



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:00 AM UTC

PDB ID : 6YFB / pdb\_00006yfb  
Title : Virus-like particle of bacteriophage AVE016  
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.  
Deposited on : 2020-03-26  
Resolution : 3.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

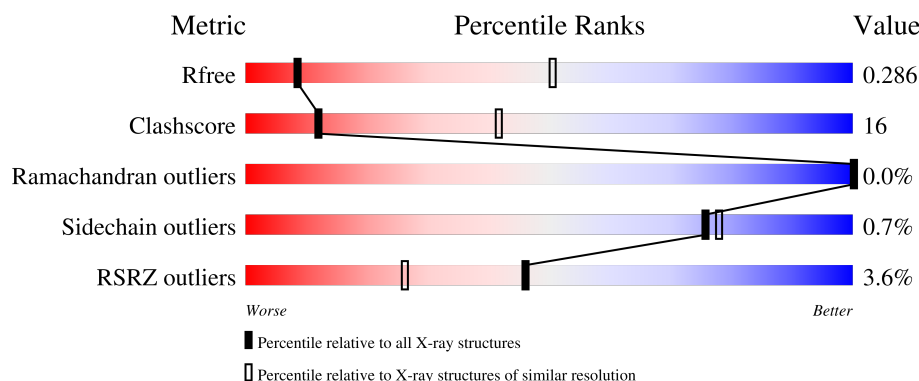
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



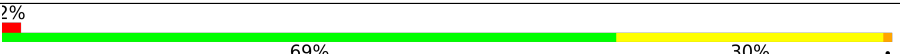
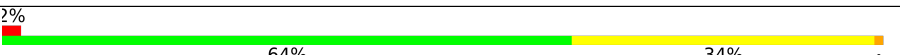
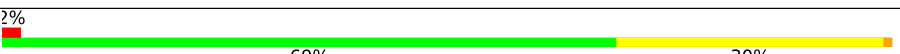
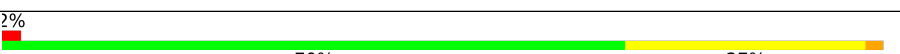
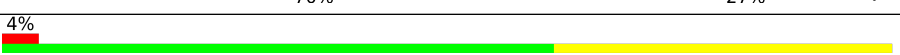
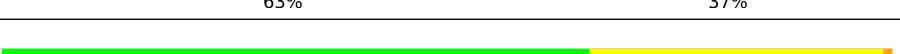
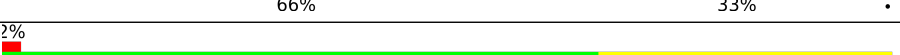
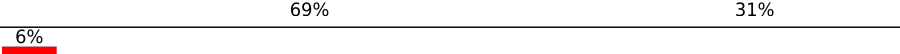
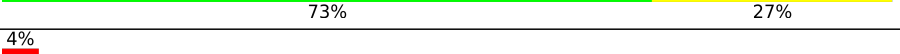
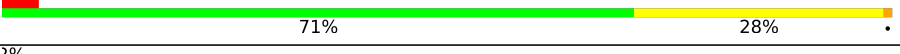
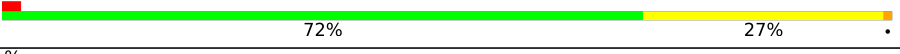
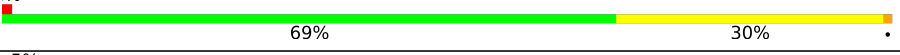
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1747 (3.70-3.50)                                      |
| Clashscore            | 190562                      | 1827 (3.70-3.50)                                      |
| Ramachandran outliers | 187476                      | 1773 (3.70-3.50)                                      |
| Sidechain outliers    | 187428                      | 1772 (3.70-3.50)                                      |
| RSRZ outliers         | 180081                      | 1745 (3.70-3.50)                                      |

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

| Mol | Chain | Length | Quality of chain                                                      |
|-----|-------|--------|-----------------------------------------------------------------------|
| 1   | AA    | 166    | <div> <div>2%</div> <div>66%</div> <div>33%</div> <div>.</div> </div> |
| 1   | AB    | 166    | <div> <div>2%</div> <div>69%</div> <div>31%</div> <div>.</div> </div> |
| 1   | AC    | 166    | <div> <div>2%</div> <div>72%</div> <div>28%</div> <div>.</div> </div> |
| 1   | AD    | 166    | <div> <div>2%</div> <div>71%</div> <div>28%</div> <div>.</div> </div> |
| 1   | AE    | 166    | <div> <div>3%</div> <div>70%</div> <div>29%</div> <div>.</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | AF    | 166    |    |
| 1   | AG    | 166    |    |
| 1   | AH    | 166    |    |
| 1   | AI    | 166    |    |
| 1   | AJ    | 166    |    |
| 1   | AK    | 166    |    |
| 1   | AL    | 166    |    |
| 1   | AM    | 166    |    |
| 1   | AN    | 166    |    |
| 1   | AO    | 166    |    |
| 1   | AP    | 166    |    |
| 1   | AQ    | 166    |    |
| 1   | AR    | 166    |   |
| 1   | AS    | 166    |  |
| 1   | AT    | 166    |  |
| 1   | AU    | 166    |  |
| 1   | AV    | 166    |  |
| 1   | AW    | 166    |  |
| 1   | AX    | 166    |  |
| 1   | AY    | 166    |  |
| 1   | AZ    | 166    |  |
| 1   | BA    | 166    |  |
| 1   | BB    | 166    |  |
| 1   | BC    | 166    |  |
| 1   | BD    | 166    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | BE    | 166    | <br>2% 67% 31%   |
| 1   | BF    | 166    | <br>2% 71% 28%   |
| 1   | BG    | 166    | <br>2% 72% 26%   |
| 1   | BH    | 166    | <br>2% 64% 36%   |
| 1   | BI    | 166    | <br>4% 65% 35%   |
| 1   | BJ    | 166    | <br>4% 66% 33%   |
| 1   | BK    | 166    | <br>7% 66% 34%   |
| 1   | BL    | 166    | <br>2% 69% 31%   |
| 1   | BM    | 166    | <br>5% 71% 29%   |
| 1   | BN    | 166    | <br>5% 65% 35%   |
| 1   | BO    | 166    | <br>2% 66% 34%   |
| 1   | BP    | 166    | <br>7% 62% 37%   |
| 1   | BQ    | 166    | <br>4% 64% 34%   |
| 1   | BR    | 166    | <br>4% 70% 30%   |
| 1   | BS    | 166    | <br>3% 71% 28%   |
| 1   | BT    | 166    | <br>2% 70% 29%   |
| 1   | BU    | 166    | <br>3% 66% 33%   |
| 1   | BV    | 166    | <br>4% 67% 33%   |
| 1   | BW    | 166    | <br>4% 72% 28%   |
| 1   | BX    | 166    | <br>3% 72% 27%   |
| 1   | BY    | 166    | <br>7% 72% 28%   |
| 1   | BZ    | 166    | <br>3% 67% 32%   |
| 1   | CA    | 166    | <br>% 70% 30%    |
| 1   | CB    | 166    | <br>2% 69% 29%   |
| 1   | CC    | 166    | <br>2% 63% 37%   |

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| Mol | Chain | Length | Quality of chain |         |
|-----|-------|--------|------------------|---------|
| 1   | CD    | 166    | 6%               | 63% 37% |
| 1   | CE    | 166    | 5%               | 64% 34% |
| 1   | CF    | 166    | 4%               | 66% 34% |
| 1   | CG    | 166    | 4%               | 68% 32% |
| 1   | CH    | 166    | 8%               | 72% 28% |
| 1   | CI    | 166    | 6%               | 64% 36% |
| 1   | CJ    | 166    | 5%               | 64% 36% |
| 1   | CK    | 166    | 5%               | 63% 36% |
| 1   | CL    | 166    | 4%               | 63% 36% |
| 1   | CM    | 166    | 3%               | 68% 32% |
| 1   | CN    | 166    | 4%               | 70% 30% |
| 1   | CO    | 166    | 2%               | 72% 28% |
| 1   | CP    | 166    | 3%               | 69% 31% |
| 1   | CQ    | 166    | 2%               | 68% 31% |
| 1   | CR    | 166    | 2%               | 68% 31% |
| 1   | CS    | 166    | 3%               | 70% 28% |
| 1   | CT    | 166    | 0%               | 72% 28% |
| 1   | CU    | 166    | 2%               | 68% 31% |
| 1   | CV    | 166    | 5%               | 70% 29% |
| 1   | CW    | 166    | 4%               | 72% 27% |
| 1   | CX    | 166    | 6%               | 66% 34% |
| 1   | CY    | 166    | 4%               | 64% 36% |
| 1   | CZ    | 166    | 6%               | 66% 33% |
| 1   | DA    | 166    | 10%              | 67% 33% |
| 1   | DB    | 166    | 4%               | 69% 31% |

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| Mol | Chain | Length | Quality of chain                                                       |
|-----|-------|--------|------------------------------------------------------------------------|
| 1   | DC    | 166    | <div> <div>5%</div> <div>72%</div> <div>28%</div> </div>               |
| 1   | DD    | 166    | <div> <div>4%</div> <div>65%</div> <div>35%</div> </div>               |
| 1   | DE    | 166    | <div> <div>3%</div> <div>66%</div> <div>34%</div> </div>               |
| 1   | DF    | 166    | <div> <div>11%</div> <div>61%</div> <div>38%</div> <div>.</div> </div> |
| 1   | DG    | 166    | <div> <div>3%</div> <div>64%</div> <div>34%</div> <div>.</div> </div>  |
| 1   | DH    | 166    | <div> <div>2%</div> <div>67%</div> <div>33%</div> </div>               |
| 1   | DI    | 166    | <div> <div>4%</div> <div>69%</div> <div>30%</div> <div>.</div> </div>  |
| 1   | DJ    | 166    | <div> <div>4%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>  |
| 1   | DK    | 166    | <div> <div>2%</div> <div>67%</div> <div>32%</div> <div>.</div> </div>  |
| 1   | DL    | 166    | <div> <div>4%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>  |
| 1   | DM    | 166    | <div> <div>4%</div> <div>70%</div> <div>29%</div> <div>.</div> </div>  |
| 1   | DN    | 166    | <div> <div>3%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>  |
| 1   | DO    | 166    | <div> <div>2%</div> <div>70%</div> <div>29%</div> <div>.</div> </div>  |
| 1   | DP    | 166    | <div> <div>2%</div> <div>67%</div> <div>33%</div> <div>.</div> </div>  |
| 1   | DQ    | 166    | <div> <div>4%</div> <div>70%</div> <div>30%</div> <div>.</div> </div>  |
| 1   | DR    | 166    | <div> <div>0%</div> <div>70%</div> <div>27%</div> <div>.</div> </div>  |
| 1   | DS    | 166    | <div> <div>5%</div> <div>63%</div> <div>37%</div> </div>               |
| 1   | DT    | 166    | <div> <div>5%</div> <div>64%</div> <div>36%</div> </div>               |
| 1   | DU    | 166    | <div> <div>4%</div> <div>67%</div> <div>32%</div> <div>.</div> </div>  |
| 1   | DV    | 166    | <div> <div>4%</div> <div>67%</div> <div>33%</div> </div>               |
| 1   | DW    | 166    | <div> <div>4%</div> <div>69%</div> <div>31%</div> </div>               |
| 1   | DX    | 166    | <div> <div>4%</div> <div>70%</div> <div>30%</div> </div>               |
| 1   | DY    | 166    | <div> <div>2%</div> <div>64%</div> <div>36%</div> </div>               |
| 1   | DZ    | 166    | <div> <div>2%</div> <div>67%</div> <div>33%</div> </div>               |
| 1   | EA    | 166    | <div> <div>0%</div> <div>65%</div> <div>34%</div> <div>.</div> </div>  |

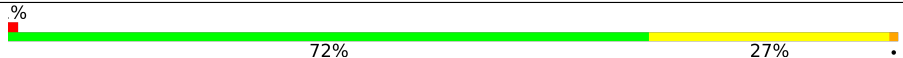
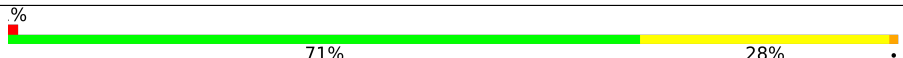
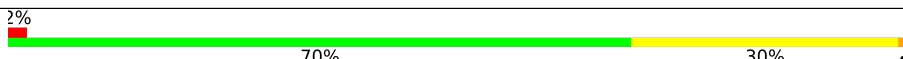
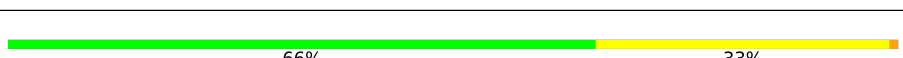
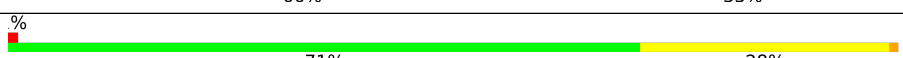
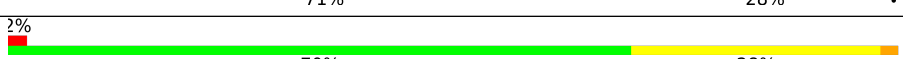
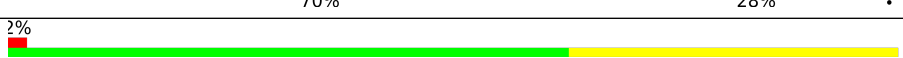
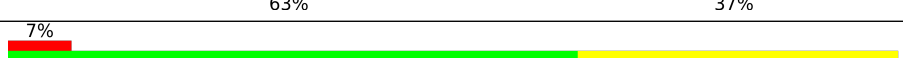
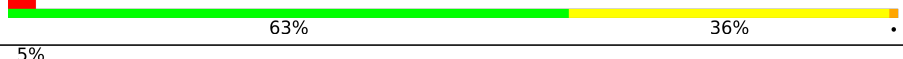
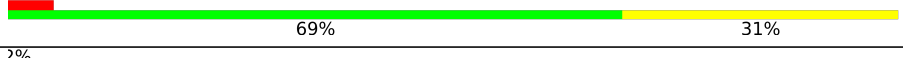
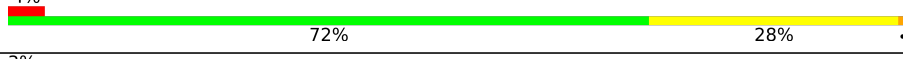
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | EB    | 166    | <br>3% 63% 36%   |
| 1   | EC    | 166    | <br>4% 70% 30%   |
| 1   | ED    | 166    | <br>2% 70% 30%   |
| 1   | EE    | 166    | <br>2% 72% 27%   |
| 1   | EF    | 166    | <br>2% 70% 30%   |
| 1   | EG    | 166    | <br>4% 70% 30%   |
| 1   | EH    | 166    | <br>2% 69% 31%   |
| 1   | EI    | 166    | <br>7% 71% 28%   |
| 1   | EJ    | 166    | <br>2% 72% 28%   |
| 1   | EK    | 166    | <br>5% 67% 32%   |
| 1   | EL    | 166    | <br>4% 69% 30%   |
| 1   | EM    | 166    | <br>2% 72% 27%   |
| 1   | EN    | 166    | <br>2% 61% 39%   |
| 1   | EO    | 166    | <br>5% 66% 34%   |
| 1   | EP    | 166    | <br>2% 67% 32%   |
| 1   | EQ    | 166    | <br>3% 65% 35%   |
| 1   | ER    | 166    | <br>6% 69% 31%   |
| 1   | ES    | 166    | <br>6% 70% 30%   |
| 1   | ET    | 166    | <br>4% 64% 36%   |
| 1   | EU    | 166    | <br>5% 64% 36%   |
| 1   | EV    | 166    | <br>7% 61% 39%   |
| 1   | EW    | 166    | <br>4% 64% 35%   |
| 1   | EX    | 166    | <br>5% 67% 33%   |
| 1   | EY    | 166    | <br>2% 70% 30%   |
| 1   | EZ    | 166    | <br>2% 72% 27%   |

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| Mol | Chain | Length | Quality of chain                                                                     |   |
|-----|-------|--------|--------------------------------------------------------------------------------------|---|
| 1   | FA    | 166    |    | • |
| 1   | FB    | 166    |    | • |
| 1   | FC    | 166    |    | • |
| 1   | FD    | 166    |    | • |
| 1   | FE    | 166    |    | • |
| 1   | FF    | 166    |    | • |
| 1   | FG    | 166    |    | • |
| 1   | FH    | 166    |    | • |
| 1   | FI    | 166    |    | • |
| 1   | FJ    | 166    |    | • |
| 1   | FK    | 166    |    | • |
| 1   | FL    | 166    |    | • |
| 1   | FM    | 166    |   | • |
| 1   | FN    | 166    |  | • |
| 1   | FO    | 166    |  | • |
| 1   | FP    | 166    |  | • |
| 1   | FQ    | 166    |  | • |
| 1   | FR    | 166    |  | • |
| 1   | FS    | 166    |  | • |
| 1   | FT    | 166    |  | • |
| 1   | FU    | 166    |  | • |
| 1   | FV    | 166    |  | • |
| 1   | FW    | 166    |  | • |
| 1   | FX    | 166    |  | • |
| 1   | FY    | 166    |  | • |

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| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 1   | FZ    | 166    | <div> <div>5%</div> <div>70%</div> <div>30%</div> </div>  |
| 1   | GA    | 166    | <div> <div>4%</div> <div>67%</div> <div>31%</div> </div>  |
| 1   | GB    | 166    | <div> <div>2%</div> <div>71%</div> <div>28%</div> </div>  |
| 1   | GC    | 166    | <div> <div>%</div> <div>72%</div> <div>26%</div> </div>   |
| 1   | GD    | 166    | <div> <div>4%</div> <div>64%</div> <div>36%</div> </div>  |
| 1   | GE    | 166    | <div> <div>3%</div> <div>64%</div> <div>36%</div> </div>  |
| 1   | GF    | 166    | <div> <div>4%</div> <div>66%</div> <div>33%</div> </div>  |
| 1   | GG    | 166    | <div> <div>4%</div> <div>66%</div> <div>34%</div> </div>  |
| 1   | GH    | 166    | <div> <div>2%</div> <div>69%</div> <div>31%</div> </div>  |
| 1   | GI    | 166    | <div> <div>5%</div> <div>72%</div> <div>28%</div> </div>  |
| 1   | GJ    | 166    | <div> <div>11%</div> <div>64%</div> <div>36%</div> </div> |
| 1   | GK    | 166    | <div> <div>7%</div> <div>69%</div> <div>31%</div> </div>  |
| 1   | GL    | 166    | <div> <div>4%</div> <div>61%</div> <div>38%</div> </div>  |
| 1   | GM    | 166    | <div> <div>4%</div> <div>64%</div> <div>34%</div> </div>  |
| 1   | GN    | 166    | <div> <div>4%</div> <div>69%</div> <div>31%</div> </div>  |
| 1   | GO    | 166    | <div> <div>3%</div> <div>72%</div> <div>28%</div> </div>  |
| 1   | GP    | 166    | <div> <div>3%</div> <div>72%</div> <div>27%</div> </div>  |
| 1   | GQ    | 166    | <div> <div>3%</div> <div>70%</div> <div>29%</div> </div>  |
| 1   | GR    | 166    | <div> <div>3%</div> <div>70%</div> <div>30%</div> </div>  |
| 1   | GS    | 166    | <div> <div>%</div> <div>69%</div> <div>31%</div> </div>   |
| 1   | GT    | 166    | <div> <div>4%</div> <div>71%</div> <div>28%</div> </div>  |
| 1   | GU    | 166    | <div> <div>4%</div> <div>71%</div> <div>28%</div> </div>  |
| 1   | GV    | 166    | <div> <div>2%</div> <div>66%</div> <div>34%</div> </div>  |
| 1   | GW    | 166    | <div> <div>2%</div> <div>70%</div> <div>29%</div> </div>  |
| 1   | GX    | 166    | <div> <div>2%</div> <div>71%</div> <div>27%</div> </div>  |

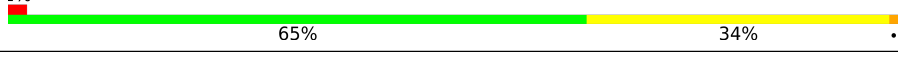
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| Mol | Chain | Length | Quality of chain                                                      |
|-----|-------|--------|-----------------------------------------------------------------------|
| 1   | GY    | 166    | <div> <div></div> <div>2%</div> <div>63%</div> <div>37%</div> </div>  |
| 1   | GZ    | 166    | <div> <div></div> <div>4%</div> <div>64%</div> <div>36%</div> </div>  |
| 1   | HA    | 166    | <div> <div></div> <div>4%</div> <div>66%</div> <div>33%</div> </div>  |
| 1   | HB    | 166    | <div> <div></div> <div>5%</div> <div>66%</div> <div>34%</div> </div>  |
| 1   | HC    | 166    | <div> <div></div> <div>2%</div> <div>70%</div> <div>30%</div> </div>  |
| 1   | HD    | 166    | <div> <div></div> <div>3%</div> <div>73%</div> <div>27%</div> </div>  |
| 1   | HE    | 166    | <div> <div></div> <div>3%</div> <div>65%</div> <div>35%</div> </div>  |
| 1   | HF    | 166    | <div> <div></div> <div>3%</div> <div>69%</div> <div>31%</div> </div>  |
| 1   | HG    | 166    | <div> <div></div> <div>11%</div> <div>58%</div> <div>41%</div> </div> |
| 1   | HH    | 166    | <div> <div></div> <div>2%</div> <div>63%</div> <div>36%</div> </div>  |
| 1   | HI    | 166    | <div> <div></div> <div>2%</div> <div>67%</div> <div>33%</div> </div>  |
| 1   | HJ    | 166    | <div> <div></div> <div>4%</div> <div>72%</div> <div>28%</div> </div>  |
| 1   | HK    | 166    | <div> <div></div> <div>5%</div> <div>72%</div> <div>27%</div> </div>  |
| 1   | HL    | 166    | <div> <div></div> <div>2%</div> <div>68%</div> <div>31%</div> </div>  |
| 1   | HM    | 166    | <div> <div></div> <div>3%</div> <div>70%</div> <div>30%</div> </div>  |
| 1   | HN    | 166    | <div> <div></div> <div>4%</div> <div>71%</div> <div>28%</div> </div>  |
| 1   | HO    | 166    | <div> <div></div> <div>2%</div> <div>70%</div> <div>29%</div> </div>  |
| 1   | HP    | 166    | <div> <div></div> <div>%</div> <div>72%</div> <div>27%</div> </div>   |
| 1   | HQ    | 166    | <div> <div></div> <div>4%</div> <div>66%</div> <div>33%</div> </div>  |
| 1   | HR    | 166    | <div> <div></div> <div>2%</div> <div>70%</div> <div>30%</div> </div>  |
| 1   | HS    | 166    | <div> <div></div> <div>2%</div> <div>70%</div> <div>28%</div> </div>  |
| 1   | HT    | 166    | <div> <div></div> <div>5%</div> <div>64%</div> <div>36%</div> </div>  |
| 1   | HU    | 166    | <div> <div></div> <div>7%</div> <div>65%</div> <div>35%</div> </div>  |
| 1   | HV    | 166    | <div> <div></div> <div>%</div> <div>66%</div> <div>33%</div> </div>   |
| 1   | HW    | 166    | <div> <div></div> <div>2%</div> <div>67%</div> <div>33%</div> </div>  |

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| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 1   | HX    | 166    | <br>3% 70% 30%   |
| 1   | HY    | 166    | <br>2% 71% 29%   |
| 1   | HZ    | 166    | <br>4% 66% 34%   |
| 1   | IA    | 166    | <br>3% 67% 33%   |
| 1   | IB    | 166    | <br>2% 65% 34% • |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 275100 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called coat protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | AA    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AB    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AC    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AD    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AE    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AF    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AG    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AH    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AI    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AJ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AK    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AL    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AM    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AN    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AO    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AP    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | AQ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AR    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AS    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AT    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AU    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AV    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AW    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AX    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AY    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | AZ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BA    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BB    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BC    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BD    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BE    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BF    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BG    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BH    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BI    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BJ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BK    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | BL    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BM    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BN    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BO    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BP    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BQ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BR    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BS    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BT    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BU    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BV    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BW    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BX    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BY    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | BZ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CA    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CB    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CC    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CD    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CE    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CF    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | CG    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CH    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CI    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CJ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CK    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CL    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CM    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CN    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CO    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CP    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CQ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CR    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CS    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CT    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CU    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CV    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CW    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CX    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CY    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | CZ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DA    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | DB    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DC    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DD    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DE    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DF    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DG    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DH    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DI    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DJ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DK    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DL    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DM    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DN    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DO    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DP    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DQ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DR    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DS    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DT    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DU    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DV    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | DW    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DX    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DY    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | DZ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EA    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EB    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EC    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | ED    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EE    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EF    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EG    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EH    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EI    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EJ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EK    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EL    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EM    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EN    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EO    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EP    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EQ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | ER    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | ES    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | ET    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EU    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EV    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EW    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EX    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EY    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | EZ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FA    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FB    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FC    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FD    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FE    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FF    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FG    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FH    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FI    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FJ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FK    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | FL    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms         |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|-------|
| 1   | FM    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FN    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FO    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FP    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FQ    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FR    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FS    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FT    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FU    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FV    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FW    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FX    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FY    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | FZ    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | GA    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | GB    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | GC    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | GD    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | GE    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | GF    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |
| 1   | GG    | 166      | Total<br>1310 | C<br>828 | N<br>215 | O<br>262 | S<br>5 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | GH    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GI    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GJ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GK    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GL    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GM    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GN    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GO    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GP    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GQ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GR    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GS    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GT    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GU    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GV    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GW    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GX    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GY    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | GZ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HA    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HB    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | HC    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HD    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HE    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HF    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HG    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HH    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HI    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HJ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HK    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HL    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HM    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HN    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HO    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HP    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HQ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HR    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HS    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HT    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HU    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HV    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HW    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |

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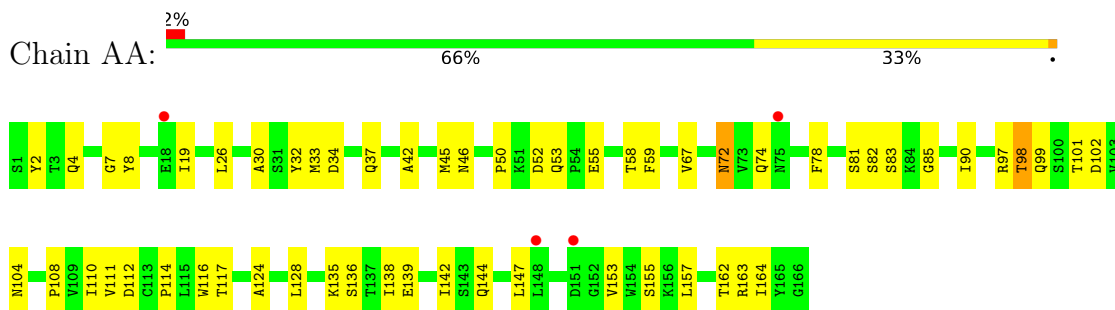
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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | HX    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HY    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | HZ    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | IA    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |
| 1   | IB    | 166      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1310  | 828 | 215 | 262 | 5 |         |         |       |

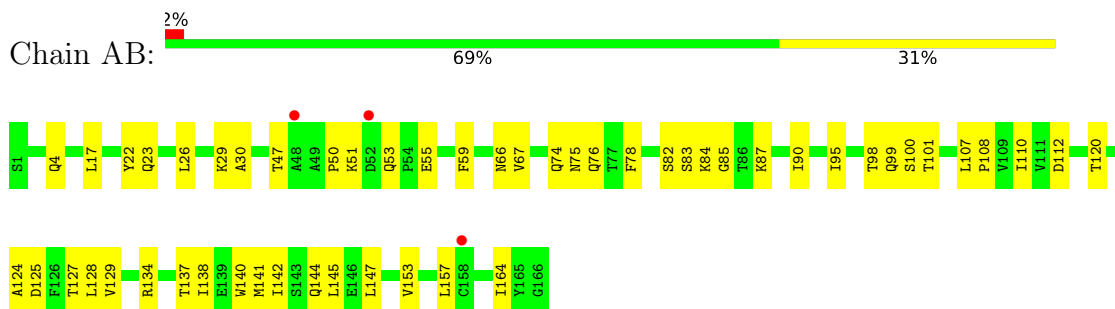
### 3 Residue-property plots [i](#)

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

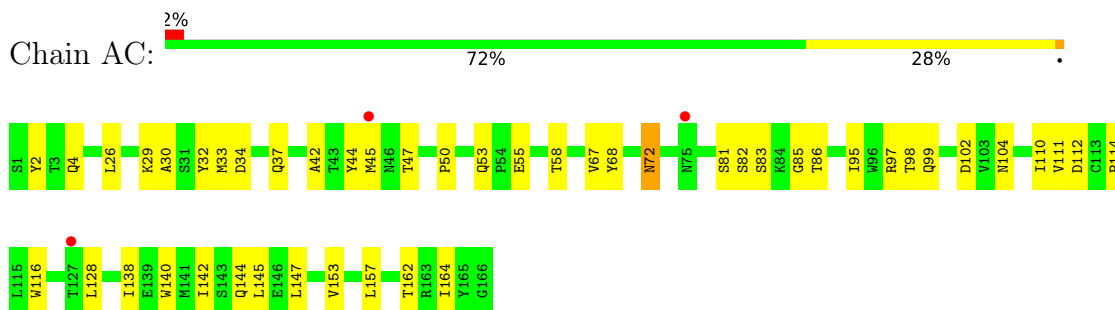
- Molecule 1: coat protein



- Molecule 1: coat protein

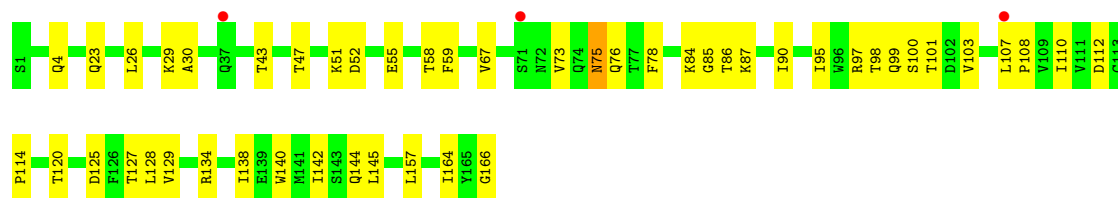


- Molecule 1: coat protein

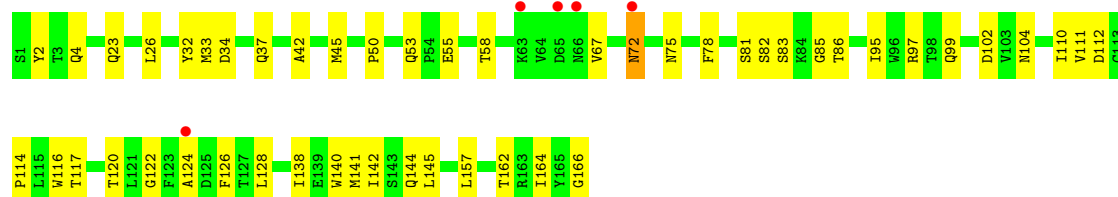


- Molecule 1: coat protein

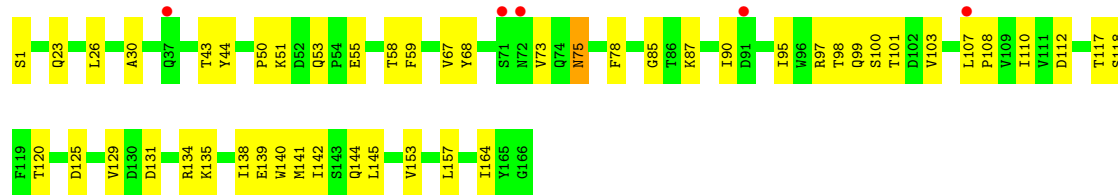




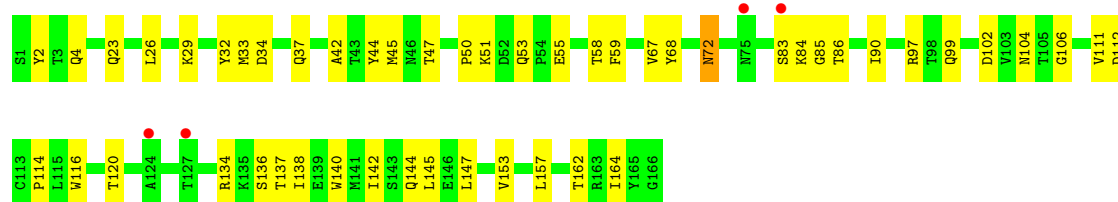
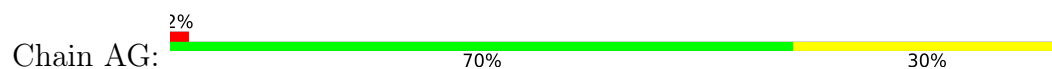
• Molecule 1: coat protein



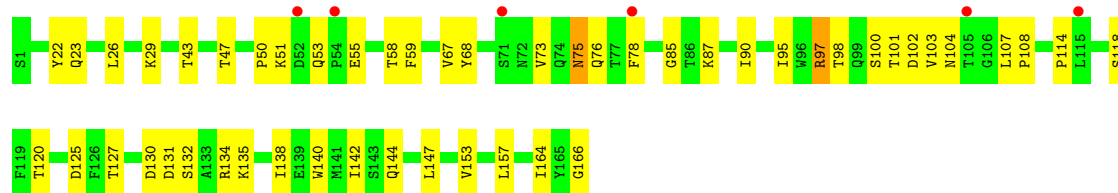
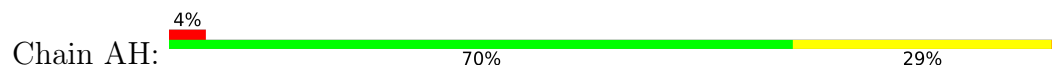
• Molecule 1: coat protein



• Molecule 1: coat protein

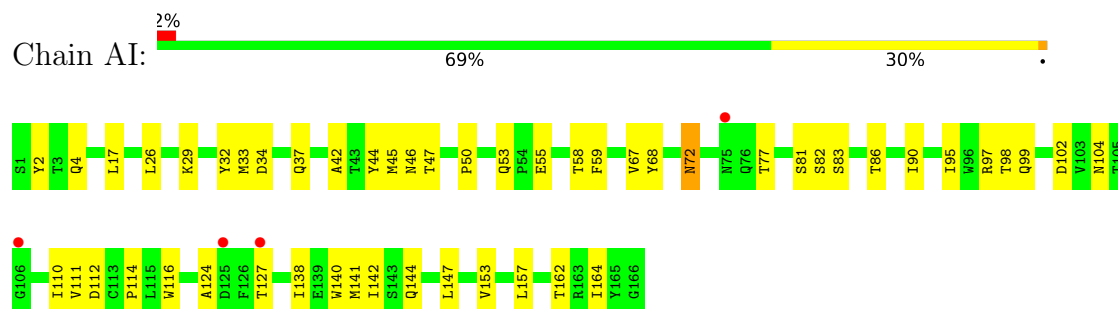


• Molecule 1: coat protein

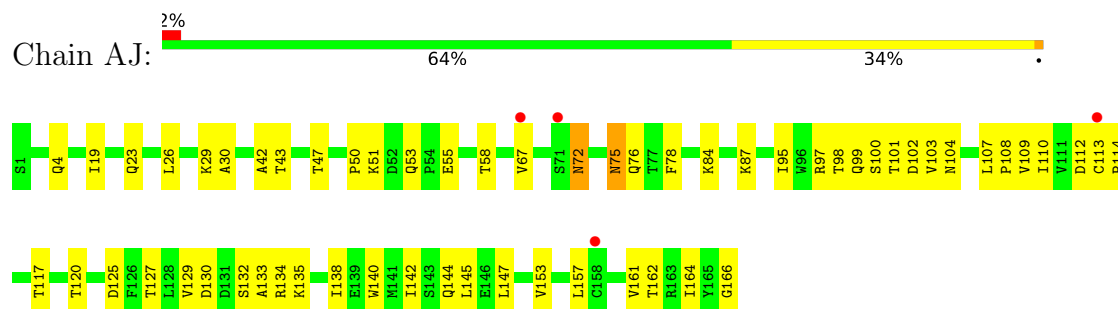




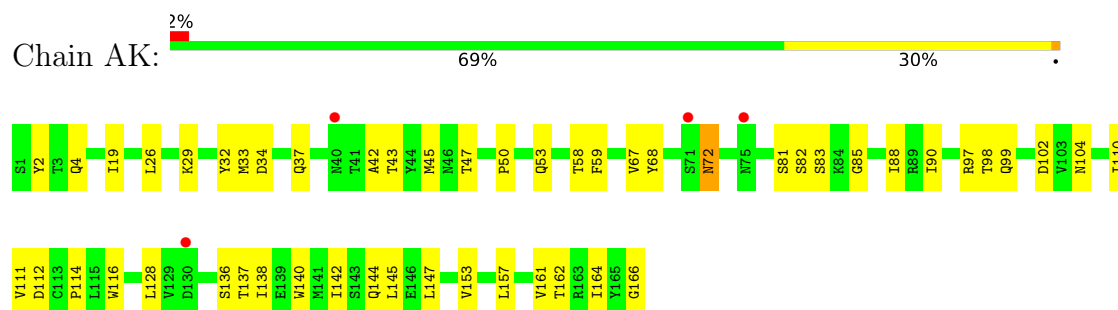
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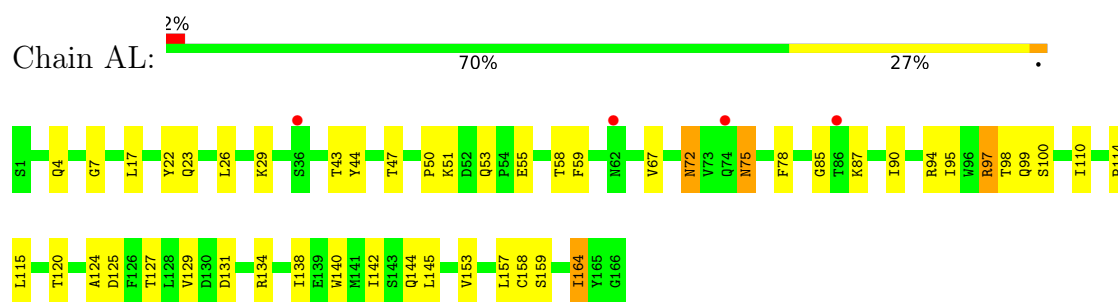
- Molecule 1: coat protein



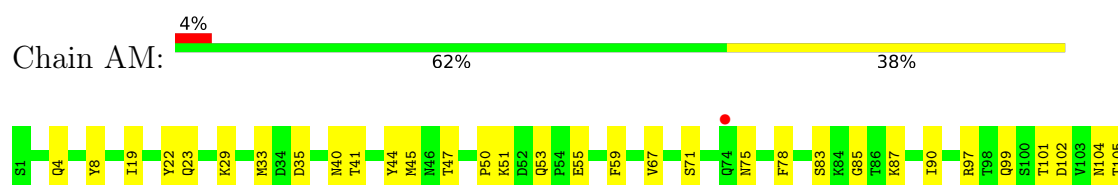
- Molecule 1: coat protein

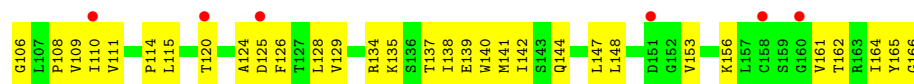


- Molecule 1: coat protein



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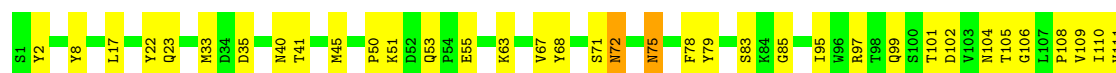




- Molecule 1: coat protein



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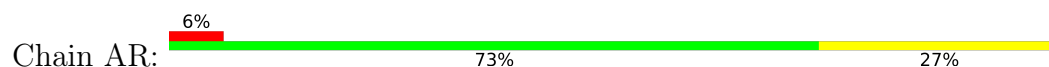
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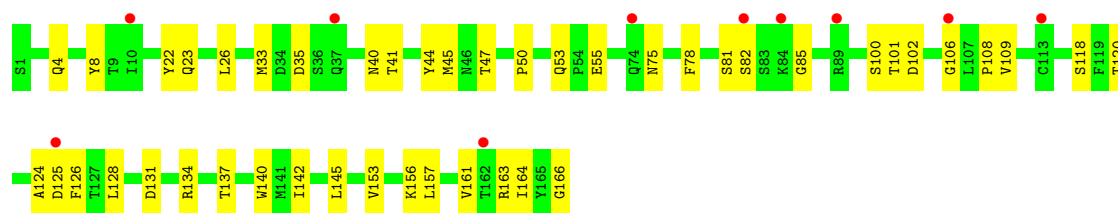


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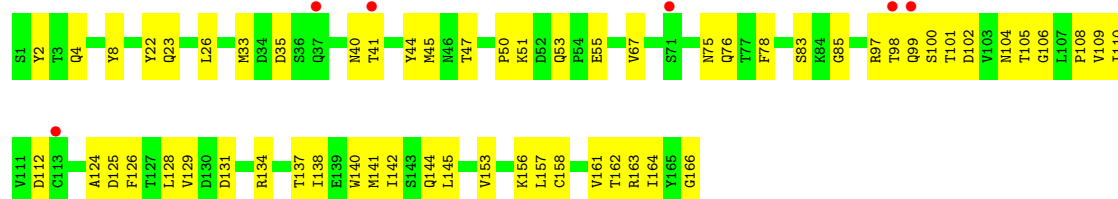


- Molecule 1: coat protein

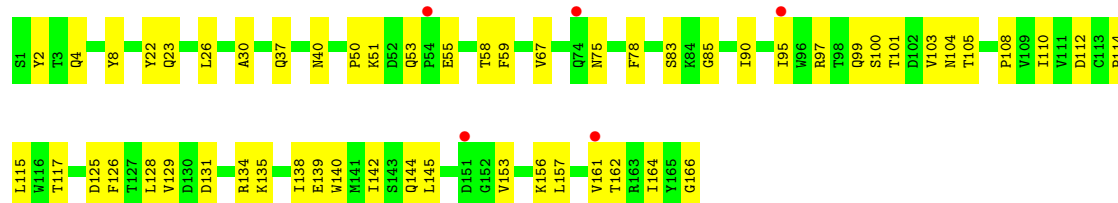




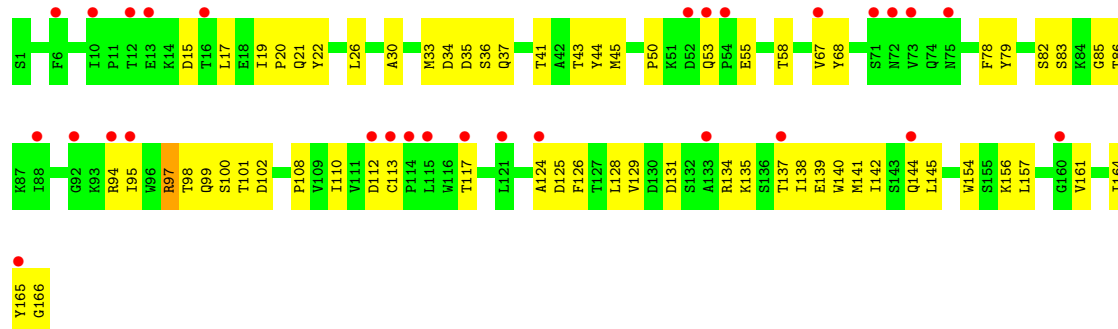
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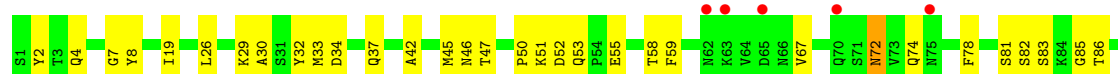
• Molecule 1: coat protein



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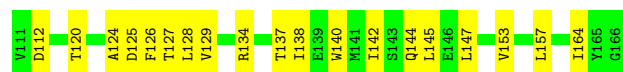
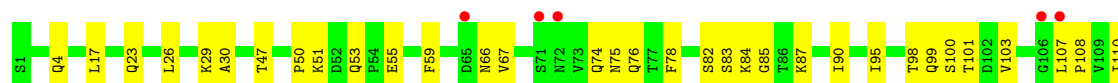
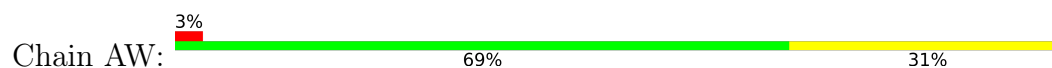


• Molecule 1: coat protein

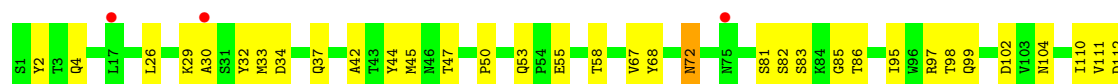




- Molecule 1: coat protein



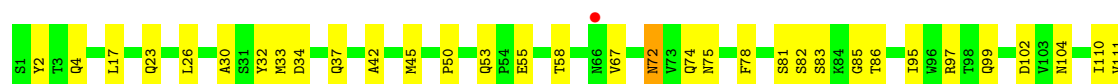
- Molecule 1: coat protein



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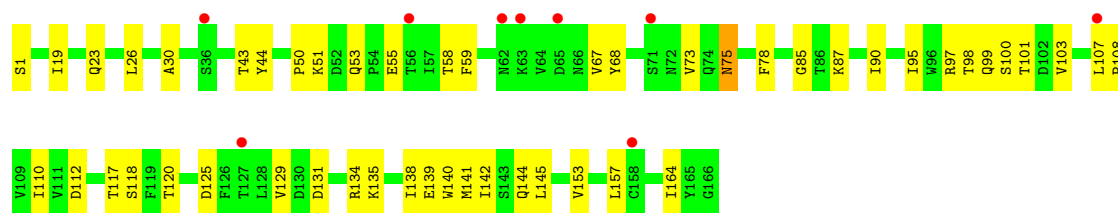


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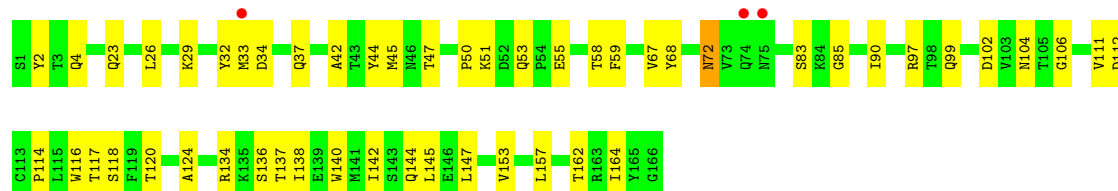


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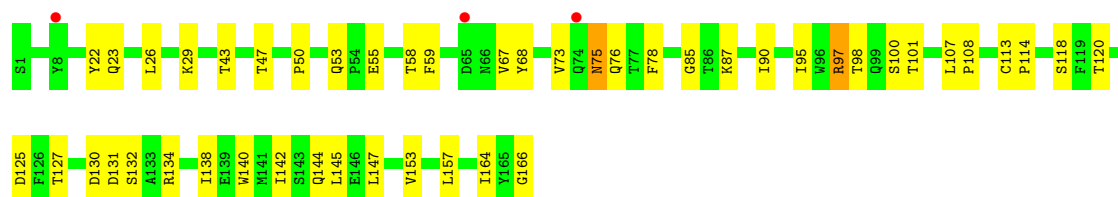
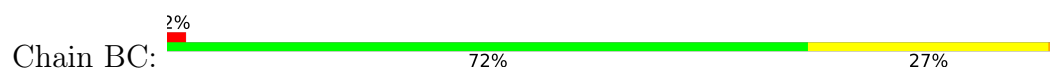




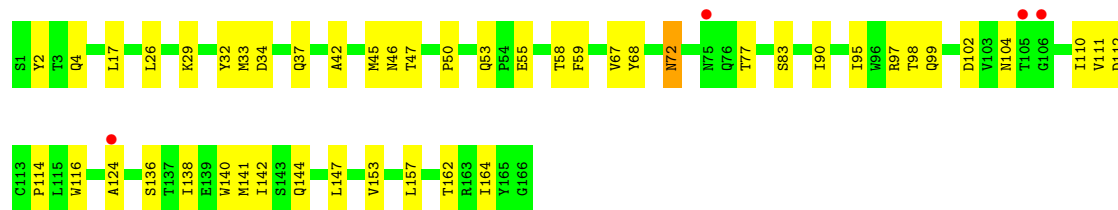
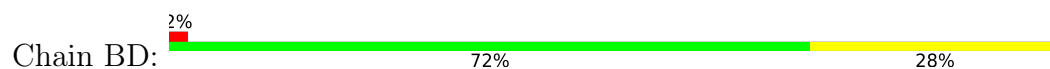
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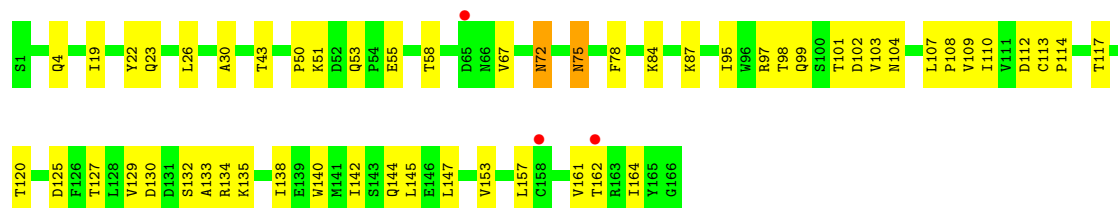
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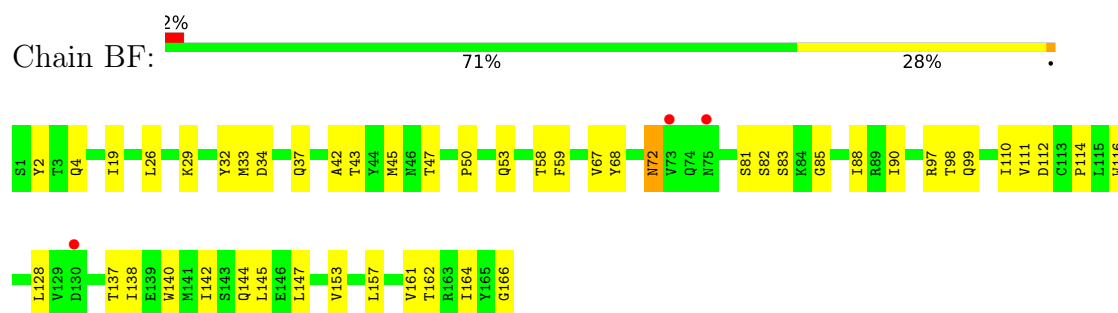
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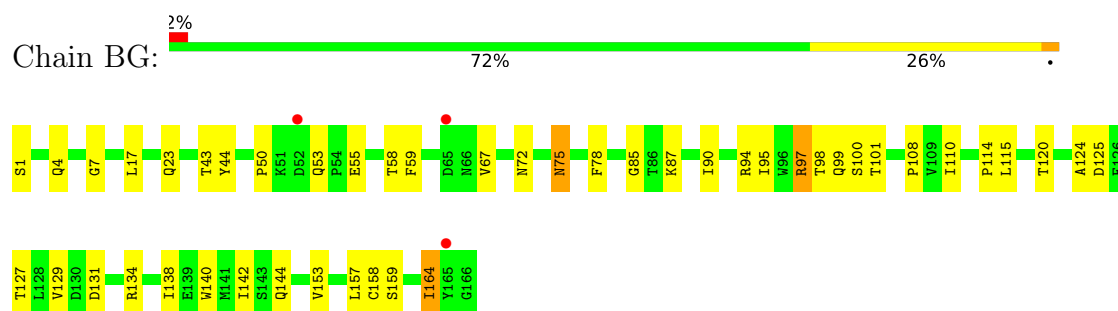
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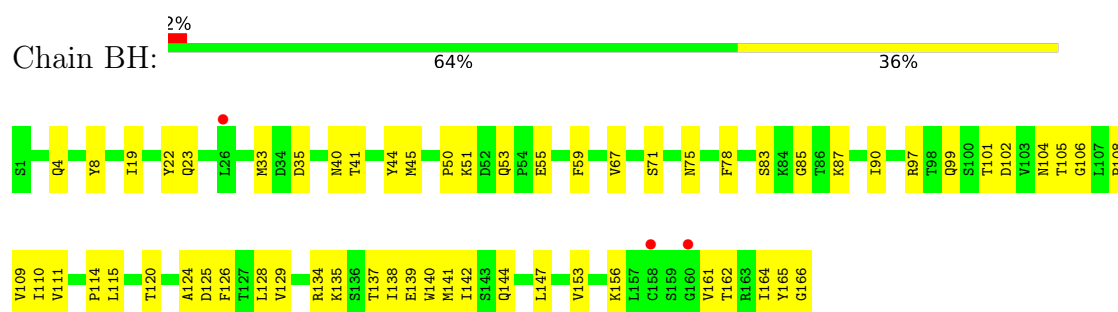
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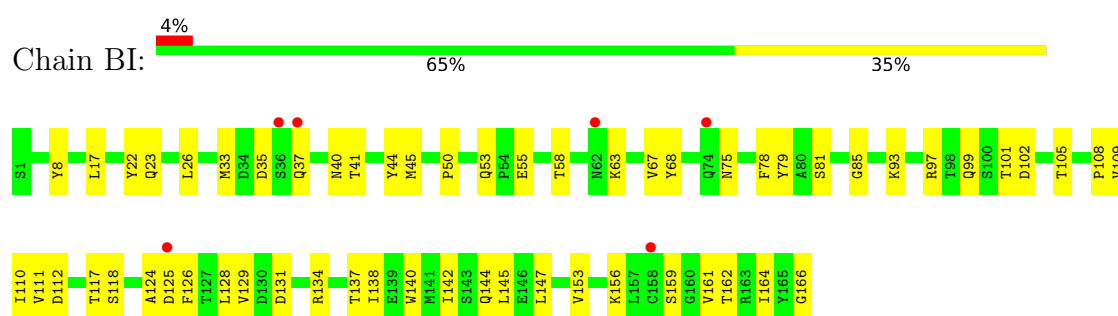
- Molecule 1: coat protein



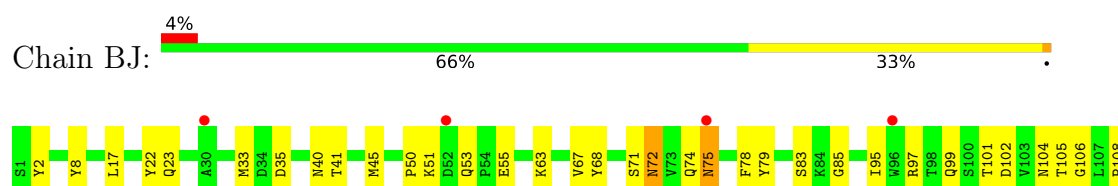
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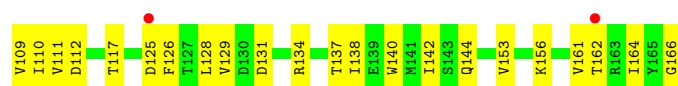


- Molecule 1: coat protein

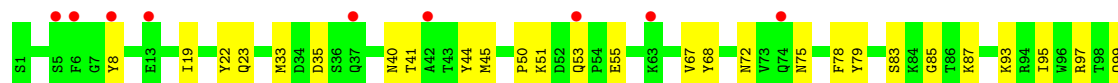


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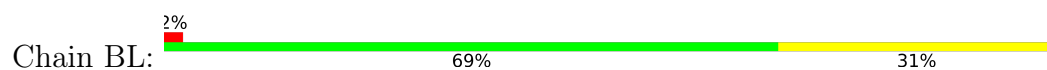




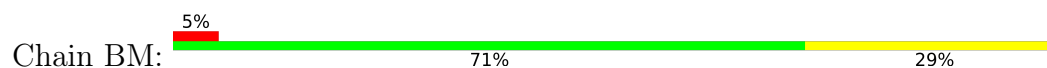
- Molecule 1: coat protein



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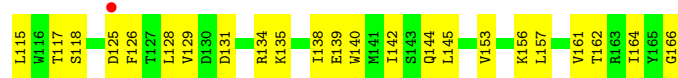
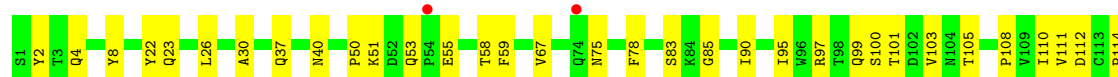


- Molecule 1: coat protein

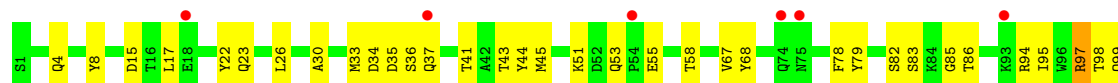


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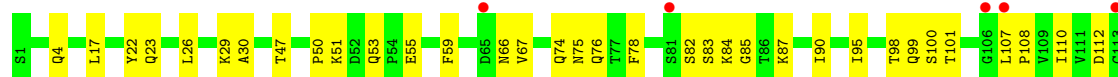
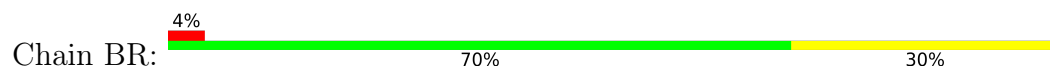
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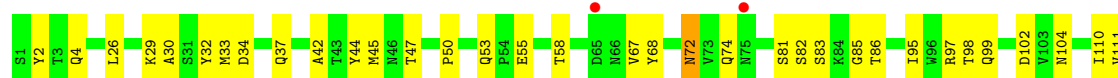
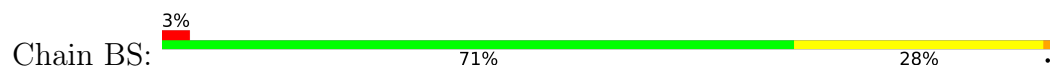
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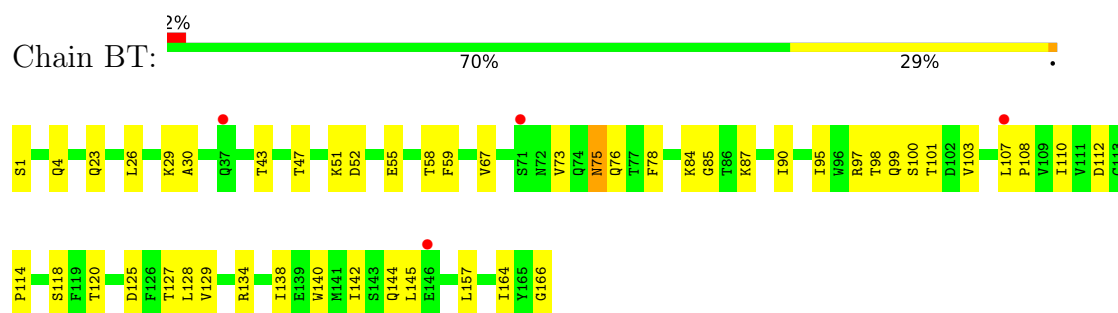


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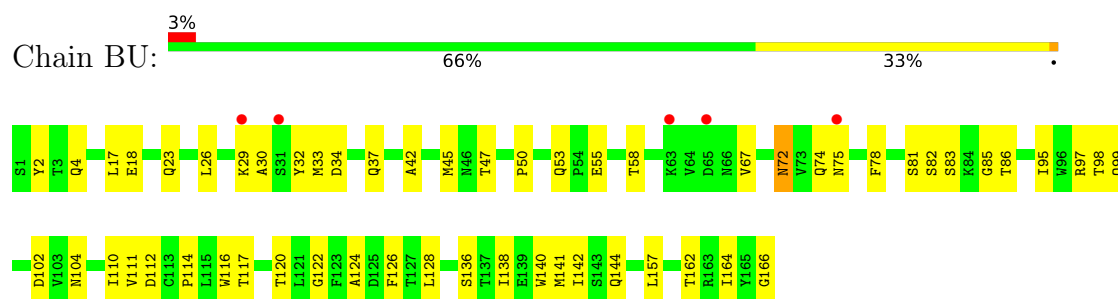




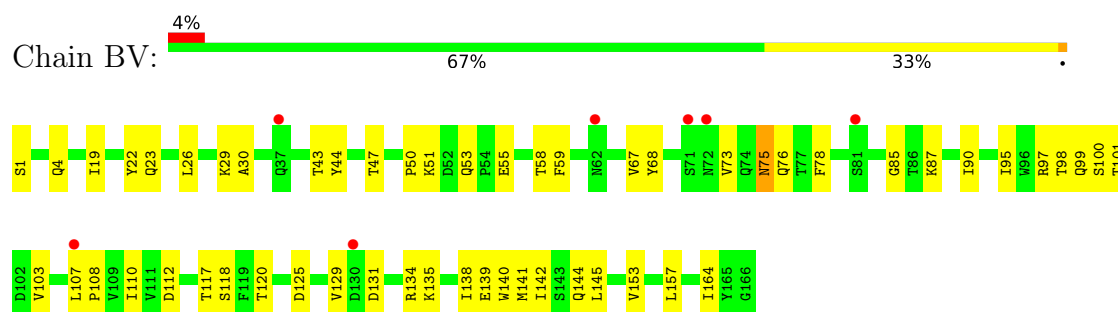
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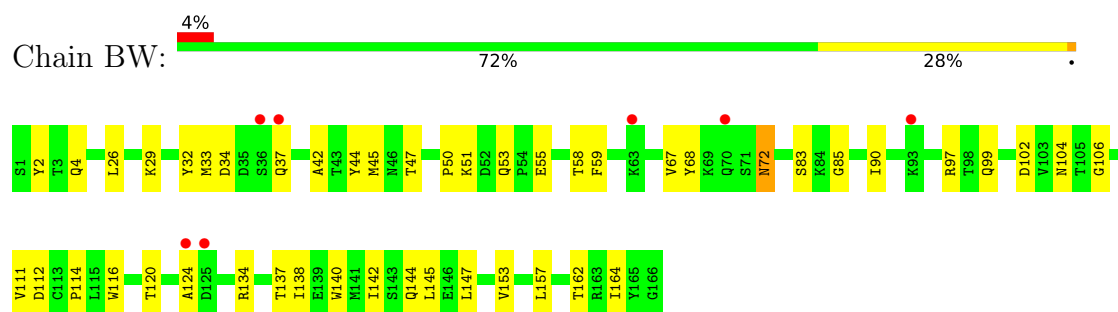
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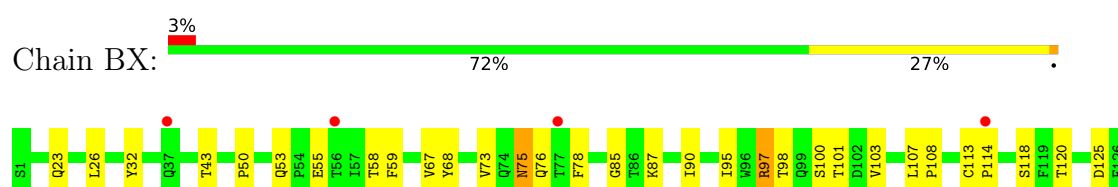
- Molecule 1: coat protein



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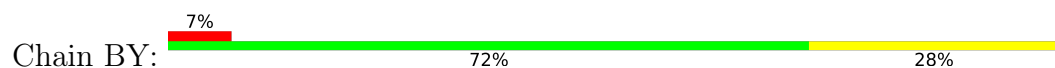


- Molecule 1: coat protein

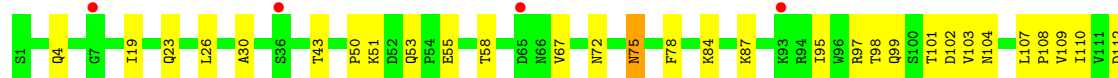




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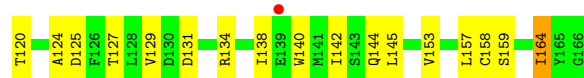
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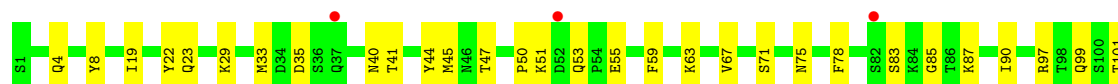


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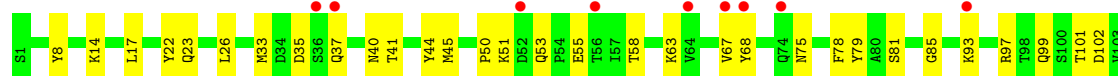


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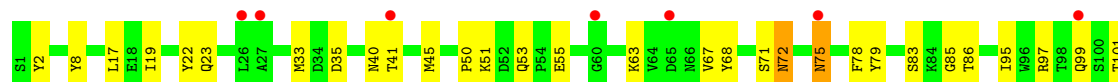




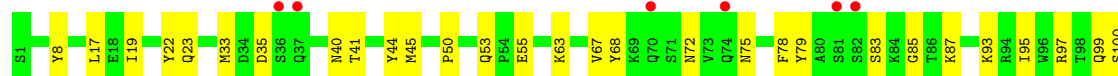
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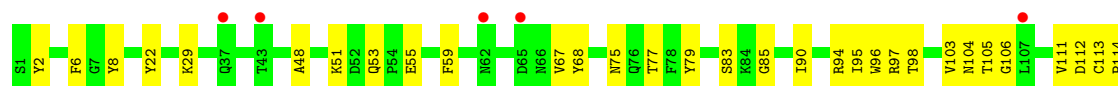
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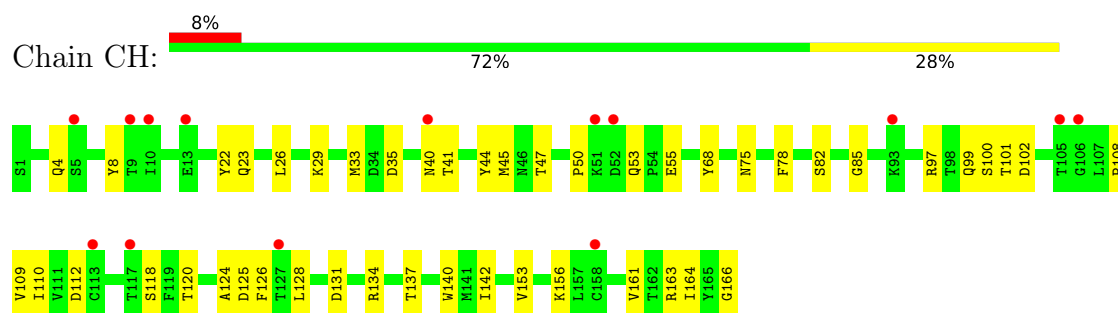
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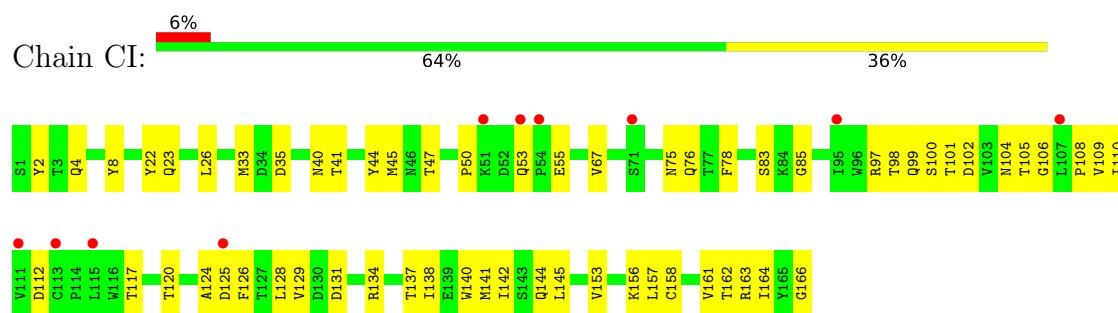
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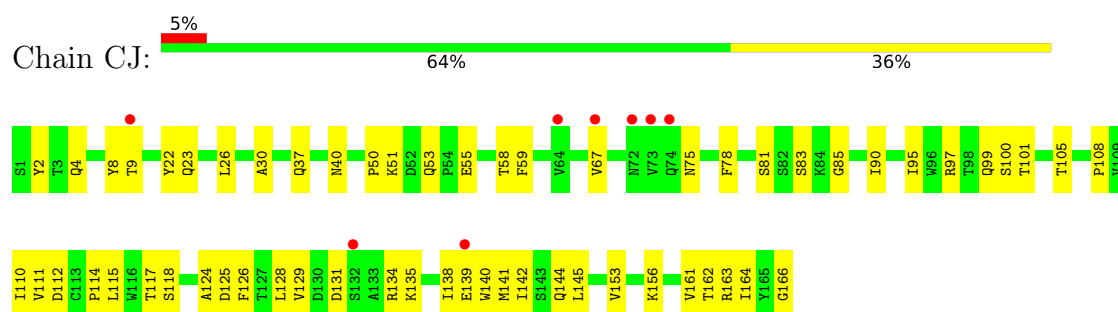
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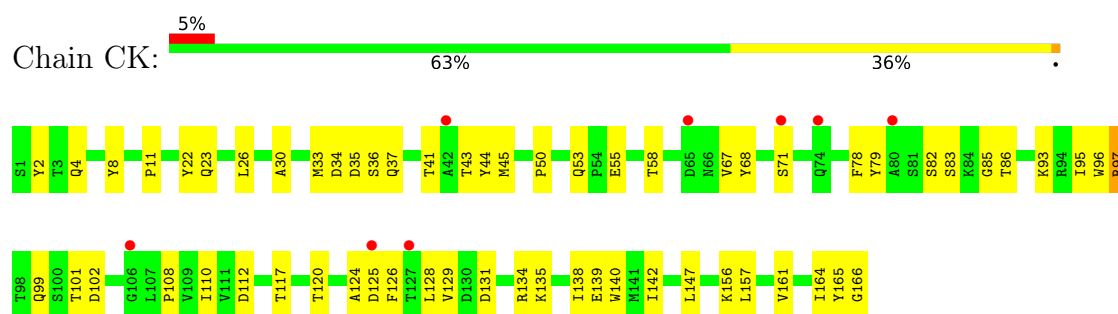
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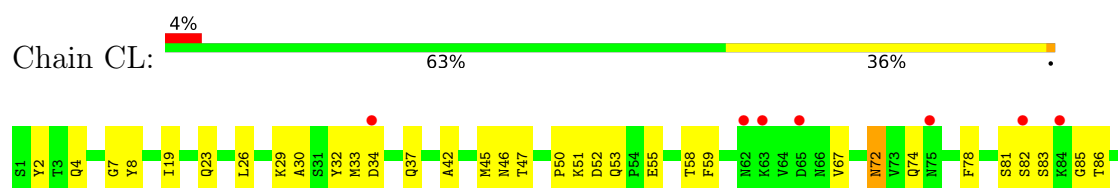
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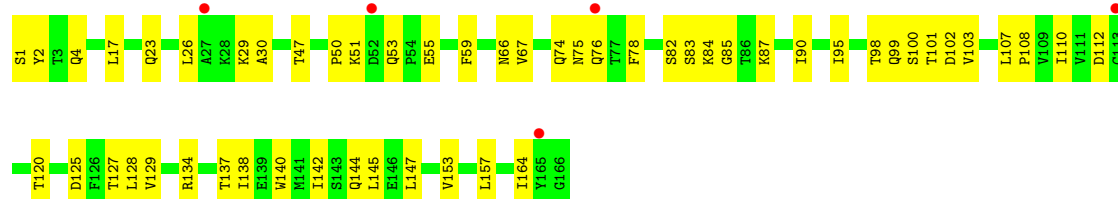
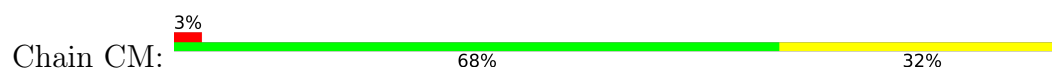


- Molecule 1: coat protein

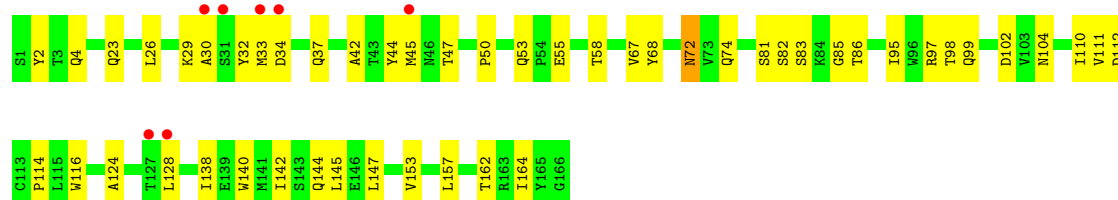
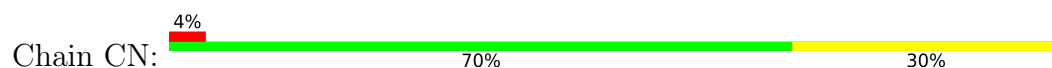




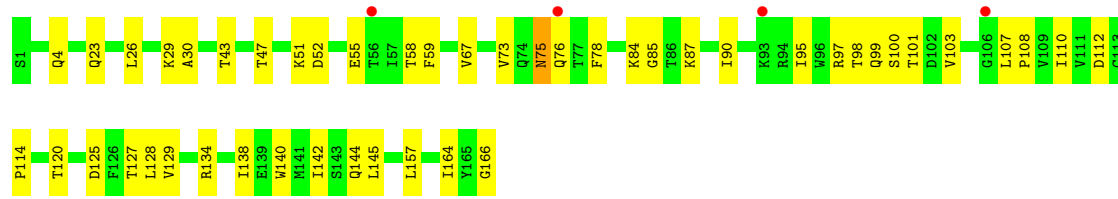
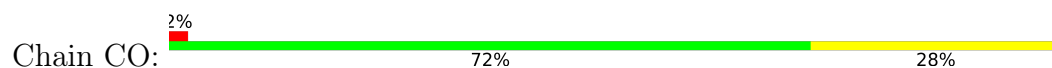
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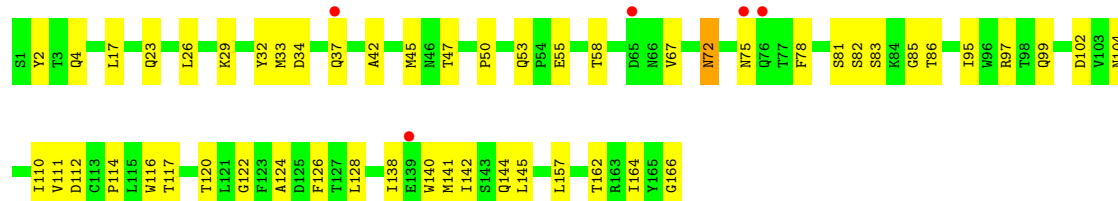
- Molecule 1: coat protein



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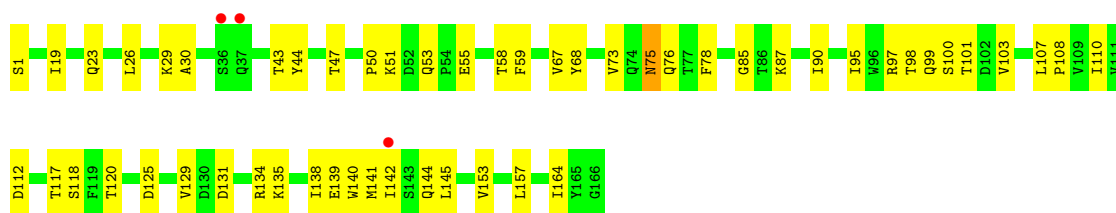


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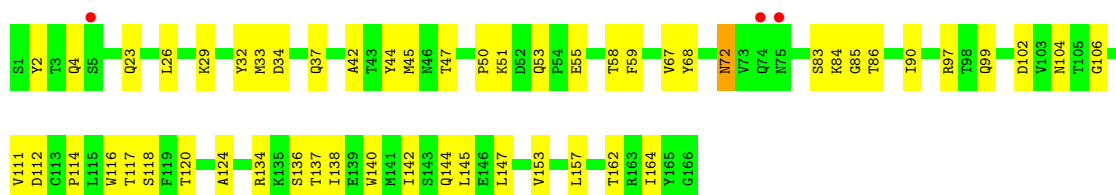


- Molecule 1: coat protein

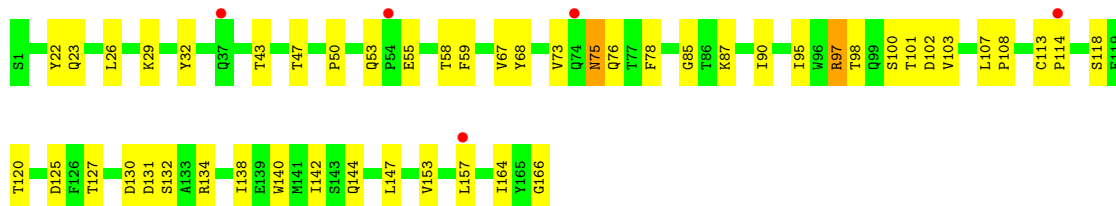
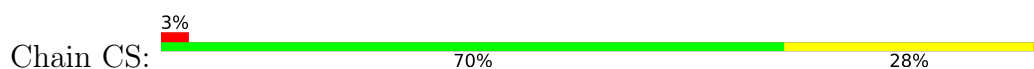




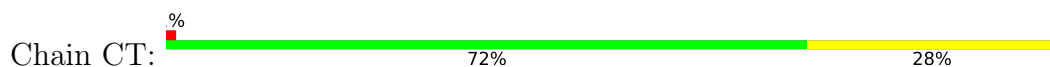
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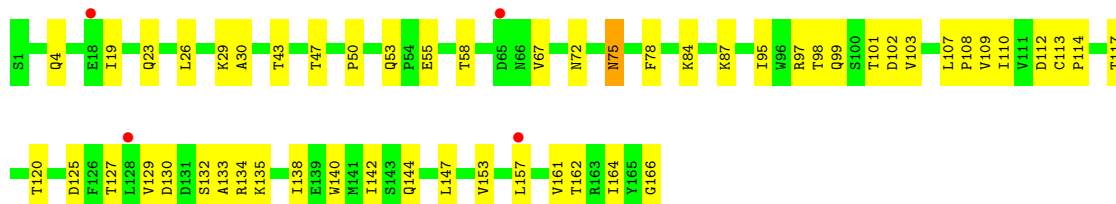
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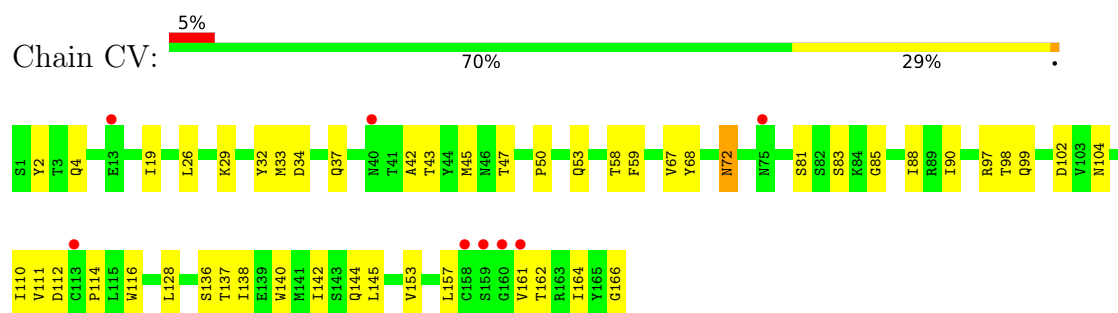
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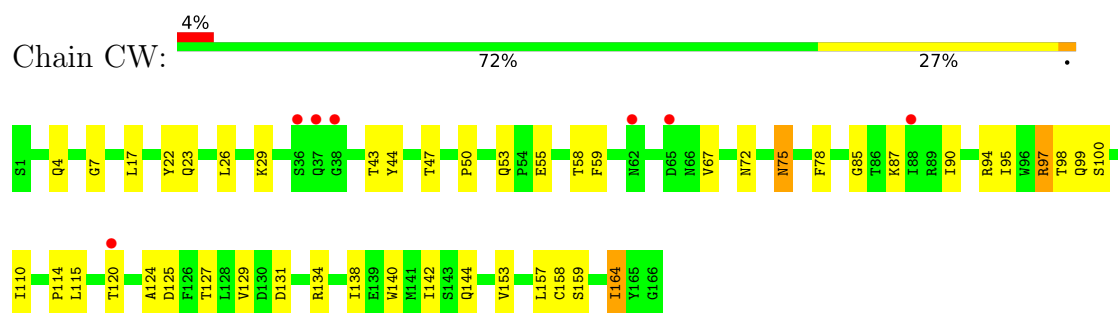
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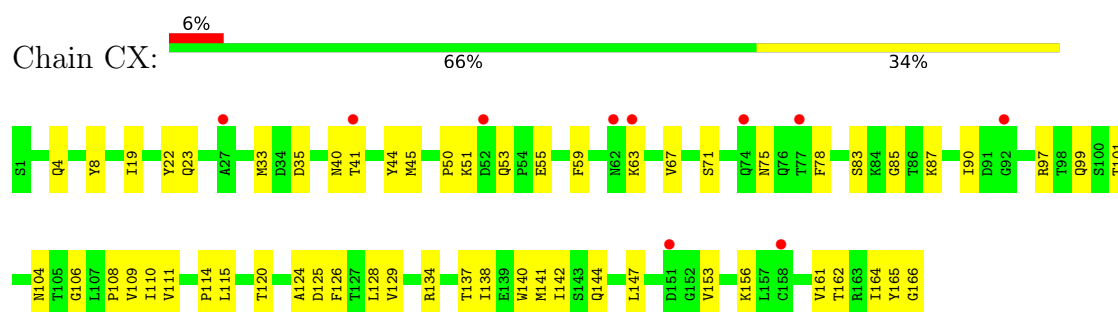
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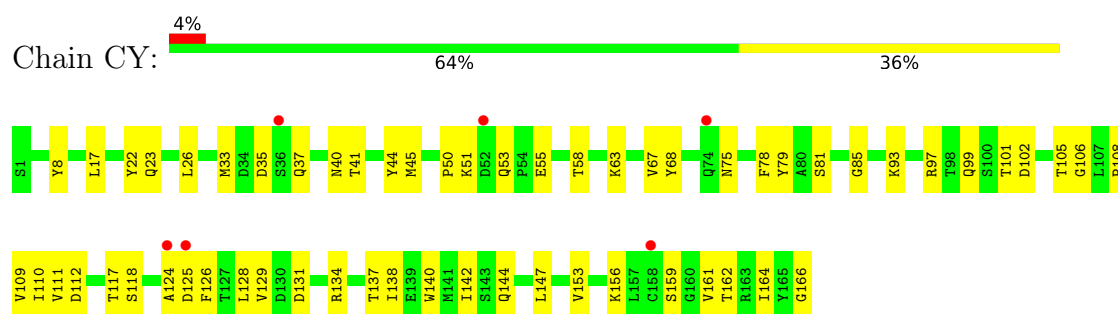
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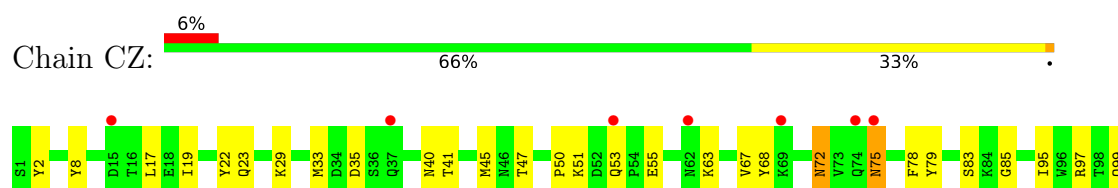
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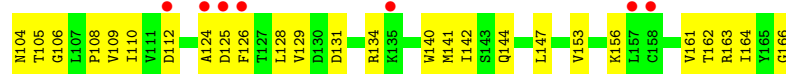
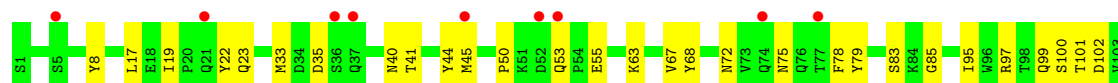


- Molecule 1: coat protein

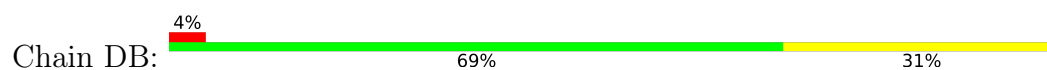




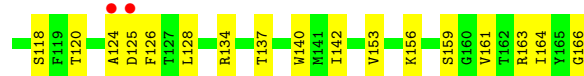
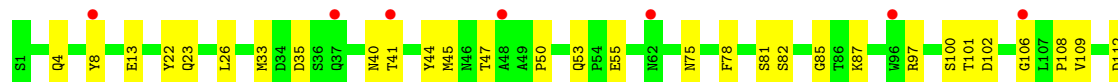
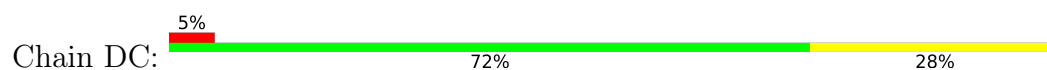
- Molecule 1: coat protein



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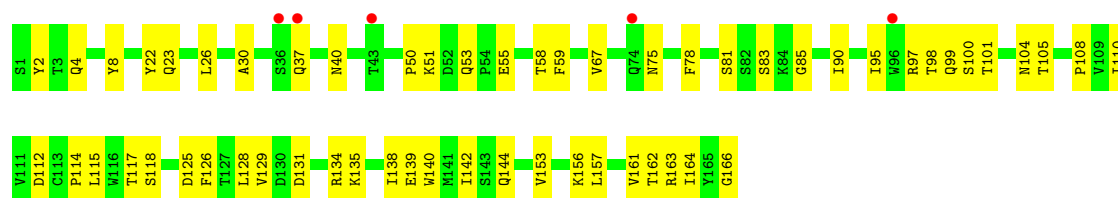
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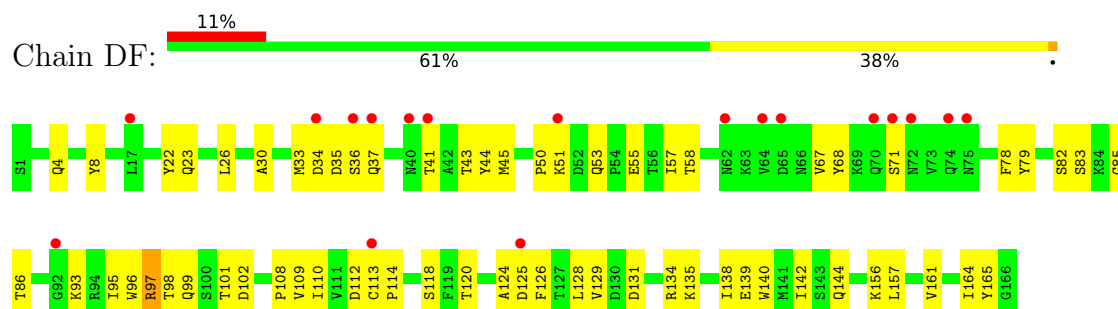
- Molecule 1: coat protein



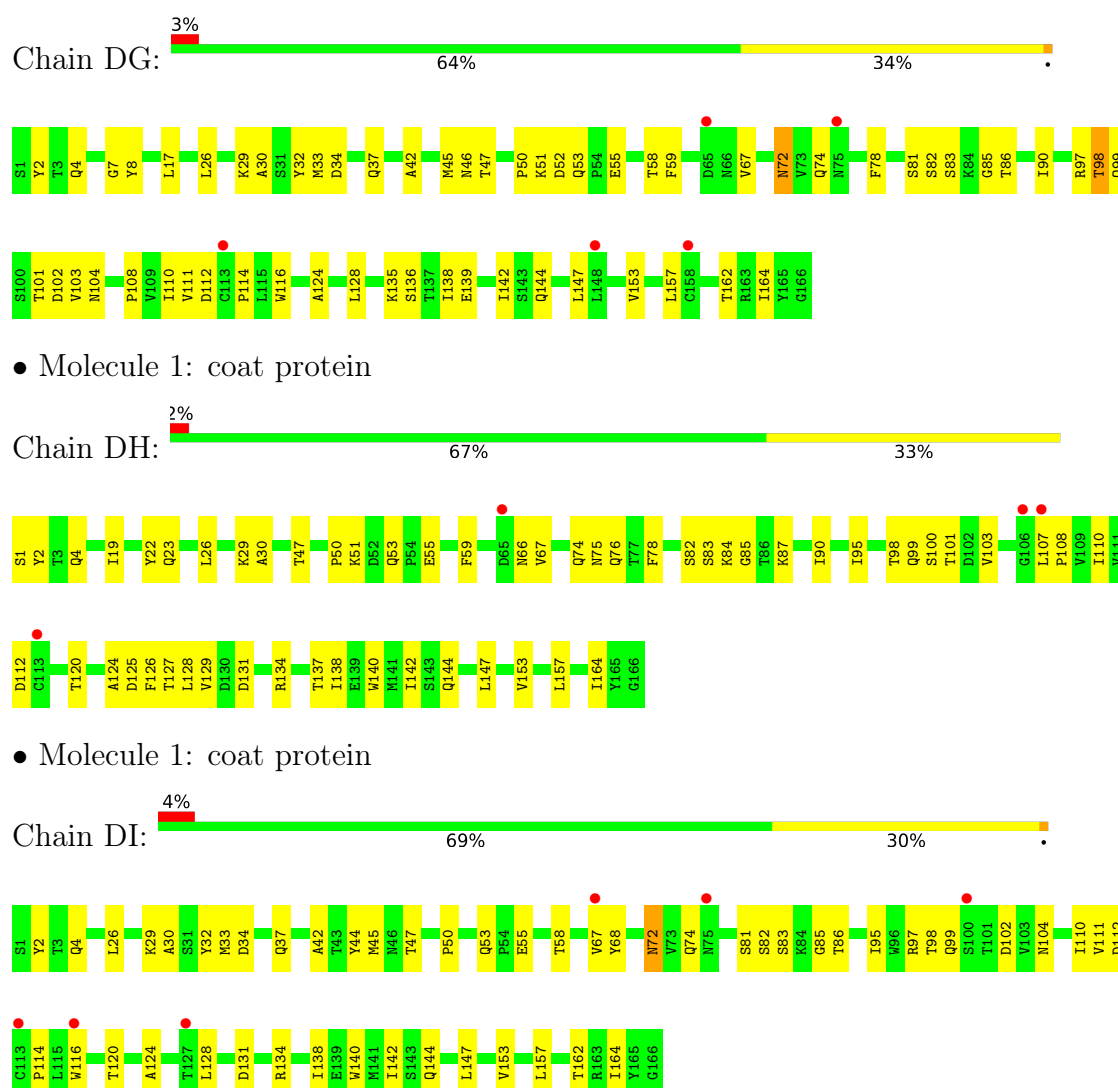




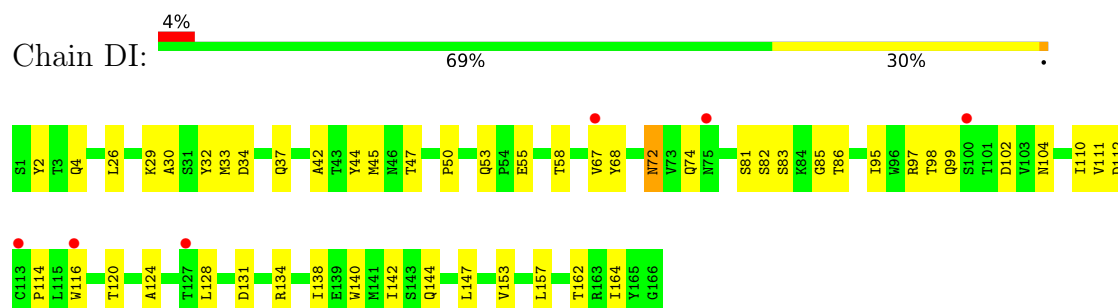
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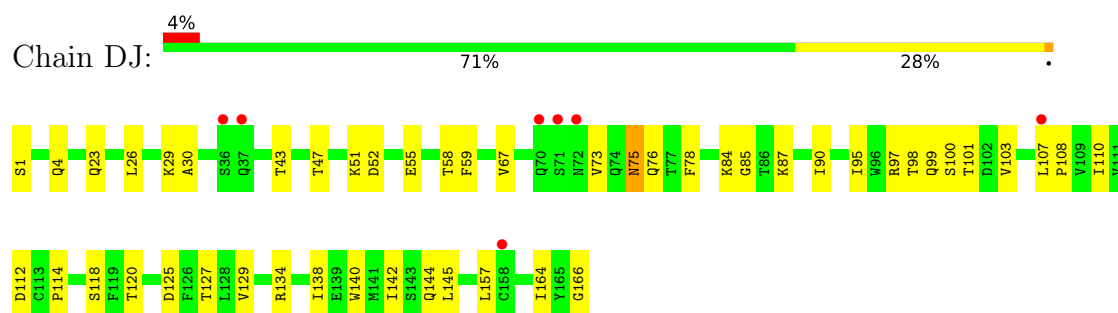
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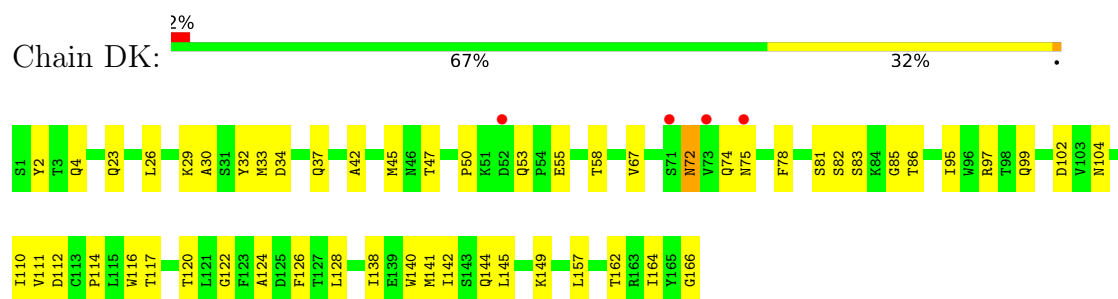
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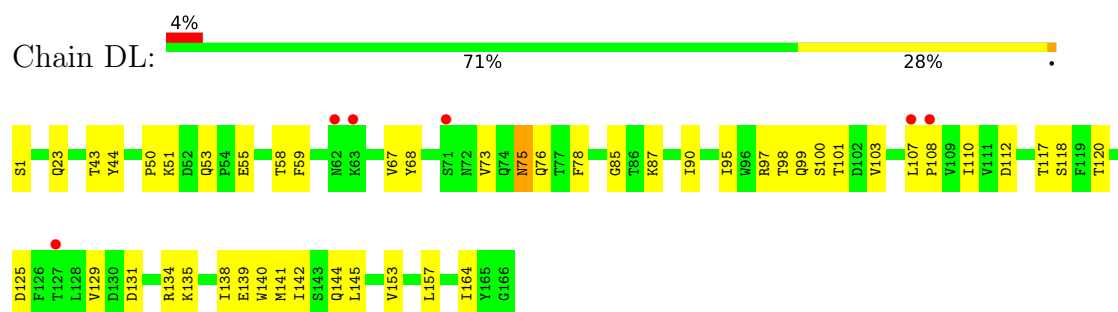
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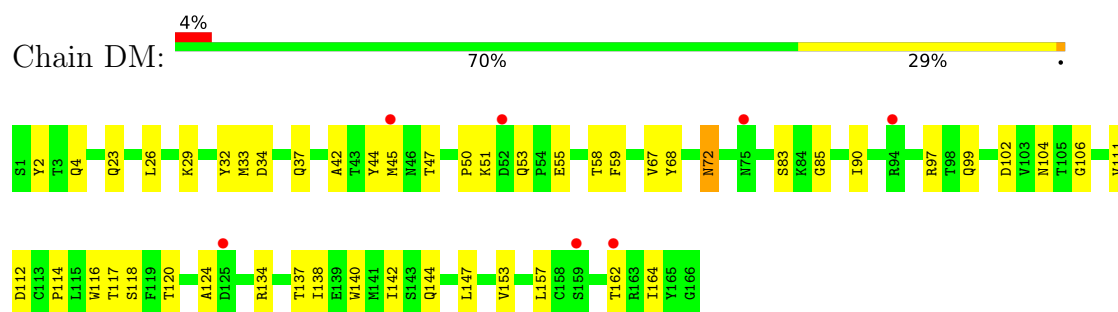
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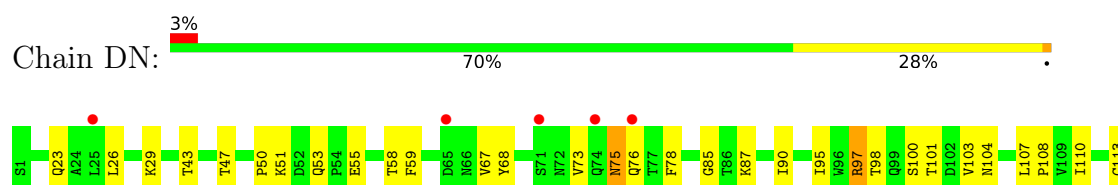
- Molecule 1: coat protein



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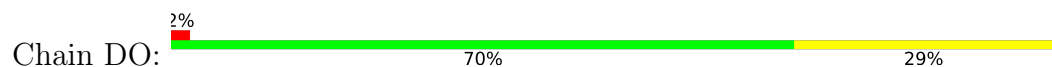


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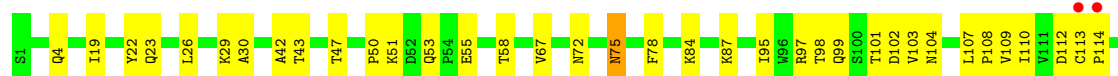




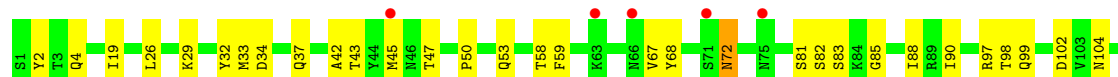
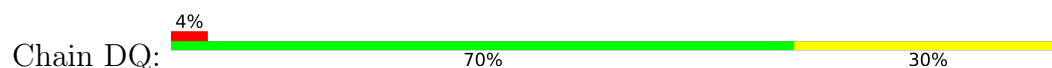
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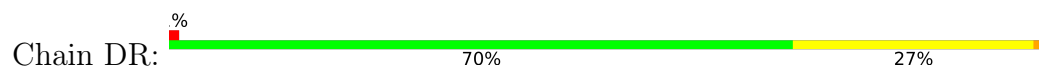
- Molecule 1: coat protein



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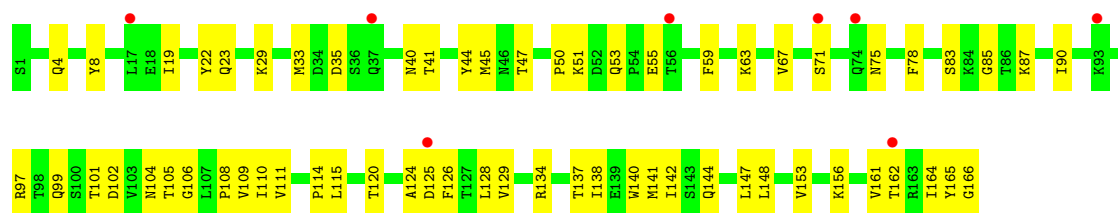


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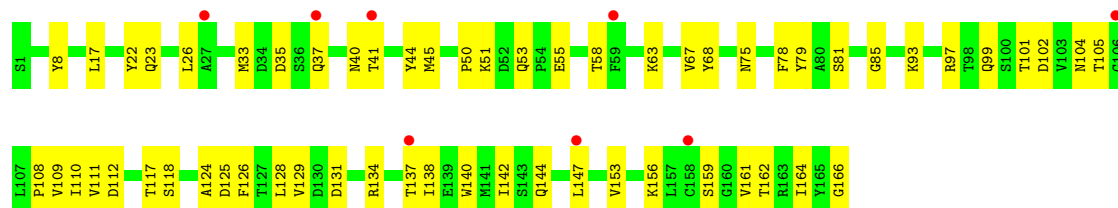


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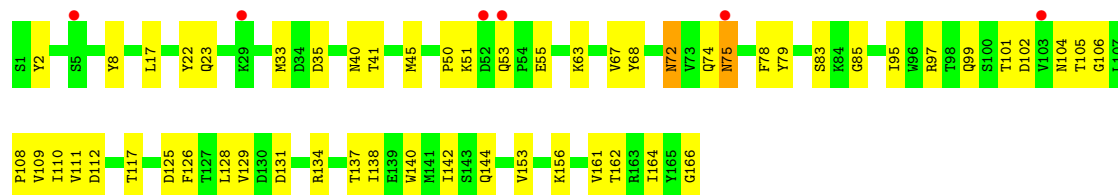




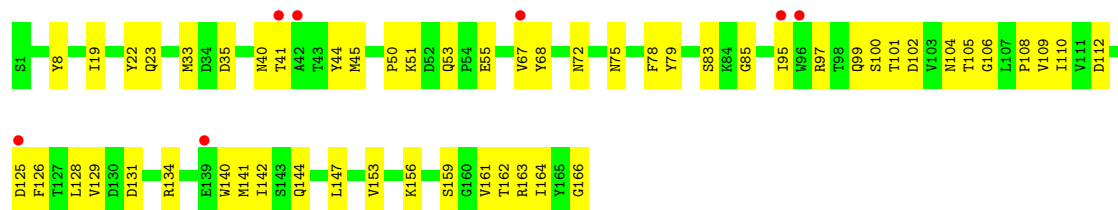
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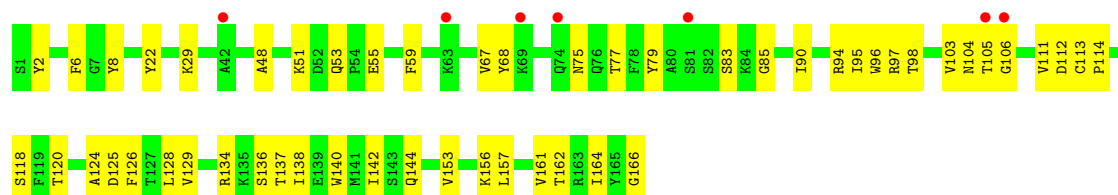
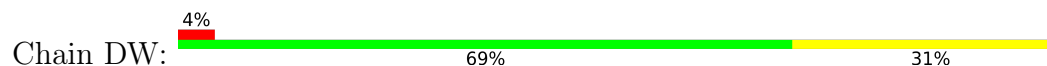
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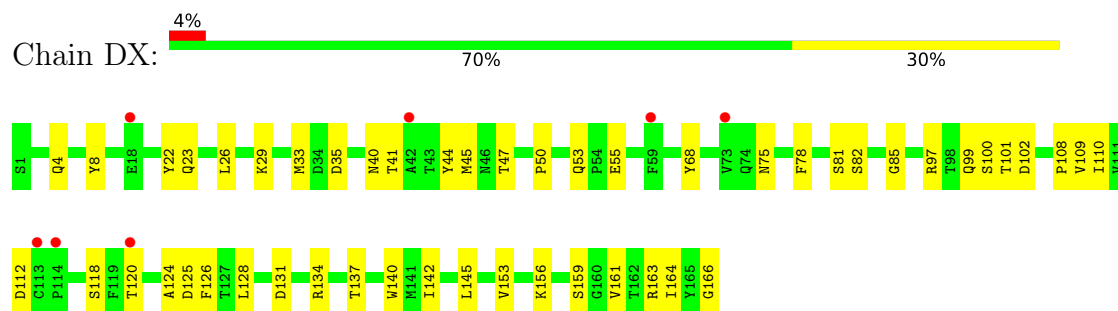
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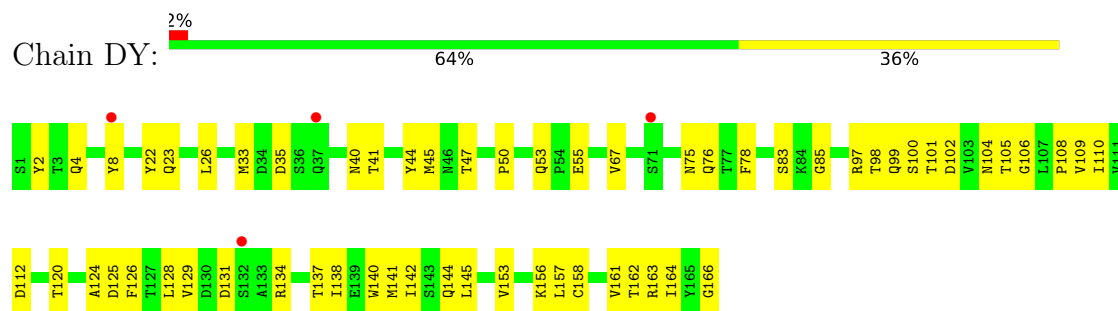
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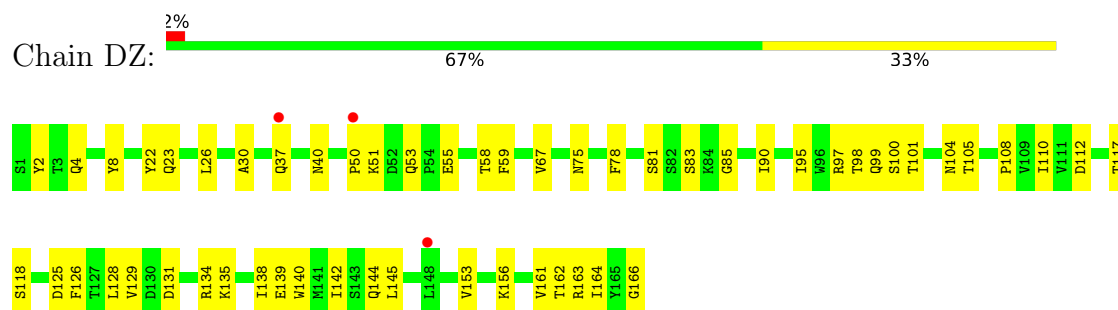
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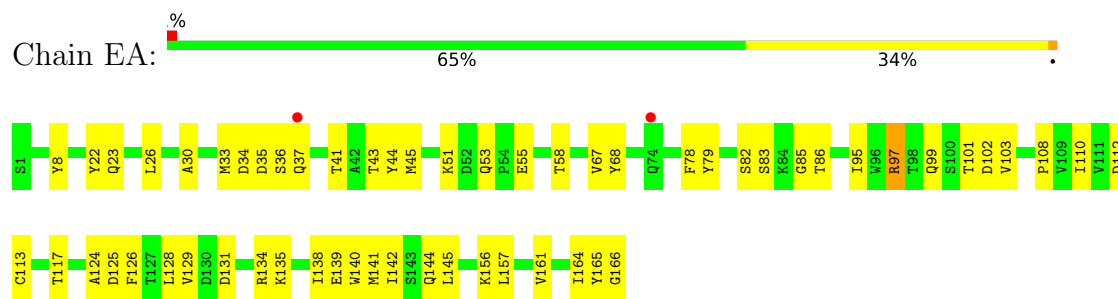
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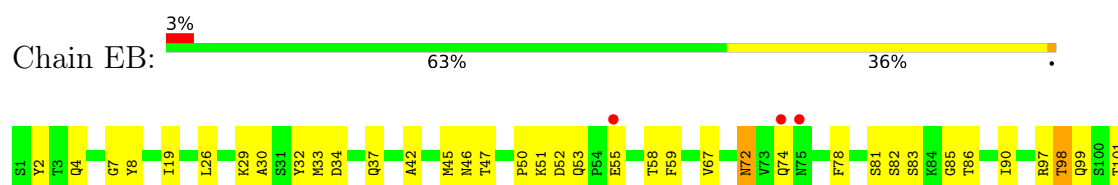
- Molecule 1: coat protein



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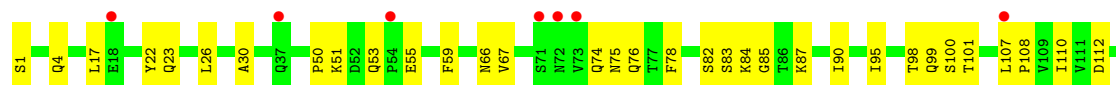
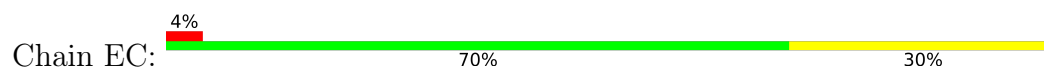


- Molecule 1: coat protein

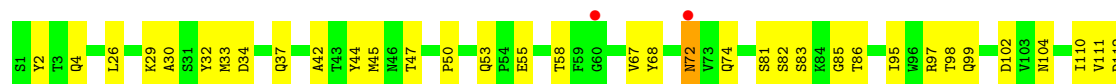
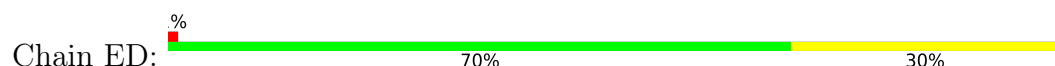




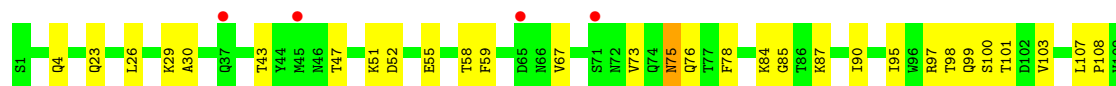
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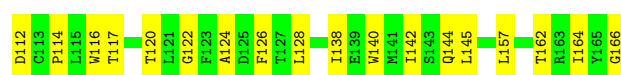
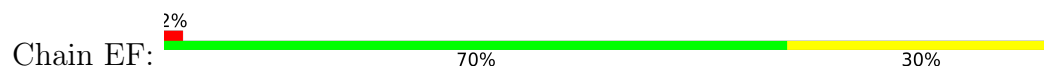
- Molecule 1: coat protein



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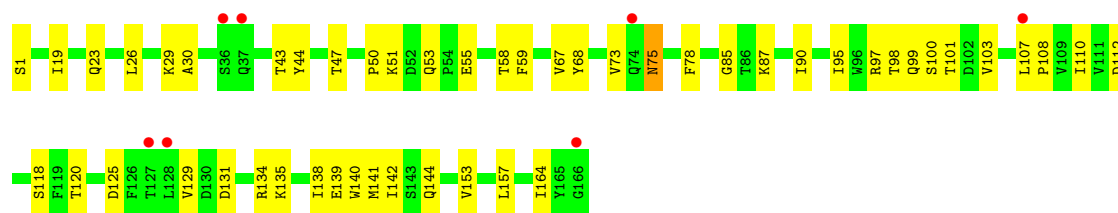


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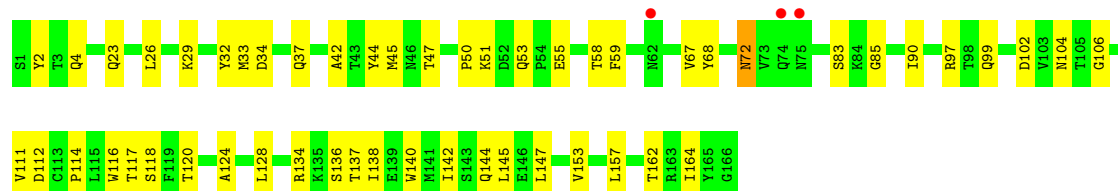


- Molecule 1: coat protein

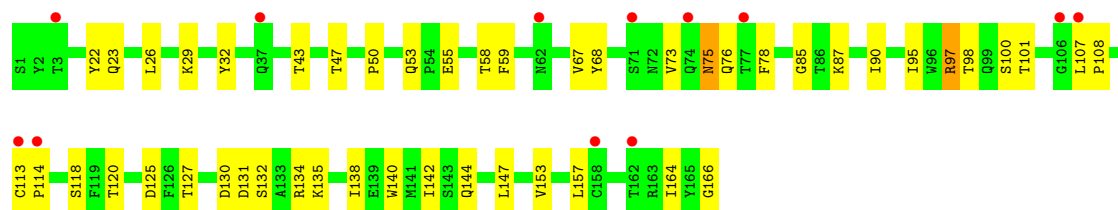




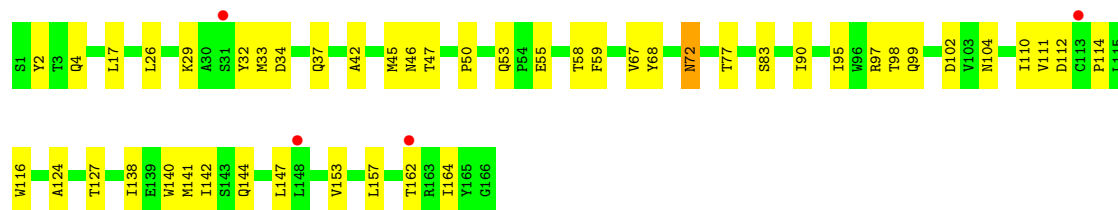
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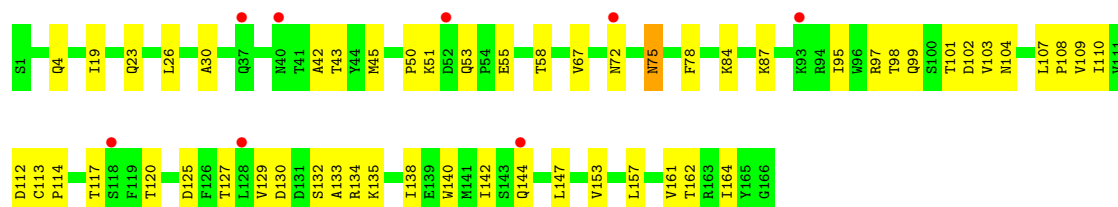
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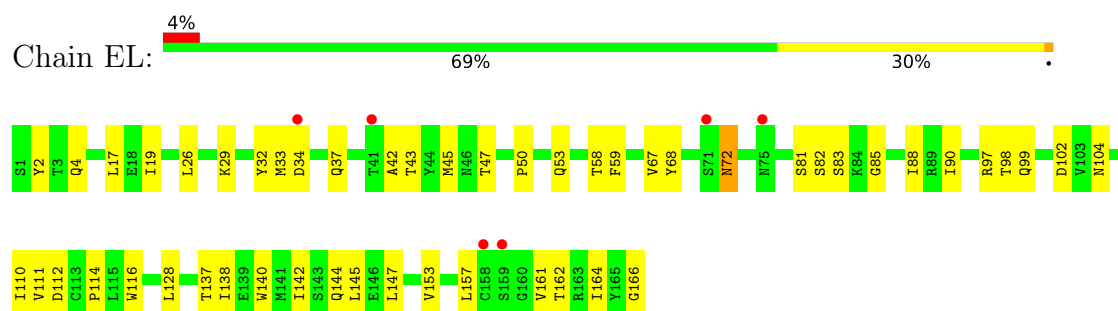
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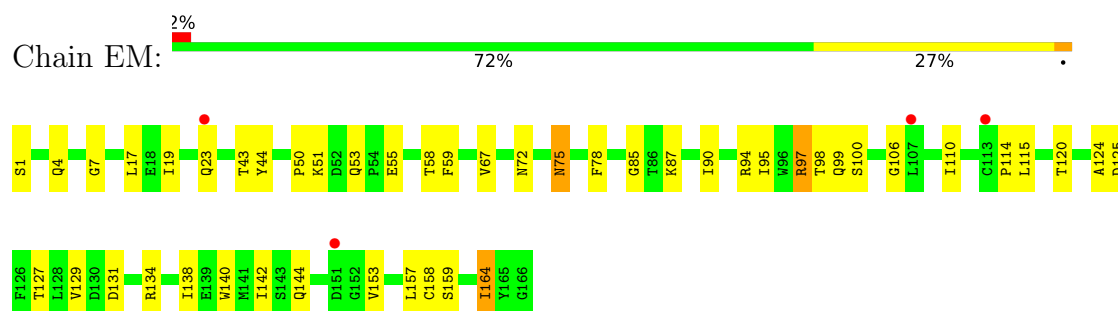
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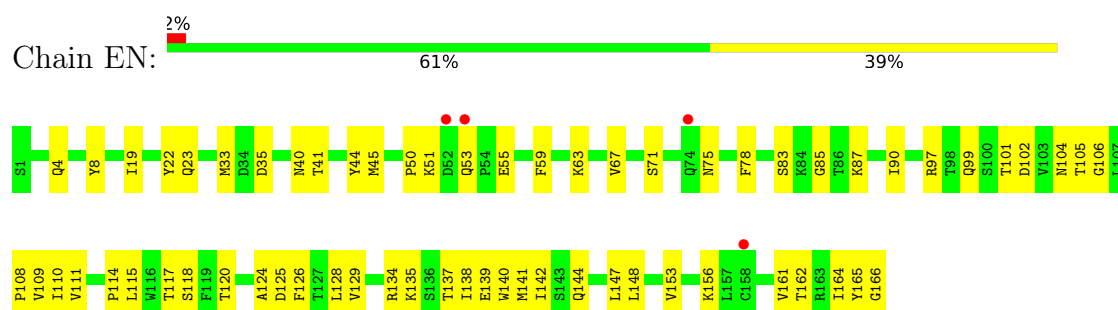
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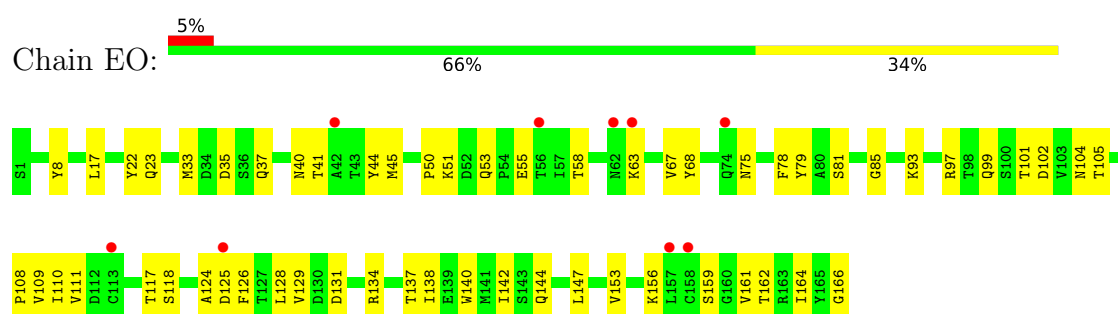
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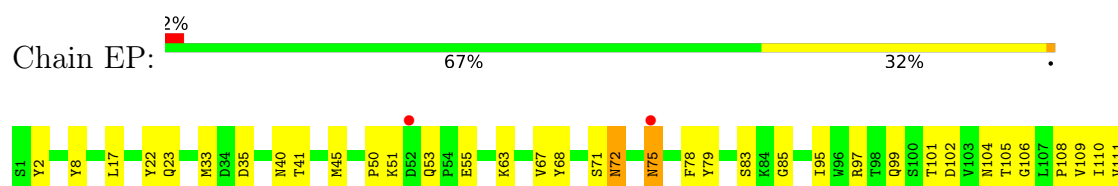
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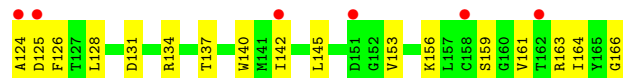
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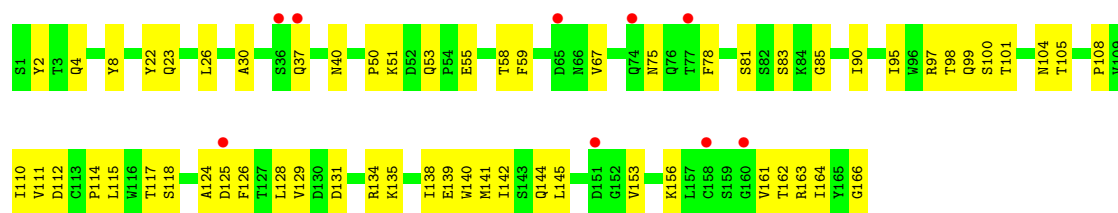


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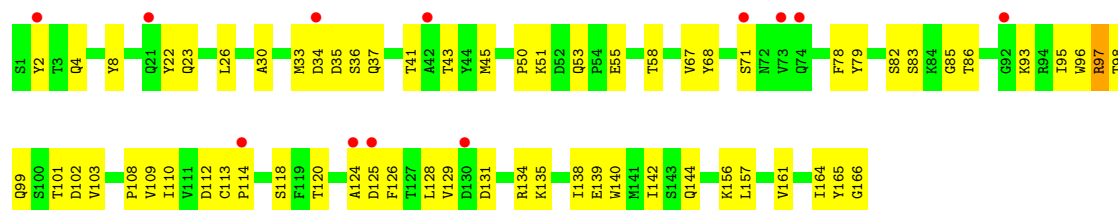


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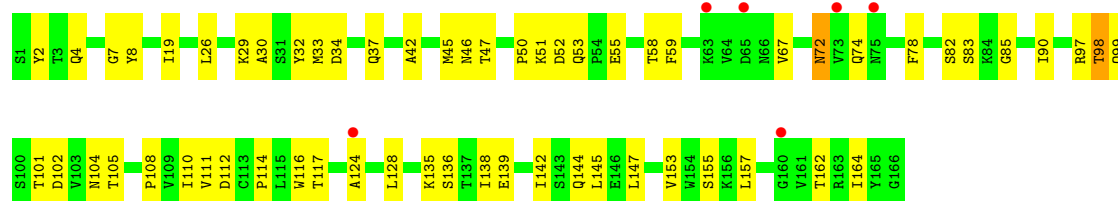




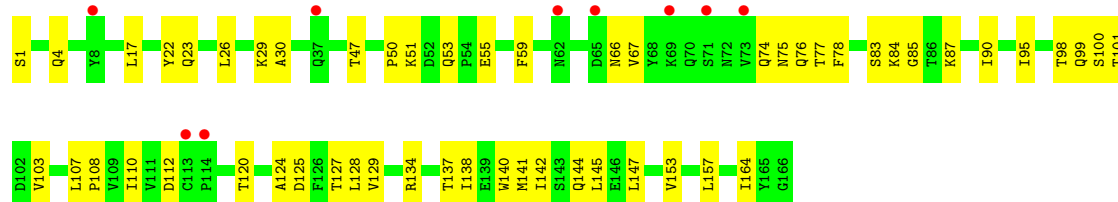
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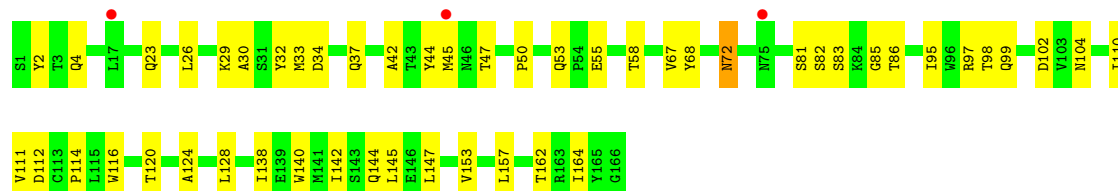
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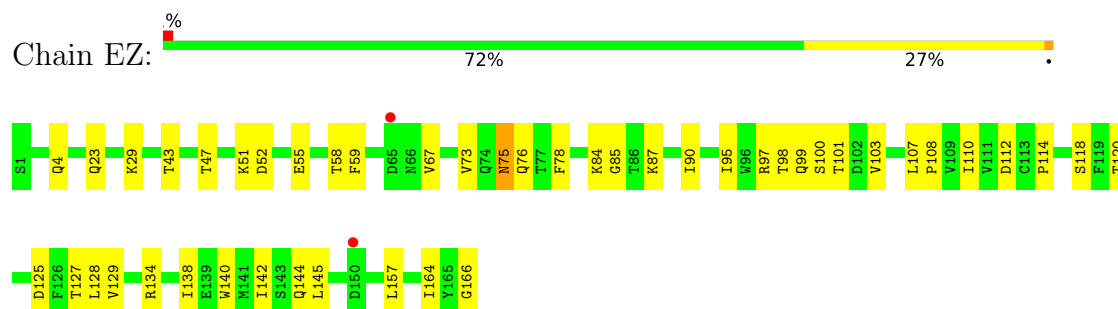
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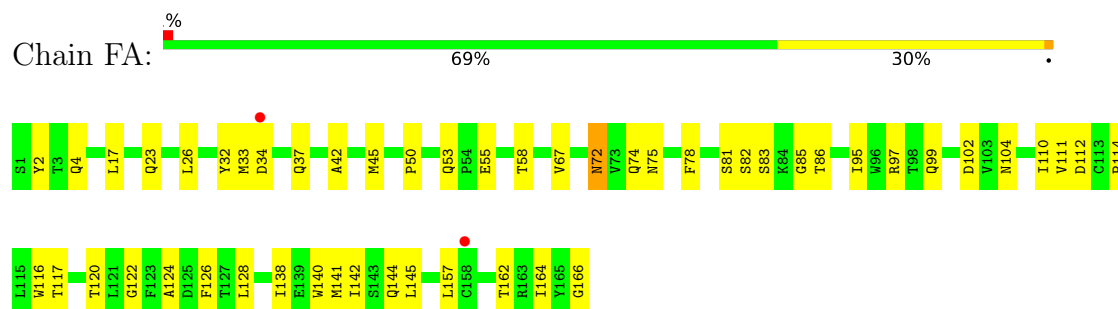
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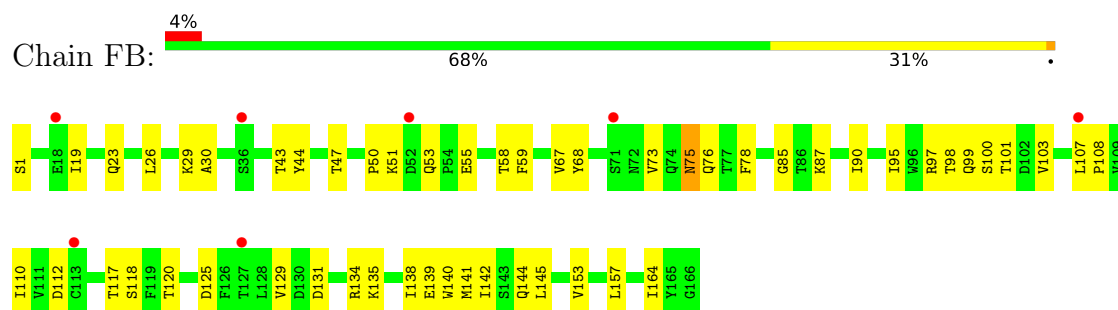
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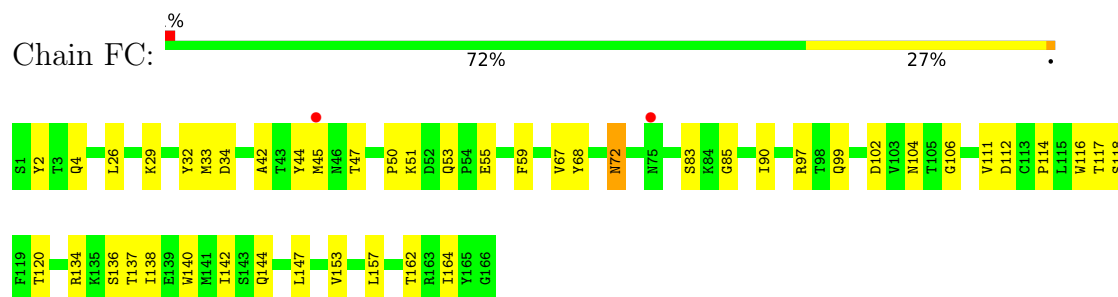
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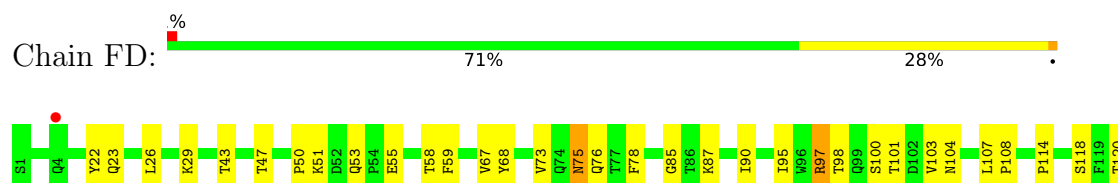
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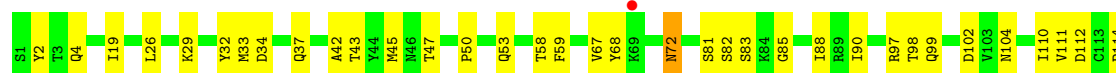
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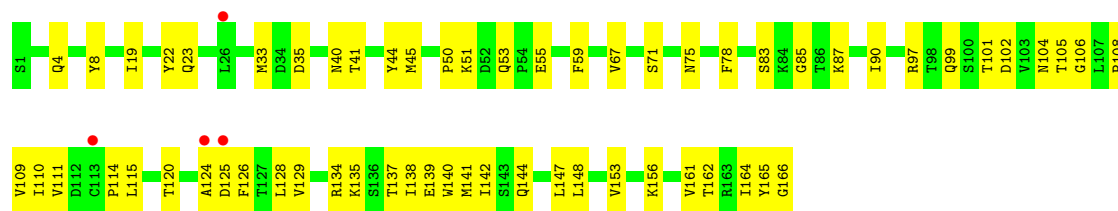


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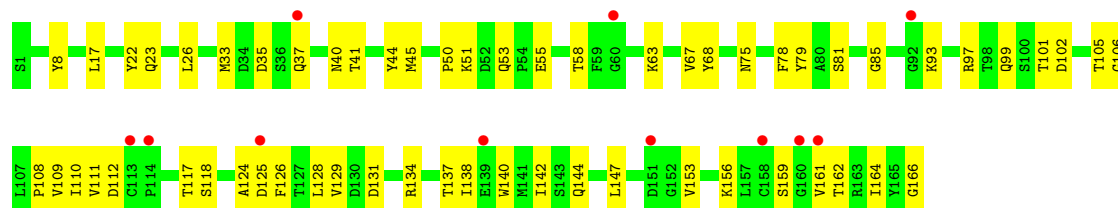


- Molecule 1: coat protein

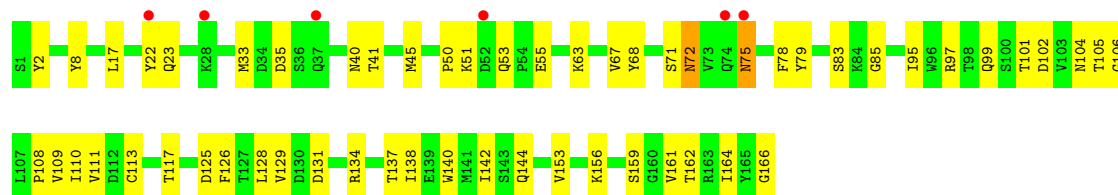




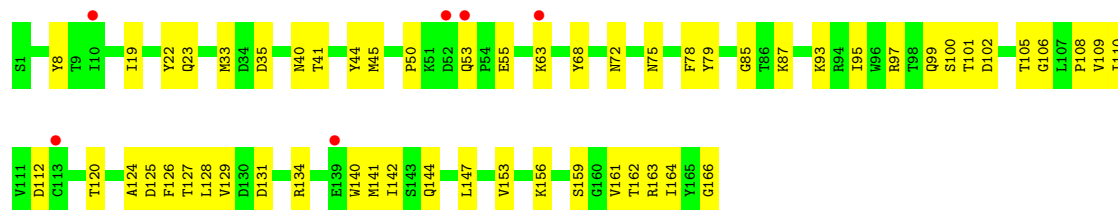
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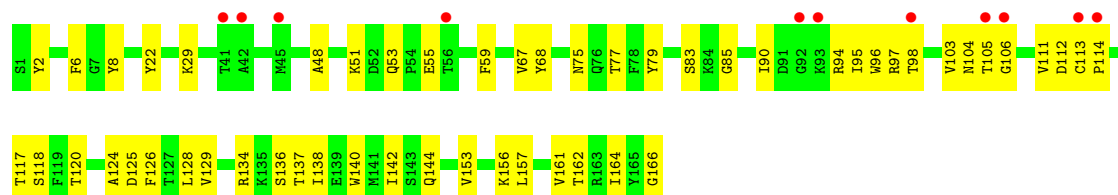
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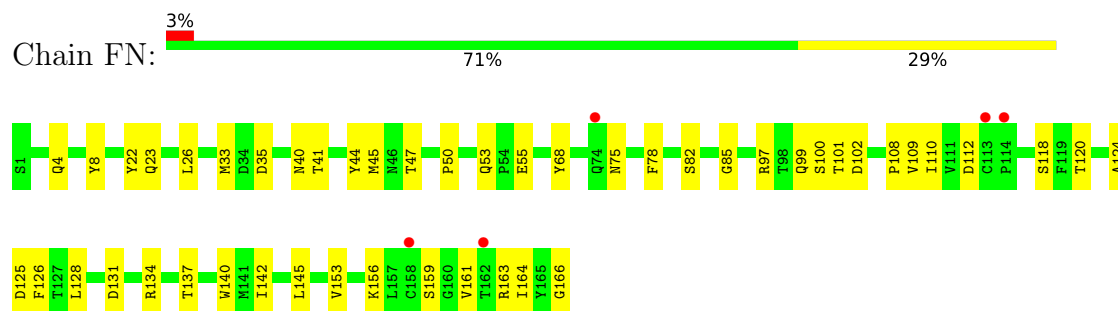
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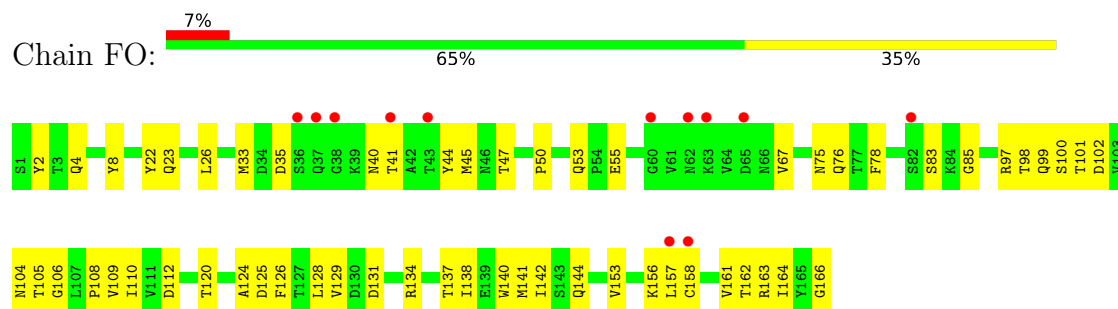
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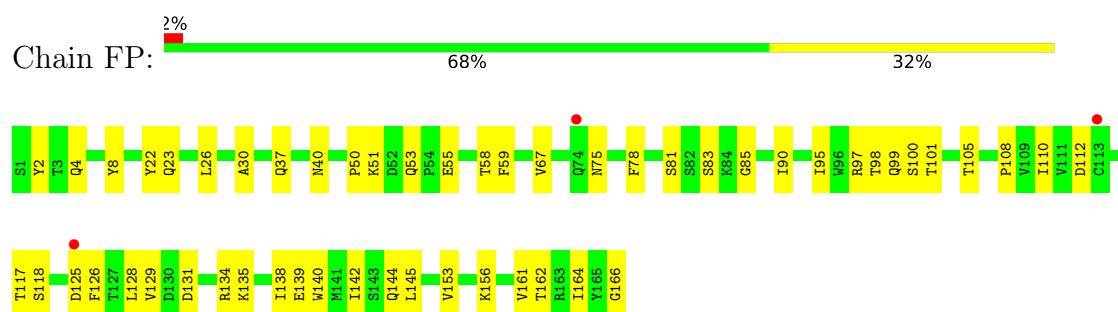
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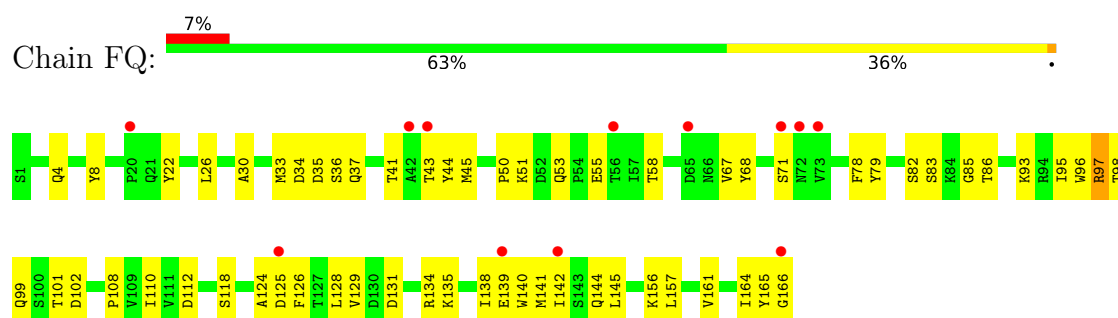
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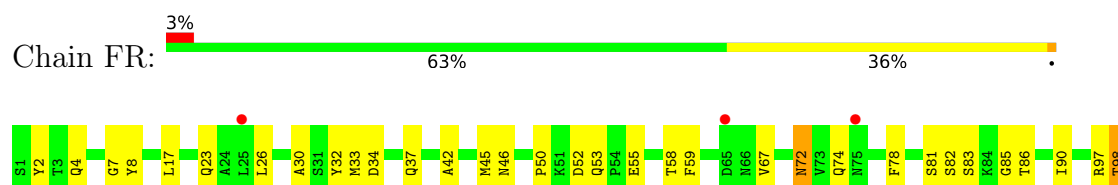
- Molecule 1: coat protein



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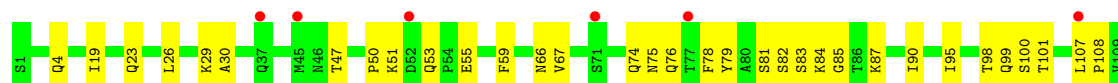


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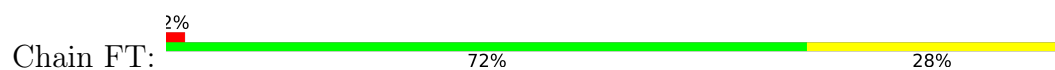




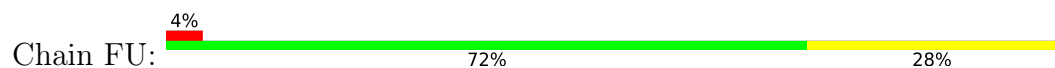
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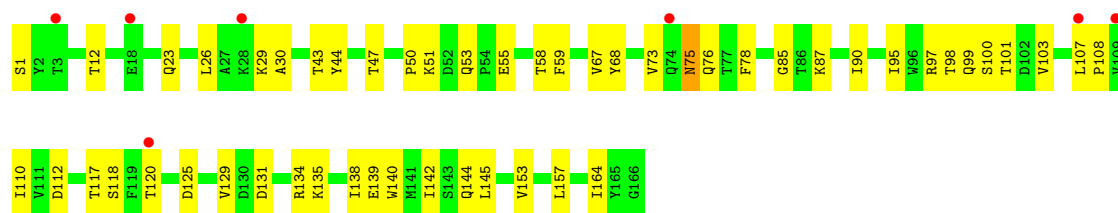


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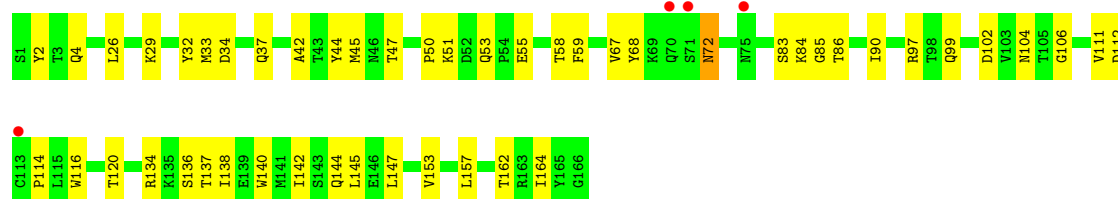
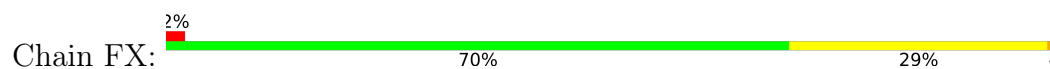


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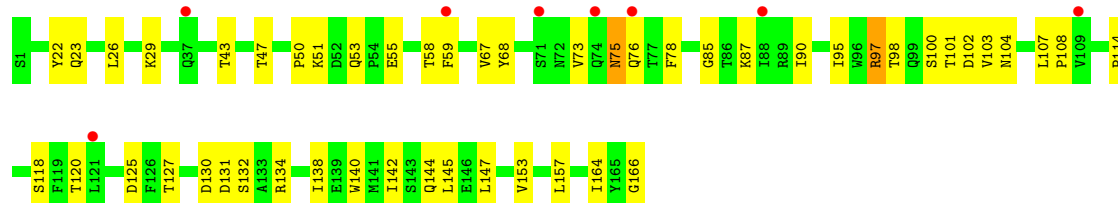




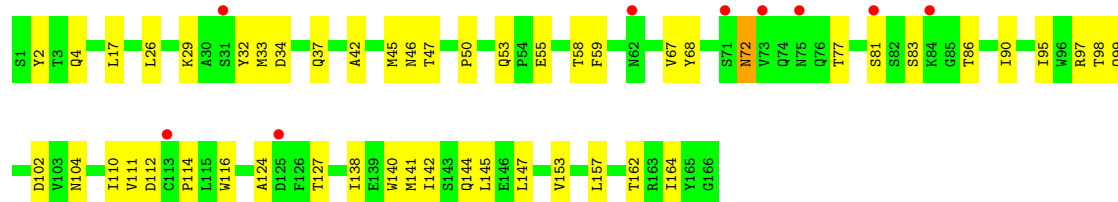
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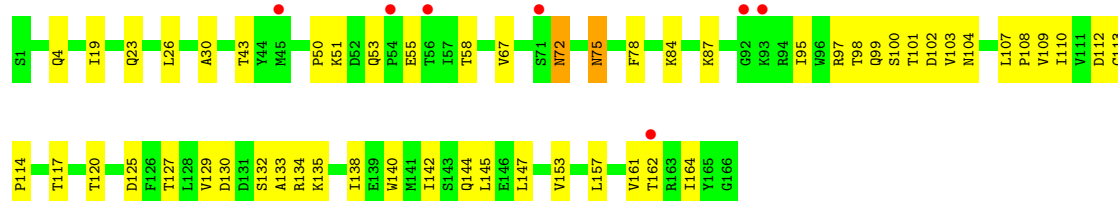
• Molecule 1: coat protein



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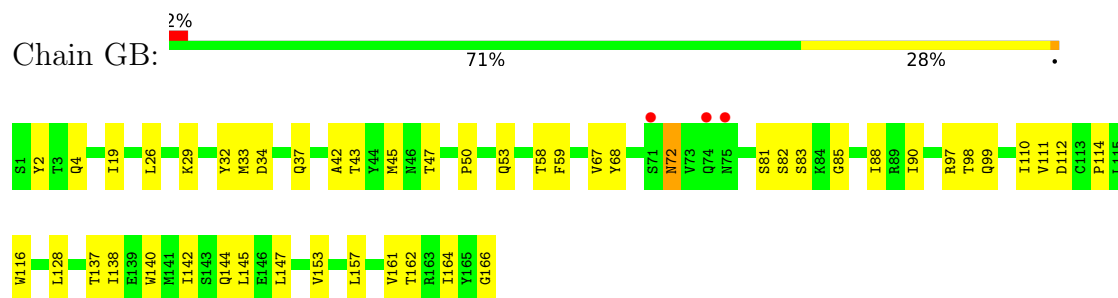


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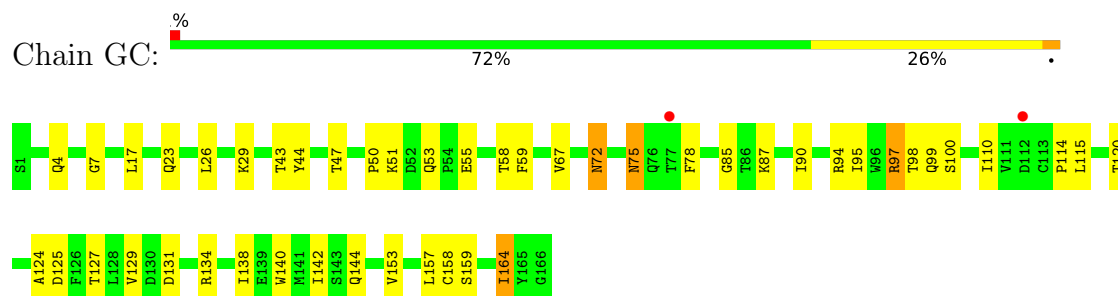




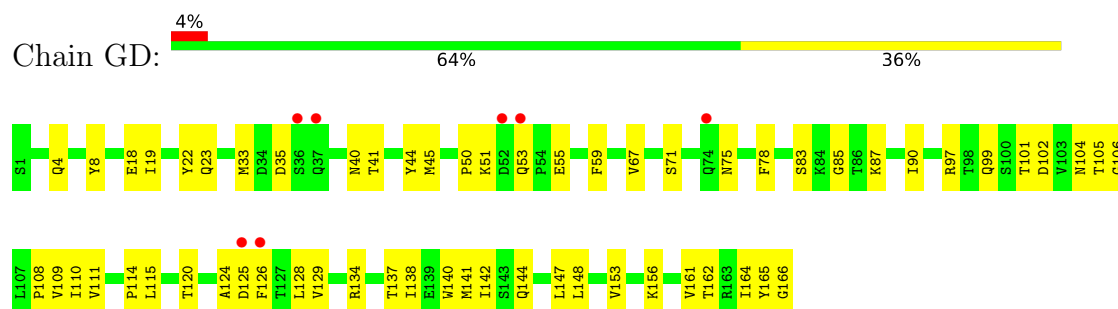
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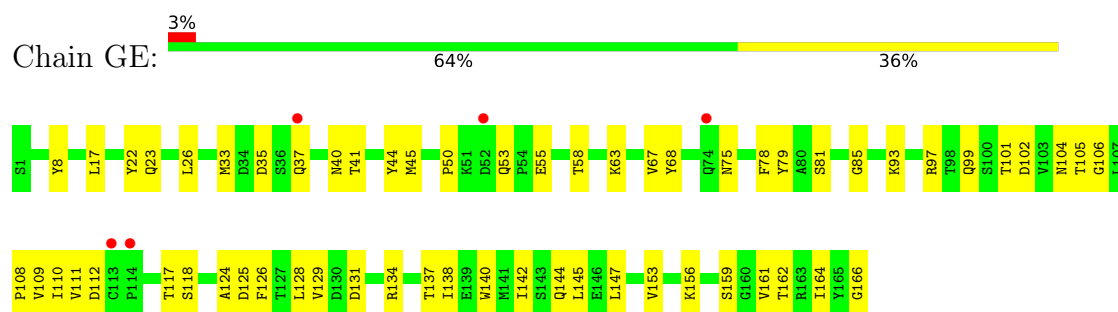
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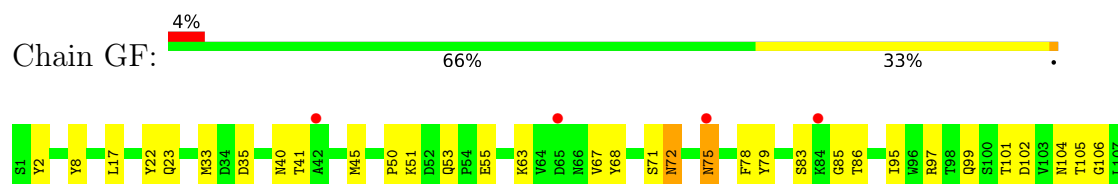
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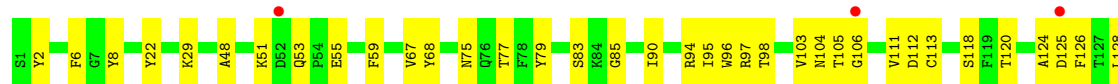
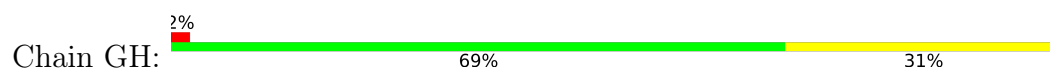




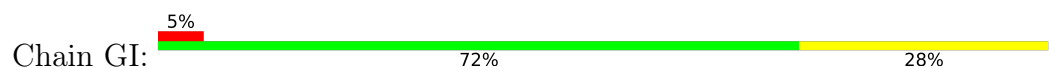
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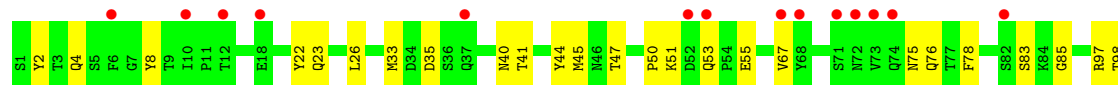
- Molecule 1: coat protein



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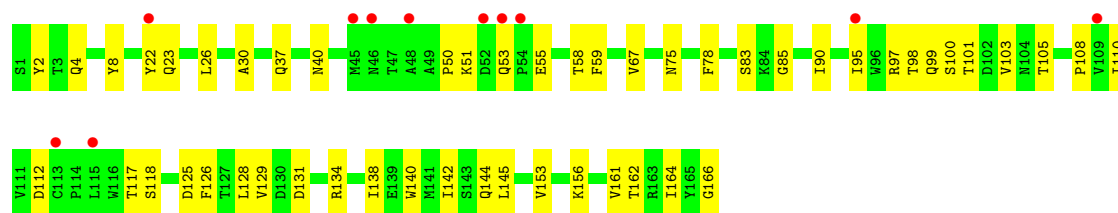


- Molecule 1: coat protein

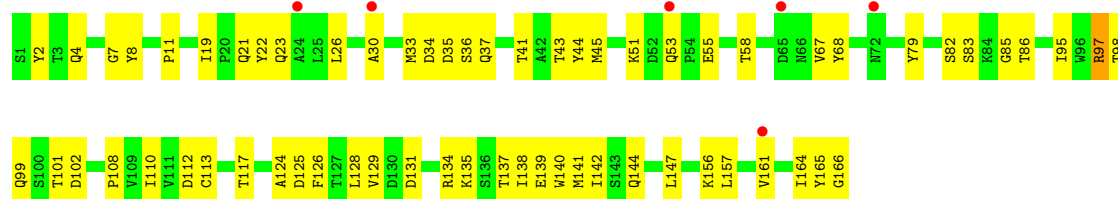


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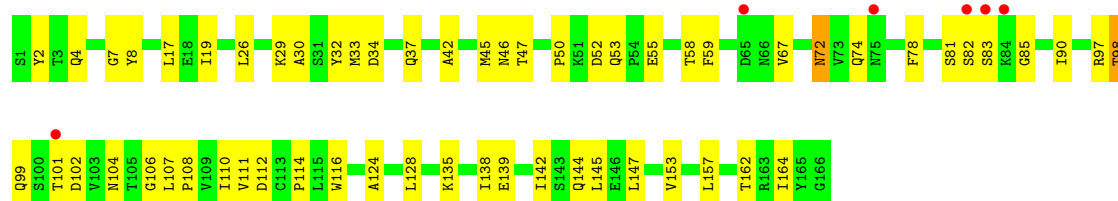




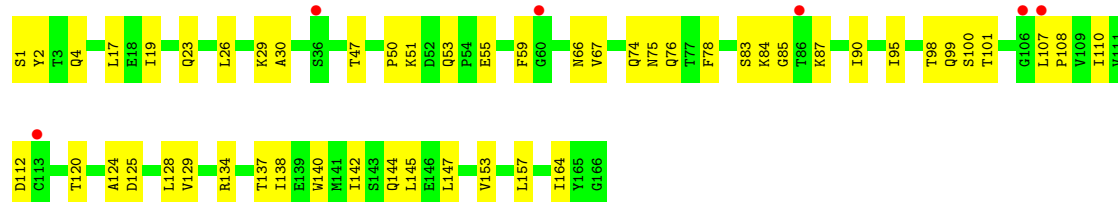
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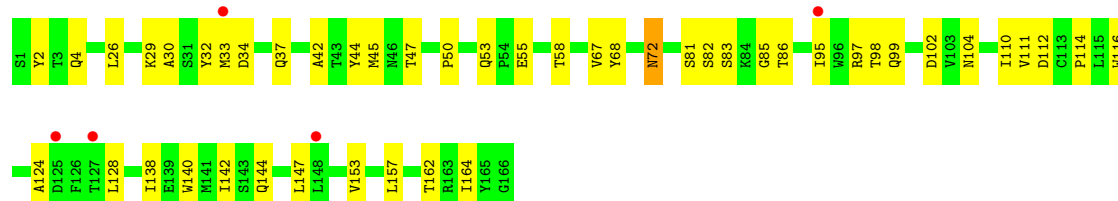
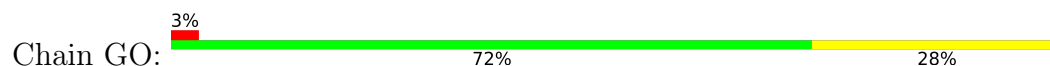
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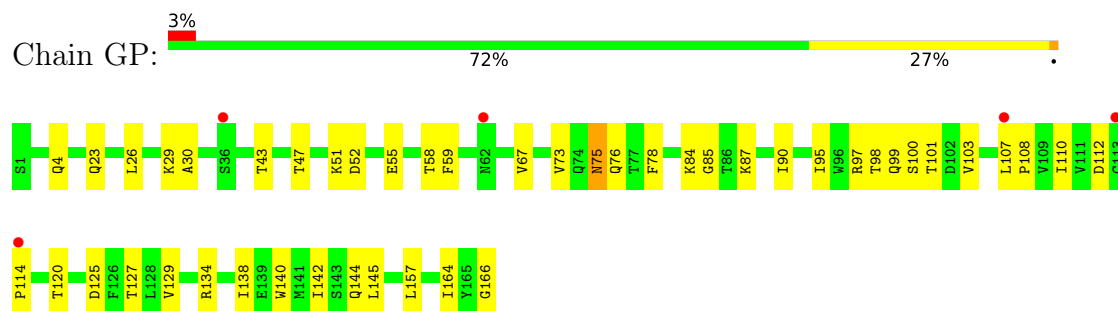
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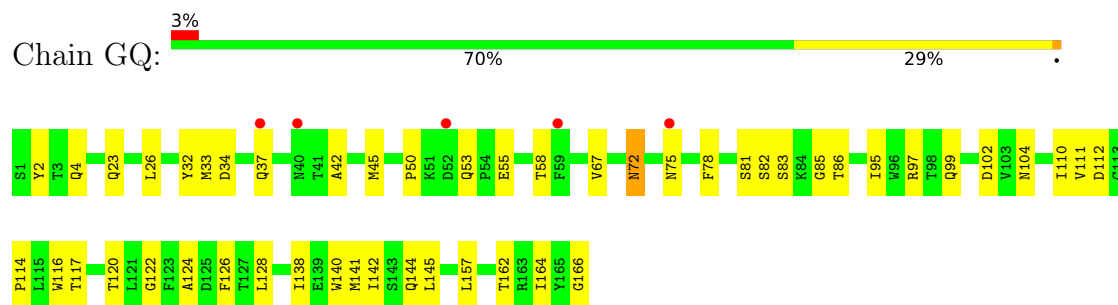
• Molecule 1: coat protein



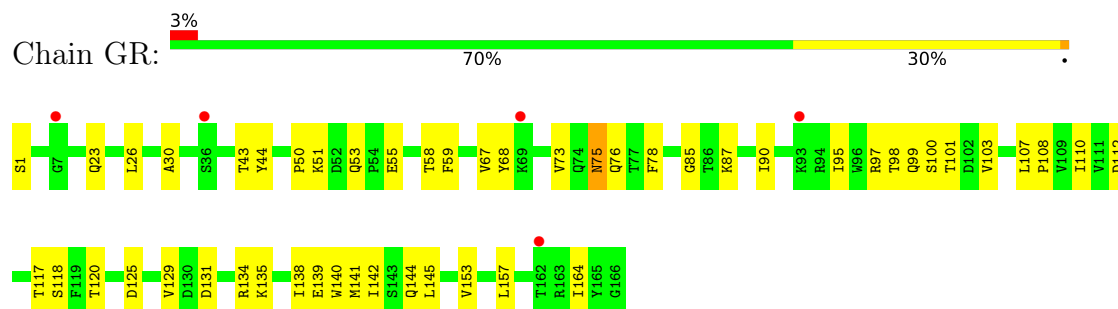
- Molecule 1: coat protein



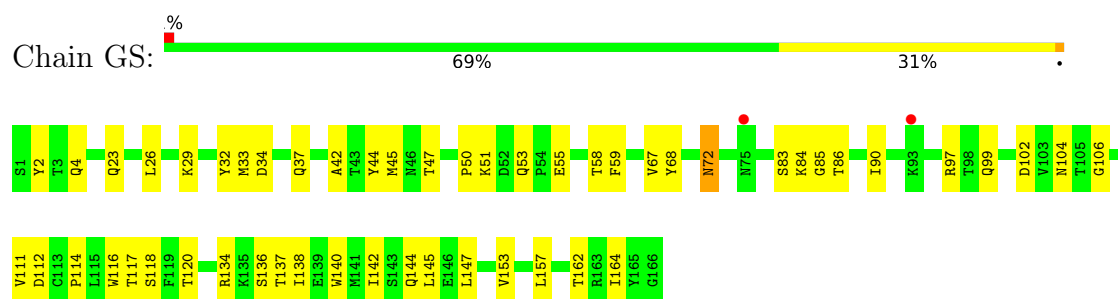
- Molecule 1: coat protein



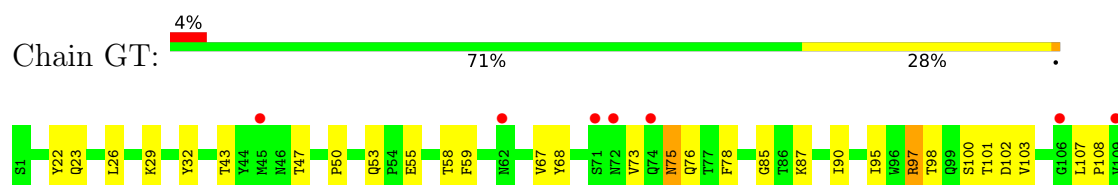
- Molecule 1: coat protein



- Molecule 1: coat protein

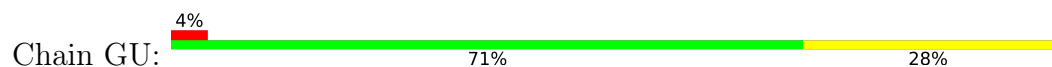


- Molecule 1: coat protein





- Molecule 1: coat protein



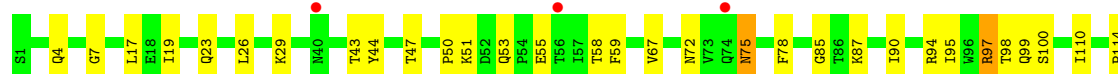
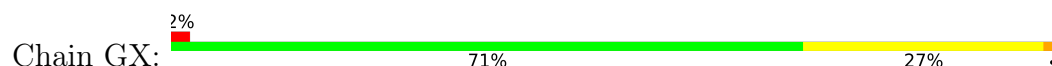
- Molecule 1: coat protein



- Molecule 1: coat protein

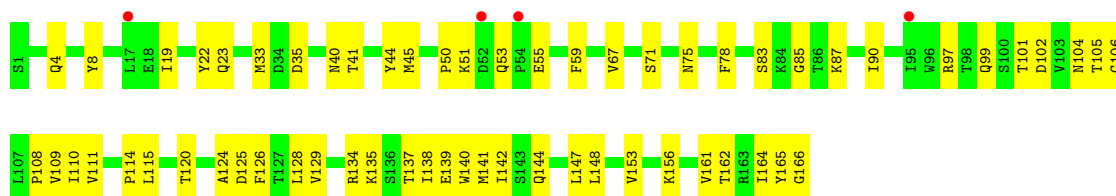


- Molecule 1: coat protein

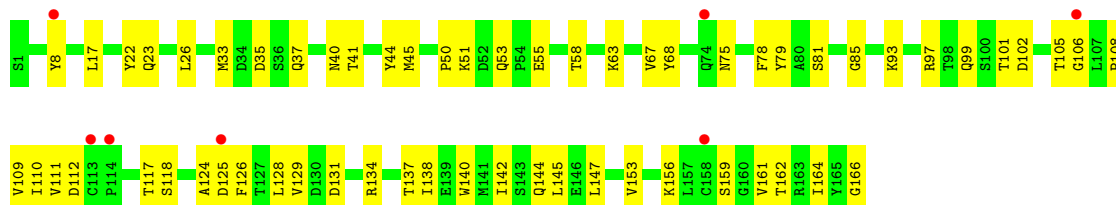


- Molecule 1: coat protein

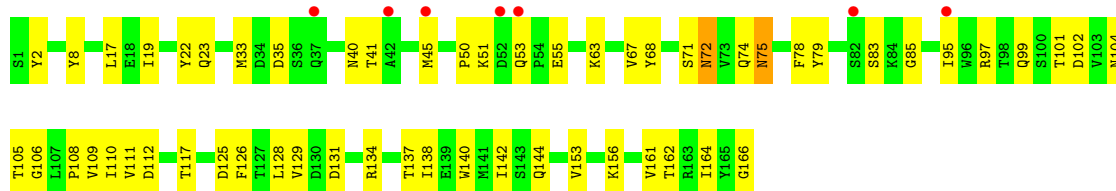




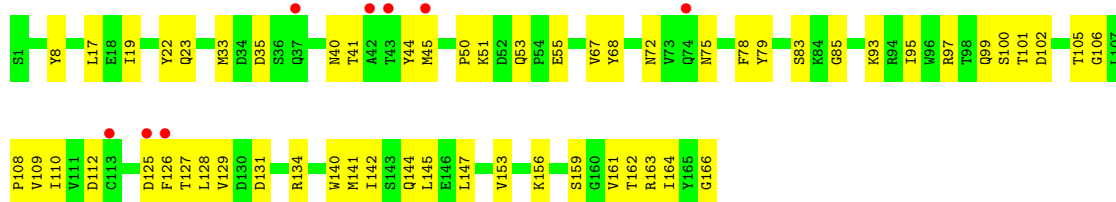
• Molecule 1: coat protein



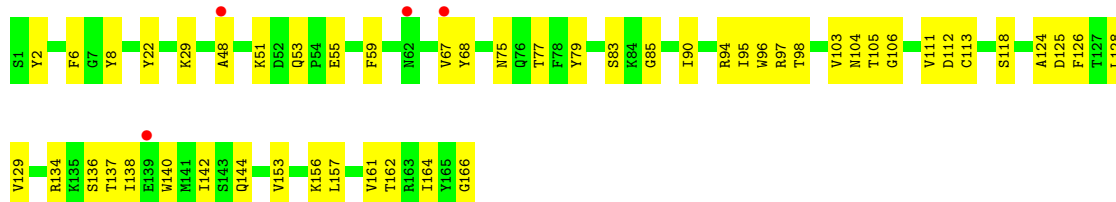
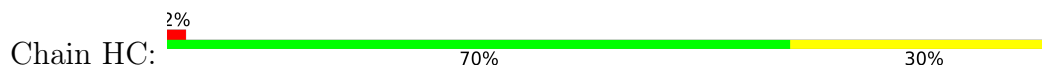
• Molecule 1: coat protein



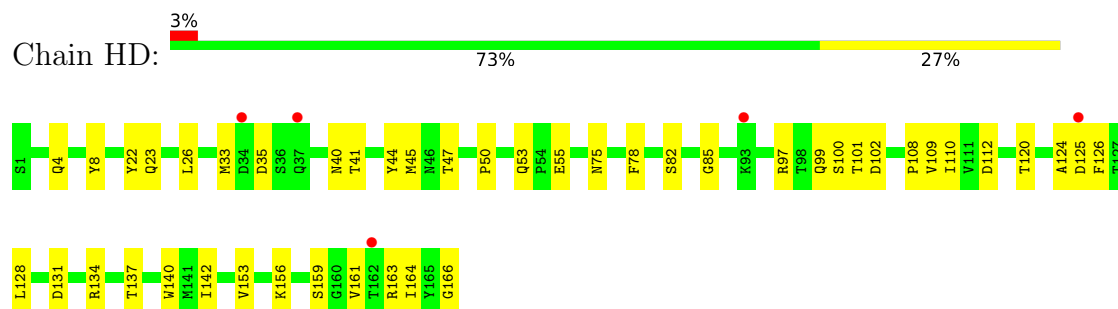
• Molecule 1: coat protein



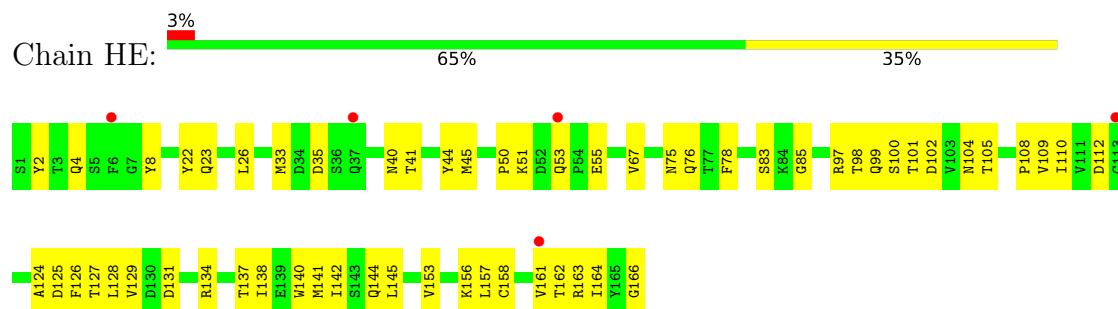
• Molecule 1: coat protein



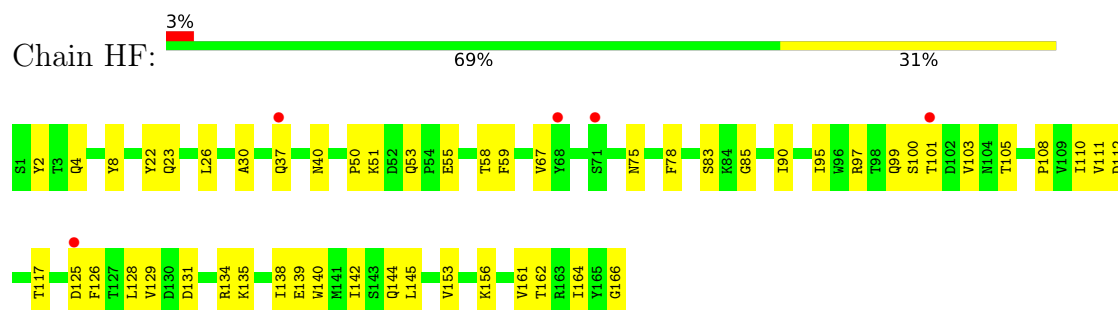
- Molecule 1: coat protein



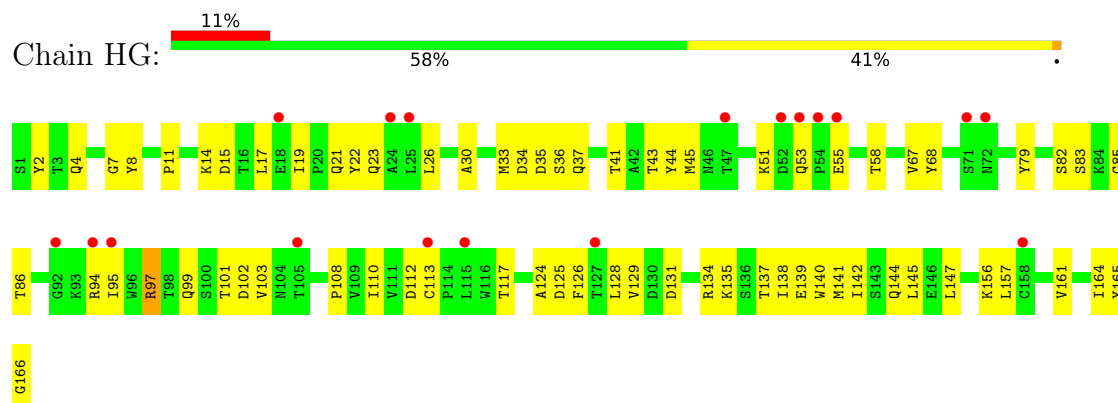
- Molecule 1: coat protein



- Molecule 1: coat protein

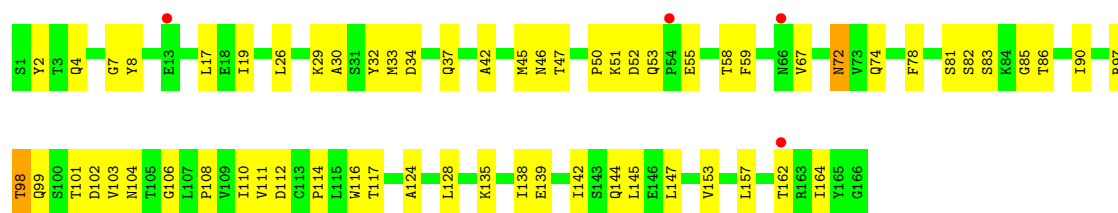


- Molecule 1: coat protein

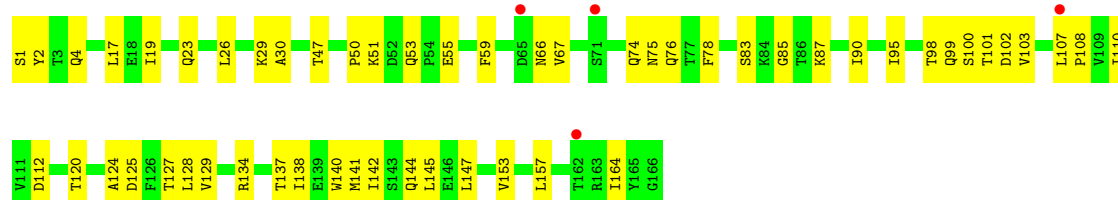


- Molecule 1: coat protein

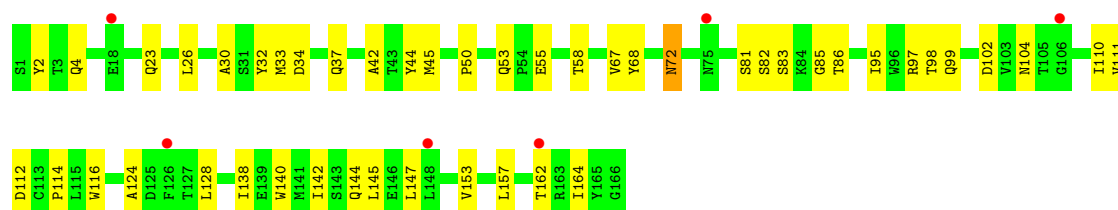
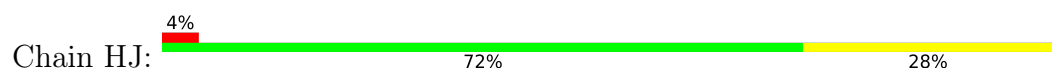




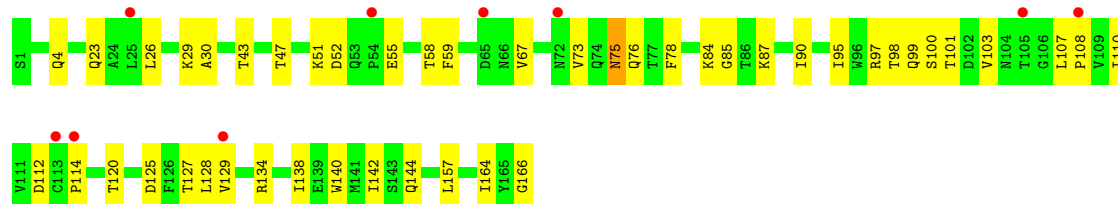
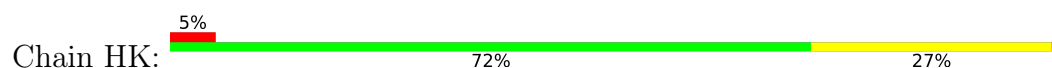
• Molecule 1: coat protein



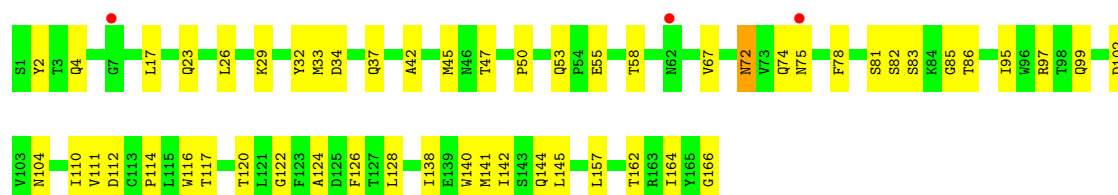
• Molecule 1: coat protein



• Molecule 1: coat protein

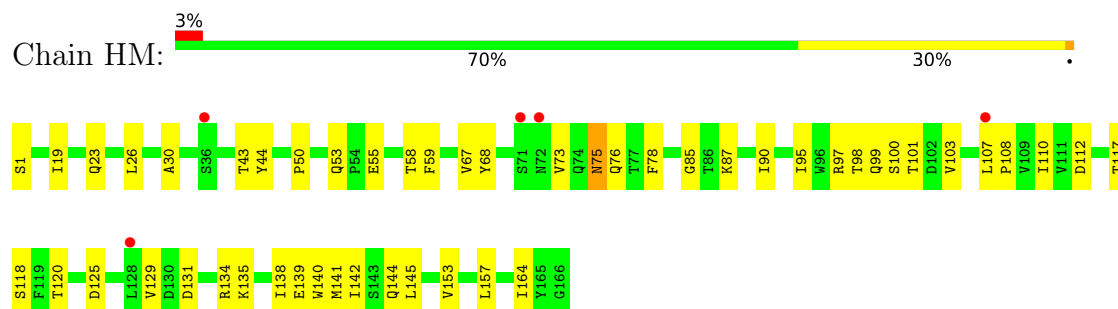


• Molecule 1: coat protein

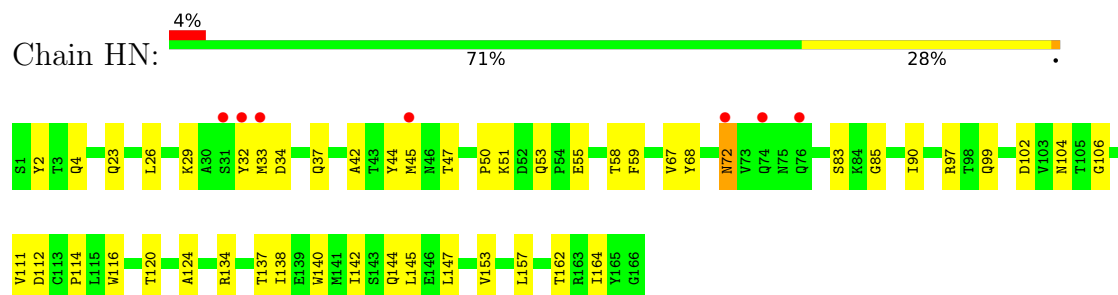




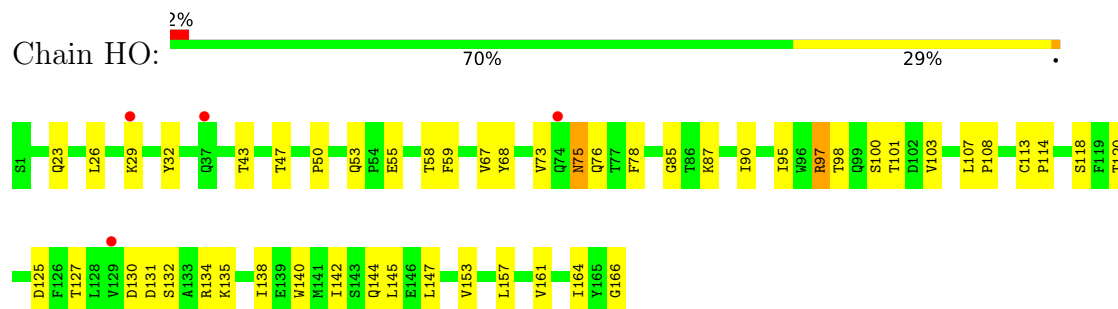
- Molecule 1: coat protein



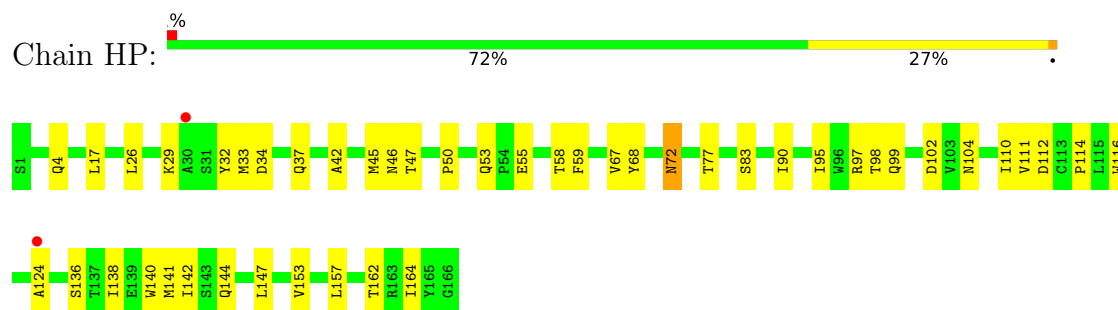
- Molecule 1: coat protein



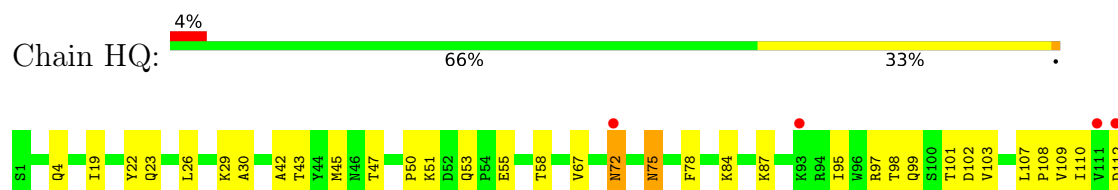
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

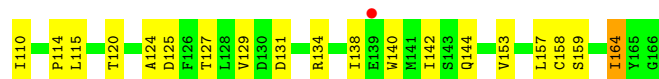
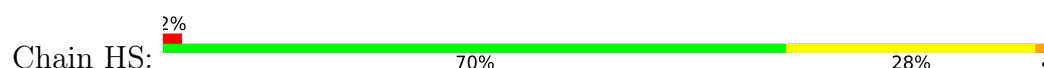




• Molecule 1: coat protein



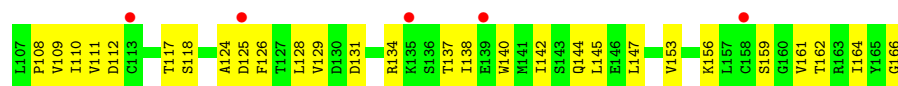
• Molecule 1: coat protein



• Molecule 1: coat protein

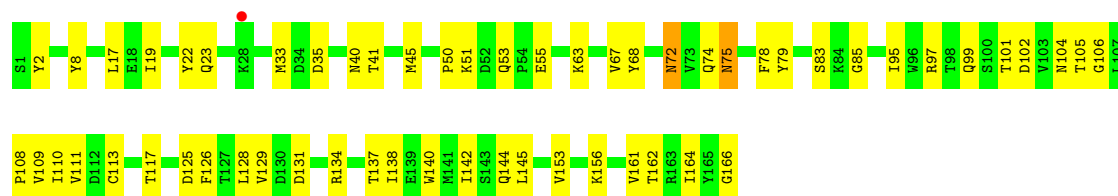


• Molecule 1: coat protein

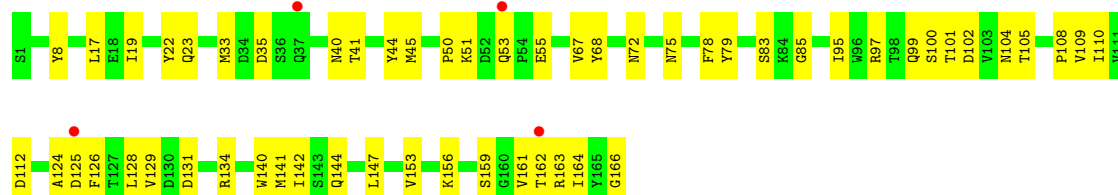


• Molecule 1: coat protein

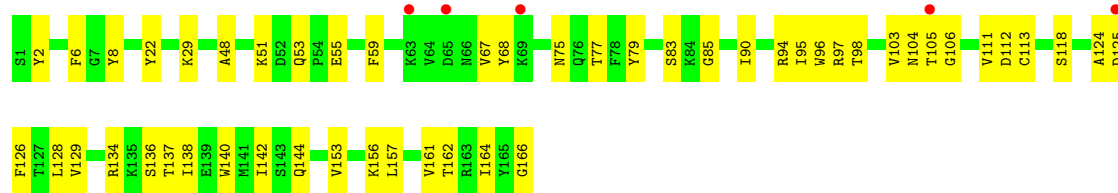
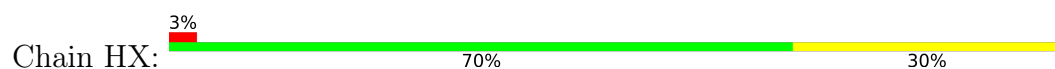




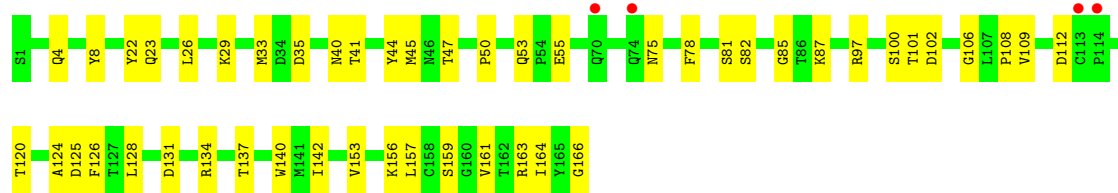
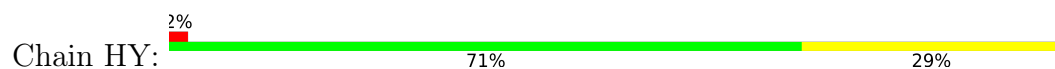
• Molecule 1: coat protein



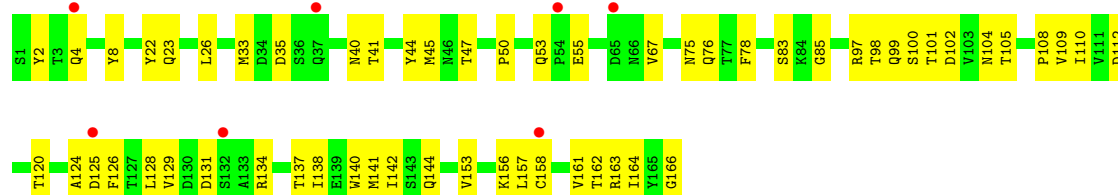
• Molecule 1: coat protein



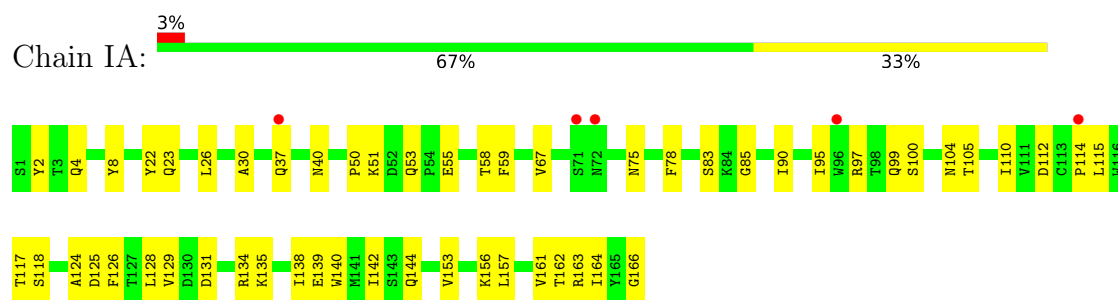
• Molecule 1: coat protein



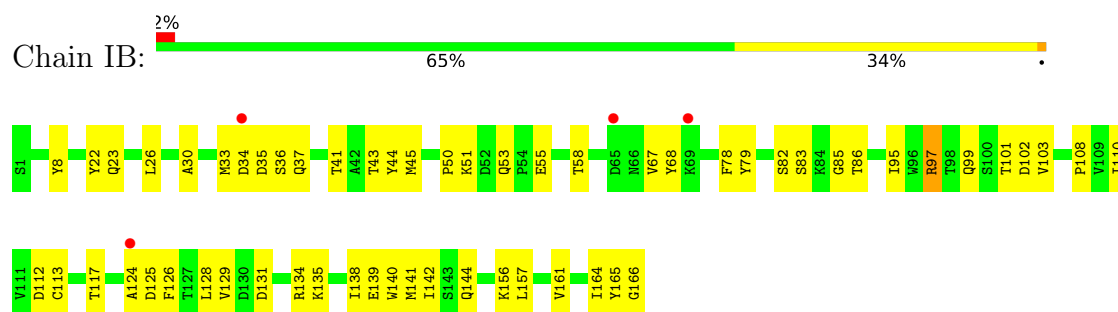
• Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 325.47Å 298.52Å 417.12Å<br>90.00° 100.00° 90.00°            | Depositor        |
| Resolution (Å)                                                          | 49.32 – 3.59<br>49.32 – 3.59                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 93.0 (49.32-3.59)<br>93.9 (49.32-3.59)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.47                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.03 (at 3.57Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.17.1_3660                                          | Depositor        |
| R, $R_{free}$                                                           | 0.278 , 0.283<br>0.281 , 0.286                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 10000 reflections (1.17%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 101.9                                                       | Xtriage          |
| Anisotropy                                                              | 0.181                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 52.5                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                        | EDS              |
| Total number of atoms                                                   | 275100                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 103.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |               | Bond angles |             |
|-----|-------|--------------|---------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$   | RMSZ        | $\# Z  > 5$ |
| 1   | AA    | 0.39         | 0/1337        | 0.59        | 0/1814      |
| 1   | AB    | 0.41         | 0/1337        | 0.63        | 0/1814      |
| 1   | AC    | 0.38         | 0/1337        | 0.60        | 0/1814      |
| 1   | AD    | 0.42         | 0/1337        | 0.65        | 0/1814      |
| 1   | AE    | 0.41         | 1/1337 (0.1%) | 0.63        | 0/1814      |
| 1   | AF    | 0.41         | 0/1337        | 0.65        | 0/1814      |
| 1   | AG    | 0.40         | 0/1337        | 0.64        | 0/1814      |
| 1   | AH    | 0.43         | 0/1337        | 0.65        | 0/1814      |
| 1   | AI    | 0.40         | 0/1337        | 0.63        | 0/1814      |
| 1   | AJ    | 0.42         | 0/1337        | 0.67        | 0/1814      |
| 1   | AK    | 0.41         | 0/1337        | 0.62        | 0/1814      |
| 1   | AL    | 0.44         | 0/1337        | 0.69        | 0/1814      |
| 1   | AM    | 0.42         | 0/1337        | 0.64        | 0/1814      |
| 1   | AN    | 0.40         | 0/1337        | 0.62        | 0/1814      |
| 1   | AO    | 0.40         | 0/1337        | 0.60        | 0/1814      |
| 1   | AP    | 0.40         | 0/1337        | 0.62        | 0/1814      |
| 1   | AQ    | 0.42         | 0/1337        | 0.64        | 0/1814      |
| 1   | AR    | 0.38         | 0/1337        | 0.60        | 0/1814      |
| 1   | AS    | 0.39         | 0/1337        | 0.63        | 0/1814      |
| 1   | AT    | 0.40         | 0/1337        | 0.62        | 0/1814      |
| 1   | AU    | 0.42         | 0/1337        | 0.63        | 0/1814      |
| 1   | AV    | 0.39         | 0/1337        | 0.59        | 0/1814      |
| 1   | AW    | 0.41         | 0/1337        | 0.63        | 0/1814      |
| 1   | AX    | 0.38         | 0/1337        | 0.60        | 0/1814      |
| 1   | AY    | 0.42         | 0/1337        | 0.65        | 0/1814      |
| 1   | AZ    | 0.41         | 1/1337 (0.1%) | 0.63        | 0/1814      |
| 1   | BA    | 0.41         | 0/1337        | 0.65        | 0/1814      |
| 1   | BB    | 0.40         | 0/1337        | 0.64        | 0/1814      |
| 1   | BC    | 0.43         | 0/1337        | 0.65        | 0/1814      |
| 1   | BD    | 0.40         | 0/1337        | 0.63        | 0/1814      |
| 1   | BE    | 0.42         | 0/1337        | 0.67        | 0/1814      |
| 1   | BF    | 0.41         | 0/1337        | 0.62        | 0/1814      |
| 1   | BG    | 0.44         | 0/1337        | 0.69        | 0/1814      |
| 1   | BH    | 0.42         | 0/1337        | 0.64        | 0/1814      |

| Mol | Chain | Bond lengths |               | Bond angles |         |
|-----|-------|--------------|---------------|-------------|---------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5 |
| 1   | BI    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | BJ    | 0.40         | 0/1337        | 0.60        | 0/1814  |
| 1   | BK    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | BL    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | BM    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | BN    | 0.39         | 0/1337        | 0.63        | 0/1814  |
| 1   | BO    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | BP    | 0.42         | 0/1337        | 0.63        | 0/1814  |
| 1   | BQ    | 0.39         | 0/1337        | 0.60        | 0/1814  |
| 1   | BR    | 0.41         | 0/1337        | 0.63        | 0/1814  |
| 1   | BS    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | BT    | 0.42         | 0/1337        | 0.65        | 0/1814  |
| 1   | BU    | 0.41         | 1/1337 (0.1%) | 0.63        | 0/1814  |
| 1   | BV    | 0.41         | 0/1337        | 0.65        | 0/1814  |
| 1   | BW    | 0.40         | 0/1337        | 0.64        | 0/1814  |
| 1   | BX    | 0.43         | 0/1337        | 0.65        | 0/1814  |
| 1   | BY    | 0.40         | 0/1337        | 0.63        | 0/1814  |
| 1   | BZ    | 0.42         | 0/1337        | 0.67        | 0/1814  |
| 1   | CA    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | CB    | 0.44         | 0/1337        | 0.69        | 0/1814  |
| 1   | CC    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | CD    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | CE    | 0.40         | 0/1337        | 0.60        | 0/1814  |
| 1   | CF    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | CG    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | CH    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | CI    | 0.39         | 0/1337        | 0.63        | 0/1814  |
| 1   | CJ    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | CK    | 0.42         | 0/1337        | 0.63        | 0/1814  |
| 1   | CL    | 0.39         | 0/1337        | 0.60        | 0/1814  |
| 1   | CM    | 0.41         | 0/1337        | 0.63        | 0/1814  |
| 1   | CN    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | CO    | 0.42         | 0/1337        | 0.65        | 0/1814  |
| 1   | CP    | 0.41         | 1/1337 (0.1%) | 0.63        | 0/1814  |
| 1   | CQ    | 0.41         | 0/1337        | 0.65        | 0/1814  |
| 1   | CR    | 0.40         | 0/1337        | 0.64        | 0/1814  |
| 1   | CS    | 0.43         | 0/1337        | 0.65        | 0/1814  |
| 1   | CT    | 0.40         | 0/1337        | 0.63        | 0/1814  |
| 1   | CU    | 0.42         | 0/1337        | 0.67        | 0/1814  |
| 1   | CV    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | CW    | 0.44         | 0/1337        | 0.69        | 0/1814  |
| 1   | CX    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | CY    | 0.40         | 0/1337        | 0.62        | 0/1814  |

| Mol | Chain | Bond lengths |               | Bond angles |         |
|-----|-------|--------------|---------------|-------------|---------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5 |
| 1   | CZ    | 0.40         | 0/1337        | 0.60        | 0/1814  |
| 1   | DA    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | DB    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | DC    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | DD    | 0.39         | 0/1337        | 0.63        | 0/1814  |
| 1   | DE    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | DF    | 0.42         | 0/1337        | 0.63        | 0/1814  |
| 1   | DG    | 0.39         | 0/1337        | 0.60        | 0/1814  |
| 1   | DH    | 0.41         | 0/1337        | 0.63        | 0/1814  |
| 1   | DI    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | DJ    | 0.42         | 0/1337        | 0.65        | 0/1814  |
| 1   | DK    | 0.41         | 1/1337 (0.1%) | 0.63        | 0/1814  |
| 1   | DL    | 0.41         | 0/1337        | 0.65        | 0/1814  |
| 1   | DM    | 0.40         | 0/1337        | 0.64        | 0/1814  |
| 1   | DN    | 0.43         | 0/1337        | 0.65        | 0/1814  |
| 1   | DO    | 0.40         | 0/1337        | 0.63        | 0/1814  |
| 1   | DP    | 0.42         | 0/1337        | 0.67        | 0/1814  |
| 1   | DQ    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | DR    | 0.44         | 0/1337        | 0.69        | 0/1814  |
| 1   | DS    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | DT    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | DU    | 0.40         | 0/1337        | 0.61        | 0/1814  |
| 1   | DV    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | DW    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | DX    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | DY    | 0.39         | 0/1337        | 0.63        | 0/1814  |
| 1   | DZ    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | EA    | 0.42         | 0/1337        | 0.63        | 0/1814  |
| 1   | EB    | 0.39         | 0/1337        | 0.60        | 0/1814  |
| 1   | EC    | 0.41         | 0/1337        | 0.63        | 0/1814  |
| 1   | ED    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | EE    | 0.42         | 0/1337        | 0.65        | 0/1814  |
| 1   | EF    | 0.41         | 1/1337 (0.1%) | 0.63        | 0/1814  |
| 1   | EG    | 0.41         | 0/1337        | 0.65        | 0/1814  |
| 1   | EH    | 0.40         | 0/1337        | 0.64        | 0/1814  |
| 1   | EI    | 0.43         | 0/1337        | 0.65        | 0/1814  |
| 1   | EJ    | 0.40         | 0/1337        | 0.63        | 0/1814  |
| 1   | EK    | 0.42         | 0/1337        | 0.67        | 0/1814  |
| 1   | EL    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | EM    | 0.44         | 0/1337        | 0.69        | 0/1814  |
| 1   | EN    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | EO    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | EP    | 0.40         | 0/1337        | 0.61        | 0/1814  |



| Mol | Chain | Bond lengths |               | Bond angles |         |
|-----|-------|--------------|---------------|-------------|---------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5 |
| 1   | EQ    | 0.40         | 0/1337        | 0.61        | 0/1814  |
| 1   | ER    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | ES    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | ET    | 0.39         | 0/1337        | 0.63        | 0/1814  |
| 1   | EU    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | EV    | 0.42         | 0/1337        | 0.63        | 0/1814  |
| 1   | EW    | 0.39         | 0/1337        | 0.60        | 0/1814  |
| 1   | EX    | 0.41         | 0/1337        | 0.63        | 0/1814  |
| 1   | EY    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | EZ    | 0.42         | 0/1337        | 0.65        | 0/1814  |
| 1   | FA    | 0.41         | 1/1337 (0.1%) | 0.63        | 0/1814  |
| 1   | FB    | 0.41         | 0/1337        | 0.65        | 0/1814  |
| 1   | FC    | 0.40         | 0/1337        | 0.64        | 0/1814  |
| 1   | FD    | 0.43         | 0/1337        | 0.65        | 0/1814  |
| 1   | FE    | 0.40         | 0/1337        | 0.63        | 0/1814  |
| 1   | FF    | 0.42         | 0/1337        | 0.67        | 0/1814  |
| 1   | FG    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | FH    | 0.44         | 0/1337        | 0.69        | 0/1814  |
| 1   | FI    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | FJ    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | FK    | 0.40         | 0/1337        | 0.60        | 0/1814  |
| 1   | FL    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | FM    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | FN    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | FO    | 0.39         | 0/1337        | 0.63        | 0/1814  |
| 1   | FP    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | FQ    | 0.42         | 0/1337        | 0.63        | 0/1814  |
| 1   | FR    | 0.39         | 0/1337        | 0.60        | 0/1814  |
| 1   | FS    | 0.41         | 0/1337        | 0.63        | 0/1814  |
| 1   | FT    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | FU    | 0.42         | 0/1337        | 0.65        | 0/1814  |
| 1   | FV    | 0.41         | 1/1337 (0.1%) | 0.63        | 0/1814  |
| 1   | FW    | 0.41         | 0/1337        | 0.65        | 0/1814  |
| 1   | FX    | 0.40         | 0/1337        | 0.64        | 0/1814  |
| 1   | FY    | 0.43         | 0/1337        | 0.65        | 0/1814  |
| 1   | FZ    | 0.40         | 0/1337        | 0.63        | 0/1814  |
| 1   | GA    | 0.42         | 0/1337        | 0.67        | 0/1814  |
| 1   | GB    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | GC    | 0.44         | 0/1337        | 0.69        | 0/1814  |
| 1   | GD    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | GE    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | GF    | 0.40         | 0/1337        | 0.61        | 0/1814  |
| 1   | GG    | 0.40         | 0/1337        | 0.62        | 0/1814  |

| Mol | Chain | Bond lengths |               | Bond angles |         |
|-----|-------|--------------|---------------|-------------|---------|
|     |       | RMSZ         | # Z  >5       | RMSZ        | # Z  >5 |
| 1   | GH    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | GI    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | GJ    | 0.39         | 0/1337        | 0.63        | 0/1814  |
| 1   | GK    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | GL    | 0.42         | 0/1337        | 0.63        | 0/1814  |
| 1   | GM    | 0.39         | 0/1337        | 0.60        | 0/1814  |
| 1   | GN    | 0.41         | 0/1337        | 0.63        | 0/1814  |
| 1   | GO    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | GP    | 0.42         | 0/1337        | 0.65        | 0/1814  |
| 1   | GQ    | 0.41         | 1/1337 (0.1%) | 0.63        | 0/1814  |
| 1   | GR    | 0.41         | 0/1337        | 0.65        | 0/1814  |
| 1   | GS    | 0.40         | 0/1337        | 0.64        | 0/1814  |
| 1   | GT    | 0.43         | 0/1337        | 0.65        | 0/1814  |
| 1   | GU    | 0.40         | 0/1337        | 0.63        | 0/1814  |
| 1   | GV    | 0.42         | 0/1337        | 0.67        | 0/1814  |
| 1   | GW    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | GX    | 0.44         | 0/1337        | 0.69        | 0/1814  |
| 1   | GY    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | GZ    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | HA    | 0.40         | 0/1337        | 0.61        | 0/1814  |
| 1   | HB    | 0.40         | 0/1337        | 0.61        | 0/1814  |
| 1   | HC    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | HD    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | HE    | 0.39         | 0/1337        | 0.63        | 0/1814  |
| 1   | HF    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | HG    | 0.42         | 0/1337        | 0.63        | 0/1814  |
| 1   | HH    | 0.39         | 0/1337        | 0.60        | 0/1814  |
| 1   | HI    | 0.41         | 0/1337        | 0.63        | 0/1814  |
| 1   | HJ    | 0.38         | 0/1337        | 0.60        | 0/1814  |
| 1   | HK    | 0.42         | 0/1337        | 0.65        | 0/1814  |
| 1   | HL    | 0.41         | 1/1337 (0.1%) | 0.63        | 0/1814  |
| 1   | HM    | 0.41         | 0/1337        | 0.65        | 0/1814  |
| 1   | HN    | 0.40         | 0/1337        | 0.64        | 0/1814  |
| 1   | HO    | 0.43         | 0/1337        | 0.65        | 0/1814  |
| 1   | HP    | 0.40         | 0/1337        | 0.63        | 0/1814  |
| 1   | HQ    | 0.42         | 0/1337        | 0.67        | 0/1814  |
| 1   | HR    | 0.41         | 0/1337        | 0.62        | 0/1814  |
| 1   | HS    | 0.44         | 0/1337        | 0.69        | 0/1814  |
| 1   | HT    | 0.42         | 0/1337        | 0.64        | 0/1814  |
| 1   | HU    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | HV    | 0.40         | 0/1337        | 0.60        | 0/1814  |
| 1   | HW    | 0.40         | 0/1337        | 0.62        | 0/1814  |
| 1   | HX    | 0.42         | 0/1337        | 0.64        | 0/1814  |

| Mol | Chain | Bond lengths |                  | Bond angles |          |
|-----|-------|--------------|------------------|-------------|----------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5  |
| 1   | HY    | 0.38         | 0/1337           | 0.60        | 0/1814   |
| 1   | HZ    | 0.39         | 0/1337           | 0.63        | 0/1814   |
| 1   | IA    | 0.40         | 0/1337           | 0.62        | 0/1814   |
| 1   | IB    | 0.42         | 0/1337           | 0.63        | 0/1814   |
| All | All   | 0.41         | 10/280770 (0.0%) | 0.63        | 0/380940 |

The worst 5 of 10 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | BU    | 122 | GLY  | CA-C  | -6.01 | 1.47        | 1.52     |
| 1   | HL    | 122 | GLY  | CA-C  | -5.95 | 1.47        | 1.52     |
| 1   | FV    | 122 | GLY  | CA-C  | -5.92 | 1.47        | 1.52     |
| 1   | GQ    | 122 | GLY  | CA-C  | -5.90 | 1.47        | 1.52     |
| 1   | DK    | 122 | GLY  | CA-C  | -5.90 | 1.47        | 1.52     |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 1310  | 0        | 1289     | 64      | 0            |
| 1   | AB    | 1310  | 0        | 1289     | 70      | 0            |
| 1   | AC    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | AD    | 1310  | 0        | 1289     | 51      | 0            |
| 1   | AE    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | AF    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | AG    | 1310  | 0        | 1289     | 55      | 0            |
| 1   | AH    | 1310  | 0        | 1289     | 50      | 0            |
| 1   | AI    | 1310  | 0        | 1289     | 57      | 0            |
| 1   | AJ    | 1310  | 0        | 1289     | 57      | 0            |
| 1   | AK    | 1310  | 0        | 1289     | 57      | 0            |
| 1   | AL    | 1310  | 0        | 1289     | 51      | 0            |
| 1   | AM    | 1310  | 0        | 1289     | 66      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AN    | 1310  | 0        | 1289     | 68      | 0            |
| 1   | AO    | 1310  | 0        | 1289     | 66      | 0            |
| 1   | AP    | 1310  | 0        | 1289     | 62      | 0            |
| 1   | AQ    | 1310  | 0        | 1289     | 61      | 0            |
| 1   | AR    | 1310  | 0        | 1289     | 46      | 0            |
| 1   | AS    | 1310  | 0        | 1289     | 77      | 0            |
| 1   | AT    | 1310  | 0        | 1289     | 64      | 0            |
| 1   | AU    | 1310  | 0        | 1289     | 76      | 0            |
| 1   | AV    | 1310  | 0        | 1289     | 67      | 0            |
| 1   | AW    | 1310  | 0        | 1289     | 65      | 0            |
| 1   | AX    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | AY    | 1310  | 0        | 1289     | 48      | 0            |
| 1   | AZ    | 1310  | 0        | 1289     | 56      | 0            |
| 1   | BA    | 1310  | 0        | 1289     | 56      | 0            |
| 1   | BB    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | BC    | 1310  | 0        | 1289     | 46      | 0            |
| 1   | BD    | 1310  | 0        | 1289     | 47      | 0            |
| 1   | BE    | 1310  | 0        | 1289     | 56      | 0            |
| 1   | BF    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | BG    | 1310  | 0        | 1289     | 47      | 0            |
| 1   | BH    | 1310  | 0        | 1289     | 63      | 0            |
| 1   | BI    | 1310  | 0        | 1289     | 63      | 0            |
| 1   | BJ    | 1310  | 0        | 1289     | 65      | 0            |
| 1   | BK    | 1310  | 0        | 1289     | 66      | 0            |
| 1   | BL    | 1310  | 0        | 1289     | 59      | 0            |
| 1   | BM    | 1310  | 0        | 1289     | 47      | 0            |
| 1   | BN    | 1310  | 0        | 1289     | 71      | 0            |
| 1   | BO    | 1310  | 0        | 1289     | 58      | 0            |
| 1   | BP    | 1310  | 0        | 1289     | 70      | 0            |
| 1   | BQ    | 1310  | 0        | 1289     | 65      | 0            |
| 1   | BR    | 1310  | 0        | 1289     | 63      | 0            |
| 1   | BS    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | BT    | 1310  | 0        | 1289     | 50      | 0            |
| 1   | BU    | 1310  | 0        | 1289     | 58      | 1            |
| 1   | BV    | 1310  | 0        | 1289     | 55      | 0            |
| 1   | BW    | 1310  | 0        | 1289     | 48      | 0            |
| 1   | BX    | 1310  | 0        | 1289     | 47      | 0            |
| 1   | BY    | 1310  | 0        | 1289     | 48      | 0            |
| 1   | BZ    | 1310  | 0        | 1289     | 50      | 0            |
| 1   | CA    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | CB    | 1310  | 0        | 1289     | 50      | 0            |
| 1   | CC    | 1310  | 0        | 1289     | 67      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | CD    | 1310  | 0        | 1289     | 67      | 1            |
| 1   | CE    | 1310  | 0        | 1289     | 68      | 0            |
| 1   | CF    | 1310  | 0        | 1289     | 65      | 0            |
| 1   | CG    | 1310  | 0        | 1289     | 61      | 0            |
| 1   | CH    | 1310  | 0        | 1289     | 45      | 0            |
| 1   | CI    | 1310  | 0        | 1289     | 73      | 0            |
| 1   | CJ    | 1310  | 0        | 1289     | 59      | 1            |
| 1   | CK    | 1310  | 0        | 1289     | 61      | 0            |
| 1   | CL    | 1310  | 0        | 1289     | 67      | 0            |
| 1   | CM    | 1310  | 0        | 1289     | 69      | 0            |
| 1   | CN    | 1310  | 0        | 1289     | 55      | 0            |
| 1   | CO    | 1310  | 0        | 1289     | 50      | 0            |
| 1   | CP    | 1310  | 0        | 1289     | 57      | 0            |
| 1   | CQ    | 1310  | 0        | 1289     | 55      | 0            |
| 1   | CR    | 1310  | 0        | 1289     | 55      | 0            |
| 1   | CS    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | CT    | 1310  | 0        | 1289     | 46      | 0            |
| 1   | CU    | 1310  | 0        | 1289     | 48      | 0            |
| 1   | CV    | 1310  | 0        | 1289     | 55      | 0            |
| 1   | CW    | 1310  | 0        | 1289     | 48      | 0            |
| 1   | CX    | 1310  | 0        | 1289     | 62      | 0            |
| 1   | CY    | 1310  | 0        | 1289     | 64      | 0            |
| 1   | CZ    | 1310  | 0        | 1289     | 65      | 0            |
| 1   | DA    | 1310  | 0        | 1289     | 63      | 0            |
| 1   | DB    | 1310  | 0        | 1289     | 59      | 0            |
| 1   | DC    | 1310  | 0        | 1289     | 45      | 1            |
| 1   | DD    | 1310  | 0        | 1289     | 71      | 0            |
| 1   | DE    | 1310  | 0        | 1289     | 60      | 0            |
| 1   | DF    | 1310  | 0        | 1289     | 71      | 0            |
| 1   | DG    | 1310  | 0        | 1289     | 73      | 0            |
| 1   | DH    | 1310  | 0        | 1289     | 74      | 0            |
| 1   | DI    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | DJ    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | DK    | 1310  | 0        | 1289     | 59      | 0            |
| 1   | DL    | 1310  | 0        | 1289     | 54      | 0            |
| 1   | DM    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | DN    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | DO    | 1310  | 0        | 1289     | 51      | 0            |
| 1   | DP    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | DQ    | 1310  | 0        | 1289     | 54      | 0            |
| 1   | DR    | 1310  | 0        | 1289     | 52      | 0            |
| 1   | DS    | 1310  | 0        | 1289     | 63      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | DT    | 1310  | 0        | 1289     | 66      | 0            |
| 1   | DU    | 1310  | 0        | 1289     | 64      | 0            |
| 1   | DV    | 1310  | 0        | 1289     | 64      | 0            |
| 1   | DW    | 1310  | 0        | 1289     | 61      | 0            |
| 1   | DX    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | DY    | 1310  | 0        | 1289     | 73      | 0            |
| 1   | DZ    | 1310  | 0        | 1289     | 57      | 0            |
| 1   | EA    | 1310  | 0        | 1289     | 59      | 0            |
| 1   | EB    | 1310  | 0        | 1289     | 67      | 0            |
| 1   | EC    | 1310  | 0        | 1289     | 67      | 0            |
| 1   | ED    | 1310  | 0        | 1289     | 55      | 0            |
| 1   | EE    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | EF    | 1310  | 0        | 1289     | 54      | 0            |
| 1   | EG    | 1310  | 0        | 1289     | 53      | 0            |
| 1   | EH    | 1310  | 0        | 1289     | 56      | 0            |
| 1   | EI    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | EJ    | 1310  | 0        | 1289     | 47      | 0            |
| 1   | EK    | 1310  | 0        | 1289     | 51      | 0            |
| 1   | EL    | 1310  | 0        | 1289     | 53      | 0            |
| 1   | EM    | 1310  | 0        | 1289     | 48      | 0            |
| 1   | EN    | 1310  | 0        | 1289     | 65      | 0            |
| 1   | EO    | 1310  | 0        | 1289     | 62      | 0            |
| 1   | EP    | 1310  | 0        | 1289     | 64      | 0            |
| 1   | EQ    | 1310  | 0        | 1289     | 66      | 0            |
| 1   | ER    | 1310  | 0        | 1289     | 61      | 0            |
| 1   | ES    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | ET    | 1310  | 0        | 1289     | 74      | 0            |
| 1   | EU    | 1310  | 0        | 1289     | 63      | 0            |
| 1   | EV    | 1310  | 0        | 1289     | 71      | 0            |
| 1   | EW    | 1310  | 0        | 1289     | 68      | 0            |
| 1   | EX    | 1310  | 0        | 1289     | 71      | 0            |
| 1   | EY    | 1310  | 0        | 1289     | 55      | 0            |
| 1   | EZ    | 1310  | 0        | 1289     | 50      | 0            |
| 1   | FA    | 1310  | 0        | 1289     | 56      | 0            |
| 1   | FB    | 1310  | 0        | 1289     | 55      | 0            |
| 1   | FC    | 1310  | 0        | 1289     | 47      | 0            |
| 1   | FD    | 1310  | 0        | 1289     | 48      | 0            |
| 1   | FE    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | FF    | 1310  | 0        | 1289     | 54      | 0            |
| 1   | FG    | 1310  | 0        | 1289     | 53      | 0            |
| 1   | FH    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | FI    | 1310  | 0        | 1289     | 64      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | FJ    | 1310  | 0        | 1289     | 65      | 0            |
| 1   | FK    | 1310  | 0        | 1289     | 66      | 0            |
| 1   | FL    | 1310  | 0        | 1289     | 66      | 0            |
| 1   | FM    | 1310  | 0        | 1289     | 62      | 0            |
| 1   | FN    | 1310  | 0        | 1289     | 47      | 0            |
| 1   | FO    | 1310  | 0        | 1289     | 71      | 0            |
| 1   | FP    | 1310  | 0        | 1289     | 57      | 0            |
| 1   | FQ    | 1310  | 0        | 1289     | 63      | 0            |
| 1   | FR    | 1310  | 0        | 1289     | 73      | 0            |
| 1   | FS    | 1310  | 0        | 1289     | 71      | 0            |
| 1   | FT    | 1310  | 0        | 1289     | 51      | 0            |
| 1   | FU    | 1310  | 0        | 1289     | 51      | 0            |
| 1   | FV    | 1310  | 0        | 1289     | 55      | 0            |
| 1   | FW    | 1310  | 0        | 1289     | 53      | 1            |
| 1   | FX    | 1310  | 0        | 1289     | 53      | 0            |
| 1   | FY    | 1310  | 0        | 1289     | 50      | 0            |
| 1   | FZ    | 1310  | 0        | 1289     | 57      | 0            |
| 1   | GA    | 1310  | 0        | 1289     | 54      | 0            |
| 1   | GB    | 1310  | 0        | 1289     | 53      | 0            |
| 1   | GC    | 1310  | 0        | 1289     | 50      | 0            |
| 1   | GD    | 1310  | 0        | 1289     | 63      | 1            |
| 1   | GE    | 1310  | 0        | 1289     | 67      | 0            |
| 1   | GF    | 1310  | 0        | 1289     | 65      | 0            |
| 1   | GG    | 1310  | 0        | 1289     | 63      | 0            |
| 1   | GH    | 1310  | 0        | 1289     | 60      | 0            |
| 1   | GI    | 1310  | 0        | 1289     | 47      | 0            |
| 1   | GJ    | 1310  | 0        | 1289     | 77      | 0            |
| 1   | GK    | 1310  | 0        | 1289     | 61      | 0            |
| 1   | GL    | 1310  | 0        | 1289     | 69      | 0            |
| 1   | GM    | 1310  | 0        | 1289     | 66      | 0            |
| 1   | GN    | 1310  | 0        | 1289     | 61      | 0            |
| 1   | GO    | 1310  | 0        | 1289     | 51      | 0            |
| 1   | GP    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | GQ    | 1310  | 0        | 1289     | 53      | 0            |
| 1   | GR    | 1310  | 0        | 1289     | 53      | 0            |
| 1   | GS    | 1310  | 0        | 1289     | 51      | 0            |
| 1   | GT    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | GU    | 1310  | 0        | 1289     | 49      | 0            |
| 1   | GV    | 1310  | 0        | 1289     | 53      | 0            |
| 1   | GW    | 1310  | 0        | 1289     | 53      | 0            |
| 1   | GX    | 1310  | 0        | 1289     | 48      | 0            |
| 1   | GY    | 1310  | 0        | 1289     | 67      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1   | GZ    | 1310   | 0        | 1289     | 66      | 0            |
| 1   | HA    | 1310   | 0        | 1289     | 67      | 0            |
| 1   | HB    | 1310   | 0        | 1289     | 69      | 0            |
| 1   | HC    | 1310   | 0        | 1289     | 58      | 0            |
| 1   | HD    | 1310   | 0        | 1289     | 44      | 0            |
| 1   | HE    | 1310   | 0        | 1289     | 70      | 0            |
| 1   | HF    | 1310   | 0        | 1289     | 57      | 0            |
| 1   | HG    | 1310   | 0        | 1289     | 77      | 0            |
| 1   | HH    | 1310   | 0        | 1289     | 66      | 0            |
| 1   | HI    | 1310   | 0        | 1289     | 77      | 0            |
| 1   | HJ    | 1310   | 0        | 1289     | 53      | 0            |
| 1   | HK    | 1310   | 0        | 1289     | 48      | 0            |
| 1   | HL    | 1310   | 0        | 1289     | 57      | 0            |
| 1   | HM    | 1310   | 0        | 1289     | 54      | 0            |
| 1   | HN    | 1310   | 0        | 1289     | 51      | 0            |
| 1   | HO    | 1310   | 0        | 1289     | 50      | 0            |
| 1   | HP    | 1310   | 0        | 1289     | 47      | 0            |
| 1   | HQ    | 1310   | 0        | 1289     | 55      | 0            |
| 1   | HR    | 1310   | 0        | 1289     | 54      | 0            |
| 1   | HS    | 1310   | 0        | 1289     | 48      | 0            |
| 1   | HT    | 1310   | 0        | 1289     | 61      | 0            |
| 1   | HU    | 1310   | 0        | 1289     | 63      | 0            |
| 1   | HV    | 1310   | 0        | 1289     | 66      | 0            |
| 1   | HW    | 1310   | 0        | 1289     | 64      | 0            |
| 1   | HX    | 1310   | 0        | 1289     | 59      | 0            |
| 1   | HY    | 1310   | 0        | 1289     | 48      | 0            |
| 1   | HZ    | 1310   | 0        | 1289     | 67      | 0            |
| 1   | IA    | 1310   | 0        | 1289     | 56      | 0            |
| 1   | IB    | 1310   | 0        | 1289     | 59      | 0            |
| All | All   | 275100 | 0        | 270690   | 8542    | 3            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 8542 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:EB:162:THR:HB | 1:HH:34:ASP:HB3 | 1.26                     | 1.14              |
| 1:AA:162:THR:HB | 1:DG:34:ASP:HB3 | 1.36                     | 1.07              |
| 1:AV:34:ASP:HB3 | 1:BQ:162:THR:HB | 1.37                     | 1.02              |
| 1:AA:155:SER:OG | 1:DG:51:LYS:NZ  | 1.92                     | 1.02              |

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| Atom-1          | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-----------------|--------------------------|-------------------|
| 1:AI:162:THR:HB | 1:AK:34:ASP:HB3 | 1.44                     | 1.00              |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1          | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------------|--------------------------|-------------------|
| 1:CD:14:LYS:NZ  | 1:FW:12:THR:OG1[1_455] | 2.03                     | 0.17              |
| 1:CJ:9:THR:OG1  | 1:DC:13:GLU:OE2[2_444] | 2.07                     | 0.13              |
| 1:BU:18:GLU:OE1 | 1:GD:18:GLU:OE1[1_455] | 2.18                     | 0.02              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | AA    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | AB    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | AC    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AD    | 164/166 (99%) | 155 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 1   | AE    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | AF    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | AG    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AH    | 164/166 (99%) | 157 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | AI    | 164/166 (99%) | 162 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | AJ    | 164/166 (99%) | 156 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 1   | AK    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | AL    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | AM    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | AN    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | AO    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | AP    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AQ    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AR    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | AS    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | AT    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | AU    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | AV    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | AW    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | AX    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | AY    | 164/166 (99%) | 155 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 1   | AZ    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | BA    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | BB    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BC    | 164/166 (99%) | 157 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | BD    | 164/166 (99%) | 162 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | BE    | 164/166 (99%) | 156 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 1   | BF    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | BG    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | BH    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | BI    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | BJ    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | BK    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BL    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BM    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | BN    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | BO    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | BP    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | BQ    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | BR    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | BS    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BT    | 164/166 (99%) | 155 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 1   | BU    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | BV    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | BW    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | BX    | 164/166 (99%) | 157 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | BY    | 164/166 (99%) | 162 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | BZ    | 164/166 (99%) | 156 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 1   | CA    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | CB    | 164/166 (99%) | 158 (96%)  | 5 (3%)  | 1 (1%)   | 21          | 54  |
| 1   | CC    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | CD    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | CE    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | CF    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CG    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CH    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | CI    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | CJ    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | CK    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | CL    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | CM    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | CN    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CO    | 164/166 (99%) | 155 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 1   | CP    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | CQ    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | CR    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | CS    | 164/166 (99%) | 157 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | CT    | 164/166 (99%) | 162 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | CU    | 164/166 (99%) | 156 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 1   | CV    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | CW    | 164/166 (99%) | 158 (96%)  | 6 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | CX    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | CY    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | CZ    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | DA    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | DB    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | DC    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | DD    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | DE    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | DF    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | DG    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | DH    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | DI    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | DJ    | 164/166 (99%) | 155 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 1   | DK    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | DL    | 164/166 (99%) | 158 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 1   | DM    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | DN    | 164/166 (99%) | 157 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | DO    | 164/166 (99%) | 162 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | DP    | 164/166 (99%) | 156 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 1   | DQ    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | DR    | 164/166 (99%) | 158 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 1   | DS    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | DT    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | DU    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | DV    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | DW    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | DX    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | DY    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | DZ    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | EA    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | EB    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | EC    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | ED    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | EE    | 164/166 (99%) | 155 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 1   | EF    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | EG    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | EH    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | EI    | 164/166 (99%) | 157 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | EJ    | 164/166 (99%) | 162 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | EK    | 164/166 (99%) | 156 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 1   | EL    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | EM    | 164/166 (99%) | 159 (97%)  | 4 (2%)  | 1 (1%)   | 21          | 54  |
| 1   | EN    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | EO    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | EP    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | EQ    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | ER    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | ES    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | ET    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | EU    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | EV    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | EW    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | EX    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | EY    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | EZ    | 164/166 (99%) | 155 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 1   | FA    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | FB    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | FC    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | FD    | 164/166 (99%) | 157 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | FE    | 164/166 (99%) | 162 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | FF    | 164/166 (99%) | 156 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 1   | FG    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | FH    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | FI    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | FJ    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | FK    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | FL    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | FM    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | FN    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | FO    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | FP    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | FQ    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | FR    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | FS    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | FT    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | FU    | 164/166 (99%) | 155 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 1   | FV    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | FW    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | FX    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | FY    | 164/166 (99%) | 157 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | FZ    | 164/166 (99%) | 162 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | GA    | 164/166 (99%) | 156 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 1   | GB    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | GC    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | GD    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | GE    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | GF    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | GG    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | GH    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | GI    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | GJ    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | GK    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | GL    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 1   | GM    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | GN    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | GO    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | GP    | 164/166 (99%) | 155 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 1   | GQ    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | GR    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | GS    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | GT    | 164/166 (99%) | 157 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | GU    | 164/166 (99%) | 162 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | GV    | 164/166 (99%) | 156 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 1   | GW    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | GX    | 164/166 (99%) | 158 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 1   | GY    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | GZ    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | HA    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | HB    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | HC    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | HD    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | HE    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | HF    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | HG    | 164/166 (99%) | 164 (100%) | 0       | 0        | 100         | 100 |
| 1   | HH    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | HI    | 164/166 (99%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 1   | HJ    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | HK    | 164/166 (99%) | 155 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 1   | HL    | 164/166 (99%) | 161 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 1   | HM    | 164/166 (99%) | 159 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 1   | HN    | 164/166 (99%) | 163 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 1   | HO    | 164/166 (99%) | 157 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 1   | HP    | 164/166 (99%) | 162 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 1   | HQ    | 164/166 (99%) | 156 (95%)  | 8 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 1   | HR    | 164/166 (99%)     | 161 (98%)   | 3 (2%)   | 0        | 100         | 100 |
| 1   | HS    | 164/166 (99%)     | 159 (97%)   | 5 (3%)   | 0        | 100         | 100 |
| 1   | HT    | 164/166 (99%)     | 164 (100%)  | 0        | 0        | 100         | 100 |
| 1   | HU    | 164/166 (99%)     | 164 (100%)  | 0        | 0        | 100         | 100 |
| 1   | HV    | 164/166 (99%)     | 164 (100%)  | 0        | 0        | 100         | 100 |
| 1   | HW    | 164/166 (99%)     | 163 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 1   | HX    | 164/166 (99%)     | 163 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 1   | HY    | 164/166 (99%)     | 164 (100%)  | 0        | 0        | 100         | 100 |
| 1   | HZ    | 164/166 (99%)     | 164 (100%)  | 0        | 0        | 100         | 100 |
| 1   | IA    | 164/166 (99%)     | 164 (100%)  | 0        | 0        | 100         | 100 |
| 1   | IB    | 164/166 (99%)     | 164 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 34440/34860 (99%) | 33906 (98%) | 532 (2%) | 2 (0%)   | 100         | 100 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CB    | 106 | GLY  |
| 1   | EM    | 106 | GLY  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | AB    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | AC    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | AD    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | AE    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | AF    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | AG    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | AH    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | AI    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | AJ    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | AK    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | AL    | 147/147 (100%) | 143 (97%)  | 4 (3%)   | 39          | 61  |
| 1   | AM    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | AN    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | AO    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | AP    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | AQ    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | AR    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | AS    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | AT    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | AU    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | AV    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | AW    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | AX    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | AY    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | AZ    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BA    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BB    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | BC    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | BD    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BE    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | BF    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BG    | 147/147 (100%) | 143 (97%)  | 4 (3%)   | 39          | 61  |
| 1   | BH    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BI    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | BJ    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | BK    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | BL    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | BM    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | BN    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | BO    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | BP    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BQ    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | BR    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | BS    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BT    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BU    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BV    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BW    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | BX    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | BY    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | BZ    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | CA    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | CB    | 147/147 (100%) | 143 (97%)  | 4 (3%)   | 39          | 61  |
| 1   | CC    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | CD    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | CE    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | CF    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | CG    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | CH    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | CI    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | CJ    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | CK    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | CL    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | CM    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | CN    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | CO    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | CP    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | CQ    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | CR    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | CS    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | CT    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | CU    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | CV    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | CW    | 147/147 (100%) | 143 (97%)  | 4 (3%)   | 39          | 61  |
| 1   | CX    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | CY    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | CZ    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | DA    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | DB    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | DC    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | DD    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | DE    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | DF    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | DG    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | DH    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | DI    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | DJ    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | DK    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | DL    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | DM    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | DN    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | DO    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | DP    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | DQ    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | DR    | 147/147 (100%) | 143 (97%)  | 4 (3%)   | 39          | 61  |
| 1   | DS    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | DT    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | DU    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | DV    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | DW    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | DX    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | DY    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | DZ    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | EA    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | EB    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | EC    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | ED    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | EE    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | EF    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | EG    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | EH    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | EI    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | EJ    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | EK    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | EL    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | EM    | 147/147 (100%) | 143 (97%)  | 4 (3%)   | 39          | 61  |
| 1   | EN    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | EO    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | EP    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | EQ    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | ER    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | ES    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | ET    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | EU    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | EV    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | EW    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | EX    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | EY    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | EZ    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | FA    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | FB    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | FC    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | FD    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | FE    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | FF    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | FG    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | FH    | 147/147 (100%) | 143 (97%)  | 4 (3%)   | 39          | 61  |
| 1   | FI    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | FJ    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | FK    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | FL    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | FM    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | FN    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | FO    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | FP    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | FQ    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | FR    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | FS    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | FT    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | FU    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | FV    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | FW    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | FX    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | FY    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | FZ    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GA    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | GB    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GC    | 147/147 (100%) | 143 (97%)  | 4 (3%)   | 39          | 61  |
| 1   | GD    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GE    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | GF    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | GG    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | GH    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | GI    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | GJ    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | GK    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | GL    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GM    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | GN    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | GO    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GP    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GQ    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GR    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GS    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | GT    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | GU    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GV    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | GW    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GX    | 147/147 (100%) | 143 (97%)  | 4 (3%)   | 39          | 61  |
| 1   | GY    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | GZ    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | HA    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | HB    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | HC    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | HD    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | HE    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | HF    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | HG    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | HH    | 147/147 (100%) | 145 (99%)  | 2 (1%)   | 59          | 71  |
| 1   | HI    | 147/147 (100%) | 147 (100%) | 0        | 100         | 100 |
| 1   | HJ    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |
| 1   | HK    | 147/147 (100%) | 146 (99%)  | 1 (1%)   | 76          | 78  |

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| Mol | Chain | Analysed           | Rotameric   | Outliers | Percentiles |     |
|-----|-------|--------------------|-------------|----------|-------------|-----|
| 1   | HL    | 147/147 (100%)     | 146 (99%)   | 1 (1%)   | 76          | 78  |
| 1   | HM    | 147/147 (100%)     | 146 (99%)   | 1 (1%)   | 76          | 78  |
| 1   | HN    | 147/147 (100%)     | 145 (99%)   | 2 (1%)   | 59          | 71  |
| 1   | HO    | 147/147 (100%)     | 145 (99%)   | 2 (1%)   | 59          | 71  |
| 1   | HP    | 147/147 (100%)     | 146 (99%)   | 1 (1%)   | 76          | 78  |
| 1   | HQ    | 147/147 (100%)     | 145 (99%)   | 2 (1%)   | 59          | 71  |
| 1   | HR    | 147/147 (100%)     | 146 (99%)   | 1 (1%)   | 76          | 78  |
| 1   | HS    | 147/147 (100%)     | 143 (97%)   | 4 (3%)   | 39          | 61  |
| 1   | HT    | 147/147 (100%)     | 146 (99%)   | 1 (1%)   | 76          | 78  |
| 1   | HU    | 147/147 (100%)     | 147 (100%)  | 0        | 100         | 100 |
| 1   | HV    | 147/147 (100%)     | 145 (99%)   | 2 (1%)   | 59          | 71  |
| 1   | HW    | 147/147 (100%)     | 147 (100%)  | 0        | 100         | 100 |
| 1   | HX    | 147/147 (100%)     | 147 (100%)  | 0        | 100         | 100 |
| 1   | HY    | 147/147 (100%)     | 147 (100%)  | 0        | 100         | 100 |
| 1   | HZ    | 147/147 (100%)     | 147 (100%)  | 0        | 100         | 100 |
| 1   | IA    | 147/147 (100%)     | 147 (100%)  | 0        | 100         | 100 |
| 1   | IB    | 147/147 (100%)     | 146 (99%)   | 1 (1%)   | 76          | 78  |
| All | All   | 30870/30870 (100%) | 30650 (99%) | 220 (1%) | 76          | 78  |

5 of 220 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | EG    | 75  | ASN  |
| 1   | FF    | 72  | ASN  |
| 1   | IB    | 97  | ARG  |
| 1   | HH    | 98  | THR  |
| 1   | EI    | 97  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | HD    | 74  | GLN  |
| 1   | HG    | 144 | GLN  |
| 1   | HY    | 99  | GLN  |
| 1   | CY    | 75  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CX    | 75  | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ > 2 |     |     | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|----------------|--------|-----------|-----|-----|-----------------------|---------|
| 1   | AA    | 166/166 (100%) | 0.44   | 4 (2%)    | 59  | 34  | 76, 102, 127, 158     | 0       |
| 1   | AB    | 166/166 (100%) | 0.45   | 3 (1%)    | 67  | 40  | 80, 103, 133, 171     | 0       |
| 1   | AC    | 166/166 (100%) | 0.35   | 3 (1%)    | 67  | 40  | 77, 99, 128, 154      | 0       |
| 1   | AD    | 166/166 (100%) | 0.33   | 3 (1%)    | 67  | 40  | 76, 101, 136, 166     | 0       |
| 1   | AE    | 166/166 (100%) | 0.31   | 5 (3%)    | 52  | 30  | 75, 99, 125, 158      | 0       |
| 1   | AF    | 166/166 (100%) | 0.43   | 5 (3%)    | 52  | 30  | 75, 100, 137, 171     | 0       |
| 1   | AG    | 166/166 (100%) | 0.64   | 4 (2%)    | 59  | 34  | 75, 98, 123, 150      | 0       |
| 1   | AH    | 166/166 (100%) | 0.60   | 6 (3%)    | 46  | 26  | 75, 97, 135, 166      | 0       |
| 1   | AI    | 166/166 (100%) | 0.41   | 4 (2%)    | 59  | 34  | 76, 97, 123, 140      | 0       |
| 1   | AJ    | 166/166 (100%) | 0.48   | 4 (2%)    | 59  | 34  | 76, 97, 127, 170      | 0       |
| 1   | AK    | 166/166 (100%) | 0.42   | 4 (2%)    | 59  | 34  | 76, 96, 121, 156      | 0       |
| 1   | AL    | 166/166 (100%) | 0.41   | 4 (2%)    | 59  | 34  | 76, 97, 133, 170      | 0       |
| 1   | AM    | 166/166 (100%) | 0.50   | 7 (4%)    | 40  | 22  | 78, 105, 138, 151     | 0       |
| 1   | AN    | 166/166 (100%) | 0.51   | 3 (1%)    | 67  | 40  | 81, 104, 137, 156     | 0       |
| 1   | AO    | 166/166 (100%) | 0.40   | 0         | 100 | 100 | 80, 100, 136, 151     | 0       |
| 1   | AP    | 166/166 (100%) | 0.38   | 4 (2%)    | 59  | 34  | 75, 103, 133, 149     | 0       |
| 1   | AQ    | 166/166 (100%) | 0.54   | 7 (4%)    | 40  | 22  | 76, 101, 138, 162     | 0       |
| 1   | AR    | 166/166 (100%) | 0.53   | 10 (6%)   | 27  | 17  | 77, 100, 138, 153     | 0       |
| 1   | AS    | 166/166 (100%) | 0.51   | 6 (3%)    | 46  | 26  | 76, 97, 138, 150      | 0       |
| 1   | AT    | 166/166 (100%) | 0.60   | 5 (3%)    | 52  | 30  | 76, 98, 134, 178      | 0       |
| 1   | AU    | 166/166 (100%) | 1.28   | 29 (17%)  | 4   | 4   | 79, 100, 130, 148     | 0       |
| 1   | AV    | 166/166 (100%) | 0.42   | 6 (3%)    | 46  | 26  | 76, 102, 127, 158     | 0       |
| 1   | AW    | 166/166 (100%) | 0.34   | 5 (3%)    | 52  | 30  | 80, 103, 133, 171     | 0       |
| 1   | AX    | 166/166 (100%) | 0.42   | 6 (3%)    | 46  | 26  | 77, 99, 128, 154      | 0       |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | AY    | 166/166 (100%) | 0.40   | 3 (1%) 67 40  | 76, 101, 136, 166     | 0     |
| 1   | AZ    | 166/166 (100%) | 0.29   | 1 (0%) 85 64  | 75, 99, 125, 158      | 0     |
| 1   | BA    | 166/166 (100%) | 0.41   | 9 (5%) 31 18  | 75, 100, 137, 171     | 0     |
| 1   | BB    | 166/166 (100%) | 0.41   | 3 (1%) 67 40  | 75, 98, 123, 150      | 0     |
| 1   | BC    | 166/166 (100%) | 0.41   | 3 (1%) 67 40  | 75, 97, 135, 166      | 0     |
| 1   | BD    | 166/166 (100%) | 0.41   | 4 (2%) 59 34  | 76, 97, 123, 140      | 0     |
| 1   | BE    | 166/166 (100%) | 0.38   | 3 (1%) 67 40  | 76, 97, 127, 170      | 0     |
| 1   | BF    | 166/166 (100%) | 0.40   | 3 (1%) 67 40  | 76, 96, 121, 156      | 0     |
| 1   | BG    | 166/166 (100%) | 0.43   | 3 (1%) 67 40  | 76, 97, 133, 170      | 0     |
| 1   | BH    | 166/166 (100%) | 0.54   | 3 (1%) 67 40  | 78, 105, 138, 151     | 0     |
| 1   | BI    | 166/166 (100%) | 0.56   | 6 (3%) 46 26  | 81, 104, 137, 156     | 0     |
| 1   | BJ    | 166/166 (100%) | 0.51   | 6 (3%) 46 26  | 80, 100, 136, 151     | 0     |
| 1   | BK    | 166/166 (100%) | 0.67   | 12 (7%) 21 14 | 75, 103, 133, 149     | 0     |
| 1   | BL    | 166/166 (100%) | 0.43   | 4 (2%) 59 34  | 76, 101, 138, 162     | 0     |
| 1   | BM    | 166/166 (100%) | 0.46   | 8 (4%) 35 20  | 77, 100, 138, 153     | 0     |
| 1   | BN    | 166/166 (100%) | 0.41   | 8 (4%) 35 20  | 76, 97, 138, 150      | 0     |
| 1   | BO    | 166/166 (100%) | 0.44   | 3 (1%) 67 40  | 76, 98, 134, 178      | 0     |
| 1   | BP    | 166/166 (100%) | 0.69   | 11 (6%) 24 15 | 79, 100, 130, 148     | 0     |
| 1   | BQ    | 166/166 (100%) | 0.56   | 7 (4%) 40 22  | 76, 102, 127, 158     | 0     |
| 1   | BR    | 166/166 (100%) | 0.44   | 6 (3%) 46 26  | 80, 103, 133, 171     | 0     |
| 1   | BS    | 166/166 (100%) | 0.50   | 5 (3%) 52 30  | 77, 99, 128, 154      | 0     |
| 1   | BT    | 166/166 (100%) | 0.50   | 4 (2%) 59 34  | 76, 101, 136, 166     | 0     |
| 1   | BU    | 166/166 (100%) | 0.49   | 5 (3%) 52 30  | 75, 99, 125, 158      | 0     |
| 1   | BV    | 166/166 (100%) | 0.60   | 7 (4%) 40 22  | 75, 100, 137, 171     | 0     |
| 1   | BW    | 166/166 (100%) | 0.54   | 7 (4%) 40 22  | 75, 98, 123, 150      | 0     |
| 1   | BX    | 166/166 (100%) | 0.57   | 5 (3%) 52 30  | 75, 97, 135, 166      | 0     |
| 1   | BY    | 166/166 (100%) | 0.61   | 12 (7%) 21 14 | 76, 97, 123, 140      | 0     |
| 1   | BZ    | 166/166 (100%) | 0.54   | 5 (3%) 52 30  | 76, 97, 127, 170      | 0     |
| 1   | CA    | 166/166 (100%) | 0.39   | 2 (1%) 76 50  | 76, 96, 121, 156      | 0     |
| 1   | CB    | 166/166 (100%) | 0.41   | 3 (1%) 67 40  | 76, 97, 133, 170      | 0     |
| 1   | CC    | 166/166 (100%) | 0.50   | 4 (2%) 59 34  | 78, 105, 138, 151     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | CD    | 166/166 (100%) | 0.62   | 10 (6%) 27 17 | 81, 104, 137, 156     | 0     |
| 1   | CE    | 166/166 (100%) | 0.51   | 8 (4%) 35 20  | 80, 100, 136, 151     | 0     |
| 1   | CF    | 166/166 (100%) | 0.54   | 6 (3%) 46 26  | 75, 103, 133, 149     | 0     |
| 1   | CG    | 166/166 (100%) | 0.59   | 6 (3%) 46 26  | 76, 101, 138, 162     | 0     |
| 1   | CH    | 166/166 (100%) | 0.69   | 14 (8%) 17 12 | 77, 100, 138, 153     | 0     |
| 1   | CI    | 166/166 (100%) | 0.68   | 10 (6%) 27 17 | 76, 97, 138, 150      | 0     |
| 1   | CJ    | 166/166 (100%) | 0.61   | 8 (4%) 35 20  | 76, 98, 134, 178      | 0     |
| 1   | CK    | 166/166 (100%) | 0.66   | 8 (4%) 35 20  | 79, 100, 130, 148     | 0     |
| 1   | CL    | 166/166 (100%) | 0.60   | 7 (4%) 40 22  | 76, 102, 127, 158     | 0     |
| 1   | CM    | 166/166 (100%) | 0.52   | 5 (3%) 52 30  | 80, 103, 133, 171     | 0     |
| 1   | CN    | 166/166 (100%) | 0.50   | 7 (4%) 40 22  | 77, 99, 128, 154      | 0     |
| 1   | CO    | 166/166 (100%) | 0.48   | 4 (2%) 59 34  | 76, 101, 136, 166     | 0     |
| 1   | CP    | 166/166 (100%) | 0.45   | 5 (3%) 52 30  | 75, 99, 125, 158      | 0     |
| 1   | CQ    | 166/166 (100%) | 0.40   | 3 (1%) 67 40  | 75, 100, 137, 171     | 0     |
| 1   | CR    | 166/166 (100%) | 0.40   | 3 (1%) 67 40  | 75, 98, 123, 150      | 0     |
| 1   | CS    | 166/166 (100%) | 0.38   | 5 (3%) 52 30  | 75, 97, 135, 166      | 0     |
| 1   | CT    | 166/166 (100%) | 0.50   | 2 (1%) 76 50  | 76, 97, 123, 140      | 0     |
| 1   | CU    | 166/166 (100%) | 0.42   | 4 (2%) 59 34  | 76, 97, 127, 170      | 0     |
| 1   | CV    | 166/166 (100%) | 0.51   | 8 (4%) 35 20  | 76, 96, 121, 156      | 0     |
| 1   | CW    | 166/166 (100%) | 0.50   | 7 (4%) 40 22  | 76, 97, 133, 170      | 0     |
| 1   | CX    | 166/166 (100%) | 0.54   | 10 (6%) 27 17 | 78, 105, 138, 151     | 0     |
| 1   | CY    | 166/166 (100%) | 0.60   | 6 (3%) 46 26  | 81, 104, 137, 156     | 0     |
| 1   | CZ    | 166/166 (100%) | 0.63   | 10 (6%) 27 17 | 80, 100, 136, 151     | 0     |
| 1   | DA    | 166/166 (100%) | 0.77   | 16 (9%) 13 10 | 75, 103, 133, 149     | 0     |
| 1   | DB    | 166/166 (100%) | 0.68   | 7 (4%) 40 22  | 76, 101, 138, 162     | 0     |
| 1   | DC    | 166/166 (100%) | 0.65   | 9 (5%) 31 18  | 77, 100, 138, 153     | 0     |
| 1   | DD    | 166/166 (100%) | 0.42   | 6 (3%) 46 26  | 76, 97, 138, 150      | 0     |
| 1   | DE    | 166/166 (100%) | 0.54   | 5 (3%) 52 30  | 76, 98, 134, 178      | 0     |
| 1   | DF    | 166/166 (100%) | 0.74   | 18 (10%) 11 9 | 79, 100, 130, 148     | 0     |
| 1   | DG    | 166/166 (100%) | 0.56   | 5 (3%) 52 30  | 76, 102, 127, 158     | 0     |
| 1   | DH    | 166/166 (100%) | 0.46   | 4 (2%) 59 34  | 80, 103, 133, 171     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2 |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------|----|----|-----------------------|-------|
| 1   | DI    | 166/166 (100%) | 0.53   | 6 (3%)  | 46 | 26 | 77, 99, 128, 154      | 0     |
| 1   | DJ    | 166/166 (100%) | 0.57   | 7 (4%)  | 40 | 22 | 76, 101, 136, 166     | 0     |
| 1   | DK    | 166/166 (100%) | 0.43   | 4 (2%)  | 59 | 34 | 75, 99, 125, 158      | 0     |
| 1   | DL    | 166/166 (100%) | 0.57   | 6 (3%)  | 46 | 26 | 75, 100, 137, 171     | 0     |
| 1   | DM    | 166/166 (100%) | 0.51   | 7 (4%)  | 40 | 22 | 75, 98, 123, 150      | 0     |
| 1   | DN    | 166/166 (100%) | 0.54   | 5 (3%)  | 52 | 30 | 75, 97, 135, 166      | 0     |
| 1   | DO    | 166/166 (100%) | 0.40   | 3 (1%)  | 67 | 40 | 76, 97, 123, 140      | 0     |
| 1   | DP    | 166/166 (100%) | 0.45   | 3 (1%)  | 67 | 40 | 76, 97, 127, 170      | 0     |
| 1   | DQ    | 166/166 (100%) | 0.54   | 6 (3%)  | 46 | 26 | 76, 96, 121, 156      | 0     |
| 1   | DR    | 166/166 (100%) | 0.53   | 2 (1%)  | 76 | 50 | 76, 97, 133, 170      | 0     |
| 1   | DS    | 166/166 (100%) | 0.61   | 8 (4%)  | 35 | 20 | 78, 105, 138, 151     | 0     |
| 1   | DT    | 166/166 (100%) | 0.63   | 8 (4%)  | 35 | 20 | 81, 104, 137, 156     | 0     |
| 1   | DU    | 166/166 (100%) | 0.48   | 6 (3%)  | 46 | 26 | 80, 100, 136, 151     | 0     |
| 1   | DV    | 166/166 (100%) | 0.57   | 7 (4%)  | 40 | 22 | 75, 103, 133, 149     | 0     |
| 1   | DW    | 166/166 (100%) | 0.60   | 7 (4%)  | 40 | 22 | 76, 101, 138, 162     | 0     |
| 1   | DX    | 166/166 (100%) | 0.58   | 7 (4%)  | 40 | 22 | 77, 100, 138, 153     | 0     |
| 1   | DY    | 166/166 (100%) | 0.45   | 4 (2%)  | 59 | 34 | 76, 97, 138, 150      | 0     |
| 1   | DZ    | 166/166 (100%) | 0.35   | 3 (1%)  | 67 | 40 | 76, 98, 134, 178      | 0     |
| 1   | EA    | 166/166 (100%) | 0.44   | 2 (1%)  | 76 | 50 | 79, 100, 130, 148     | 0     |
| 1   | EB    | 166/166 (100%) | 0.45   | 5 (3%)  | 52 | 30 | 76, 102, 127, 158     | 0     |
| 1   | EC    | 166/166 (100%) | 0.54   | 7 (4%)  | 40 | 22 | 80, 103, 133, 171     | 0     |
| 1   | ED    | 166/166 (100%) | 0.36   | 2 (1%)  | 76 | 50 | 77, 99, 128, 154      | 0     |
| 1   | EE    | 166/166 (100%) | 0.33   | 4 (2%)  | 59 | 34 | 76, 101, 136, 166     | 0     |
| 1   | EF    | 166/166 (100%) | 0.25   | 4 (2%)  | 59 | 34 | 75, 99, 125, 158      | 0     |
| 1   | EG    | 166/166 (100%) | 0.42   | 7 (4%)  | 40 | 22 | 75, 100, 137, 171     | 0     |
| 1   | EH    | 166/166 (100%) | 0.43   | 3 (1%)  | 67 | 40 | 75, 98, 123, 150      | 0     |
| 1   | EI    | 166/166 (100%) | 0.61   | 12 (7%) | 21 | 14 | 75, 97, 135, 166      | 0     |
| 1   | EJ    | 166/166 (100%) | 0.60   | 4 (2%)  | 59 | 34 | 76, 97, 123, 140      | 0     |
| 1   | EK    | 166/166 (100%) | 0.73   | 8 (4%)  | 35 | 20 | 76, 97, 127, 170      | 0     |
| 1   | EL    | 166/166 (100%) | 0.42   | 6 (3%)  | 46 | 26 | 76, 96, 121, 156      | 0     |
| 1   | EM    | 166/166 (100%) | 0.41   | 4 (2%)  | 59 | 34 | 76, 97, 133, 170      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2 |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------|-----|-----|-----------------------|-------|
| 1   | EN    | 166/166 (100%) | 0.52   | 4 (2%)  | 59  | 34  | 78, 105, 138, 151     | 0     |
| 1   | EO    | 166/166 (100%) | 0.61   | 9 (5%)  | 31  | 18  | 81, 104, 137, 156     | 0     |
| 1   | EP    | 166/166 (100%) | 0.45   | 4 (2%)  | 59  | 34  | 80, 100, 136, 151     | 0     |
| 1   | EQ    | 166/166 (100%) | 0.48   | 5 (3%)  | 52  | 30  | 75, 103, 133, 149     | 0     |
| 1   | ER    | 166/166 (100%) | 0.74   | 10 (6%) | 27  | 17  | 76, 101, 138, 162     | 0     |
| 1   | ES    | 166/166 (100%) | 0.64   | 10 (6%) | 27  | 17  | 77, 100, 138, 153     | 0     |
| 1   | ET    | 166/166 (100%) | 0.67   | 6 (3%)  | 46  | 26  | 76, 97, 138, 150      | 0     |
| 1   | EU    | 166/166 (100%) | 0.67   | 9 (5%)  | 31  | 18  | 76, 98, 134, 178      | 0     |
| 1   | EV    | 166/166 (100%) | 0.80   | 12 (7%) | 21  | 14  | 79, 100, 130, 148     | 0     |
| 1   | EW    | 166/166 (100%) | 0.57   | 6 (3%)  | 46  | 26  | 76, 102, 127, 158     | 0     |
| 1   | EX    | 166/166 (100%) | 0.50   | 9 (5%)  | 31  | 18  | 80, 103, 133, 171     | 0     |
| 1   | EY    | 166/166 (100%) | 0.30   | 3 (1%)  | 67  | 40  | 77, 99, 128, 154      | 0     |
| 1   | EZ    | 166/166 (100%) | 0.41   | 2 (1%)  | 76  | 50  | 76, 101, 136, 166     | 0     |
| 1   | FA    | 166/166 (100%) | 0.24   | 2 (1%)  | 76  | 50  | 75, 99, 125, 158      | 0     |
| 1   | FB    | 166/166 (100%) | 0.31   | 7 (4%)  | 40  | 22  | 75, 100, 137, 171     | 0     |
| 1   | FC    | 166/166 (100%) | 0.33   | 2 (1%)  | 76  | 50  | 75, 98, 123, 150      | 0     |
| 1   | FD    | 166/166 (100%) | 0.37   | 2 (1%)  | 76  | 50  | 75, 97, 135, 166      | 0     |
| 1   | FE    | 166/166 (100%) | 0.35   | 4 (2%)  | 59  | 34  | 76, 97, 123, 140      | 0     |
| 1   | FF    | 166/166 (100%) | 0.35   | 0       | 100 | 100 | 76, 97, 127, 170      | 0     |
| 1   | FG    | 166/166 (100%) | 0.41   | 2 (1%)  | 76  | 50  | 76, 96, 121, 156      | 0     |
| 1   | FH    | 166/166 (100%) | 0.41   | 4 (2%)  | 59  | 34  | 76, 97, 133, 170      | 0     |
| 1   | FI    | 166/166 (100%) | 0.49   | 4 (2%)  | 59  | 34  | 78, 105, 138, 151     | 0     |
| 1   | FJ    | 166/166 (100%) | 0.68   | 11 (6%) | 24  | 15  | 81, 104, 137, 156     | 0     |
| 1   | FK    | 166/166 (100%) | 0.46   | 6 (3%)  | 46  | 26  | 80, 100, 136, 151     | 0     |
| 1   | FL    | 166/166 (100%) | 0.52   | 6 (3%)  | 46  | 26  | 75, 103, 133, 149     | 0     |
| 1   | FM    | 166/166 (100%) | 0.57   | 11 (6%) | 24  | 15  | 76, 101, 138, 162     | 0     |
| 1   | FN    | 166/166 (100%) | 0.50   | 5 (3%)  | 52  | 30  | 77, 100, 138, 153     | 0     |
| 1   | FO    | 166/166 (100%) | 0.56   | 12 (7%) | 21  | 14  | 76, 97, 138, 150      | 0     |
| 1   | FP    | 166/166 (100%) | 0.46   | 3 (1%)  | 67  | 40  | 76, 98, 134, 178      | 0     |
| 1   | FQ    | 166/166 (100%) | 0.66   | 12 (7%) | 21  | 14  | 79, 100, 130, 148     | 0     |
| 1   | FR    | 166/166 (100%) | 0.41   | 5 (3%)  | 52  | 30  | 76, 102, 127, 158     | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|----|----|-----------------------|-------|
| 1   | FS    | 166/166 (100%) | 0.53   | 8 (4%)   | 35 | 20 | 80, 103, 133, 171     | 0     |
| 1   | FT    | 166/166 (100%) | 0.42   | 4 (2%)   | 59 | 34 | 77, 99, 128, 154      | 0     |
| 1   | FU    | 166/166 (100%) | 0.49   | 7 (4%)   | 40 | 22 | 76, 101, 136, 166     | 0     |
| 1   | FV    | 166/166 (100%) | 0.39   | 5 (3%)   | 52 | 30 | 75, 99, 125, 158      | 0     |
| 1   | FW    | 166/166 (100%) | 0.48   | 7 (4%)   | 40 | 22 | 75, 100, 137, 171     | 0     |
| 1   | FX    | 166/166 (100%) | 0.34   | 4 (2%)   | 59 | 34 | 75, 98, 123, 150      | 0     |
| 1   | FY    | 166/166 (100%) | 0.57   | 8 (4%)   | 35 | 20 | 75, 97, 135, 166      | 0     |
| 1   | FZ    | 166/166 (100%) | 0.55   | 9 (5%)   | 31 | 18 | 76, 97, 123, 140      | 0     |
| 1   | GA    | 166/166 (100%) | 0.63   | 7 (4%)   | 40 | 22 | 76, 97, 127, 170      | 0     |
| 1   | GB    | 166/166 (100%) | 0.37   | 3 (1%)   | 67 | 40 | 76, 96, 121, 156      | 0     |
| 1   | GC    | 166/166 (100%) | 0.37   | 2 (1%)   | 76 | 50 | 76, 97, 133, 170      | 0     |
| 1   | GD    | 166/166 (100%) | 0.47   | 7 (4%)   | 40 | 22 | 78, 105, 138, 151     | 0     |
| 1   | GE    | 166/166 (100%) | 0.47   | 5 (3%)   | 52 | 30 | 81, 104, 137, 156     | 0     |
| 1   | GF    | 166/166 (100%) | 0.42   | 6 (3%)   | 46 | 26 | 80, 100, 136, 151     | 0     |
| 1   | GG    | 166/166 (100%) | 0.39   | 6 (3%)   | 46 | 26 | 75, 103, 133, 149     | 0     |
| 1   | GH    | 166/166 (100%) | 0.34   | 3 (1%)   | 67 | 40 | 76, 101, 138, 162     | 0     |
| 1   | GI    | 166/166 (100%) | 0.57   | 9 (5%)   | 31 | 18 | 77, 100, 138, 153     | 0     |
| 1   | GJ    | 166/166 (100%) | 0.88   | 19 (11%) | 10 | 8  | 76, 97, 138, 150      | 0     |
| 1   | GK    | 166/166 (100%) | 0.80   | 11 (6%)  | 24 | 15 | 76, 98, 134, 178      | 0     |
| 1   | GL    | 166/166 (100%) | 0.50   | 6 (3%)   | 46 | 26 | 79, 100, 130, 148     | 0     |
| 1   | GM    | 166/166 (100%) | 0.55   | 6 (3%)   | 46 | 26 | 76, 102, 127, 158     | 0     |
| 1   | GN    | 166/166 (100%) | 0.49   | 6 (3%)   | 46 | 26 | 80, 103, 133, 171     | 0     |
| 1   | GO    | 166/166 (100%) | 0.49   | 5 (3%)   | 52 | 30 | 77, 99, 128, 154      | 0     |
| 1   | GP    | 166/166 (100%) | 0.48   | 5 (3%)   | 52 | 30 | 76, 101, 136, 166     | 0     |
| 1   | GQ    | 166/166 (100%) | 0.44   | 5 (3%)   | 52 | 30 | 75, 99, 125, 158      | 0     |
| 1   | GR    | 166/166 (100%) | 0.40   | 5 (3%)   | 52 | 30 | 75, 100, 137, 171     | 0     |
| 1   | GS    | 166/166 (100%) | 0.36   | 2 (1%)   | 76 | 50 | 75, 98, 123, 150      | 0     |
| 1   | GT    | 166/166 (100%) | 0.45   | 7 (4%)   | 40 | 22 | 75, 97, 135, 166      | 0     |
| 1   | GU    | 166/166 (100%) | 0.41   | 6 (3%)   | 46 | 26 | 76, 97, 123, 140      | 0     |
| 1   | GV    | 166/166 (100%) | 0.39   | 4 (2%)   | 59 | 34 | 76, 97, 127, 170      | 0     |
| 1   | GW    | 166/166 (100%) | 0.39   | 3 (1%)   | 67 | 40 | 76, 96, 121, 156      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|----|----|-----------------------|-------|
| 1   | GX    | 166/166 (100%) | 0.41   | 4 (2%)   | 59 | 34 | 76, 97, 133, 170      | 0     |
| 1   | GY    | 166/166 (100%) | 0.39   | 4 (2%)   | 59 | 34 | 78, 105, 138, 151     | 0     |
| 1   | GZ    | 166/166 (100%) | 0.44   | 7 (4%)   | 40 | 22 | 81, 104, 137, 156     | 0     |
| 1   | HA    | 166/166 (100%) | 0.55   | 7 (4%)   | 40 | 22 | 80, 100, 136, 151     | 0     |
| 1   | HB    | 166/166 (100%) | 0.57   | 8 (4%)   | 35 | 20 | 75, 103, 133, 149     | 0     |
| 1   | HC    | 166/166 (100%) | 0.63   | 4 (2%)   | 59 | 34 | 76, 101, 138, 162     | 0     |
| 1   | HD    | 166/166 (100%) | 0.63   | 5 (3%)   | 52 | 30 | 77, 100, 138, 153     | 0     |
| 1   | HE    | 166/166 (100%) | 0.53   | 5 (3%)   | 52 | 30 | 76, 97, 138, 150      | 0     |
| 1   | HF    | 166/166 (100%) | 0.49   | 5 (3%)   | 52 | 30 | 76, 98, 134, 178      | 0     |
| 1   | HG    | 166/166 (100%) | 0.93   | 18 (10%) | 11 | 9  | 79, 100, 130, 148     | 0     |
| 1   | HH    | 166/166 (100%) | 0.52   | 4 (2%)   | 59 | 34 | 76, 102, 127, 158     | 0     |
| 1   | HI    | 166/166 (100%) | 0.47   | 4 (2%)   | 59 | 34 | 80, 103, 133, 171     | 0     |
| 1   | HJ    | 166/166 (100%) | 0.50   | 6 (3%)   | 46 | 26 | 77, 99, 128, 154      | 0     |
| 1   | HK    | 166/166 (100%) | 0.51   | 9 (5%)   | 31 | 18 | 76, 101, 136, 166     | 0     |
| 1   | HL    | 166/166 (100%) | 0.31   | 3 (1%)   | 67 | 40 | 75, 99, 125, 158      | 0     |
| 1   | HM    | 166/166 (100%) | 0.34   | 5 (3%)   | 52 | 30 | 75, 100, 137, 171     | 0     |
| 1   | HN    | 166/166 (100%) | 0.44   | 7 (4%)   | 40 | 22 | 75, 98, 123, 150      | 0     |
| 1   | HO    | 166/166 (100%) | 0.36   | 4 (2%)   | 59 | 34 | 75, 97, 135, 166      | 0     |
| 1   | HP    | 166/166 (100%) | 0.28   | 2 (1%)   | 76 | 50 | 76, 97, 123, 140      | 0     |
| 1   | HQ    | 166/166 (100%) | 0.39   | 6 (3%)   | 46 | 26 | 76, 97, 127, 170      | 0     |
| 1   | HR    | 166/166 (100%) | 0.36   | 3 (1%)   | 67 | 40 | 76, 96, 121, 156      | 0     |
| 1   | HS    | 166/166 (100%) | 0.41   | 4 (2%)   | 59 | 34 | 76, 97, 133, 170      | 0     |
| 1   | HT    | 166/166 (100%) | 0.53   | 8 (4%)   | 35 | 20 | 78, 105, 138, 151     | 0     |
| 1   | HU    | 166/166 (100%) | 0.56   | 11 (6%)  | 24 | 15 | 81, 104, 137, 156     | 0     |
| 1   | HV    | 166/166 (100%) | 0.43   | 1 (0%)   | 85 | 64 | 80, 100, 136, 151     | 0     |
| 1   | HW    | 166/166 (100%) | 0.44   | 4 (2%)   | 59 | 34 | 75, 103, 133, 149     | 0     |
| 1   | HX    | 166/166 (100%) | 0.42   | 5 (3%)   | 52 | 30 | 76, 101, 138, 162     | 0     |
| 1   | HY    | 166/166 (100%) | 0.34   | 4 (2%)   | 59 | 34 | 77, 100, 138, 153     | 0     |
| 1   | HZ    | 166/166 (100%) | 0.38   | 7 (4%)   | 40 | 22 | 76, 97, 138, 150      | 0     |
| 1   | IA    | 166/166 (100%) | 0.38   | 5 (3%)   | 52 | 30 | 76, 98, 134, 178      | 0     |
| 1   | IB    | 166/166 (100%) | 0.49   | 4 (2%)   | 59 | 34 | 79, 100, 130, 148     | 0     |

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| Mol | Chain | Analysed           | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|--------------------|--------|-----------------|-----------------------|-------|
| All | All   | 34860/34860 (100%) | 0.49   | 1245 (3%) 46 26 | 75, 100, 135, 178     | 0     |

The worst 5 of 1245 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | DA    | 37  | GLN  | 6.6  |
| 1   | FJ    | 160 | GLY  | 6.0  |
| 1   | HB    | 37  | GLN  | 5.7  |
| 1   | DE    | 36  | SER  | 5.6  |
| 1   | DE    | 37  | GLN  | 5.5  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.