 165/192 (85%) | -0.49  | 2 (1%) 79 77 | 9, 28, 81, 105        | 0     |
| 1   | As    | 161/192 (83%) | -0.51  | 3 (1%) 66 64 | 9, 32, 60, 109        | 0     |
| 1   | At    | 160/192 (83%) | -0.60  | 2 (1%) 77 75 | 9, 31, 67, 107        | 0     |
| 1   | Au    | 160/192 (83%) | -0.30  | 2 (1%) 77 75 | 19, 40, 66, 104       | 0     |
| 1   | Av    | 165/192 (85%) | -0.31  | 5 (3%) 50 45 | 16, 39, 85, 110       | 0     |
| 1   | Aw    | 161/192 (83%) | -0.47  | 3 (1%) 66 64 | 8, 31, 58, 109        | 0     |
| 1   | Ax    | 155/192 (80%) | -0.71  | 1 (0%) 89 88 | 11, 31, 45, 76        | 0     |
| 1   | BA    | 166/192 (86%) | -0.25  | 2 (1%) 79 77 | 30, 51, 87, 108       | 0     |
| 1   | BB    | 157/192 (81%) | 0.47   | 8 (5%) 28 23 | 68, 86, 98, 109       | 0     |
| 1   | BC    | 155/192 (80%) | 0.24   | 4 (2%) 56 52 | 64, 84, 94, 103       | 0     |
| 1   | BD    | 160/192 (83%) | -0.30  | 1 (0%) 89 88 | 22, 52, 76, 105       | 0     |
| 1   | BE    | 159/192 (82%) | -0.38  | 2 (1%) 77 75 | 26, 46, 72, 111       | 0     |
| 1   | BF    | 159/192 (82%) | -0.63  | 0 100 100    | 13, 32, 53, 102       | 0     |
| 1   | BG    | 156/192 (81%) | -0.22  | 2 (1%) 77 75 | 31, 58, 70, 94        | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1   | BH    | 154/192 (80%) | 0.05   | 3 (1%) 66 64 | 40, 70, 86, 99        | 0     |
| 1   | BI    | 155/192 (80%) | -0.36  | 0 100 100    | 19, 52, 73, 97        | 0     |
| 1   | BJ    | 157/192 (81%) | -0.06  | 2 (1%) 77 75 | 50, 69, 91, 111       | 0     |
| 1   | BK    | 156/192 (81%) | 0.49   | 8 (5%) 28 23 | 71, 87, 98, 105       | 0     |
| 1   | BL    | 155/192 (80%) | 0.04   | 0 100 100    | 57, 74, 89, 92        | 0     |
| 1   | BM    | 158/192 (82%) | -0.33  | 2 (1%) 77 75 | 9, 33, 54, 102        | 0     |
| 1   | BN    | 159/192 (82%) | -0.36  | 0 100 100    | 20, 41, 63, 114       | 0     |
| 1   | BO    | 160/192 (83%) | -0.11  | 4 (2%) 57 54 | 37, 62, 86, 114       | 0     |
| 1   | BP    | 159/192 (82%) | -0.26  | 5 (3%) 49 43 | 29, 55, 83, 114       | 0     |
| 1   | BQ    | 160/192 (83%) | -0.49  | 1 (0%) 89 88 | 17, 37, 63, 114       | 0     |
| 1   | BR    | 161/192 (83%) | -0.44  | 3 (1%) 66 64 | 18, 42, 68, 103       | 0     |
| 1   | BS    | 159/192 (82%) | -0.41  | 0 100 100    | 18, 34, 54, 98        | 0     |
| 1   | BT    | 157/192 (81%) | 0.20   | 5 (3%) 47 42 | 58, 74, 92, 118       | 0     |
| 1   | BU    | 162/192 (84%) | 0.05   | 1 (0%) 89 88 | 55, 78, 91, 115       | 0     |
| 1   | BV    | 156/192 (81%) | 0.27   | 7 (4%) 33 28 | 69, 87, 96, 111       | 0     |
| 1   | BW    | 161/192 (83%) | -0.15  | 4 (2%) 57 54 | 38, 60, 81, 117       | 0     |
| 1   | BX    | 163/192 (84%) | 0.31   | 6 (3%) 41 35 | 61, 78, 91, 110       | 0     |
| 1   | Ba    | 158/192 (82%) | -0.11  | 4 (2%) 57 54 | 52, 71, 88, 111       | 0     |
| 1   | Bb    | 159/192 (82%) | -0.01  | 3 (1%) 66 64 | 49, 72, 90, 118       | 0     |
| 1   | Bc    | 161/192 (83%) | -0.41  | 1 (0%) 89 88 | 15, 38, 69, 109       | 0     |
| 1   | Bd    | 161/192 (83%) | -0.47  | 3 (1%) 66 64 | 21, 40, 64, 114       | 0     |
| 1   | Be    | 163/192 (84%) | -0.47  | 1 (0%) 89 88 | 13, 36, 77, 107       | 0     |
| 1   | Bf    | 165/192 (85%) | -0.31  | 6 (3%) 42 36 | 14, 44, 85, 110       | 0     |
| 1   | Bg    | 156/192 (81%) | 0.11   | 4 (2%) 56 52 | 54, 76, 89, 108       | 0     |
| 1   | Bh    | 159/192 (82%) | -0.45  | 3 (1%) 66 64 | 30, 48, 72, 108       | 0     |
| 1   | Bi    | 157/192 (81%) | -0.22  | 1 (0%) 89 88 | 32, 58, 70, 94        | 0     |
| 1   | Bj    | 154/192 (80%) | 0.09   | 0 100 100    | 55, 76, 85, 96        | 0     |
| 1   | Bk    | 159/192 (82%) | -0.20  | 2 (1%) 77 75 | 37, 57, 80, 114       | 0     |
| 1   | Bl    | 159/192 (82%) | -0.53  | 1 (0%) 89 88 | 12, 38, 61, 109       | 0     |
| 1   | Bm    | 159/192 (82%) | -0.52  | 3 (1%) 66 64 | 18, 36, 59, 113       | 0     |
| 1   | Bn    | 165/192 (85%) | -0.09  | 4 (2%) 59 55 | 33, 61, 89, 111       | 0     |

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| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1   | Bo    | 156/192 (81%) | -0.19  | 3 (1%) 66 64 | 44, 65, 84, 96        | 0     |
| 1   | Bp    | 162/192 (84%) | -0.39  | 7 (4%) 35 30 | 17, 41, 79, 116       | 0     |
| 1   | Bq    | 160/192 (83%) | -0.11  | 3 (1%) 66 64 | 26, 55, 76, 111       | 0     |
| 1   | Br    | 161/192 (83%) | -0.58  | 2 (1%) 79 77 | 8, 28, 57, 105        | 0     |
| 1   | Bs    | 155/192 (80%) | -0.24  | 2 (1%) 77 75 | 37, 57, 80, 97        | 0     |
| 1   | Bt    | 158/192 (82%) | 0.14   | 4 (2%) 57 54 | 61, 79, 93, 110       | 0     |
| 1   | Bu    | 165/192 (85%) | -0.40  | 6 (3%) 42 36 | 14, 36, 83, 106       | 0     |
| 1   | Bv    | 160/192 (83%) | -0.43  | 5 (3%) 49 43 | 23, 45, 72, 120       | 0     |
| 1   | Bw    | 159/192 (82%) | -0.40  | 3 (1%) 66 64 | 11, 29, 55, 112       | 0     |
| 1   | Bx    | 157/192 (81%) | 0.23   | 7 (4%) 33 28 | 62, 83, 95, 113       | 0     |
| 1   | CA    | 160/192 (83%) | -0.51  | 1 (0%) 89 88 | 12, 36, 61, 111       | 0     |
| 1   | CB    | 161/192 (83%) | -0.25  | 4 (2%) 57 54 | 19, 52, 79, 108       | 0     |
| 1   | CC    | 157/192 (81%) | -0.24  | 2 (1%) 77 75 | 45, 65, 78, 109       | 0     |
| 1   | CD    | 161/192 (83%) | -0.49  | 2 (1%) 79 77 | 13, 39, 68, 107       | 0     |
| 1   | CE    | 160/192 (83%) | -0.27  | 1 (0%) 89 88 | 29, 52, 80, 112       | 0     |
| 1   | CF    | 160/192 (83%) | -0.48  | 3 (1%) 66 64 | 11, 35, 53, 101       | 0     |
| 1   | CG    | 160/192 (83%) | -0.41  | 2 (1%) 77 75 | 21, 45, 72, 112       | 0     |
| 1   | CH    | 159/192 (82%) | -0.13  | 3 (1%) 66 64 | 33, 62, 79, 119       | 0     |
| 1   | CI    | 160/192 (83%) | -0.21  | 3 (1%) 66 64 | 15, 35, 74, 107       | 0     |
| 1   | CJ    | 165/192 (85%) | -0.38  | 5 (3%) 50 45 | 24, 44, 85, 105       | 0     |
| 1   | CK    | 160/192 (83%) | -0.28  | 2 (1%) 77 75 | 22, 60, 77, 115       | 0     |
| 1   | CL    | 159/192 (82%) | -0.35  | 3 (1%) 66 64 | 38, 57, 73, 121       | 0     |
| 1   | CM    | 159/192 (82%) | -0.46  | 3 (1%) 66 64 | 16, 42, 63, 112       | 0     |
| 1   | CN    | 161/192 (83%) | -0.51  | 1 (0%) 89 88 | 16, 40, 77, 110       | 0     |
| 1   | CO    | 159/192 (82%) | -0.37  | 2 (1%) 77 75 | 38, 58, 74, 99        | 0     |
| 1   | CP    | 158/192 (82%) | -0.38  | 2 (1%) 77 75 | 25, 57, 76, 110       | 0     |
| 1   | CQ    | 162/192 (84%) | -0.48  | 3 (1%) 66 64 | 9, 31, 61, 104        | 0     |
| 1   | CR    | 166/192 (86%) | -0.40  | 5 (3%) 50 45 | 24, 42, 82, 107       | 0     |
| 1   | CS    | 161/192 (83%) | -0.34  | 4 (2%) 57 54 | 10, 35, 65, 114       | 0     |
| 1   | CT    | 158/192 (82%) | -0.40  | 3 (1%) 66 64 | 26, 50, 66, 106       | 0     |
| 1   | CU    | 159/192 (82%) | -0.23  | 1 (0%) 89 88 | 51, 67, 82, 120       | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 1   | CV    | 158/192 (82%)     | -0.21  | 4 (2%) 57 54   | 55, 68, 84, 120       | 0     |
| 1   | CW    | 155/192 (80%)     | -0.49  | 1 (0%) 89 88   | 27, 47, 69, 87        | 0     |
| 1   | CX    | 161/192 (83%)     | -0.47  | 3 (1%) 66 64   | 20, 48, 70, 107       | 0     |
| 1   | Ca    | 158/192 (82%)     | 0.62   | 18 (11%) 5 3   | 58, 89, 103, 121      | 0     |
| 1   | Cb    | 159/192 (82%)     | 0.02   | 6 (3%) 40 34   | 37, 69, 87, 109       | 0     |
| 1   | Cc    | 157/192 (81%)     | -0.12  | 4 (2%) 57 54   | 40, 69, 86, 118       | 0     |
| 1   | Cd    | 153/192 (79%)     | 0.65   | 16 (10%) 6 4   | 76, 91, 104, 109      | 0     |
| 1   | Ce    | 154/192 (80%)     | 0.26   | 8 (5%) 27 22   | 59, 81, 92, 95        | 0     |
| 1   | Cf    | 153/192 (79%)     | 0.84   | 17 (11%) 5 3   | 83, 97, 107, 110      | 0     |
| 1   | Cg    | 160/192 (83%)     | 0.02   | 7 (4%) 34 29   | 48, 68, 93, 126       | 0     |
| 1   | Ch    | 159/192 (82%)     | -0.43  | 2 (1%) 77 75   | 23, 49, 66, 114       | 0     |
| 1   | Ci    | 153/192 (79%)     | 0.62   | 15 (9%) 7 5    | 69, 89, 104, 111      | 0     |
| 1   | Cj    | 156/192 (81%)     | 0.31   | 9 (5%) 23 18   | 61, 81, 100, 112      | 0     |
| 1   | Ck    | 154/192 (80%)     | -0.08  | 2 (1%) 77 75   | 45, 74, 92, 104       | 0     |
| 1   | Cl    | 155/192 (80%)     | 0.18   | 5 (3%) 47 42   | 56, 85, 97, 113       | 0     |
| 1   | Cm    | 159/192 (82%)     | 0.42   | 16 (10%) 7 5   | 71, 88, 100, 113      | 0     |
| 1   | Cn    | 155/192 (80%)     | 0.22   | 7 (4%) 33 28   | 65, 86, 101, 104      | 0     |
| 1   | Co    | 155/192 (80%)     | -0.34  | 2 (1%) 77 75   | 26, 52, 71, 100       | 0     |
| 1   | Cp    | 158/192 (82%)     | -0.08  | 7 (4%) 34 29   | 46, 67, 89, 109       | 0     |
| 1   | Cq    | 155/192 (80%)     | 0.75   | 21 (13%) 3 2   | 83, 96, 106, 112      | 0     |
| 1   | Cr    | 154/192 (80%)     | 0.20   | 8 (5%) 27 22   | 78, 91, 103, 111      | 0     |
| 1   | Cs    | 154/192 (80%)     | 0.57   | 16 (10%) 6 4   | 83, 98, 106, 107      | 0     |
| 1   | Ct    | 160/192 (83%)     | -0.38  | 4 (2%) 57 54   | 34, 51, 79, 115       | 0     |
| 1   | Cu    | 159/192 (82%)     | -0.23  | 6 (3%) 40 34   | 44, 62, 81, 119       | 0     |
| 1   | Cv    | 161/192 (83%)     | -0.13  | 3 (1%) 66 64   | 39, 59, 81, 119       | 0     |
| 1   | Cw    | 155/192 (80%)     | 0.19   | 4 (2%) 56 52   | 71, 89, 98, 107       | 0     |
| 1   | Cx    | 156/192 (81%)     | -0.21  | 2 (1%) 77 75   | 39, 59, 78, 99        | 0     |
| All | All   | 22946/27648 (82%) | -0.23  | 578 (2%) 57 54 | 7, 52, 95, 126        | 0     |

The worst 5 of 578 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Ci    | 155 | LEU  | 6.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | Bn    | 159 | GLU  | 6.2  |
| 1   | Ar    | 162 | LEU  | 6.1  |
| 1   | Av    | 159 | GLU  | 5.6  |
| 1   | Av    | 162 | LEU  | 5.6  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | CA   | BN    | 201 | 1/1   | 0.55 | 0.35 | 73,73,73,73                 | 0     |
| 2   | CA   | An    | 201 | 1/1   | 0.58 | 0.30 | 61,61,61,61                 | 0     |
| 2   | CA   | Cl    | 201 | 1/1   | 0.59 | 0.45 | 85,85,85,85                 | 1     |
| 2   | CA   | Cn    | 201 | 1/1   | 0.65 | 0.17 | 108,108,108,108             | 0     |
| 2   | CA   | BB    | 201 | 1/1   | 0.71 | 0.12 | 86,86,86,86                 | 0     |
| 2   | CA   | AC    | 201 | 1/1   | 0.72 | 0.32 | 86,86,86,86                 | 0     |
| 2   | CA   | BG    | 201 | 1/1   | 0.73 | 0.27 | 94,94,94,94                 | 0     |
| 2   | CA   | BR    | 201 | 1/1   | 0.76 | 0.31 | 72,72,72,72                 | 0     |
| 2   | CA   | Bb    | 201 | 1/1   | 0.76 | 0.26 | 98,98,98,98                 | 0     |
| 2   | CA   | Cg    | 201 | 1/1   | 0.78 | 0.18 | 85,85,85,85                 | 0     |
| 2   | CA   | Bd    | 201 | 1/1   | 0.79 | 0.27 | 61,61,61,61                 | 0     |
| 2   | CA   | Ac    | 201 | 1/1   | 0.79 | 0.27 | 70,70,70,70                 | 0     |
| 2   | CA   | Ag    | 201 | 1/1   | 0.79 | 0.25 | 55,55,55,55                 | 0     |
| 2   | CA   | CE    | 201 | 1/1   | 0.80 | 0.31 | 83,83,83,83                 | 0     |
| 2   | CA   | BA    | 201 | 1/1   | 0.83 | 0.24 | 78,78,78,78                 | 0     |
| 2   | CA   | CA    | 201 | 1/1   | 0.83 | 0.32 | 67,67,67,67                 | 0     |
| 2   | CA   | Aa    | 201 | 1/1   | 0.84 | 0.24 | 58,58,58,58                 | 0     |
| 2   | CA   | AB    | 201 | 1/1   | 0.84 | 0.21 | 75,75,75,75                 | 0     |
| 2   | CA   | BC    | 201 | 1/1   | 0.84 | 0.45 | 73,73,73,73                 | 1     |

*Continued on next page...*



*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | CA   | Ck    | 201 | 1/1   | 0.85 | 0.18 | 78,78,78,78                 | 0     |
| 2   | CA   | AF    | 201 | 1/1   | 0.85 | 0.25 | 68,68,68,68                 | 0     |
| 2   | CA   | CC    | 201 | 1/1   | 0.85 | 0.20 | 96,96,96,96                 | 0     |
| 2   | CA   | BD    | 201 | 1/1   | 0.85 | 0.19 | 81,81,81,81                 | 0     |
| 2   | CA   | Ba    | 201 | 1/1   | 0.85 | 0.18 | 80,80,80,80                 | 0     |
| 2   | CA   | CO    | 201 | 1/1   | 0.86 | 0.21 | 68,68,68,68                 | 0     |
| 2   | CA   | AA    | 201 | 1/1   | 0.86 | 0.18 | 106,106,106,106             | 0     |
| 2   | CA   | AL    | 201 | 1/1   | 0.87 | 0.17 | 84,84,84,84                 | 0     |
| 2   | CA   | AO    | 201 | 1/1   | 0.88 | 0.24 | 67,67,67,67                 | 0     |
| 2   | CA   | Ce    | 201 | 1/1   | 0.88 | 0.27 | 106,106,106,106             | 0     |
| 2   | CA   | Bc    | 201 | 1/1   | 0.88 | 0.31 | 73,73,73,73                 | 0     |
| 2   | CA   | Be    | 201 | 1/1   | 0.88 | 0.31 | 66,66,66,66                 | 0     |
| 2   | CA   | Bg    | 201 | 1/1   | 0.90 | 0.24 | 88,88,88,88                 | 0     |
| 2   | CA   | AM    | 201 | 1/1   | 0.90 | 0.24 | 68,68,68,68                 | 0     |
| 2   | CA   | Ae    | 201 | 1/1   | 0.90 | 0.26 | 70,70,70,70                 | 0     |
| 2   | CA   | Aj    | 201 | 1/1   | 0.90 | 0.29 | 56,56,56,56                 | 0     |
| 2   | CA   | AH    | 201 | 1/1   | 0.91 | 0.28 | 62,62,62,62                 | 0     |
| 2   | CA   | Ad    | 201 | 1/1   | 0.91 | 0.23 | 54,54,54,54                 | 0     |
| 2   | CA   | Cb    | 201 | 1/1   | 0.91 | 0.26 | 80,80,80,80                 | 0     |
| 2   | CA   | Bf    | 201 | 1/1   | 0.92 | 0.27 | 68,68,68,68                 | 0     |
| 2   | CA   | CB    | 201 | 1/1   | 0.92 | 0.24 | 60,60,60,60                 | 0     |
| 2   | CA   | CF    | 201 | 1/1   | 0.93 | 0.33 | 63,63,63,63                 | 0     |
| 2   | CA   | BH    | 201 | 1/1   | 0.95 | 0.26 | 96,96,96,96                 | 0     |
| 2   | CA   | CH    | 201 | 1/1   | 0.96 | 0.15 | 69,69,69,69                 | 0     |
| 2   | CA   | Cp    | 201 | 1/1   | 0.96 | 0.25 | 69,69,69,69                 | 0     |
| 2   | CA   | Bu    | 201 | 1/1   | 0.97 | 0.27 | 61,61,61,61                 | 0     |
| 2   | CA   | Ah    | 201 | 1/1   | 0.97 | 0.28 | 56,56,56,56                 | 0     |
| 2   | CA   | Ca    | 201 | 1/1   | 0.97 | 0.42 | 87,87,87,87                 | 1     |
| 2   | CA   | CD    | 201 | 1/1   | 0.97 | 0.17 | 68,68,68,68                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.