



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:20 PM UTC

PDB ID : 4V5W / pdb_00004v5w
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 X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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>.

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

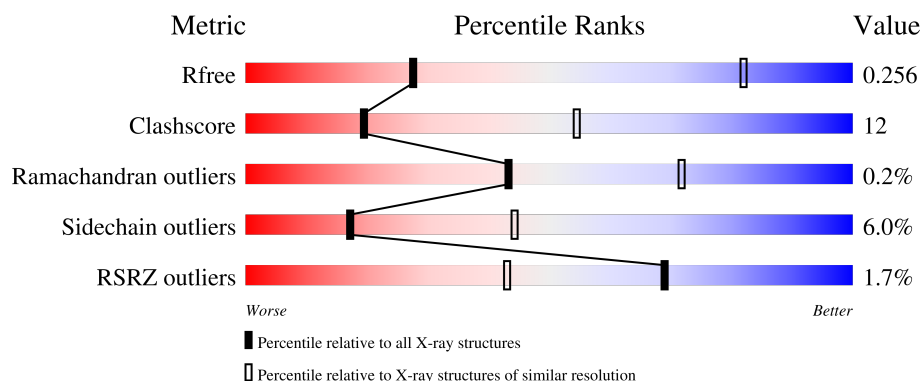
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.



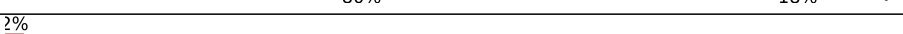
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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 ≥ 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	504	79% 19% .
1	AB	504	78% 18% .
1	AC	504	79% 18% .
1	AD	504	81% 17% .
1	AE	504	81% 17% .

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Mol	Chain	Length	Quality of chain
1	AF	504	 79% 19% .
1	AG	504	 76% 19% 5% .
1	AH	504	 77% 20% .
1	AI	504	 78% 18% .
1	AJ	504	 78% 19% .
1	AK	504	 78% 19% .
1	AL	504	 79% 19% .
1	AM	504	 80% 18% .
1	AN	504	 77% 20% .
1	AO	504	 77% 19% .
1	AP	504	 80% 17% .
1	AQ	504	 77% 20% .
1	AR	504	 79% 18% .
1	AS	504	 81% 16% .
1	AT	504	 80% 18% .
1	BA	504	 2% 79% 19% .
1	BB	504	 4% 81% 16% .
1	BC	504	 5% 79% 18% .
1	BD	504	 3% 79% 18% .
1	BE	504	 1% 79% 18% .
1	BF	504	 2% 77% 20% .
1	BG	504	 2% 80% 18% .
1	BH	504	 2% 80% 17% .
1	BI	504	 2% 81% 17% .
1	BJ	504	 3% 80% 17% .

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Mol	Chain	Length	Quality of chain
1	BK	504	 82% 16% .
1	BL	504	 79% 18% .
1	BM	504	 80% 17% .
1	BN	504	 80% 17% .
1	BO	504	 79% 18% .
1	BP	504	 81% 16% .
1	BQ	504	 81% 17% .
1	BR	504	 80% 17% .
1	BS	504	 80% 18% .
1	BT	504	 79% 19% .
1	CA	504	 81% 16% .
1	CB	504	 79% 18% .
1	CC	504	 81% 16% .
1	CD	504	 80% 17% .
1	CE	504	 78% 19% .
1	CF	504	 80% 17% .
1	CG	504	 80% 18% .
1	CH	504	 78% 19% .
1	CI	504	 77% 19% .
1	CJ	504	 78% 19% .
1	CK	504	 79% 19% .
1	CL	504	 81% 17% .
1	CM	504	 79% 19% .
1	CN	504	 81% 17% .
1	CO	504	 79% 19% .

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Mol	Chain	Length	Quality of chain
1	CP	504	 80% 17% .
1	CQ	504	%  80% 18% .
1	CR	504	%  77% 20% .
1	CS	504	%  80% 17% .
1	CT	504	 81% 16% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 237060 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	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			

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

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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

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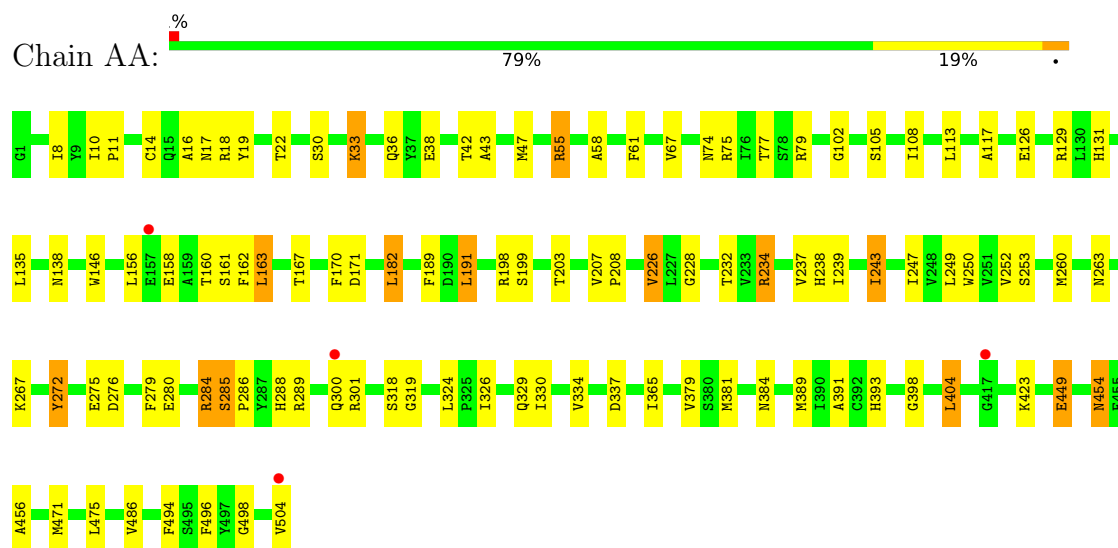
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CS	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			
1	CT	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			

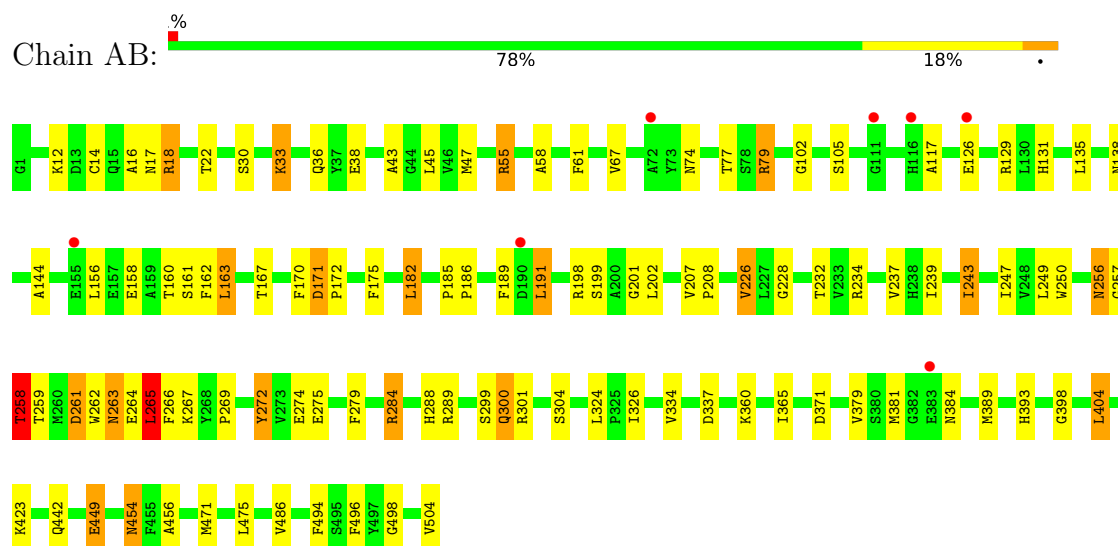
3 Residue-property plots [i](#)

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

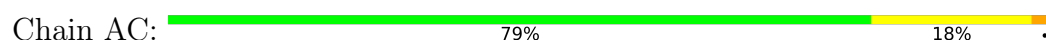
• Molecule 1: COAT PROTEIN

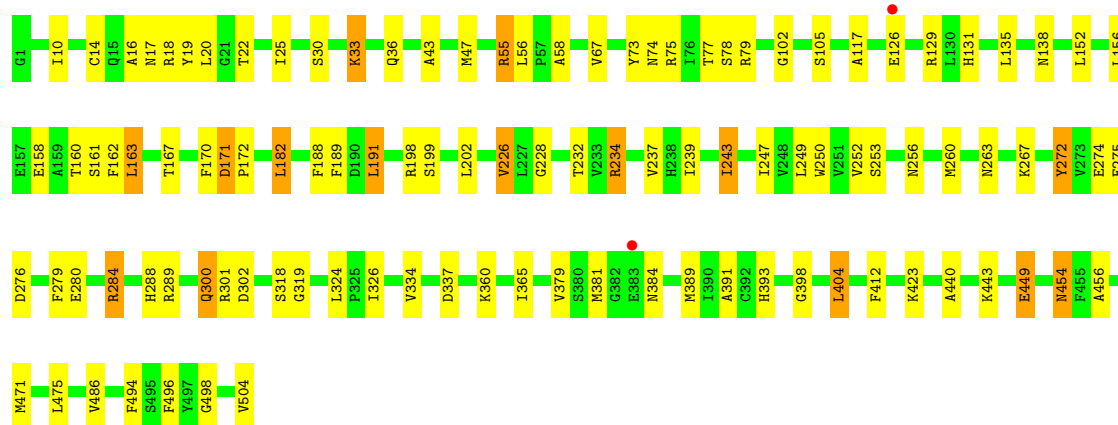


• Molecule 1: COAT PROTEIN



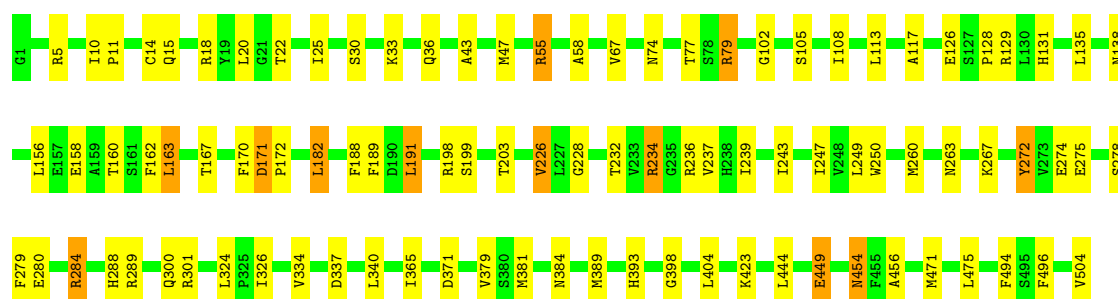
• Molecule 1: COAT PROTEIN





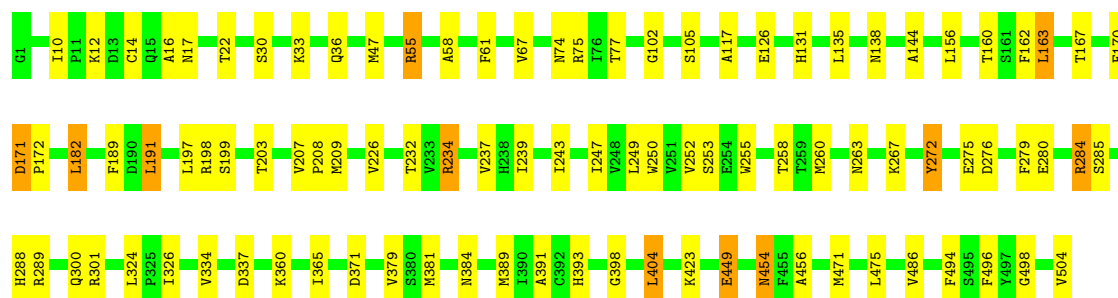
• Molecule 1: COAT PROTEIN

Chain AD: 81% 17% .



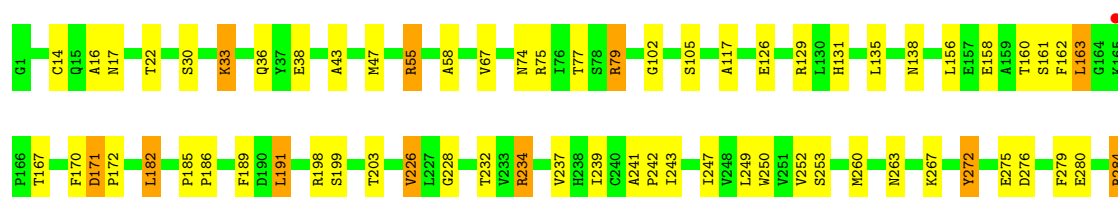
• Molecule 1: COAT PROTEIN

Chain AE: 81% 17% .



• Molecule 1: COAT PROTEIN

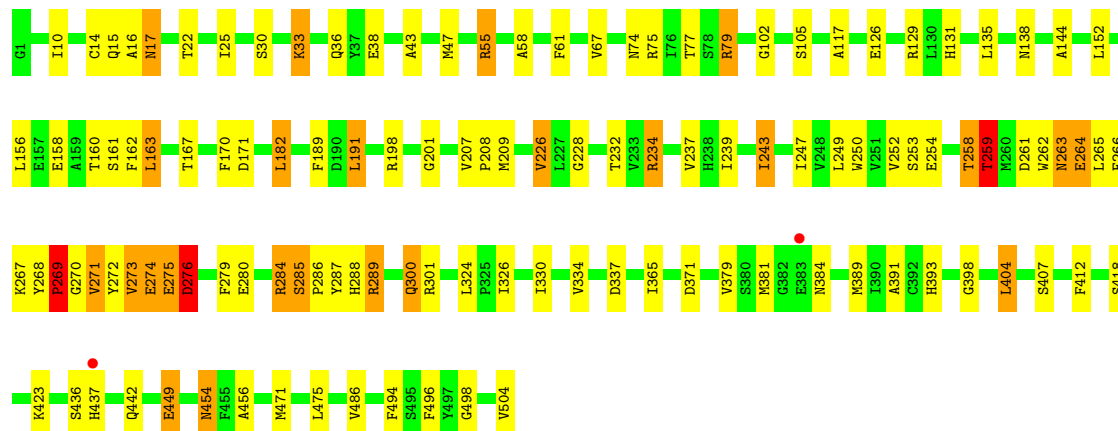
Chain AF: 79% 19% .





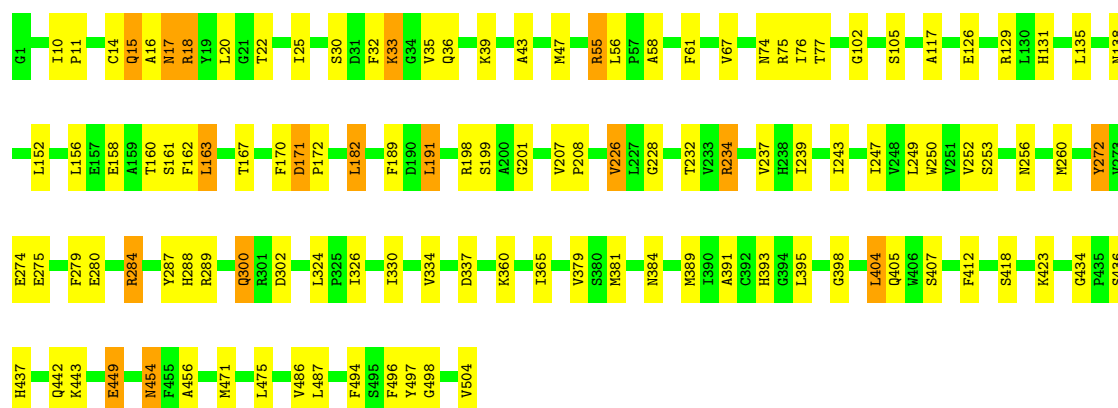
• Molecule 1: COAT PROTEIN

Chain AG: 76% 19% 5% •



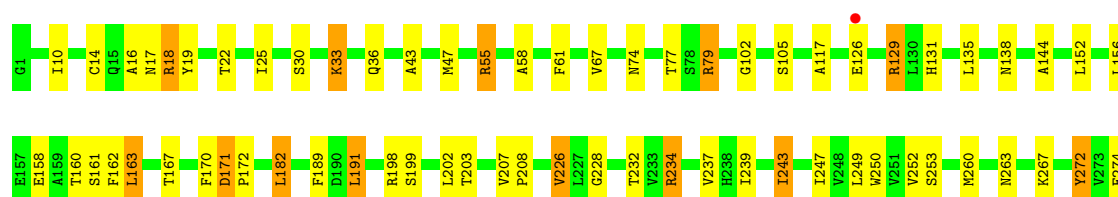
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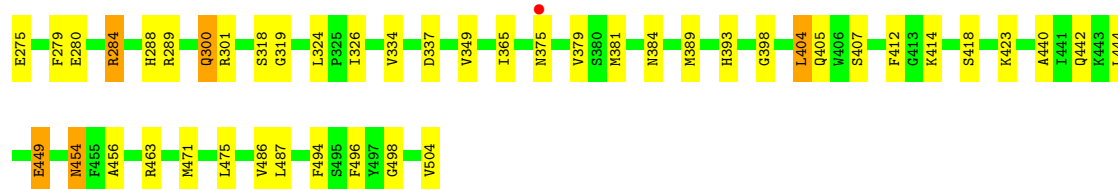
Chain AH: 77% 20% •



• Molecule 1: COAT PROTEIN

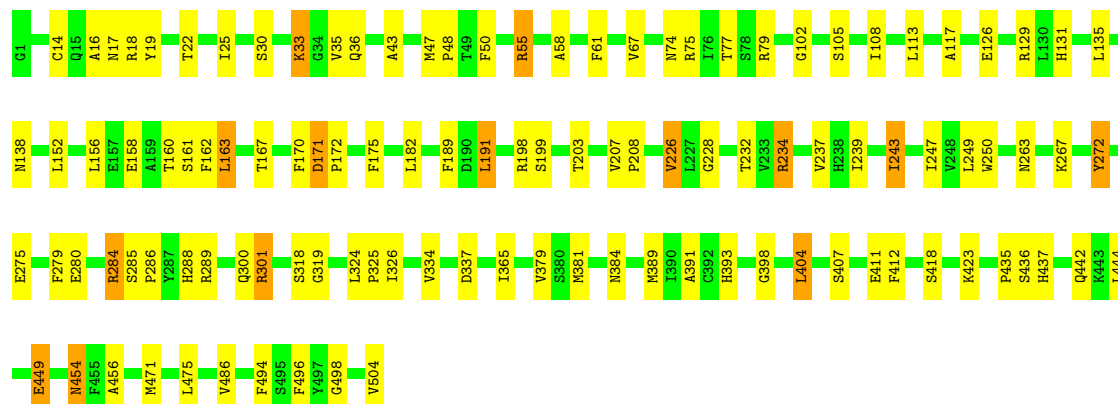
Chain AI: 78% 18% •





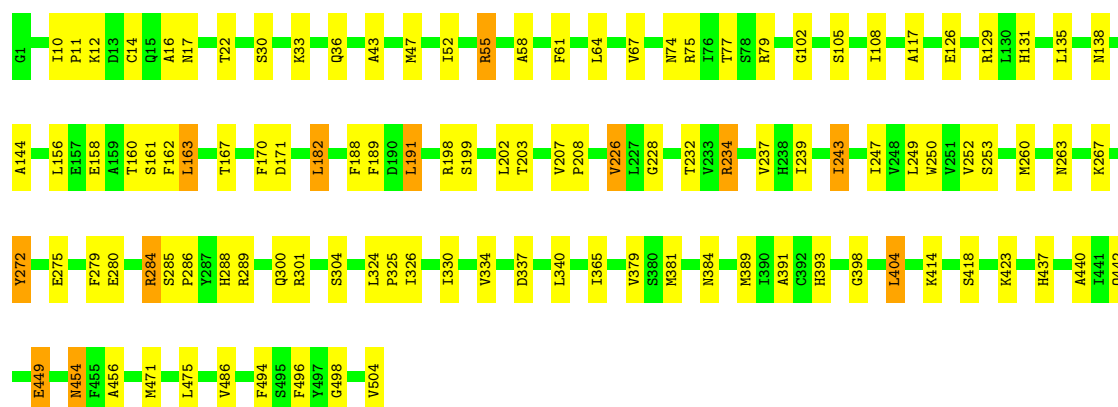
• Molecule 1: COAT PROTEIN

Chain AJ: 78% 19% .



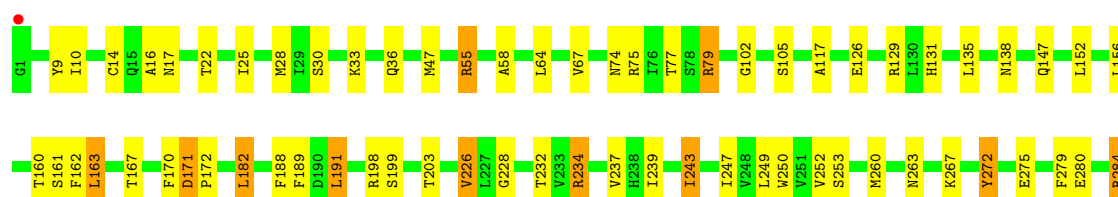
• Molecule 1: COAT PROTEIN

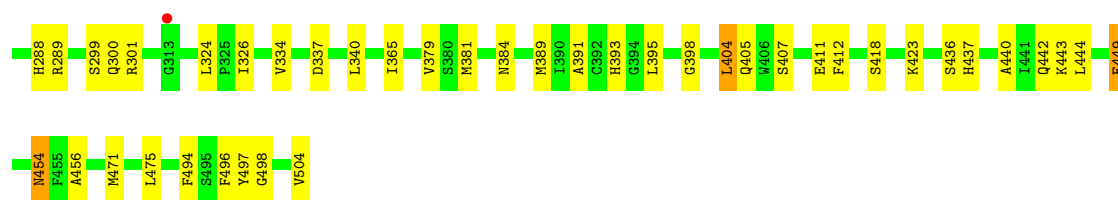
Chain AK: 78% 19% .



• Molecule 1: COAT PROTEIN

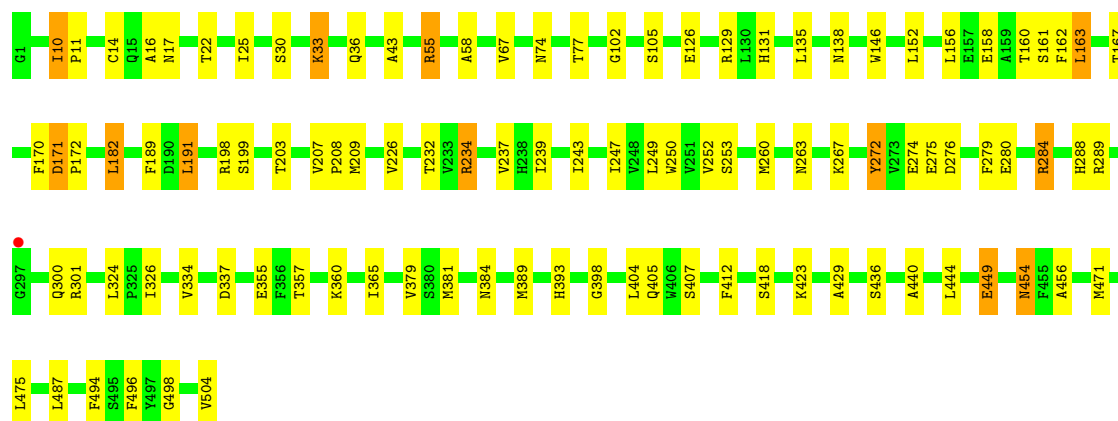
Chain AL: 79% 19% .





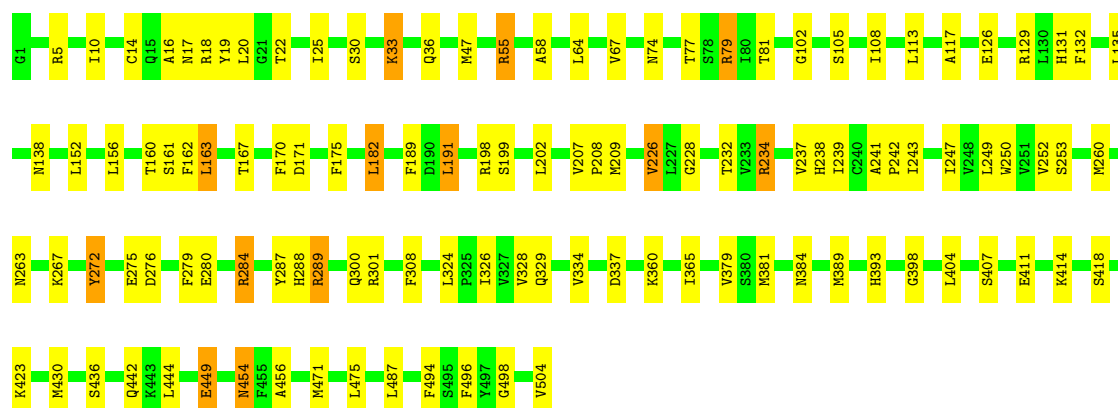
• Molecule 1: COAT PROTEIN

Chain AM: 80% 18% .



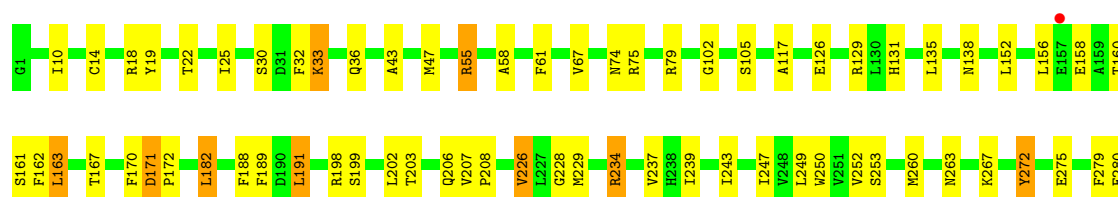
• Molecule 1: COAT PROTEIN

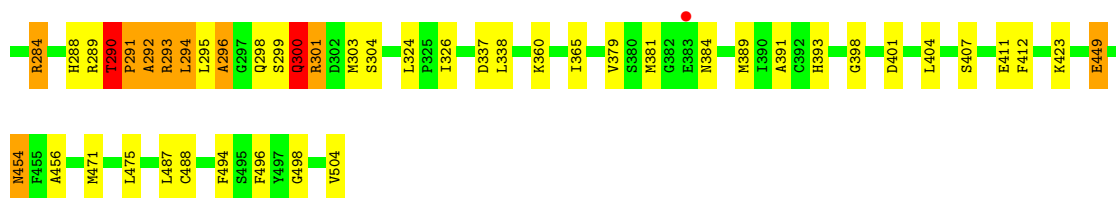
Chain AN: 77% 20% .



• Molecule 1: COAT PROTEIN

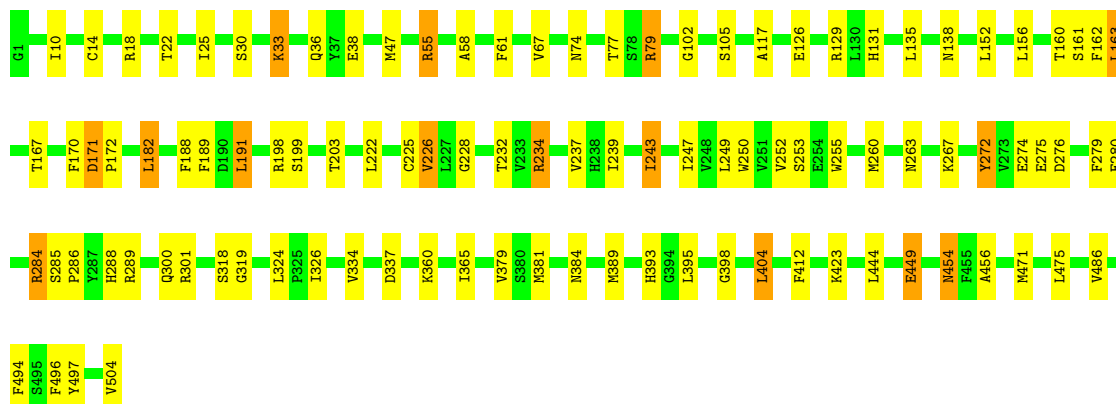
Chain AO: 77% 19% .





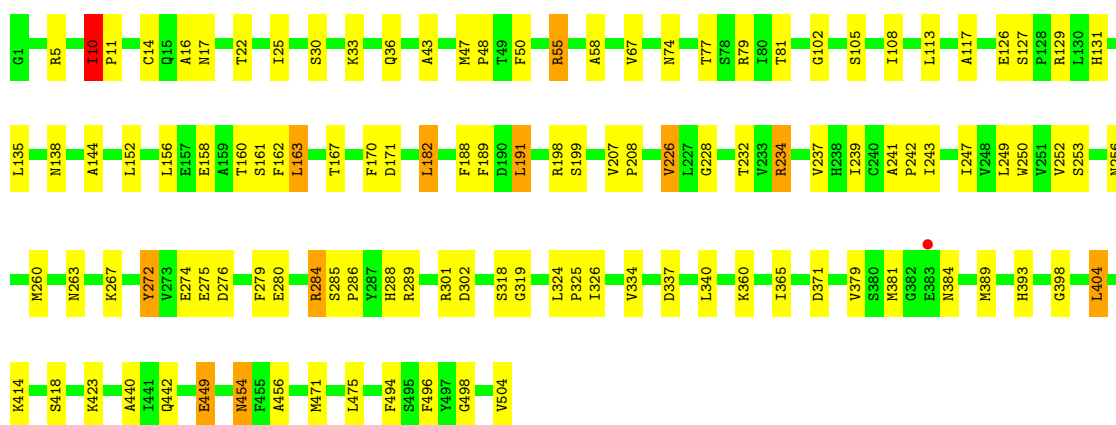
• Molecule 1: COAT PROTEIN

Chain AP: 80% 17% .



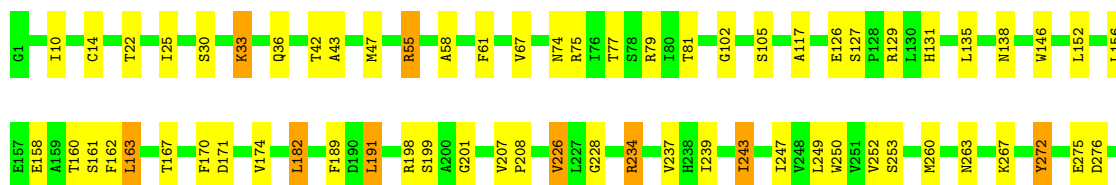
• Molecule 1: COAT PROTEIN

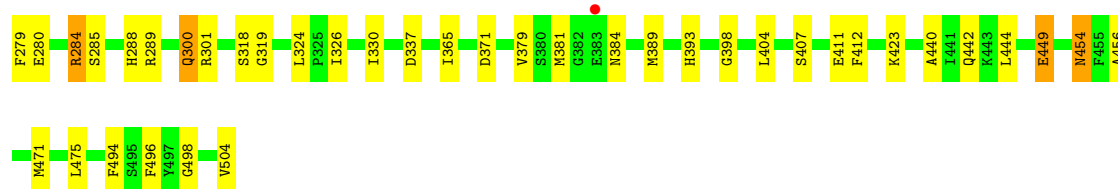
Chain AQ: 77% 20% .



• Molecule 1: COAT PROTEIN

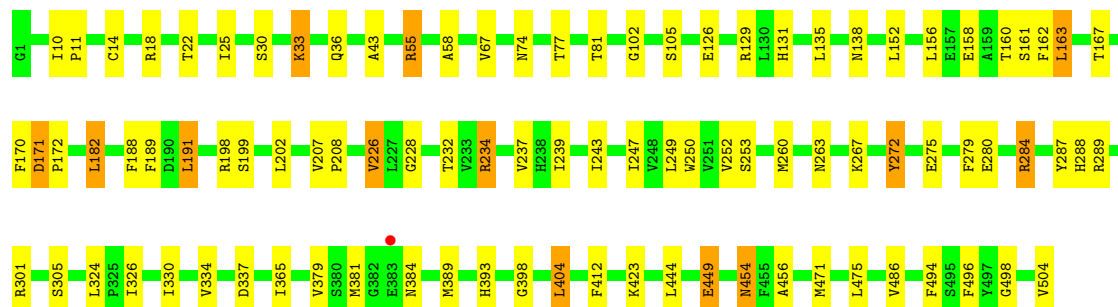
Chain AR: 79% 18% .





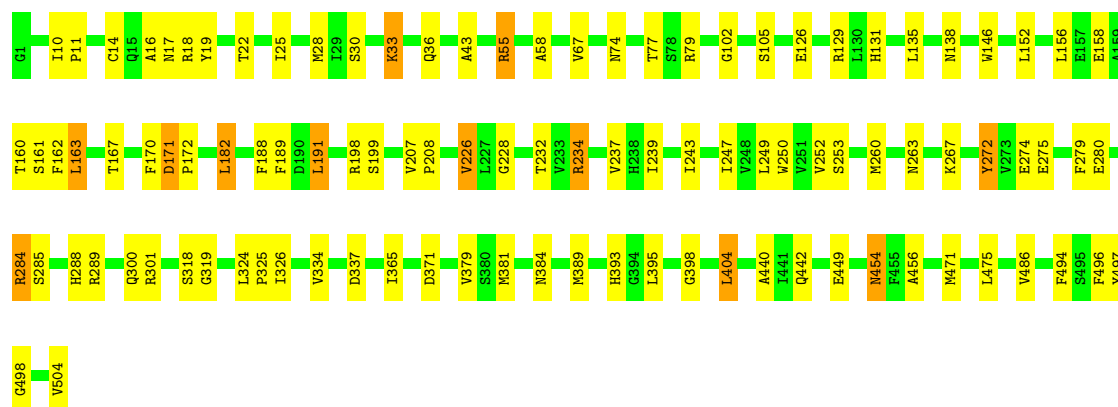
• Molecule 1: COAT PROTEIN

Chain AS: 81% 16% .



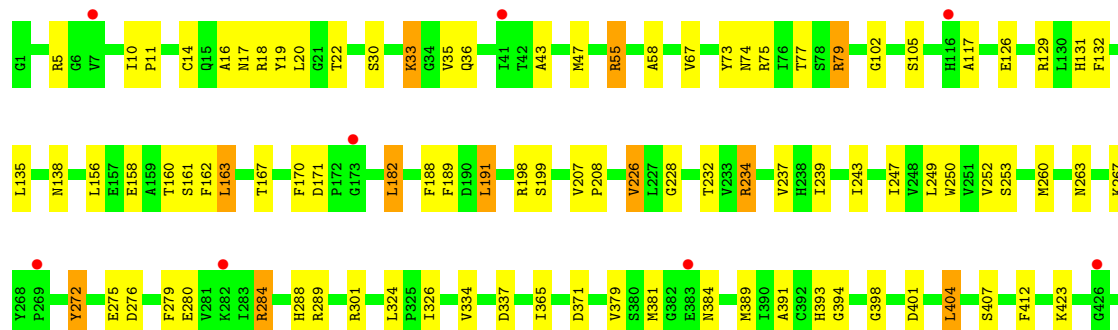
• Molecule 1: COAT PROTEIN

Chain AT: 80% 18% .



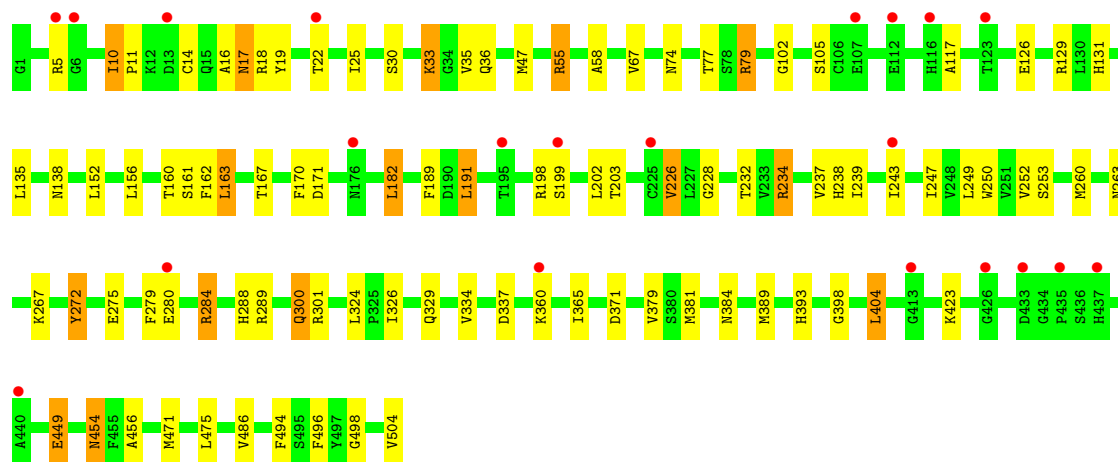
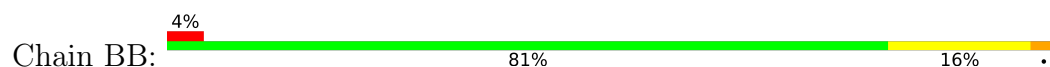
• Molecule 1: COAT PROTEIN

Chain BA: 2% 79% 19% .

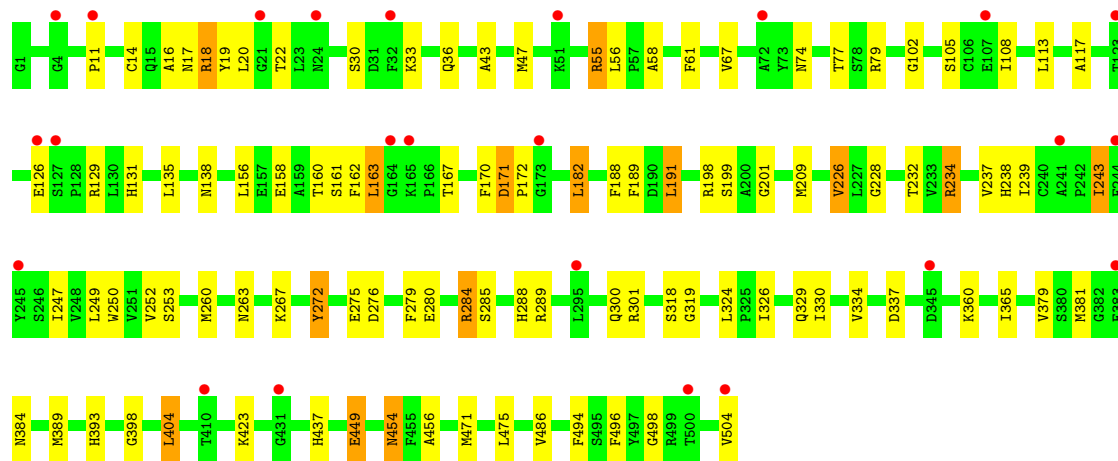
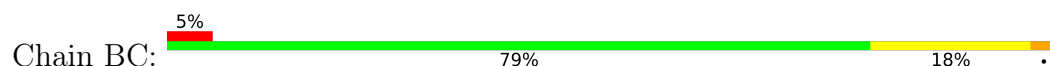




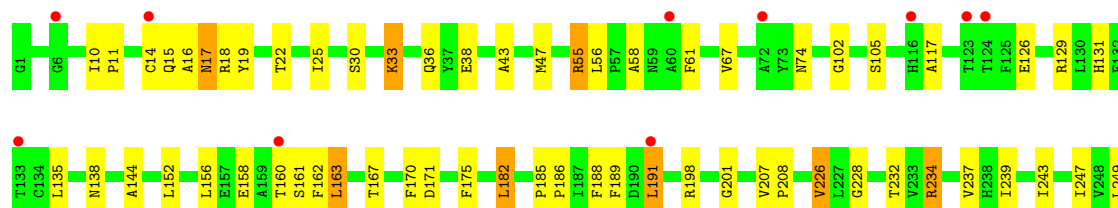
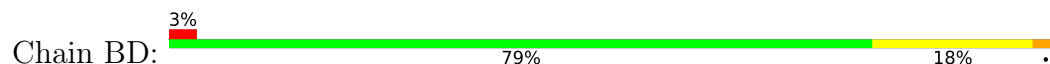
• Molecule 1: COAT PROTEIN

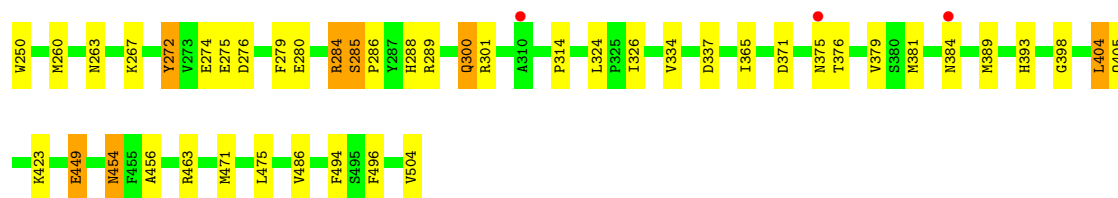


• Molecule 1: COAT PROTEIN

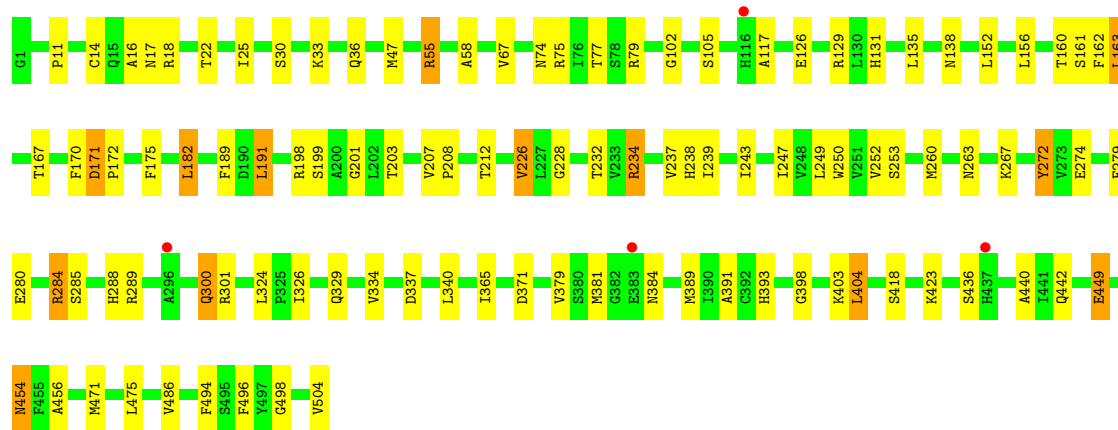
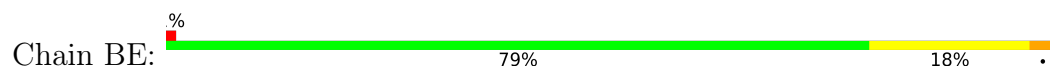


• Molecule 1: COAT PROTEIN

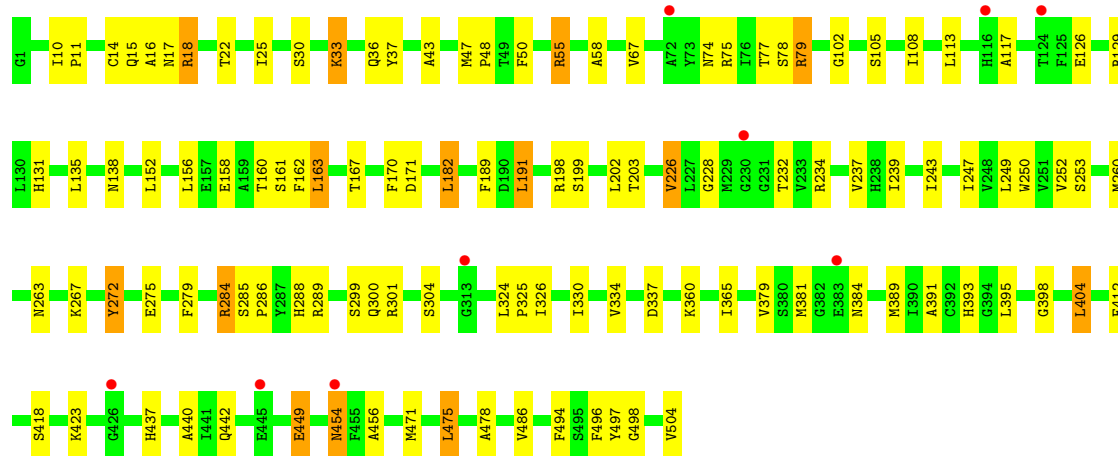
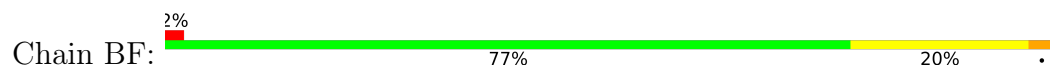




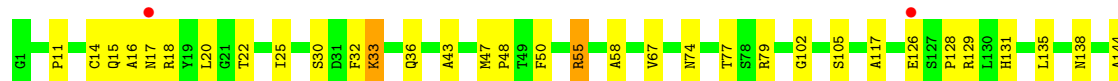
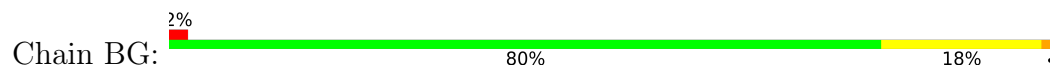
• Molecule 1: COAT PROTEIN

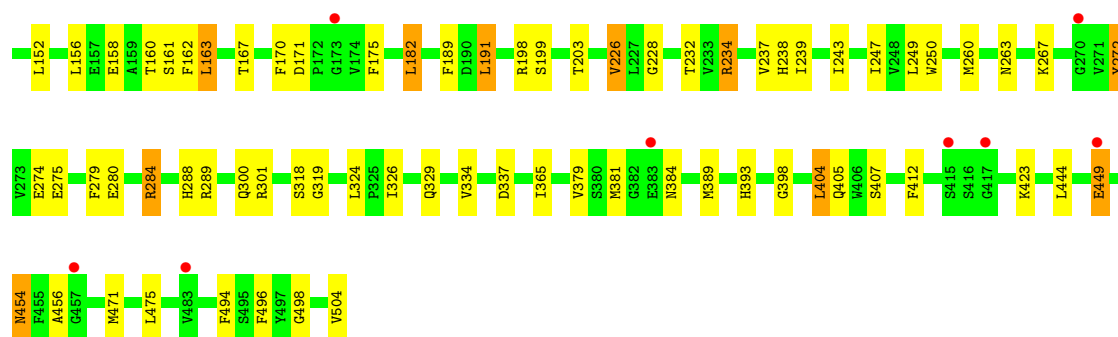


• Molecule 1: COAT PROTEIN

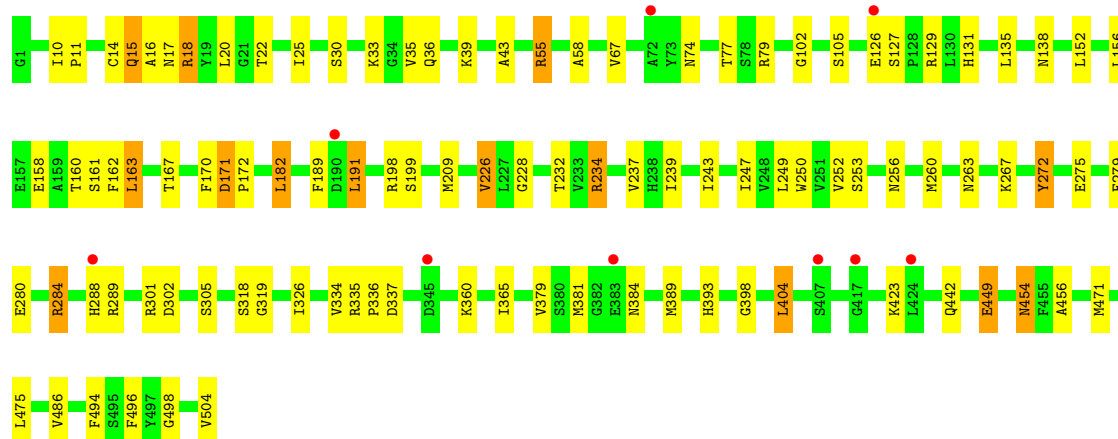
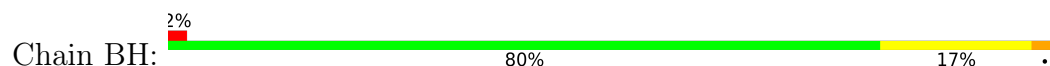


• Molecule 1: COAT PROTEIN

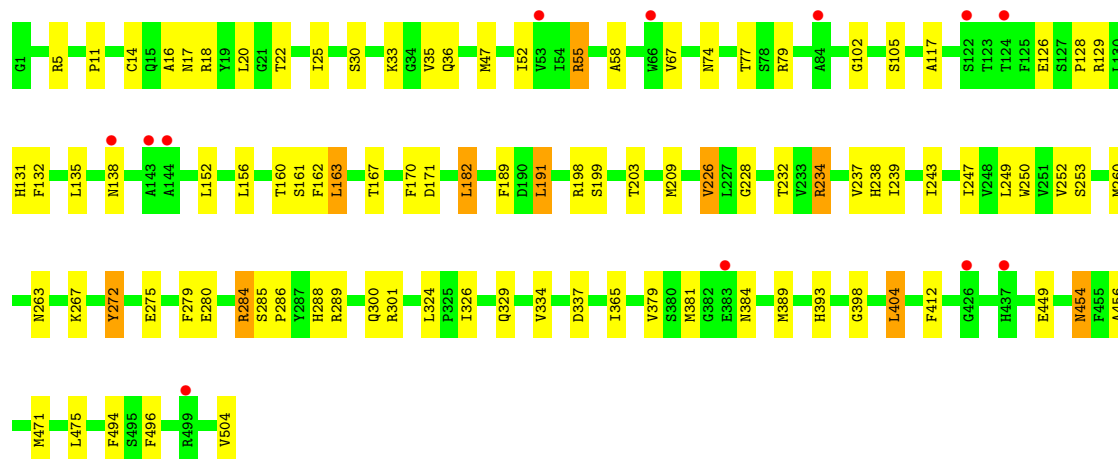
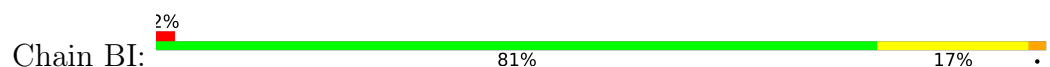




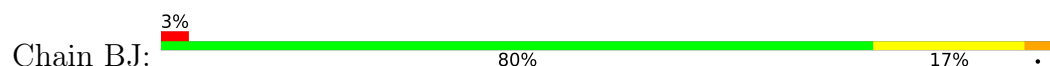
• Molecule 1: COAT PROTEIN

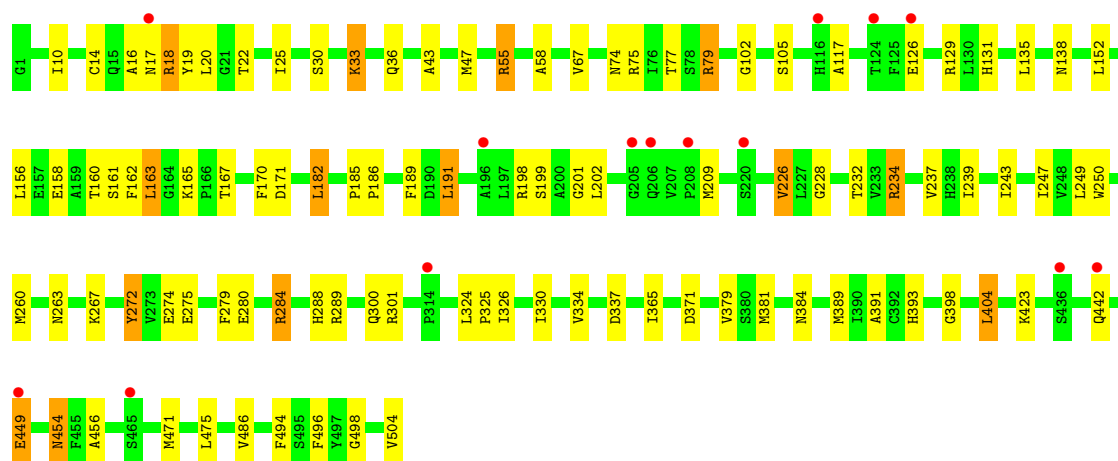


• Molecule 1: COAT PROTEIN



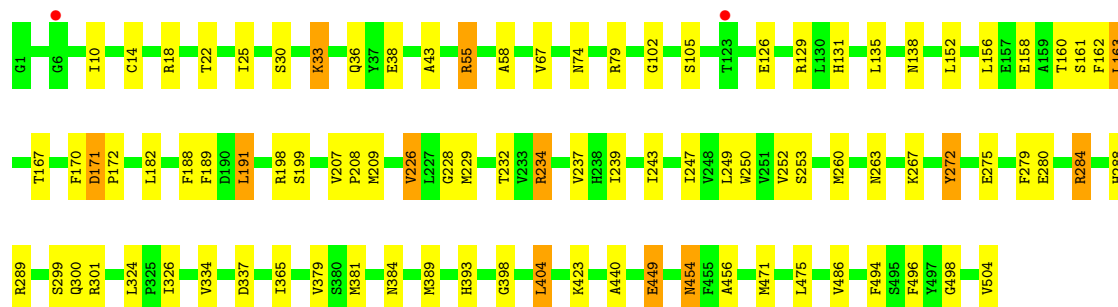
• Molecule 1: COAT PROTEIN





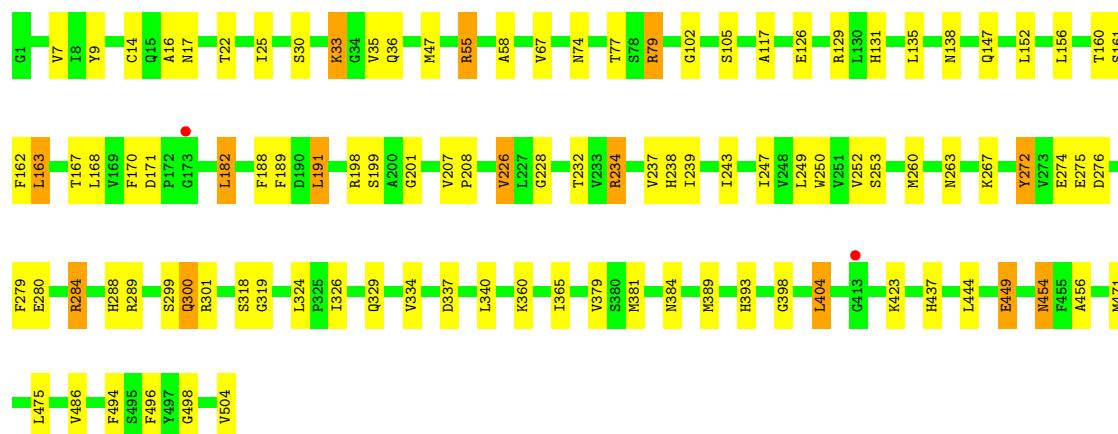
• Molecule 1: COAT PROTEIN

Chain BK: 82% 16% 2%



• Molecule 1: COAT PROTEIN

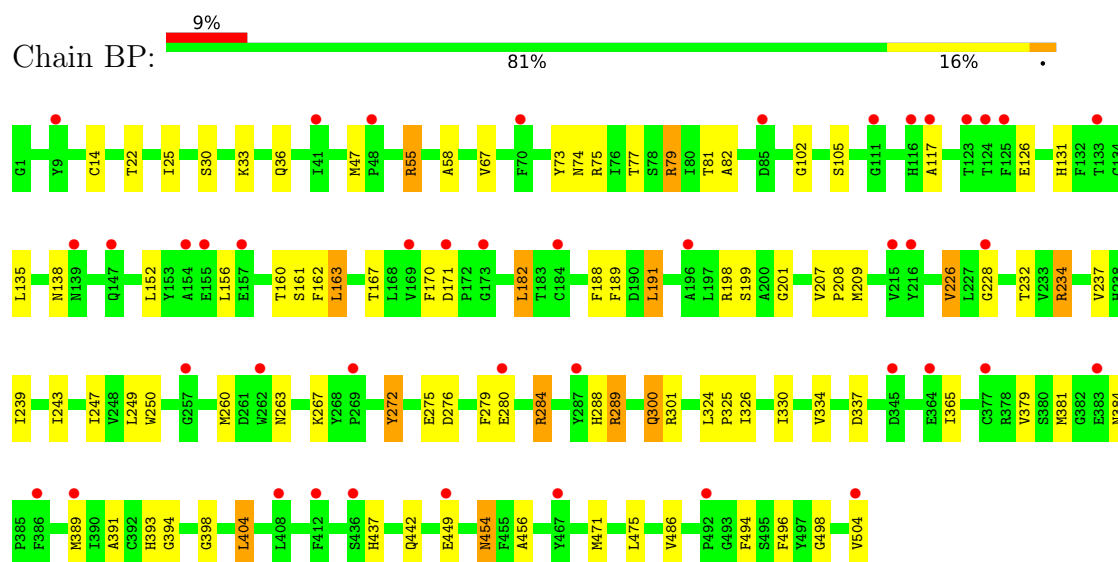
Chain BL: 79% 18% 2%



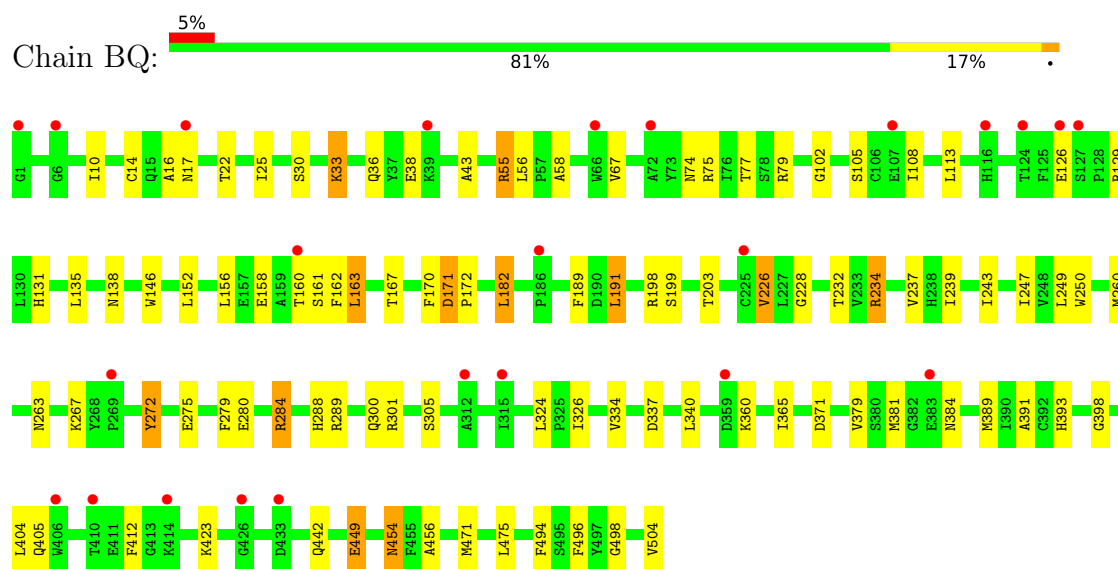
• Molecule 1: COAT PROTEIN

Chain BM: 80% 17% 2%

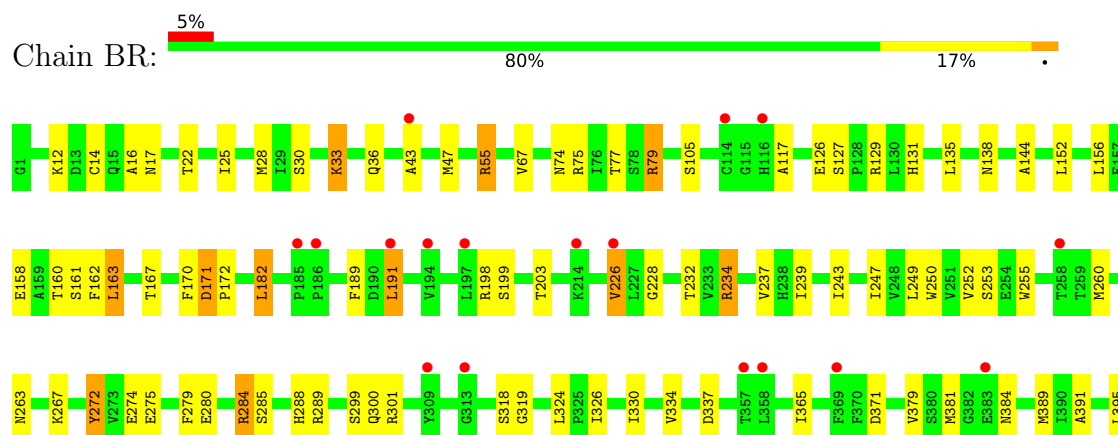


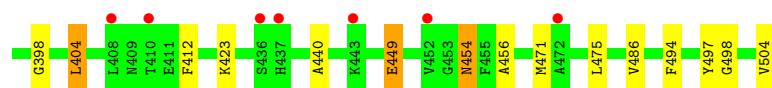


• Molecule 1: COAT PROTEIN

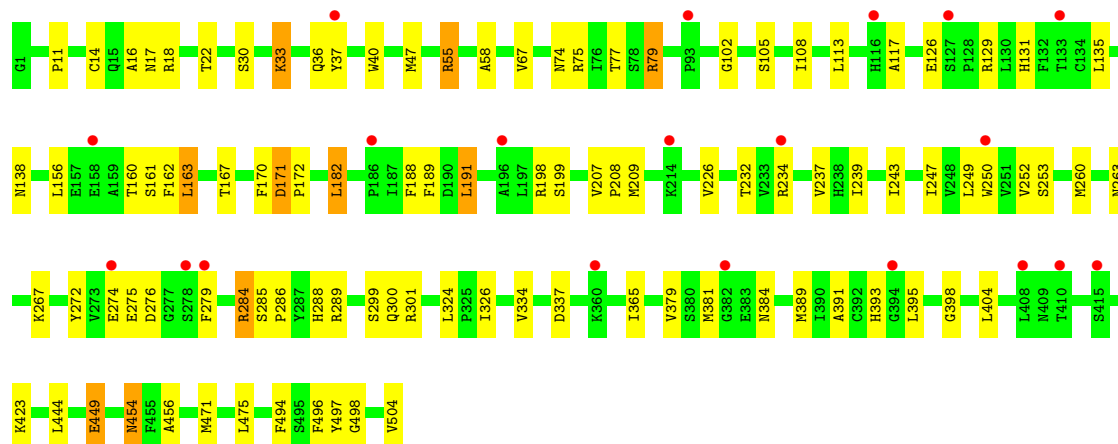
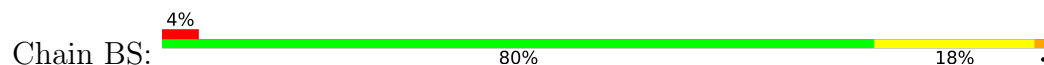


• Molecule 1: COAT PROTEIN

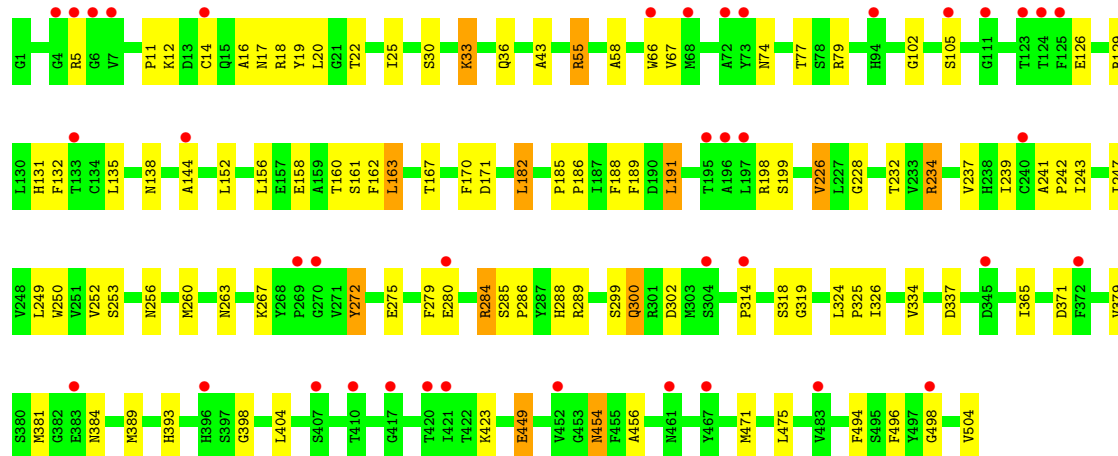
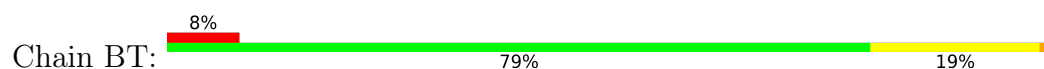




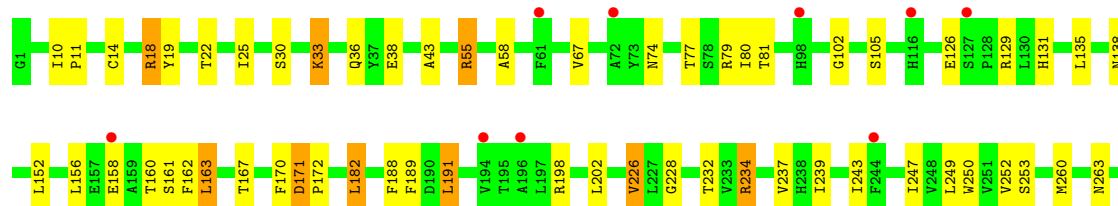
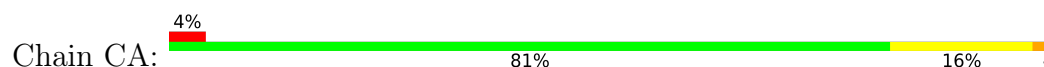
• Molecule 1: COAT PROTEIN

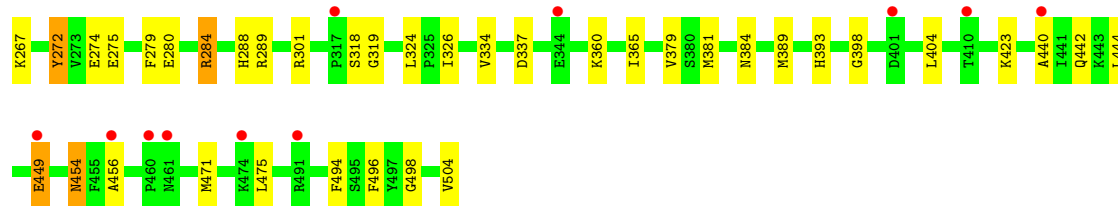


• Molecule 1: COAT PROTEIN

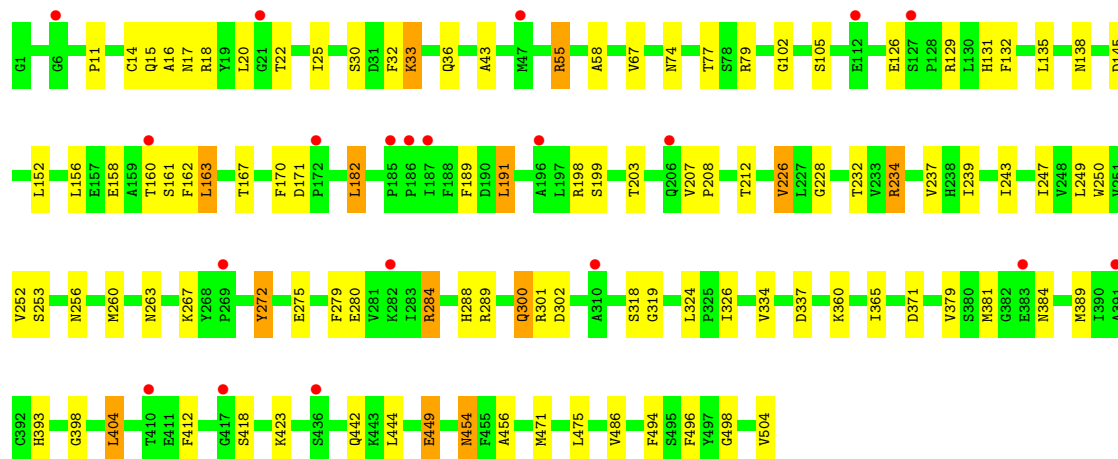
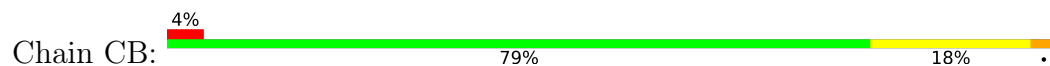


• Molecule 1: COAT PROTEIN

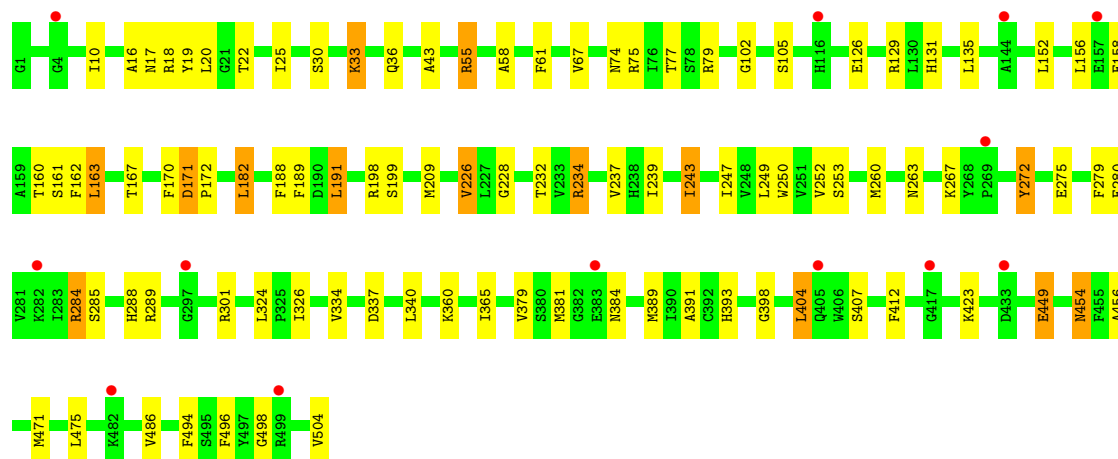
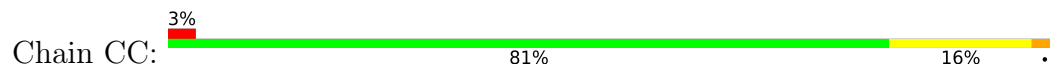




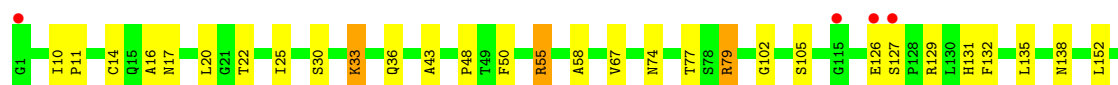
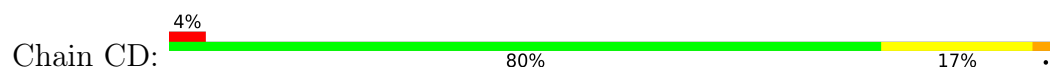
• Molecule 1: COAT PROTEIN

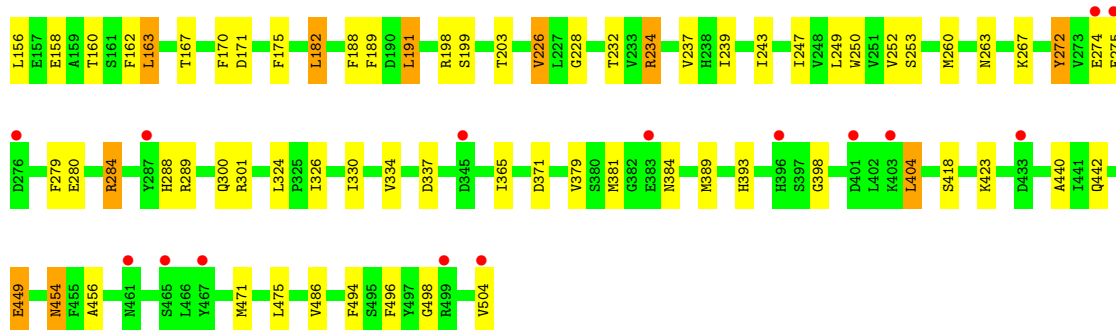


• Molecule 1: COAT PROTEIN

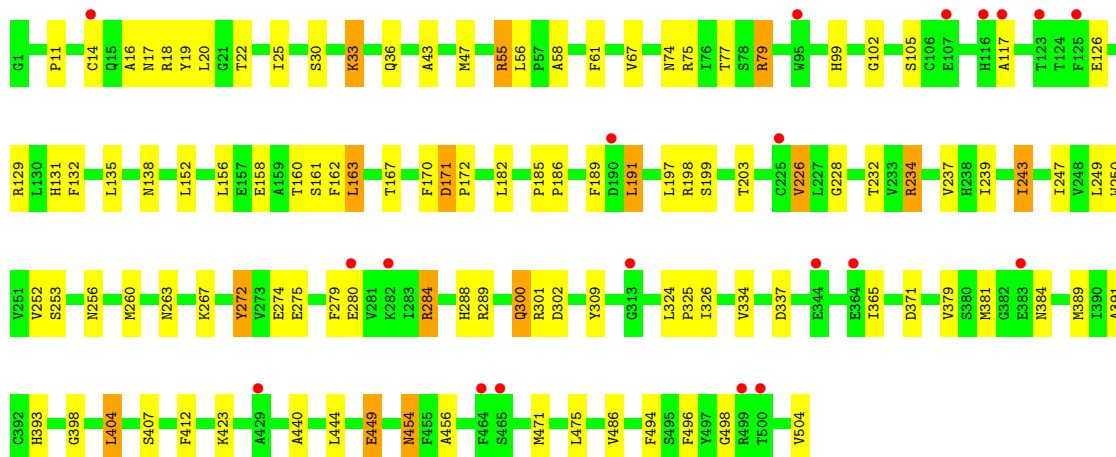
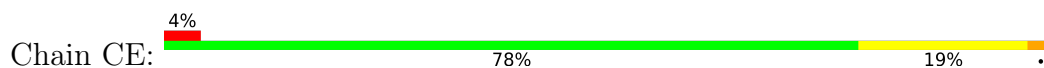


• Molecule 1: COAT PROTEIN

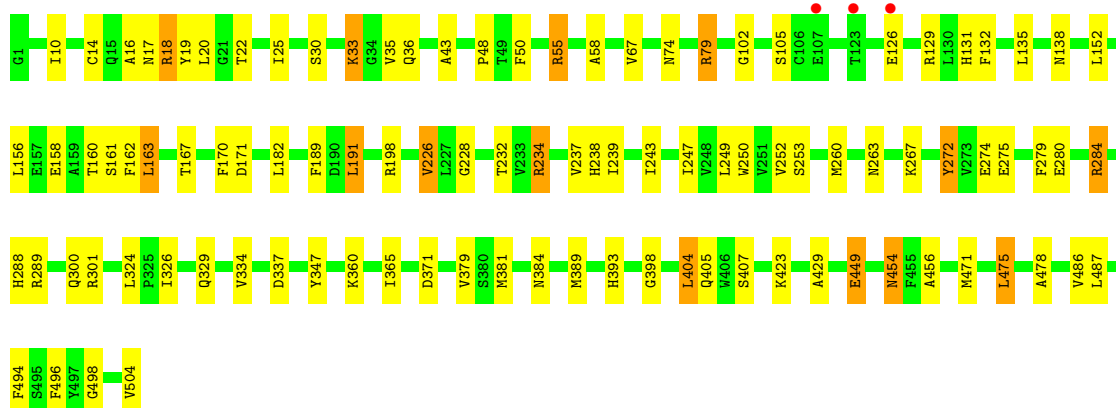
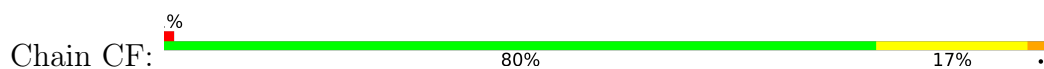




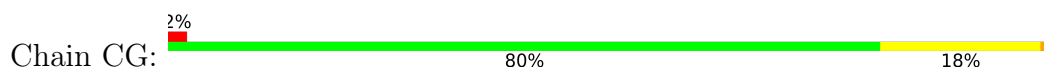
● Molecule 1: COAT PROTEIN

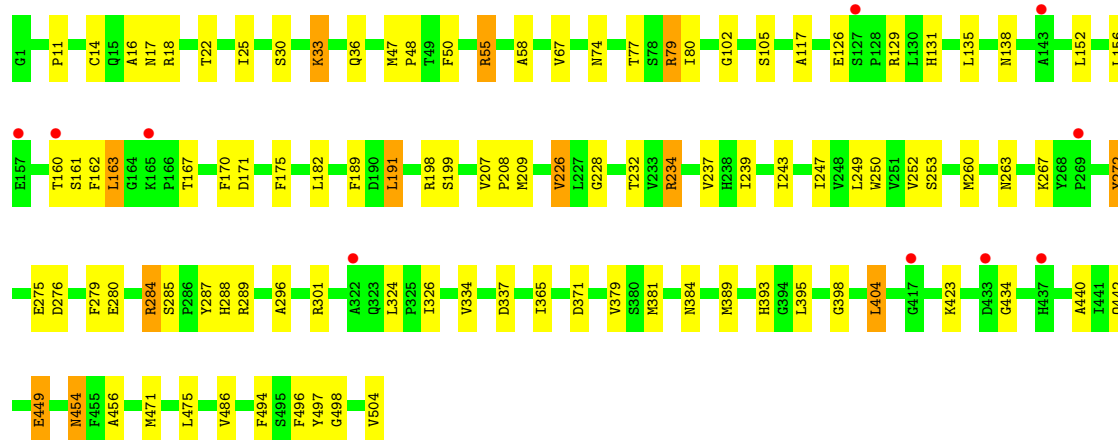


● Molecule 1: COAT PROTEIN

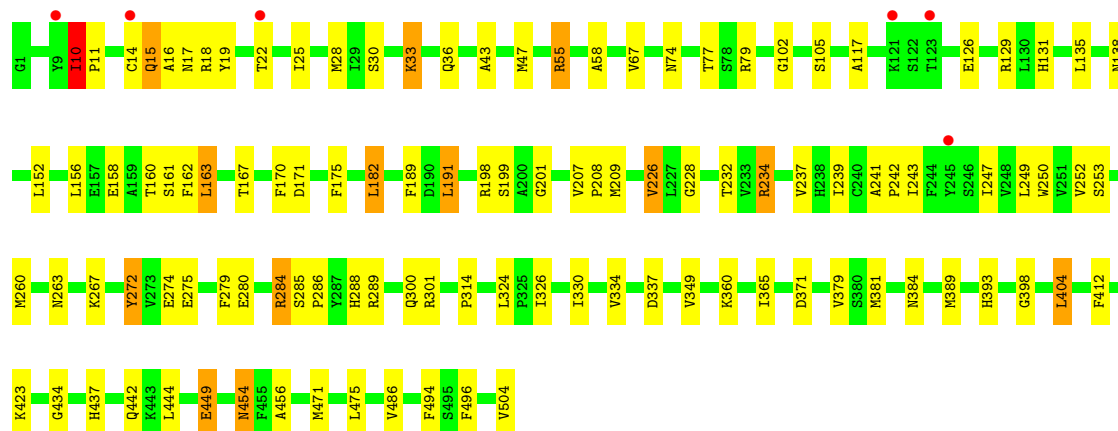
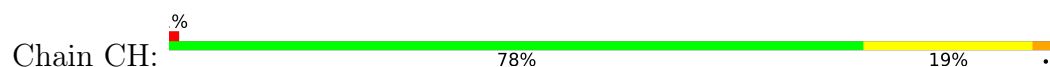


● Molecule 1: COAT PROTEIN

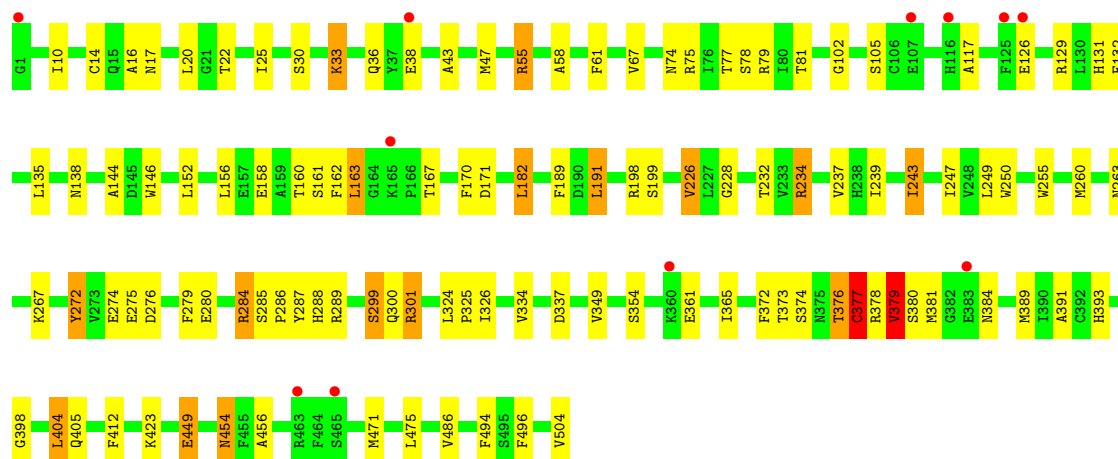
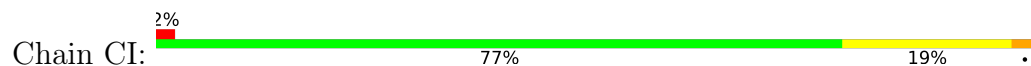




• Molecule 1: COAT PROTEIN

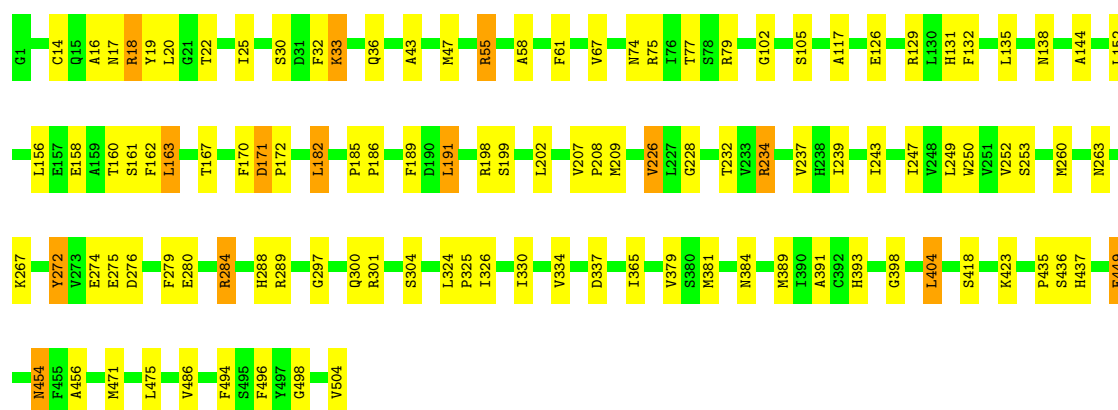


• Molecule 1: COAT PROTEIN



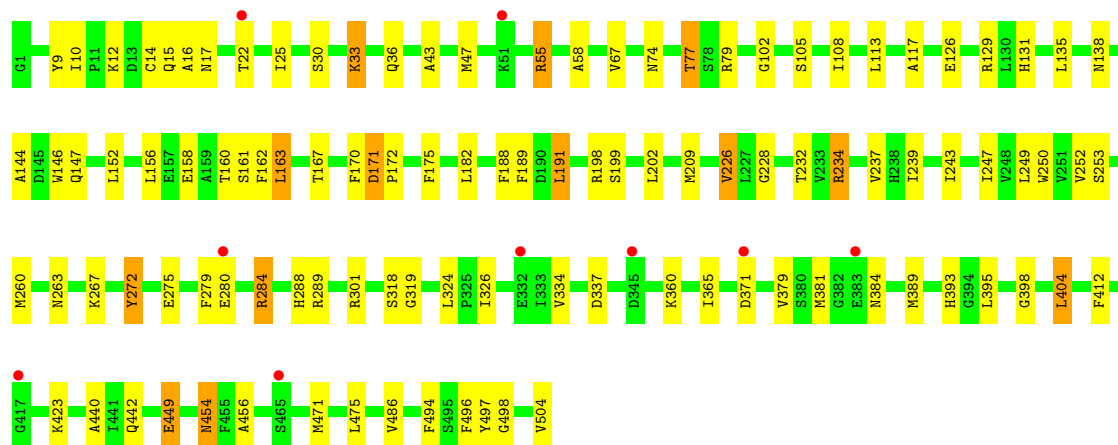
• Molecule 1: COAT PROTEIN

Chain CJ:  78% 19%



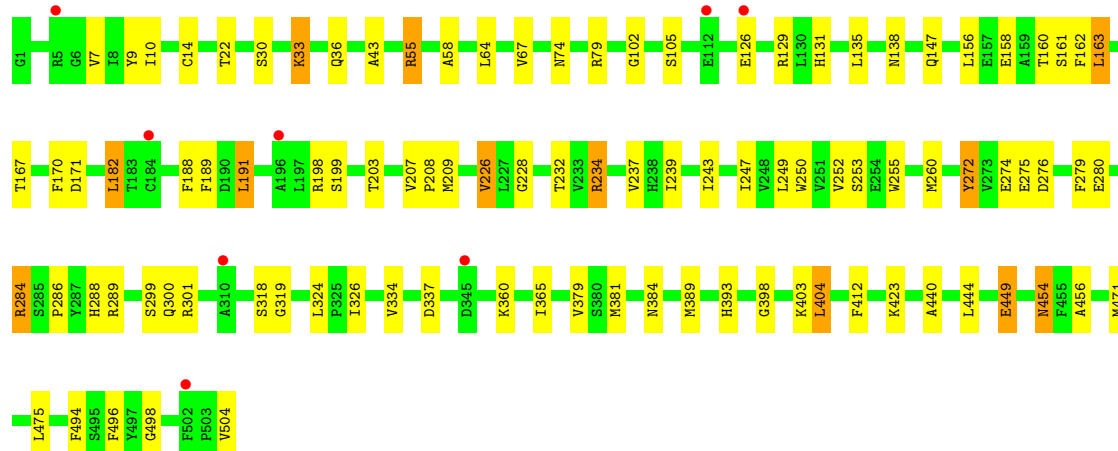
• Molecule 1: COAT PROTEIN

Chain CK:  79% 19%

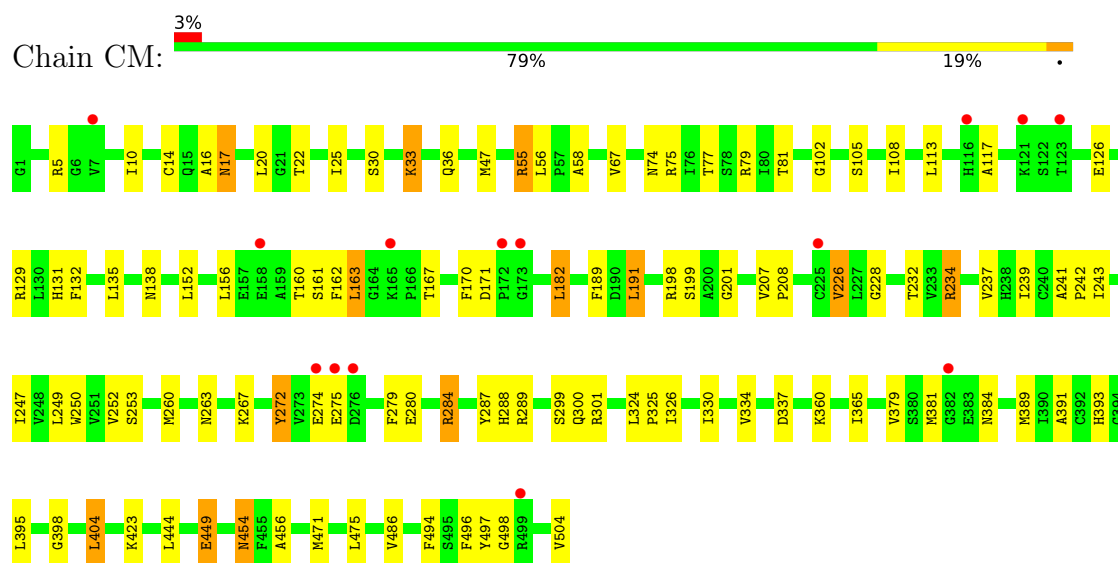


• Molecule 1: COAT PROTEIN

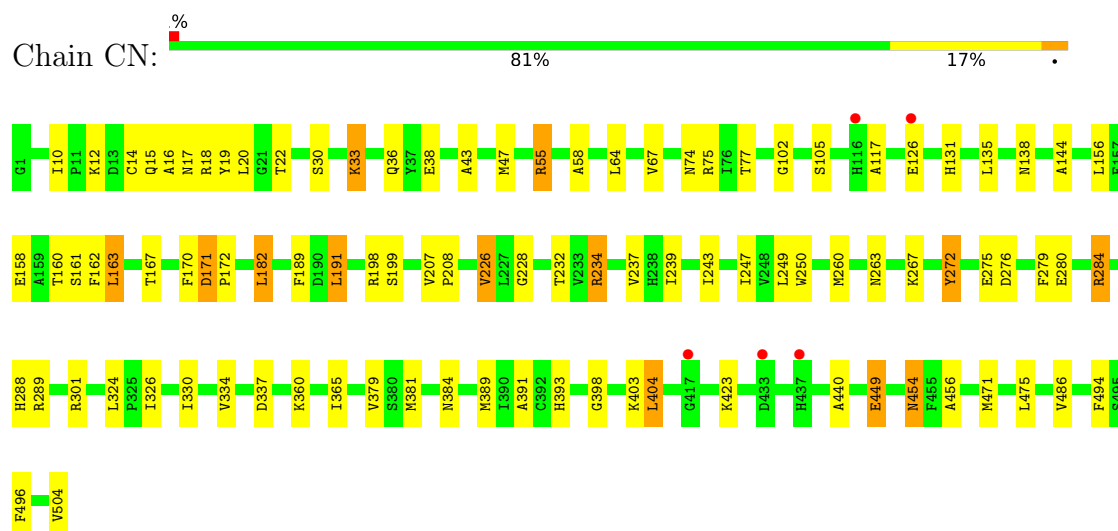
Chain CL:  81% 17%



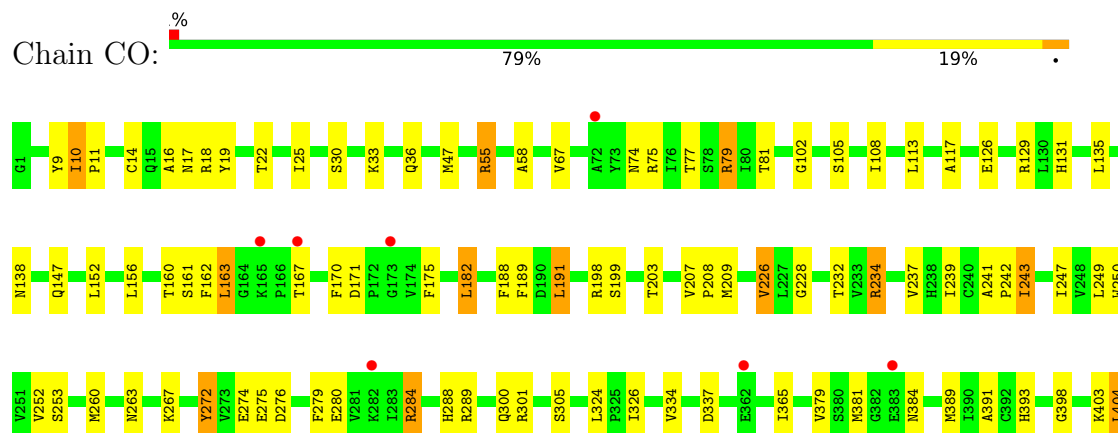
• Molecule 1: COAT PROTEIN

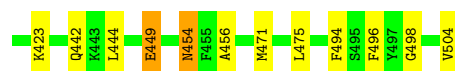


• Molecule 1: COAT PROTEIN

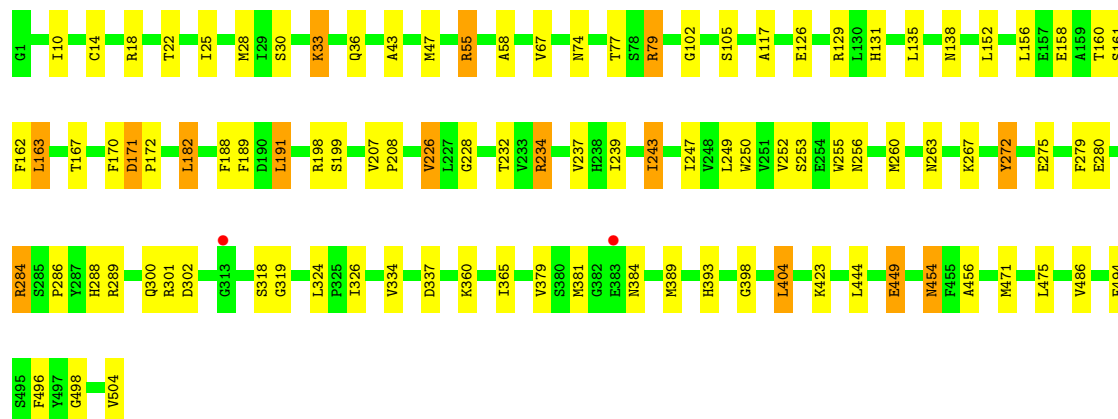


• Molecule 1: COAT PROTEIN

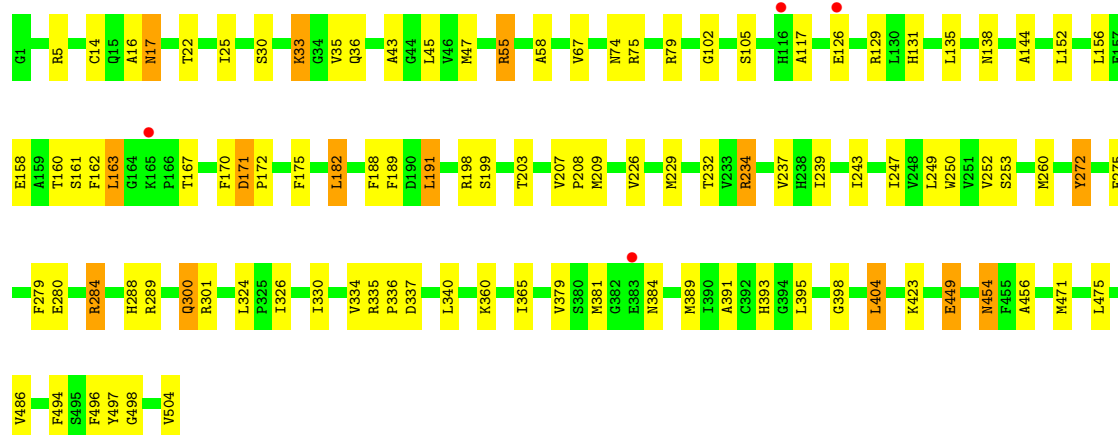




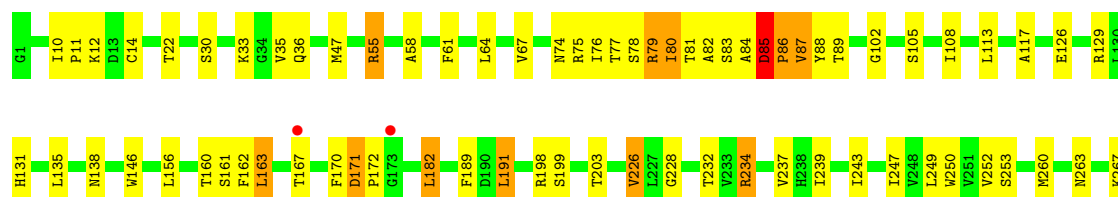
• Molecule 1: COAT PROTEIN

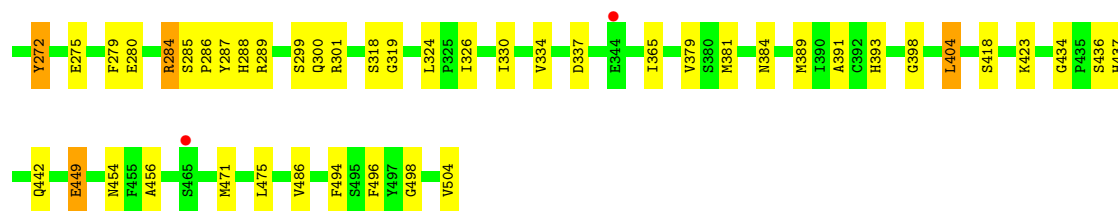
Chain CP:  80% 17%

• Molecule 1: COAT PROTEIN

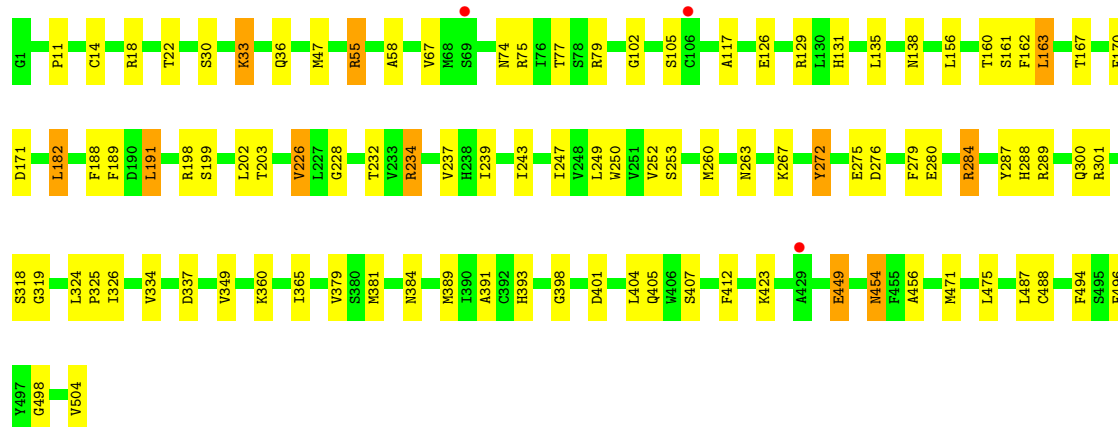
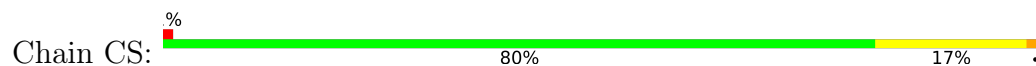
Chain CQ:  80% 18%

• Molecule 1: COAT PROTEIN

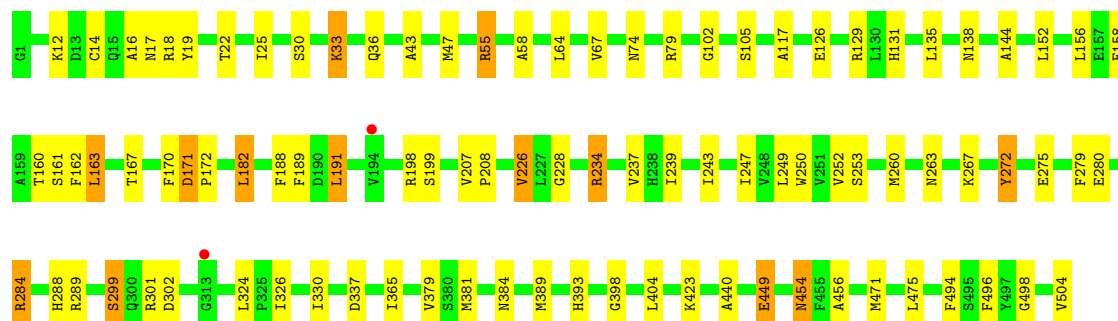
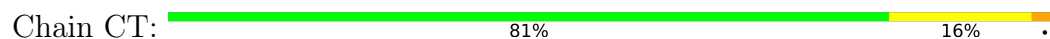
Chain CR:  77% 20%



• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants 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 49.80 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.80-3.70) 99.0 (49.80-3.70)	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 0.244 , 0.256	Depositor DCC
R_{free} test set	34196 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 81.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.088 for -k,-h,-l 0.087 for k,h,-l 0.089 for h,-k,-l	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.

²Theoretical 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	0.57	0/4058	0.88	4/5517 (0.1%)
1	AB	0.65	1/4058 (0.0%)	0.91	5/5517 (0.1%)
1	AC	0.57	0/4058	0.88	3/5517 (0.1%)
1	AD	0.57	0/4058	0.88	2/5517 (0.0%)
1	AE	0.63	0/4058	0.90	2/5517 (0.0%)
1	AF	0.57	0/4058	0.89	2/5517 (0.0%)
1	AG	0.69	2/4058 (0.0%)	0.94	9/5517 (0.2%)
1	AH	0.58	0/4058	0.89	3/5517 (0.1%)
1	AI	0.58	0/4058	0.89	4/5517 (0.1%)
1	AJ	0.56	0/4058	0.87	2/5517 (0.0%)
1	AK	0.55	0/4058	0.88	2/5517 (0.0%)
1	AL	0.59	0/4058	0.89	2/5517 (0.0%)
1	AM	0.60	0/4058	0.89	4/5517 (0.1%)
1	AN	0.58	0/4058	0.89	2/5517 (0.0%)
1	AO	0.69	3/4058 (0.1%)	0.92	8/5517 (0.1%)
1	AP	0.60	0/4058	0.89	4/5517 (0.1%)
1	AQ	0.57	0/4058	0.89	5/5517 (0.1%)
1	AR	0.60	0/4058	0.89	7/5517 (0.1%)
1	AS	0.58	0/4058	0.87	2/5517 (0.0%)
1	AT	0.56	0/4058	0.87	4/5517 (0.1%)
1	BA	0.56	0/4058	0.88	2/5517 (0.0%)
1	BB	0.58	0/4058	0.90	4/5517 (0.1%)
1	BC	0.55	0/4058	0.88	4/5517 (0.1%)
1	BD	0.55	0/4058	0.88	6/5517 (0.1%)
1	BE	0.57	0/4058	0.88	4/5517 (0.1%)
1	BF	0.57	0/4058	0.89	2/5517 (0.0%)
1	BG	0.56	0/4058	0.87	2/5517 (0.0%)
1	BH	0.58	0/4058	0.88	4/5517 (0.1%)
1	BI	0.61	0/4058	0.89	2/5517 (0.0%)
1	BJ	0.56	0/4058	0.88	3/5517 (0.1%)
1	BK	0.56	0/4058	0.87	4/5517 (0.1%)
1	BL	0.59	0/4058	0.89	2/5517 (0.0%)
1	BM	0.62	0/4058	0.90	2/5517 (0.0%)
1	BN	0.58	0/4058	0.89	2/5517 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BO	0.60	0/4058	0.89	4/5517 (0.1%)
1	BP	0.62	0/4058	0.91	2/5517 (0.0%)
1	BQ	0.58	0/4058	0.89	2/5517 (0.0%)
1	BR	0.58	0/4058	0.89	4/5517 (0.1%)
1	BS	0.57	0/4058	0.89	2/5517 (0.0%)
1	BT	0.56	0/4058	0.87	2/5517 (0.0%)
1	CA	0.56	0/4058	0.89	3/5517 (0.1%)
1	CB	0.56	0/4058	0.88	2/5517 (0.0%)
1	CC	0.56	0/4058	0.87	4/5517 (0.1%)
1	CD	0.57	0/4058	0.88	2/5517 (0.0%)
1	CE	0.58	1/4058 (0.0%)	0.89	2/5517 (0.0%)
1	CF	0.55	0/4058	0.88	3/5517 (0.1%)
1	CG	0.56	0/4058	0.89	6/5517 (0.1%)
1	CH	0.55	0/4058	0.88	4/5517 (0.1%)
1	CI	0.64	2/4058 (0.0%)	0.90	2/5517 (0.0%)
1	CJ	0.57	0/4058	0.89	2/5517 (0.0%)
1	CK	0.56	0/4058	0.87	2/5517 (0.0%)
1	CL	0.58	0/4058	0.89	4/5517 (0.1%)
1	CM	0.59	0/4058	0.87	2/5517 (0.0%)
1	CN	0.59	0/4058	0.89	2/5517 (0.0%)
1	CO	0.59	0/4058	0.89	4/5517 (0.1%)
1	CP	0.61	0/4058	0.89	2/5517 (0.0%)
1	CQ	0.58	0/4058	0.89	2/5517 (0.0%)
1	CR	0.67	0/4058	0.93	8/5517 (0.1%)
1	CS	0.58	0/4058	0.89	2/5517 (0.0%)
1	CT	0.58	0/4058	0.87	2/5517 (0.0%)
All	All	0.59	9/243480 (0.0%)	0.89	195/331020 (0.1%)

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

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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

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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 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CI	379	VAL	CA-CB	-10.58	1.44	1.55
1	AG	271	VAL	CA-CB	-6.26	1.46	1.55
1	AO	290	THR	CA-CB	-6.10	1.42	1.54
1	AG	259	THR	CA-C	-5.78	1.45	1.53
1	AO	292	ALA	CA-CB	-5.76	1.43	1.53

The worst 5 of 195 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AG	263	ASN	N-CA-C	-11.97	98.23	111.28
1	AG	259	THR	N-CA-C	-9.31	98.24	110.43
1	AB	258	THR	N-CA-C	-8.29	96.11	108.79
1	AB	263	ASN	N-CA-C	-7.61	102.13	111.33
1	CR	80	ILE	N-CA-C	7.54	118.33	110.72

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 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	3951	0	3909	103	0
1	AB	3951	0	3909	124	0
1	AC	3951	0	3909	97	0
1	AD	3951	0	3909	96	0
1	AE	3951	0	3909	96	0
1	AF	3951	0	3909	105	0
1	AG	3951	0	3907	155	1
1	AH	3951	0	3909	114	0
1	AI	3951	0	3909	119	5
1	AJ	3951	0	3909	116	1
1	AK	3951	0	3909	113	0
1	AL	3951	0	3909	116	0
1	AM	3951	0	3909	100	5
1	AN	3951	0	3909	119	1
1	AO	3951	0	3909	132	0
1	AP	3951	0	3909	92	0
1	AQ	3951	0	3909	107	0
1	AR	3951	0	3909	103	0
1	AS	3951	0	3909	97	0
1	AT	3951	0	3909	100	0
1	BA	3951	0	3909	106	0
1	BB	3951	0	3909	95	0
1	BC	3951	0	3909	88	0
1	BD	3951	0	3909	93	2
1	BE	3951	0	3909	99	1
1	BF	3951	0	3909	106	0
1	BG	3951	0	3909	112	2
1	BH	3951	0	3909	95	0
1	BI	3951	0	3909	92	0
1	BJ	3951	0	3909	100	0
1	BK	3951	0	3909	78	0
1	BL	3951	0	3909	101	0
1	BM	3951	0	3909	95	0
1	BN	3951	0	3909	95	0
1	BO	3951	0	3909	107	0
1	BP	3951	0	3909	102	0
1	BQ	3951	0	3909	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	3951	0	3909	102	0
1	BS	3951	0	3909	89	0
1	BT	3951	0	3909	95	0
1	CA	3951	0	3909	93	0
1	CB	3951	0	3909	100	3
1	CC	3951	0	3909	91	0
1	CD	3951	0	3909	100	0
1	CE	3951	0	3909	112	0
1	CF	3951	0	3909	106	0
1	CG	3951	0	3909	94	0
1	CH	3951	0	3909	104	0
1	CI	3951	0	3909	122	1
1	CJ	3951	0	3909	116	2
1	CK	3951	0	3909	92	0
1	CL	3951	0	3909	92	0
1	CM	3951	0	3909	94	0
1	CN	3951	0	3909	92	0
1	CO	3951	0	3909	104	0
1	CP	3951	0	3909	98	0
1	CQ	3951	0	3909	96	0
1	CR	3951	0	3909	129	0
1	CS	3951	0	3909	92	0
1	CT	3951	0	3909	84	0
All	All	237060	0	234538	5473	12

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 12.

The worst 5 of 5473 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: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	Interatomic distance (Å)	Clash overlap (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 [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	502/504 (100%)	478 (95%)	23 (5%)	1 (0%)	43	72
1	AB	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	72
1	AC	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	30	60
1	AD	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AE	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	72
1	AF	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AG	502/504 (100%)	480 (96%)	18 (4%)	4 (1%)	16	48
1	AH	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	30	60
1	AI	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	AJ	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	72
1	AK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	AL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	AM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	72
1	AN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	AO	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	72
1	AP	502/504 (100%)	483 (96%)	19 (4%)	0	100	100
1	AQ	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	72
1	AR	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AS	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	72
1	AT	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	43	72
1	BA	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	72
1	BB	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	30	60
1	BC	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	BD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	BE	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	BF	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	30	60
1	BG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	72
1	BH	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	BI	502/504 (100%)	479 (95%)	23 (5%)	0	100	100
1	BJ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	BK	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	72
1	BL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	BM	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	BN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	BO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	BP	502/504 (100%)	479 (95%)	21 (4%)	2 (0%)	30	60
1	BQ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	BR	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	BS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	BT	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	72
1	CA	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	CB	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	72
1	CC	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	CD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	CE	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	72
1	CF	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	72
1	CG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	72
1	CH	502/504 (100%)	481 (96%)	21 (4%)	0	100	100
1	CI	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CJ	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	43	72
1	CK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	72
1	CL	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	CM	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	30	60
1	CN	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	CO	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	CP	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	72
1	CQ	502/504 (100%)	482 (96%)	18 (4%)	2 (0%)	30	60
1	CR	502/504 (100%)	479 (95%)	21 (4%)	2 (0%)	30	60
1	CS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	72
1	CT	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	43	72
All	All	30120/30240 (100%)	28873 (96%)	1181 (4%)	66 (0%)	43	72

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%)	20	46
1	AB	430/430 (100%)	399 (93%)	31 (7%)	13	40
1	AC	430/430 (100%)	402 (94%)	28 (6%)	15	43
1	AD	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	AE	430/430 (100%)	407 (95%)	23 (5%)	20	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AF	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	AG	430/430 (100%)	402 (94%)	28 (6%)	15	43
1	AH	430/430 (100%)	401 (93%)	29 (7%)	15	42
1	AI	430/430 (100%)	403 (94%)	27 (6%)	16	43
1	AJ	430/430 (100%)	408 (95%)	22 (5%)	21	47
1	AK	430/430 (100%)	407 (95%)	23 (5%)	20	46
1	AL	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	AM	430/430 (100%)	406 (94%)	24 (6%)	19	46
1	AN	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	AO	430/430 (100%)	403 (94%)	27 (6%)	16	43
1	AP	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	AQ	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	AR	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	AS	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	AT	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	BA	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	BB	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	BC	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	BD	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	BE	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	BF	430/430 (100%)	402 (94%)	28 (6%)	15	43
1	BG	430/430 (100%)	406 (94%)	24 (6%)	19	46
1	BH	430/430 (100%)	403 (94%)	27 (6%)	16	43
1	BI	430/430 (100%)	407 (95%)	23 (5%)	20	46
1	BJ	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	BK	430/430 (100%)	403 (94%)	27 (6%)	16	43
1	BL	430/430 (100%)	402 (94%)	28 (6%)	15	43
1	BM	430/430 (100%)	403 (94%)	27 (6%)	16	43
1	BN	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	BO	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	BP	430/430 (100%)	406 (94%)	24 (6%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BQ	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	BR	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	BS	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	BT	430/430 (100%)	406 (94%)	24 (6%)	19	46
1	CA	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	CB	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	CC	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	CD	430/430 (100%)	406 (94%)	24 (6%)	19	46
1	CE	430/430 (100%)	403 (94%)	27 (6%)	16	43
1	CF	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	CG	430/430 (100%)	406 (94%)	24 (6%)	19	46
1	CH	430/430 (100%)	403 (94%)	27 (6%)	16	43
1	CI	430/430 (100%)	402 (94%)	28 (6%)	15	43
1	CJ	430/430 (100%)	405 (94%)	25 (6%)	18	45
1	CK	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	CL	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	CM	430/430 (100%)	402 (94%)	28 (6%)	15	43
1	CN	430/430 (100%)	407 (95%)	23 (5%)	20	46
1	CO	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	CP	430/430 (100%)	403 (94%)	27 (6%)	16	43
1	CQ	430/430 (100%)	404 (94%)	26 (6%)	17	44
1	CR	430/430 (100%)	403 (94%)	27 (6%)	16	43
1	CS	430/430 (100%)	406 (94%)	24 (6%)	19	46
1	CT	430/430 (100%)	406 (94%)	24 (6%)	19	46
All	All	25800/25800 (100%)	24258 (94%)	1542 (6%)	17	44

5 of 1542 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BQ	56	LEU
1	CE	289	ARG
1	BR	105	SER
1	BP	504	VAL
1	CA	260	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 742 such sidechains are listed below:

Mol	Chain	Res	Type
1	BR	98	HIS
1	CG	147	GLN
1	BS	98	HIS
1	BR	74	ASN
1	CB	454	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.05	4 (0%) 82 60	51, 87, 117, 148	0
1	AB	504/504 (100%)	0.15	7 (1%) 73 48	55, 90, 122, 148	0
1	AC	504/504 (100%)	-0.00	2 (0%) 88 72	42, 76, 104, 147	0
1	AD	504/504 (100%)	-0.11	0 100 100	33, 68, 99, 130	0
1	AE	504/504 (100%)	-0.08	0 100 100	46, 75, 105, 119	0
1	AF	504/504 (100%)	-0.02	1 (0%) 91 80	41, 80, 110, 166	0
1	AG	504/504 (100%)	0.06	2 (0%) 88 72	46, 83, 118, 165	0
1	AH	504/504 (100%)	-0.07	0 100 100	44, 74, 105, 131	0
1	AI	504/504 (100%)	-0.11	2 (0%) 88 72	29, 65, 98, 141	0
1	AJ	504/504 (100%)	-0.11	0 100 100	34, 67, 99, 137	0
1	AK	504/504 (100%)	-0.04	0 100 100	37, 72, 104, 142	0
1	AL	504/504 (100%)	-0.08	2 (0%) 88 72	31, 67, 94, 131	0
1	AM	504/504 (100%)	-0.11	1 (0%) 91 80	32, 65, 96, 117	0
1	AN	504/504 (100%)	-0.16	0 100 100	29, 64, 94, 128	0
1	AO	504/504 (100%)	-0.13	2 (0%) 88 72	34, 66, 93, 124	0
1	AP	504/504 (100%)	-0.09	0 100 100	34, 69, 96, 124	0
1	AQ	504/504 (100%)	-0.16	1 (0%) 91 80	28, 60, 88, 111	0
1	AR	504/504 (100%)	-0.19	1 (0%) 91 80	23, 57, 89, 120	0
1	AS	504/504 (100%)	-0.20	1 (0%) 91 80	30, 60, 92, 124	0
1	AT	504/504 (100%)	-0.13	0 100 100	35, 69, 100, 141	0
1	BA	504/504 (100%)	0.39	9 (1%) 67 42	47, 90, 125, 207	0
1	BB	504/504 (100%)	0.71	21 (4%) 40 25	67, 105, 138, 173	0
1	BC	504/504 (100%)	0.84	24 (4%) 35 23	71, 114, 149, 205	0
1	BD	504/504 (100%)	0.64	13 (2%) 57 35	62, 104, 133, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	BE	504/504 (100%)	0.44	4 (0%) 82 60	48, 89, 122, 158	0
1	BF	504/504 (100%)	0.68	9 (1%) 67 42	63, 99, 131, 191	0
1	BG	504/504 (100%)	0.62	10 (1%) 65 41	59, 93, 125, 154	0
1	BH	504/504 (100%)	0.54	9 (1%) 67 42	48, 95, 130, 160	0
1	BI	504/504 (100%)	0.70	12 (2%) 59 37	65, 108, 143, 170	0
1	BJ	504/504 (100%)	0.76	14 (2%) 55 34	70, 109, 140, 195	0
1	BK	504/504 (100%)	0.30	2 (0%) 88 72	47, 85, 116, 178	0
1	BL	504/504 (100%)	0.10	2 (0%) 88 72	42, 75, 105, 152	0
1	BM	504/504 (100%)	0.42	11 (2%) 62 39	45, 84, 121, 181	0
1	BN	504/504 (100%)	0.55	6 (1%) 76 51	59, 98, 129, 176	0
1	BO	504/504 (100%)	0.49	7 (1%) 73 48	56, 98, 127, 161	0
1	BP	504/504 (100%)	0.94	43 (8%) 16 14	77, 124, 163, 199	0
1	BQ	504/504 (100%)	0.89	24 (4%) 35 23	78, 122, 162, 199	0
1	BR	504/504 (100%)	0.84	24 (4%) 35 23	76, 116, 149, 189	0
1	BS	504/504 (100%)	0.89	20 (3%) 42 27	72, 117, 152, 210	0
1	BT	504/504 (100%)	1.04	40 (7%) 18 15	87, 127, 161, 200	0
1	CA	504/504 (100%)	0.86	20 (3%) 42 27	76, 120, 153, 177	0
1	CB	504/504 (100%)	0.72	20 (3%) 42 27	68, 106, 141, 177	0
1	CC	504/504 (100%)	0.64	13 (2%) 57 35	55, 102, 137, 204	0
1	CD	504/504 (100%)	0.59	19 (3%) 44 28	68, 105, 141, 172	0
1	CE	504/504 (100%)	0.79	20 (3%) 42 27	72, 119, 149, 191	0
1	CF	504/504 (100%)	0.27	3 (0%) 85 66	41, 85, 115, 151	0
1	CG	504/504 (100%)	0.49	10 (1%) 65 41	57, 88, 121, 163	0
1	CH	504/504 (100%)	0.44	6 (1%) 76 51	58, 90, 124, 179	0
1	CI	504/504 (100%)	0.32	11 (2%) 62 39	44, 84, 121, 188	0
1	CJ	504/504 (100%)	0.12	0 100 100	44, 77, 110, 151	0
1	CK	504/504 (100%)	0.58	9 (1%) 67 42	61, 103, 133, 150	0
1	CL	504/504 (100%)	0.65	8 (1%) 70 45	68, 114, 148, 184	0
1	CM	504/504 (100%)	0.61	14 (2%) 55 34	64, 111, 141, 186	0
1	CN	504/504 (100%)	0.41	5 (0%) 79 55	62, 97, 127, 171	0
1	CO	504/504 (100%)	0.35	7 (1%) 73 48	59, 91, 126, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	CP	504/504 (100%)	0.05	2 (0%)	88 72	41, 73, 105, 133	0
1	CQ	504/504 (100%)	0.17	4 (0%)	82 60	46, 76, 112, 171	0
1	CR	504/504 (100%)	0.23	4 (0%)	82 60	45, 84, 114, 172	0
1	CS	504/504 (100%)	0.24	3 (0%)	85 66	45, 86, 119, 153	0
1	CT	504/504 (100%)	0.26	2 (0%)	88 72	52, 82, 111, 136	0
All	All	30240/30240 (100%)	0.33	510 (1%)	69 43	23, 89, 135, 210	0

The worst 5 of 510 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BD	116	HIS	4.6
1	BG	383	GLU	4.1
1	BF	426	GLY	4.0
1	BI	143	ALA	3.9
1	BP	155	GLU	3.8

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.