



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:36 PM BST

PDB ID : 4V5W
Title : Grapevine Fanleaf virus
Authors : Schellenberger, P.; Demangeat, G.; Ritzenthaler, C.; Lorber, B.; Sauter, C.
Deposited on : 2011-05-10
Resolution : 3.70 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

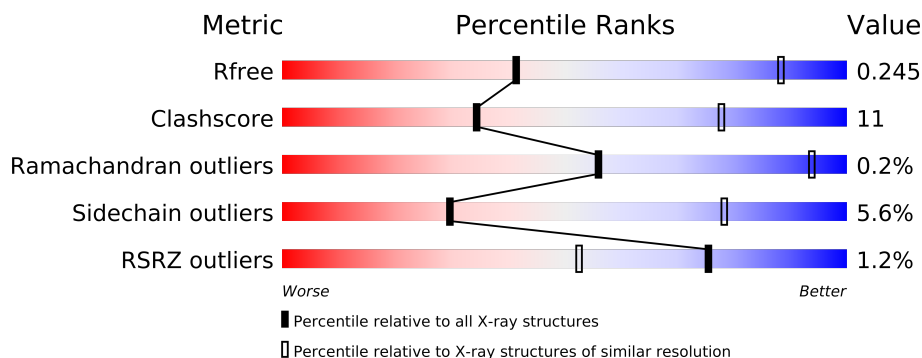
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 3.70 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 66092 | 1098 (4.00-3.40) |
| Clashscore | 79885 | 1009 (3.94-3.46) |
| Ramachandran outliers | 78287 | 1016 (3.98-3.42) |
| Sidechain outliers | 78261 | 1014 (3.98-3.42) |
| RSRZ outliers | 66119 | 1099 (4.00-3.40) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | AA | 504 | |
| 1 | AB | 504 | |
| 1 | AC | 504 | |
| 1 | AD | 504 | |
| 1 | AE | 504 | |
| 1 | AF | 504 | |
| 1 | AG | 504 | |
| 1 | AH | 504 | |
| 1 | AI | 504 | |
| 1 | AJ | 504 | |
| 1 | AK | 504 | |
| 1 | AL | 504 | |
| 1 | AM | 504 | |
| 1 | AN | 504 | |





Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | AO | 504 | |
| 1 | AP | 504 | |
| 1 | AQ | 504 | |
| 1 | AR | 504 | |
| 1 | AS | 504 | |
| 1 | AT | 504 | |
| 1 | BA | 504 | |
| 1 | BB | 504 | |
| 1 | BC | 504 | |
| 1 | BD | 504 | |
| 1 | BE | 504 | |
| 1 | BF | 504 | |
| 1 | BG | 504 | |
| 1 | BH | 504 | |
| 1 | BI | 504 | |
| 1 | BJ | 504 | |
| 1 | BK | 504 | |
| 1 | BL | 504 | |
| 1 | BM | 504 | |
| 1 | BN | 504 | |
| 1 | BO | 504 | |
| 1 | BP | 504 | |
| 1 | BQ | 504 | |
| 1 | BR | 504 | |
| 1 | BS | 504 | |
| 1 | BT | 504 | |
| 1 | CA | 504 | |
| 1 | CB | 504 | |
| 1 | CC | 504 | |
| 1 | CD | 504 | |
| 1 | CE | 504 | |
| 1 | CF | 504 | |
| 1 | CG | 504 | |
| 1 | CH | 504 | |
| 1 | CI | 504 | |
| 1 | CJ | 504 | |
| 1 | CK | 504 | |
| 1 | CL | 504 | |
| 1 | CM | 504 | |
| 1 | CN | 504 | |
| 1 | CO | 504 | |
| 1 | CP | 504 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | CQ | 504 |  |
| 1 | CR | 504 |  |
| 1 | CS | 504 |  |
| 1 | CT | 504 |  |

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 237060 atoms, of which 0 are hydrogen and 0 are deuterium.

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 | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AB | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AC | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AD | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AE | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AF | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AG | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AH | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AI | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AJ | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AK | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AL | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AM | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AN | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AO | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | AP | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
| 1 | AQ | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | AR | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | AS | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | AT | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BA | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BB | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BC | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BD | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BE | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BF | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BG | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BH | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BI | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BJ | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BK | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BL | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BM | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BN | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BO | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BP | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BQ | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
| 1 | BR | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BS | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | BT | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CA | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CB | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CC | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CD | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CE | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CF | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CG | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CH | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CI | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CJ | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CK | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CL | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CM | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CN | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CO | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CP | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CQ | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |
| 1 | CR | 504 | Total 3951 | C 2555 | N 653 | O 721 | S 22 | 0 | 0 | 0 |

Continued on next page...

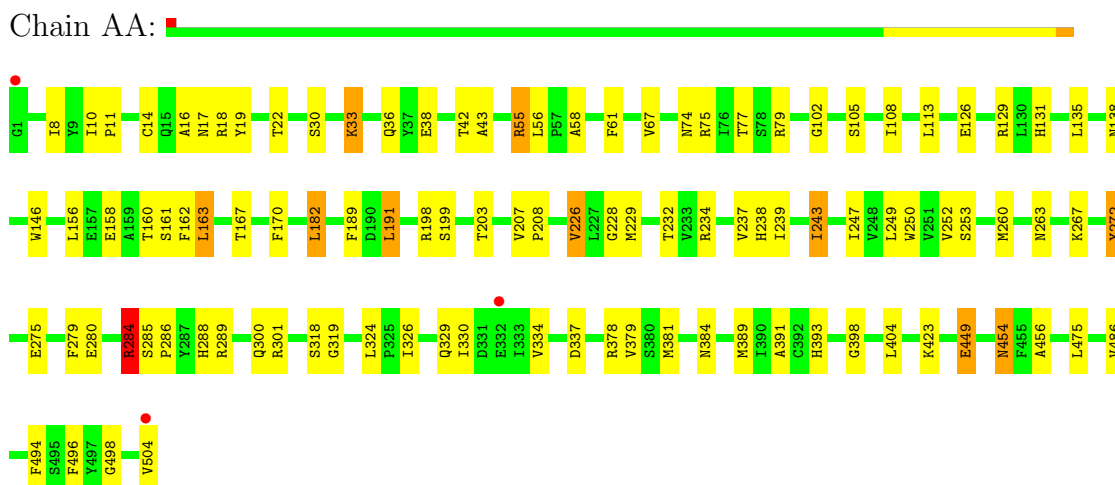
Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | CS | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |
| 1 | CT | 504 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3951 | 2555 | 653 | 721 | 22 | | | |

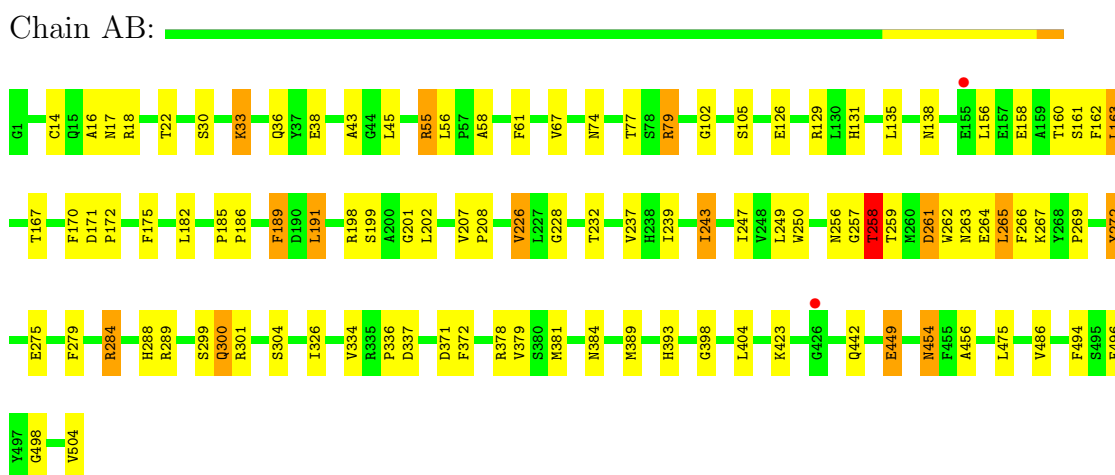
3 Residue-property plots

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

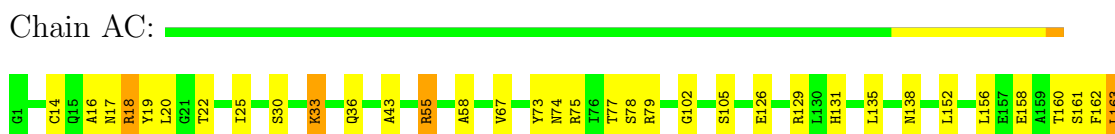
• Molecule 1: COAT PROTEIN

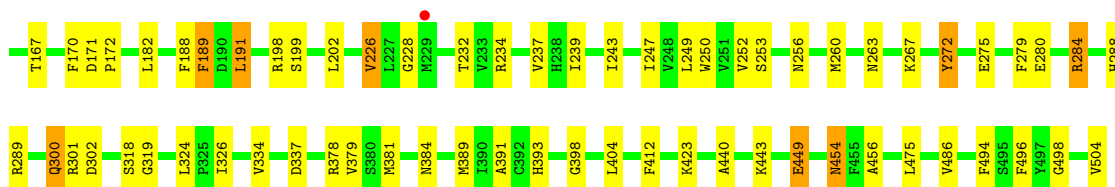


• Molecule 1: COAT PROTEIN



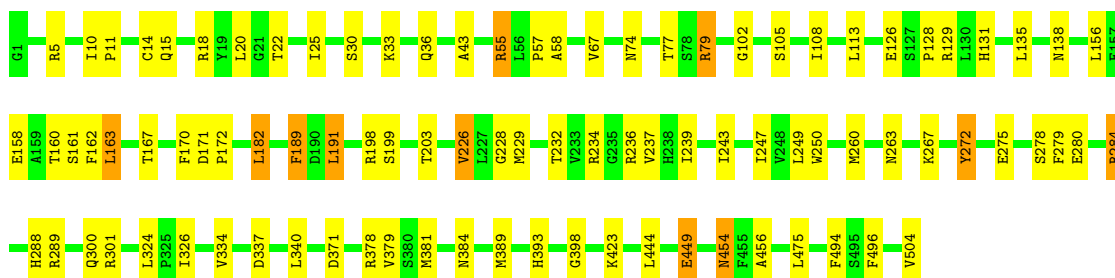
• Molecule 1: COAT PROTEIN





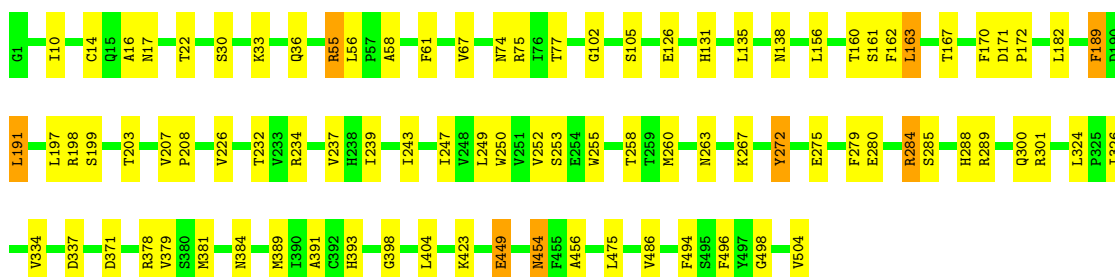
• Molecule 1: COAT PROTEIN

Chain AD:



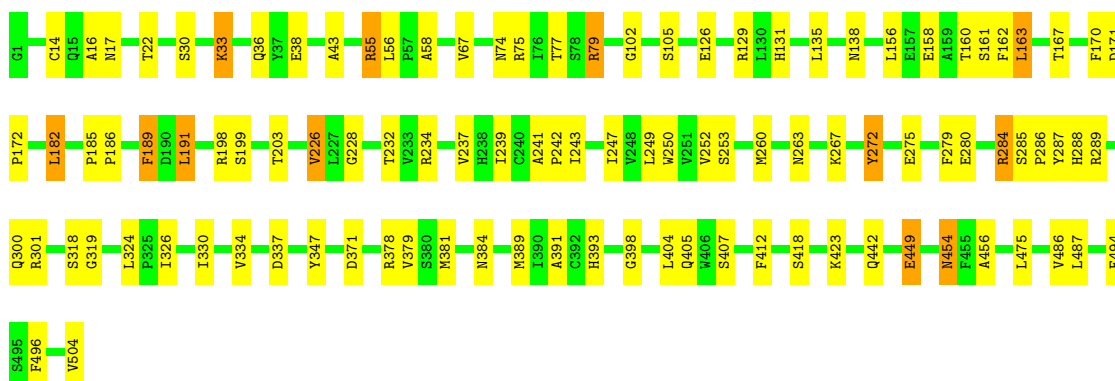
• Molecule 1: COAT PROTEIN

Chain AE:



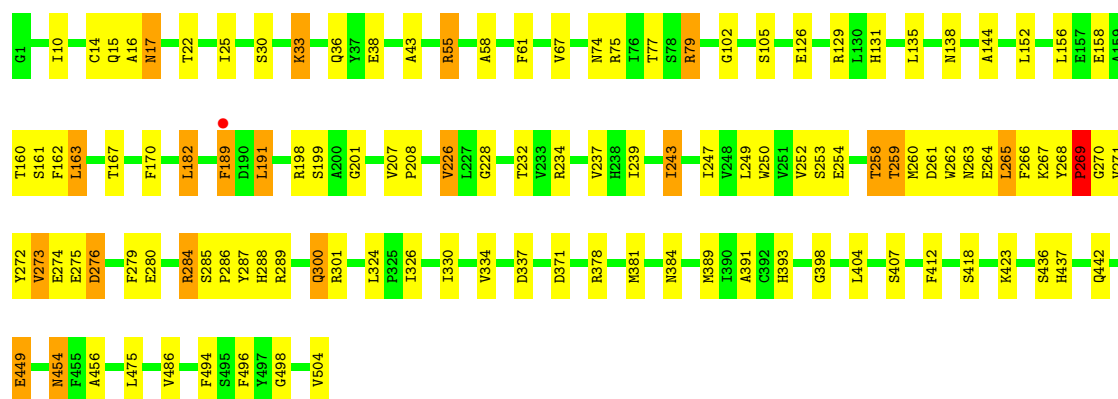
• Molecule 1: COAT PROTEIN

Chain AF:



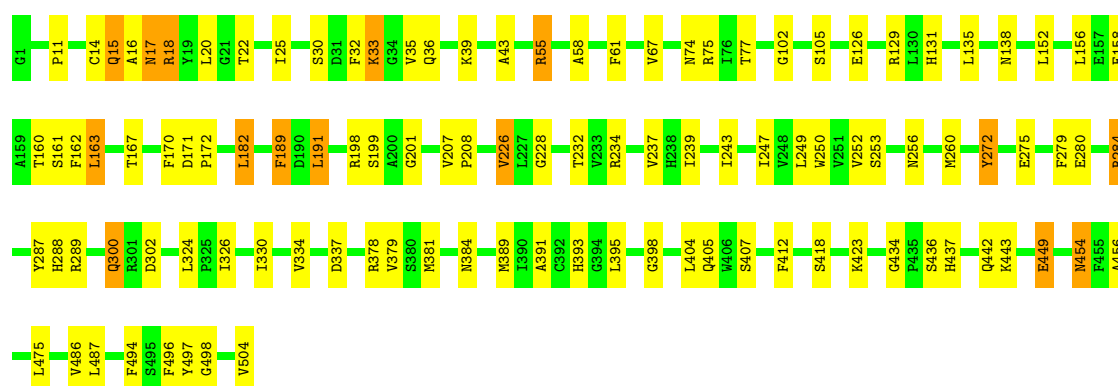
• Molecule 1: COAT PROTEIN

Chain AG:



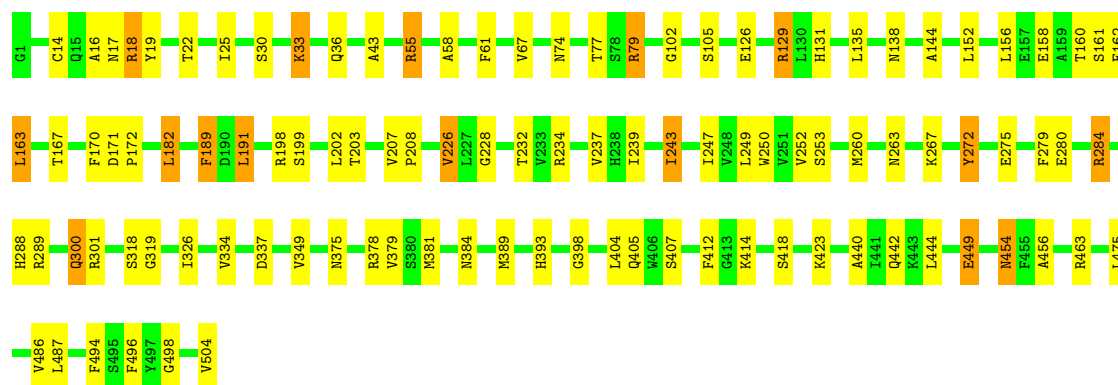
• Molecule 1: COAT PROTEIN

Chain AH: 



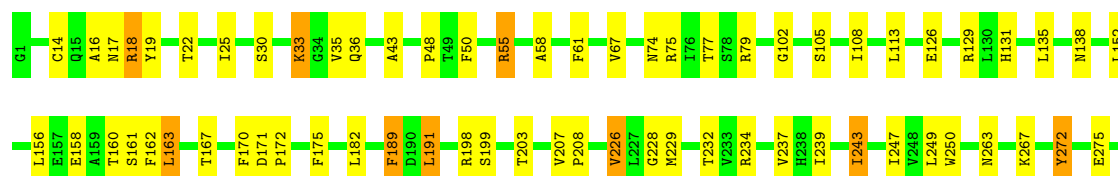
• Molecule 1: COAT PROTEIN

Chain AI: 



• Molecule 1: COAT PROTEIN

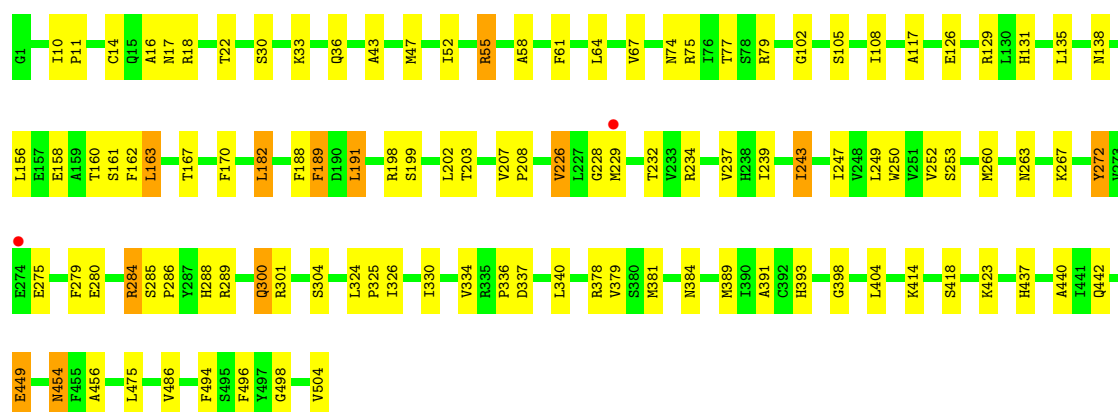
Chain AJ: 





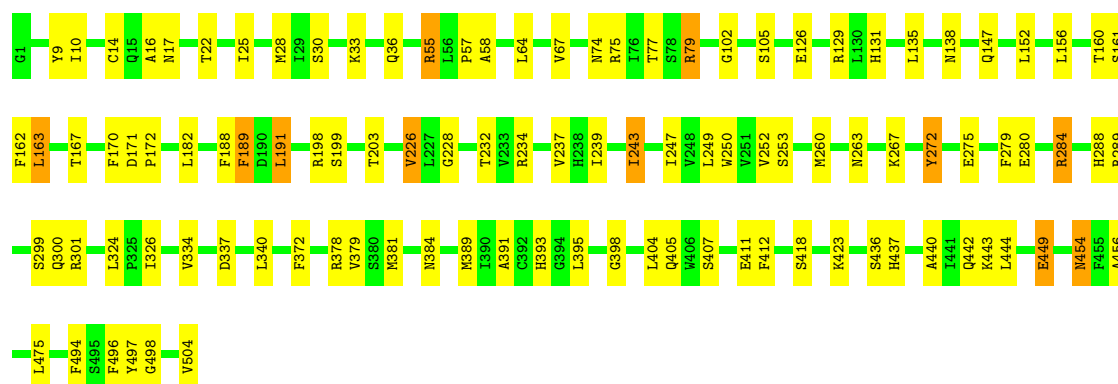
• Molecule 1: COAT PROTEIN

Chain AK:



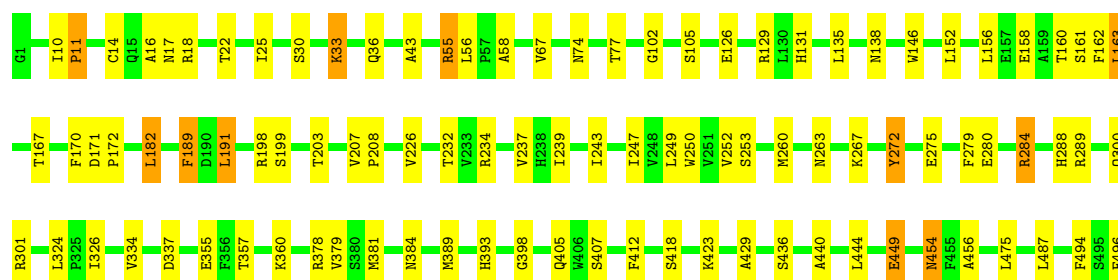
• Molecule 1: COAT PROTEIN

Chain AL:



• Molecule 1: COAT PROTEIN

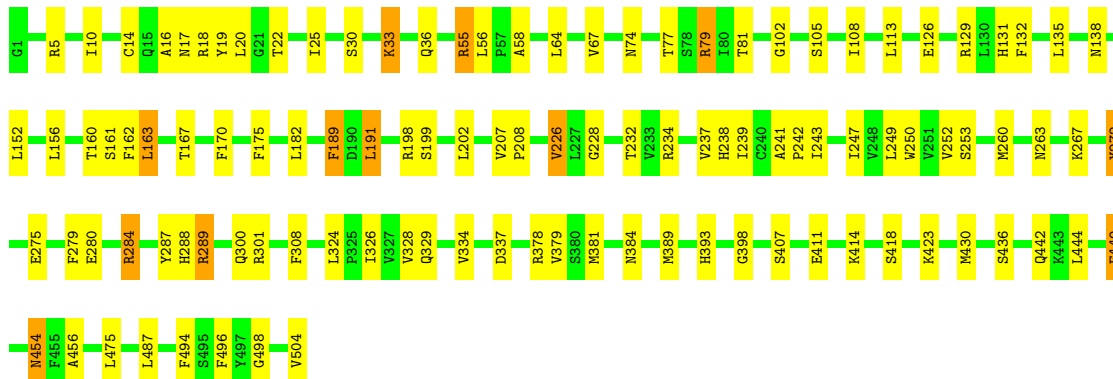
Chain AM:





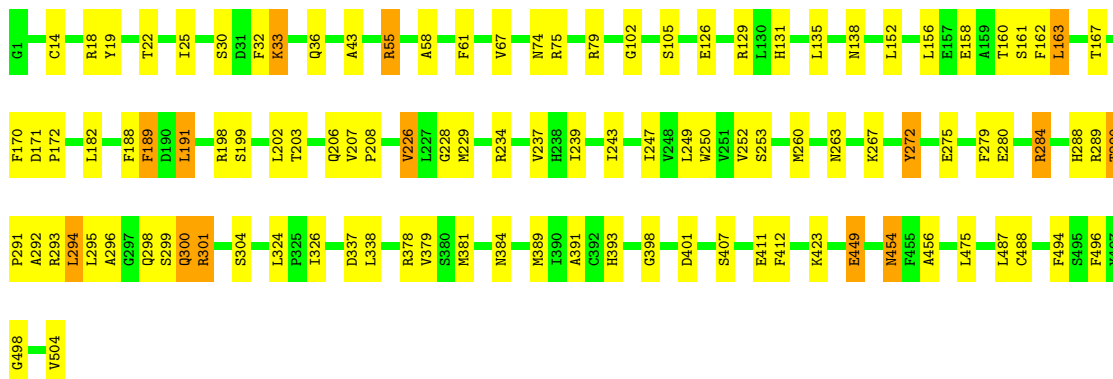
• Molecule 1: COAT PROTEIN

Chain AN:



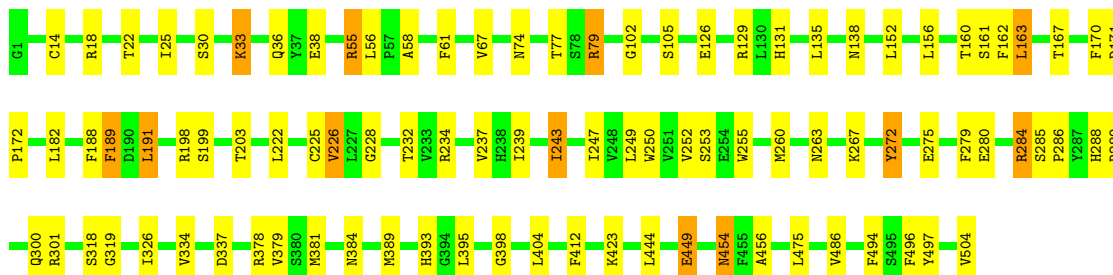
• Molecule 1: COAT PROTEIN

Chain AO:



• Molecule 1: COAT PROTEIN

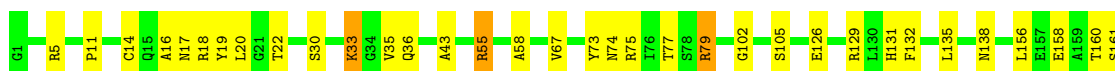
Chain AP:

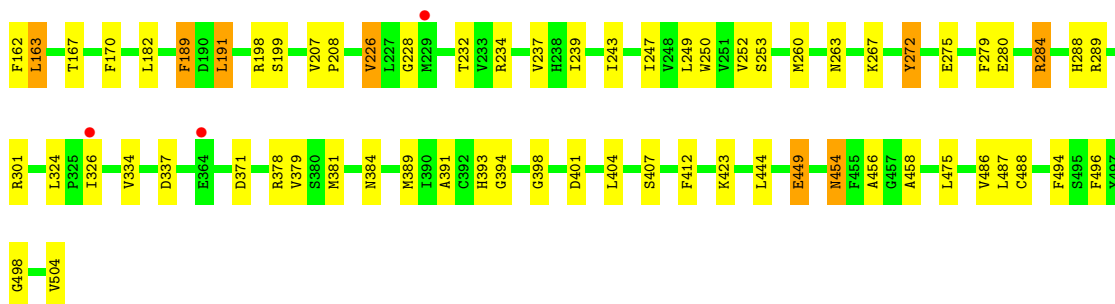


• Molecule 1: COAT PROTEIN

Chain AQ:

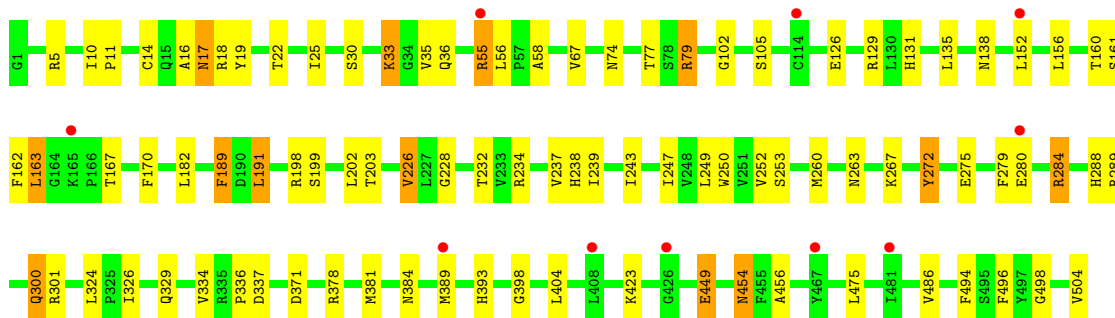






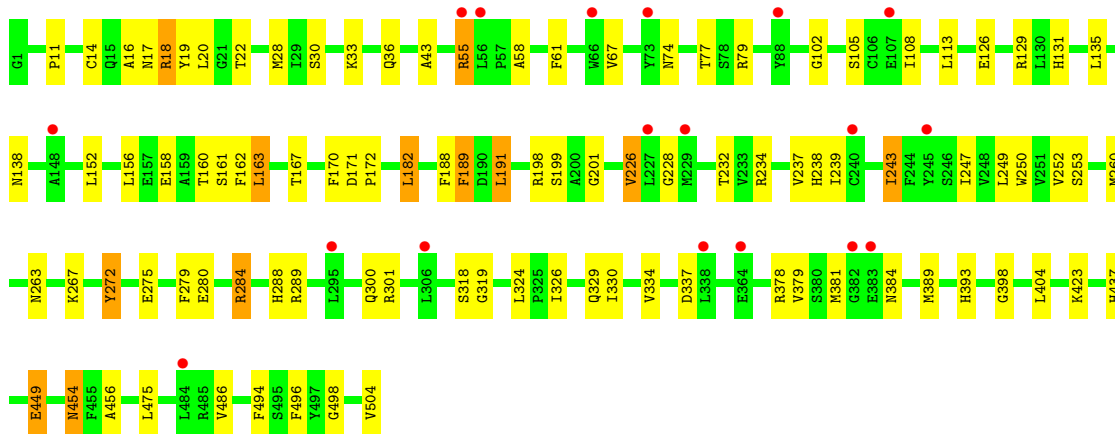
• Molecule 1: COAT PROTEIN

Chain BB: 



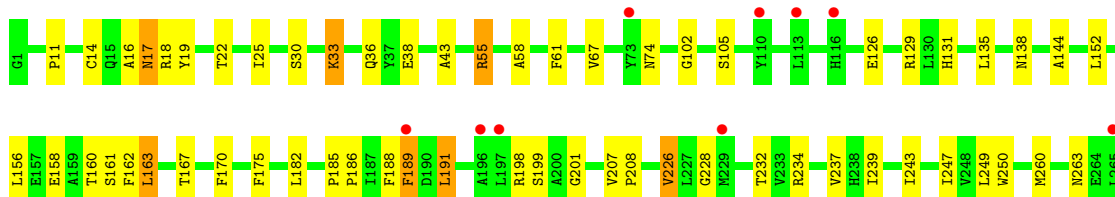
• Molecule 1: COAT PROTEIN

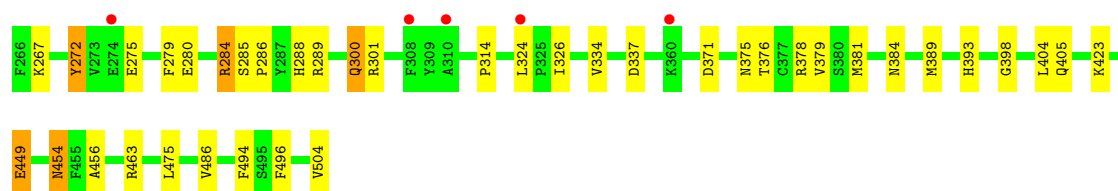
Chain BC: 



• Molecule 1: COAT PROTEIN

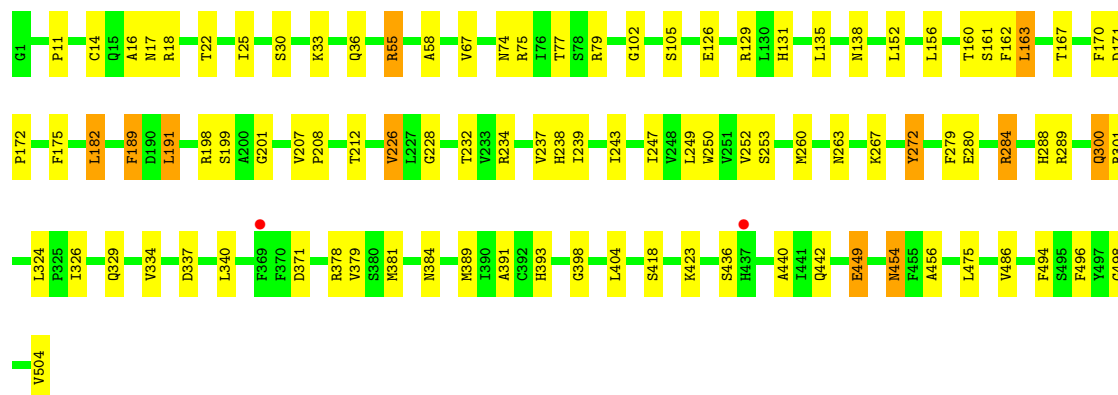
Chain BD: 





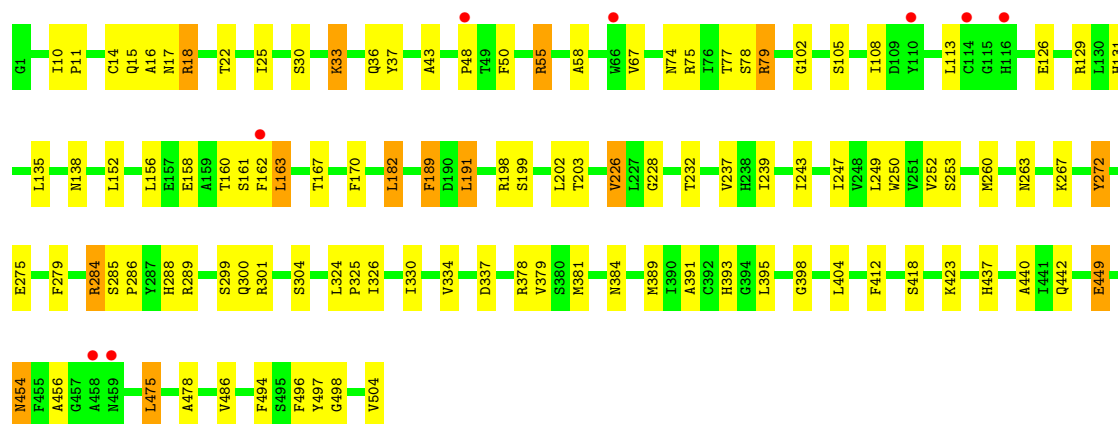
• Molecule 1: COAT PROTEIN

Chain BE:



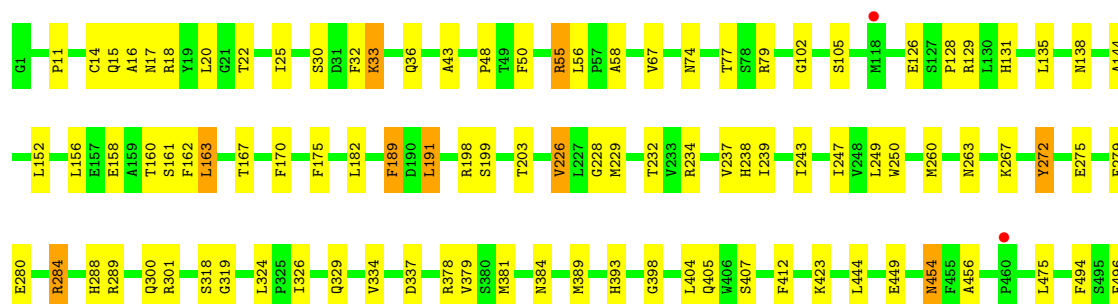
• Molecule 1: COAT PROTEIN

Chain BF:



• Molecule 1: COAT PROTEIN

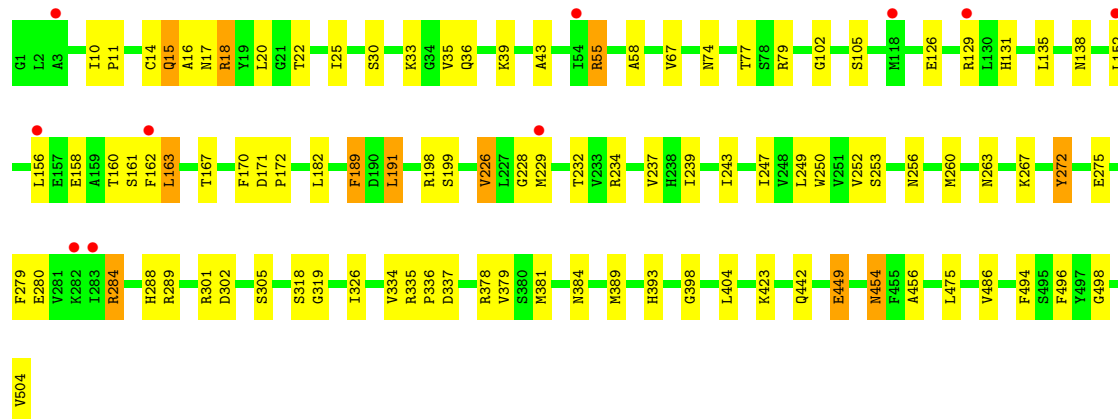
Chain BG:





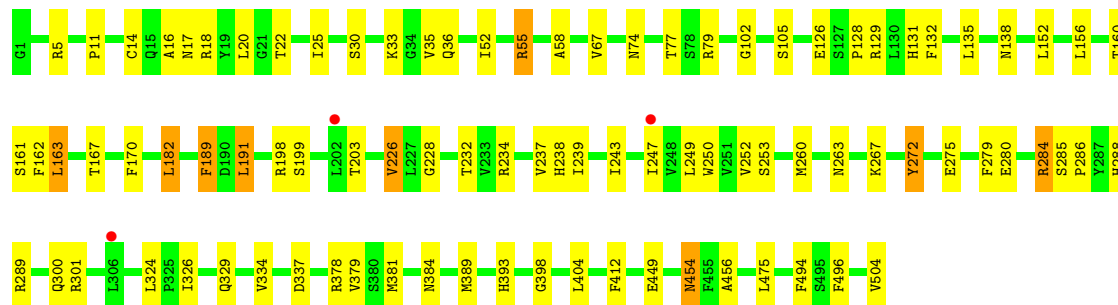
• Molecule 1: COAT PROTEIN

Chain BH:



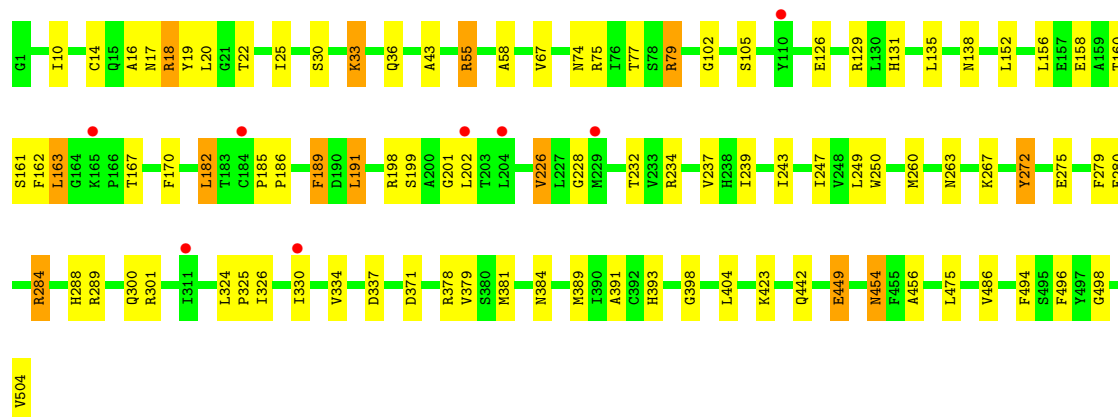
• Molecule 1: COAT PROTEIN

Chain BI:



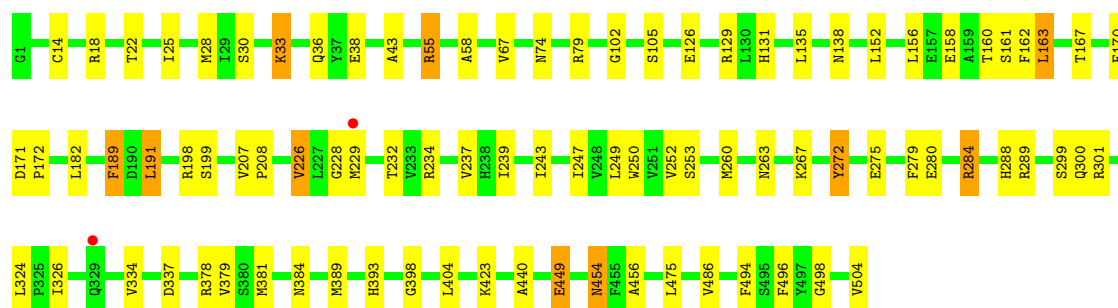
• Molecule 1: COAT PROTEIN

Chain BJ:



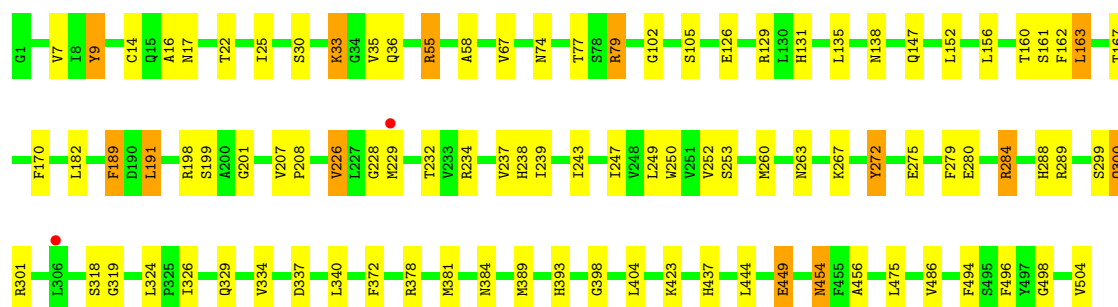
• Molecule 1: COAT PROTEIN

Chain BK:



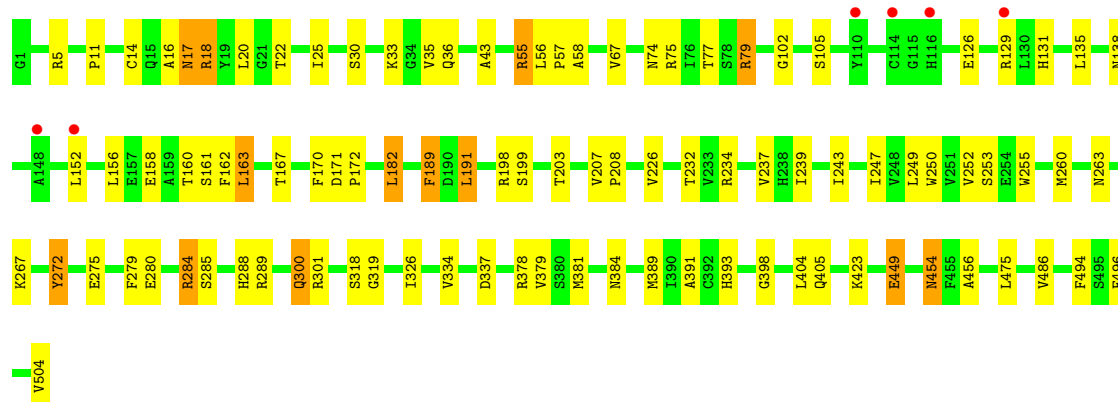
• Molecule 1: COAT PROTEIN

Chain BL:



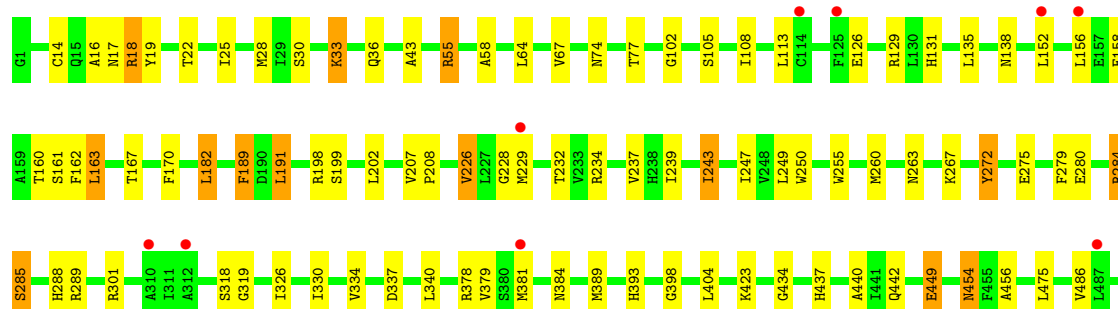
• Molecule 1: COAT PROTEIN

Chain BM:



• Molecule 1: COAT PROTEIN

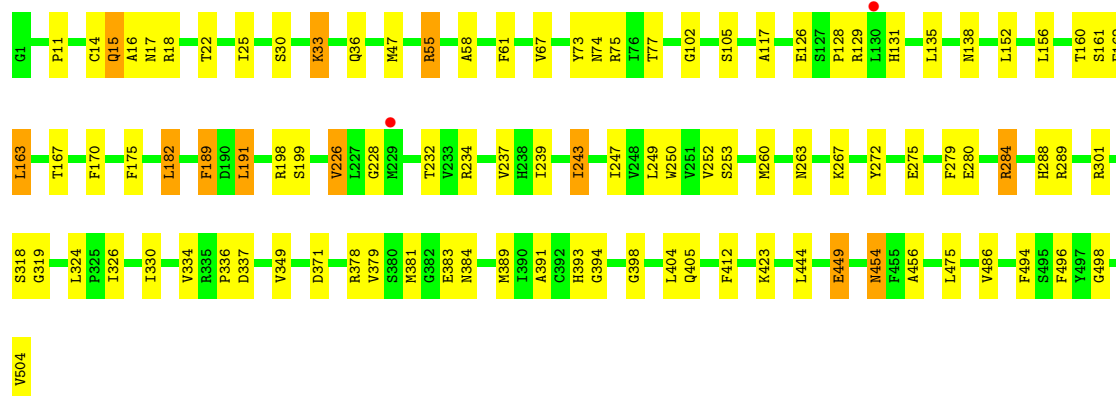
Chain BN:





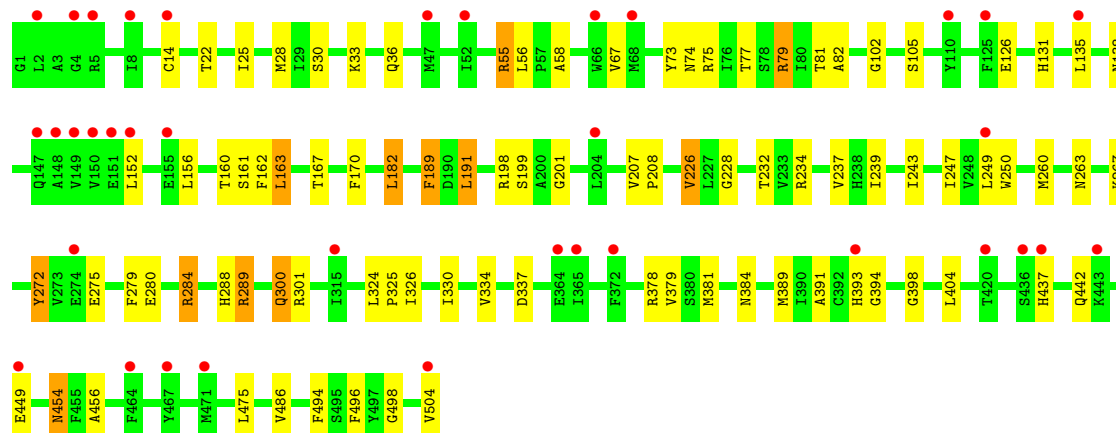
• Molecule 1: COAT PROTEIN

Chain BO:



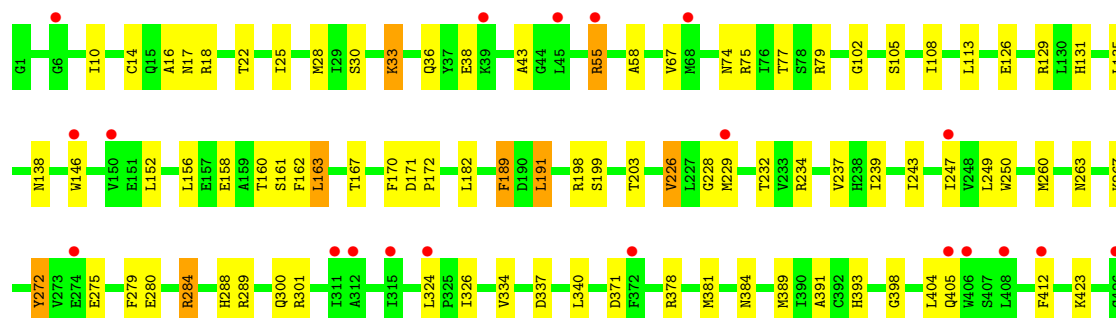
• Molecule 1: COAT PROTEIN

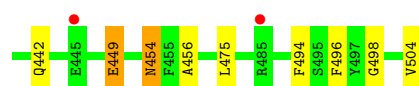
Chain BP:



• Molecule 1: COAT PROTEIN

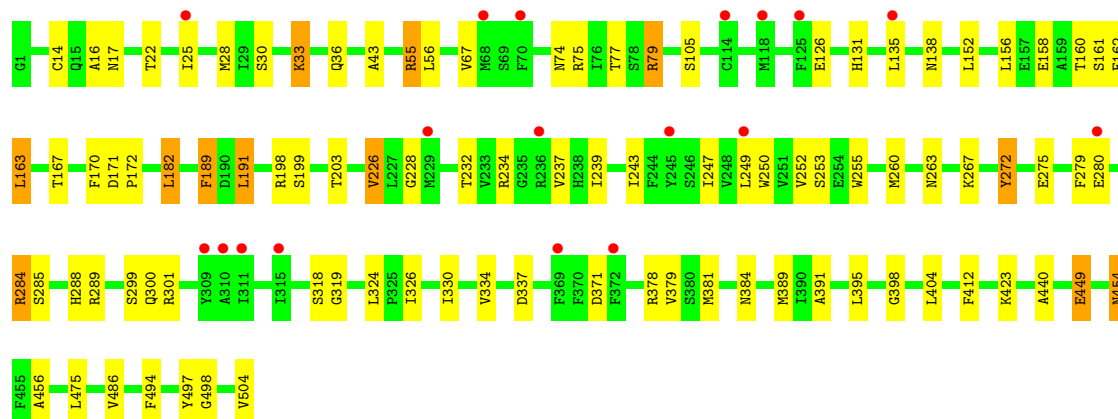
Chain BQ:





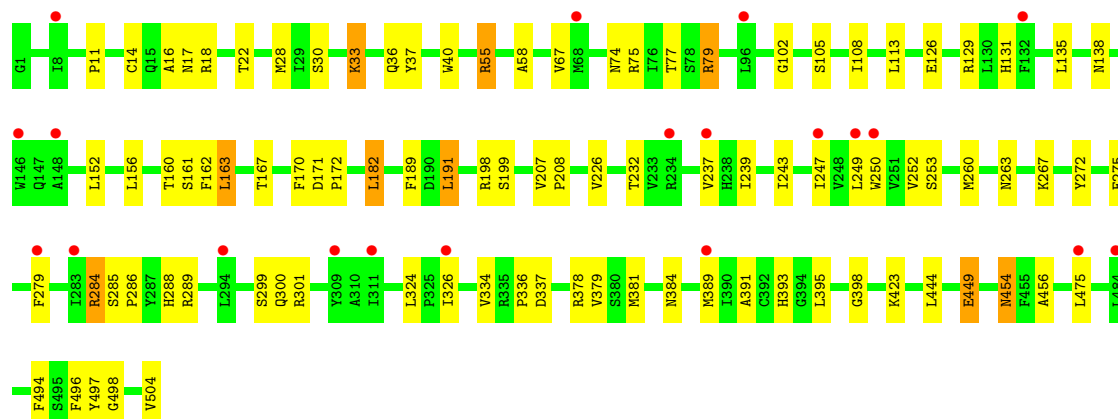
• Molecule 1: COAT PROTEIN

Chain BR:



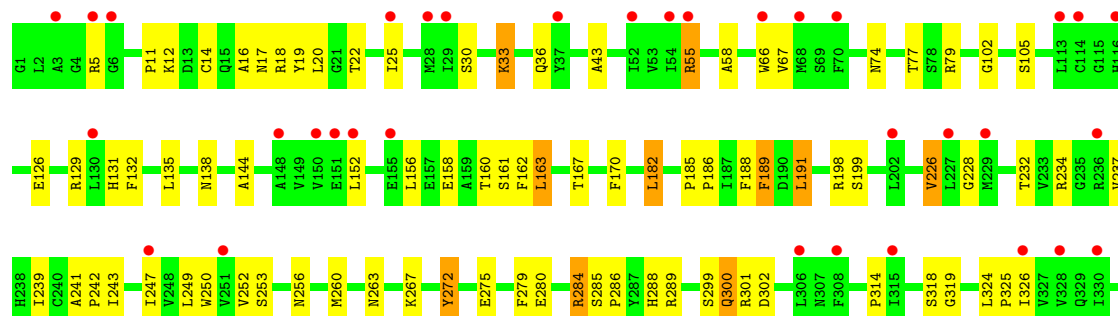
• Molecule 1: COAT PROTEIN

Chain BS:



• Molecule 1: COAT PROTEIN

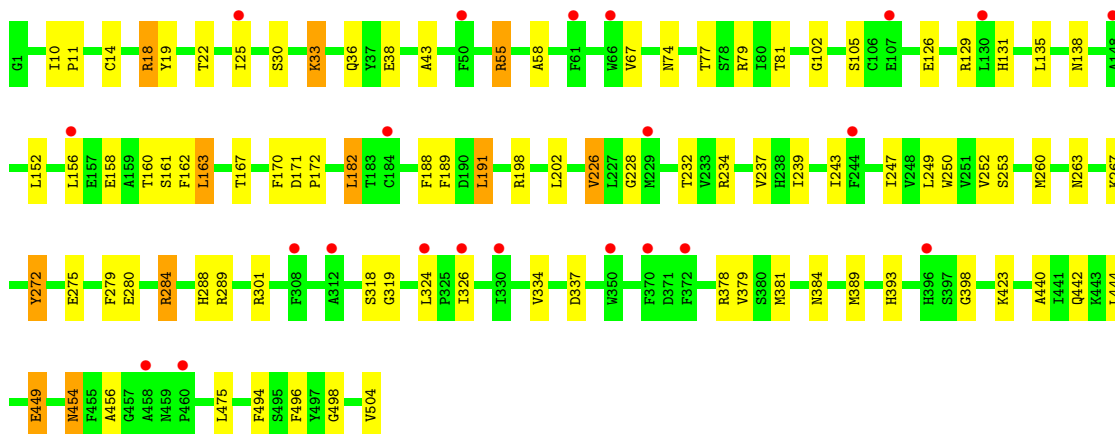
Chain BT:





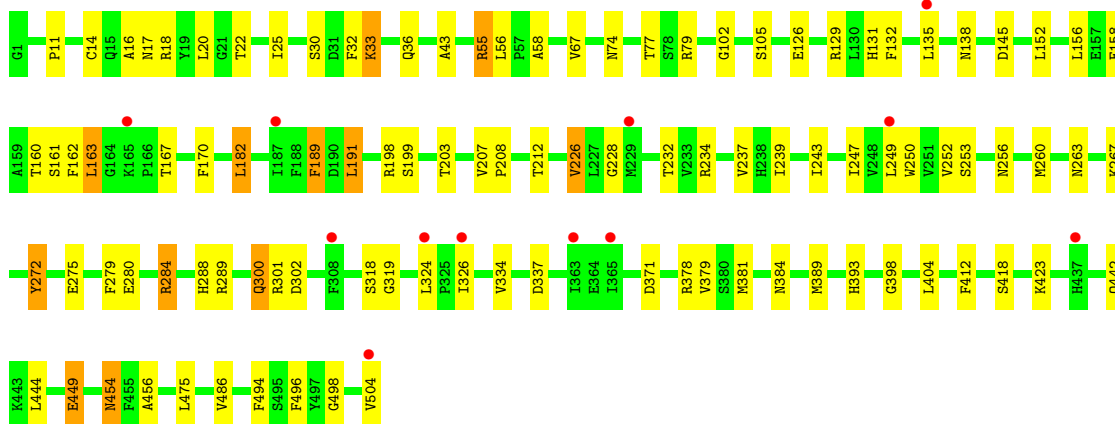
• Molecule 1: COAT PROTEIN

Chain CA:



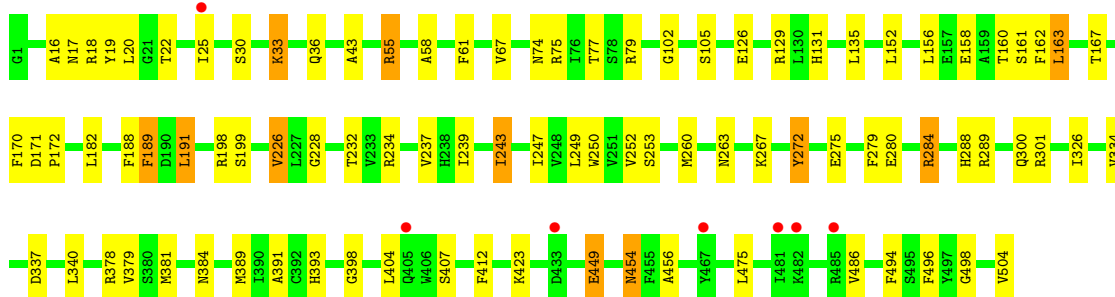
• Molecule 1: COAT PROTEIN

Chain CB:



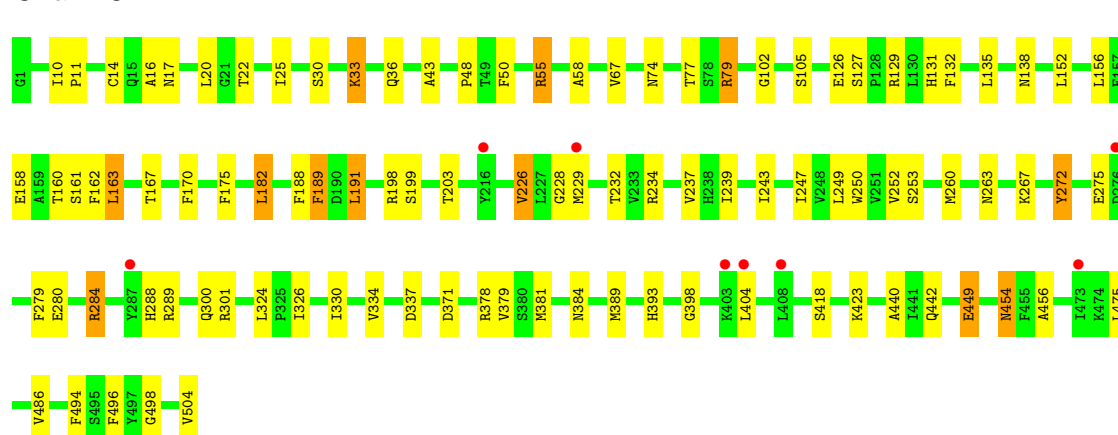
• Molecule 1: COAT PROTEIN

Chain CC:



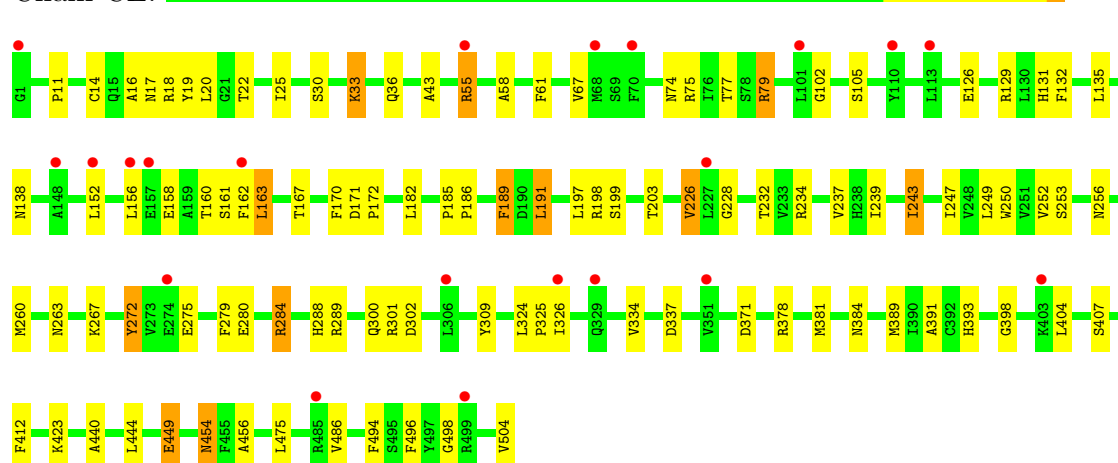
• Molecule 1: COAT PROTEIN

Chain CD:



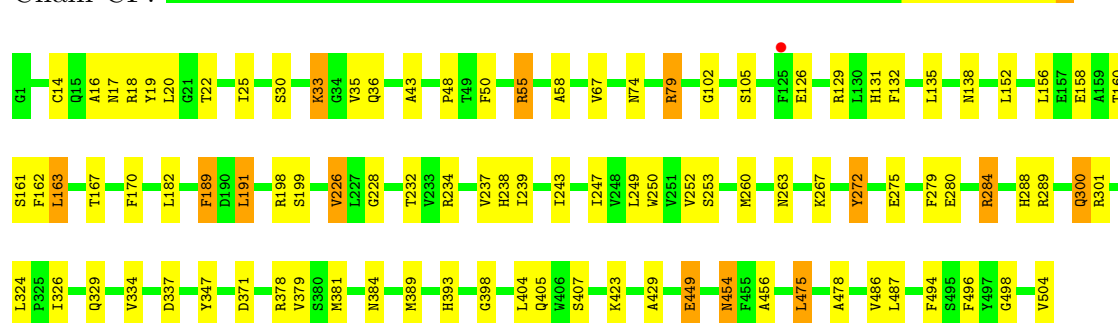
• Molecule 1: COAT PROTEIN

Chain CE:



• Molecule 1: COAT PROTEIN

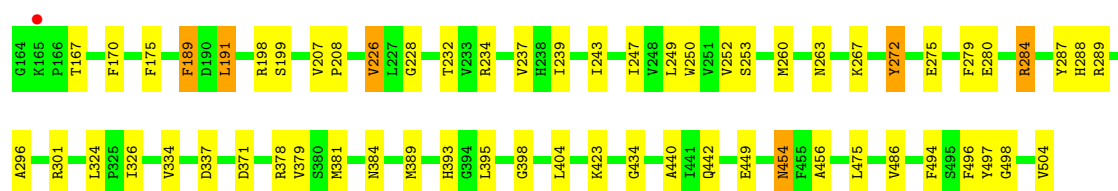
Chain CF:



• Molecule 1: COAT PROTEIN

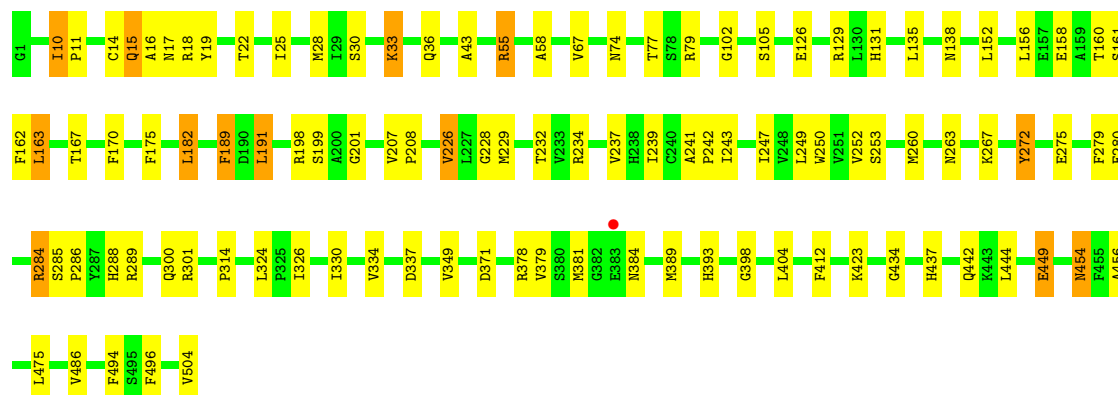
Chain CG:





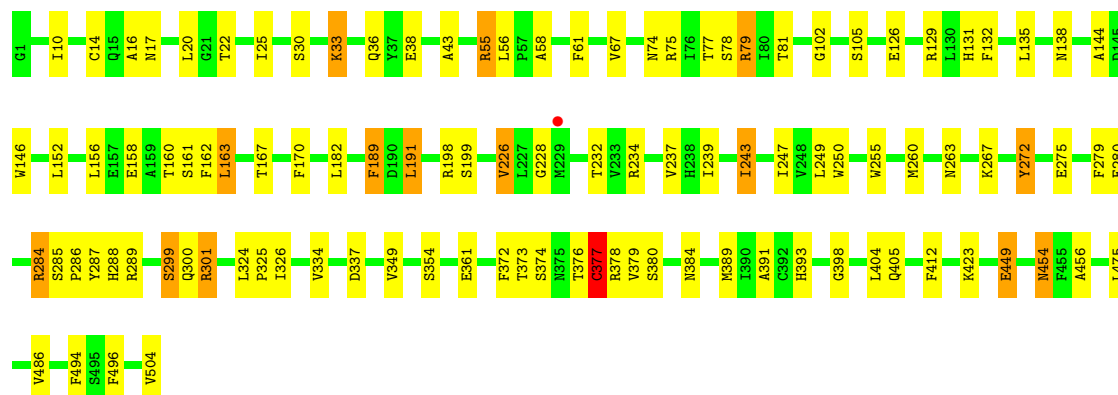
• Molecule 1: COAT PROTEIN

Chain CH:



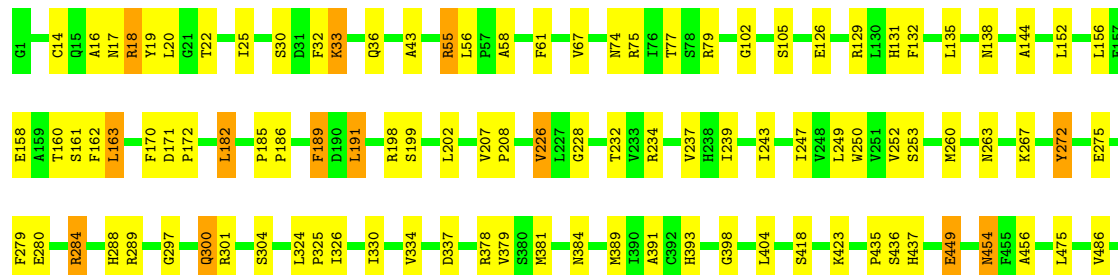
• Molecule 1: COAT PROTEIN

Chain CI:



• Molecule 1: COAT PROTEIN

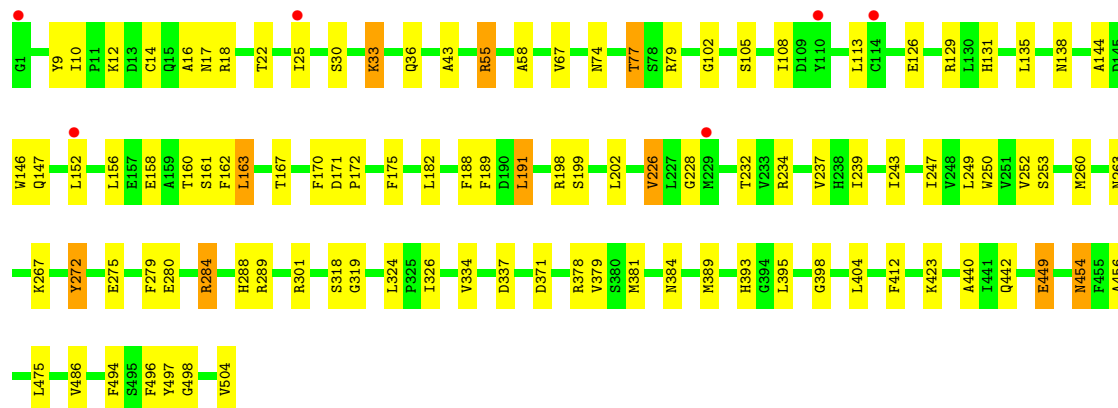
Chain CJ:





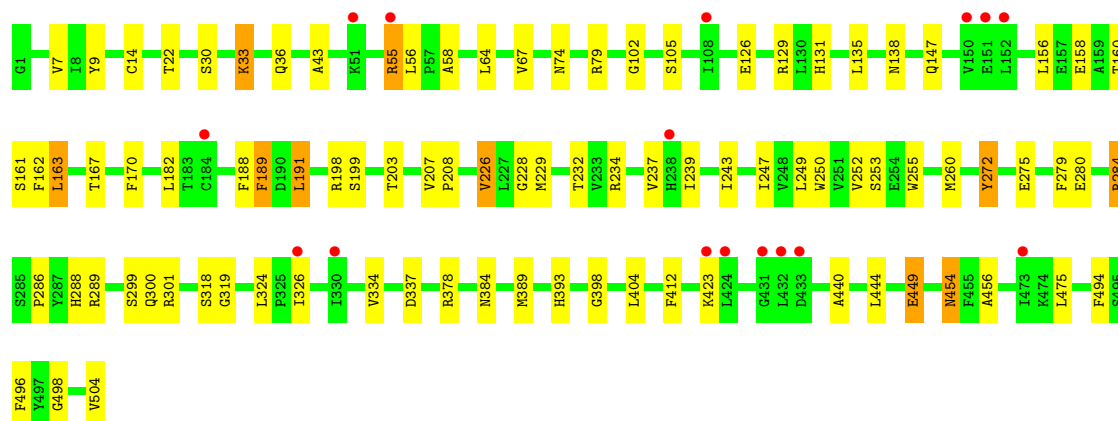
• Molecule 1: COAT PROTEIN

Chain CK:



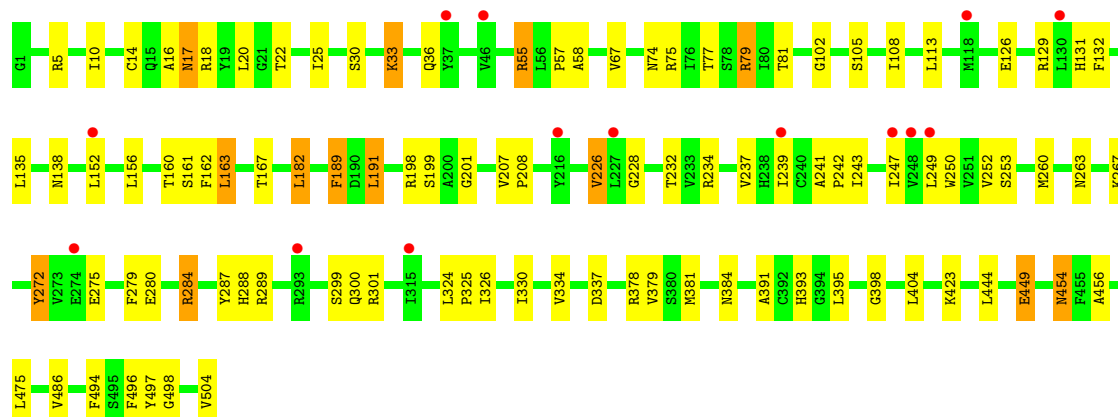
• Molecule 1: COAT PROTEIN

Chain CL:



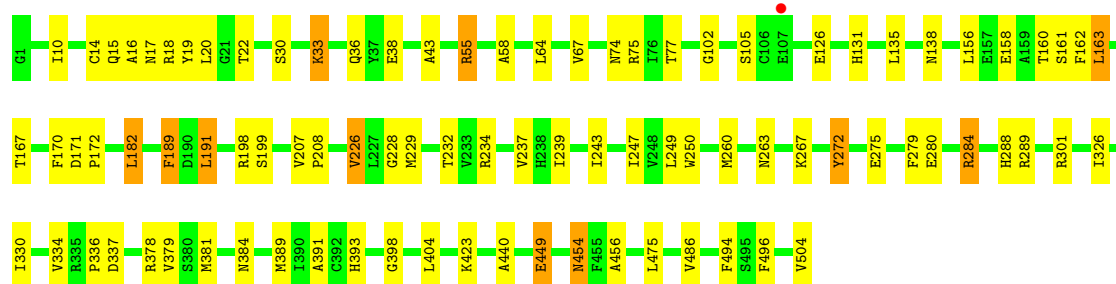
• Molecule 1: COAT PROTEIN

Chain CM:



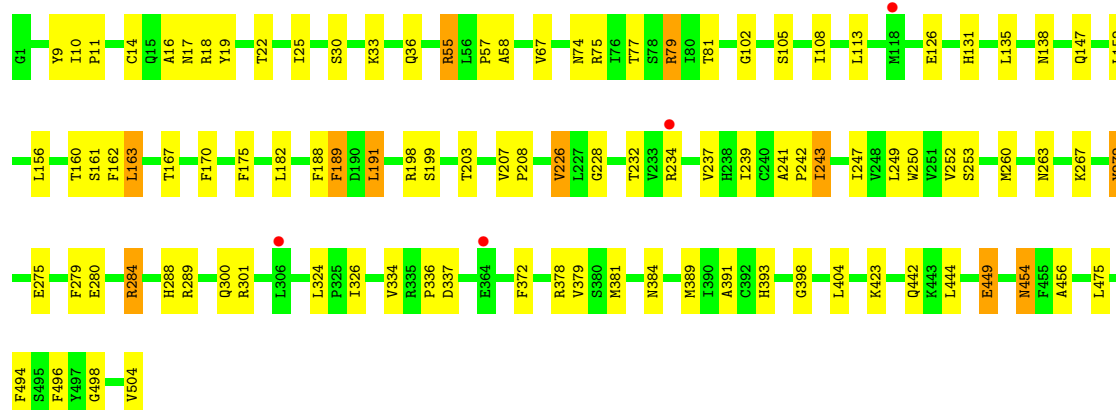
- Molecule 1: COAT PROTEIN

Chain CN:



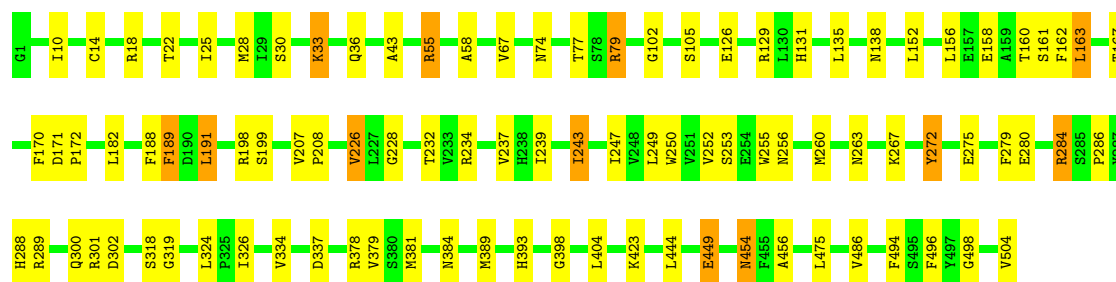
- Molecule 1: COAT PROTEIN

Chain CO:



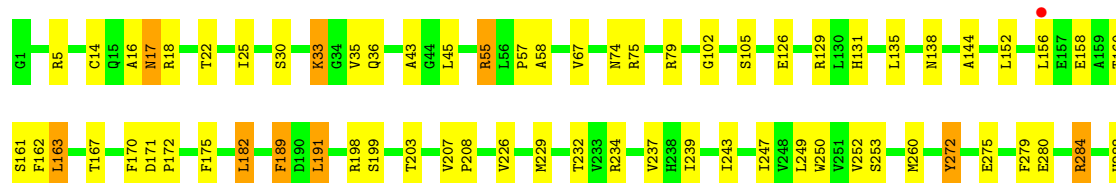
- Molecule 1: COAT PROTEIN

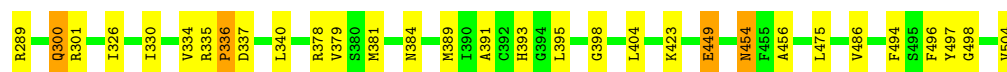
Chain CP:



- Molecule 1: COAT PROTEIN

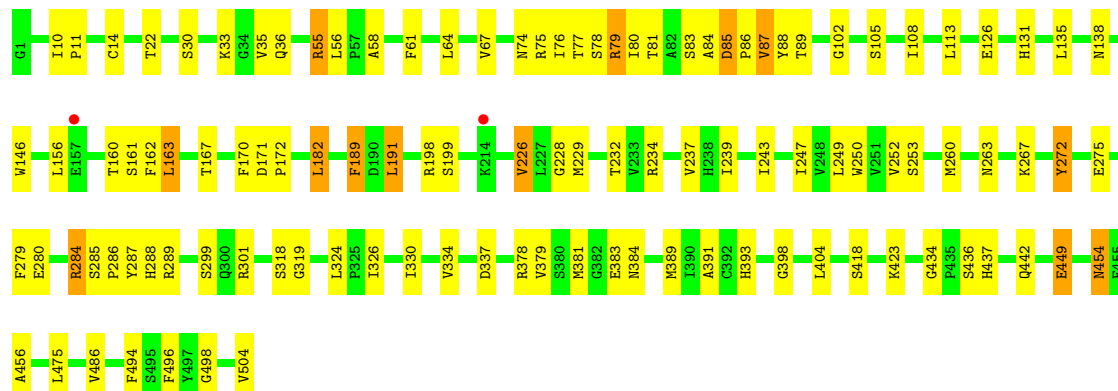
Chain CQ:





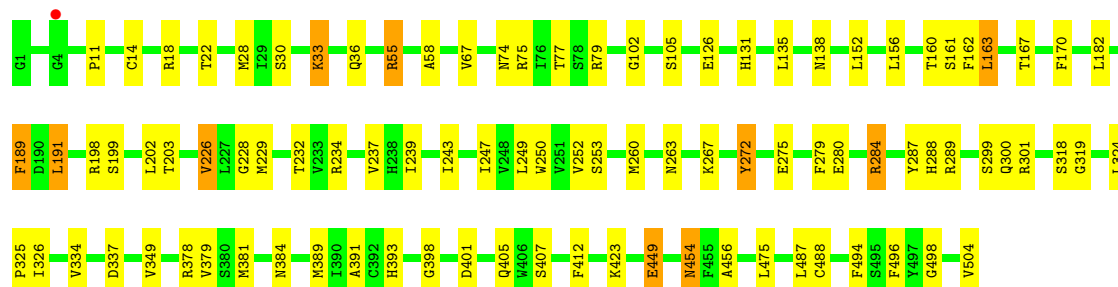
• Molecule 1: COAT PROTEIN

Chain CR:



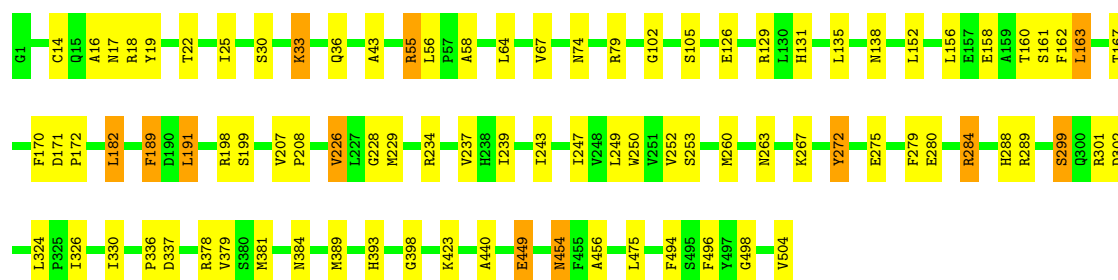
• Molecule 1: COAT PROTEIN

Chain CS:



• Molecule 1: COAT PROTEIN

Chain CT:



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 283.60Å 295.50Å 394.30Å 90.00° 91.60° 90.00° | Depositor |
| Resolution (Å) | 49.80 – 3.70 98.52 – 3.70 | Depositor EDS |
| % Data completeness (in resolution range) | 99.0 (49.80-3.70) 91.4 (98.52-3.70) | Depositor EDS |
| R_{merge} | 0.27 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.88 (at 3.67Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE) | Depositor |
| R, R_{free} | 0.232 , 0.247 0.240 , 0.245 | Depositor DCC |
| R_{free} test set | 34196 reflections (5.28%) | DCC |
| Wilson B-factor (Å ²) | 66.2 | Xtriage |
| Anisotropy | 0.406 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.33 , 42.6 | EDS |
| Estimated twinning fraction | 0.088 for -k,-h,-l 0.087 for k,h,-l 0.089 for h,-k,-l | Xtriage |
| L-test for twinning | $\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$ | Xtriage |
| Outliers | 0 of 682381 reflections | Xtriage |
| F_o, F_c correlation | 0.83 | EDS |
| Total number of atoms | 237060 | wwPDB-VP |
| Average B, all atoms (Å ²) | 91.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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 | 0.50 | 0/4058 | 0.62 | 2/5517 (0.0%) |
| 1 | AB | 0.56 | 2/4058 (0.0%) | 0.64 | 2/5517 (0.0%) |
| 1 | AC | 0.49 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AD | 0.50 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AE | 0.53 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | AF | 0.49 | 1/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | AG | 0.59 | 1/4058 (0.0%) | 0.65 | 2/5517 (0.0%) |
| 1 | AH | 0.51 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AI | 0.50 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AJ | 0.49 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AK | 0.49 | 2/4058 (0.0%) | 0.61 | 0/5517 |
| 1 | AL | 0.53 | 2/4058 (0.0%) | 0.64 | 0/5517 |
| 1 | AM | 0.51 | 2/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | AN | 0.50 | 1/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | AO | 0.57 | 2/4058 (0.0%) | 0.66 | 0/5517 |
| 1 | AP | 0.51 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | AQ | 0.50 | 1/4058 (0.0%) | 0.61 | 0/5517 |
| 1 | AR | 0.52 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | AS | 0.51 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | AT | 0.49 | 1/4058 (0.0%) | 0.61 | 0/5517 |
| 1 | BA | 0.49 | 1/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | BB | 0.52 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | BC | 0.49 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BD | 0.48 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BE | 0.50 | 2/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | BF | 0.51 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BG | 0.50 | 2/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | BH | 0.49 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BI | 0.51 | 1/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | BJ | 0.50 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BK | 0.49 | 2/4058 (0.0%) | 0.61 | 0/5517 |
| 1 | BL | 0.52 | 3/4058 (0.1%) | 0.62 | 0/5517 |
| 1 | BM | 0.53 | 3/4058 (0.1%) | 0.64 | 1/5517 (0.0%) |
| 1 | BN | 0.51 | 2/4058 (0.0%) | 0.63 | 0/5517 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|------------------|-------------|------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | BO | 0.51 | 3/4058 (0.1%) | 0.63 | 0/5517 |
| 1 | BP | 0.53 | 2/4058 (0.0%) | 0.65 | 1/5517 (0.0%) |
| 1 | BQ | 0.51 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | BR | 0.51 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | BS | 0.50 | 0/4058 | 0.62 | 0/5517 |
| 1 | BT | 0.48 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CA | 0.50 | 0/4058 | 0.62 | 0/5517 |
| 1 | CB | 0.51 | 2/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| 1 | CC | 0.49 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CD | 0.50 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CE | 0.50 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CF | 0.48 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CG | 0.51 | 1/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | CH | 0.49 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CI | 0.55 | 1/4058 (0.0%) | 0.64 | 1/5517 (0.0%) |
| 1 | CJ | 0.50 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | CK | 0.48 | 0/4058 | 0.62 | 0/5517 |
| 1 | CL | 0.52 | 2/4058 (0.0%) | 0.63 | 1/5517 (0.0%) |
| 1 | CM | 0.51 | 1/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CN | 0.51 | 1/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | CO | 0.51 | 2/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | CP | 0.52 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CQ | 0.50 | 2/4058 (0.0%) | 0.62 | 0/5517 |
| 1 | CR | 0.54 | 3/4058 (0.1%) | 0.64 | 1/5517 (0.0%) |
| 1 | CS | 0.52 | 2/4058 (0.0%) | 0.63 | 0/5517 |
| 1 | CT | 0.50 | 1/4058 (0.0%) | 0.62 | 1/5517 (0.0%) |
| All | All | 0.51 | 95/243480 (0.0%) | 0.63 | 23/331020 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | AA | 0 | 2 |
| 1 | AB | 0 | 2 |
| 1 | AC | 0 | 2 |
| 1 | AD | 0 | 1 |
| 1 | AE | 0 | 1 |
| 1 | AF | 0 | 2 |
| 1 | AG | 0 | 2 |
| 1 | AH | 0 | 2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | AI | 0 | 2 |
| 1 | AJ | 0 | 2 |
| 1 | AK | 0 | 1 |
| 1 | AL | 0 | 1 |
| 1 | AM | 0 | 2 |
| 1 | AN | 0 | 2 |
| 1 | AO | 0 | 2 |
| 1 | AP | 0 | 2 |
| 1 | AQ | 0 | 1 |
| 1 | AR | 0 | 2 |
| 1 | AS | 0 | 2 |
| 1 | AT | 0 | 2 |
| 1 | BA | 0 | 2 |
| 1 | BB | 0 | 2 |
| 1 | BC | 0 | 1 |
| 1 | BD | 0 | 2 |
| 1 | BE | 0 | 1 |
| 1 | BF | 0 | 2 |
| 1 | BG | 0 | 2 |
| 1 | BH | 0 | 1 |
| 1 | BI | 0 | 1 |
| 1 | BJ | 0 | 2 |
| 1 | BK | 0 | 2 |
| 1 | BL | 0 | 2 |
| 1 | BM | 0 | 1 |
| 1 | BN | 0 | 2 |
| 1 | BO | 0 | 2 |
| 1 | BP | 0 | 1 |
| 1 | BQ | 0 | 2 |
| 1 | BR | 0 | 2 |
| 1 | BS | 0 | 2 |
| 1 | BT | 0 | 2 |
| 1 | CA | 0 | 2 |
| 1 | CB | 0 | 2 |
| 1 | CC | 0 | 2 |
| 1 | CD | 0 | 2 |
| 1 | CE | 0 | 2 |
| 1 | CF | 0 | 2 |
| 1 | CG | 0 | 2 |
| 1 | CH | 0 | 2 |
| 1 | CI | 0 | 3 |
| 1 | CJ | 0 | 2 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | CK | 0 | 2 |
| 1 | CL | 0 | 2 |
| 1 | CM | 0 | 2 |
| 1 | CN | 0 | 2 |
| 1 | CO | 0 | 1 |
| 1 | CP | 0 | 2 |
| 1 | CQ | 0 | 2 |
| 1 | CR | 0 | 1 |
| 1 | CS | 0 | 2 |
| 1 | CT | 0 | 2 |
| All | All | 0 | 108 |

The worst 5 of 95 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | BM | 189 | PHE | CE1-CZ | -6.81 | 1.24 | 1.37 |
| 1 | AL | 189 | PHE | CE1-CZ | -6.43 | 1.25 | 1.37 |
| 1 | CJ | 189 | PHE | CE1-CZ | -6.33 | 1.25 | 1.37 |
| 1 | BL | 189 | PHE | CE1-CZ | -6.28 | 1.25 | 1.37 |
| 1 | BR | 189 | PHE | CE1-CZ | -6.26 | 1.25 | 1.37 |

The worst 5 of 23 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | AA | 284 | ARG | NE-CZ-NH2 | -5.70 | 117.45 | 120.30 |
| 1 | AG | 265 | LEU | CA-CB-CG | -5.59 | 102.45 | 115.30 |
| 1 | AB | 258 | THR | N-CA-C | -5.51 | 96.11 | 111.00 |
| 1 | CJ | 56 | LEU | CA-CB-CG | 5.46 | 127.86 | 115.30 |
| 1 | AF | 56 | LEU | CA-CB-CG | 5.33 | 127.57 | 115.30 |

There are no chirality outliers.

5 of 108 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | AA | 33 | LYS | Peptide |
| 1 | AA | 55 | ARG | Peptide |
| 1 | AB | 33 | LYS | Peptide |
| 1 | AB | 55 | ARG | Peptide |
| 1 | AC | 33 | LYS | Peptide |

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | AA | 3951 | 0 | 3909 | 93 | 0 |
| 1 | AB | 3951 | 0 | 3909 | 116 | 0 |
| 1 | AC | 3951 | 0 | 3909 | 92 | 0 |
| 1 | AD | 3951 | 0 | 3909 | 89 | 0 |
| 1 | AE | 3951 | 0 | 3909 | 89 | 0 |
| 1 | AF | 3951 | 0 | 3909 | 99 | 0 |
| 1 | AG | 3951 | 0 | 3907 | 149 | 1 |
| 1 | AH | 3951 | 0 | 3909 | 108 | 0 |
| 1 | AI | 3951 | 0 | 3909 | 113 | 5 |
| 1 | AJ | 3951 | 0 | 3909 | 109 | 1 |
| 1 | AK | 3951 | 0 | 3909 | 106 | 0 |
| 1 | AL | 3951 | 0 | 3909 | 110 | 0 |
| 1 | AM | 3951 | 0 | 3909 | 94 | 5 |
| 1 | AN | 3951 | 0 | 3909 | 111 | 1 |
| 1 | AO | 3951 | 0 | 3909 | 129 | 0 |
| 1 | AP | 3951 | 0 | 3909 | 84 | 0 |
| 1 | AQ | 3951 | 0 | 3909 | 101 | 0 |
| 1 | AR | 3951 | 0 | 3909 | 96 | 0 |
| 1 | AS | 3951 | 0 | 3909 | 92 | 0 |
| 1 | AT | 3951 | 0 | 3909 | 96 | 0 |
| 1 | BA | 3951 | 0 | 3909 | 97 | 0 |
| 1 | BB | 3951 | 0 | 3909 | 87 | 0 |
| 1 | BC | 3951 | 0 | 3909 | 80 | 0 |
| 1 | BD | 3951 | 0 | 3909 | 86 | 2 |
| 1 | BE | 3951 | 0 | 3909 | 93 | 1 |
| 1 | BF | 3951 | 0 | 3909 | 101 | 0 |
| 1 | BG | 3951 | 0 | 3909 | 108 | 2 |
| 1 | BH | 3951 | 0 | 3909 | 90 | 0 |
| 1 | BI | 3951 | 0 | 3909 | 86 | 0 |
| 1 | BJ | 3951 | 0 | 3909 | 91 | 0 |
| 1 | BK | 3951 | 0 | 3909 | 72 | 0 |
| 1 | BL | 3951 | 0 | 3909 | 90 | 0 |
| 1 | BM | 3951 | 0 | 3909 | 90 | 0 |
| 1 | BN | 3951 | 0 | 3909 | 90 | 0 |
| 1 | BO | 3951 | 0 | 3909 | 100 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 1 | BP | 3951 | 0 | 3909 | 93 | 0 |
| 1 | BQ | 3951 | 0 | 3909 | 85 | 0 |
| 1 | BR | 3951 | 0 | 3909 | 97 | 0 |
| 1 | BS | 3951 | 0 | 3909 | 81 | 0 |
| 1 | BT | 3951 | 0 | 3909 | 91 | 0 |
| 1 | CA | 3951 | 0 | 3909 | 89 | 0 |
| 1 | CB | 3951 | 0 | 3909 | 96 | 3 |
| 1 | CC | 3951 | 0 | 3909 | 85 | 0 |
| 1 | CD | 3951 | 0 | 3909 | 94 | 0 |
| 1 | CE | 3951 | 0 | 3909 | 105 | 0 |
| 1 | CF | 3951 | 0 | 3909 | 103 | 0 |
| 1 | CG | 3951 | 0 | 3909 | 89 | 0 |
| 1 | CH | 3951 | 0 | 3909 | 95 | 0 |
| 1 | CI | 3951 | 0 | 3909 | 115 | 1 |
| 1 | CJ | 3951 | 0 | 3909 | 109 | 2 |
| 1 | CK | 3951 | 0 | 3909 | 86 | 0 |
| 1 | CL | 3951 | 0 | 3909 | 83 | 0 |
| 1 | CM | 3951 | 0 | 3909 | 89 | 0 |
| 1 | CN | 3951 | 0 | 3909 | 81 | 0 |
| 1 | CO | 3951 | 0 | 3909 | 95 | 0 |
| 1 | CP | 3951 | 0 | 3909 | 94 | 0 |
| 1 | CQ | 3951 | 0 | 3909 | 88 | 0 |
| 1 | CR | 3951 | 0 | 3909 | 122 | 0 |
| 1 | CS | 3951 | 0 | 3909 | 85 | 0 |
| 1 | CT | 3951 | 0 | 3909 | 77 | 0 |
| All | All | 237060 | 0 | 234538 | 5081 | 12 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 5081 close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:AG:263:ASN:ND2 | 1:BG:32:PHE:CA | 1.68 | 1.50 |
| 1:AG:272:TYR:CE2 | 1:BG:55:ARG:CZ | 2.02 | 1.43 |
| 1:AG:272:TYR:HE2 | 1:BG:55:ARG:NE | 1.23 | 1.37 |
| 1:AN:430:MET:CE | 1:AO:296:ALA:HB2 | 1.62 | 1.29 |
| 1:AG:272:TYR:HE2 | 1:BG:55:ARG:CZ | 1.36 | 1.25 |

The worst 5 of 12 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 | Distance(Å) | Clash(Å) |
|------------------|-------------------------|-------------|----------|
| 1:BG:18:ARG:NH2 | 1:CJ:297:GLY:CA[2.646] | 1.46 | 0.74 |
| 1:BD:463:ARG:NH2 | 1:CB:145:ASP:OD2[2.545] | 1.54 | 0.66 |
| 1:AI:463:ARG:NH2 | 1:AM:360:LYS:CE[2.546] | 1.57 | 0.63 |
| 1:AJ:301:ARG:NH2 | 1:AN:411:GLU:OE2[2.546] | 1.59 | 0.61 |
| 1:AG:15:GLN:OE1 | 1:CI:81:THR:OG1[2.646] | 1.80 | 0.40 |

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | AA | 502/504 (100%) | 478 (95%) | 23 (5%) | 1 (0%) | 56 | 94 |
| 1 | AB | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 56 | 94 |
| 1 | AC | 502/504 (100%) | 480 (96%) | 20 (4%) | 2 (0%) | 43 | 90 |
| 1 | AD | 502/504 (100%) | 482 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | AE | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 56 | 94 |
| 1 | AF | 502/504 (100%) | 482 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | AG | 502/504 (100%) | 480 (96%) | 18 (4%) | 4 (1%) | 27 | 83 |
| 1 | AH | 502/504 (100%) | 481 (96%) | 19 (4%) | 2 (0%) | 43 | 90 |
| 1 | AI | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | AJ | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 56 | 94 |
| 1 | AK | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | AL | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | AM | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 56 | 94 |
| 1 | AN | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | AO | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 56 | 94 |
| 1 | AP | 502/504 (100%) | 483 (96%) | 19 (4%) | 0 | 100 | 100 |
| 1 | AQ | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 56 | 94 |
| 1 | AR | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 56 | 94 |
| 1 | AS | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 56 | 94 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 1 | AT | 502/504 (100%) | 484 (96%) | 17 (3%) | 1 (0%) | 56 | 94 |
| 1 | BA | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 56 | 94 |
| 1 | BB | 502/504 (100%) | 481 (96%) | 19 (4%) | 2 (0%) | 43 | 90 |
| 1 | BC | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | BD | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | BE | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | BF | 502/504 (100%) | 481 (96%) | 19 (4%) | 2 (0%) | 43 | 90 |
| 1 | BG | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 56 | 94 |
| 1 | BH | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | BI | 502/504 (100%) | 479 (95%) | 23 (5%) | 0 | 100 | 100 |
| 1 | BJ | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | BK | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 56 | 94 |
| 1 | BL | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | BM | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | BN | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | BO | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | BP | 502/504 (100%) | 479 (95%) | 21 (4%) | 2 (0%) | 43 | 90 |
| 1 | BQ | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | BR | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | BS | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | BT | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 56 | 94 |
| 1 | CA | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | CB | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 56 | 94 |
| 1 | CC | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | CD | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | CE | 502/504 (100%) | 483 (96%) | 18 (4%) | 1 (0%) | 56 | 94 |
| 1 | CF | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 56 | 94 |
| 1 | CG | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 56 | 94 |
| 1 | CH | 502/504 (100%) | 481 (96%) | 21 (4%) | 0 | 100 | 100 |
| 1 | CI | 502/504 (100%) | 481 (96%) | 19 (4%) | 2 (0%) | 43 | 90 |
| 1 | CJ | 502/504 (100%) | 484 (96%) | 17 (3%) | 1 (0%) | 56 | 94 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|--------------------|-------------|-----------|----------|-------------|-----|
| 1 | CK | 502/504 (100%) | 482 (96%) | 19 (4%) | 1 (0%) | 56 | 94 |
| 1 | CL | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | CM | 502/504 (100%) | 480 (96%) | 20 (4%) | 2 (0%) | 43 | 90 |
| 1 | CN | 502/504 (100%) | 482 (96%) | 20 (4%) | 0 | 100 | 100 |
| 1 | CO | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | CP | 502/504 (100%) | 480 (96%) | 21 (4%) | 1 (0%) | 56 | 94 |
| 1 | CQ | 502/504 (100%) | 482 (96%) | 18 (4%) | 2 (0%) | 43 | 90 |
| 1 | CR | 502/504 (100%) | 479 (95%) | 21 (4%) | 2 (0%) | 43 | 90 |
| 1 | CS | 502/504 (100%) | 481 (96%) | 20 (4%) | 1 (0%) | 56 | 94 |
| 1 | CT | 502/504 (100%) | 479 (95%) | 22 (4%) | 1 (0%) | 56 | 94 |
| All | All | 30120/30240 (100%) | 28873 (96%) | 1181 (4%) | 66 (0%) | 56 | 94 |

5 of 66 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BP | 82 | ALA |
| 1 | CR | 87 | VAL |
| 1 | AG | 273 | VAL |
| 1 | CI | 377 | CYS |
| 1 | BM | 17 | ASN |

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 | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | AB | 430/430 (100%) | 402 (94%) | 28 (6%) | 24 | 73 |
| 1 | AC | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | AD | 430/430 (100%) | 404 (94%) | 26 (6%) | 27 | 76 |
| 1 | AE | 430/430 (100%) | 409 (95%) | 21 (5%) | 35 | 82 |
| 1 | AF | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | AG | 430/430 (100%) | 403 (94%) | 27 (6%) | 25 | 75 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | AH | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | AI | 430/430 (100%) | 405 (94%) | 25 (6%) | 28 | 76 |
| 1 | AJ | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | AK | 430/430 (100%) | 404 (94%) | 26 (6%) | 27 | 76 |
| 1 | AL | 430/430 (100%) | 404 (94%) | 26 (6%) | 27 | 76 |
| 1 | AM | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | AN | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | AO | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | AP | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | AQ | 430/430 (100%) | 405 (94%) | 25 (6%) | 28 | 76 |
| 1 | AR | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | AS | 430/430 (100%) | 405 (94%) | 25 (6%) | 28 | 76 |
| 1 | AT | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | BA | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | BB | 430/430 (100%) | 405 (94%) | 25 (6%) | 28 | 76 |
| 1 | BC | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | BD | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | BE | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | BF | 430/430 (100%) | 404 (94%) | 26 (6%) | 27 | 76 |
| 1 | BG | 430/430 (100%) | 408 (95%) | 22 (5%) | 33 | 81 |
| 1 | BH | 430/430 (100%) | 404 (94%) | 26 (6%) | 27 | 76 |
| 1 | BI | 430/430 (100%) | 408 (95%) | 22 (5%) | 33 | 81 |
| 1 | BJ | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | BK | 430/430 (100%) | 404 (94%) | 26 (6%) | 27 | 76 |
| 1 | BL | 430/430 (100%) | 404 (94%) | 26 (6%) | 27 | 76 |
| 1 | BM | 430/430 (100%) | 404 (94%) | 26 (6%) | 27 | 76 |
| 1 | BN | 430/430 (100%) | 405 (94%) | 25 (6%) | 28 | 76 |
| 1 | BO | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | BP | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | BQ | 430/430 (100%) | 405 (94%) | 25 (6%) | 28 | 76 |
| 1 | BR | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------------|-------------|-----------|-------------|----|
| 1 | BS | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | BT | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | CA | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | CB | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | CC | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | CD | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | CE | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | CF | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | CG | 430/430 (100%) | 409 (95%) | 21 (5%) | 35 | 82 |
| 1 | CH | 430/430 (100%) | 405 (94%) | 25 (6%) | 28 | 76 |
| 1 | CI | 430/430 (100%) | 405 (94%) | 25 (6%) | 28 | 76 |
| 1 | CJ | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | CK | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | CL | 430/430 (100%) | 406 (94%) | 24 (6%) | 30 | 78 |
| 1 | CM | 430/430 (100%) | 403 (94%) | 27 (6%) | 25 | 75 |
| 1 | CN | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | CO | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | CP | 430/430 (100%) | 405 (94%) | 25 (6%) | 28 | 76 |
| 1 | CQ | 430/430 (100%) | 403 (94%) | 27 (6%) | 25 | 75 |
| 1 | CR | 430/430 (100%) | 404 (94%) | 26 (6%) | 27 | 76 |
| 1 | CS | 430/430 (100%) | 407 (95%) | 23 (5%) | 32 | 80 |
| 1 | CT | 430/430 (100%) | 405 (94%) | 25 (6%) | 28 | 76 |
| All | All | 25800/25800 (100%) | 24348 (94%) | 1452 (6%) | 30 | 78 |

5 of 1452 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BH | 105 | SER |
| 1 | BN | 191 | LEU |
| 1 | CP | 284 | ARG |
| 1 | BH | 449 | GLU |
| 1 | BK | 229 | MET |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 653 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | BG | 300 | GLN |
| 1 | BN | 238 | HIS |
| 1 | CP | 263 | ASN |
| 1 | BH | 256 | ASN |
| 1 | BK | 138 | ASN |

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1 | AA | 504/504 (100%) | 0.41 | 3 (0%) 86 69 | 51, 87, 117, 148 | 0 |
| 1 | AB | 504/504 (100%) | 0.42 | 2 (0%) 90 78 | 55, 90, 122, 148 | 0 |
| 1 | AC | 504/504 (100%) | 0.35 | 1 (0%) 93 86 | 42, 76, 104, 147 | 0 |
| 1 | AD | 504/504 (100%) | 0.36 | 0 100 100 | 33, 68, 99, 130 | 0 |
| 1 | AE | 504/504 (100%) | 0.34 | 0 100 100 | 46, 75, 105, 119 | 0 |
| 1 | AF | 504/504 (100%) | 0.37 | 0 100 100 | 41, 80, 110, 166 | 0 |
| 1 | AG | 504/504 (100%) | 0.35 | 1 (0%) 93 86 | 46, 83, 118, 165 | 0 |
| 1 | AH | 504/504 (100%) | 0.34 | 0 100 100 | 44, 74, 105, 131 | 0 |
| 1 | AI | 504/504 (100%) | 0.35 | 0 100 100 | 29, 65, 98, 141 | 0 |
| 1 | AJ | 504/504 (100%) | 0.32 | 0 100 100 | 34, 67, 99, 137 | 0 |
| 1 | AK | 504/504 (100%) | 0.31 | 2 (0%) 90 78 | 37, 72, 104, 142 | 0 |
| 1 | AL | 504/504 (100%) | 0.34 | 0 100 100 | 31, 67, 94, 131 | 0 |
| 1 | AM | 504/504 (100%) | 0.35 | 0 100 100 | 32, 65, 96, 117 | 0 |
| 1 | AN | 504/504 (100%) | 0.34 | 0 100 100 | 29, 64, 94, 128 | 0 |
| 1 | AO | 504/504 (100%) | 0.35 | 0 100 100 | 34, 66, 93, 124 | 0 |
| 1 | AP | 504/504 (100%) | 0.30 | 0 100 100 | 34, 69, 97, 124 | 0 |
| 1 | AQ | 504/504 (100%) | 0.31 | 0 100 100 | 28, 60, 88, 111 | 0 |
| 1 | AR | 504/504 (100%) | 0.30 | 0 100 100 | 23, 57, 89, 120 | 0 |
| 1 | AS | 504/504 (100%) | 0.27 | 0 100 100 | 30, 60, 92, 124 | 0 |
| 1 | AT | 504/504 (100%) | 0.31 | 0 100 100 | 35, 69, 100, 141 | 0 |
| 1 | BA | 504/504 (100%) | 0.47 | 3 (0%) 86 69 | 47, 90, 125, 207 | 0 |
| 1 | BB | 504/504 (100%) | 0.57 | 10 (1%) 62 39 | 67, 105, 138, 173 | 0 |
| 1 | BC | 504/504 (100%) | 0.67 | 18 (3%) 41 26 | 71, 114, 149, 205 | 0 |
| 1 | BD | 504/504 (100%) | 0.61 | 14 (2%) 50 31 | 62, 104, 133, 170 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1 | BE | 504/504 (100%) | 0.50 | 2 (0%) 90 78 | 48, 89, 122, 158 | 0 |
| 1 | BF | 504/504 (100%) | 0.62 | 8 (1%) 68 45 | 63, 99, 131, 191 | 0 |
| 1 | BG | 504/504 (100%) | 0.53 | 2 (0%) 90 78 | 59, 93, 125, 154 | 0 |
| 1 | BH | 504/504 (100%) | 0.62 | 10 (1%) 62 39 | 48, 95, 130, 160 | 0 |
| 1 | BI | 504/504 (100%) | 0.56 | 3 (0%) 86 69 | 65, 108, 143, 170 | 0 |
| 1 | BJ | 504/504 (100%) | 0.64 | 8 (1%) 68 45 | 70, 109, 140, 195 | 0 |
| 1 | BK | 504/504 (100%) | 0.43 | 2 (0%) 90 78 | 47, 85, 116, 178 | 0 |
| 1 | BL | 504/504 (100%) | 0.46 | 2 (0%) 90 78 | 42, 75, 105, 152 | 0 |
| 1 | BM | 504/504 (100%) | 0.55 | 6 (1%) 75 52 | 45, 85, 121, 181 | 0 |
| 1 | BN | 504/504 (100%) | 0.57 | 10 (1%) 62 39 | 59, 98, 129, 176 | 0 |
| 1 | BO | 504/504 (100%) | 0.49 | 2 (0%) 90 78 | 56, 98, 127, 161 | 0 |
| 1 | BP | 504/504 (100%) | 0.82 | 36 (7%) 16 11 | 77, 124, 163, 199 | 0 |
| 1 | BQ | 504/504 (100%) | 0.70 | 22 (4%) 33 21 | 78, 122, 162, 199 | 0 |
| 1 | BR | 504/504 (100%) | 0.70 | 18 (3%) 41 26 | 76, 116, 149, 189 | 0 |
| 1 | BS | 504/504 (100%) | 0.70 | 20 (3%) 36 23 | 73, 117, 152, 210 | 0 |
| 1 | BT | 504/504 (100%) | 0.90 | 52 (10%) 7 7 | 87, 127, 161, 200 | 0 |
| 1 | CA | 504/504 (100%) | 0.69 | 22 (4%) 33 21 | 76, 120, 153, 177 | 0 |
| 1 | CB | 504/504 (100%) | 0.62 | 12 (2%) 56 35 | 68, 106, 141, 177 | 0 |
| 1 | CC | 504/504 (100%) | 0.66 | 7 (1%) 72 48 | 55, 102, 137, 204 | 0 |
| 1 | CD | 504/504 (100%) | 0.61 | 8 (1%) 68 45 | 68, 105, 141, 173 | 0 |
| 1 | CE | 504/504 (100%) | 0.69 | 21 (4%) 35 22 | 72, 119, 149, 191 | 0 |
| 1 | CF | 504/504 (100%) | 0.43 | 1 (0%) 93 86 | 41, 85, 115, 151 | 0 |
| 1 | CG | 504/504 (100%) | 0.47 | 2 (0%) 90 78 | 57, 88, 121, 163 | 0 |
| 1 | CH | 504/504 (100%) | 0.47 | 1 (0%) 93 86 | 58, 90, 124, 179 | 0 |
| 1 | CI | 504/504 (100%) | 0.47 | 1 (0%) 93 86 | 44, 84, 121, 188 | 0 |
| 1 | CJ | 504/504 (100%) | 0.40 | 0 100 100 | 44, 77, 110, 151 | 0 |
| 1 | CK | 504/504 (100%) | 0.54 | 6 (1%) 75 52 | 61, 103, 133, 150 | 0 |
| 1 | CL | 504/504 (100%) | 0.64 | 16 (3%) 45 28 | 68, 114, 148, 184 | 0 |
| 1 | CM | 504/504 (100%) | 0.61 | 14 (2%) 50 31 | 64, 111, 141, 187 | 0 |
| 1 | CN | 504/504 (100%) | 0.46 | 1 (0%) 93 86 | 62, 97, 127, 171 | 0 |
| 1 | CO | 504/504 (100%) | 0.54 | 4 (0%) 83 63 | 59, 91, 126, 157 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|--------------------|--------|----------------|-----------------------|-------|
| 1 | CP | 504/504 (100%) | 0.38 | 0 100 100 | 41, 73, 105, 133 | 0 |
| 1 | CQ | 504/504 (100%) | 0.42 | 1 (0%) 93 86 | 46, 76, 112, 171 | 0 |
| 1 | CR | 504/504 (100%) | 0.49 | 2 (0%) 90 78 | 45, 84, 114, 172 | 0 |
| 1 | CS | 504/504 (100%) | 0.49 | 1 (0%) 93 86 | 45, 86, 119, 153 | 0 |
| 1 | CT | 504/504 (100%) | 0.42 | 0 100 100 | 52, 82, 111, 136 | 0 |
| All | All | 30240/30240 (100%) | 0.49 | 377 (1%) 75 52 | 23, 89, 135, 210 | 0 |

The worst 5 of 377 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | CC | 405 | GLN | 4.2 |
| 1 | BT | 6 | GLY | 4.1 |
| 1 | BC | 383 | GLU | 4.1 |
| 1 | CL | 432 | LEU | 4.1 |
| 1 | BC | 56 | LEU | 4.0 |

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.