



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:39 AM UTC

PDB ID : 6YFT / pdb\_00006yft  
Title : Virus-like particle of Wenzhou levi-like virus 1  
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.  
Deposited on : 2020-03-26  
Resolution : 3.50 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                                                             |

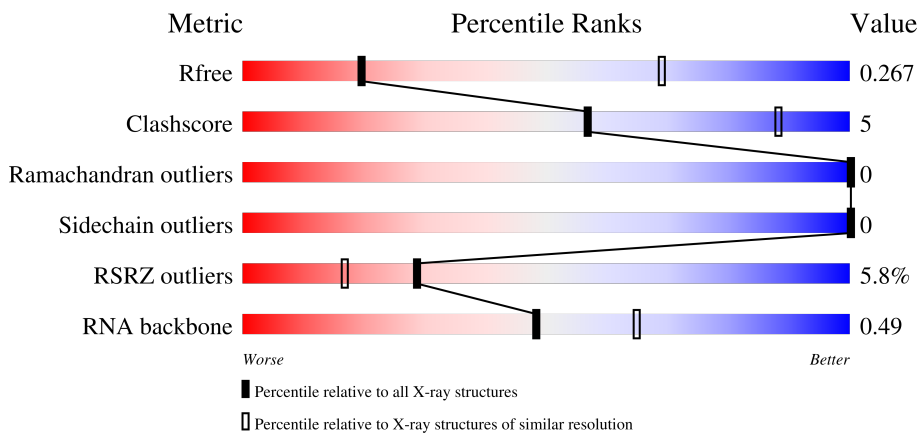
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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                      | 1085 (3.54-3.46)                                      |
| Clashscore            | 190562                      | 1140 (3.54-3.46)                                      |
| Ramachandran outliers | 187476                      | 1113 (3.54-3.46)                                      |
| Sidechain outliers    | 187428                      | 1114 (3.54-3.46)                                      |
| RSRZ outliers         | 180081                      | 1084 (3.54-3.46)                                      |
| RNA backbone          | 3983                        | 1010 (3.98-3.02)                                      |

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    | 113    | <div> <div>6%</div> <div>86%</div> <div>14%</div> </div> |
| 1   | AB    | 113    | <div> <div>2%</div> <div>92%</div> <div>8%</div> </div>  |
| 1   | AC    | 113    | <div> <div>4%</div> <div>90%</div> <div>10%</div> </div> |
| 1   | AD    | 113    | <div> <div>5%</div> <div>87%</div> <div>13%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                      |
|-----|-------|--------|-----------------------------------------------------------------------|
| 1   | AE    | 113    | <div> <div></div> <div>5%</div> <div>94%</div> <div>6%</div> </div>   |
| 1   | AF    | 113    | <div> <div></div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | AG    | 113    | <div> <div></div> <div>3%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | AH    | 113    | <div> <div></div> <div>5%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | AI    | 113    | <div> <div></div> <div>13%</div> <div>86%</div> <div>14%</div> </div> |
| 1   | AJ    | 113    | <div> <div></div> <div>9%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | AK    | 113    | <div> <div></div> <div>3%</div> <div>94%</div> <div>6%</div> </div>   |
| 1   | AL    | 113    | <div> <div></div> <div>9%</div> <div>84%</div> <div>16%</div> </div>  |
| 1   | AM    | 113    | <div> <div></div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | AN    | 113    | <div> <div></div> <div>%</div> <div>93%</div> <div>7%</div> </div>    |
| 1   | AO    | 113    | <div> <div></div> <div>4%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | AP    | 113    | <div> <div></div> <div>11%</div> <div>87%</div> <div>13%</div> </div> |
| 1   | AQ    | 113    | <div> <div></div> <div>4%</div> <div>92%</div> <div>8%</div> </div>   |
| 1   | AR    | 113    | <div> <div></div> <div>8%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | AS    | 113    | <div> <div></div> <div>4%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | AT    | 113    | <div> <div></div> <div>3%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | AU    | 113    | <div> <div></div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | AV    | 113    | <div> <div></div> <div>5%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | AW    | 113    | <div> <div></div> <div>4%</div> <div>91%</div> <div>9%</div> </div>   |
| 1   | AX    | 113    | <div> <div></div> <div>7%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | AY    | 113    | <div> <div></div> <div>3%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | AZ    | 113    | <div> <div></div> <div>5%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | BA    | 113    | <div> <div></div> <div>7%</div> <div>83%</div> <div>17%</div> </div>  |
| 1   | BB    | 113    | <div> <div></div> <div>7%</div> <div>81%</div> <div>19%</div> </div>  |
| 1   | BC    | 113    | <div> <div></div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | BD    | 113    |                  |
| 1   | BE    | 113    |                  |
| 1   | BF    | 113    |                  |
| 1   | BG    | 113    |                  |
| 1   | BH    | 113    |                  |
| 1   | BI    | 113    |                  |
| 1   | BJ    | 113    |                  |
| 1   | BK    | 113    |                  |
| 1   | BL    | 113    |                  |
| 1   | BM    | 113    |                  |
| 1   | BN    | 113    |                  |
| 1   | BO    | 113    |                  |
| 1   | BP    | 113    |                  |
| 1   | BQ    | 113    |                  |
| 1   | BR    | 113    |                  |
| 1   | BS    | 113    |                  |
| 1   | BT    | 113    |                  |
| 1   | BU    | 113    |                  |
| 1   | BV    | 113    |                  |
| 1   | BW    | 113    |                  |
| 1   | BX    | 113    |                  |
| 1   | BY    | 113    |                  |
| 1   | BZ    | 113    |                  |
| 1   | CA    | 113    |                  |
| 1   | CB    | 113    |                  |

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| Mol | Chain | Length | Quality of chain                                                      |
|-----|-------|--------|-----------------------------------------------------------------------|
| 1   | CC    | 113    | <div> <div></div> <div>9%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | CD    | 113    | <div> <div></div> <div>5%</div> <div>94%</div> <div>6%</div> </div>   |
| 1   | CE    | 113    | <div> <div></div> <div>13%</div> <div>88%</div> <div>12%</div> </div> |
| 1   | CF    | 113    | <div> <div></div> <div>5%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | CG    | 113    | <div> <div></div> <div>5%</div> <div>93%</div> <div>7%</div> </div>   |
| 1   | CH    | 113    | <div> <div></div> <div>11%</div> <div>87%</div> <div>13%</div> </div> |
| 1   | CI    | 113    | <div> <div></div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | CJ    | 113    | <div> <div></div> <div>5%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | CK    | 113    | <div> <div></div> <div>4%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | CL    | 113    | <div> <div></div> <div>5%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | CM    | 113    | <div> <div></div> <div>4%</div> <div>93%</div> <div>7%</div> </div>   |
| 1   | CN    | 113    | <div> <div></div> <div>10%</div> <div>89%</div> <div>11%</div> </div> |
| 1   | CO    | 113    | <div> <div></div> <div>4%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | CP    | 113    | <div> <div></div> <div>12%</div> <div>87%</div> <div>13%</div> </div> |
| 1   | CQ    | 113    | <div> <div></div> <div>4%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | CR    | 113    | <div> <div></div> <div>8%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | CS    | 113    | <div> <div></div> <div>4%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | CT    | 113    | <div> <div></div> <div>6%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | CU    | 113    | <div> <div></div> <div>6%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | CV    | 113    | <div> <div></div> <div>6%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | CW    | 113    | <div> <div></div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | CX    | 113    | <div> <div></div> <div>12%</div> <div>81%</div> <div>19%</div> </div> |
| 1   | CY    | 113    | <div> <div></div> <div>6%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | CZ    | 113    | <div> <div></div> <div>12%</div> <div>85%</div> <div>15%</div> </div> |
| 1   | DA    | 113    | <div> <div></div> <div>4%</div> <div>87%</div> <div>13%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | DB    | 113    |                  |
| 1   | DC    | 113    |                  |
| 1   | DD    | 113    |                  |
| 1   | DE    | 113    |                  |
| 1   | DF    | 113    |                  |
| 1   | DG    | 113    |                  |
| 1   | DH    | 113    |                  |
| 1   | DI    | 113    |                  |
| 1   | DJ    | 113    |                  |
| 1   | DK    | 113    |                  |
| 1   | DL    | 113    |                  |
| 1   | DM    | 113    |                  |
| 1   | DN    | 113    |                  |
| 1   | DO    | 113    |                  |
| 1   | DP    | 113    |                  |
| 1   | DQ    | 113    |                  |
| 1   | DR    | 113    |                  |
| 1   | DS    | 113    |                  |
| 1   | DT    | 113    |                  |
| 1   | DU    | 113    |                  |
| 1   | DV    | 113    |                  |
| 1   | DW    | 113    |                  |
| 1   | DX    | 113    |                  |
| 1   | DY    | 113    |                  |
| 1   | DZ    | 113    |                  |

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| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 1   | EA    | 113    | <div> <div></div> <div>87%</div> <div>13%</div> </div>    |
| 1   | EB    | 113    | <div> <div>8%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | EC    | 113    | <div> <div>9%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | ED    | 113    | <div> <div>5%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | EE    | 113    | <div> <div>9%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | EF    | 113    | <div> <div></div> <div>92%</div> <div>8%</div> </div>     |
| 1   | EG    | 113    | <div> <div>7%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | EH    | 113    | <div> <div>6%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | EI    | 113    | <div> <div>3%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | EJ    | 113    | <div> <div>6%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | EK    | 113    | <div> <div>7%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | EL    | 113    | <div> <div>10%</div> <div>90%</div> <div>10%</div> </div> |
| 1   | EM    | 113    | <div> <div>8%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | EN    | 113    | <div> <div>4%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | EO    | 113    | <div> <div>7%</div> <div>91%</div> <div>9%</div> </div>   |
| 1   | EP    | 113    | <div> <div>10%</div> <div>89%</div> <div>11%</div> </div> |
| 1   | EQ    | 113    | <div> <div>5%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | ER    | 113    | <div> <div>4%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | ES    | 113    | <div> <div>8%</div> <div>85%</div> <div>15%</div> </div>  |
| 1   | ET    | 113    | <div> <div>6%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | EU    | 113    | <div> <div>10%</div> <div>90%</div> <div>10%</div> </div> |
| 1   | EV    | 113    | <div> <div>4%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | EW    | 113    | <div> <div>8%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | EX    | 113    | <div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | EY    | 113    | <div> <div>5%</div> <div>88%</div> <div>12%</div> </div>  |

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| Mol | Chain | Length | Quality of chain                                                      |
|-----|-------|--------|-----------------------------------------------------------------------|
| 1   | EZ    | 113    | <div> <div></div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | FA    | 113    | <div> <div></div> <div>5%</div> <div>91%</div> <div>9%</div> </div>   |
| 1   | FB    | 113    | <div> <div></div> <div>5%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | FC    | 113    | <div> <div></div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | FD    | 113    | <div> <div></div> <div>4%</div> <div>93%</div> <div>7%</div> </div>   |
| 1   | FE    | 113    | <div> <div></div> <div>12%</div> <div>87%</div> <div>13%</div> </div> |
| 1   | FF    | 113    | <div> <div></div> <div>9%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | FG    | 113    | <div> <div></div> <div>4%</div> <div>93%</div> <div>7%</div> </div>   |
| 1   | FH    | 113    | <div> <div></div> <div>3%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | FI    | 113    | <div> <div></div> <div>3%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | FJ    | 113    | <div> <div></div> <div>4%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | FK    | 113    | <div> <div></div> <div>4%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | FL    | 113    | <div> <div></div> <div>5%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | FM    | 113    | <div> <div></div> <div>2%</div> <div>91%</div> <div>9%</div> </div>   |
| 1   | FN    | 113    | <div> <div></div> <div>%</div> <div>89%</div> <div>11%</div> </div>   |
| 1   | FO    | 113    | <div> <div></div> <div>3%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | FP    | 113    | <div> <div></div> <div>4%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | FQ    | 113    | <div> <div></div> <div>5%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | FR    | 113    | <div> <div></div> <div>6%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | FS    | 113    | <div> <div></div> <div>6%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | FT    | 113    | <div> <div></div> <div>5%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | FU    | 113    | <div> <div></div> <div>5%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | FV    | 113    | <div> <div></div> <div>3%</div> <div>93%</div> <div>7%</div> </div>   |
| 1   | FW    | 113    | <div> <div></div> <div>4%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | FX    | 113    | <div> <div></div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | FY    | 113    |                  |
| 1   | FZ    | 113    |                  |
| 1   | GA    | 113    |                  |
| 1   | GB    | 113    |                  |
| 1   | GC    | 113    |                  |
| 1   | GD    | 113    |                  |
| 1   | GE    | 113    |                  |
| 1   | GF    | 113    |                  |
| 1   | GG    | 113    |                  |
| 1   | GH    | 113    |                  |
| 1   | GI    | 113    |                  |
| 1   | GJ    | 113    |                  |
| 1   | GK    | 113    |                  |
| 1   | GL    | 113    |                  |
| 1   | GM    | 113    |                  |
| 1   | GN    | 113    |                  |
| 1   | GO    | 113    |                  |
| 1   | GP    | 113    |                  |
| 1   | GQ    | 113    |                  |
| 1   | GR    | 113    |                  |
| 1   | GS    | 113    |                  |
| 1   | GT    | 113    |                  |
| 1   | GU    | 113    |                  |
| 1   | GV    | 113    |                  |
| 1   | GW    | 113    |                  |

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| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 1   | GX    | 113    | <div> <div>8%</div> <div>82%</div> <div>18%</div> </div>  |
| 1   | GY    | 113    | <div> <div>10%</div> <div>88%</div> <div>12%</div> </div> |
| 1   | GZ    | 113    | <div> <div>4%</div> <div>91%</div> <div>9%</div> </div>   |
| 1   | HA    | 113    | <div> <div>7%</div> <div>82%</div> <div>18%</div> </div>  |
| 1   | HB    | 113    | <div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | HC    | 113    | <div> <div>7%</div> <div>91%</div> <div>9%</div> </div>   |
| 1   | HD    | 113    | <div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | HE    | 113    | <div> <div>8%</div> <div>83%</div> <div>17%</div> </div>  |
| 1   | HF    | 113    | <div> <div>2%</div> <div>91%</div> <div>9%</div> </div>   |
| 1   | HG    | 113    | <div> <div>5%</div> <div>90%</div> <div>10%</div> </div>  |
| 1   | HH    | 113    | <div> <div>9%</div> <div>86%</div> <div>14%</div> </div>  |
| 1   | HI    | 113    | <div> <div>10%</div> <div>86%</div> <div>14%</div> </div> |
| 1   | HJ    | 113    | <div> <div>11%</div> <div>88%</div> <div>12%</div> </div> |
| 1   | HK    | 113    | <div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | HL    | 113    | <div> <div>2%</div> <div>91%</div> <div>9%</div> </div>   |
| 1   | HM    | 113    | <div> <div>8%</div> <div>83%</div> <div>17%</div> </div>  |
| 1   | HN    | 113    | <div> <div>0%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | HO    | 113    | <div> <div>6%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | HP    | 113    | <div> <div>4%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | HQ    | 113    | <div> <div>2%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | HR    | 113    | <div> <div>10%</div> <div>91%</div> <div>9%</div> </div>  |
| 1   | HS    | 113    | <div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | HT    | 113    | <div> <div>2%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | HU    | 113    | <div> <div>2%</div> <div>92%</div> <div>8%</div> </div>   |
| 1   | HV    | 113    | <div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | HW    | 113    |                  |
| 1   | HX    | 113    |                  |
| 1   | HY    | 113    |                  |
| 1   | HZ    | 113    |                  |
| 1   | IA    | 113    |                  |
| 1   | IB    | 113    |                  |
| 1   | IC    | 113    |                  |
| 1   | ID    | 113    |                  |
| 1   | IE    | 113    |                  |
| 1   | IF    | 113    |                  |
| 1   | IG    | 113    |                  |
| 1   | IH    | 113    |                  |
| 1   | II    | 113    |                  |
| 1   | IJ    | 113    |                  |
| 1   | IK    | 113    |                  |
| 1   | IL    | 113    |                  |
| 1   | IM    | 113    |                  |
| 1   | IN    | 113    |                  |
| 1   | IO    | 113    |                  |
| 1   | IP    | 113    |                  |
| 1   | IQ    | 113    |                  |
| 1   | IR    | 113    |                  |
| 1   | IS    | 113    |                  |
| 1   | IT    | 113    |                  |
| 1   | IU    | 113    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | IV    | 113    |                  |
| 1   | IW    | 113    |                  |
| 1   | IX    | 113    |                  |
| 1   | IY    | 113    |                  |
| 1   | IZ    | 113    |                  |
| 1   | JA    | 113    |                  |
| 1   | JB    | 113    |                  |
| 1   | JC    | 113    |                  |
| 1   | JD    | 113    |                  |
| 1   | JE    | 113    |                  |
| 1   | JF    | 113    |                  |
| 1   | JG    | 113    |                  |
| 1   | JH    | 113    |                  |
| 1   | JI    | 113    |                  |
| 1   | JJ    | 113    |                  |
| 1   | JK    | 113    |                  |
| 1   | JL    | 113    |                  |
| 1   | JM    | 113    |                  |
| 1   | JN    | 113    |                  |
| 1   | JO    | 113    |                  |
| 1   | JP    | 113    |                  |
| 1   | JQ    | 113    |                  |
| 1   | JR    | 113    |                  |
| 1   | JS    | 113    |                  |
| 1   | JT    | 113    |                  |

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| Mol | Chain | Length | Quality of chain                                          |
|-----|-------|--------|-----------------------------------------------------------|
| 1   | JU    | 113    | <div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | JV    | 113    | <div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | JW    | 113    | <div> <div>4%</div> <div>93%</div> <div>7%</div> </div>   |
| 1   | JX    | 113    | <div> <div>10%</div> <div>88%</div> <div>12%</div> </div> |
| 1   | JY    | 113    | <div> <div>5%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | JZ    | 113    | <div> <div>4%</div> <div>93%</div> <div>7%</div> </div>   |
| 1   | KA    | 113    | <div> <div>4%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | KB    | 113    | <div> <div>5%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | KC    | 113    | <div> <div>4%</div> <div>92%</div> <div>8%</div> </div>   |
| 1   | KD    | 113    | <div> <div>7%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | KE    | 113    | <div> <div>4%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | KF    | 113    | <div> <div>5%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | KG    | 113    | <div> <div>8%</div> <div>88%</div> <div>12%</div> </div>  |
| 1   | KH    | 113    | <div> <div>4%</div> <div>85%</div> <div>15%</div> </div>  |
| 1   | KI    | 113    | <div> <div>8%</div> <div>91%</div> <div>9%</div> </div>   |
| 1   | KJ    | 113    | <div> <div>11%</div> <div>86%</div> <div>14%</div> </div> |
| 1   | KK    | 113    | <div> <div>3%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | KL    | 113    | <div> <div>4%</div> <div>92%</div> <div>8%</div> </div>   |
| 1   | KM    | 113    | <div> <div>7%</div> <div>81%</div> <div>19%</div> </div>  |
| 1   | KN    | 113    | <div> <div>10%</div> <div>87%</div> <div>13%</div> </div> |
| 1   | KO    | 113    | <div> <div>4%</div> <div>92%</div> <div>8%</div> </div>   |
| 1   | KP    | 113    | <div> <div>2%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | KQ    | 113    | <div> <div>4%</div> <div>87%</div> <div>13%</div> </div>  |
| 1   | KR    | 113    | <div> <div>2%</div> <div>89%</div> <div>11%</div> </div>  |
| 1   | KS    | 113    | <div> <div>4%</div> <div>89%</div> <div>11%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | KT    | 113    |                  |
| 1   | KU    | 113    |                  |
| 1   | KV    | 113    |                  |
| 1   | KW    | 113    |                  |
| 1   | KX    | 113    |                  |
| 1   | KY    | 113    |                  |
| 1   | KZ    | 113    |                  |
| 1   | LA    | 113    |                  |
| 1   | LB    | 113    |                  |
| 1   | LC    | 113    |                  |
| 1   | LD    | 113    |                  |
| 1   | LE    | 113    |                  |
| 1   | LF    | 113    |                  |
| 1   | LG    | 113    |                  |
| 1   | LH    | 113    |                  |
| 1   | LI    | 113    |                  |
| 1   | LJ    | 113    |                  |
| 1   | LK    | 113    |                  |
| 1   | LL    | 113    |                  |
| 1   | LM    | 113    |                  |
| 1   | LN    | 113    |                  |
| 1   | LO    | 113    |                  |
| 1   | LP    | 113    |                  |
| 1   | LQ    | 113    |                  |
| 1   | LR    | 113    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | LS    | 113    |                  |
| 1   | LT    | 113    |                  |
| 1   | LU    | 113    |                  |
| 1   | LV    | 113    |                  |
| 1   | LW    | 113    |                  |
| 1   | LX    | 113    |                  |
| 1   | LY    | 113    |                  |
| 1   | LZ    | 113    |                  |
| 1   | MA    | 113    |                  |
| 1   | MB    | 113    |                  |
| 1   | MC    | 113    |                  |
| 1   | MD    | 113    |                  |
| 1   | ME    | 113    |                  |
| 1   | MF    | 113    |                  |
| 1   | MG    | 113    |                  |
| 1   | MH    | 113    |                  |
| 1   | MI    | 113    |                  |
| 1   | MJ    | 113    |                  |
| 1   | MK    | 113    |                  |
| 1   | ML    | 113    |                  |
| 1   | MM    | 113    |                  |
| 1   | MN    | 113    |                  |
| 1   | MO    | 113    |                  |
| 1   | MP    | 113    |                  |
| 1   | MQ    | 113    |                  |

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| Mol | Chain | Length | Quality of chain |         |
|-----|-------|--------|------------------|---------|
| 1   | MR    | 113    | 6%               | 85% 15% |
| 1   | MS    | 113    | 4%               | 84% 16% |
| 1   | MT    | 113    | 4%               | 89% 11% |
| 1   | MU    | 113    | 4%               | 85% 15% |
| 1   | MV    | 113    | 5%               | 87% 13% |
| 1   | MW    | 113    | 4%               | 88% 12% |
| 1   | MX    | 113    | 8%               | 88% 12% |
| 1   | MY    | 113    | 7%               | 87% 13% |
| 1   | MZ    | 113    | 7%               | 92% 8%  |
| 1   | NA    | 113    | 6%               | 85% 15% |
| 1   | NB    | 113    | 3%               | 88% 12% |
| 1   | NC    | 113    | 5%               | 92% 8%  |
| 1   | ND    | 113    | 4%               | 89% 11% |
| 1   | NE    | 113    | 8%               | 88% 12% |
| 1   | NF    | 113    | 4%               | 93% 7%  |
| 1   | NG    | 113    | 4%               | 88% 12% |
| 1   | NH    | 113    | 4%               | 88% 12% |
| 1   | NI    | 113    | 3%               | 89% 11% |
| 1   | NJ    | 113    | 7%               | 88% 12% |
| 1   | NK    | 113    | 6%               | 88% 12% |
| 1   | NL    | 113    | 5%               | 91% 9%  |
| 1   | NM    | 113    | 12%              | 88% 12% |
| 1   | NN    | 113    | 4%               | 87% 13% |
| 1   | NO    | 113    | 4%               | 89% 11% |
| 1   | NP    | 113    | 4%               | 89% 11% |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1   | NQ    | 113    | <div> <div></div> <div>4%</div> <div>86%</div> <div>14%</div> </div>                 |
| 1   | NR    | 113    | <div> <div></div> <div>%</div> <div>91%</div> <div>9%</div> </div>                   |
| 1   | NS    | 113    | <div> <div></div> <div>6%</div> <div>89%</div> <div>11%</div> </div>                 |
| 1   | NT    | 113    | <div> <div></div> <div>4%</div> <div>85%</div> <div>15%</div> </div>                 |
| 1   | NU    | 113    | <div> <div></div> <div>4%</div> <div>88%</div> <div>12%</div> </div>                 |
| 1   | NV    | 113    | <div> <div></div> <div>14%</div> <div>85%</div> <div>15%</div> </div>                |
| 2   | RA    | 30     | <div> <div></div> <div>10%</div> <div>47%</div> <div>20%</div> <div>33%</div> </div> |
| 2   | RB    | 30     | <div> <div></div> <div>7%</div> <div>47%</div> <div>20%</div> <div>33%</div> </div>  |
| 2   | RC    | 30     | <div> <div></div> <div>7%</div> <div>57%</div> <div>10%</div> <div>33%</div> </div>  |
| 2   | RD    | 30     | <div> <div></div> <div>7%</div> <div>57%</div> <div>10%</div> <div>33%</div> </div>  |
| 2   | RE    | 30     | <div> <div></div> <div>3%</div> <div>57%</div> <div>10%</div> <div>33%</div> </div>  |
| 2   | RF    | 30     | <div> <div></div> <div>10%</div> <div>50%</div> <div>17%</div> <div>33%</div> </div> |
| 2   | RG    | 30     | <div> <div></div> <div>3%</div> <div>50%</div> <div>17%</div> <div>33%</div> </div>  |
| 2   | RH    | 30     | <div> <div></div> <div></div> <div>57%</div> <div>10%</div> <div>33%</div> </div>    |
| 2   | RI    | 30     | <div> <div></div> <div>7%</div> <div>47%</div> <div>20%</div> <div>33%</div> </div>  |
| 2   | RJ    | 30     | <div> <div></div> <div>7%</div> <div>47%</div> <div>20%</div> <div>33%</div> </div>  |
| 2   | RK    | 30     | <div> <div></div> <div>10%</div> <div>47%</div> <div>20%</div> <div>33%</div> </div> |
| 2   | RL    | 30     | <div> <div></div> <div>7%</div> <div>50%</div> <div>17%</div> <div>33%</div> </div>  |
| 2   | RM    | 30     | <div> <div></div> <div>7%</div> <div>57%</div> <div>10%</div> <div>33%</div> </div>  |
| 2   | RN    | 30     | <div> <div></div> <div>7%</div> <div>53%</div> <div>13%</div> <div>33%</div> </div>  |
| 2   | RO    | 30     | <div> <div></div> <div>17%</div> <div>47%</div> <div>20%</div> <div>33%</div> </div> |
| 2   | RP    | 30     | <div> <div></div> <div>3%</div> <div>57%</div> <div>10%</div> <div>33%</div> </div>  |
| 2   | RQ    | 30     | <div> <div></div> <div>3%</div> <div>57%</div> <div>10%</div> <div>33%</div> </div>  |
| 2   | RR    | 30     | <div> <div></div> <div>10%</div> <div>53%</div> <div>13%</div> <div>33%</div> </div> |
| 2   | RS    | 30     | <div> <div></div> <div>10%</div> <div>53%</div> <div>13%</div> <div>33%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | RT    | 30     |                  |
| 2   | RU    | 30     |                  |
| 2   | RV    | 30     |                  |
| 2   | RW    | 30     |                  |
| 2   | RX    | 30     |                  |
| 2   | RY    | 30     |                  |
| 2   | RZ    | 30     |                  |
| 2   | SA    | 30     |                  |
| 2   | SB    | 30     |                  |
| 2   | SC    | 30     |                  |
| 2   | SD    | 30     |                  |
| 2   | SE    | 30     |                  |
| 2   | SF    | 30     |                  |
| 2   | SG    | 30     |                  |
| 2   | SH    | 30     |                  |
| 2   | SI    | 30     |                  |
| 2   | SJ    | 30     |                  |
| 2   | SK    | 30     |                  |
| 2   | SL    | 30     |                  |
| 2   | SM    | 30     |                  |
| 2   | SN    | 30     |                  |
| 2   | SO    | 30     |                  |
| 2   | SP    | 30     |                  |
| 2   | SQ    | 30     |                  |
| 2   | SR    | 30     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | SS    | 30     |                  |
| 2   | ST    | 30     |                  |
| 2   | SU    | 30     |                  |
| 2   | SV    | 30     |                  |
| 2   | SW    | 30     |                  |
| 2   | SX    | 30     |                  |
| 2   | SY    | 30     |                  |
| 2   | SZ    | 30     |                  |
| 2   | TA    | 30     |                  |
| 2   | TB    | 30     |                  |
| 2   | TC    | 30     |                  |
| 2   | TD    | 30     |                  |
| 2   | TE    | 30     |                  |
| 2   | TF    | 30     |                  |
| 2   | TG    | 30     |                  |
| 2   | TH    | 30     |                  |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 327240 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    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AD    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AI    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AL    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | AQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AT    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AX    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AY    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | AZ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BA    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BD    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BI    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | BL    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BT    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BX    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BY    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | BZ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CA    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CD    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | CG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CI    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CL    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CT    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CX    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CY    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | CZ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DA    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | DB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DD    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DI    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DL    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DT    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | DW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DX    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DY    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | DZ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EA    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | ED    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EI    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EL    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | ER    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | ES    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | ET    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EX    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EY    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | EZ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FA    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FD    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FI    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FL    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | FM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FT    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FX    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FY    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | FZ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | GA    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | GB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | GC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | GD    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | GE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | GF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | GG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 1   | GH    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GI    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GJ    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GK    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GL    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GM    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GN    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GO    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GP    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GQ    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GR    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GS    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GT    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GU    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GV    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GW    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GX    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GY    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | GZ    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | HA    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | HB    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | HC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HD    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HI    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HL    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HT    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | HX    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HY    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | HZ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IA    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | ID    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | II    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IL    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | IR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 1   | IS    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | IT    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | IU    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | IV    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | IW    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | IX    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | IY    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | IZ    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JA    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JB    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JC    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JD    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JE    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JF    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JG    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JH    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JI    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JJ    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JK    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JL    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | JM    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | JN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JT    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JX    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JY    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | JZ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | KA    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | KB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | KC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | KD    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | KE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | KF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | KG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | KH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 1   | KI    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KJ    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KK    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KL    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KM    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KN    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KO    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KP    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KQ    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KR    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KS    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KT    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KU    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KV    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KW    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KX    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KY    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | KZ    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | LA    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | LB    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |
| 1   | LC    | 113      | Total<br>839 | C<br>529 | N<br>146 | O<br>163 | S<br>1 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | LD    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LI    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LL    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LT    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LX    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | LY    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | LZ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MA    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MD    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | ME    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MI    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | ML    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | MT    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MW    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MX    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MY    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | MZ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NA    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NB    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NC    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | ND    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NE    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NF    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NG    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NH    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NI    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NJ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NK    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NL    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NM    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NN    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 1   | NO    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NP    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NQ    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NR    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NS    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NT    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NU    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |
| 1   | NV    | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 839   | 529 | 146 | 163 | 1 |         |         |       |

- Molecule 2 is a RNA chain called RNA.

| Mol | Chain | Residues | Atoms |     |    |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 2   | RA    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |
| 2   | RB    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |
| 2   | RC    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |
| 2   | RD    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |
| 2   | RE    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |
| 2   | RF    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |
| 2   | RG    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |
| 2   | RH    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |
| 2   | RI    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |
| 2   | RJ    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |
| 2   | RK    | 20       | Total | C   | N  | O   | P  | 0       | 0       | 0     |
|     |       |          | 420   | 190 | 70 | 140 | 20 |         |         |       |

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| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 2   | RL    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RM    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RN    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RO    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RP    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RQ    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RR    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RS    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RT    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RU    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RV    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RW    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RX    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RY    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | RZ    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SA    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SB    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SC    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SD    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SE    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SF    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 2   | SG    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SH    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SI    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SJ    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SK    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SL    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SM    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SN    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SO    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SP    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SQ    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SR    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SS    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | ST    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SU    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SV    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SW    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SX    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SY    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | SZ    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | TA    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |

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| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 2   | TB    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | TC    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | TD    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | TE    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | TF    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | TG    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |
| 2   | TH    | 20       | Total<br>420 | C<br>190 | N<br>70 | O<br>140 | P<br>20 | 0       | 0       | 0     |

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

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

- Molecule 1: coat protein



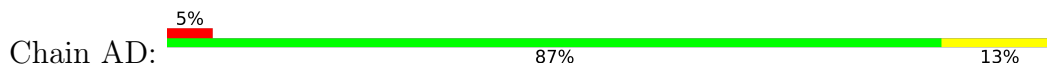
- Molecule 1: coat protein



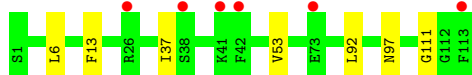
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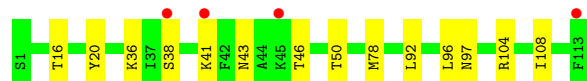
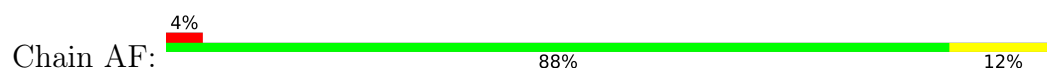
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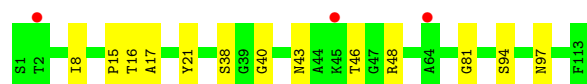
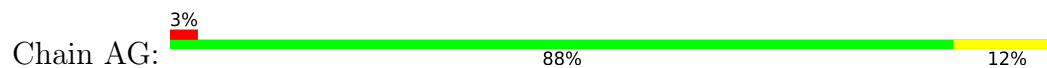
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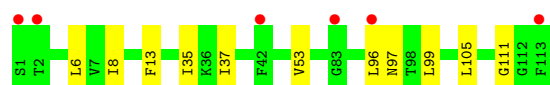
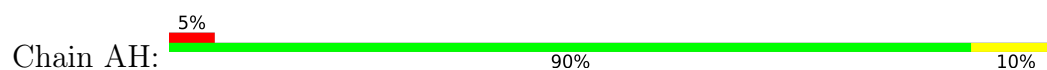
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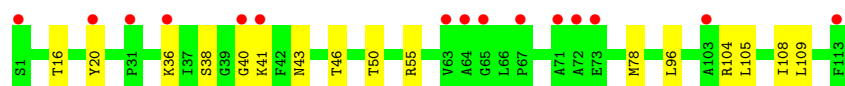
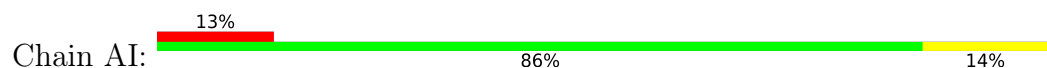
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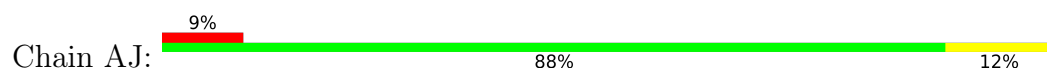
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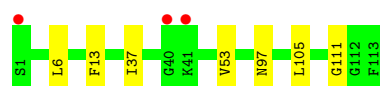
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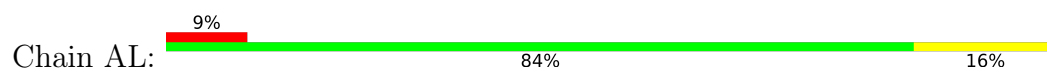
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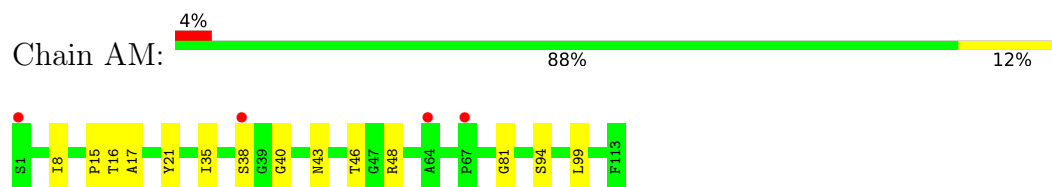
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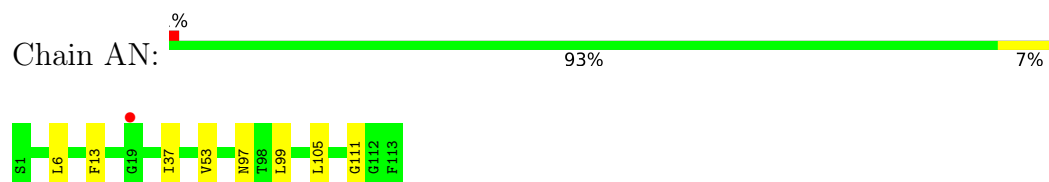
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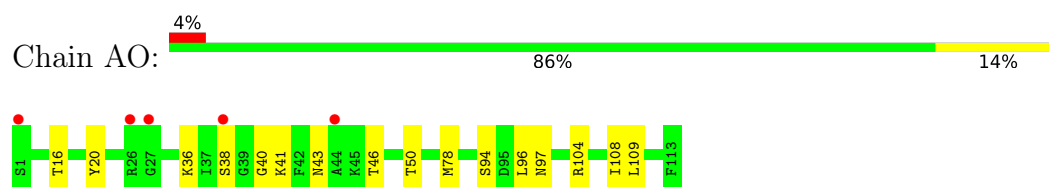
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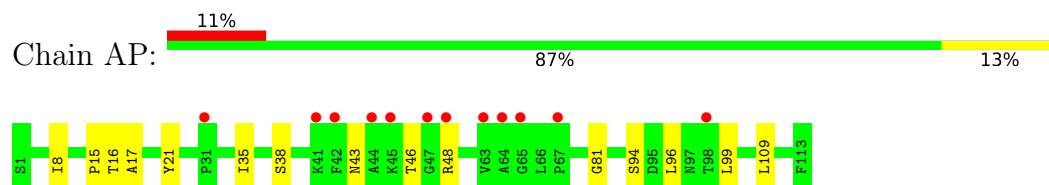
## ● Molecule 1: coat protein



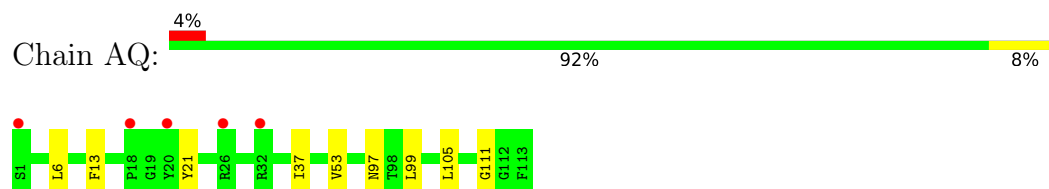
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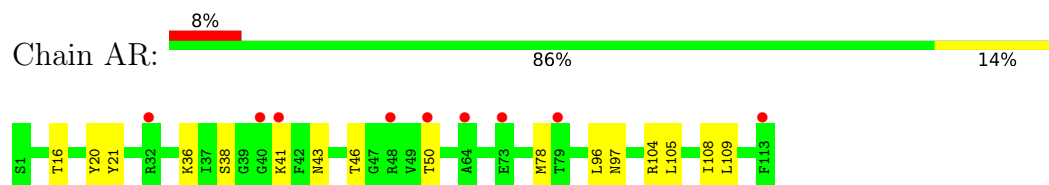
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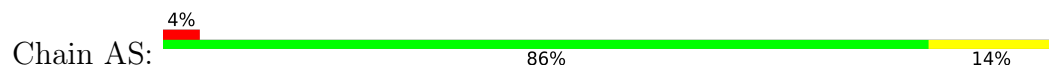
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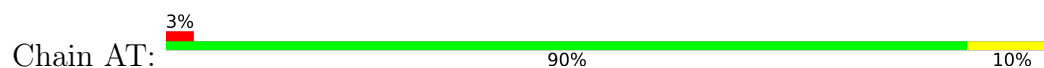


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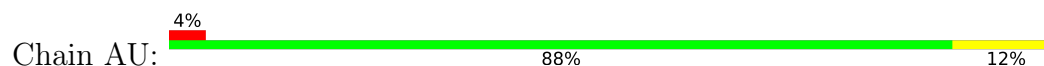




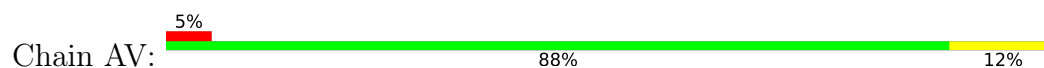
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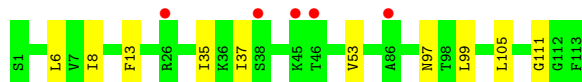
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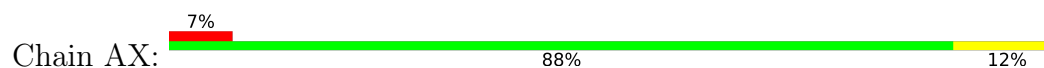
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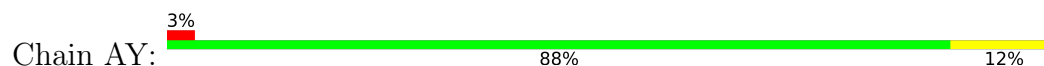
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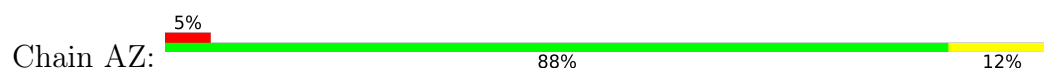
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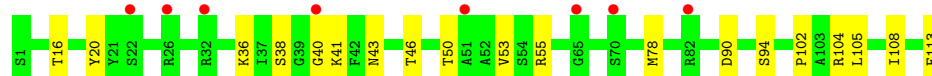
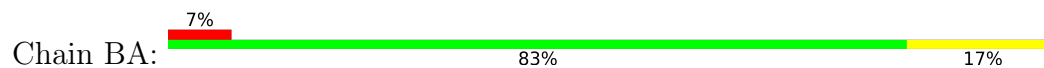
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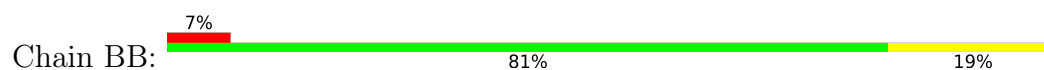
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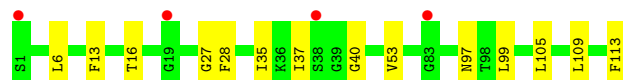
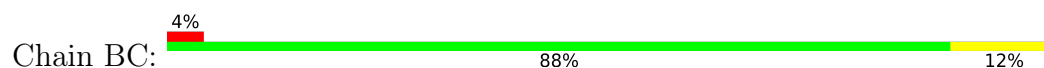
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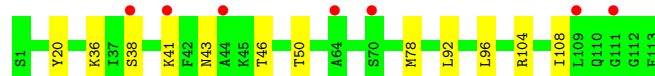
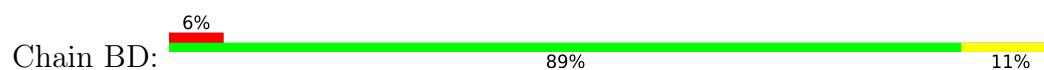
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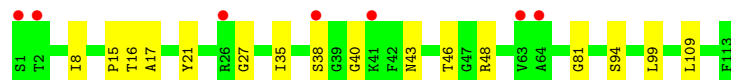
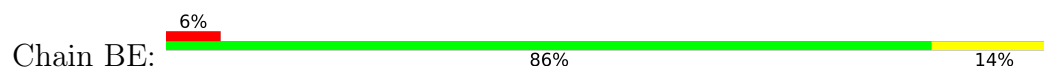
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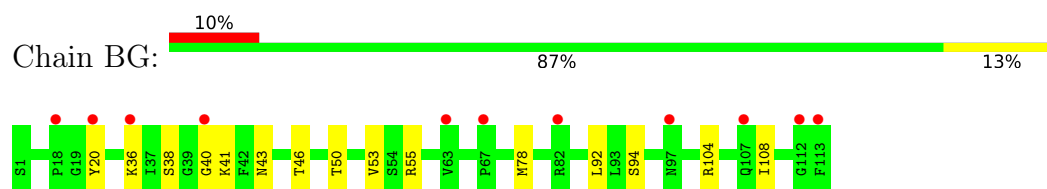
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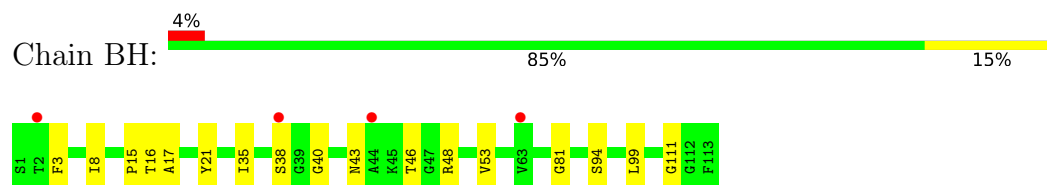
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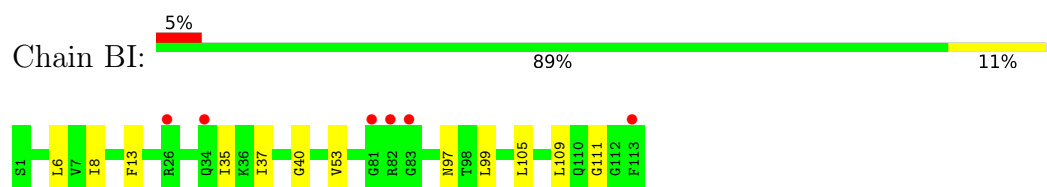
## ● Molecule 1: coat protein



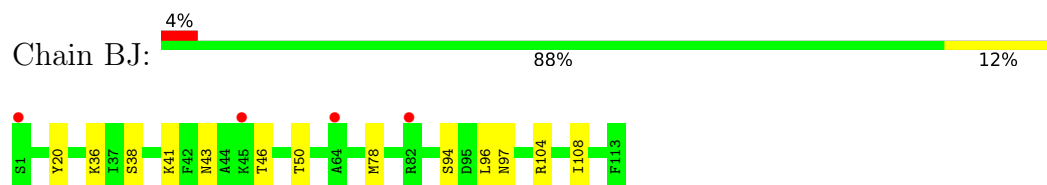
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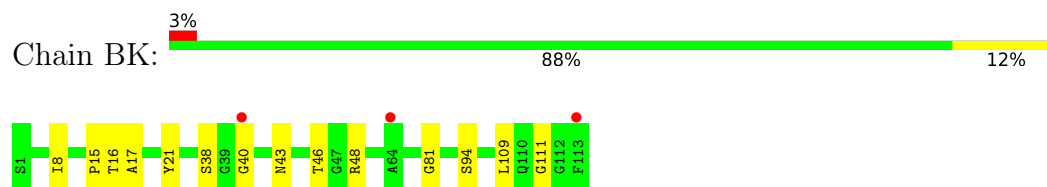
## ● Molecule 1: coat protein



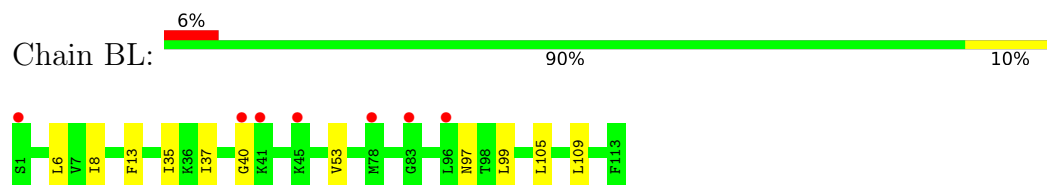
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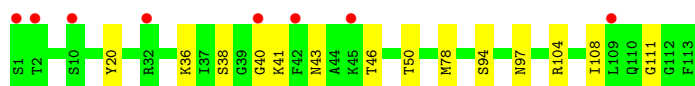


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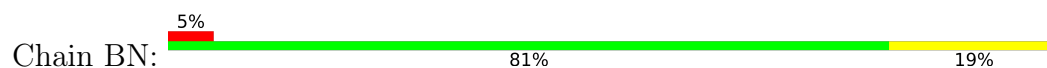


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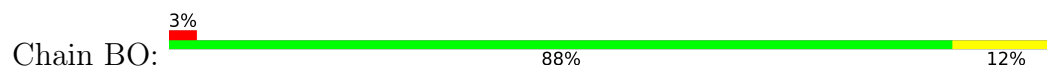




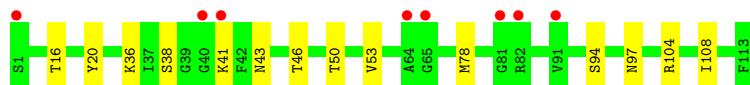
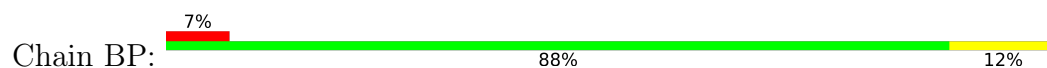
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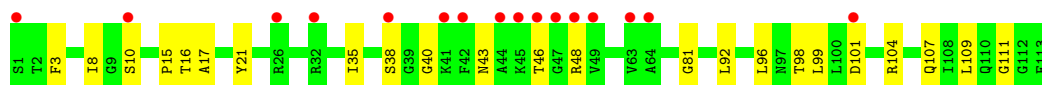
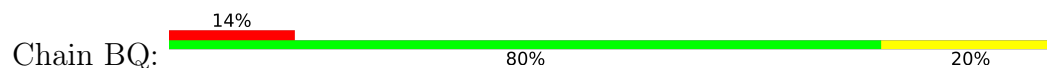
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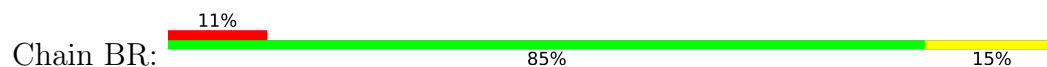
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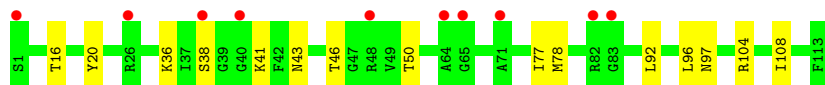
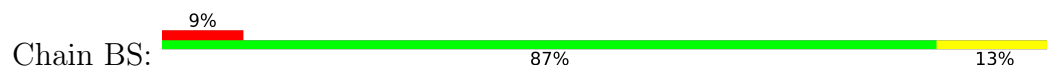
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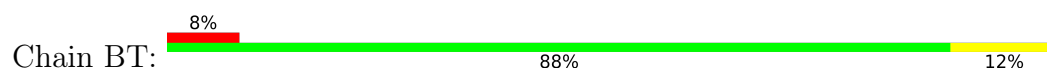
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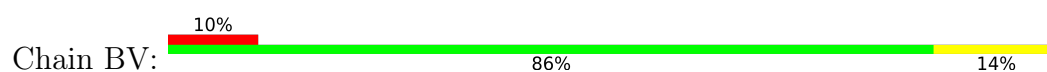
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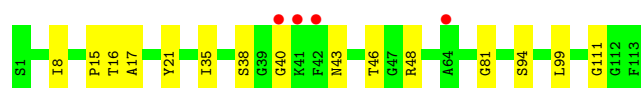
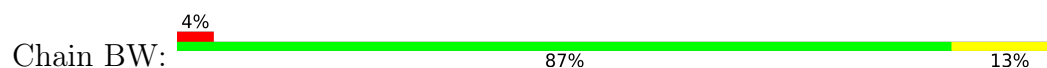
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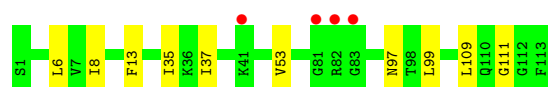
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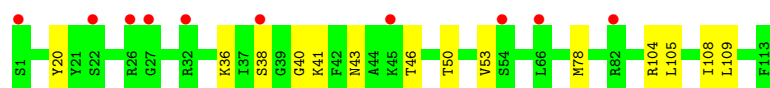
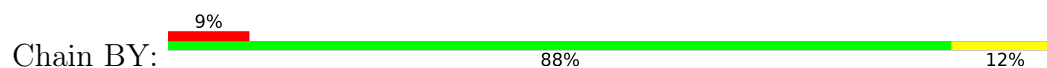
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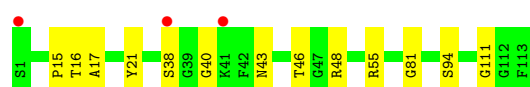
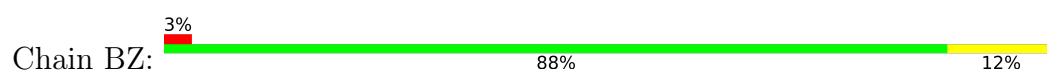
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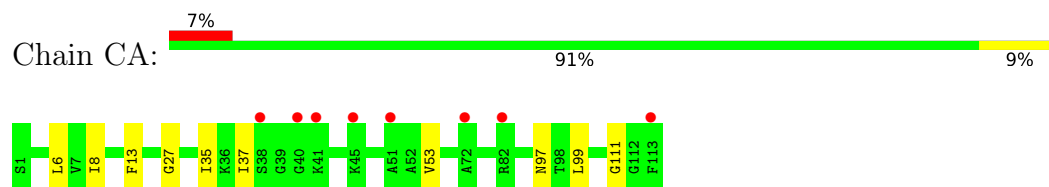
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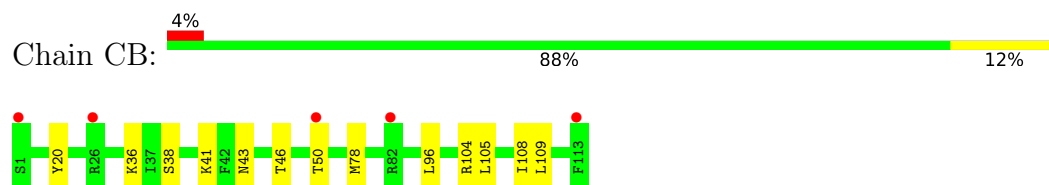
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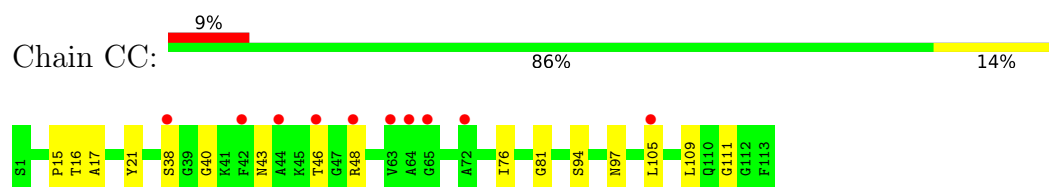
## ● Molecule 1: coat protein



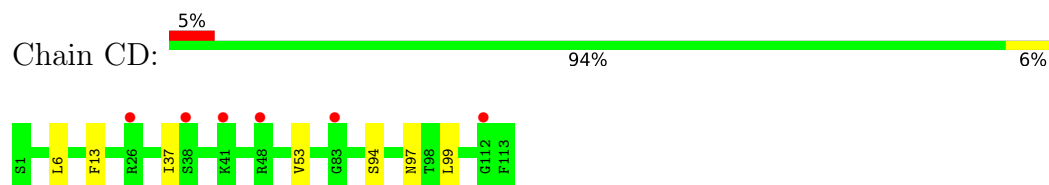
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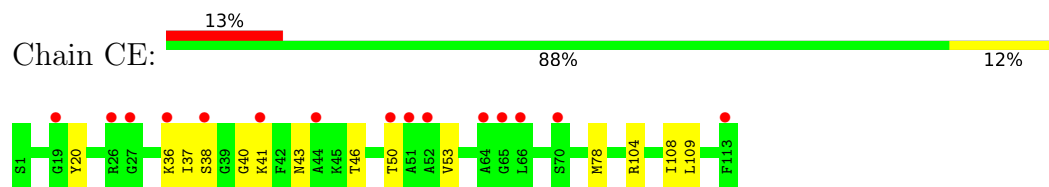
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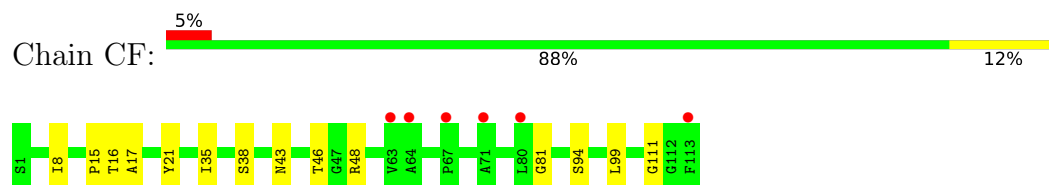
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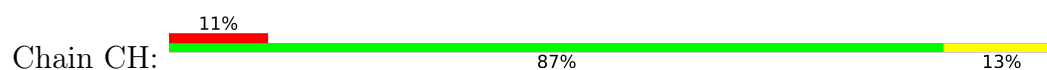


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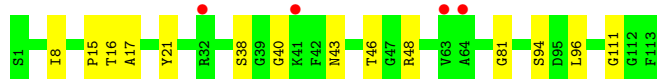
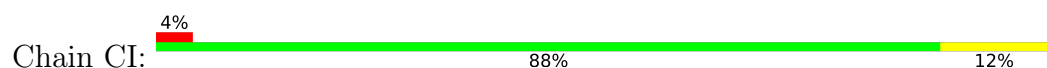




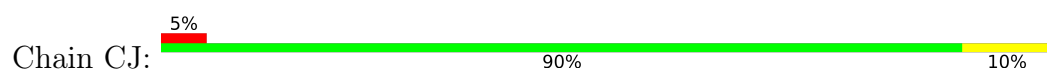
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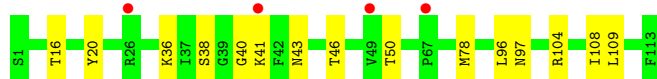
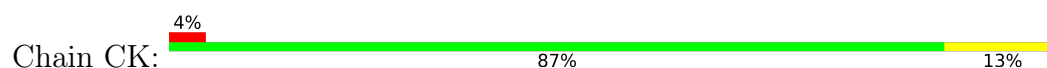
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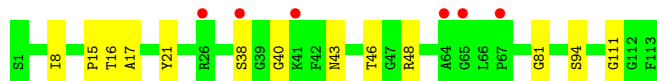
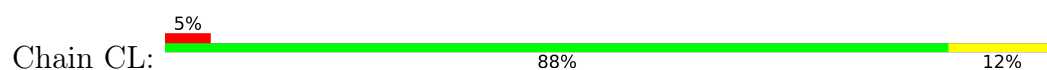
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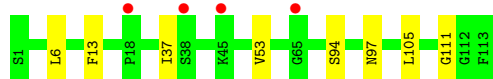
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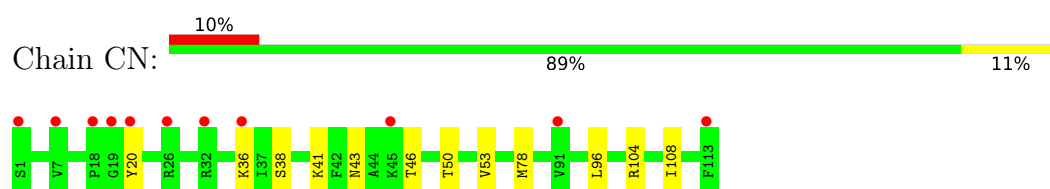
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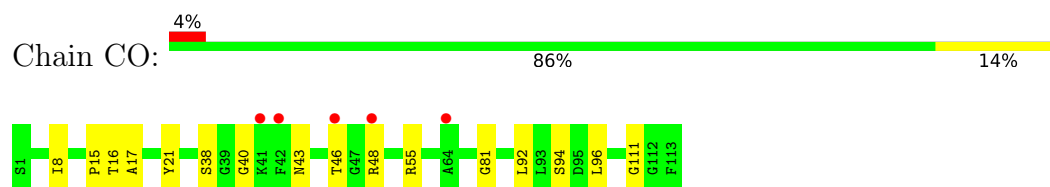
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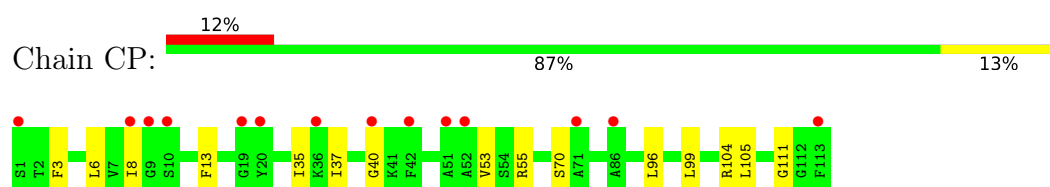
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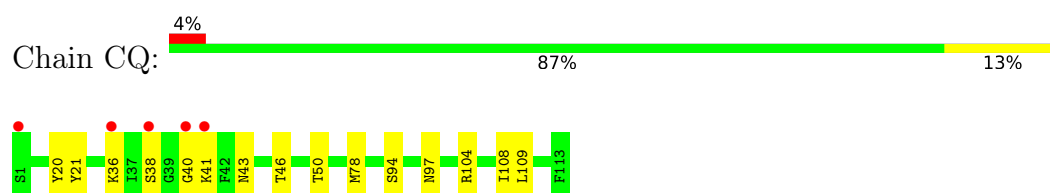
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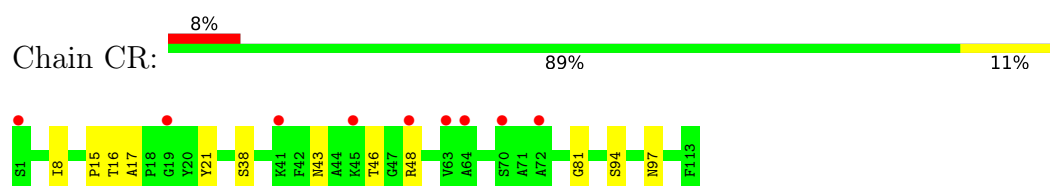
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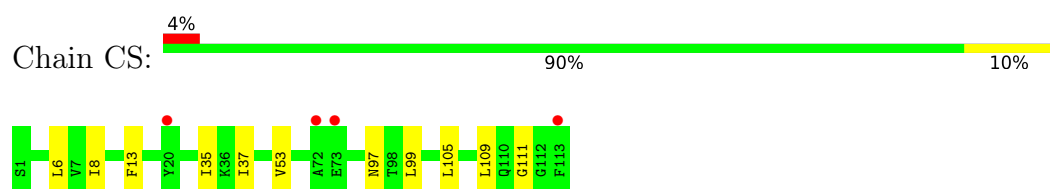
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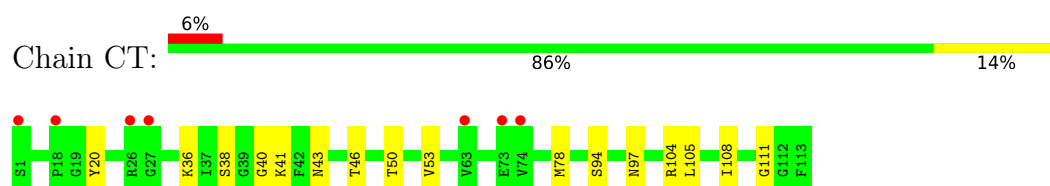
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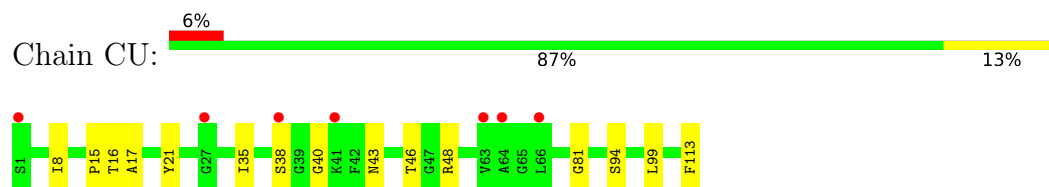
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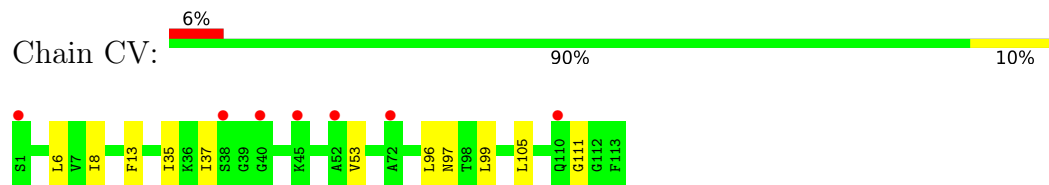
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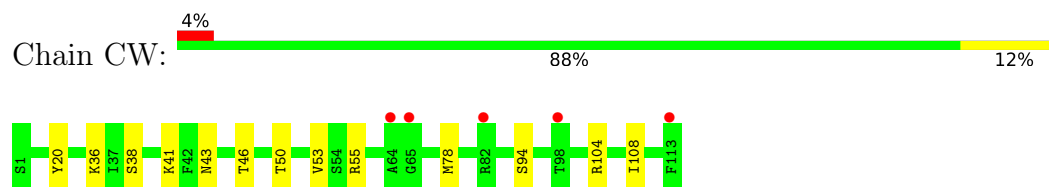
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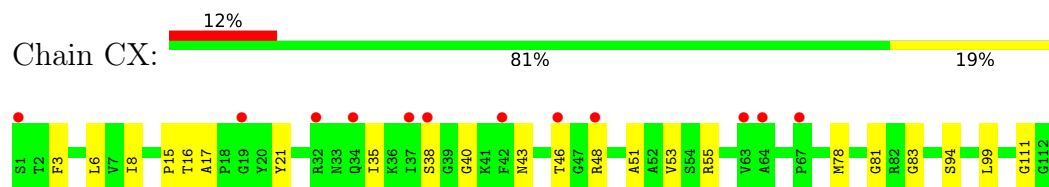
- Molecule 1: coat protein



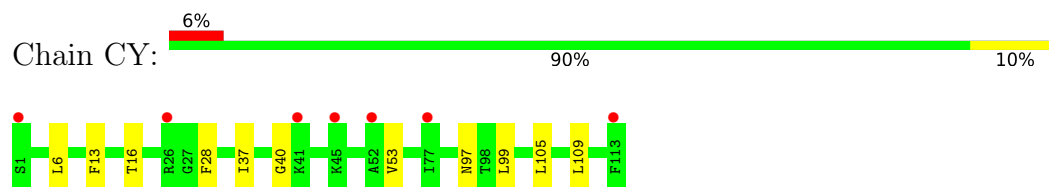
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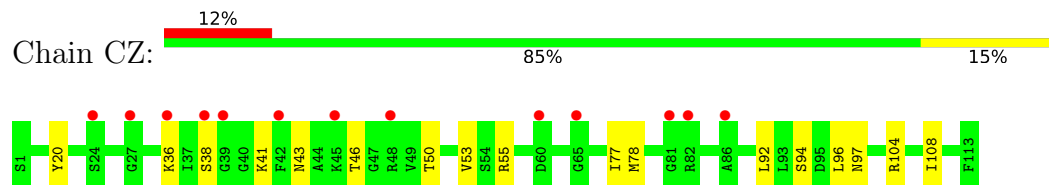
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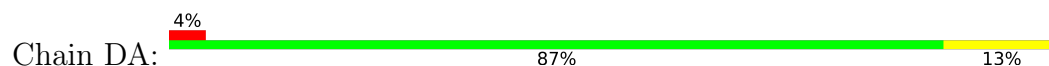
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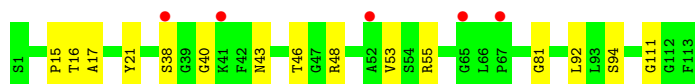


- Molecule 1: coat protein

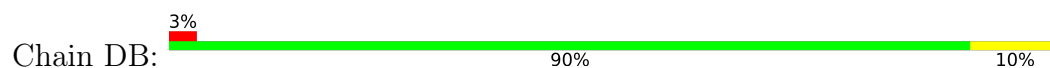


- Molecule 1: coat protein

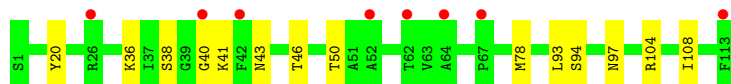
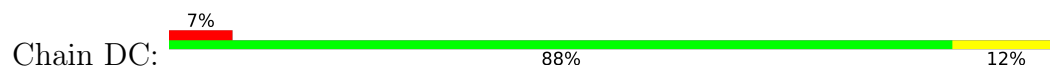




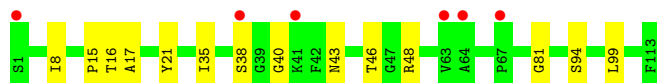
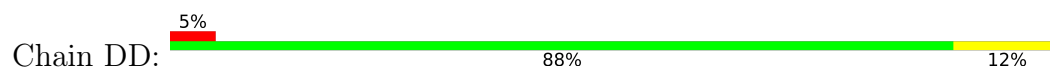
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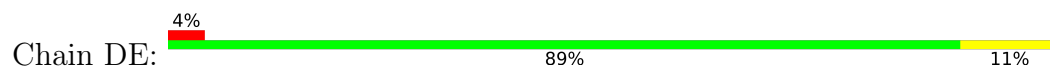
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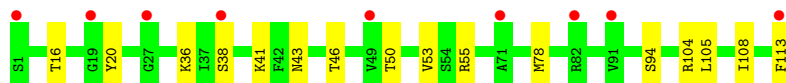
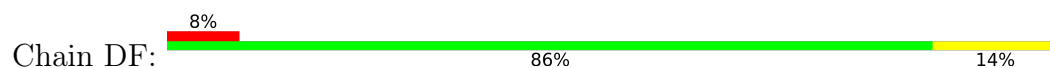
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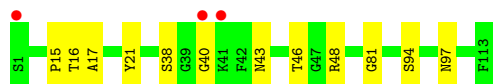
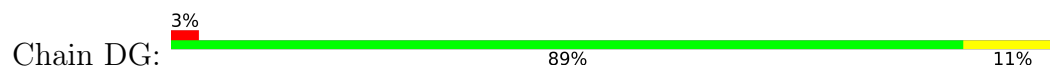
- Molecule 1: coat protein



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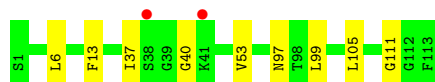


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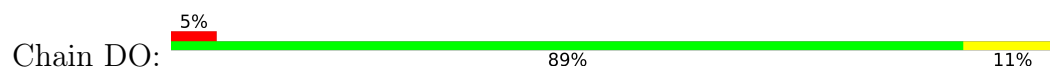


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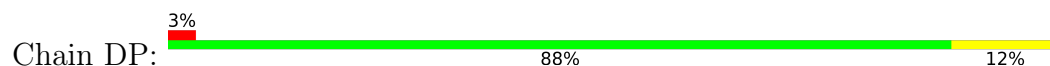




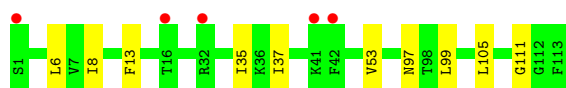
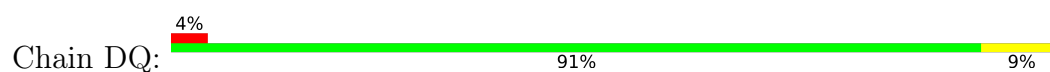
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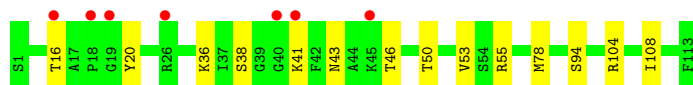
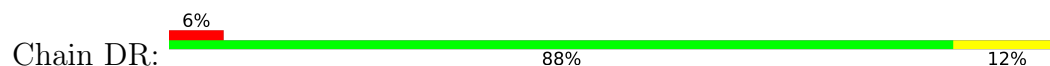
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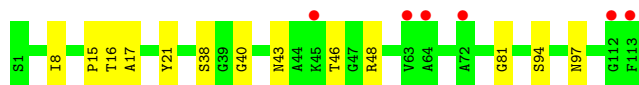
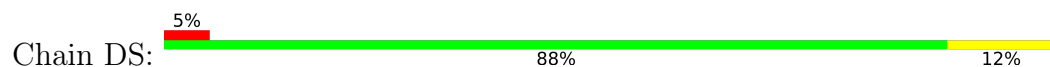
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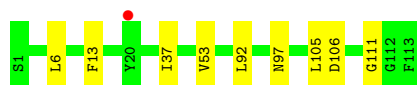
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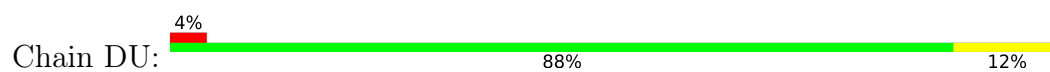
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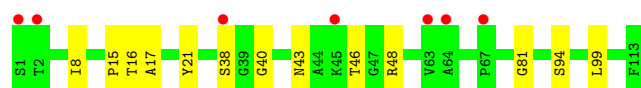
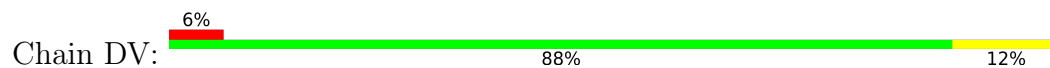
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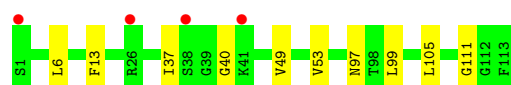
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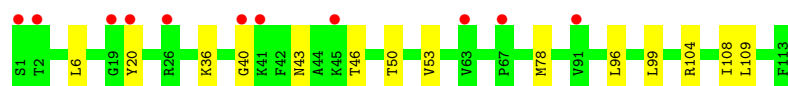
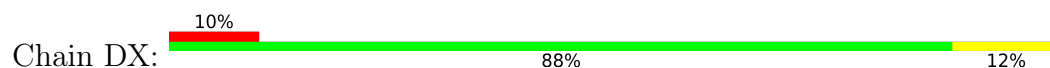
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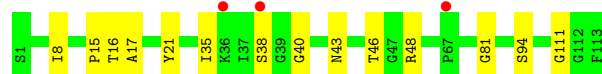
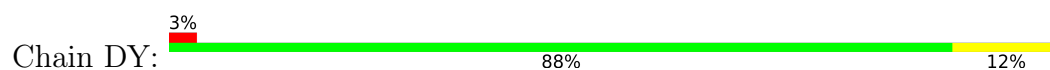
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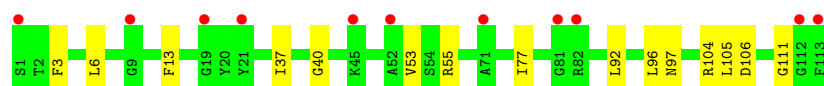
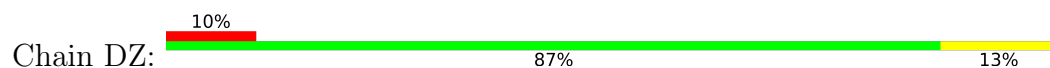
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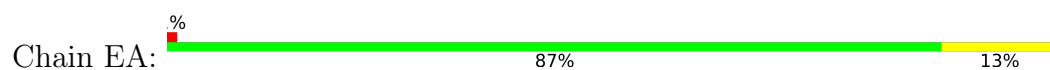
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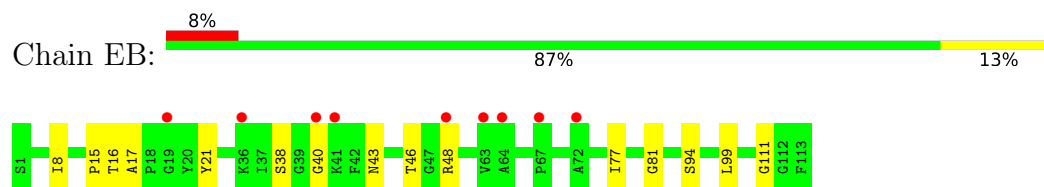
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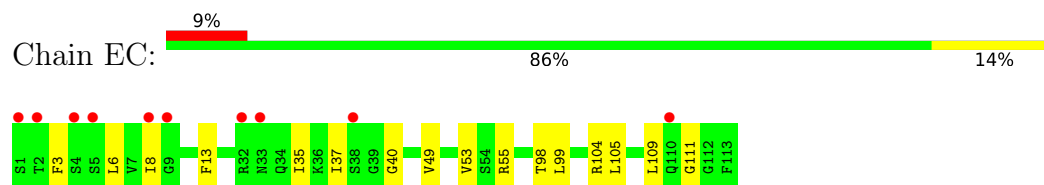
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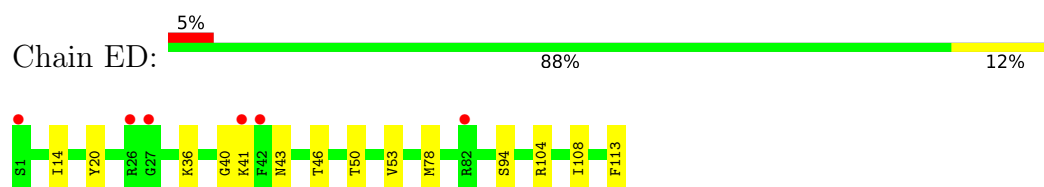
## ● Molecule 1: coat protein



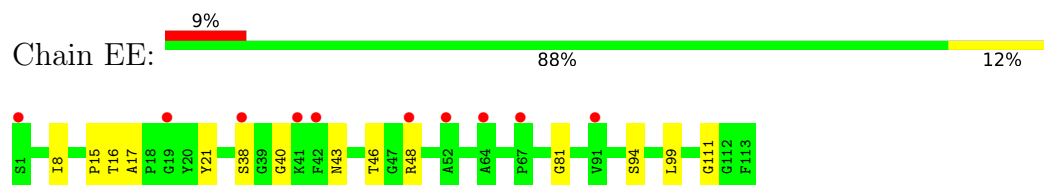
## ● Molecule 1: coat protein



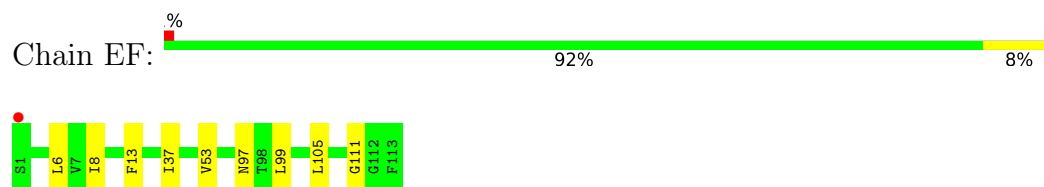
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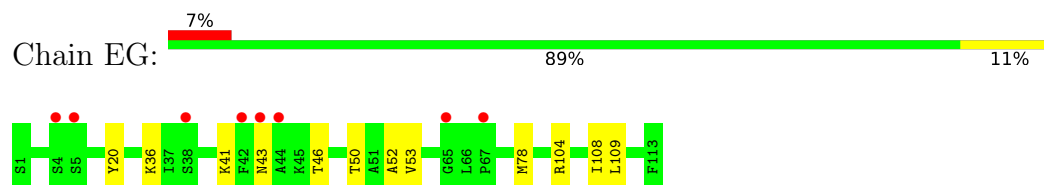
## ● Molecule 1: coat protein



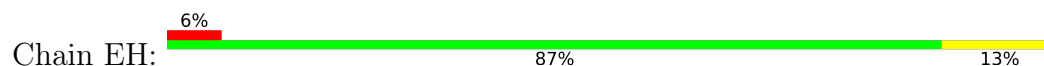
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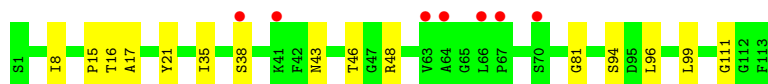


## ● Molecule 1: coat protein

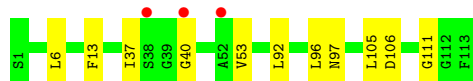
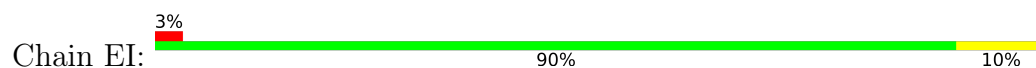


## ● Molecule 1: coat protein

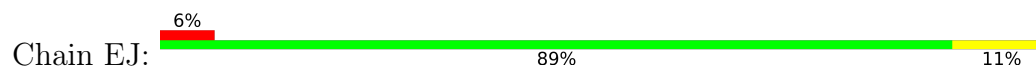




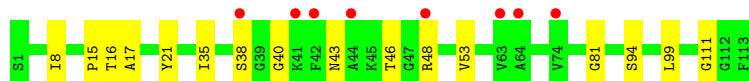
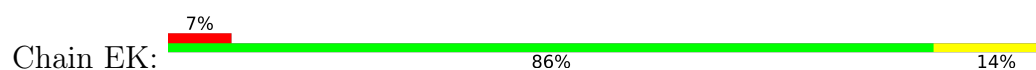
- Molecule 1: coat protein



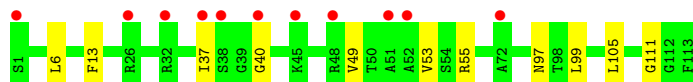
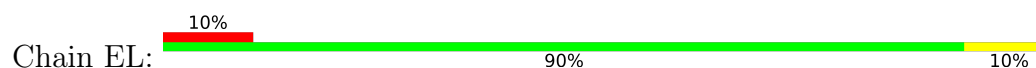
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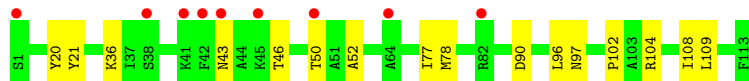
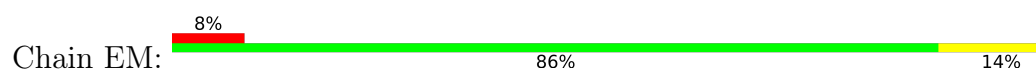
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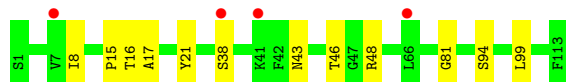
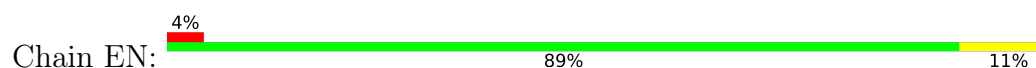
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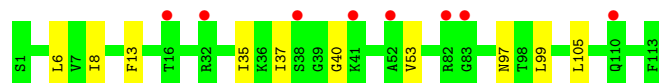
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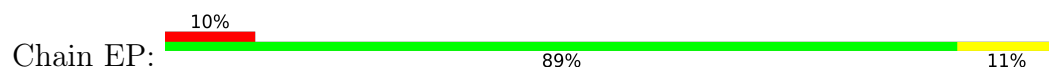
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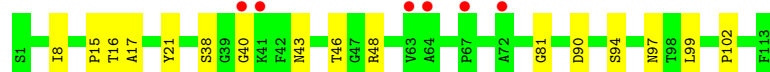
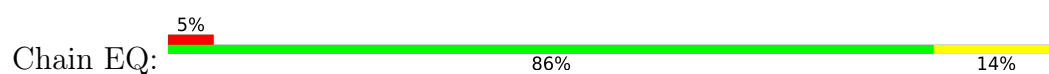
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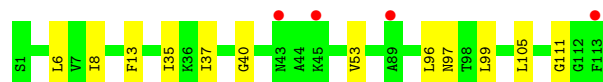
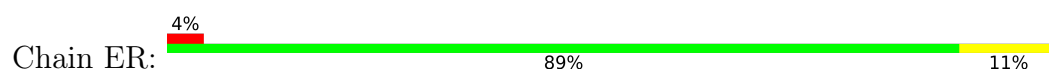
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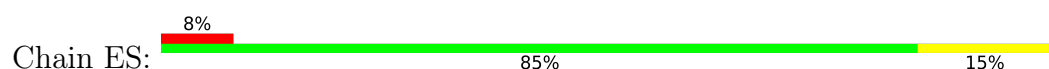
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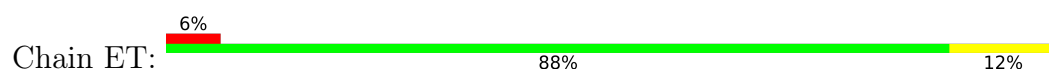
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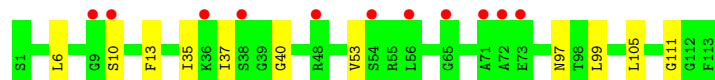
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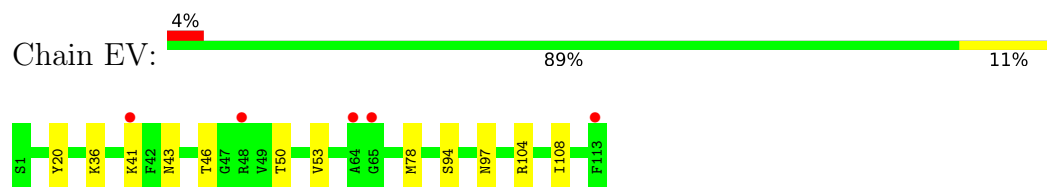
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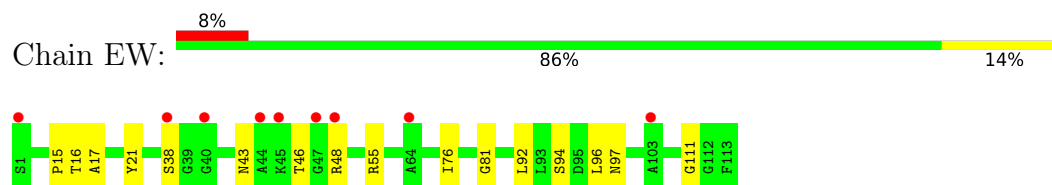
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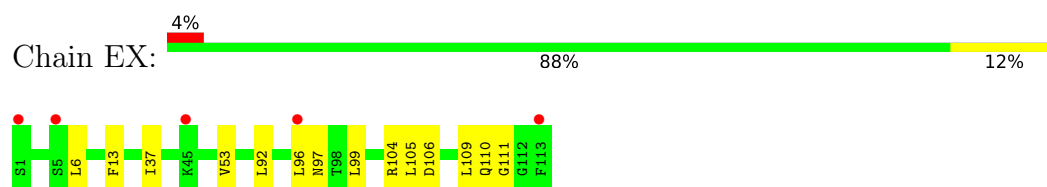
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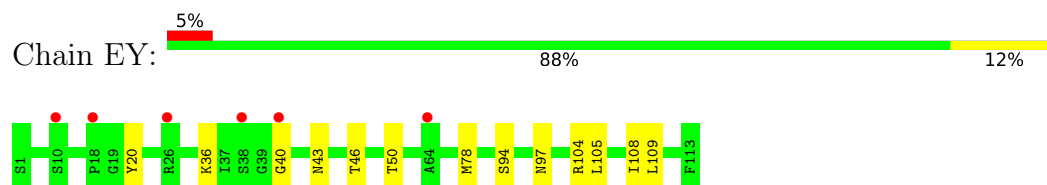
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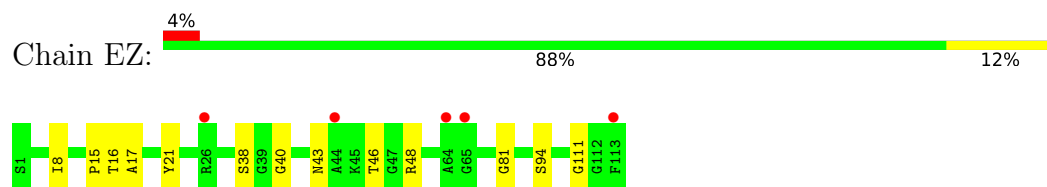
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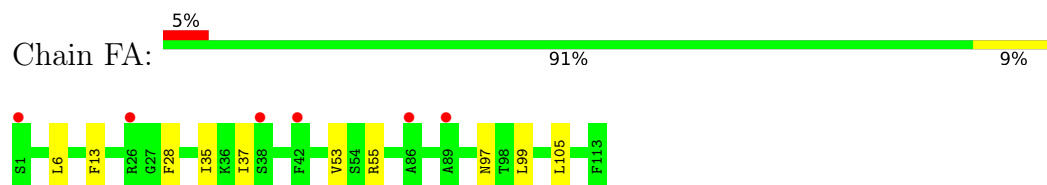
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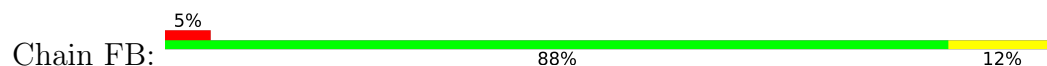
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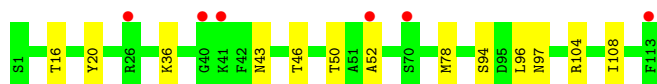


- Molecule 1: coat protein

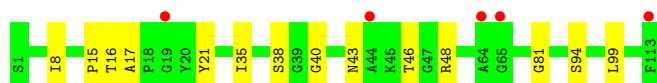
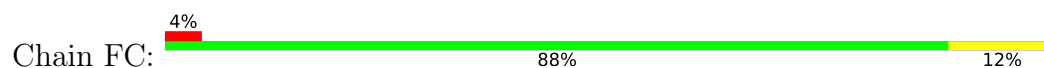


- Molecule 1: coat protein





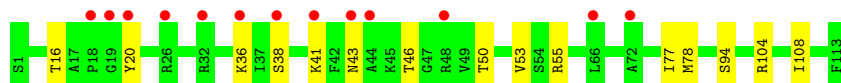
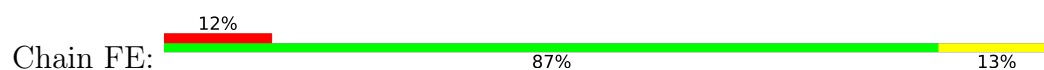
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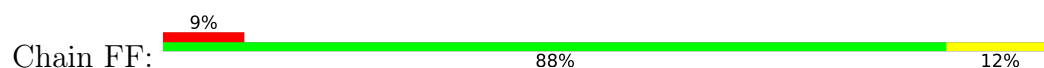
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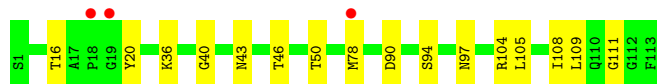
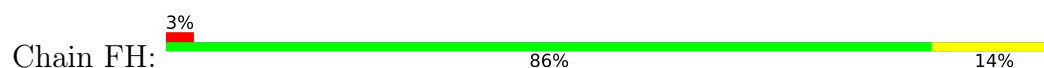
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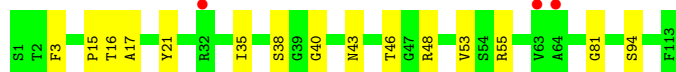
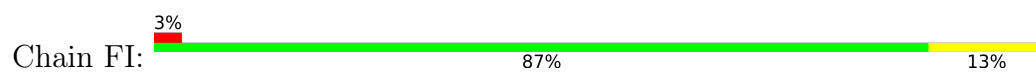
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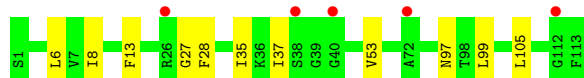
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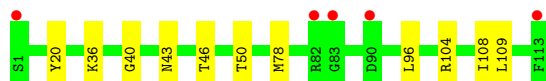
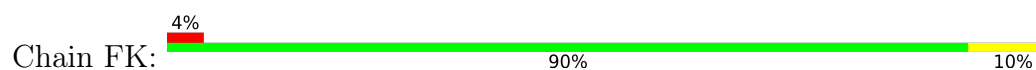
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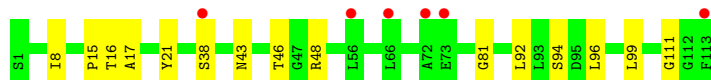
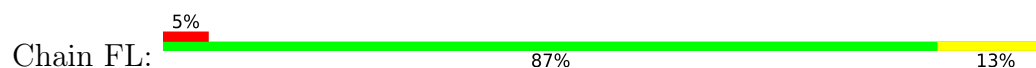
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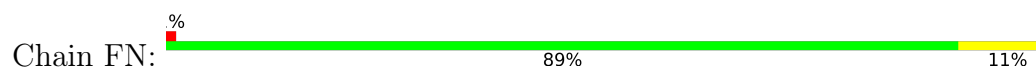
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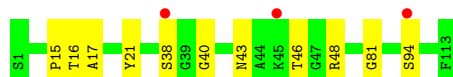
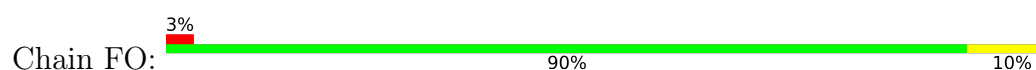
- Molecule 1: coat protein



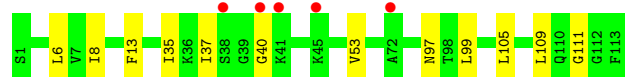
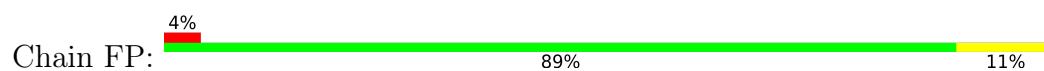
- Molecule 1: coat protein



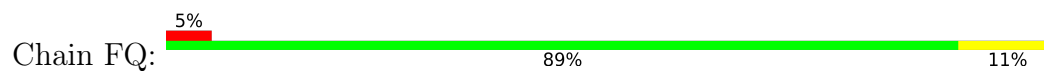
- Molecule 1: coat protein



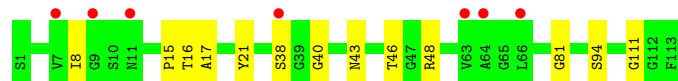
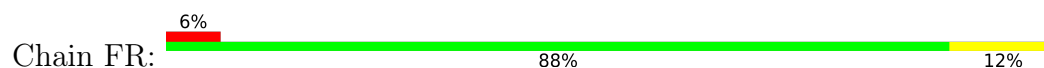
## ● Molecule 1: coat protein



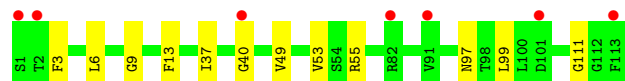
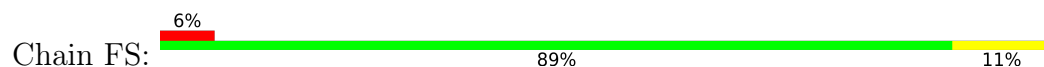
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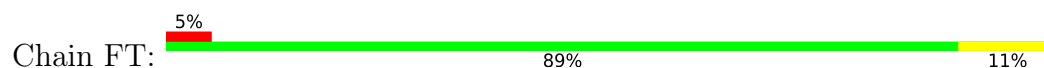
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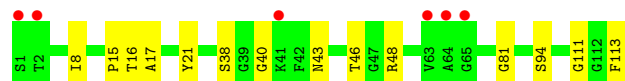
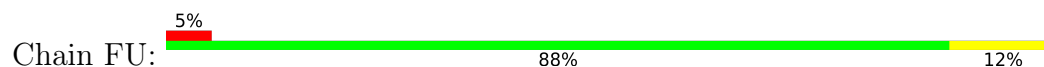
## ● Molecule 1: coat protein



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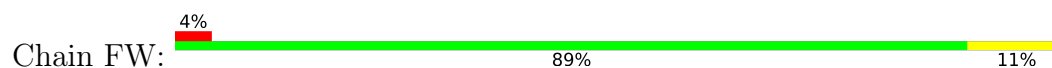


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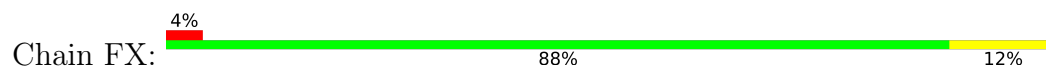




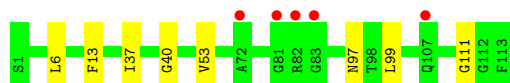
- Molecule 1: coat protein



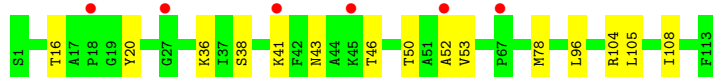
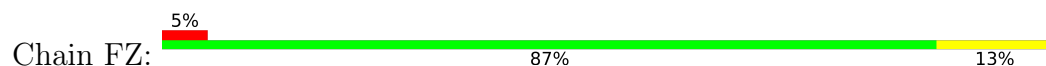
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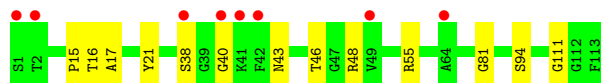
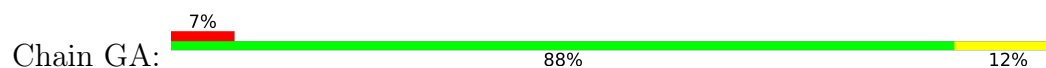
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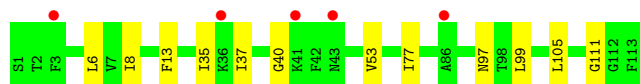
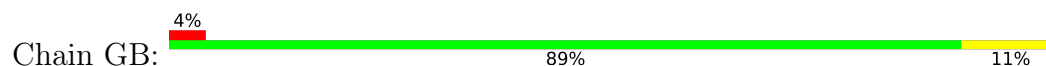
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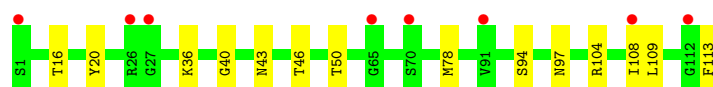
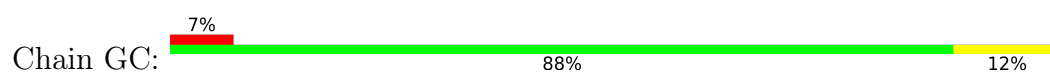
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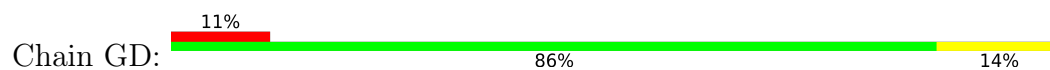
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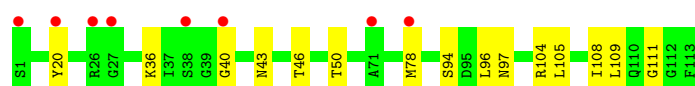
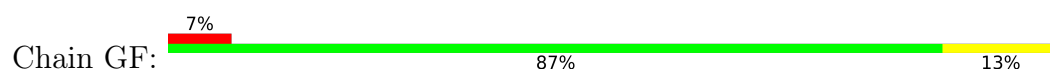
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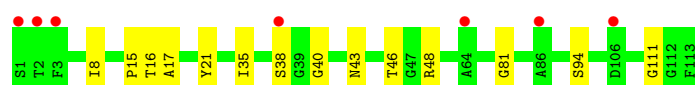
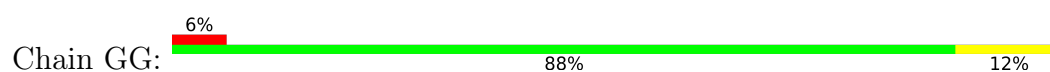
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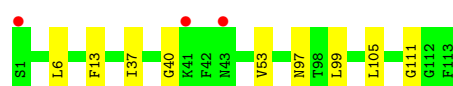
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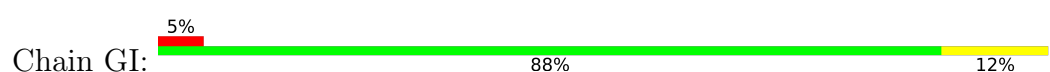
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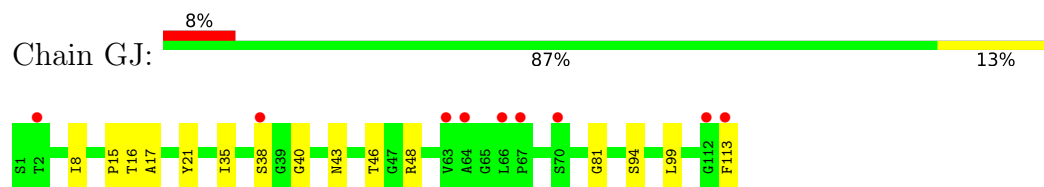
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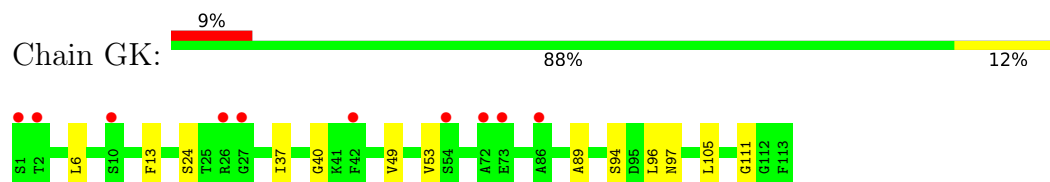
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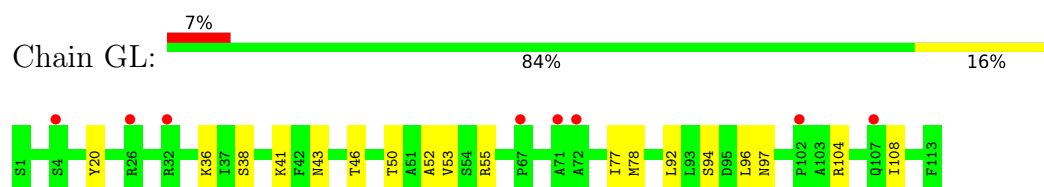
## ● Molecule 1: coat protein



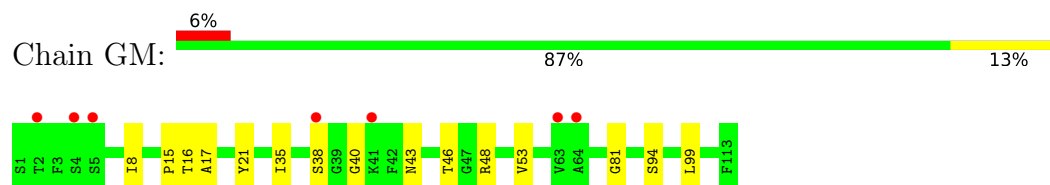
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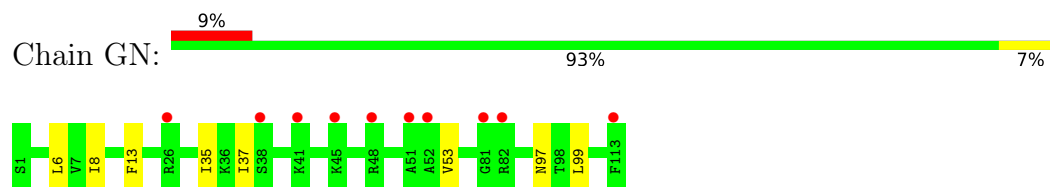
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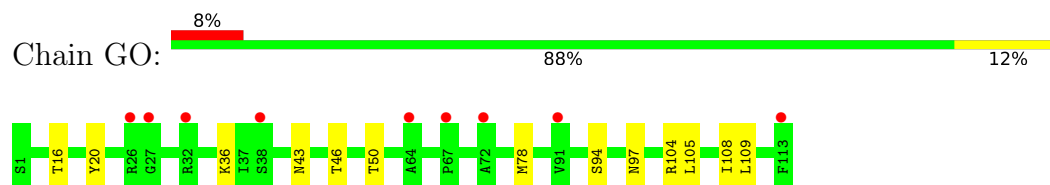
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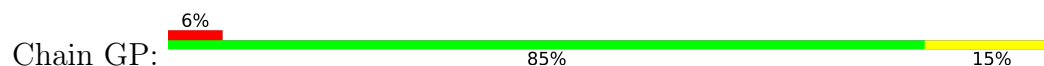
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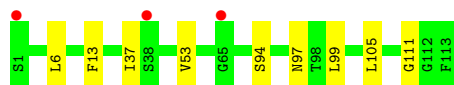


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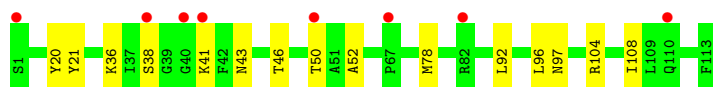




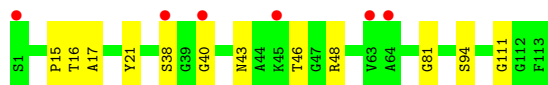
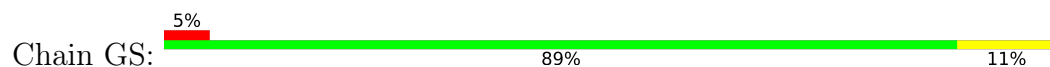
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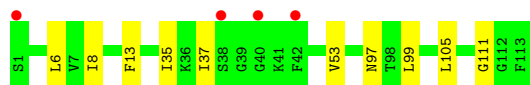
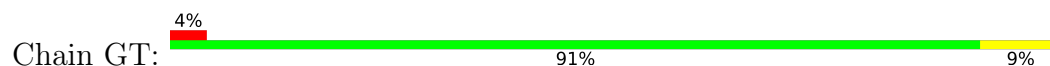
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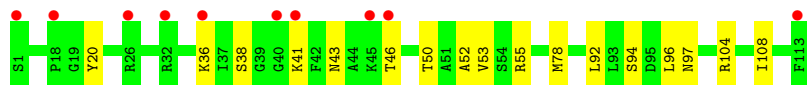
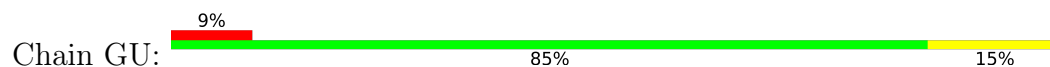
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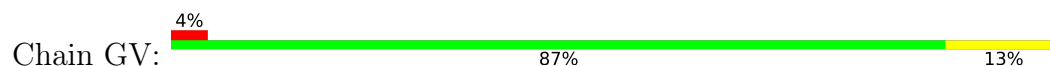
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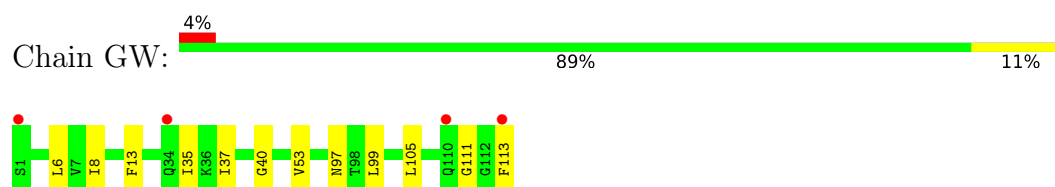
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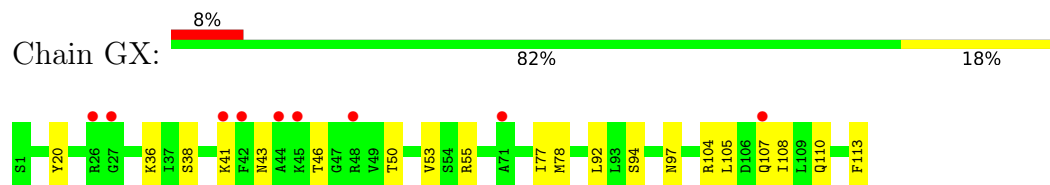
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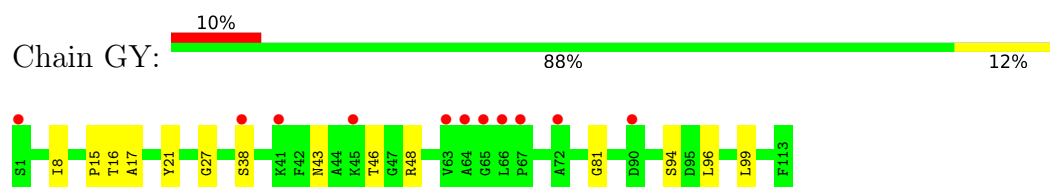
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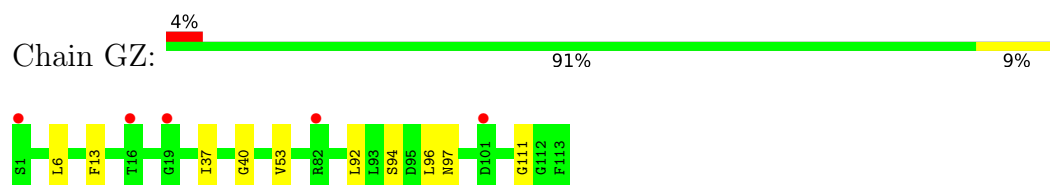
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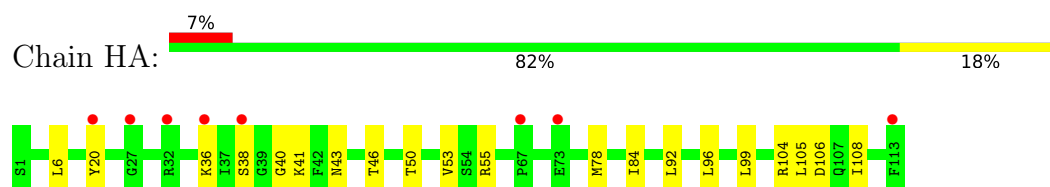
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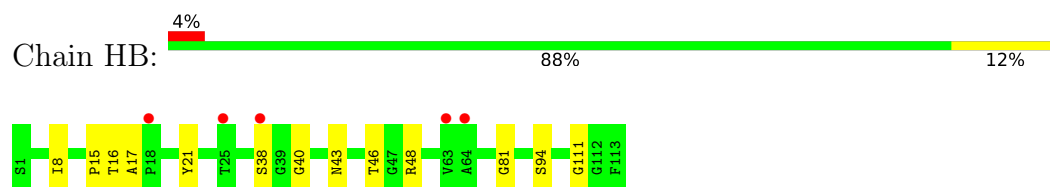
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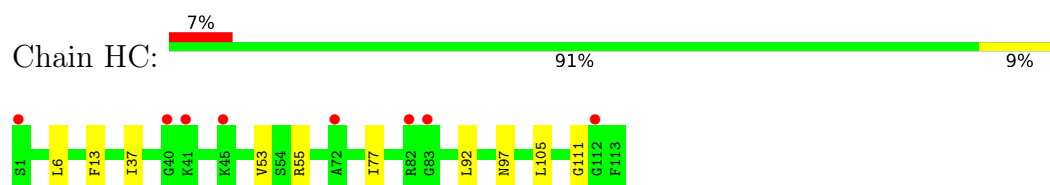
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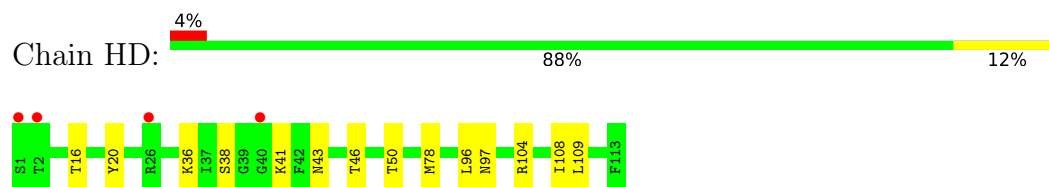
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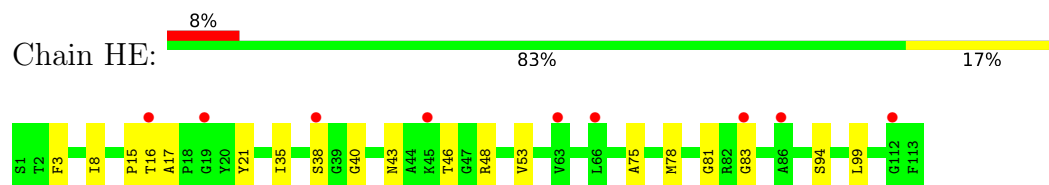
- Molecule 1: coat protein



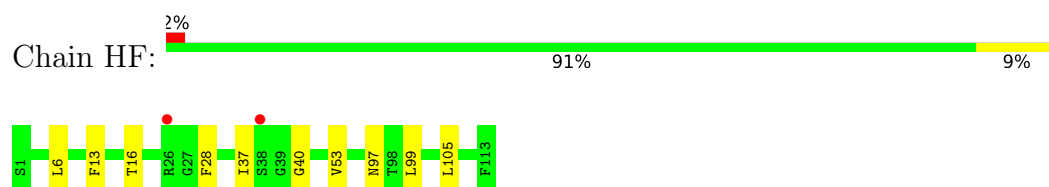
## ● Molecule 1: coat protein



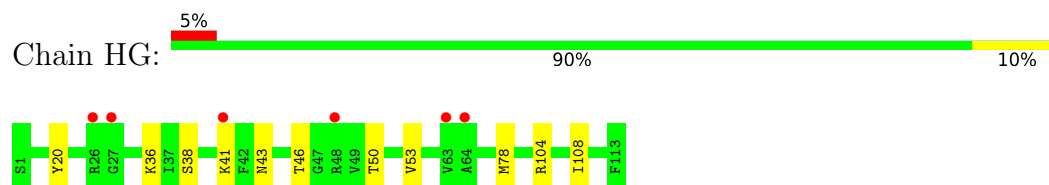
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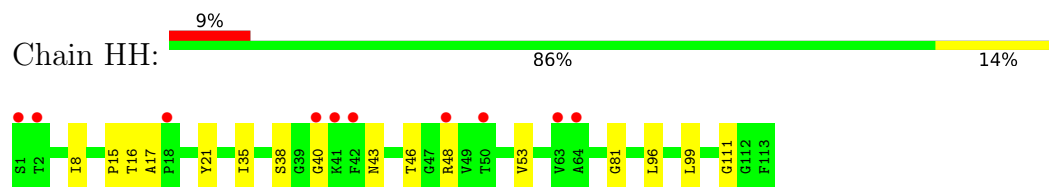
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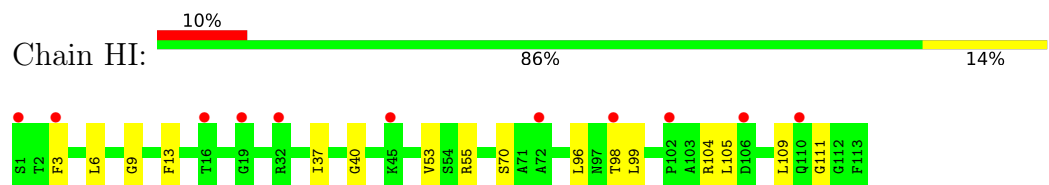
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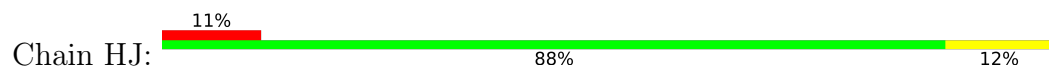
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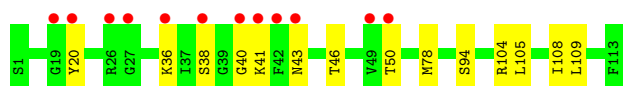


## ● Molecule 1: coat protein

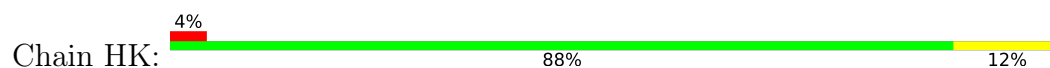


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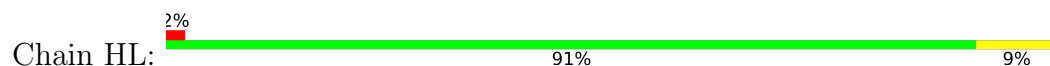




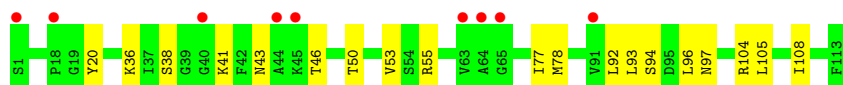
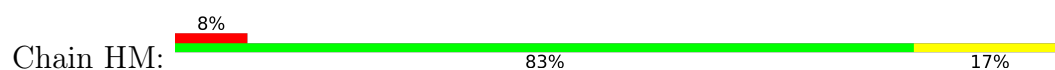
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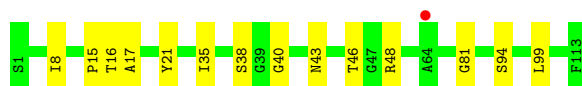
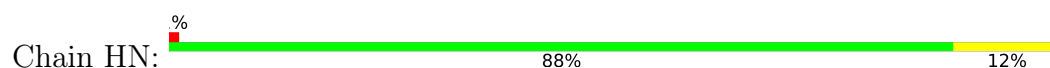
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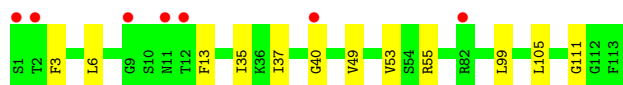
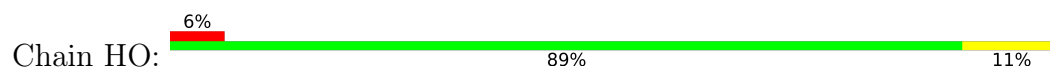
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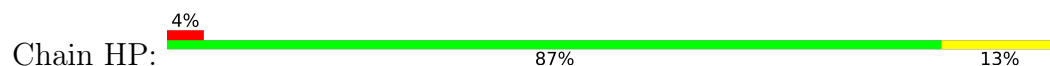
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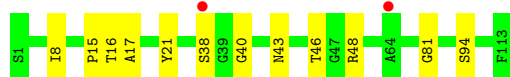
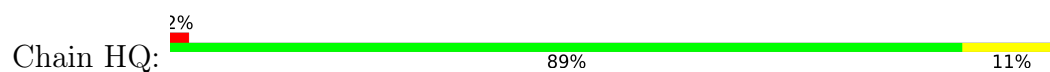
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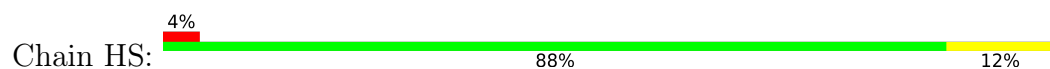
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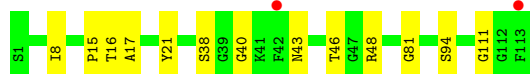
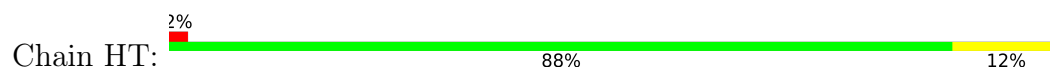
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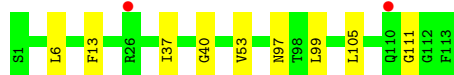
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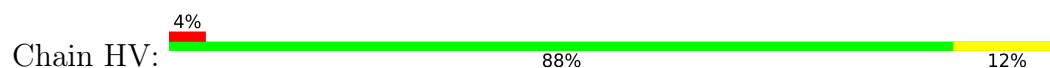
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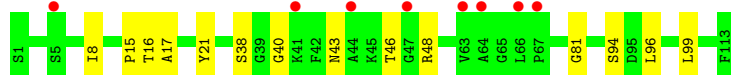
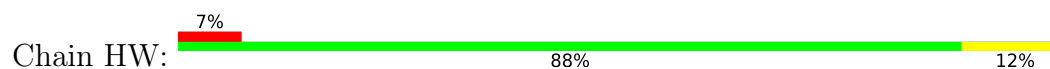
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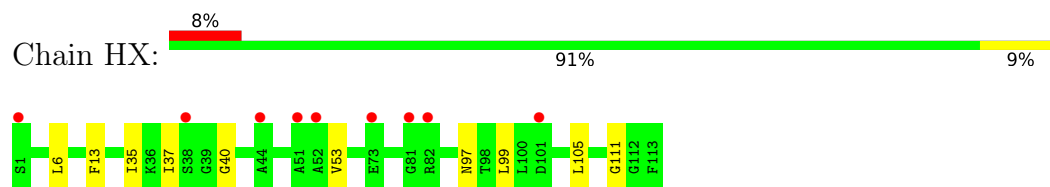
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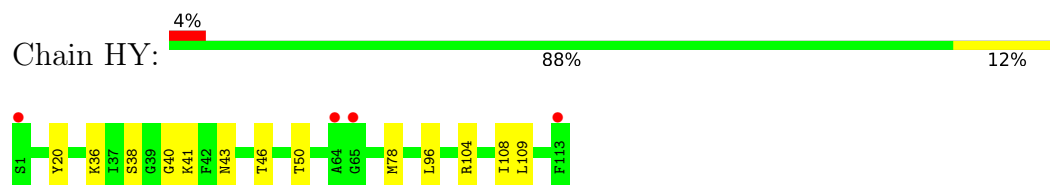
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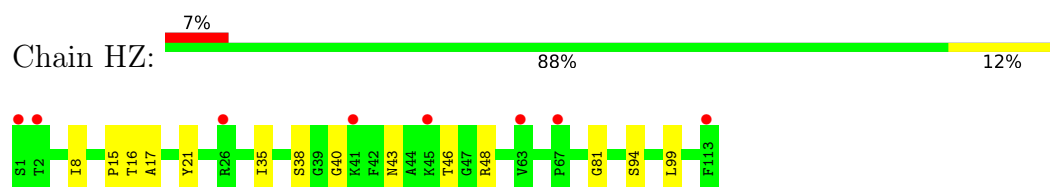
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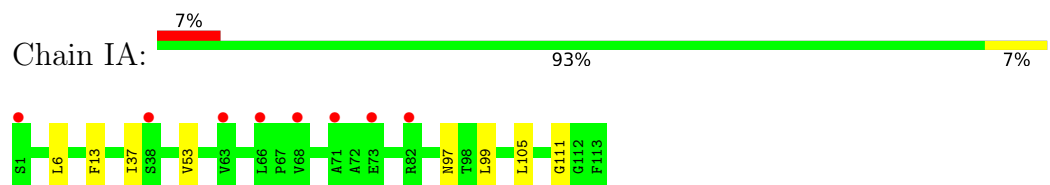
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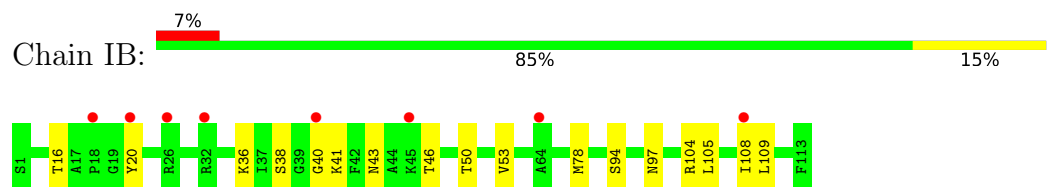
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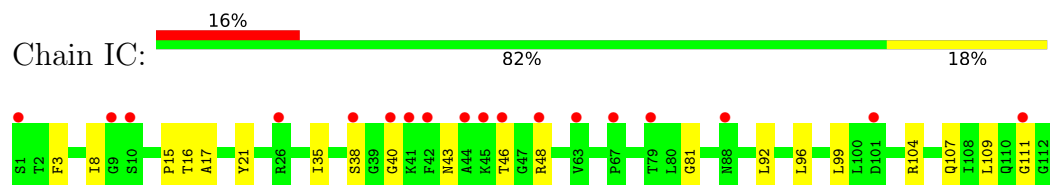
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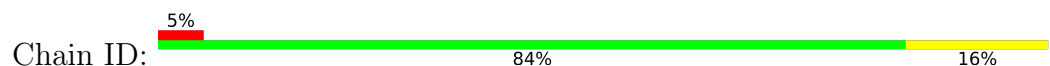
- Molecule 1: coat protein



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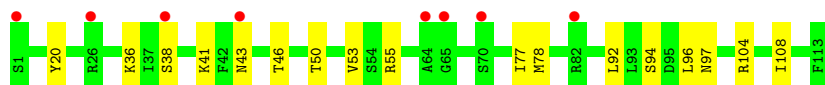
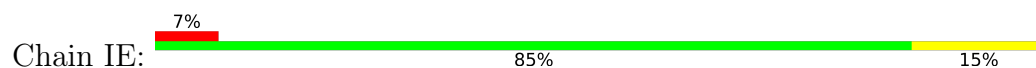


- Molecule 1: coat protein

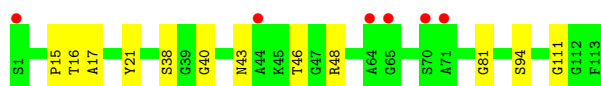
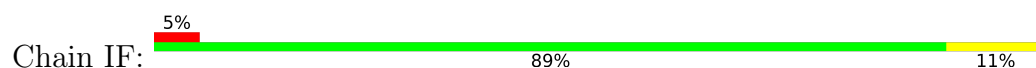




- Molecule 1: coat protein



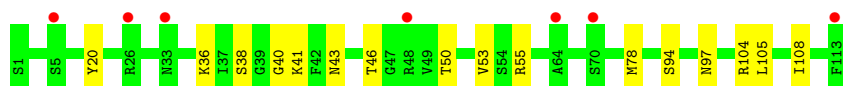
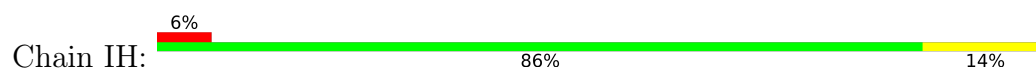
- Molecule 1: coat protein



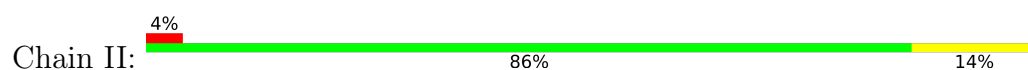
- Molecule 1: coat protein



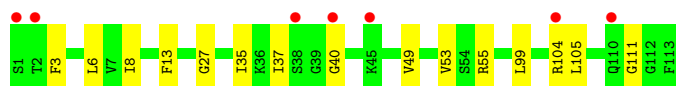
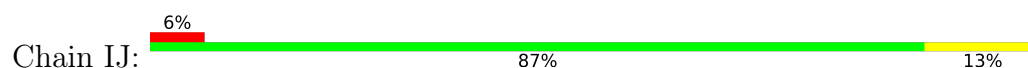
- Molecule 1: coat protein



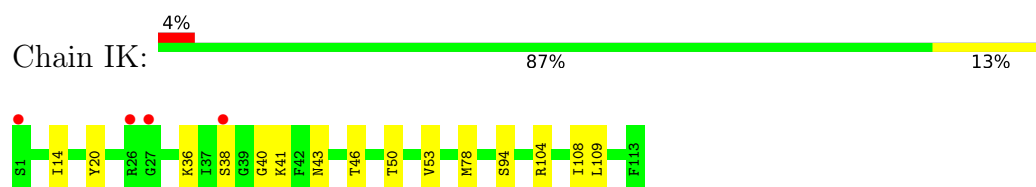
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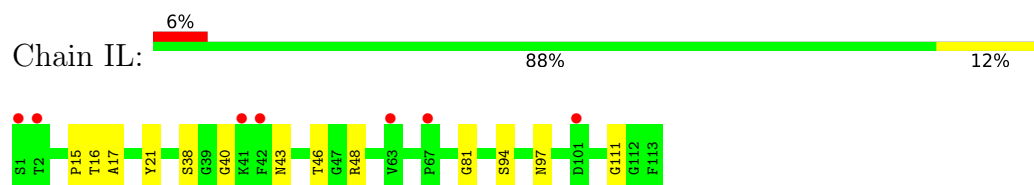
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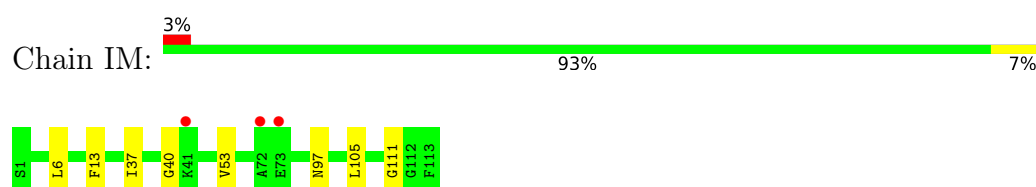
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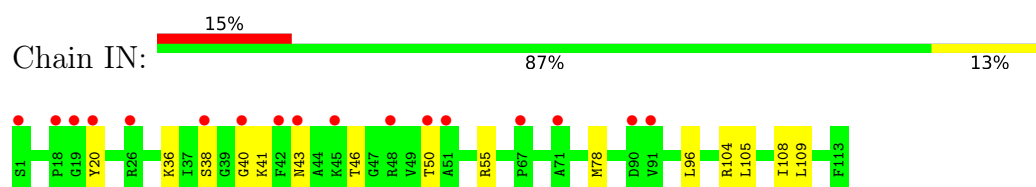
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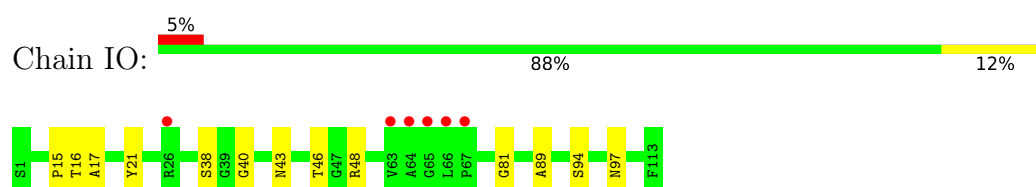
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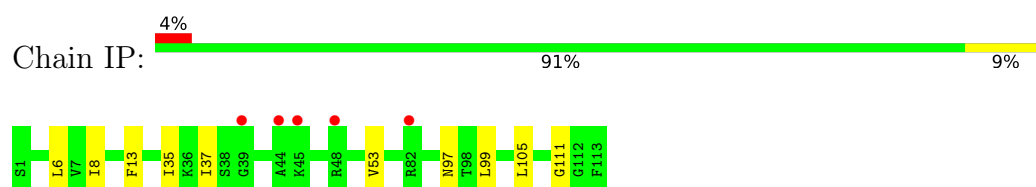
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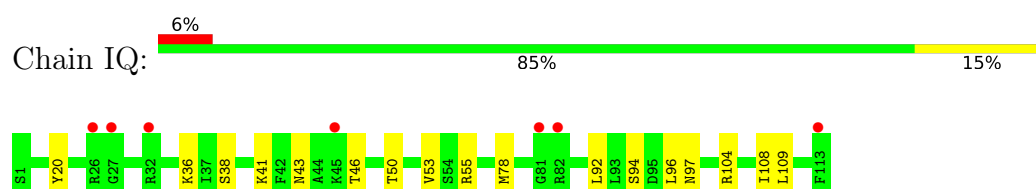
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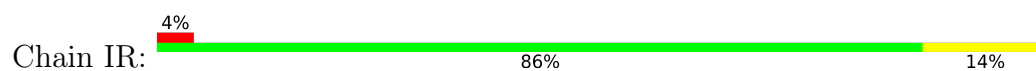
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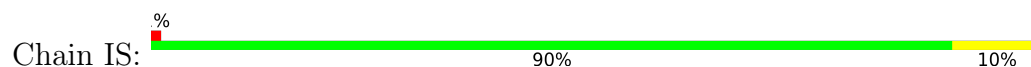
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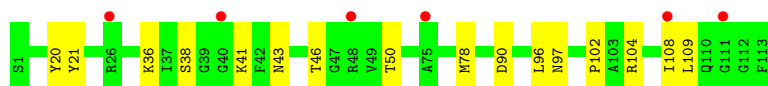
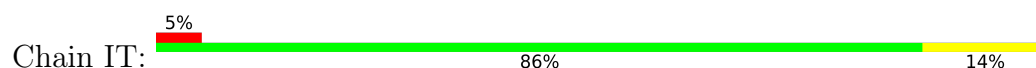
## ● Molecule 1: coat protein



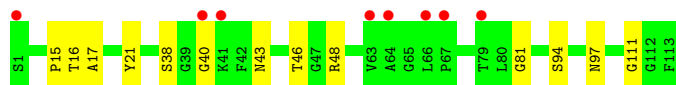
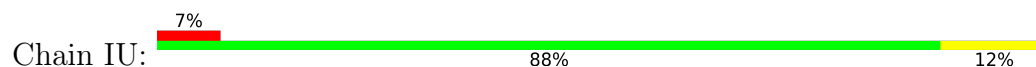
## ● Molecule 1: coat protein



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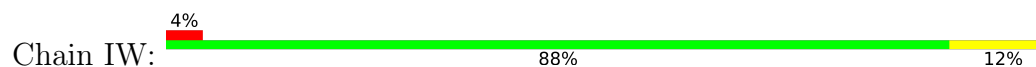
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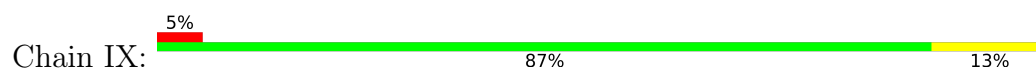
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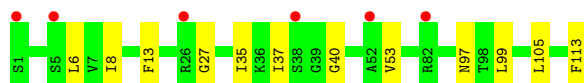
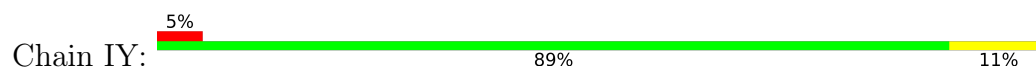


## ● Molecule 1: coat protein

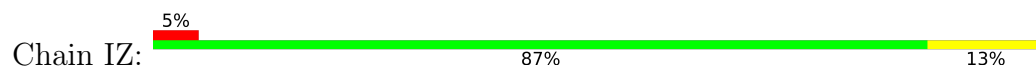




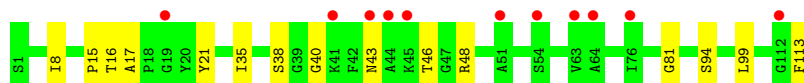
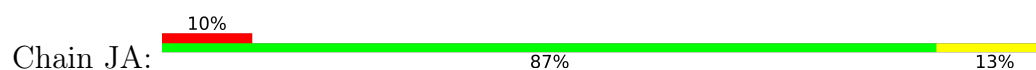
- Molecule 1: coat protein



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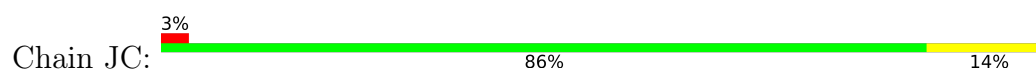
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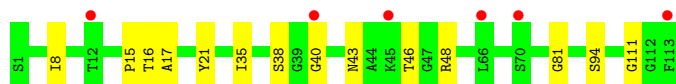
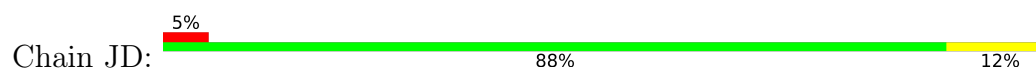
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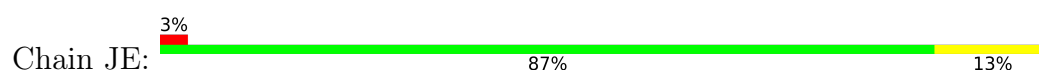
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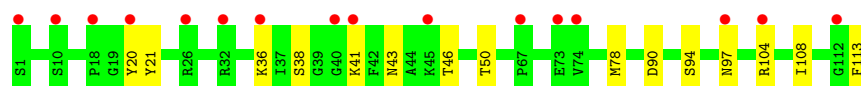
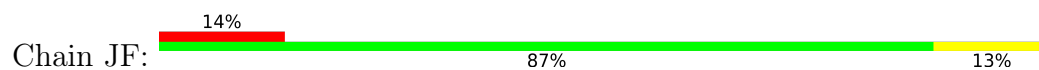
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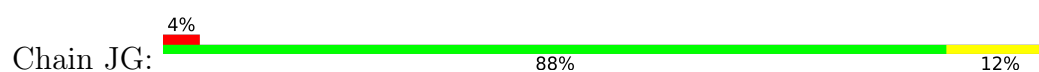
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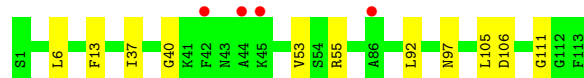
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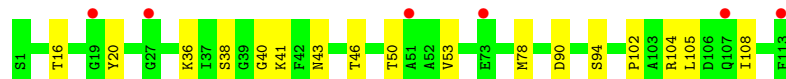
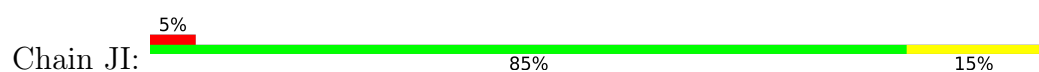
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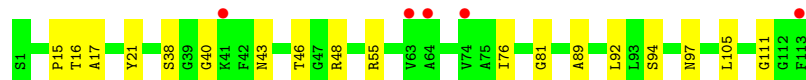
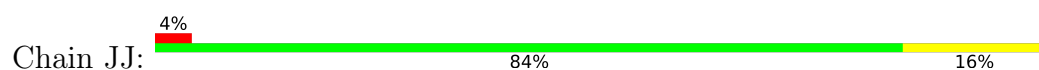
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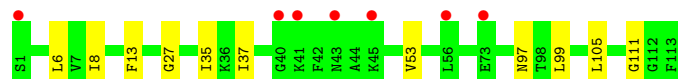
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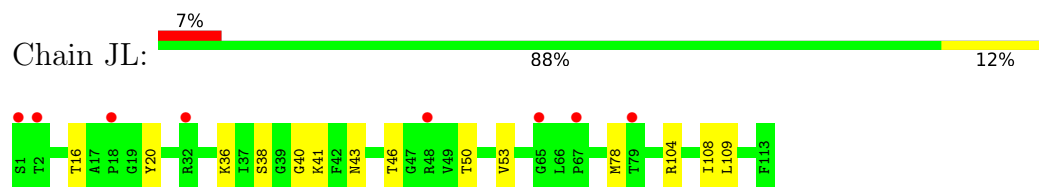
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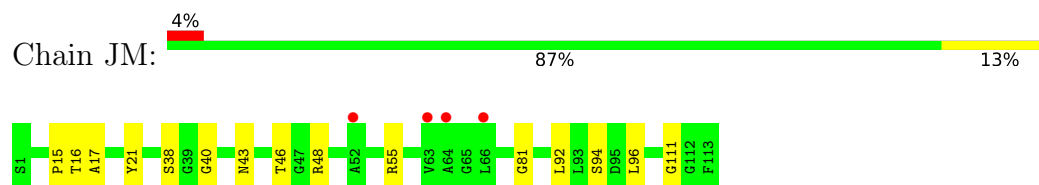
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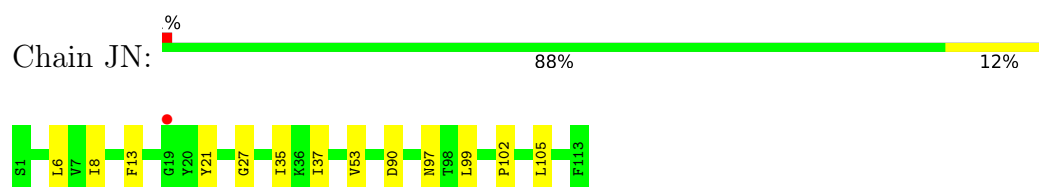
## ● Molecule 1: coat protein



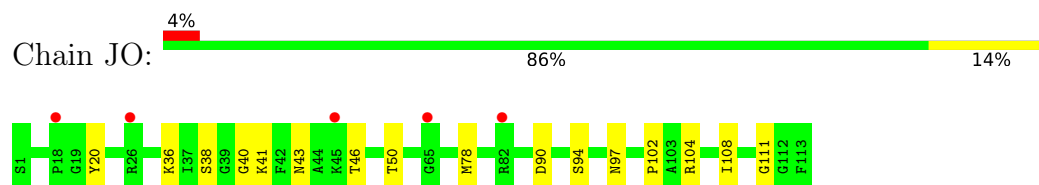
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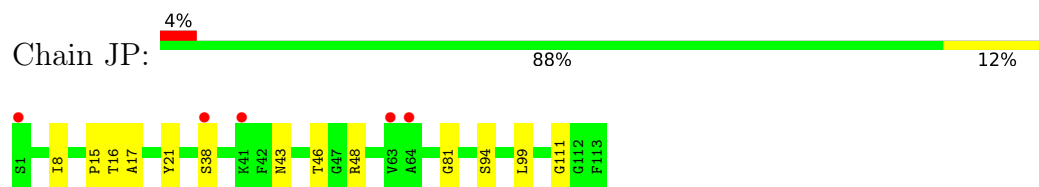
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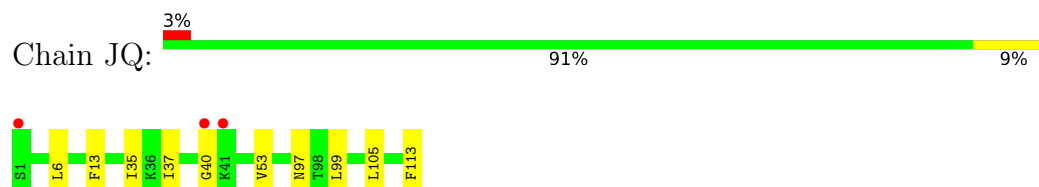
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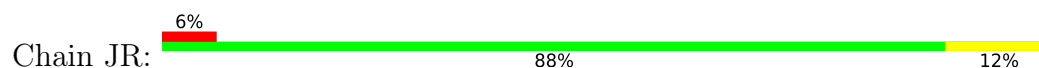
## ● Molecule 1: coat protein



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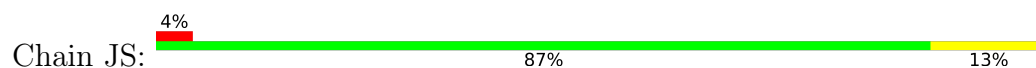


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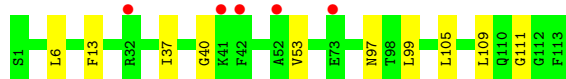




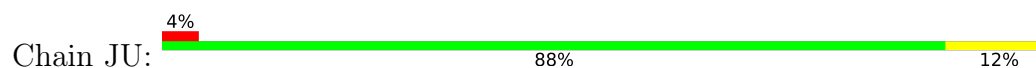
- Molecule 1: coat protein



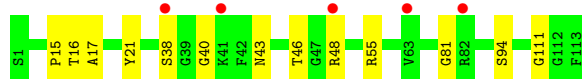
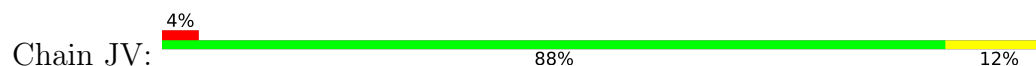
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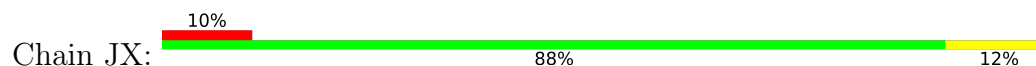
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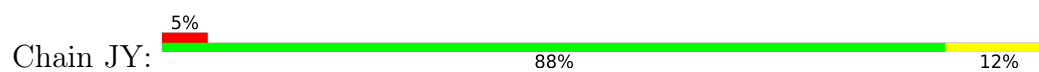
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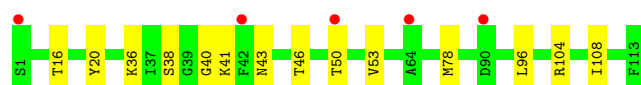
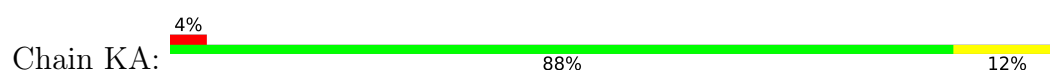
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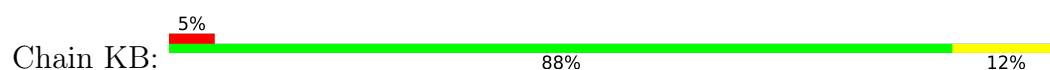
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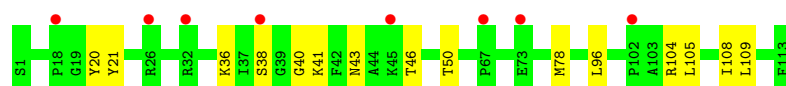
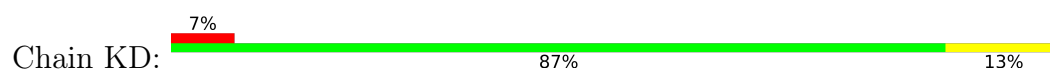
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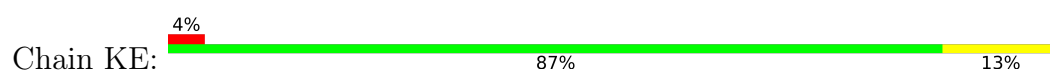
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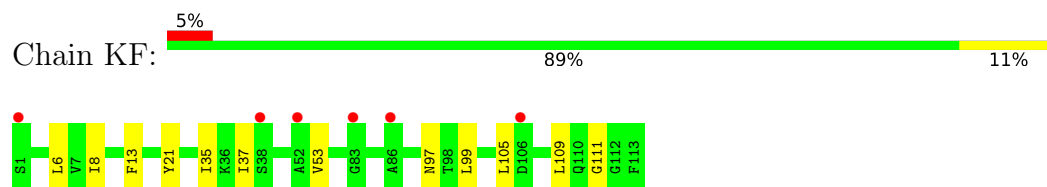
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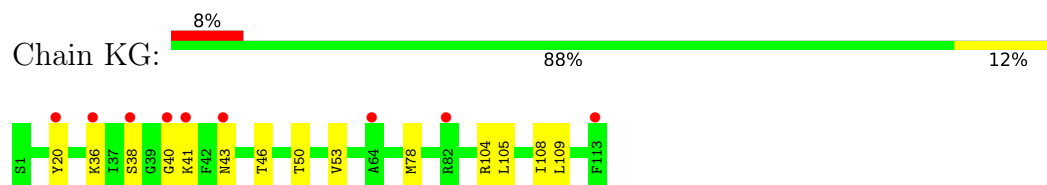
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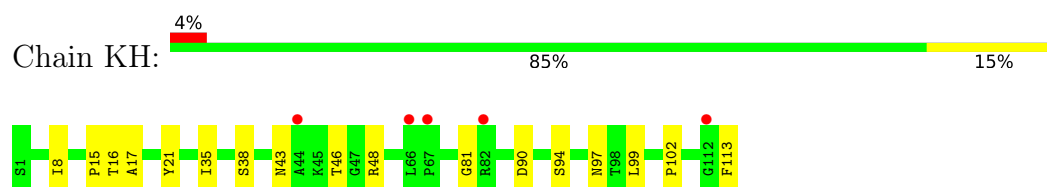
## ● Molecule 1: coat protein



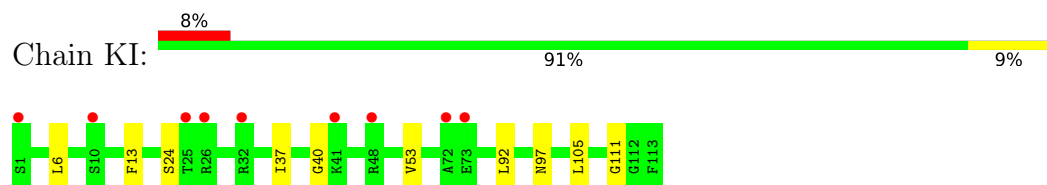
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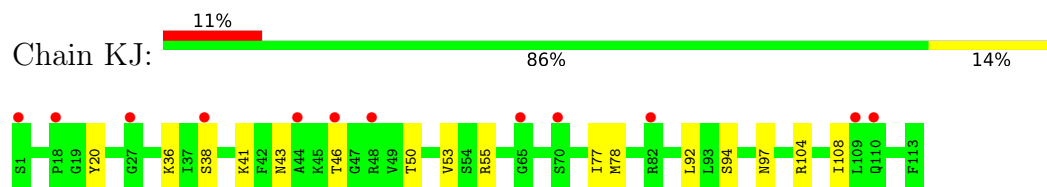
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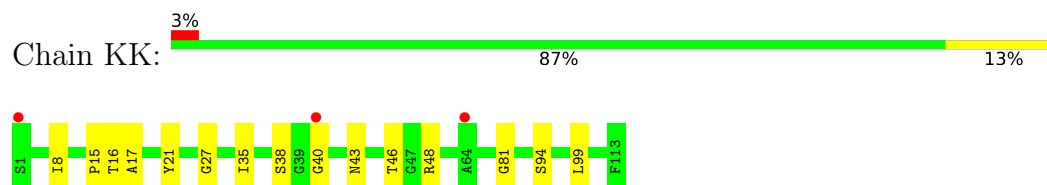
## ● Molecule 1: coat protein



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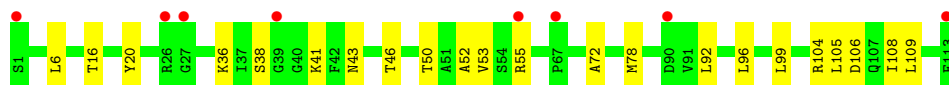
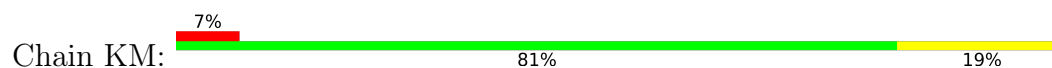


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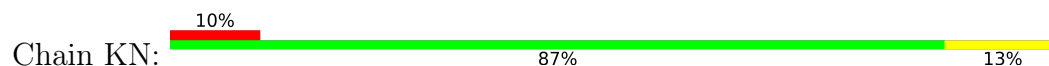




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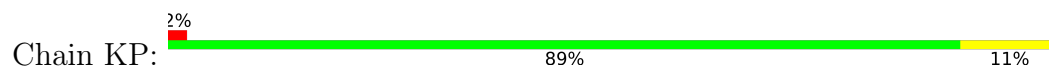
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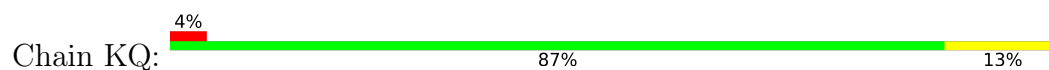
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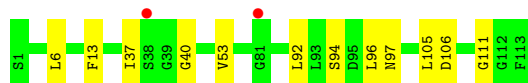
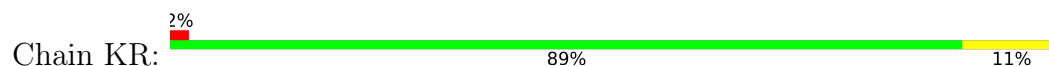
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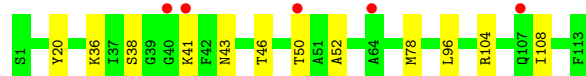
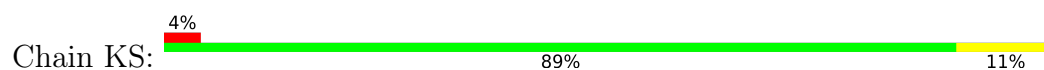
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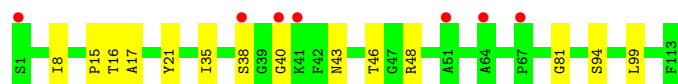
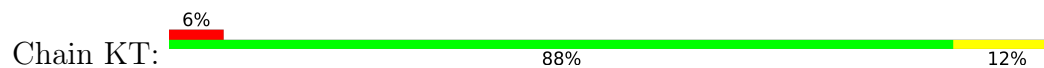
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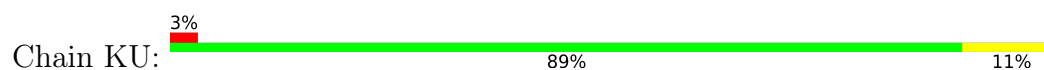
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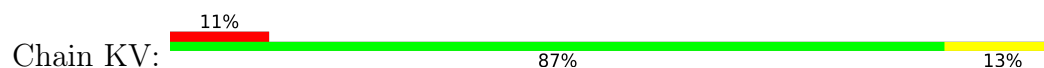
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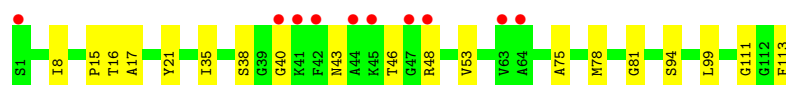
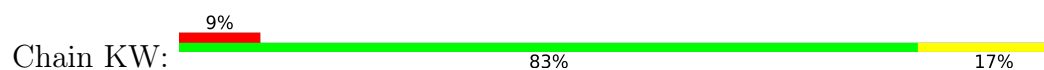
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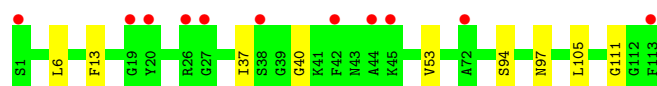
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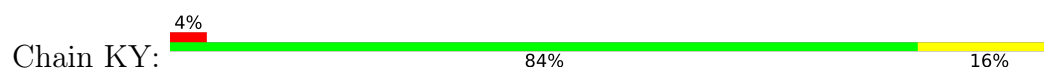
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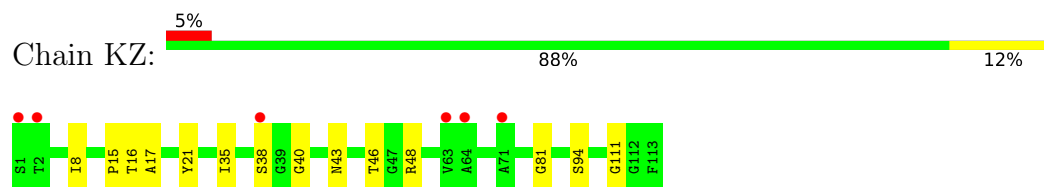
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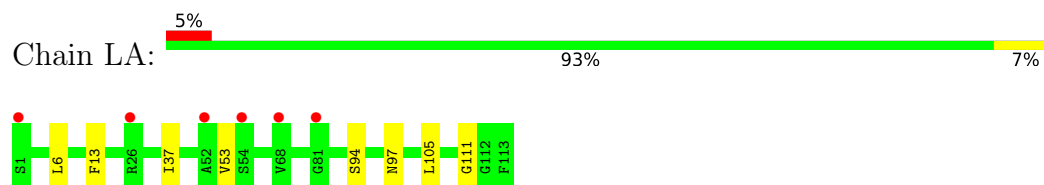
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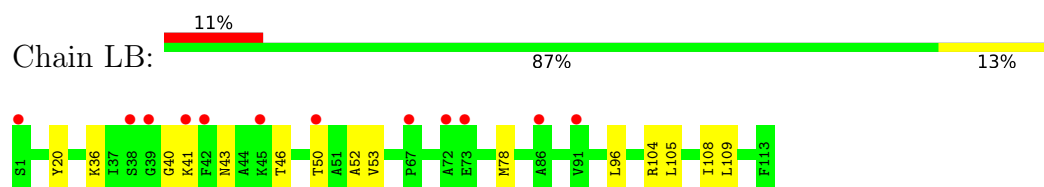
## ● Molecule 1: coat protein



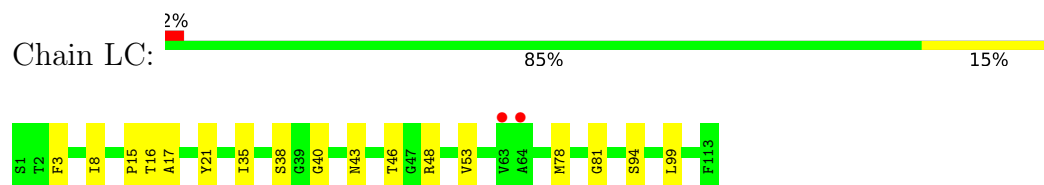
## ● Molecule 1: coat protein



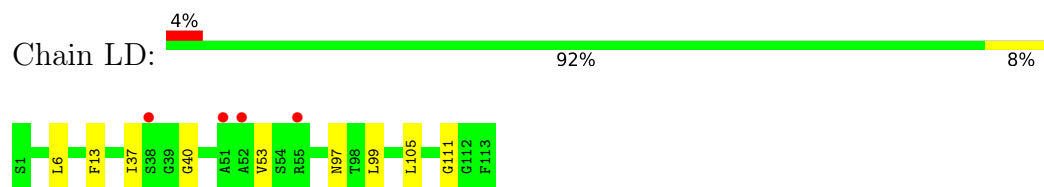
## ● Molecule 1: coat protein



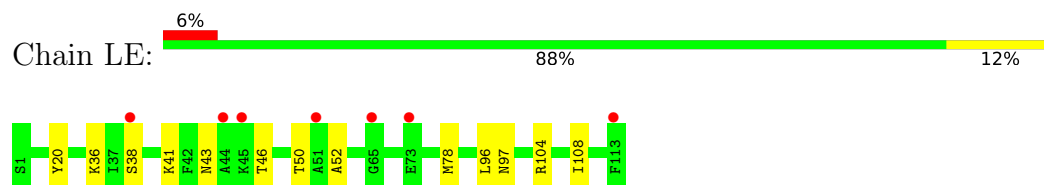
## ● Molecule 1: coat protein



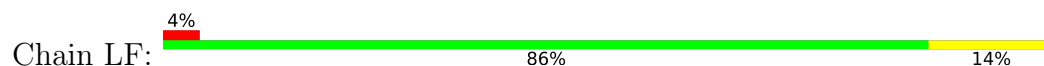
## ● Molecule 1: coat protein

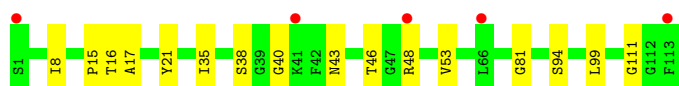


## ● Molecule 1: coat protein

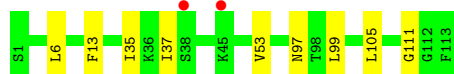


## ● Molecule 1: coat protein

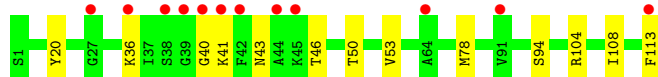
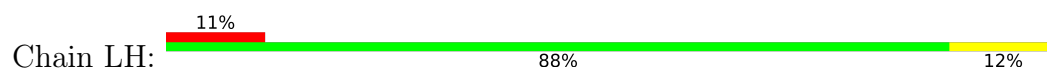




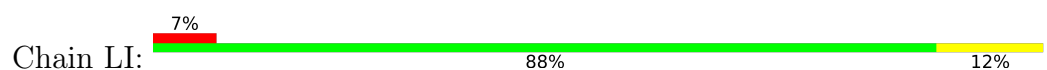
- Molecule 1: coat protein



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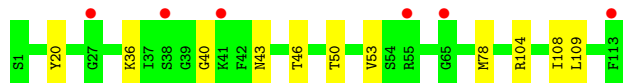
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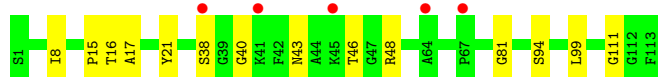
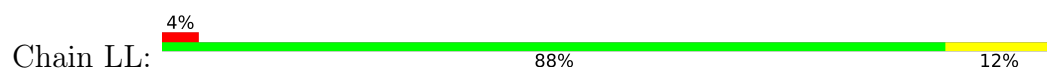
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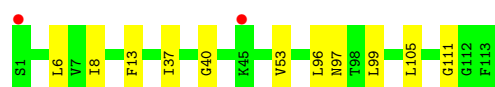
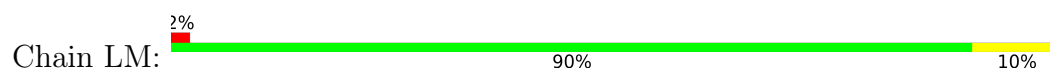
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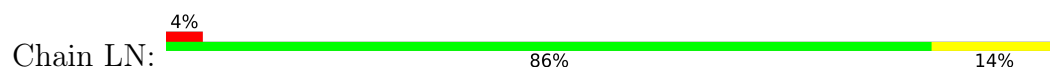
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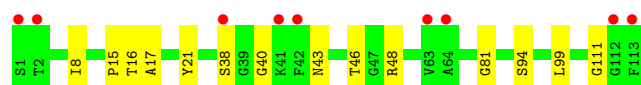
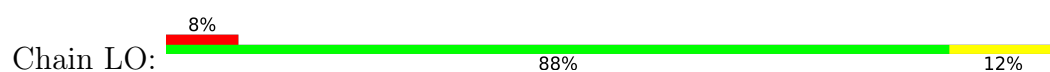
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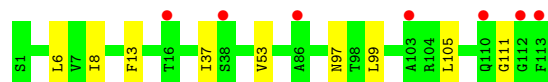
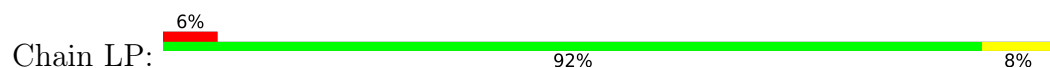
• Molecule 1: coat protein



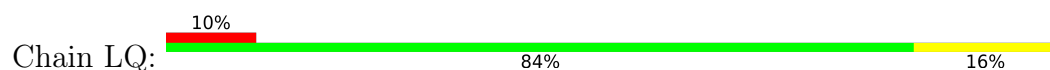
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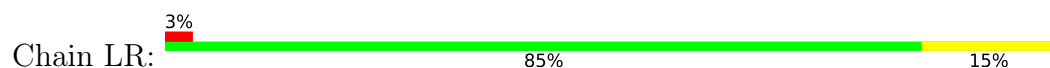
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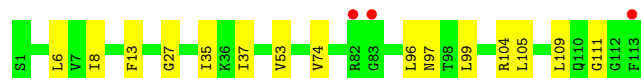
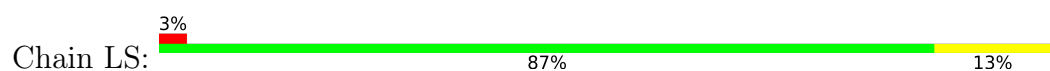
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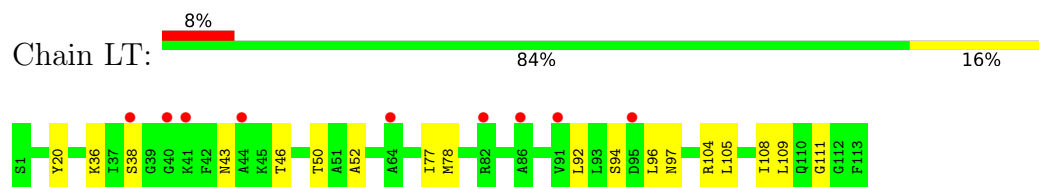
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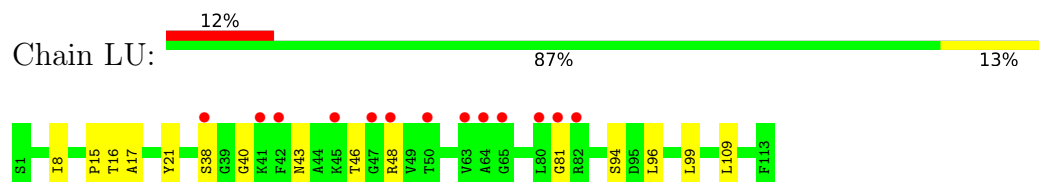
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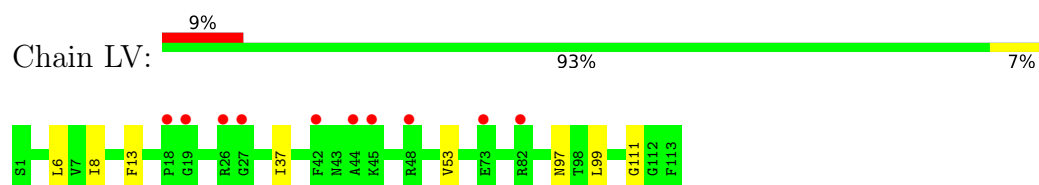
## ● Molecule 1: coat protein



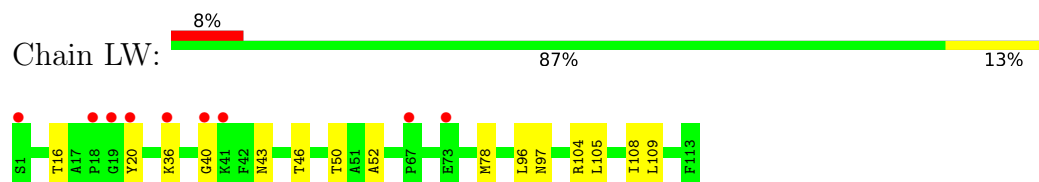
## ● Molecule 1: coat protein



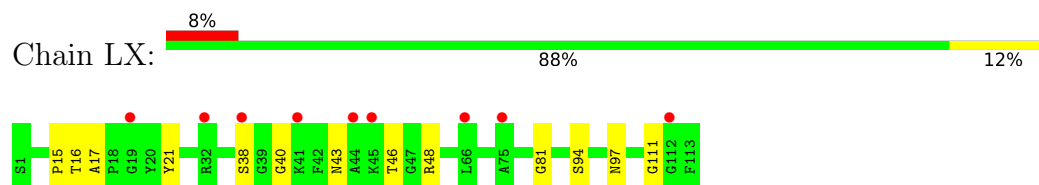
## ● Molecule 1: coat protein



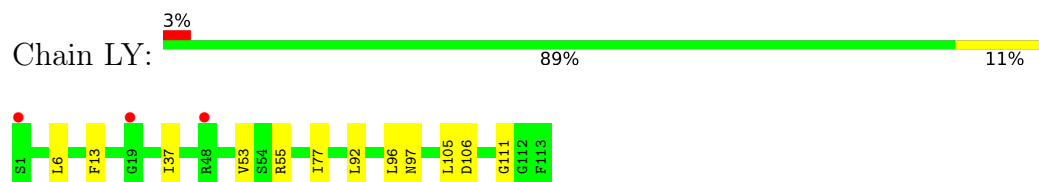
## ● Molecule 1: coat protein



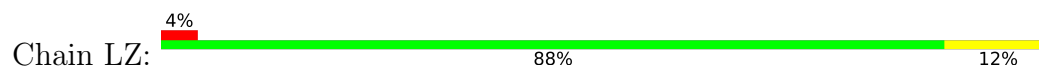
## ● Molecule 1: coat protein



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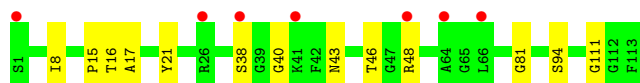
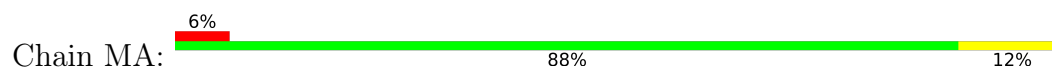


## ● Molecule 1: coat protein





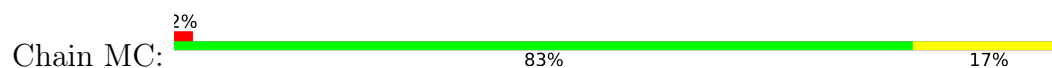
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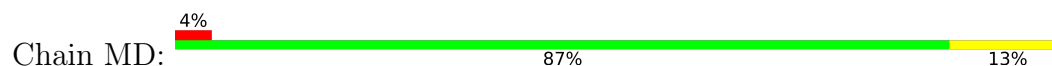
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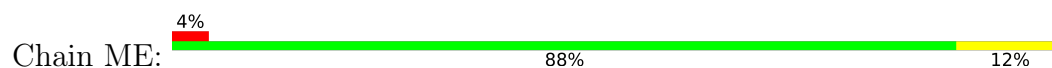
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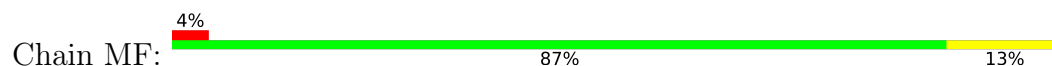
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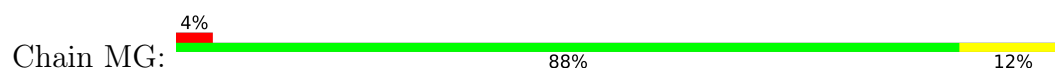
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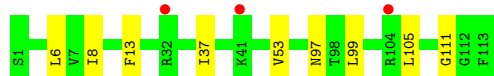
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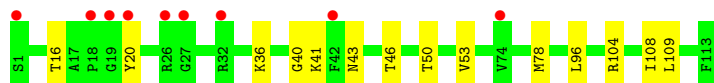
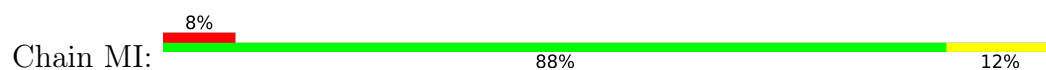
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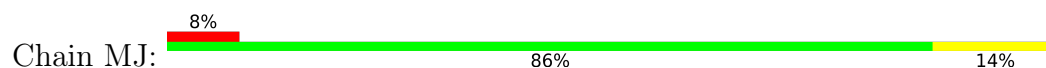
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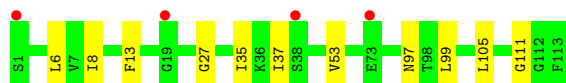
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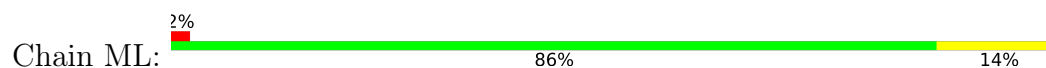
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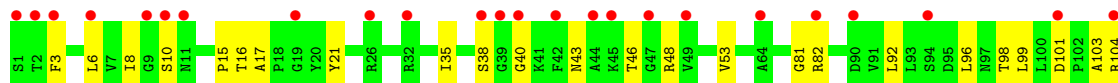
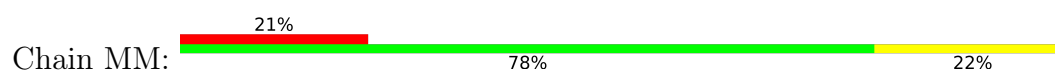
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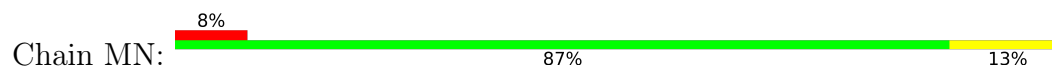


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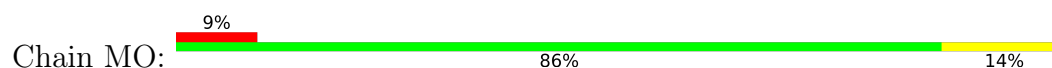




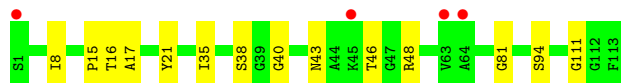
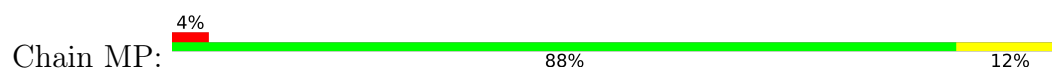
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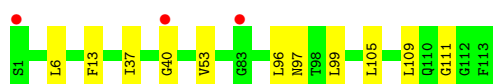
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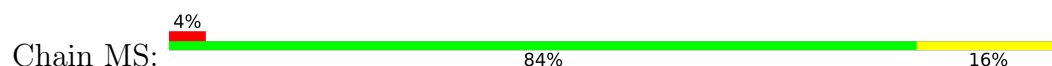
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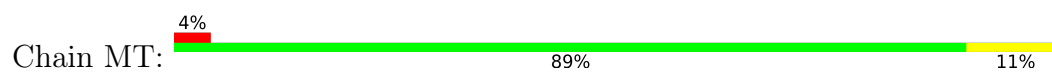
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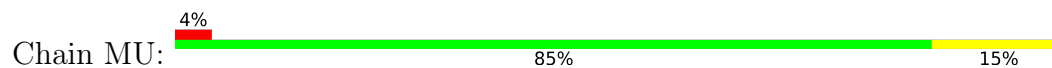
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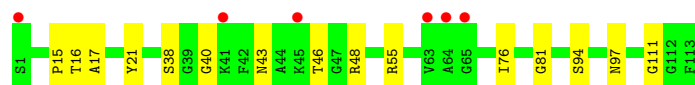
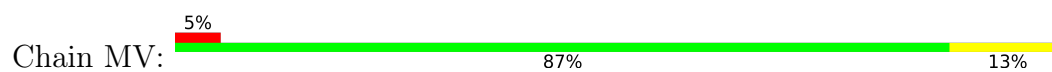
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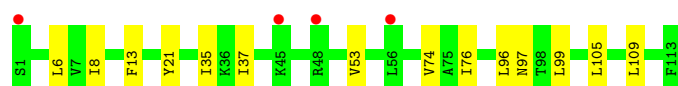
• Molecule 1: coat protein



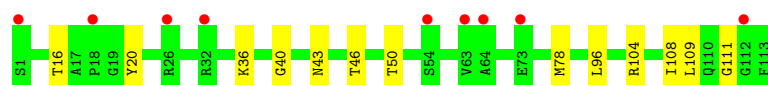
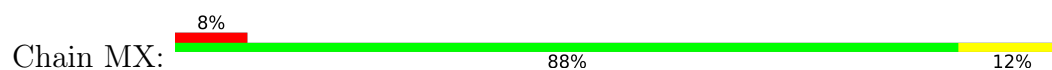
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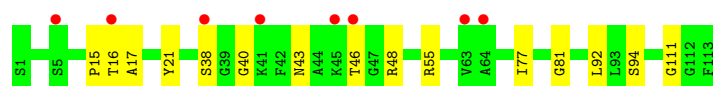
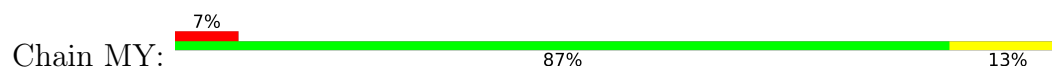
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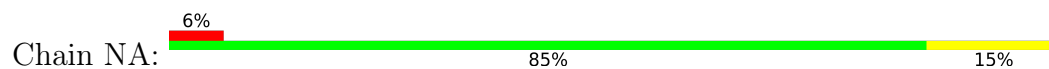
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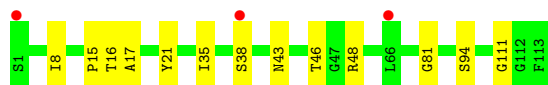
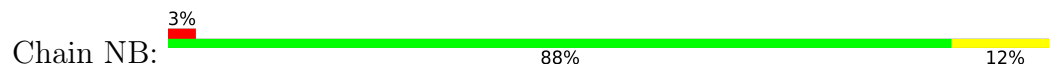
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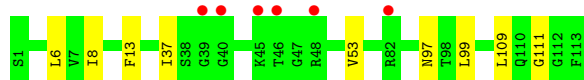
## ● Molecule 1: coat protein



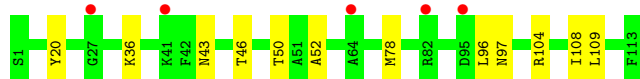
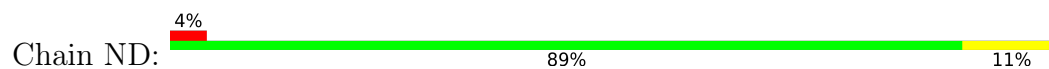
## ● Molecule 1: coat protein



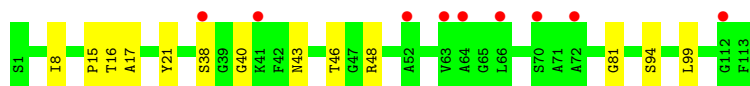
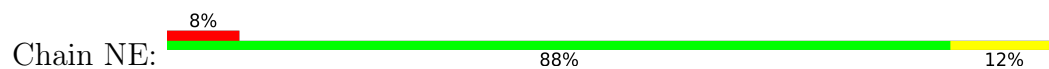
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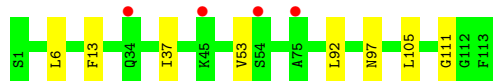
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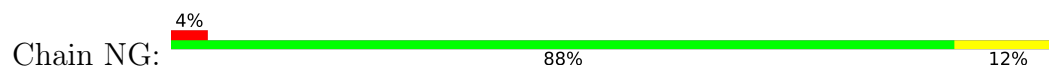
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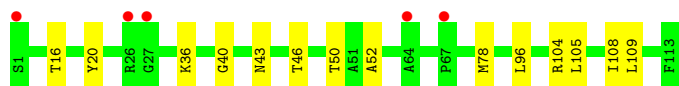


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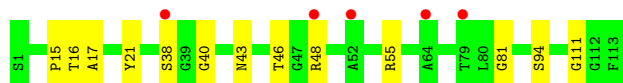
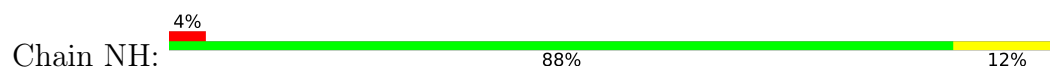


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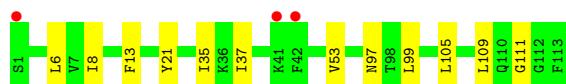
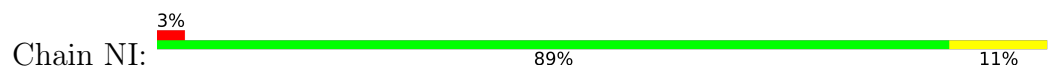




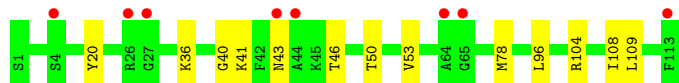
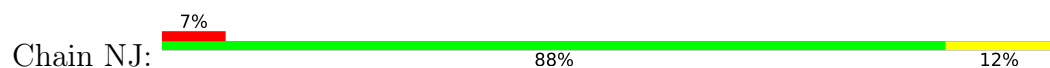
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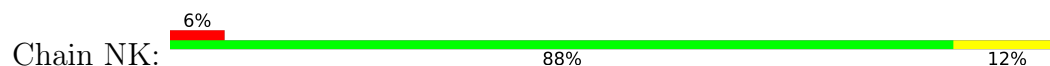
- Molecule 1: coat protein



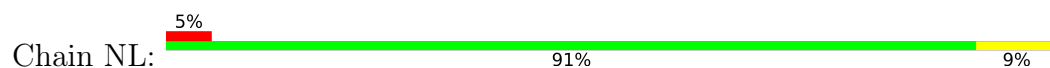
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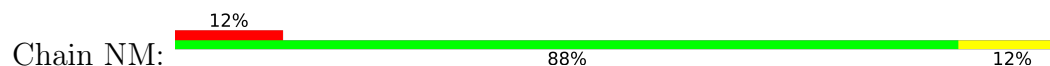
- Molecule 1: coat protein



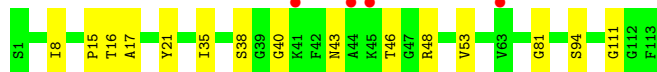
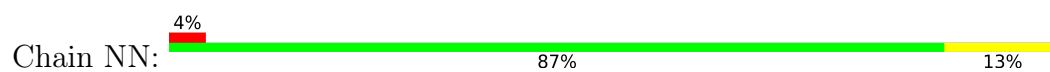
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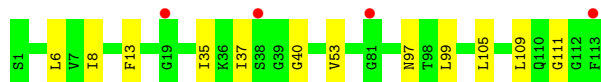
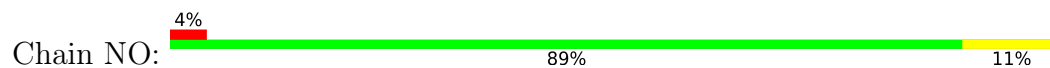
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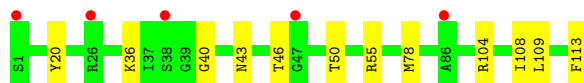
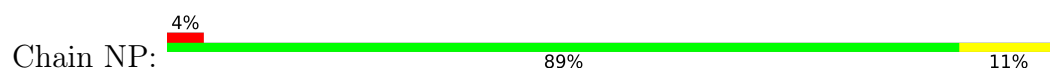
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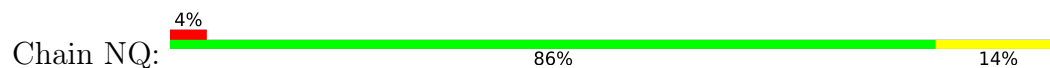
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- Molecule 1: coat protein



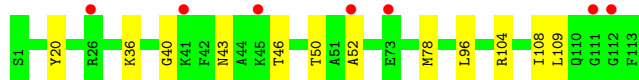
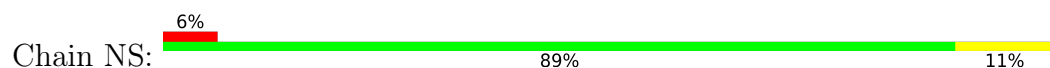
- Molecule 1: coat protein



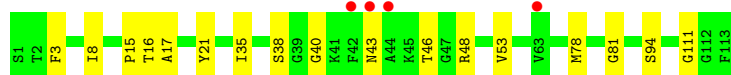
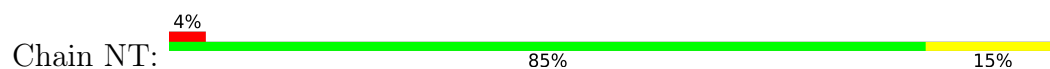
- Molecule 1: coat protein



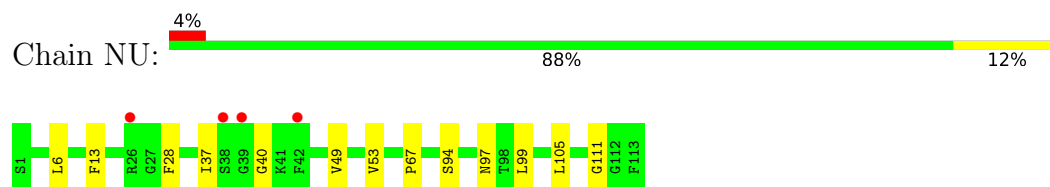
- Molecule 1: coat protein



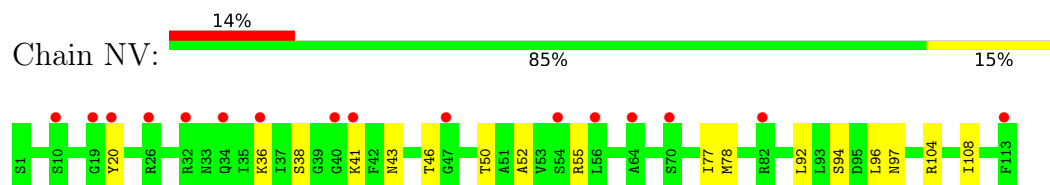
- Molecule 1: coat protein



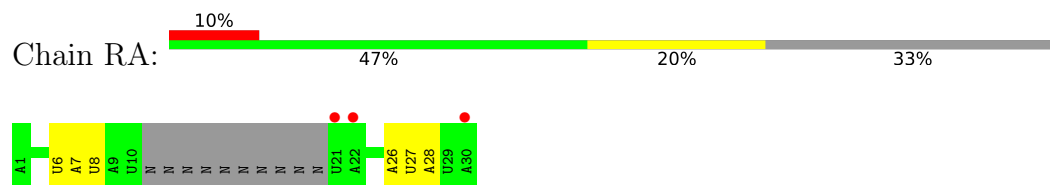
## • Molecule 1: coat protein



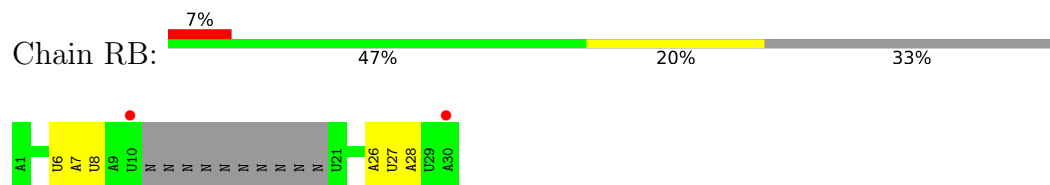
## • Molecule 1: coat protein



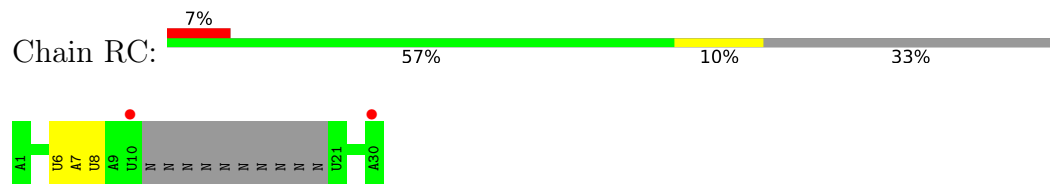
## • Molecule 2: RNA



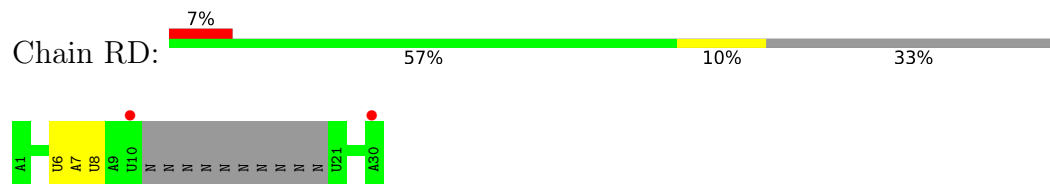
## • Molecule 2: RNA



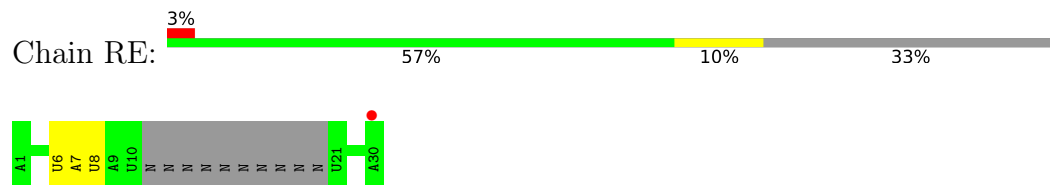
## • Molecule 2: RNA



## • Molecule 2: RNA



## • Molecule 2: RNA



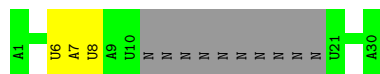
## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA

Chain RM:  7% 57% 10% 33%



## ● Molecule 2: RNA

Chain RN:  7% 53% 13% 33%



## ● Molecule 2: RNA

Chain RO:  17% 47% 20% 33%



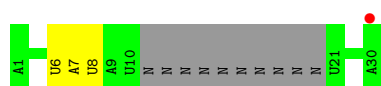
## ● Molecule 2: RNA

Chain RP:  3% 57% 10% 33%



## ● Molecule 2: RNA

Chain RQ:  3% 57% 10% 33%



## ● Molecule 2: RNA

Chain RR:  10% 53% 13% 33%



## ● Molecule 2: RNA

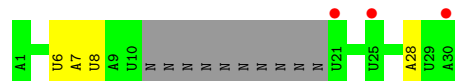
Chain RS:  10% 53% 13% 33%



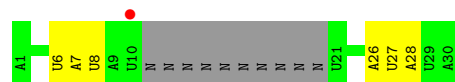
## ● Molecule 2: RNA



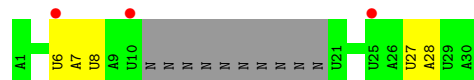
## ● Molecule 2: RNA



## ● Molecule 2: RNA



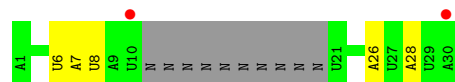
## ● Molecule 2: RNA



## ● Molecule 2: RNA



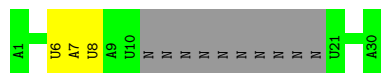
## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA

Chain SA:  57% 10% 33%

## ● Molecule 2: RNA

Chain SB:  10% 47% 20% 33%

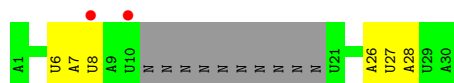
## ● Molecule 2: RNA

Chain SC:  3% 50% 17% 33%

## ● Molecule 2: RNA

Chain SD:  3% 47% 20% 33%

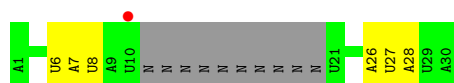
## ● Molecule 2: RNA

Chain SE:  7% 47% 20% 33%

## ● Molecule 2: RNA

Chain SF:  3% 50% 17% 33%

## ● Molecule 2: RNA

Chain SG:  3% 47% 20% 33%

## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



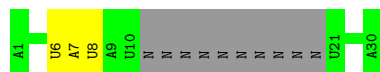
## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



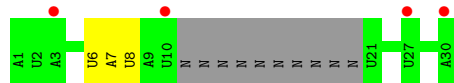
## ● Molecule 2: RNA



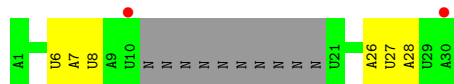
## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



## ● Molecule 2: RNA



## • Molecule 2: RNA



## • Molecule 2: RNA



## • Molecule 2: RNA



## • Molecule 2: RNA



## • Molecule 2: RNA



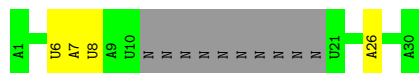
## • Molecule 2: RNA



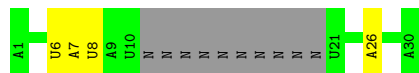
## • Molecule 2: RNA



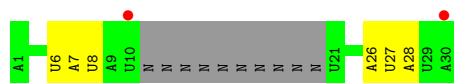
## • Molecule 2: RNA

Chain TC:  53% 13% 33%

## • Molecule 2: RNA

Chain TD:  53% 13% 33%

## • Molecule 2: RNA

Chain TE:  7% 47% 20% 33%

## • Molecule 2: RNA

Chain TF:  7% 53% 13% 33%

## • Molecule 2: RNA

Chain TG:  7% 53% 13% 33%

## • Molecule 2: RNA

Chain TH:  10% 47% 20% 33%

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 277.47Å 396.64Å 399.87Å<br>69.66° 83.65° 83.49°             | Depositor        |
| Resolution (Å)                                                          | 61.15 – 3.50<br>61.15 – 3.50                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 87.2 (61.15-3.50)<br>87.6 (61.15-3.50)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.31                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.26 (at 3.49Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.17.1_3660                                          | Depositor        |
| R, $R_{free}$                                                           | 0.261 , 0.261<br>0.268 , 0.267                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 20000 reflections (1.14%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 72.4                                                        | Xtriage          |
| Anisotropy                                                              | 0.317                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.29 , 60.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$ | Xtriage          |
| Estimated twinning fraction                                             | 0.096 for -h,-l,-k                                          | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.85                                                        | EDS              |
| Total number of atoms                                                   | 327240                                                      | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 100.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | AB    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | AC    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | AD    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | AE    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | AF    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | AG    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | AH    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | AI    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | AJ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | AK    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | AL    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | AM    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | AN    | 0.37         | 0/852   | 0.58        | 0/1158        |
| 1   | AO    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | AP    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | AQ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | AR    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | AS    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | AT    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | AU    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | AV    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | AW    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | AX    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | AY    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | AZ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | BA    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | BB    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | BC    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | BD    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | BE    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | BF    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | BG    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | BH    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | BI    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | BJ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | BK    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | BL    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | BM    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | BN    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | BO    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | BP    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | BQ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | BR    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | BS    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | BT    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | BU    | 0.36         | 0/852   | 0.57        | 0/1158        |
| 1   | BV    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | BW    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | BX    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | BY    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | BZ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | CA    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | CB    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | CC    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | CD    | 0.37         | 0/852   | 0.58        | 0/1158        |
| 1   | CE    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | CF    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | CG    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | CH    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | CI    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | CJ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | CK    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | CL    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | CM    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | CN    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | CO    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | CP    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | CQ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | CR    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | CS    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | CT    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | CU    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | CV    | 0.37         | 0/852   | 0.58        | 0/1158        |
| 1   | CW    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | CX    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | CY    | 0.37         | 0/852   | 0.57        | 0/1158        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | CZ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | DA    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | DB    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | DC    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | DD    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | DE    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | DF    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | DG    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | DH    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | DI    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | DJ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | DK    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | DL    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | DM    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | DN    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | DO    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | DP    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | DQ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | DR    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | DS    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | DT    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | DU    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | DV    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | DW    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | DX    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | DY    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | DZ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | EA    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | EB    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | EC    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | ED    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | EE    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | EF    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | EG    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | EH    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | EI    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | EJ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | EK    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | EL    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | EM    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | EN    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | EO    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | EP    | 0.38         | 0/852   | 0.55        | 0/1158        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | EQ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | ER    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | ES    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | ET    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | EU    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | EV    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | EW    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | EX    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | EY    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | EZ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | FA    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | FB    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | FC    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | FD    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | FE    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | FF    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | FG    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | FH    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | FI    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | FJ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | FK    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | FL    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | FM    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | FN    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | FO    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | FP    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | FQ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | FR    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | FS    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | FT    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | FU    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | FV    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | FW    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | FX    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | FY    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | FZ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | GA    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | GB    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | GC    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | GD    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | GE    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | GF    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | GG    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | GH    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | GI    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | GJ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | GK    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | GL    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | GM    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | GN    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | GO    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | GP    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | GQ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | GR    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | GS    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | GT    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | GU    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | GV    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | GW    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | GX    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | GY    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | GZ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | HA    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | HB    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | HC    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | HD    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | HE    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | HF    | 0.37         | 0/852   | 0.58        | 0/1158        |
| 1   | HG    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | HH    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | HI    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | HJ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | HK    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | HL    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | HM    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | HN    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | HO    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | HP    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | HQ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | HR    | 0.37         | 0/852   | 0.58        | 0/1158        |
| 1   | HS    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | HT    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | HU    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | HV    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | HW    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | HX    | 0.37         | 0/852   | 0.57        | 0/1158        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | HY    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | HZ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | IA    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | IB    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | IC    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | ID    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | IE    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | IF    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | IG    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | IH    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | II    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | IJ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | IK    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | IL    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | IM    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | IN    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | IO    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | IP    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | IQ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | IR    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | IS    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | IT    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | IU    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | IV    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | IW    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | IX    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | IY    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | IZ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | JA    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | JB    | 0.37         | 0/852   | 0.58        | 0/1158        |
| 1   | JC    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | JD    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | JE    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | JF    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | JG    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | JH    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | JI    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | JJ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | JK    | 0.37         | 0/852   | 0.58        | 0/1158        |
| 1   | JL    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | JM    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | JN    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | JO    | 0.38         | 0/852   | 0.55        | 0/1158        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | JP    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | JQ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | JR    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | JS    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | JT    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | JU    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | JV    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | JW    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | JX    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | JY    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | JZ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | KA    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | KB    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | KC    | 0.37         | 0/852   | 0.58        | 0/1158        |
| 1   | KD    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | KE    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | KF    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | KG    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | KH    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | KI    | 0.37         | 0/852   | 0.58        | 0/1158        |
| 1   | KJ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | KK    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | KL    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | KM    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | KN    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | KO    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | KP    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | KQ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | KR    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | KS    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | KT    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | KU    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | KV    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | KW    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | KX    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | KY    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | KZ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | LA    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | LB    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | LC    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | LD    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | LE    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | LF    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | LG    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | LH    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | LI    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | LJ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | LK    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | LL    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | LM    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | LN    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | LO    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | LP    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | LQ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | LR    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | LS    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | LT    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | LU    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | LV    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | LW    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | LX    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | LY    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | LZ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | MA    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | MB    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | MC    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | MD    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | ME    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | MF    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | MG    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | MH    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | MI    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | MJ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | MK    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | ML    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | MM    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | MN    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | MO    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | MP    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | MQ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | MR    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | MS    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | MT    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | MU    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | MV    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | MW    | 0.37         | 0/852   | 0.57        | 0/1158        |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 1   | MX    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | MY    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | MZ    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | NA    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | NB    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | NC    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | ND    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | NE    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | NF    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | NG    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | NH    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | NI    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | NJ    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | NK    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | NL    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | NM    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | NN    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | NO    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | NP    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | NQ    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | NR    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | NS    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 1   | NT    | 0.38         | 0/852   | 0.60        | 2/1158 (0.2%) |
| 1   | NU    | 0.37         | 0/852   | 0.57        | 0/1158        |
| 1   | NV    | 0.38         | 0/852   | 0.55        | 0/1158        |
| 2   | RA    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RB    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RC    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RD    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RE    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RF    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RG    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RH    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RI    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RJ    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RK    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RL    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RM    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RN    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RO    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RP    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RQ    | 0.35         | 0/468   | 0.45        | 0/722         |
| 2   | RR    | 0.35         | 0/468   | 0.45        | 0/722         |

| Mol | Chain | Bond lengths |          | Bond angles |                   |
|-----|-------|--------------|----------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5           |
| 2   | RS    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | RT    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | RU    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | RV    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | RW    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | RX    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | RY    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | RZ    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SA    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SB    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SC    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SD    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SE    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SF    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SG    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SH    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SI    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SJ    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SK    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SL    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SM    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SN    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SO    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SP    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SQ    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SR    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SS    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | ST    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SU    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SV    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SW    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SX    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SY    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | SZ    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | TA    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | TB    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | TC    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | TD    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | TE    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | TF    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | TG    | 0.35         | 0/468    | 0.45        | 0/722             |
| 2   | TH    | 0.35         | 0/468    | 0.45        | 0/722             |
| All | All   | 0.37         | 0/334800 | 0.56        | 240/460200 (0.1%) |

There are no bond length outliers.

The worst 5 of 240 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | GJ    | 38  | SER  | CA-C-N | -5.56 | 112.07      | 121.47   |
| 1   | GJ    | 38  | SER  | C-N-CA | -5.56 | 112.07      | 121.47   |
| 1   | DM    | 38  | SER  | CA-C-N | -5.56 | 112.08      | 121.47   |
| 1   | DM    | 38  | SER  | C-N-CA | -5.56 | 112.08      | 121.47   |
| 1   | KQ    | 38  | SER  | CA-C-N | -5.55 | 112.08      | 121.47   |

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    | 839   | 0        | 858      | 14      | 0            |
| 1   | AB    | 839   | 0        | 858      | 8       | 0            |
| 1   | AC    | 839   | 0        | 858      | 8       | 0            |
| 1   | AD    | 839   | 0        | 858      | 12      | 0            |
| 1   | AE    | 839   | 0        | 858      | 6       | 0            |
| 1   | AF    | 839   | 0        | 858      | 13      | 0            |
| 1   | AG    | 839   | 0        | 858      | 9       | 0            |
| 1   | AH    | 839   | 0        | 858      | 12      | 0            |
| 1   | AI    | 839   | 0        | 858      | 14      | 0            |
| 1   | AJ    | 839   | 0        | 858      | 12      | 0            |
| 1   | AK    | 839   | 0        | 858      | 6       | 0            |
| 1   | AL    | 839   | 0        | 858      | 15      | 0            |
| 1   | AM    | 839   | 0        | 858      | 11      | 0            |
| 1   | AN    | 839   | 0        | 858      | 7       | 0            |
| 1   | AO    | 839   | 0        | 858      | 15      | 0            |
| 1   | AP    | 839   | 0        | 858      | 11      | 0            |
| 1   | AQ    | 839   | 0        | 858      | 8       | 0            |
| 1   | AR    | 839   | 0        | 858      | 14      | 0            |
| 1   | AS    | 839   | 0        | 858      | 12      | 0            |
| 1   | AT    | 839   | 0        | 858      | 10      | 0            |
| 1   | AU    | 839   | 0        | 858      | 10      | 0            |
| 1   | AV    | 839   | 0        | 858      | 10      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AW    | 839   | 0        | 858      | 10      | 0            |
| 1   | AX    | 839   | 0        | 858      | 12      | 0            |
| 1   | AY    | 839   | 0        | 858      | 12      | 0            |
| 1   | AZ    | 839   | 0        | 858      | 14      | 2            |
| 1   | BA    | 839   | 0        | 858      | 18      | 0            |
| 1   | BB    | 839   | 0        | 858      | 20      | 0            |
| 1   | BC    | 839   | 0        | 858      | 14      | 0            |
| 1   | BD    | 839   | 0        | 858      | 10      | 0            |
| 1   | BE    | 839   | 0        | 858      | 12      | 0            |
| 1   | BF    | 839   | 0        | 858      | 8       | 0            |
| 1   | BG    | 839   | 0        | 858      | 16      | 0            |
| 1   | BH    | 839   | 0        | 858      | 16      | 0            |
| 1   | BI    | 839   | 0        | 858      | 13      | 0            |
| 1   | BJ    | 839   | 0        | 858      | 11      | 0            |
| 1   | BK    | 839   | 0        | 858      | 10      | 0            |
| 1   | BL    | 839   | 0        | 858      | 10      | 0            |
| 1   | BM    | 839   | 0        | 858      | 13      | 0            |
| 1   | BN    | 839   | 0        | 858      | 25      | 0            |
| 1   | BO    | 839   | 0        | 858      | 15      | 0            |
| 1   | BP    | 839   | 0        | 858      | 13      | 0            |
| 1   | BQ    | 839   | 0        | 858      | 31      | 0            |
| 1   | BR    | 839   | 0        | 858      | 21      | 0            |
| 1   | BS    | 839   | 0        | 858      | 16      | 0            |
| 1   | BT    | 839   | 0        | 858      | 9       | 0            |
| 1   | BU    | 839   | 0        | 858      | 10      | 0            |
| 1   | BV    | 839   | 0        | 858      | 16      | 0            |
| 1   | BW    | 839   | 0        | 858      | 12      | 0            |
| 1   | BX    | 839   | 0        | 858      | 10      | 0            |
| 1   | BY    | 839   | 0        | 858      | 11      | 0            |
| 1   | BZ    | 839   | 0        | 858      | 9       | 0            |
| 1   | CA    | 839   | 0        | 858      | 10      | 0            |
| 1   | CB    | 839   | 0        | 858      | 10      | 0            |
| 1   | CC    | 839   | 0        | 858      | 12      | 0            |
| 1   | CD    | 839   | 0        | 858      | 6       | 0            |
| 1   | CE    | 839   | 0        | 858      | 11      | 0            |
| 1   | CF    | 839   | 0        | 858      | 11      | 0            |
| 1   | CG    | 839   | 0        | 858      | 7       | 0            |
| 1   | CH    | 839   | 0        | 858      | 12      | 0            |
| 1   | CI    | 839   | 0        | 858      | 10      | 0            |
| 1   | CJ    | 839   | 0        | 858      | 12      | 0            |
| 1   | CK    | 839   | 0        | 858      | 13      | 0            |
| 1   | CL    | 839   | 0        | 858      | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | CM    | 839   | 0        | 858      | 7       | 0            |
| 1   | CN    | 839   | 0        | 858      | 9       | 0            |
| 1   | CO    | 839   | 0        | 858      | 14      | 0            |
| 1   | CP    | 839   | 0        | 858      | 18      | 0            |
| 1   | CQ    | 839   | 0        | 858      | 15      | 0            |
| 1   | CR    | 839   | 0        | 858      | 8       | 0            |
| 1   | CS    | 839   | 0        | 858      | 11      | 0            |
| 1   | CT    | 839   | 0        | 858      | 16      | 0            |
| 1   | CU    | 839   | 0        | 858      | 12      | 0            |
| 1   | CV    | 839   | 0        | 858      | 11      | 0            |
| 1   | CW    | 839   | 0        | 858      | 11      | 0            |
| 1   | CX    | 839   | 0        | 858      | 23      | 0            |
| 1   | CY    | 839   | 0        | 858      | 11      | 0            |
| 1   | CZ    | 839   | 0        | 858      | 16      | 0            |
| 1   | DA    | 839   | 0        | 858      | 13      | 0            |
| 1   | DB    | 839   | 0        | 858      | 11      | 0            |
| 1   | DC    | 839   | 0        | 858      | 13      | 0            |
| 1   | DD    | 839   | 0        | 858      | 12      | 0            |
| 1   | DE    | 839   | 0        | 858      | 12      | 0            |
| 1   | DF    | 839   | 0        | 858      | 14      | 0            |
| 1   | DG    | 839   | 0        | 858      | 8       | 0            |
| 1   | DH    | 839   | 0        | 858      | 11      | 0            |
| 1   | DI    | 839   | 0        | 858      | 16      | 0            |
| 1   | DJ    | 839   | 0        | 858      | 21      | 0            |
| 1   | DK    | 839   | 0        | 858      | 24      | 0            |
| 1   | DL    | 839   | 0        | 858      | 17      | 0            |
| 1   | DM    | 839   | 0        | 858      | 11      | 0            |
| 1   | DN    | 839   | 0        | 858      | 8       | 0            |
| 1   | DO    | 839   | 0        | 858      | 9       | 0            |
| 1   | DP    | 839   | 0        | 858      | 12      | 0            |
| 1   | DQ    | 839   | 0        | 858      | 10      | 0            |
| 1   | DR    | 839   | 0        | 858      | 13      | 0            |
| 1   | DS    | 839   | 0        | 858      | 9       | 0            |
| 1   | DT    | 839   | 0        | 858      | 8       | 0            |
| 1   | DU    | 839   | 0        | 858      | 10      | 0            |
| 1   | DV    | 839   | 0        | 858      | 10      | 0            |
| 1   | DW    | 839   | 0        | 858      | 9       | 0            |
| 1   | DX    | 839   | 0        | 858      | 12      | 0            |
| 1   | DY    | 839   | 0        | 858      | 11      | 0            |
| 1   | DZ    | 839   | 0        | 858      | 23      | 0            |
| 1   | EA    | 839   | 0        | 858      | 13      | 0            |
| 1   | EB    | 839   | 0        | 858      | 13      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | EC    | 839   | 0        | 858      | 23      | 0            |
| 1   | ED    | 839   | 0        | 858      | 12      | 0            |
| 1   | EE    | 839   | 0        | 858      | 10      | 0            |
| 1   | EF    | 839   | 0        | 858      | 9       | 0            |
| 1   | EG    | 839   | 0        | 858      | 9       | 0            |
| 1   | EH    | 839   | 0        | 858      | 11      | 0            |
| 1   | EI    | 839   | 0        | 858      | 11      | 0            |
| 1   | EJ    | 839   | 0        | 858      | 9       | 0            |
| 1   | EK    | 839   | 0        | 858      | 13      | 0            |
| 1   | EL    | 839   | 0        | 858      | 11      | 0            |
| 1   | EM    | 839   | 0        | 858      | 18      | 0            |
| 1   | EN    | 839   | 0        | 858      | 9       | 0            |
| 1   | EO    | 839   | 0        | 858      | 10      | 0            |
| 1   | EP    | 839   | 0        | 858      | 10      | 0            |
| 1   | EQ    | 839   | 0        | 858      | 12      | 0            |
| 1   | ER    | 839   | 0        | 858      | 12      | 0            |
| 1   | ES    | 839   | 0        | 858      | 18      | 0            |
| 1   | ET    | 839   | 0        | 858      | 9       | 0            |
| 1   | EU    | 839   | 0        | 858      | 9       | 1            |
| 1   | EV    | 839   | 0        | 858      | 10      | 0            |
| 1   | EW    | 839   | 0        | 858      | 15      | 0            |
| 1   | EX    | 839   | 0        | 858      | 14      | 0            |
| 1   | EY    | 839   | 0        | 858      | 11      | 0            |
| 1   | EZ    | 839   | 0        | 858      | 10      | 0            |
| 1   | FA    | 839   | 0        | 858      | 10      | 0            |
| 1   | FB    | 839   | 0        | 858      | 11      | 0            |
| 1   | FC    | 839   | 0        | 858      | 11      | 0            |
| 1   | FD    | 839   | 0        | 858      | 7       | 0            |
| 1   | FE    | 839   | 0        | 858      | 16      | 0            |
| 1   | FF    | 839   | 0        | 858      | 9       | 0            |
| 1   | FG    | 839   | 0        | 858      | 7       | 0            |
| 1   | FH    | 839   | 0        | 858      | 15      | 0            |
| 1   | FI    | 839   | 0        | 858      | 13      | 0            |
| 1   | FJ    | 839   | 0        | 858      | 10      | 0            |
| 1   | FK    | 839   | 0        | 858      | 7       | 0            |
| 1   | FL    | 839   | 0        | 858      | 11      | 0            |
| 1   | FM    | 839   | 0        | 858      | 10      | 0            |
| 1   | FN    | 839   | 0        | 858      | 8       | 0            |
| 1   | FO    | 839   | 0        | 858      | 7       | 0            |
| 1   | FP    | 839   | 0        | 858      | 12      | 0            |
| 1   | FQ    | 839   | 0        | 858      | 9       | 0            |
| 1   | FR    | 839   | 0        | 858      | 9       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | FS    | 839   | 0        | 858      | 12      | 1            |
| 1   | FT    | 839   | 0        | 858      | 9       | 0            |
| 1   | FU    | 839   | 0        | 858      | 10      | 0            |
| 1   | FV    | 839   | 0        | 858      | 7       | 0            |
| 1   | FW    | 839   | 0        | 858      | 10      | 0            |
| 1   | FX    | 839   | 0        | 858      | 9       | 0            |
| 1   | FY    | 839   | 0        | 858      | 8       | 0            |
| 1   | FZ    | 839   | 0        | 858      | 12      | 0            |
| 1   | GA    | 839   | 0        | 858      | 9       | 0            |
| 1   | GB    | 839   | 0        | 858      | 11      | 0            |
| 1   | GC    | 839   | 0        | 858      | 15      | 0            |
| 1   | GD    | 839   | 0        | 858      | 14      | 0            |
| 1   | GE    | 839   | 0        | 858      | 8       | 0            |
| 1   | GF    | 839   | 0        | 858      | 13      | 0            |
| 1   | GG    | 839   | 0        | 858      | 10      | 0            |
| 1   | GH    | 839   | 0        | 858      | 9       | 0            |
| 1   | GI    | 839   | 0        | 858      | 11      | 0            |
| 1   | GJ    | 839   | 0        | 858      | 11      | 0            |
| 1   | GK    | 839   | 0        | 858      | 11      | 1            |
| 1   | GL    | 839   | 0        | 858      | 17      | 0            |
| 1   | GM    | 839   | 0        | 858      | 12      | 0            |
| 1   | GN    | 839   | 0        | 858      | 8       | 0            |
| 1   | GO    | 839   | 0        | 858      | 11      | 0            |
| 1   | GP    | 839   | 0        | 858      | 14      | 0            |
| 1   | GQ    | 839   | 0        | 858      | 8       | 0            |
| 1   | GR    | 839   | 0        | 858      | 13      | 0            |
| 1   | GS    | 839   | 0        | 858      | 8       | 0            |
| 1   | GT    | 839   | 0        | 858      | 10      | 0            |
| 1   | GU    | 839   | 0        | 858      | 15      | 0            |
| 1   | GV    | 839   | 0        | 858      | 13      | 0            |
| 1   | GW    | 839   | 0        | 858      | 11      | 0            |
| 1   | GX    | 839   | 0        | 858      | 19      | 0            |
| 1   | GY    | 839   | 0        | 858      | 12      | 0            |
| 1   | GZ    | 839   | 0        | 858      | 9       | 0            |
| 1   | HA    | 839   | 0        | 858      | 21      | 0            |
| 1   | HB    | 839   | 0        | 858      | 9       | 0            |
| 1   | HC    | 839   | 0        | 858      | 9       | 0            |
| 1   | HD    | 839   | 0        | 858      | 11      | 0            |
| 1   | HE    | 839   | 0        | 858      | 18      | 0            |
| 1   | HF    | 839   | 0        | 858      | 10      | 0            |
| 1   | HG    | 839   | 0        | 858      | 8       | 0            |
| 1   | HH    | 839   | 0        | 858      | 12      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | HI    | 839   | 0        | 858      | 25      | 0            |
| 1   | HJ    | 839   | 0        | 858      | 11      | 0            |
| 1   | HK    | 839   | 0        | 858      | 12      | 0            |
| 1   | HL    | 839   | 0        | 858      | 10      | 0            |
| 1   | HM    | 839   | 0        | 858      | 20      | 0            |
| 1   | HN    | 839   | 0        | 858      | 12      | 0            |
| 1   | HO    | 839   | 0        | 858      | 16      | 0            |
| 1   | HP    | 839   | 0        | 858      | 12      | 0            |
| 1   | HQ    | 839   | 0        | 858      | 8       | 0            |
| 1   | HR    | 839   | 0        | 858      | 8       | 1            |
| 1   | HS    | 839   | 0        | 858      | 11      | 0            |
| 1   | HT    | 839   | 0        | 858      | 9       | 0            |
| 1   | HU    | 839   | 0        | 858      | 8       | 0            |
| 1   | HV    | 839   | 0        | 858      | 11      | 0            |
| 1   | HW    | 839   | 0        | 858      | 10      | 0            |
| 1   | HX    | 839   | 0        | 858      | 10      | 0            |
| 1   | HY    | 839   | 0        | 858      | 10      | 0            |
| 1   | HZ    | 839   | 0        | 858      | 10      | 0            |
| 1   | IA    | 839   | 0        | 858      | 7       | 0            |
| 1   | IB    | 839   | 0        | 858      | 17      | 0            |
| 1   | IC    | 839   | 0        | 858      | 22      | 0            |
| 1   | ID    | 839   | 0        | 858      | 19      | 0            |
| 1   | IE    | 839   | 0        | 858      | 16      | 0            |
| 1   | IF    | 839   | 0        | 858      | 8       | 0            |
| 1   | IG    | 839   | 0        | 858      | 10      | 0            |
| 1   | IH    | 839   | 0        | 858      | 16      | 0            |
| 1   | II    | 839   | 0        | 858      | 12      | 0            |
| 1   | IJ    | 839   | 0        | 858      | 21      | 0            |
| 1   | IK    | 839   | 0        | 858      | 12      | 0            |
| 1   | IL    | 839   | 0        | 858      | 9       | 0            |
| 1   | IM    | 839   | 0        | 858      | 7       | 0            |
| 1   | IN    | 839   | 0        | 858      | 13      | 0            |
| 1   | IO    | 839   | 0        | 858      | 9       | 0            |
| 1   | IP    | 839   | 0        | 858      | 9       | 0            |
| 1   | IQ    | 839   | 0        | 858      | 15      | 0            |
| 1   | IR    | 839   | 0        | 858      | 13      | 0            |
| 1   | IS    | 839   | 0        | 858      | 11      | 0            |
| 1   | IT    | 839   | 0        | 858      | 14      | 0            |
| 1   | IU    | 839   | 0        | 858      | 9       | 0            |
| 1   | IV    | 839   | 0        | 858      | 11      | 0            |
| 1   | IW    | 839   | 0        | 858      | 11      | 0            |
| 1   | IX    | 839   | 0        | 858      | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | IY    | 839   | 0        | 858      | 12      | 0            |
| 1   | IZ    | 839   | 0        | 858      | 13      | 0            |
| 1   | JA    | 839   | 0        | 858      | 13      | 0            |
| 1   | JB    | 839   | 0        | 858      | 7       | 0            |
| 1   | JC    | 839   | 0        | 858      | 15      | 0            |
| 1   | JD    | 839   | 0        | 858      | 10      | 0            |
| 1   | JE    | 839   | 0        | 858      | 17      | 0            |
| 1   | JF    | 839   | 0        | 858      | 15      | 0            |
| 1   | JG    | 839   | 0        | 858      | 9       | 0            |
| 1   | JH    | 839   | 0        | 858      | 11      | 0            |
| 1   | JI    | 839   | 0        | 858      | 16      | 0            |
| 1   | JJ    | 839   | 0        | 858      | 17      | 0            |
| 1   | JK    | 839   | 0        | 858      | 11      | 0            |
| 1   | JL    | 839   | 0        | 858      | 12      | 0            |
| 1   | JM    | 839   | 0        | 858      | 12      | 0            |
| 1   | JN    | 839   | 0        | 858      | 17      | 0            |
| 1   | JO    | 839   | 0        | 858      | 16      | 0            |
| 1   | JP    | 839   | 0        | 858      | 9       | 0            |
| 1   | JQ    | 839   | 0        | 858      | 10      | 0            |
| 1   | JR    | 839   | 0        | 858      | 11      | 0            |
| 1   | JS    | 839   | 0        | 858      | 13      | 0            |
| 1   | JT    | 839   | 0        | 858      | 9       | 0            |
| 1   | JU    | 839   | 0        | 858      | 11      | 0            |
| 1   | JV    | 839   | 0        | 858      | 9       | 0            |
| 1   | JW    | 839   | 0        | 858      | 7       | 0            |
| 1   | JX    | 839   | 0        | 858      | 11      | 0            |
| 1   | JY    | 839   | 0        | 858      | 11      | 0            |
| 1   | JZ    | 839   | 0        | 858      | 7       | 0            |
| 1   | KA    | 839   | 0        | 858      | 11      | 0            |
| 1   | KB    | 839   | 0        | 858      | 11      | 0            |
| 1   | KC    | 839   | 0        | 858      | 9       | 0            |
| 1   | KD    | 839   | 0        | 858      | 13      | 0            |
| 1   | KE    | 839   | 0        | 858      | 12      | 0            |
| 1   | KF    | 839   | 0        | 858      | 12      | 0            |
| 1   | KG    | 839   | 0        | 858      | 11      | 0            |
| 1   | KH    | 839   | 0        | 858      | 17      | 0            |
| 1   | KI    | 839   | 0        | 858      | 8       | 1            |
| 1   | KJ    | 839   | 0        | 858      | 16      | 0            |
| 1   | KK    | 839   | 0        | 858      | 11      | 0            |
| 1   | KL    | 839   | 0        | 858      | 10      | 0            |
| 1   | KM    | 839   | 0        | 858      | 23      | 0            |
| 1   | KN    | 839   | 0        | 858      | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | KO    | 839   | 0        | 858      | 8       | 0            |
| 1   | KP    | 839   | 0        | 858      | 9       | 0            |
| 1   | KQ    | 839   | 0        | 858      | 13      | 0            |
| 1   | KR    | 839   | 0        | 858      | 11      | 0            |
| 1   | KS    | 839   | 0        | 858      | 9       | 0            |
| 1   | KT    | 839   | 0        | 858      | 11      | 0            |
| 1   | KU    | 839   | 0        | 858      | 11      | 0            |
| 1   | KV    | 839   | 0        | 858      | 13      | 0            |
| 1   | KW    | 839   | 0        | 858      | 15      | 0            |
| 1   | KX    | 839   | 0        | 858      | 8       | 0            |
| 1   | KY    | 839   | 0        | 858      | 19      | 0            |
| 1   | KZ    | 839   | 0        | 858      | 12      | 0            |
| 1   | LA    | 839   | 0        | 858      | 8       | 0            |
| 1   | LB    | 839   | 0        | 858      | 12      | 0            |
| 1   | LC    | 839   | 0        | 858      | 14      | 0            |
| 1   | LD    | 839   | 0        | 858      | 8       | 0            |
| 1   | LE    | 839   | 0        | 858      | 11      | 0            |
| 1   | LF    | 839   | 0        | 858      | 13      | 0            |
| 1   | LG    | 839   | 0        | 858      | 9       | 0            |
| 1   | LH    | 839   | 0        | 858      | 10      | 0            |
| 1   | LI    | 839   | 0        | 858      | 10      | 0            |
| 1   | LJ    | 839   | 0        | 858      | 7       | 0            |
| 1   | LK    | 839   | 0        | 858      | 7       | 0            |
| 1   | LL    | 839   | 0        | 858      | 10      | 0            |
| 1   | LM    | 839   | 0        | 858      | 12      | 0            |
| 1   | LN    | 839   | 0        | 858      | 14      | 0            |
| 1   | LO    | 839   | 0        | 858      | 11      | 0            |
| 1   | LP    | 839   | 0        | 858      | 8       | 0            |
| 1   | LQ    | 839   | 0        | 858      | 17      | 0            |
| 1   | LR    | 839   | 0        | 858      | 17      | 0            |
| 1   | LS    | 839   | 0        | 858      | 14      | 0            |
| 1   | LT    | 839   | 0        | 858      | 16      | 0            |
| 1   | LU    | 839   | 0        | 858      | 11      | 0            |
| 1   | LV    | 839   | 0        | 858      | 7       | 0            |
| 1   | LW    | 839   | 0        | 858      | 12      | 0            |
| 1   | LX    | 839   | 0        | 858      | 10      | 0            |
| 1   | LY    | 839   | 0        | 858      | 12      | 0            |
| 1   | LZ    | 839   | 0        | 858      | 10      | 0            |
| 1   | MA    | 839   | 0        | 858      | 9       | 0            |
| 1   | MB    | 839   | 0        | 858      | 8       | 0            |
| 1   | MC    | 839   | 0        | 858      | 17      | 0            |
| 1   | MD    | 839   | 0        | 858      | 11      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | ME    | 839   | 0        | 858      | 16      | 1            |
| 1   | MF    | 839   | 0        | 858      | 13      | 0            |
| 1   | MG    | 839   | 0        | 858      | 10      | 0            |
| 1   | MH    | 839   | 0        | 858      | 8       | 0            |
| 1   | MI    | 839   | 0        | 858      | 10      | 0            |
| 1   | MJ    | 839   | 0        | 858      | 13      | 0            |
| 1   | MK    | 839   | 0        | 858      | 10      | 0            |
| 1   | ML    | 839   | 0        | 858      | 14      | 0            |
| 1   | MM    | 839   | 0        | 858      | 32      | 0            |
| 1   | MN    | 839   | 0        | 858      | 17      | 0            |
| 1   | MO    | 839   | 0        | 858      | 15      | 0            |
| 1   | MP    | 839   | 0        | 858      | 11      | 0            |
| 1   | MQ    | 839   | 0        | 858      | 11      | 0            |
| 1   | MR    | 839   | 0        | 858      | 20      | 0            |
| 1   | MS    | 839   | 0        | 858      | 17      | 0            |
| 1   | MT    | 839   | 0        | 858      | 11      | 0            |
| 1   | MU    | 839   | 0        | 858      | 14      | 0            |
| 1   | MV    | 839   | 0        | 858      | 11      | 0            |
| 1   | MW    | 839   | 0        | 858      | 13      | 0            |
| 1   | MX    | 839   | 0        | 858      | 9       | 0            |
| 1   | MY    | 839   | 0        | 858      | 11      | 0            |
| 1   | MZ    | 839   | 0        | 858      | 9       | 0            |
| 1   | NA    | 839   | 0        | 858      | 15      | 0            |
| 1   | NB    | 839   | 0        | 858      | 9       | 0            |
| 1   | NC    | 839   | 0        | 858      | 9       | 0            |
| 1   | ND    | 839   | 0        | 858      | 9       | 0            |
| 1   | NE    | 839   | 0        | 858      | 9       | 0            |
| 1   | NF    | 839   | 0        | 858      | 7       | 0            |
| 1   | NG    | 839   | 0        | 858      | 10      | 0            |
| 1   | NH    | 839   | 0        | 858      | 9       | 0            |
| 1   | NI    | 839   | 0        | 858      | 12      | 0            |
| 1   | NJ    | 839   | 0        | 858      | 9       | 0            |
| 1   | NK    | 839   | 0        | 858      | 10      | 0            |
| 1   | NL    | 839   | 0        | 858      | 9       | 2            |
| 1   | NM    | 839   | 0        | 858      | 10      | 0            |
| 1   | NN    | 839   | 0        | 858      | 12      | 0            |
| 1   | NO    | 839   | 0        | 858      | 12      | 0            |
| 1   | NP    | 839   | 0        | 858      | 10      | 0            |
| 1   | NQ    | 839   | 0        | 858      | 12      | 0            |
| 1   | NR    | 839   | 0        | 858      | 10      | 0            |
| 1   | NS    | 839   | 0        | 858      | 8       | 0            |
| 1   | NT    | 839   | 0        | 858      | 16      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | NU    | 839   | 0        | 858      | 12      | 0            |
| 1   | NV    | 839   | 0        | 858      | 17      | 0            |
| 2   | RA    | 420   | 0        | 212      | 7       | 0            |
| 2   | RB    | 420   | 0        | 212      | 6       | 0            |
| 2   | RC    | 420   | 0        | 212      | 3       | 0            |
| 2   | RD    | 420   | 0        | 212      | 3       | 0            |
| 2   | RE    | 420   | 0        | 212      | 3       | 0            |
| 2   | RF    | 420   | 0        | 212      | 5       | 0            |
| 2   | RG    | 420   | 0        | 212      | 6       | 0            |
| 2   | RH    | 420   | 0        | 212      | 3       | 0            |
| 2   | RI    | 420   | 0        | 212      | 8       | 0            |
| 2   | RJ    | 420   | 0        | 212      | 6       | 0            |
| 2   | RK    | 420   | 0        | 212      | 7       | 0            |
| 2   | RL    | 420   | 0        | 212      | 5       | 0            |
| 2   | RM    | 420   | 0        | 212      | 3       | 0            |
| 2   | RN    | 420   | 0        | 212      | 4       | 0            |
| 2   | RO    | 420   | 0        | 212      | 6       | 0            |
| 2   | RP    | 420   | 0        | 212      | 3       | 0            |
| 2   | RQ    | 420   | 0        | 212      | 3       | 0            |
| 2   | RR    | 420   | 0        | 212      | 4       | 0            |
| 2   | RS    | 420   | 0        | 212      | 4       | 0            |
| 2   | RT    | 420   | 0        | 212      | 4       | 0            |
| 2   | RU    | 420   | 0        | 212      | 4       | 0            |
| 2   | RV    | 420   | 0        | 212      | 7       | 0            |
| 2   | RW    | 420   | 0        | 212      | 5       | 0            |
| 2   | RX    | 420   | 0        | 212      | 3       | 0            |
| 2   | RY    | 420   | 0        | 212      | 6       | 0            |
| 2   | RZ    | 420   | 0        | 212      | 7       | 0            |
| 2   | SA    | 420   | 0        | 212      | 3       | 0            |
| 2   | SB    | 420   | 0        | 212      | 7       | 0            |
| 2   | SC    | 420   | 0        | 212      | 6       | 0            |
| 2   | SD    | 420   | 0        | 212      | 6       | 0            |
| 2   | SE    | 420   | 0        | 212      | 7       | 0            |
| 2   | SF    | 420   | 0        | 212      | 5       | 0            |
| 2   | SG    | 420   | 0        | 212      | 7       | 0            |
| 2   | SH    | 420   | 0        | 212      | 7       | 0            |
| 2   | SI    | 420   | 0        | 212      | 6       | 0            |
| 2   | SJ    | 420   | 0        | 212      | 6       | 0            |
| 2   | SK    | 420   | 0        | 212      | 7       | 0            |
| 2   | SL    | 420   | 0        | 212      | 5       | 0            |
| 2   | SM    | 420   | 0        | 212      | 3       | 0            |
| 2   | SN    | 420   | 0        | 212      | 4       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 2   | SO    | 420    | 0        | 212      | 6       | 0            |
| 2   | SP    | 420    | 0        | 212      | 6       | 0            |
| 2   | SQ    | 420    | 0        | 212      | 5       | 0            |
| 2   | SR    | 420    | 0        | 212      | 3       | 0            |
| 2   | SS    | 420    | 0        | 212      | 6       | 0            |
| 2   | ST    | 420    | 0        | 212      | 4       | 0            |
| 2   | SU    | 420    | 0        | 212      | 4       | 0            |
| 2   | SV    | 420    | 0        | 212      | 5       | 0            |
| 2   | SW    | 420    | 0        | 212      | 7       | 0            |
| 2   | SX    | 420    | 0        | 212      | 10      | 0            |
| 2   | SY    | 420    | 0        | 212      | 5       | 0            |
| 2   | SZ    | 420    | 0        | 212      | 3       | 0            |
| 2   | TA    | 420    | 0        | 212      | 4       | 0            |
| 2   | TB    | 420    | 0        | 212      | 4       | 0            |
| 2   | TC    | 420    | 0        | 212      | 4       | 0            |
| 2   | TD    | 420    | 0        | 212      | 4       | 0            |
| 2   | TE    | 420    | 0        | 212      | 6       | 0            |
| 2   | TF    | 420    | 0        | 212      | 4       | 0            |
| 2   | TG    | 420    | 0        | 212      | 4       | 0            |
| 2   | TH    | 420    | 0        | 212      | 7       | 0            |
| All | All   | 327240 | 0        | 321600   | 2967    | 5            |

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 5.

The worst 5 of 2967 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:EC:98:THR:HG23 | 1:MM:98:THR:HG23 | 1.36                     | 1.05              |
| 1:EC:98:THR:CG2  | 1:MM:98:THR:HG23 | 1.95                     | 0.96              |
| 1:CX:40:GLY:HA2  | 1:DK:109:LEU:O   | 1.71                     | 0.90              |
| 1:EC:98:THR:HG23 | 1:MM:98:THR:CG2  | 2.06                     | 0.83              |
| 1:HE:40:GLY:HA2  | 1:ID:109:LEU:O   | 1.78                     | 0.83              |

All (5) 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:HR:10:SER:OG   | 1:KI:24:SER:CB[1_655] | 1.58                     | 0.62              |
| 1:AZ:101:ASP:OD2 | 1:NL:10:SER:N[1_545]  | 2.02                     | 0.18              |

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| Atom-1           | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 1:AZ:101:ASP:OD2 | 1:NL:10:SER:OG[1_545]   | 2.11                     | 0.09              |
| 1:EU:10:SER:OG   | 1:GK:24:SER:CB[1_655]   | 2.13                     | 0.07              |
| 1:FS:9:GLY:O     | 1:ME:104:ARG:NH2[1_446] | 2.13                     | 0.07              |

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | AA    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AB    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AC    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | AD    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AE    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AF    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | AG    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AH    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AI    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | AJ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AK    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AL    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | AM    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AN    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AO    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | AP    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AQ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AR    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | AS    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | AT    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AU    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | AV    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AW    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AX    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | AY    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | AZ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BA    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | BB    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BC    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BD    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | BE    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BF    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BG    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | BH    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BI    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BJ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | BK    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BL    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BM    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | BN    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BO    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BP    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | BQ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BR    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BS    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | BT    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BU    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BV    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | BW    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | BX    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | BY    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | BZ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CA    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CB    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | CC    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CD    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CE    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | CF    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CG    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CH    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | CI    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CJ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CK    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | CL    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CM    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CN    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | CO    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CP    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CQ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | CR    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CS    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CT    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | CU    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CV    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CW    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | CX    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CY    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | CZ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | DA    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DB    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DC    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | DD    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DE    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DF    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | DG    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DH    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DI    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | DJ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DK    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DL    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | DM    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DN    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DO    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | DP    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DQ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DR    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | DS    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DT    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DU    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | DV    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DW    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DX    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | DY    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | DZ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EA    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | EB    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EC    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | ED    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | EE    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EF    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EG    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | EH    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | EI    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EJ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | EK    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EL    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EM    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | EN    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EO    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EP    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | EQ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | ER    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | ES    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | ET    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EU    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EV    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | EW    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EX    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | EY    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | EZ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FA    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FB    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | FC    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FD    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FE    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | FF    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FG    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FH    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | FI    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FJ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FK    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | FL    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FM    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | FN    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | FO    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FP    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FQ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | FR    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FS    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FT    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | FU    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FV    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FW    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | FX    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FY    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | FZ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | GA    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GB    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GC    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | GD    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GE    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GF    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | GG    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GH    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GI    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | GJ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GK    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GL    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | GM    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GN    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GO    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | GP    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GQ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GR    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | GS    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GT    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GU    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | GV    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GW    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GX    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | GY    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | GZ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HA    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | HB    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HC    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HD    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | HE    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HF    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HG    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | HH    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HI    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HJ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | HK    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HL    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HM    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | HN    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HO    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HP    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | HQ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HR    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HS    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | HT    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HU    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HV    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | HW    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | HX    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | HY    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | HZ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IA    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IB    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | IC    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | ID    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IE    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | IF    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IG    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IH    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | II    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IJ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IK    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | IL    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IM    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IN    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | IO    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IP    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IQ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | IR    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IS    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IT    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | IU    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IV    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IW    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | IX    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IY    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | IZ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | JA    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JB    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | JC    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | JD    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JE    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JF    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | JG    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JH    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JI    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | JJ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JK    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JL    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | JM    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JN    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JO    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | JP    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JQ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JR    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | JS    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JT    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JU    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | JV    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JW    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JX    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | JY    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | JZ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KA    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | KB    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KC    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KD    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | KE    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KF    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KG    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | KH    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KI    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KJ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | KK    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KL    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KM    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | KN    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KO    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KP    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | KQ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KR    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KS    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | KT    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KU    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KV    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | KW    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KX    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | KY    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | KZ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LA    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LB    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | LC    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LD    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LE    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | LF    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LG    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LH    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | LI    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LJ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LK    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | LL    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | LM    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LN    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | LO    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LP    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LQ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | LR    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LS    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LT    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | LU    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LV    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LW    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | LX    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LY    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | LZ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | MA    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MB    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MC    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | MD    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | ME    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MF    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | MG    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MH    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MI    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | MJ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MK    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | ML    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | MM    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MN    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MO    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | MP    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MQ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | MR    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | MS    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MT    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MU    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | MV    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MW    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MX    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | MY    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | MZ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NA    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | NB    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NC    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | ND    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | NE    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NF    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NG    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | NH    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NI    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NJ    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | NK    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NL    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NM    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | NN    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NO    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NP    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | NQ    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NR    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NS    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 1   | NT    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NU    | 111/113 (98%) | 109 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 1   | NV    | 111/113 (98%) | 110 (99%) | 1 (1%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| All | All   | 39960/40680 (98%) | 39360 (98%) | 600 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | AA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | AV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | AZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | BZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | CA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | CZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | DF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | DZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | ED    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | EK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | ER    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | ES    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | ET    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | EZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | FP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | FZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | GU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | GZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | HY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | HZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | ID    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | II    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | IZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | JE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | JZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | KJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | KZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LE    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LL    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |     |
|-----|-------|--------------|-----------|----------|-------------|-----|
| 1   | LO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LT    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LU    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LV    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LW    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LX    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LY    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | LZ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MA    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MB    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MC    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MD    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | ME    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MF    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MG    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MH    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MI    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MJ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MK    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | ML    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MM    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MN    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MO    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MP    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MQ    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MR    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |
| 1   | MS    | 91/91 (100%) | 91 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed           | Rotameric    | Outliers | Percentiles |     |
|-----|-------|--------------------|--------------|----------|-------------|-----|
| 1   | MT    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | MU    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | MV    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | MW    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | MX    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | MY    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | MZ    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NA    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NB    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NC    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | ND    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NE    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NF    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NG    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NH    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NI    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NJ    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NK    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NL    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NM    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NN    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NO    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NP    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NQ    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NR    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NS    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NT    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NU    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| 1   | NV    | 91/91 (100%)       | 91 (100%)    | 0        | 100         | 100 |
| All | All   | 32760/32760 (100%) | 32760 (100%) | 0        | 100         | 100 |

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 346 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | JN    | 97  | ASN  |
| 1   | LU    | 107 | GLN  |
| 1   | JV    | 97  | ASN  |
| 1   | KT    | 97  | ASN  |
| 1   | MI    | 97  | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2   | RA    | 18/30 (60%) | 0                 | 0               |
| 2   | RB    | 18/30 (60%) | 0                 | 0               |
| 2   | RC    | 18/30 (60%) | 0                 | 0               |
| 2   | RD    | 18/30 (60%) | 0                 | 0               |
| 2   | RE    | 18/30 (60%) | 0                 | 0               |
| 2   | RF    | 18/30 (60%) | 0                 | 0               |
| 2   | RG    | 18/30 (60%) | 0                 | 0               |
| 2   | RH    | 18/30 (60%) | 0                 | 0               |
| 2   | RI    | 18/30 (60%) | 0                 | 0               |
| 2   | RJ    | 18/30 (60%) | 0                 | 0               |
| 2   | RK    | 18/30 (60%) | 0                 | 0               |
| 2   | RL    | 18/30 (60%) | 0                 | 0               |
| 2   | RM    | 18/30 (60%) | 0                 | 0               |
| 2   | RN    | 18/30 (60%) | 0                 | 0               |
| 2   | RO    | 18/30 (60%) | 0                 | 0               |
| 2   | RP    | 18/30 (60%) | 0                 | 0               |
| 2   | RQ    | 18/30 (60%) | 0                 | 0               |
| 2   | RR    | 18/30 (60%) | 0                 | 0               |
| 2   | RS    | 18/30 (60%) | 0                 | 0               |
| 2   | RT    | 18/30 (60%) | 0                 | 0               |
| 2   | RU    | 18/30 (60%) | 0                 | 0               |
| 2   | RV    | 18/30 (60%) | 0                 | 0               |
| 2   | RW    | 18/30 (60%) | 0                 | 0               |
| 2   | RX    | 18/30 (60%) | 0                 | 0               |
| 2   | RY    | 18/30 (60%) | 0                 | 0               |
| 2   | RZ    | 18/30 (60%) | 0                 | 0               |
| 2   | SA    | 18/30 (60%) | 0                 | 0               |
| 2   | SB    | 18/30 (60%) | 0                 | 0               |
| 2   | SC    | 18/30 (60%) | 0                 | 0               |
| 2   | SD    | 18/30 (60%) | 0                 | 0               |
| 2   | SE    | 18/30 (60%) | 0                 | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 2   | SF    | 18/30 (60%)     | 0                 | 0               |
| 2   | SG    | 18/30 (60%)     | 0                 | 0               |
| 2   | SH    | 18/30 (60%)     | 0                 | 0               |
| 2   | SI    | 18/30 (60%)     | 0                 | 0               |
| 2   | SJ    | 18/30 (60%)     | 0                 | 0               |
| 2   | SK    | 18/30 (60%)     | 0                 | 0               |
| 2   | SL    | 18/30 (60%)     | 0                 | 0               |
| 2   | SM    | 18/30 (60%)     | 0                 | 0               |
| 2   | SN    | 18/30 (60%)     | 0                 | 0               |
| 2   | SO    | 18/30 (60%)     | 0                 | 0               |
| 2   | SP    | 18/30 (60%)     | 0                 | 0               |
| 2   | SQ    | 18/30 (60%)     | 0                 | 0               |
| 2   | SR    | 18/30 (60%)     | 0                 | 0               |
| 2   | SS    | 18/30 (60%)     | 0                 | 0               |
| 2   | ST    | 18/30 (60%)     | 0                 | 0               |
| 2   | SU    | 18/30 (60%)     | 0                 | 0               |
| 2   | SV    | 18/30 (60%)     | 0                 | 0               |
| 2   | SW    | 18/30 (60%)     | 0                 | 0               |
| 2   | SX    | 18/30 (60%)     | 0                 | 0               |
| 2   | SY    | 18/30 (60%)     | 0                 | 0               |
| 2   | SZ    | 18/30 (60%)     | 0                 | 0               |
| 2   | TA    | 18/30 (60%)     | 0                 | 0               |
| 2   | TB    | 18/30 (60%)     | 0                 | 0               |
| 2   | TC    | 18/30 (60%)     | 0                 | 0               |
| 2   | TD    | 18/30 (60%)     | 0                 | 0               |
| 2   | TE    | 18/30 (60%)     | 0                 | 0               |
| 2   | TF    | 18/30 (60%)     | 0                 | 0               |
| 2   | TG    | 18/30 (60%)     | 0                 | 0               |
| 2   | TH    | 18/30 (60%)     | 0                 | 0               |
| All | All   | 1080/1800 (60%) | 0                 | 0               |

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no 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    | 113/113 (100%) | 0.45   | 7 (6%)   | 26 | 16 | 51, 87, 163, 193      | 0     |
| 1   | AB    | 113/113 (100%) | 0.31   | 2 (1%)   | 67 | 42 | 49, 83, 126, 154      | 0     |
| 1   | AC    | 113/113 (100%) | 0.42   | 5 (4%)   | 39 | 21 | 54, 96, 147, 177      | 0     |
| 1   | AD    | 113/113 (100%) | 0.52   | 6 (5%)   | 32 | 18 | 51, 87, 163, 193      | 0     |
| 1   | AE    | 113/113 (100%) | 0.46   | 6 (5%)   | 32 | 18 | 49, 83, 126, 154      | 0     |
| 1   | AF    | 113/113 (100%) | 0.56   | 4 (3%)   | 47 | 26 | 54, 96, 147, 177      | 0     |
| 1   | AG    | 113/113 (100%) | 0.40   | 3 (2%)   | 56 | 33 | 51, 87, 163, 193      | 0     |
| 1   | AH    | 113/113 (100%) | 0.55   | 6 (5%)   | 32 | 18 | 49, 83, 126, 154      | 0     |
| 1   | AI    | 113/113 (100%) | 0.69   | 15 (13%) | 7  | 6  | 54, 96, 147, 177      | 0     |
| 1   | AJ    | 113/113 (100%) | 0.49   | 10 (8%)  | 15 | 10 | 51, 87, 163, 193      | 0     |
| 1   | AK    | 113/113 (100%) | 0.28   | 3 (2%)   | 56 | 33 | 49, 83, 126, 154      | 0     |
| 1   | AL    | 113/113 (100%) | 0.67   | 10 (8%)  | 15 | 10 | 54, 96, 147, 177      | 0     |
| 1   | AM    | 113/113 (100%) | 0.34   | 4 (3%)   | 47 | 26 | 51, 87, 163, 193      | 0     |
| 1   | AN    | 113/113 (100%) | 0.48   | 1 (0%)   | 81 | 58 | 49, 83, 126, 154      | 0     |
| 1   | AO    | 113/113 (100%) | 0.40   | 5 (4%)   | 39 | 21 | 54, 96, 147, 177      | 0     |
| 1   | AP    | 113/113 (100%) | 0.78   | 12 (10%) | 11 | 8  | 51, 87, 163, 193      | 0     |
| 1   | AQ    | 113/113 (100%) | 0.55   | 5 (4%)   | 39 | 21 | 49, 83, 126, 154      | 0     |
| 1   | AR    | 113/113 (100%) | 0.71   | 9 (7%)   | 18 | 12 | 54, 96, 147, 177      | 0     |
| 1   | AS    | 113/113 (100%) | 0.48   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | AT    | 113/113 (100%) | 0.33   | 3 (2%)   | 56 | 33 | 49, 83, 126, 154      | 0     |
| 1   | AU    | 113/113 (100%) | 0.53   | 4 (3%)   | 47 | 26 | 54, 96, 147, 177      | 0     |
| 1   | AV    | 113/113 (100%) | 0.48   | 6 (5%)   | 32 | 18 | 51, 87, 163, 193      | 0     |
| 1   | AW    | 113/113 (100%) | 0.44   | 5 (4%)   | 39 | 21 | 49, 83, 126, 154      | 0     |
| 1   | AX    | 113/113 (100%) | 0.63   | 8 (7%)   | 22 | 14 | 54, 96, 147, 177      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | AY    | 113/113 (100%) | 0.35   | 3 (2%) 56 33  | 51, 87, 163, 193      | 0     |
| 1   | AZ    | 113/113 (100%) | 0.71   | 6 (5%) 32 18  | 49, 83, 126, 154      | 0     |
| 1   | BA    | 113/113 (100%) | 0.65   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | BB    | 113/113 (100%) | 0.72   | 8 (7%) 22 14  | 51, 87, 163, 193      | 0     |
| 1   | BC    | 113/113 (100%) | 0.31   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | BD    | 113/113 (100%) | 0.55   | 7 (6%) 26 16  | 54, 96, 147, 177      | 0     |
| 1   | BE    | 113/113 (100%) | 0.50   | 7 (6%) 26 16  | 51, 87, 163, 193      | 0     |
| 1   | BF    | 113/113 (100%) | 0.47   | 6 (5%) 32 18  | 49, 83, 126, 154      | 0     |
| 1   | BG    | 113/113 (100%) | 0.68   | 11 (9%) 13 9  | 54, 96, 147, 177      | 0     |
| 1   | BH    | 113/113 (100%) | 0.36   | 4 (3%) 47 26  | 51, 87, 163, 193      | 0     |
| 1   | BI    | 113/113 (100%) | 0.47   | 6 (5%) 32 18  | 49, 83, 126, 154      | 0     |
| 1   | BJ    | 113/113 (100%) | 0.57   | 4 (3%) 47 26  | 54, 96, 147, 177      | 0     |
| 1   | BK    | 113/113 (100%) | 0.42   | 3 (2%) 56 33  | 51, 87, 163, 193      | 0     |
| 1   | BL    | 113/113 (100%) | 0.45   | 7 (6%) 26 16  | 49, 83, 126, 154      | 0     |
| 1   | BM    | 113/113 (100%) | 0.66   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | BN    | 113/113 (100%) | 0.54   | 6 (5%) 32 18  | 51, 87, 163, 193      | 0     |
| 1   | BO    | 113/113 (100%) | 0.42   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | BP    | 113/113 (100%) | 0.54   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | BQ    | 113/113 (100%) | 1.14   | 16 (14%) 6 5  | 51, 87, 163, 193      | 0     |
| 1   | BR    | 113/113 (100%) | 0.77   | 12 (10%) 11 8 | 49, 83, 126, 154      | 0     |
| 1   | BS    | 113/113 (100%) | 0.82   | 10 (8%) 15 10 | 54, 96, 147, 177      | 0     |
| 1   | BT    | 113/113 (100%) | 0.51   | 9 (7%) 18 12  | 51, 87, 163, 193      | 0     |
| 1   | BU    | 113/113 (100%) | 0.56   | 7 (6%) 26 16  | 49, 83, 126, 154      | 0     |
| 1   | BV    | 113/113 (100%) | 0.80   | 11 (9%) 13 9  | 54, 96, 147, 177      | 0     |
| 1   | BW    | 113/113 (100%) | 0.35   | 4 (3%) 47 26  | 51, 87, 163, 193      | 0     |
| 1   | BX    | 113/113 (100%) | 0.40   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | BY    | 113/113 (100%) | 0.64   | 10 (8%) 15 10 | 54, 96, 147, 177      | 0     |
| 1   | BZ    | 113/113 (100%) | 0.33   | 3 (2%) 56 33  | 51, 87, 163, 193      | 0     |
| 1   | CA    | 113/113 (100%) | 0.42   | 8 (7%) 22 14  | 49, 83, 126, 154      | 0     |
| 1   | CB    | 113/113 (100%) | 0.45   | 5 (4%) 39 21  | 54, 96, 147, 177      | 0     |
| 1   | CC    | 113/113 (100%) | 0.56   | 10 (8%) 15 10 | 51, 87, 163, 193      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | CD    | 113/113 (100%) | 0.54   | 6 (5%) 32 18  | 49, 83, 126, 154      | 0     |
| 1   | CE    | 113/113 (100%) | 0.68   | 15 (13%) 7 6  | 54, 96, 147, 177      | 0     |
| 1   | CF    | 113/113 (100%) | 0.51   | 6 (5%) 32 18  | 51, 87, 163, 193      | 0     |
| 1   | CG    | 113/113 (100%) | 0.63   | 6 (5%) 32 18  | 49, 83, 126, 154      | 0     |
| 1   | CH    | 113/113 (100%) | 0.65   | 12 (10%) 11 8 | 54, 96, 147, 177      | 0     |
| 1   | CI    | 113/113 (100%) | 0.46   | 4 (3%) 47 26  | 51, 87, 163, 193      | 0     |
| 1   | CJ    | 113/113 (100%) | 0.55   | 6 (5%) 32 18  | 49, 83, 126, 154      | 0     |
| 1   | CK    | 113/113 (100%) | 0.60   | 4 (3%) 47 26  | 54, 96, 147, 177      | 0     |
| 1   | CL    | 113/113 (100%) | 0.49   | 6 (5%) 32 18  | 51, 87, 163, 193      | 0     |
| 1   | CM    | 113/113 (100%) | 0.51   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | CN    | 113/113 (100%) | 0.66   | 11 (9%) 13 9  | 54, 96, 147, 177      | 0     |
| 1   | CO    | 113/113 (100%) | 0.49   | 5 (4%) 39 21  | 51, 87, 163, 193      | 0     |
| 1   | CP    | 113/113 (100%) | 0.93   | 14 (12%) 8 6  | 49, 83, 126, 154      | 0     |
| 1   | CQ    | 113/113 (100%) | 0.76   | 5 (4%) 39 21  | 54, 96, 147, 177      | 0     |
| 1   | CR    | 113/113 (100%) | 0.63   | 9 (7%) 18 12  | 51, 87, 163, 193      | 0     |
| 1   | CS    | 113/113 (100%) | 0.54   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | CT    | 113/113 (100%) | 0.64   | 7 (6%) 26 16  | 54, 96, 147, 177      | 0     |
| 1   | CU    | 113/113 (100%) | 0.65   | 7 (6%) 26 16  | 51, 87, 163, 193      | 0     |
| 1   | CV    | 113/113 (100%) | 0.53   | 7 (6%) 26 16  | 49, 83, 126, 154      | 0     |
| 1   | CW    | 113/113 (100%) | 0.55   | 5 (4%) 39 21  | 54, 96, 147, 177      | 0     |
| 1   | CX    | 113/113 (100%) | 0.70   | 13 (11%) 9 6  | 51, 87, 163, 193      | 0     |
| 1   | CY    | 113/113 (100%) | 0.51   | 7 (6%) 26 16  | 49, 83, 126, 154      | 0     |
| 1   | CZ    | 113/113 (100%) | 0.73   | 13 (11%) 9 6  | 54, 96, 147, 177      | 0     |
| 1   | DA    | 113/113 (100%) | 0.36   | 5 (4%) 39 21  | 51, 87, 163, 193      | 0     |
| 1   | DB    | 113/113 (100%) | 0.39   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | DC    | 113/113 (100%) | 0.65   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | DD    | 113/113 (100%) | 0.47   | 6 (5%) 32 18  | 51, 87, 163, 193      | 0     |
| 1   | DE    | 113/113 (100%) | 0.40   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | DF    | 113/113 (100%) | 0.80   | 9 (7%) 18 12  | 54, 96, 147, 177      | 0     |
| 1   | DG    | 113/113 (100%) | 0.41   | 3 (2%) 56 33  | 51, 87, 163, 193      | 0     |
| 1   | DH    | 113/113 (100%) | 0.49   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | DI    | 113/113 (100%) | 0.67   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | DJ    | 113/113 (100%) | 1.13   | 19 (16%) 4 4  | 51, 87, 163, 193      | 0     |
| 1   | DK    | 113/113 (100%) | 0.80   | 7 (6%) 26 16  | 49, 83, 126, 154      | 0     |
| 1   | DL    | 113/113 (100%) | 0.62   | 4 (3%) 47 26  | 54, 96, 147, 177      | 0     |
| 1   | DM    | 113/113 (100%) | 0.42   | 5 (4%) 39 21  | 51, 87, 163, 193      | 0     |
| 1   | DN    | 113/113 (100%) | 0.25   | 2 (1%) 67 42  | 49, 83, 126, 154      | 0     |
| 1   | DO    | 113/113 (100%) | 0.52   | 6 (5%) 32 18  | 54, 96, 147, 177      | 0     |
| 1   | DP    | 113/113 (100%) | 0.42   | 3 (2%) 56 33  | 51, 87, 163, 193      | 0     |
| 1   | DQ    | 113/113 (100%) | 0.38   | 5 (4%) 39 21  | 49, 83, 126, 154      | 0     |
| 1   | DR    | 113/113 (100%) | 0.54   | 7 (6%) 26 16  | 54, 96, 147, 177      | 0     |
| 1   | DS    | 113/113 (100%) | 0.59   | 6 (5%) 32 18  | 51, 87, 163, 193      | 0     |
| 1   | DT    | 113/113 (100%) | 0.30   | 1 (0%) 81 58  | 49, 83, 126, 154      | 0     |
| 1   | DU    | 113/113 (100%) | 0.68   | 5 (4%) 39 21  | 54, 96, 147, 177      | 0     |
| 1   | DV    | 113/113 (100%) | 0.50   | 7 (6%) 26 16  | 51, 87, 163, 193      | 0     |
| 1   | DW    | 113/113 (100%) | 0.29   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | DX    | 113/113 (100%) | 0.75   | 11 (9%) 13 9  | 54, 96, 147, 177      | 0     |
| 1   | DY    | 113/113 (100%) | 0.47   | 3 (2%) 56 33  | 51, 87, 163, 193      | 0     |
| 1   | DZ    | 113/113 (100%) | 0.57   | 11 (9%) 13 9  | 49, 83, 126, 154      | 0     |
| 1   | EA    | 113/113 (100%) | 0.32   | 1 (0%) 81 58  | 54, 96, 147, 177      | 0     |
| 1   | EB    | 113/113 (100%) | 0.81   | 9 (7%) 18 12  | 51, 87, 163, 193      | 0     |
| 1   | EC    | 113/113 (100%) | 0.99   | 10 (8%) 15 10 | 49, 83, 126, 154      | 0     |
| 1   | ED    | 113/113 (100%) | 0.74   | 6 (5%) 32 18  | 54, 96, 147, 177      | 0     |
| 1   | EE    | 113/113 (100%) | 0.65   | 10 (8%) 15 10 | 51, 87, 163, 193      | 0     |
| 1   | EF    | 113/113 (100%) | 0.33   | 1 (0%) 81 58  | 49, 83, 126, 154      | 0     |
| 1   | EG    | 113/113 (100%) | 0.57   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | EH    | 113/113 (100%) | 0.46   | 7 (6%) 26 16  | 51, 87, 163, 193      | 0     |
| 1   | EI    | 113/113 (100%) | 0.44   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | EJ    | 113/113 (100%) | 0.64   | 7 (6%) 26 16  | 54, 96, 147, 177      | 0     |
| 1   | EK    | 113/113 (100%) | 0.60   | 8 (7%) 22 14  | 51, 87, 163, 193      | 0     |
| 1   | EL    | 113/113 (100%) | 0.54   | 11 (9%) 13 9  | 49, 83, 126, 154      | 0     |
| 1   | EM    | 113/113 (100%) | 0.54   | 9 (7%) 18 12  | 54, 96, 147, 177      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|----|----|-----------------------|-------|
| 1   | EN    | 113/113 (100%) | 0.44   | 4 (3%)   | 47 | 26 | 51, 87, 163, 193      | 0     |
| 1   | EO    | 113/113 (100%) | 0.43   | 8 (7%)   | 22 | 14 | 49, 83, 126, 154      | 0     |
| 1   | EP    | 113/113 (100%) | 0.57   | 11 (9%)  | 13 | 9  | 54, 96, 147, 177      | 0     |
| 1   | EQ    | 113/113 (100%) | 0.61   | 6 (5%)   | 32 | 18 | 51, 87, 163, 193      | 0     |
| 1   | ER    | 113/113 (100%) | 0.45   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |
| 1   | ES    | 113/113 (100%) | 0.80   | 9 (7%)   | 18 | 12 | 54, 96, 147, 177      | 0     |
| 1   | ET    | 113/113 (100%) | 0.51   | 7 (6%)   | 26 | 16 | 51, 87, 163, 193      | 0     |
| 1   | EU    | 113/113 (100%) | 0.75   | 11 (9%)  | 13 | 9  | 49, 83, 126, 154      | 0     |
| 1   | EV    | 113/113 (100%) | 0.43   | 5 (4%)   | 39 | 21 | 54, 96, 147, 177      | 0     |
| 1   | EW    | 113/113 (100%) | 0.61   | 9 (7%)   | 18 | 12 | 51, 87, 163, 193      | 0     |
| 1   | EX    | 113/113 (100%) | 0.55   | 5 (4%)   | 39 | 21 | 49, 83, 126, 154      | 0     |
| 1   | EY    | 113/113 (100%) | 0.69   | 6 (5%)   | 32 | 18 | 54, 96, 147, 177      | 0     |
| 1   | EZ    | 113/113 (100%) | 0.51   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | FA    | 113/113 (100%) | 0.44   | 6 (5%)   | 32 | 18 | 49, 83, 126, 154      | 0     |
| 1   | FB    | 113/113 (100%) | 0.48   | 6 (5%)   | 32 | 18 | 54, 96, 147, 177      | 0     |
| 1   | FC    | 113/113 (100%) | 0.55   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | FD    | 113/113 (100%) | 0.56   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |
| 1   | FE    | 113/113 (100%) | 0.82   | 13 (11%) | 9  | 6  | 54, 96, 147, 177      | 0     |
| 1   | FF    | 113/113 (100%) | 0.60   | 10 (8%)  | 15 | 10 | 51, 87, 163, 193      | 0     |
| 1   | FG    | 113/113 (100%) | 0.49   | 5 (4%)   | 39 | 21 | 49, 83, 126, 154      | 0     |
| 1   | FH    | 113/113 (100%) | 0.63   | 3 (2%)   | 56 | 33 | 54, 96, 147, 177      | 0     |
| 1   | FI    | 113/113 (100%) | 0.46   | 3 (2%)   | 56 | 33 | 51, 87, 163, 193      | 0     |
| 1   | FJ    | 113/113 (100%) | 0.44   | 5 (4%)   | 39 | 21 | 49, 83, 126, 154      | 0     |
| 1   | FK    | 113/113 (100%) | 0.44   | 5 (4%)   | 39 | 21 | 54, 96, 147, 177      | 0     |
| 1   | FL    | 113/113 (100%) | 0.44   | 6 (5%)   | 32 | 18 | 51, 87, 163, 193      | 0     |
| 1   | FM    | 113/113 (100%) | 0.41   | 2 (1%)   | 67 | 42 | 49, 83, 126, 154      | 0     |
| 1   | FN    | 113/113 (100%) | 0.46   | 1 (0%)   | 81 | 58 | 54, 96, 147, 177      | 0     |
| 1   | FO    | 113/113 (100%) | 0.39   | 3 (2%)   | 56 | 33 | 51, 87, 163, 193      | 0     |
| 1   | FP    | 113/113 (100%) | 0.53   | 5 (4%)   | 39 | 21 | 49, 83, 126, 154      | 0     |
| 1   | FQ    | 113/113 (100%) | 0.51   | 6 (5%)   | 32 | 18 | 54, 96, 147, 177      | 0     |
| 1   | FR    | 113/113 (100%) | 0.52   | 7 (6%)   | 26 | 16 | 51, 87, 163, 193      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | FS    | 113/113 (100%) | 0.65   | 7 (6%) 26 16  | 49, 83, 126, 154      | 0     |
| 1   | FT    | 113/113 (100%) | 0.49   | 6 (5%) 32 18  | 54, 96, 147, 177      | 0     |
| 1   | FU    | 113/113 (100%) | 0.53   | 6 (5%) 32 18  | 51, 87, 163, 193      | 0     |
| 1   | FV    | 113/113 (100%) | 0.50   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | FW    | 113/113 (100%) | 0.64   | 5 (4%) 39 21  | 54, 96, 147, 177      | 0     |
| 1   | FX    | 113/113 (100%) | 0.44   | 4 (3%) 47 26  | 51, 87, 163, 193      | 0     |
| 1   | FY    | 113/113 (100%) | 0.35   | 5 (4%) 39 21  | 49, 83, 126, 154      | 0     |
| 1   | FZ    | 113/113 (100%) | 0.67   | 6 (5%) 32 18  | 54, 96, 147, 177      | 0     |
| 1   | GA    | 113/113 (100%) | 0.59   | 8 (7%) 22 14  | 51, 87, 163, 193      | 0     |
| 1   | GB    | 113/113 (100%) | 0.76   | 5 (4%) 39 21  | 49, 83, 126, 154      | 0     |
| 1   | GC    | 113/113 (100%) | 0.81   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | GD    | 113/113 (100%) | 0.64   | 12 (10%) 11 8 | 51, 87, 163, 193      | 0     |
| 1   | GE    | 113/113 (100%) | 0.52   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | GF    | 113/113 (100%) | 0.63   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | GG    | 113/113 (100%) | 0.50   | 7 (6%) 26 16  | 51, 87, 163, 193      | 0     |
| 1   | GH    | 113/113 (100%) | 0.50   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | GI    | 113/113 (100%) | 0.54   | 6 (5%) 32 18  | 54, 96, 147, 177      | 0     |
| 1   | GJ    | 113/113 (100%) | 0.58   | 9 (7%) 18 12  | 51, 87, 163, 193      | 0     |
| 1   | GK    | 113/113 (100%) | 0.74   | 10 (8%) 15 10 | 49, 83, 126, 154      | 0     |
| 1   | GL    | 113/113 (100%) | 0.69   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | GM    | 113/113 (100%) | 0.44   | 7 (6%) 26 16  | 51, 87, 163, 193      | 0     |
| 1   | GN    | 113/113 (100%) | 0.52   | 10 (8%) 15 10 | 49, 83, 126, 154      | 0     |
| 1   | GO    | 113/113 (100%) | 0.62   | 9 (7%) 18 12  | 54, 96, 147, 177      | 0     |
| 1   | GP    | 113/113 (100%) | 0.81   | 7 (6%) 26 16  | 51, 87, 163, 193      | 0     |
| 1   | GQ    | 113/113 (100%) | 0.41   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | GR    | 113/113 (100%) | 0.79   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | GS    | 113/113 (100%) | 0.47   | 6 (5%) 32 18  | 51, 87, 163, 193      | 0     |
| 1   | GT    | 113/113 (100%) | 0.44   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | GU    | 113/113 (100%) | 0.68   | 10 (8%) 15 10 | 54, 96, 147, 177      | 0     |
| 1   | GV    | 113/113 (100%) | 0.45   | 5 (4%) 39 21  | 51, 87, 163, 193      | 0     |
| 1   | GW    | 113/113 (100%) | 0.40   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|-------|-----------------------|-------|
| 1   | GX    | 113/113 (100%) | 0.72   | 9 (7%)   | 18 12 | 54, 96, 147, 177      | 0     |
| 1   | GY    | 113/113 (100%) | 0.63   | 11 (9%)  | 13 9  | 51, 87, 163, 193      | 0     |
| 1   | GZ    | 113/113 (100%) | 0.51   | 5 (4%)   | 39 21 | 49, 83, 126, 154      | 0     |
| 1   | HA    | 113/113 (100%) | 0.63   | 8 (7%)   | 22 14 | 54, 96, 147, 177      | 0     |
| 1   | HB    | 113/113 (100%) | 0.41   | 5 (4%)   | 39 21 | 51, 87, 163, 193      | 0     |
| 1   | HC    | 113/113 (100%) | 0.46   | 8 (7%)   | 22 14 | 49, 83, 126, 154      | 0     |
| 1   | HD    | 113/113 (100%) | 0.52   | 4 (3%)   | 47 26 | 54, 96, 147, 177      | 0     |
| 1   | HE    | 113/113 (100%) | 0.69   | 9 (7%)   | 18 12 | 51, 87, 163, 193      | 0     |
| 1   | HF    | 113/113 (100%) | 0.35   | 2 (1%)   | 67 42 | 49, 83, 126, 154      | 0     |
| 1   | HG    | 113/113 (100%) | 0.59   | 6 (5%)   | 32 18 | 54, 96, 147, 177      | 0     |
| 1   | HH    | 113/113 (100%) | 0.75   | 10 (8%)  | 15 10 | 51, 87, 163, 193      | 0     |
| 1   | HI    | 113/113 (100%) | 1.03   | 11 (9%)  | 13 9  | 49, 83, 126, 154      | 0     |
| 1   | HJ    | 113/113 (100%) | 0.97   | 12 (10%) | 11 8  | 54, 96, 147, 177      | 0     |
| 1   | HK    | 113/113 (100%) | 0.30   | 5 (4%)   | 39 21 | 51, 87, 163, 193      | 0     |
| 1   | HL    | 113/113 (100%) | 0.43   | 2 (1%)   | 67 42 | 49, 83, 126, 154      | 0     |
| 1   | HM    | 113/113 (100%) | 0.64   | 9 (7%)   | 18 12 | 54, 96, 147, 177      | 0     |
| 1   | HN    | 113/113 (100%) | 0.35   | 1 (0%)   | 81 58 | 51, 87, 163, 193      | 0     |
| 1   | HO    | 113/113 (100%) | 0.57   | 7 (6%)   | 26 16 | 49, 83, 126, 154      | 0     |
| 1   | HP    | 113/113 (100%) | 0.46   | 5 (4%)   | 39 21 | 54, 96, 147, 177      | 0     |
| 1   | HQ    | 113/113 (100%) | 0.46   | 2 (1%)   | 67 42 | 51, 87, 163, 193      | 0     |
| 1   | HR    | 113/113 (100%) | 0.78   | 11 (9%)  | 13 9  | 49, 83, 126, 154      | 0     |
| 1   | HS    | 113/113 (100%) | 0.58   | 5 (4%)   | 39 21 | 54, 96, 147, 177      | 0     |
| 1   | HT    | 113/113 (100%) | 0.44   | 2 (1%)   | 67 42 | 51, 87, 163, 193      | 0     |
| 1   | HU    | 113/113 (100%) | 0.37   | 2 (1%)   | 67 42 | 49, 83, 126, 154      | 0     |
| 1   | HV    | 113/113 (100%) | 0.52   | 5 (4%)   | 39 21 | 54, 96, 147, 177      | 0     |
| 1   | HW    | 113/113 (100%) | 0.48   | 8 (7%)   | 22 14 | 51, 87, 163, 193      | 0     |
| 1   | HX    | 113/113 (100%) | 0.62   | 9 (7%)   | 18 12 | 49, 83, 126, 154      | 0     |
| 1   | HY    | 113/113 (100%) | 0.68   | 4 (3%)   | 47 26 | 54, 96, 147, 177      | 0     |
| 1   | HZ    | 113/113 (100%) | 0.43   | 8 (7%)   | 22 14 | 51, 87, 163, 193      | 0     |
| 1   | IA    | 113/113 (100%) | 0.56   | 8 (7%)   | 22 14 | 49, 83, 126, 154      | 0     |
| 1   | IB    | 113/113 (100%) | 0.65   | 8 (7%)   | 22 14 | 54, 96, 147, 177      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|--------------|-----------------------|-------|
| 1   | IC    | 113/113 (100%) | 1.08   | 18 (15%) 5 4 | 51, 87, 163, 193      | 0     |
| 1   | ID    | 113/113 (100%) | 0.70   | 6 (5%) 32 18 | 49, 83, 126, 154      | 0     |
| 1   | IE    | 113/113 (100%) | 0.81   | 8 (7%) 22 14 | 54, 96, 147, 177      | 0     |
| 1   | IF    | 113/113 (100%) | 0.37   | 6 (5%) 32 18 | 51, 87, 163, 193      | 0     |
| 1   | IG    | 113/113 (100%) | 0.56   | 4 (3%) 47 26 | 49, 83, 126, 154      | 0     |
| 1   | IH    | 113/113 (100%) | 0.80   | 7 (6%) 26 16 | 54, 96, 147, 177      | 0     |
| 1   | II    | 113/113 (100%) | 0.59   | 4 (3%) 47 26 | 51, 87, 163, 193      | 0     |
| 1   | IJ    | 113/113 (100%) | 0.85   | 7 (6%) 26 16 | 49, 83, 126, 154      | 0     |
| 1   | IK    | 113/113 (100%) | 0.57   | 4 (3%) 47 26 | 54, 96, 147, 177      | 0     |
| 1   | IL    | 113/113 (100%) | 0.45   | 7 (6%) 26 16 | 51, 87, 163, 193      | 0     |
| 1   | IM    | 113/113 (100%) | 0.42   | 3 (2%) 56 33 | 49, 83, 126, 154      | 0     |
| 1   | IN    | 113/113 (100%) | 0.86   | 17 (15%) 5 5 | 54, 96, 147, 177      | 0     |
| 1   | IO    | 113/113 (100%) | 0.57   | 6 (5%) 32 18 | 51, 87, 163, 193      | 0     |
| 1   | IP    | 113/113 (100%) | 0.56   | 5 (4%) 39 21 | 49, 83, 126, 154      | 0     |
| 1   | IQ    | 113/113 (100%) | 0.60   | 7 (6%) 26 16 | 54, 96, 147, 177      | 0     |
| 1   | IR    | 113/113 (100%) | 0.46   | 4 (3%) 47 26 | 51, 87, 163, 193      | 0     |
| 1   | IS    | 113/113 (100%) | 0.34   | 1 (0%) 81 58 | 49, 83, 126, 154      | 0     |
| 1   | IT    | 113/113 (100%) | 0.64   | 6 (5%) 32 18 | 54, 96, 147, 177      | 0     |
| 1   | IU    | 113/113 (100%) | 0.56   | 8 (7%) 22 14 | 51, 87, 163, 193      | 0     |
| 1   | IV    | 113/113 (100%) | 0.63   | 7 (6%) 26 16 | 49, 83, 126, 154      | 0     |
| 1   | IW    | 113/113 (100%) | 0.68   | 4 (3%) 47 26 | 54, 96, 147, 177      | 0     |
| 1   | IX    | 113/113 (100%) | 0.43   | 6 (5%) 32 18 | 51, 87, 163, 193      | 0     |
| 1   | IY    | 113/113 (100%) | 0.50   | 6 (5%) 32 18 | 49, 83, 126, 154      | 0     |
| 1   | IZ    | 113/113 (100%) | 0.53   | 6 (5%) 32 18 | 54, 96, 147, 177      | 0     |
| 1   | JA    | 113/113 (100%) | 0.70   | 11 (9%) 13 9 | 51, 87, 163, 193      | 0     |
| 1   | JB    | 113/113 (100%) | 0.37   | 4 (3%) 47 26 | 49, 83, 126, 154      | 0     |
| 1   | JC    | 113/113 (100%) | 0.67   | 3 (2%) 56 33 | 54, 96, 147, 177      | 0     |
| 1   | JD    | 113/113 (100%) | 0.75   | 6 (5%) 32 18 | 51, 87, 163, 193      | 0     |
| 1   | JE    | 113/113 (100%) | 0.46   | 3 (2%) 56 33 | 49, 83, 126, 154      | 0     |
| 1   | JF    | 113/113 (100%) | 0.87   | 16 (14%) 6 5 | 54, 96, 147, 177      | 0     |
| 1   | JG    | 113/113 (100%) | 0.37   | 4 (3%) 47 26 | 51, 87, 163, 193      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|----|----|-----------------------|-------|
| 1   | JH    | 113/113 (100%) | 0.35   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |
| 1   | JI    | 113/113 (100%) | 0.69   | 6 (5%)   | 32 | 18 | 54, 96, 147, 177      | 0     |
| 1   | JJ    | 113/113 (100%) | 0.56   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | JK    | 113/113 (100%) | 0.51   | 7 (6%)   | 26 | 16 | 49, 83, 126, 154      | 0     |
| 1   | JL    | 113/113 (100%) | 0.66   | 8 (7%)   | 22 | 14 | 54, 96, 147, 177      | 0     |
| 1   | JM    | 113/113 (100%) | 0.32   | 4 (3%)   | 47 | 26 | 51, 87, 163, 193      | 0     |
| 1   | JN    | 113/113 (100%) | 0.35   | 1 (0%)   | 81 | 58 | 49, 83, 126, 154      | 0     |
| 1   | JO    | 113/113 (100%) | 0.54   | 5 (4%)   | 39 | 21 | 54, 96, 147, 177      | 0     |
| 1   | JP    | 113/113 (100%) | 0.53   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | JQ    | 113/113 (100%) | 0.47   | 3 (2%)   | 56 | 33 | 49, 83, 126, 154      | 0     |
| 1   | JR    | 113/113 (100%) | 0.67   | 7 (6%)   | 26 | 16 | 54, 96, 147, 177      | 0     |
| 1   | JS    | 113/113 (100%) | 0.45   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | JT    | 113/113 (100%) | 0.45   | 5 (4%)   | 39 | 21 | 49, 83, 126, 154      | 0     |
| 1   | JU    | 113/113 (100%) | 0.56   | 5 (4%)   | 39 | 21 | 54, 96, 147, 177      | 0     |
| 1   | JV    | 113/113 (100%) | 0.55   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | JW    | 113/113 (100%) | 0.46   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |
| 1   | JX    | 113/113 (100%) | 0.63   | 11 (9%)  | 13 | 9  | 54, 96, 147, 177      | 0     |
| 1   | JY    | 113/113 (100%) | 0.39   | 6 (5%)   | 32 | 18 | 51, 87, 163, 193      | 0     |
| 1   | JZ    | 113/113 (100%) | 0.35   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |
| 1   | KA    | 113/113 (100%) | 0.65   | 5 (4%)   | 39 | 21 | 54, 96, 147, 177      | 0     |
| 1   | KB    | 113/113 (100%) | 0.40   | 6 (5%)   | 32 | 18 | 51, 87, 163, 193      | 0     |
| 1   | KC    | 113/113 (100%) | 0.43   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |
| 1   | KD    | 113/113 (100%) | 0.50   | 8 (7%)   | 22 | 14 | 54, 96, 147, 177      | 0     |
| 1   | KE    | 113/113 (100%) | 0.46   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | KF    | 113/113 (100%) | 0.55   | 6 (5%)   | 32 | 18 | 49, 83, 126, 154      | 0     |
| 1   | KG    | 113/113 (100%) | 0.51   | 9 (7%)   | 18 | 12 | 54, 96, 147, 177      | 0     |
| 1   | KH    | 113/113 (100%) | 0.57   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | KI    | 113/113 (100%) | 0.59   | 9 (7%)   | 18 | 12 | 49, 83, 126, 154      | 0     |
| 1   | KJ    | 113/113 (100%) | 0.74   | 12 (10%) | 11 | 8  | 54, 96, 147, 177      | 0     |
| 1   | KK    | 113/113 (100%) | 0.45   | 3 (2%)   | 56 | 33 | 51, 87, 163, 193      | 0     |
| 1   | KL    | 113/113 (100%) | 0.37   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | KM    | 113/113 (100%) | 0.66   | 8 (7%) 22 14  | 54, 96, 147, 177      | 0     |
| 1   | KN    | 113/113 (100%) | 0.53   | 11 (9%) 13 9  | 51, 87, 163, 193      | 0     |
| 1   | KO    | 113/113 (100%) | 0.50   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | KP    | 113/113 (100%) | 0.57   | 2 (1%) 67 42  | 54, 96, 147, 177      | 0     |
| 1   | KQ    | 113/113 (100%) | 0.33   | 5 (4%) 39 21  | 51, 87, 163, 193      | 0     |
| 1   | KR    | 113/113 (100%) | 0.33   | 2 (1%) 67 42  | 49, 83, 126, 154      | 0     |
| 1   | KS    | 113/113 (100%) | 0.51   | 5 (4%) 39 21  | 54, 96, 147, 177      | 0     |
| 1   | KT    | 113/113 (100%) | 0.64   | 7 (6%) 26 16  | 51, 87, 163, 193      | 0     |
| 1   | KU    | 113/113 (100%) | 0.65   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | KV    | 113/113 (100%) | 0.77   | 12 (10%) 11 8 | 54, 96, 147, 177      | 0     |
| 1   | KW    | 113/113 (100%) | 0.66   | 10 (8%) 15 10 | 51, 87, 163, 193      | 0     |
| 1   | KX    | 113/113 (100%) | 0.59   | 11 (9%) 13 9  | 49, 83, 126, 154      | 0     |
| 1   | KY    | 113/113 (100%) | 0.55   | 5 (4%) 39 21  | 54, 96, 147, 177      | 0     |
| 1   | KZ    | 113/113 (100%) | 0.39   | 6 (5%) 32 18  | 51, 87, 163, 193      | 0     |
| 1   | LA    | 113/113 (100%) | 0.59   | 6 (5%) 32 18  | 49, 83, 126, 154      | 0     |
| 1   | LB    | 113/113 (100%) | 0.71   | 12 (10%) 11 8 | 54, 96, 147, 177      | 0     |
| 1   | LC    | 113/113 (100%) | 0.51   | 2 (1%) 67 42  | 51, 87, 163, 193      | 0     |
| 1   | LD    | 113/113 (100%) | 0.49   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | LE    | 113/113 (100%) | 0.54   | 7 (6%) 26 16  | 54, 96, 147, 177      | 0     |
| 1   | LF    | 113/113 (100%) | 0.66   | 5 (4%) 39 21  | 51, 87, 163, 193      | 0     |
| 1   | LG    | 113/113 (100%) | 0.30   | 2 (1%) 67 42  | 49, 83, 126, 154      | 0     |
| 1   | LH    | 113/113 (100%) | 0.66   | 12 (10%) 11 8 | 54, 96, 147, 177      | 0     |
| 1   | LI    | 113/113 (100%) | 0.47   | 8 (7%) 22 14  | 51, 87, 163, 193      | 0     |
| 1   | LJ    | 113/113 (100%) | 0.55   | 1 (0%) 81 58  | 49, 83, 126, 154      | 0     |
| 1   | LK    | 113/113 (100%) | 0.64   | 6 (5%) 32 18  | 54, 96, 147, 177      | 0     |
| 1   | LL    | 113/113 (100%) | 0.60   | 5 (4%) 39 21  | 51, 87, 163, 193      | 0     |
| 1   | LM    | 113/113 (100%) | 0.41   | 2 (1%) 67 42  | 49, 83, 126, 154      | 0     |
| 1   | LN    | 113/113 (100%) | 0.55   | 4 (3%) 47 26  | 54, 96, 147, 177      | 0     |
| 1   | LO    | 113/113 (100%) | 0.58   | 9 (7%) 18 12  | 51, 87, 163, 193      | 0     |
| 1   | LP    | 113/113 (100%) | 0.53   | 7 (6%) 26 16  | 49, 83, 126, 154      | 0     |
| 1   | LQ    | 113/113 (100%) | 0.81   | 11 (9%) 13 9  | 54, 96, 147, 177      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | LR    | 113/113 (100%) | 0.59   | 3 (2%) 56 33  | 51, 87, 163, 193      | 0     |
| 1   | LS    | 113/113 (100%) | 0.44   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | LT    | 113/113 (100%) | 0.62   | 9 (7%) 18 12  | 54, 96, 147, 177      | 0     |
| 1   | LU    | 113/113 (100%) | 0.64   | 13 (11%) 9 6  | 51, 87, 163, 193      | 0     |
| 1   | LV    | 113/113 (100%) | 0.59   | 10 (8%) 15 10 | 49, 83, 126, 154      | 0     |
| 1   | LW    | 113/113 (100%) | 0.68   | 9 (7%) 18 12  | 54, 96, 147, 177      | 0     |
| 1   | LX    | 113/113 (100%) | 0.78   | 9 (7%) 18 12  | 51, 87, 163, 193      | 0     |
| 1   | LY    | 113/113 (100%) | 0.31   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | LZ    | 113/113 (100%) | 0.58   | 5 (4%) 39 21  | 54, 96, 147, 177      | 0     |
| 1   | MA    | 113/113 (100%) | 0.49   | 7 (6%) 26 16  | 51, 87, 163, 193      | 0     |
| 1   | MB    | 113/113 (100%) | 0.46   | 2 (1%) 67 42  | 49, 83, 126, 154      | 0     |
| 1   | MC    | 113/113 (100%) | 0.50   | 2 (1%) 67 42  | 54, 96, 147, 177      | 0     |
| 1   | MD    | 113/113 (100%) | 0.44   | 5 (4%) 39 21  | 51, 87, 163, 193      | 0     |
| 1   | ME    | 113/113 (100%) | 0.55   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | MF    | 113/113 (100%) | 0.59   | 4 (3%) 47 26  | 54, 96, 147, 177      | 0     |
| 1   | MG    | 113/113 (100%) | 0.41   | 4 (3%) 47 26  | 51, 87, 163, 193      | 0     |
| 1   | MH    | 113/113 (100%) | 0.52   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | MI    | 113/113 (100%) | 0.72   | 9 (7%) 18 12  | 54, 96, 147, 177      | 0     |
| 1   | MJ    | 113/113 (100%) | 0.44   | 9 (7%) 18 12  | 51, 87, 163, 193      | 0     |
| 1   | MK    | 113/113 (100%) | 0.52   | 4 (3%) 47 26  | 49, 83, 126, 154      | 0     |
| 1   | ML    | 113/113 (100%) | 0.53   | 2 (1%) 67 42  | 54, 96, 147, 177      | 0     |
| 1   | MM    | 113/113 (100%) | 1.20   | 24 (21%) 2 3  | 51, 87, 163, 193      | 0     |
| 1   | MN    | 113/113 (100%) | 0.82   | 9 (7%) 18 12  | 49, 83, 126, 154      | 0     |
| 1   | MO    | 113/113 (100%) | 0.66   | 10 (8%) 15 10 | 54, 96, 147, 177      | 0     |
| 1   | MP    | 113/113 (100%) | 0.49   | 4 (3%) 47 26  | 51, 87, 163, 193      | 0     |
| 1   | MQ    | 113/113 (100%) | 0.42   | 3 (2%) 56 33  | 49, 83, 126, 154      | 0     |
| 1   | MR    | 113/113 (100%) | 0.72   | 7 (6%) 26 16  | 54, 96, 147, 177      | 0     |
| 1   | MS    | 113/113 (100%) | 0.63   | 4 (3%) 47 26  | 51, 87, 163, 193      | 0     |
| 1   | MT    | 113/113 (100%) | 0.38   | 5 (4%) 39 21  | 49, 83, 126, 154      | 0     |
| 1   | MU    | 113/113 (100%) | 0.54   | 4 (3%) 47 26  | 54, 96, 147, 177      | 0     |
| 1   | MV    | 113/113 (100%) | 0.56   | 6 (5%) 32 18  | 51, 87, 163, 193      | 0     |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2  |    |    | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|----------|----|----|-----------------------|-------|
| 1   | MW    | 113/113 (100%) | 0.52   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |
| 1   | MX    | 113/113 (100%) | 0.63   | 9 (7%)   | 18 | 12 | 54, 96, 147, 177      | 0     |
| 1   | MY    | 113/113 (100%) | 0.44   | 8 (7%)   | 22 | 14 | 51, 87, 163, 193      | 0     |
| 1   | MZ    | 113/113 (100%) | 0.64   | 8 (7%)   | 22 | 14 | 49, 83, 126, 154      | 0     |
| 1   | NA    | 113/113 (100%) | 0.58   | 7 (6%)   | 26 | 16 | 54, 96, 147, 177      | 0     |
| 1   | NB    | 113/113 (100%) | 0.48   | 3 (2%)   | 56 | 33 | 51, 87, 163, 193      | 0     |
| 1   | NC    | 113/113 (100%) | 0.44   | 6 (5%)   | 32 | 18 | 49, 83, 126, 154      | 0     |
| 1   | ND    | 113/113 (100%) | 0.55   | 5 (4%)   | 39 | 21 | 54, 96, 147, 177      | 0     |
| 1   | NE    | 113/113 (100%) | 0.60   | 9 (7%)   | 18 | 12 | 51, 87, 163, 193      | 0     |
| 1   | NF    | 113/113 (100%) | 0.57   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |
| 1   | NG    | 113/113 (100%) | 0.40   | 5 (4%)   | 39 | 21 | 54, 96, 147, 177      | 0     |
| 1   | NH    | 113/113 (100%) | 0.30   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | NI    | 113/113 (100%) | 0.49   | 3 (2%)   | 56 | 33 | 49, 83, 126, 154      | 0     |
| 1   | NJ    | 113/113 (100%) | 0.62   | 8 (7%)   | 22 | 14 | 54, 96, 147, 177      | 0     |
| 1   | NK    | 113/113 (100%) | 0.60   | 7 (6%)   | 26 | 16 | 51, 87, 163, 193      | 0     |
| 1   | NL    | 113/113 (100%) | 0.78   | 6 (5%)   | 32 | 18 | 49, 83, 126, 154      | 0     |
| 1   | NM    | 113/113 (100%) | 0.78   | 13 (11%) | 9  | 6  | 54, 96, 147, 177      | 0     |
| 1   | NN    | 113/113 (100%) | 0.40   | 4 (3%)   | 47 | 26 | 51, 87, 163, 193      | 0     |
| 1   | NO    | 113/113 (100%) | 0.54   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |
| 1   | NP    | 113/113 (100%) | 0.49   | 5 (4%)   | 39 | 21 | 54, 96, 147, 177      | 0     |
| 1   | NQ    | 113/113 (100%) | 0.53   | 5 (4%)   | 39 | 21 | 51, 87, 163, 193      | 0     |
| 1   | NR    | 113/113 (100%) | 0.43   | 1 (0%)   | 81 | 58 | 49, 83, 126, 154      | 0     |
| 1   | NS    | 113/113 (100%) | 0.49   | 7 (6%)   | 26 | 16 | 54, 96, 147, 177      | 0     |
| 1   | NT    | 113/113 (100%) | 0.66   | 4 (3%)   | 47 | 26 | 51, 87, 163, 193      | 0     |
| 1   | NU    | 113/113 (100%) | 0.54   | 4 (3%)   | 47 | 26 | 49, 83, 126, 154      | 0     |
| 1   | NV    | 113/113 (100%) | 0.83   | 16 (14%) | 6  | 5  | 54, 96, 147, 177      | 0     |
| 2   | RA    | 20/30 (66%)    | 0.96   | 3 (15%)  | 5  | 5  | 137, 172, 234, 256    | 0     |
| 2   | RB    | 20/30 (66%)    | 0.98   | 2 (10%)  | 12 | 8  | 137, 172, 234, 256    | 0     |
| 2   | RC    | 20/30 (66%)    | 0.87   | 2 (10%)  | 12 | 8  | 137, 172, 234, 256    | 0     |
| 2   | RD    | 20/30 (66%)    | 0.63   | 2 (10%)  | 12 | 8  | 137, 172, 234, 256    | 0     |
| 2   | RE    | 20/30 (66%)    | 0.63   | 1 (5%)   | 34 | 19 | 137, 172, 234, 256    | 0     |

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| Mol | Chain | Analysed    | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------|--------|--------------|-----------------------|-------|
| 2   | RF    | 20/30 (66%) | 1.15   | 3 (15%) 5 5  | 137, 172, 234, 256    | 0     |
| 2   | RG    | 20/30 (66%) | 0.61   | 1 (5%) 34 19 | 137, 172, 234, 256    | 0     |
| 2   | RH    | 20/30 (66%) | 0.52   | 0 100 100    | 137, 172, 234, 256    | 0     |
| 2   | RI    | 20/30 (66%) | 0.73   | 2 (10%) 12 8 | 137, 172, 234, 256    | 0     |
| 2   | RJ    | 20/30 (66%) | 0.84   | 2 (10%) 12 8 | 137, 172, 234, 256    | 0     |
| 2   | RK    | 20/30 (66%) | 0.91   | 3 (15%) 5 5  | 137, 172, 234, 256    | 0     |
| 2   | RL    | 20/30 (66%) | 0.88   | 2 (10%) 12 8 | 137, 172, 234, 256    | 0     |
| 2   | RM    | 20/30 (66%) | 1.14   | 2 (10%) 12 8 | 137, 172, 234, 256    | 0     |
| 2   | RN    | 20/30 (66%) | 0.62   | 2 (10%) 12 8 | 137, 172, 234, 256    | 0     |
| 2   | RO    | 20/30 (66%) | 1.44   | 5 (25%) 2 2  | 137, 172, 234, 256    | 0     |
| 2   | RP    | 20/30 (66%) | 0.84   | 1 (5%) 34 19 | 137, 172, 234, 256    | 0     |
| 2   | RQ    | 20/30 (66%) | 0.87   | 1 (5%) 34 19 | 137, 172, 234, 256    | 0     |
| 2   | RR    | 20/30 (66%) | 0.90   | 3 (15%) 5 5  | 137, 172, 234, 256    | 0     |
| 2   | RS    | 20/30 (66%) | 1.03   | 3 (15%) 5 5  | 137, 172, 234, 256    | 0     |
| 2   | RT    | 20/30 (66%) | 0.92   | 2 (10%) 12 8 | 137, 172, 234, 256    | 0     |
| 2   | RU    | 20/30 (66%) | 1.40   | 3 (15%) 5 5  | 137, 172, 234, 256    | 0     |
| 2   | RV    | 20/30 (66%) | 0.78   | 1 (5%) 34 19 | 137, 172, 234, 256    | 0     |
| 2   | RW    | 20/30 (66%) | 1.08   | 3 (15%) 5 5  | 137, 172, 234, 256    | 0     |
| 2   | RX    | 20/30 (66%) | 0.76   | 0 100 100    | 137, 172, 234, 256    | 0     |
| 2   | RY    | 20/30 (66%) | 0.92   | 2 (10%) 12 8 | 137, 172, 234, 256    | 0     |
| 2   | RZ    | 20/30 (66%) | 0.85   | 4 (20%) 3 3  | 137, 172, 234, 256    | 0     |
| 2   | SA    | 20/30 (66%) | 0.51   | 0 100 100    | 137, 172, 234, 256    | 0     |
| 2   | SB    | 20/30 (66%) | 1.03   | 3 (15%) 5 5  | 137, 172, 234, 256    | 0     |
| 2   | SC    | 20/30 (66%) | 0.63   | 1 (5%) 34 19 | 137, 172, 234, 256    | 0     |
| 2   | SD    | 20/30 (66%) | 0.93   | 1 (5%) 34 19 | 137, 172, 234, 256    | 0     |
| 2   | SE    | 20/30 (66%) | 0.88   | 2 (10%) 12 8 | 137, 172, 234, 256    | 0     |
| 2   | SF    | 20/30 (66%) | 1.08   | 1 (5%) 34 19 | 137, 172, 234, 256    | 0     |
| 2   | SG    | 20/30 (66%) | 0.59   | 1 (5%) 34 19 | 137, 172, 234, 256    | 0     |
| 2   | SH    | 20/30 (66%) | 1.24   | 4 (20%) 3 3  | 137, 172, 234, 256    | 0     |
| 2   | SI    | 20/30 (66%) | 0.80   | 2 (10%) 12 8 | 137, 172, 234, 256    | 0     |
| 2   | SJ    | 20/30 (66%) | 0.96   | 2 (10%) 12 8 | 137, 172, 234, 256    | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2         | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|-----------------|-----------------------|-------|
| 2   | SK    | 20/30 (66%)       | 0.94   | 5 (25%) 2 2     | 137, 172, 234, 256    | 0     |
| 2   | SL    | 20/30 (66%)       | 1.08   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | SM    | 20/30 (66%)       | 0.64   | 0 100 100       | 137, 172, 234, 256    | 0     |
| 2   | SN    | 20/30 (66%)       | 0.86   | 3 (15%) 5 5     | 137, 172, 234, 256    | 0     |
| 2   | SO    | 20/30 (66%)       | 1.15   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | SP    | 20/30 (66%)       | 0.76   | 1 (5%) 34 19    | 137, 172, 234, 256    | 0     |
| 2   | SQ    | 20/30 (66%)       | 1.17   | 4 (20%) 3 3     | 137, 172, 234, 256    | 0     |
| 2   | SR    | 20/30 (66%)       | 1.45   | 4 (20%) 3 3     | 137, 172, 234, 256    | 0     |
| 2   | SS    | 20/30 (66%)       | 0.71   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | ST    | 20/30 (66%)       | 0.78   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | SU    | 20/30 (66%)       | 1.05   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | SV    | 20/30 (66%)       | 0.94   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | SW    | 20/30 (66%)       | 0.99   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | SX    | 20/30 (66%)       | 1.43   | 3 (15%) 5 5     | 137, 172, 234, 256    | 0     |
| 2   | SY    | 20/30 (66%)       | 0.75   | 1 (5%) 34 19    | 137, 172, 234, 256    | 0     |
| 2   | SZ    | 20/30 (66%)       | 0.93   | 1 (5%) 34 19    | 137, 172, 234, 256    | 0     |
| 2   | TA    | 20/30 (66%)       | 0.74   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | TB    | 20/30 (66%)       | 1.01   | 4 (20%) 3 3     | 137, 172, 234, 256    | 0     |
| 2   | TC    | 20/30 (66%)       | 0.83   | 0 100 100       | 137, 172, 234, 256    | 0     |
| 2   | TD    | 20/30 (66%)       | 0.60   | 0 100 100       | 137, 172, 234, 256    | 0     |
| 2   | TE    | 20/30 (66%)       | 0.75   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | TF    | 20/30 (66%)       | 0.66   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | TG    | 20/30 (66%)       | 0.77   | 2 (10%) 12 8    | 137, 172, 234, 256    | 0     |
| 2   | TH    | 20/30 (66%)       | 0.96   | 3 (15%) 5 5     | 137, 172, 234, 256    | 0     |
| All | All   | 41880/42480 (98%) | 0.57   | 2425 (5%) 29 17 | 49, 89, 154, 256      | 0     |

The worst 5 of 2425 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | BS    | 65  | GLY  | 9.4  |
| 1   | IE    | 65  | GLY  | 7.8  |
| 1   | GJ    | 64  | ALA  | 7.2  |
| 1   | JX    | 65  | GLY  | 6.6  |
| 1   | GG    | 64  | ALA  | 6.1  |

## 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.