



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 02:34 PM UTC

PDB ID : 4V5T / pdb_00004v5t
Title : X-ray structure of the Grapevine Fanleaf virus
Authors : Schellenberger, P.; Sauter, C.; Lorber, B.; Bron, P.; Trapani, S.; Bergdoll, M.; Marmonier, A.; Schmitt-Keichinger, C.; Lemaire, O.; Demangeat, G.; Ritzenthaler, C.
Deposited on : 2011-02-01
Resolution : 3.00 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

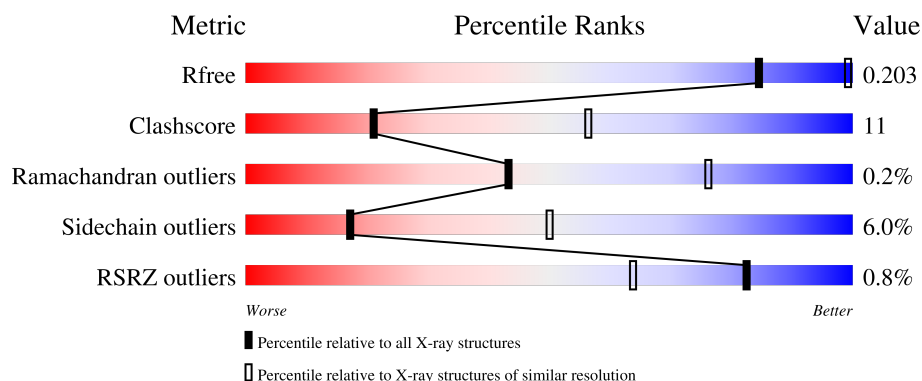
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



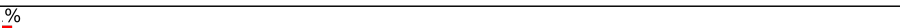
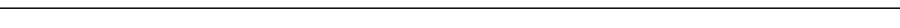
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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% 18% .
1	AB	504	% 80% 17% .
1	AC	504	79% 19% .
1	AD	504	% 80% 18% .
1	AE	504	% 81% 17% .

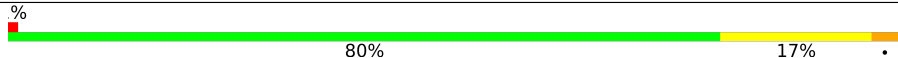
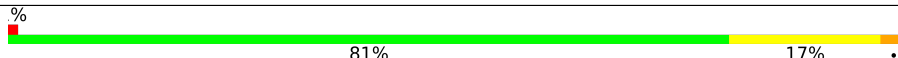
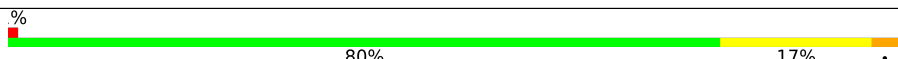
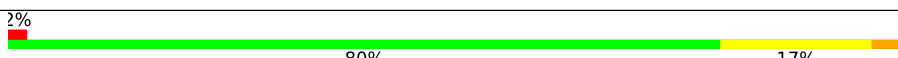
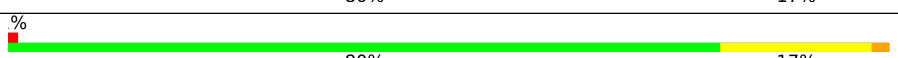
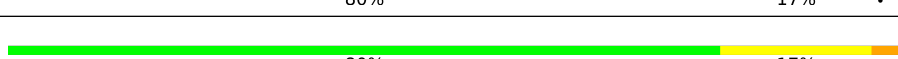
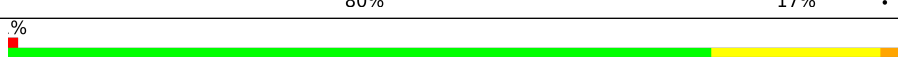
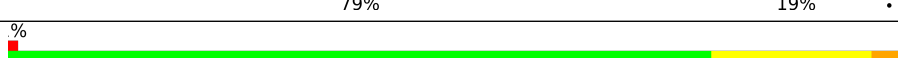
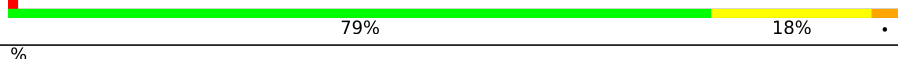
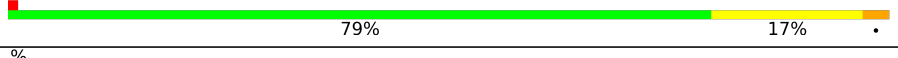
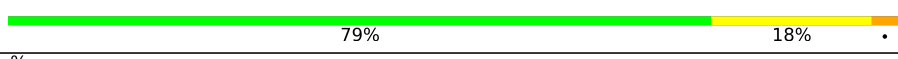
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Mol	Chain	Length	Quality of chain	
1	AF	504		.
1	AG	504		.
1	AH	504		.
1	AI	504		.
1	AJ	504		.
1	AK	504		.
1	AL	504		.
1	AM	504		.
1	AN	504		.
1	AO	504		.
1	AP	504		.
1	AQ	504		.
1	AR	504		.
1	AS	504		.
1	AT	504		.
1	BA	504		.
1	BB	504		.
1	BC	504		.
1	BD	504		.
1	BE	504		.
1	BF	504		.
1	BG	504		.
1	BH	504		.
1	BI	504		.
1	BJ	504		.

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Mol	Chain	Length	Quality of chain	
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		.

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Mol	Chain	Length	Quality of chain
1	CP	504	% 80% 17%
1	CQ	504	81% 17%
1	CR	504	% 80% 18%
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 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

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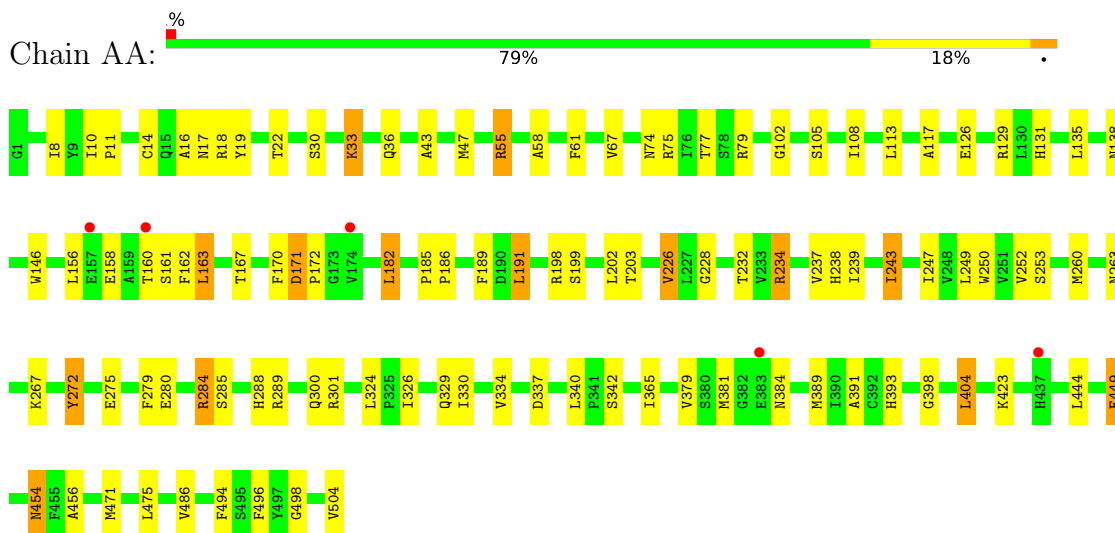
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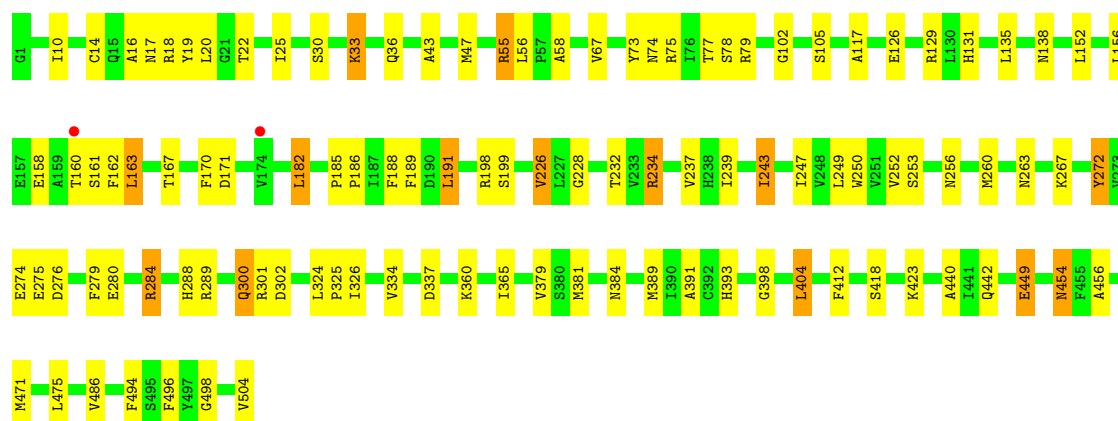
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CS	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			
1	CT	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			

3 Residue-property plots

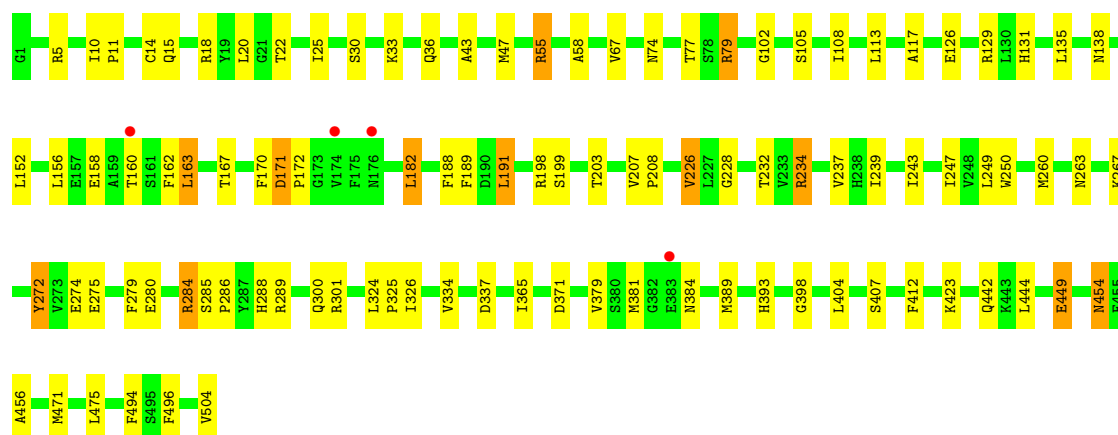
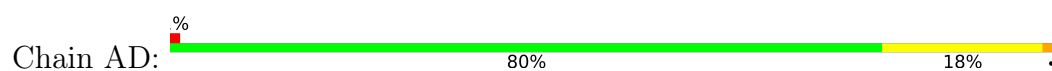
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

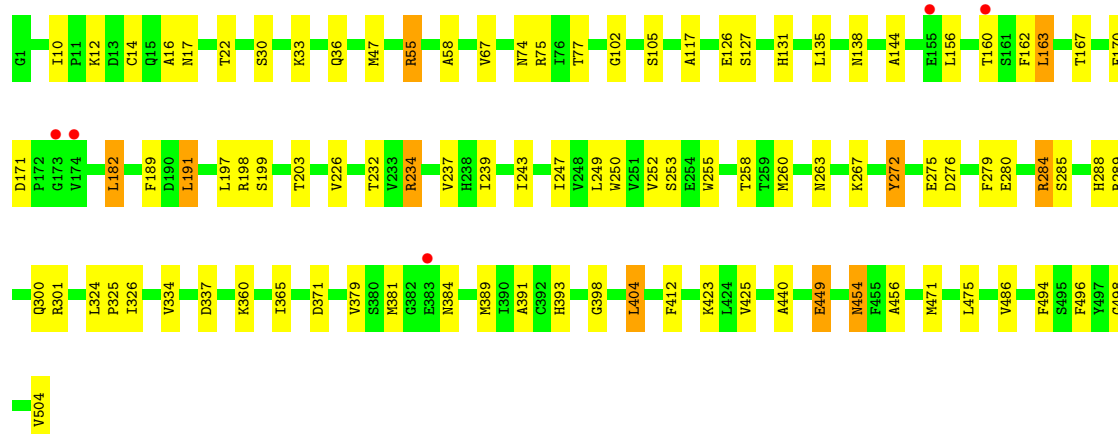
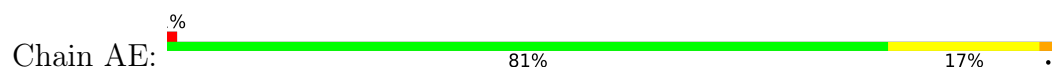




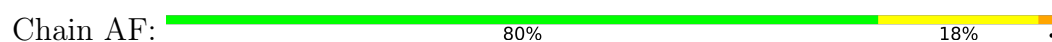
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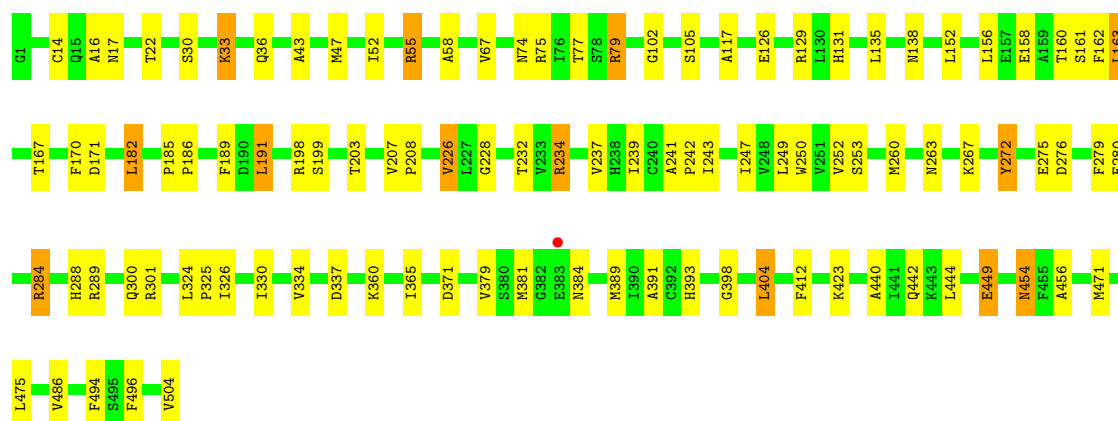


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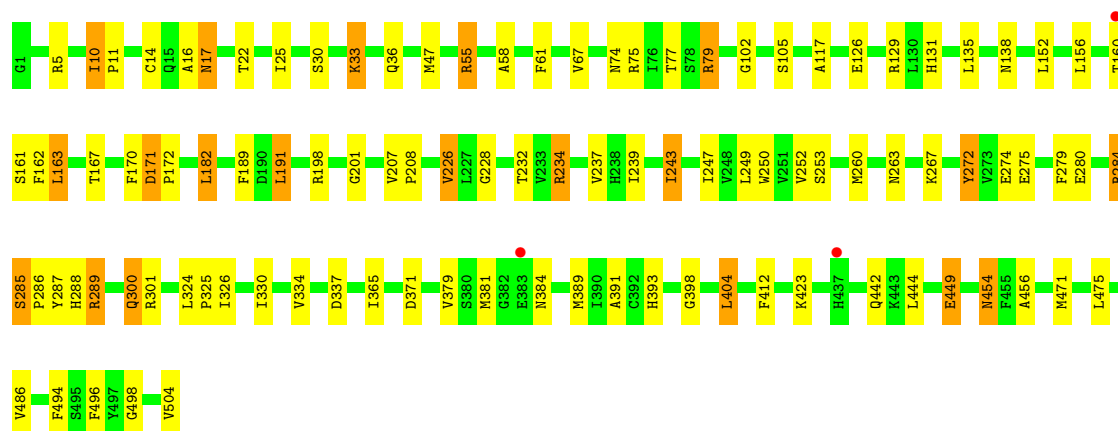
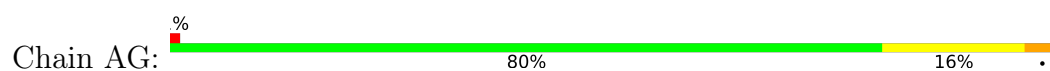


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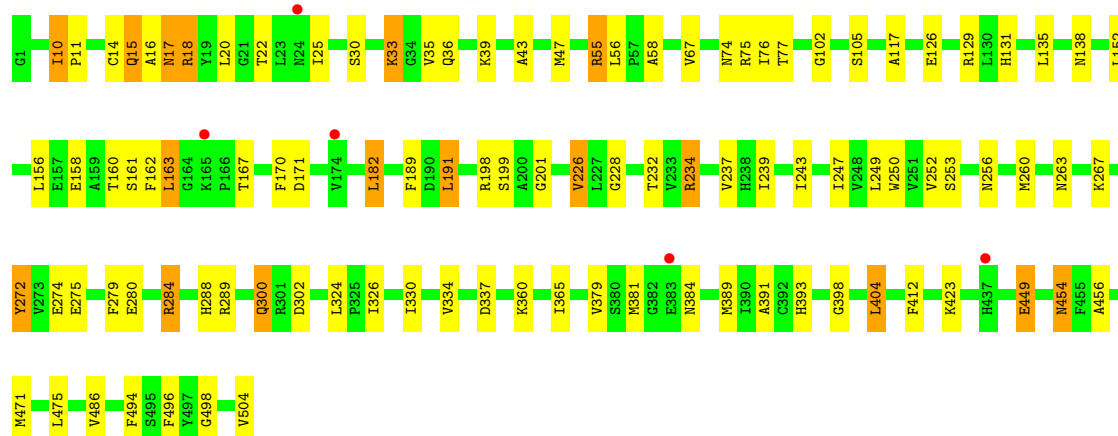
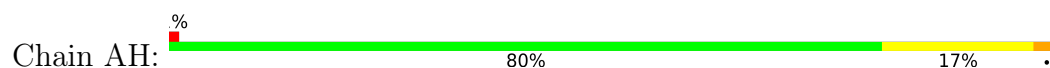




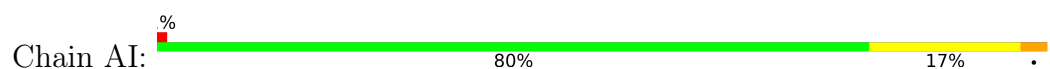
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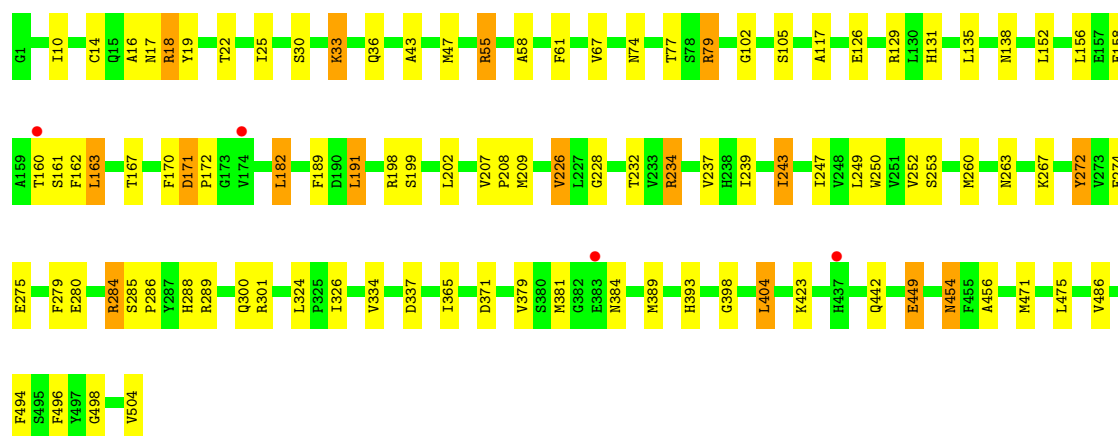


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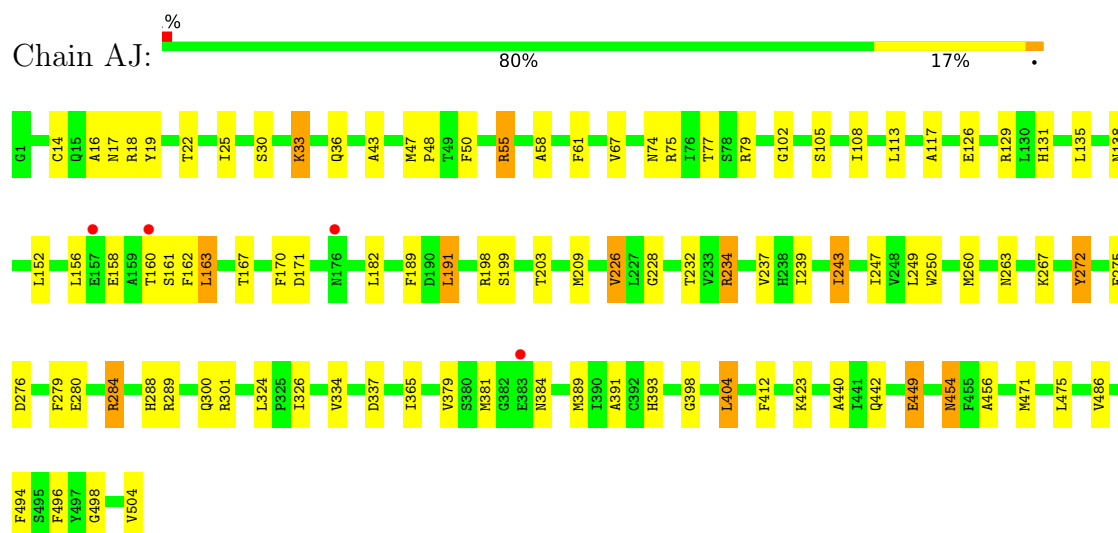


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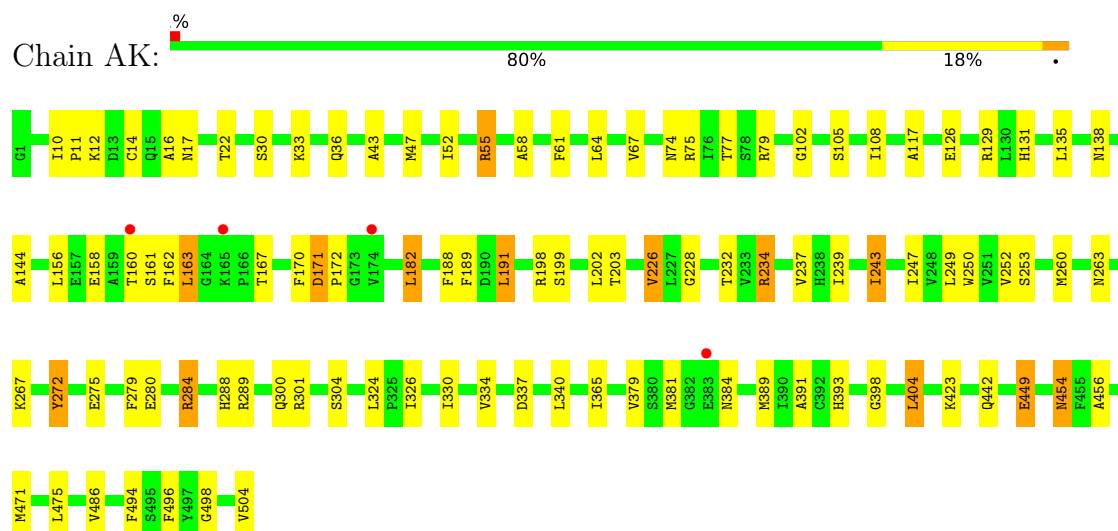




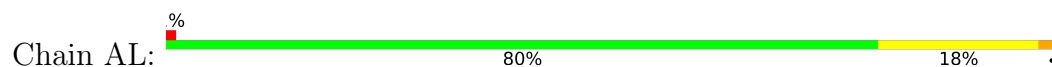
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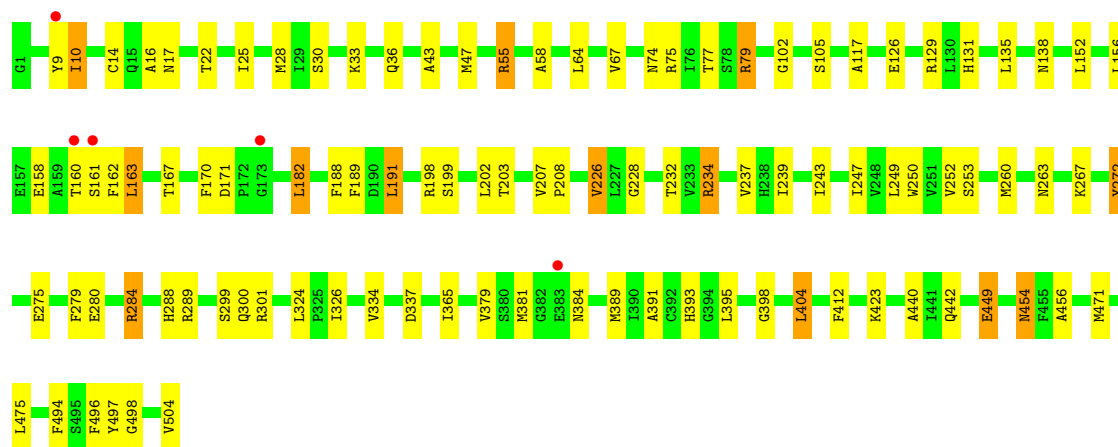


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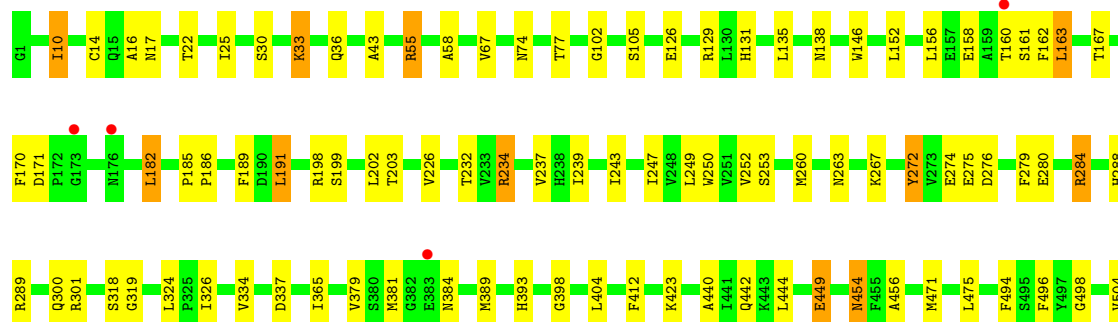
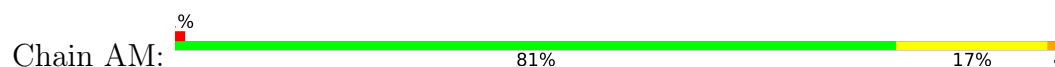


• Molecule 1: COAT PROTEIN

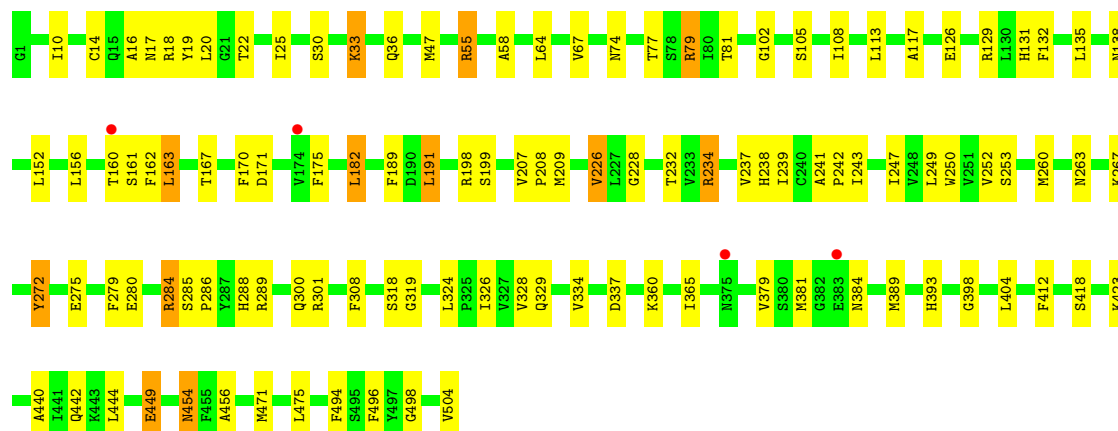
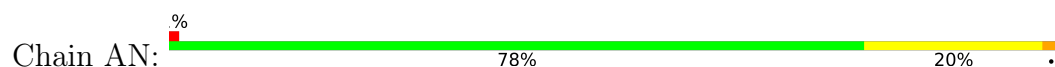




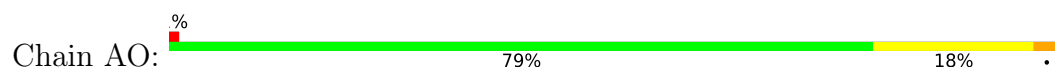
• Molecule 1: COAT PROTEIN

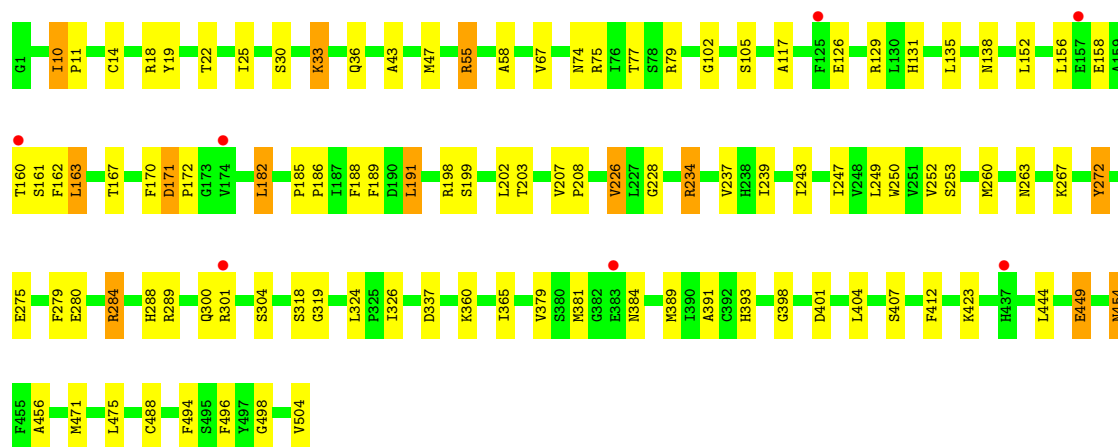


• Molecule 1: COAT PROTEIN



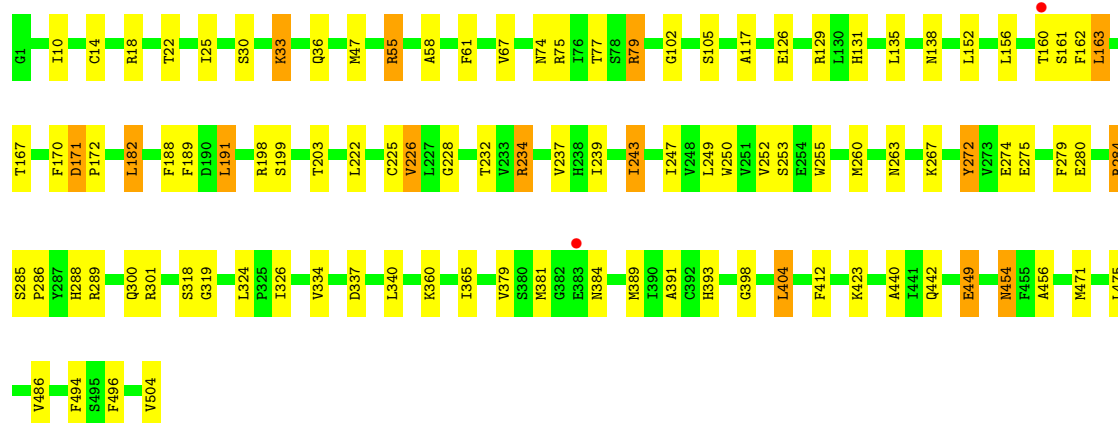
• Molecule 1: COAT PROTEIN





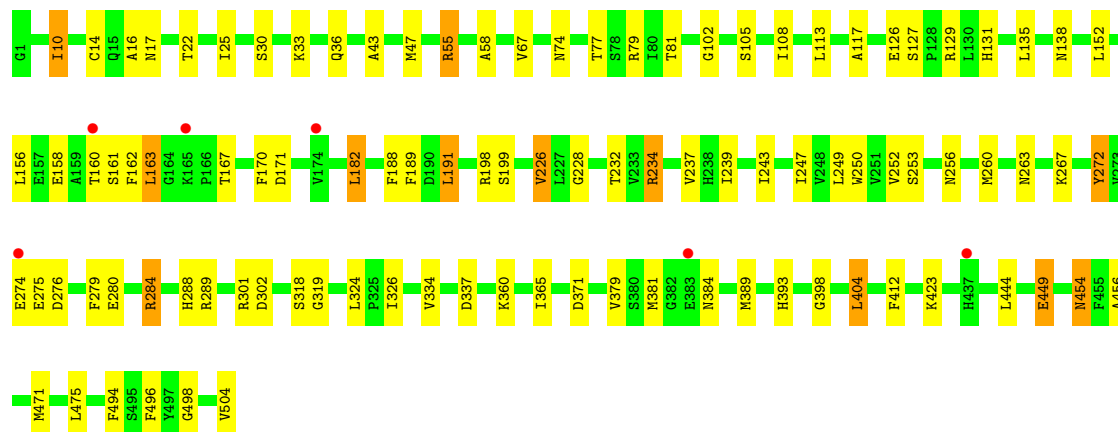
• Molecule 1: COAT PROTEIN

Chain AP: 80% 17% .

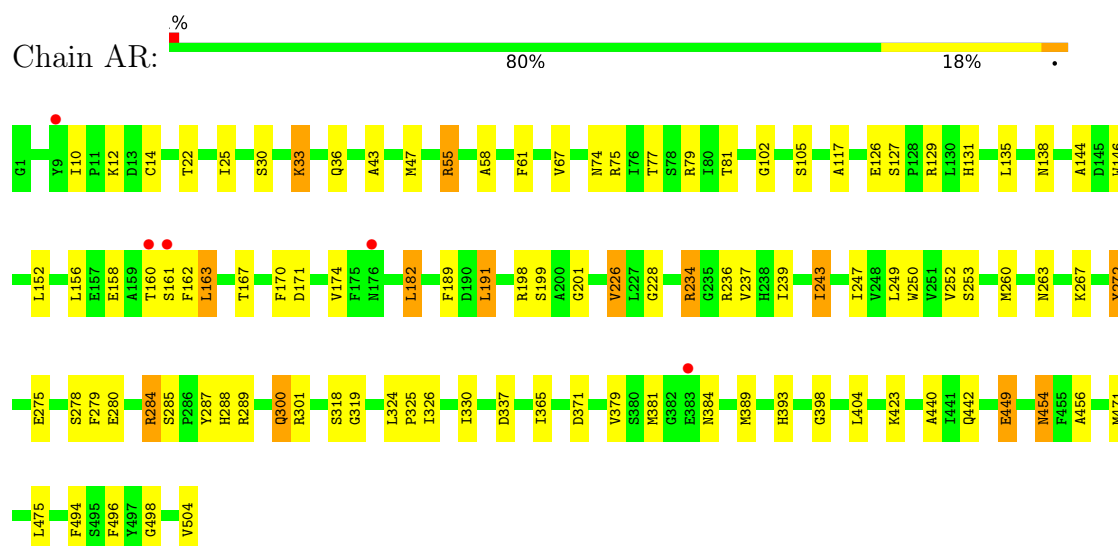


• Molecule 1: COAT PROTEIN

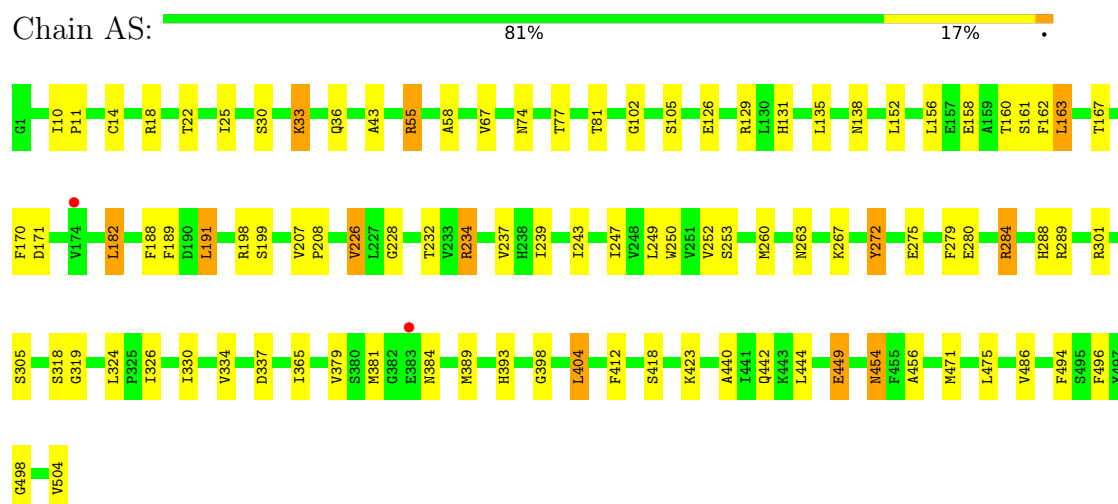
Chain AQ: 80% 17% .



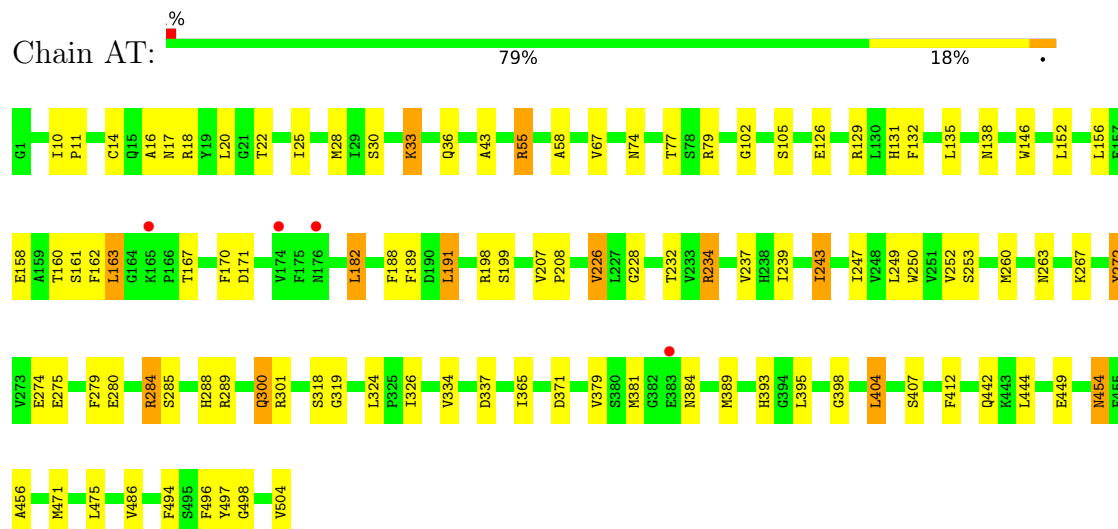
• Molecule 1: COAT PROTEIN



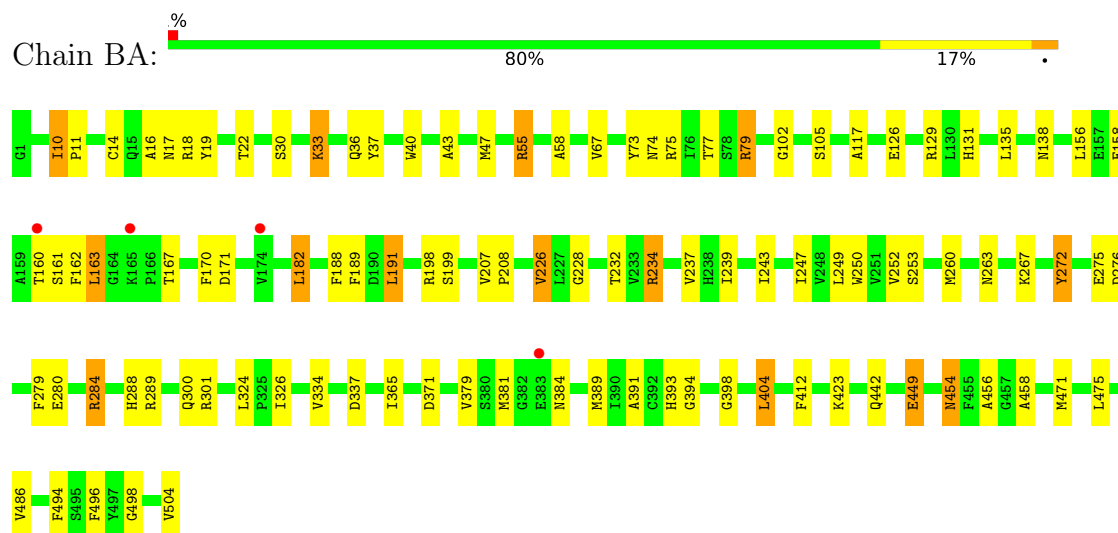
• Molecule 1: COAT PROTEIN



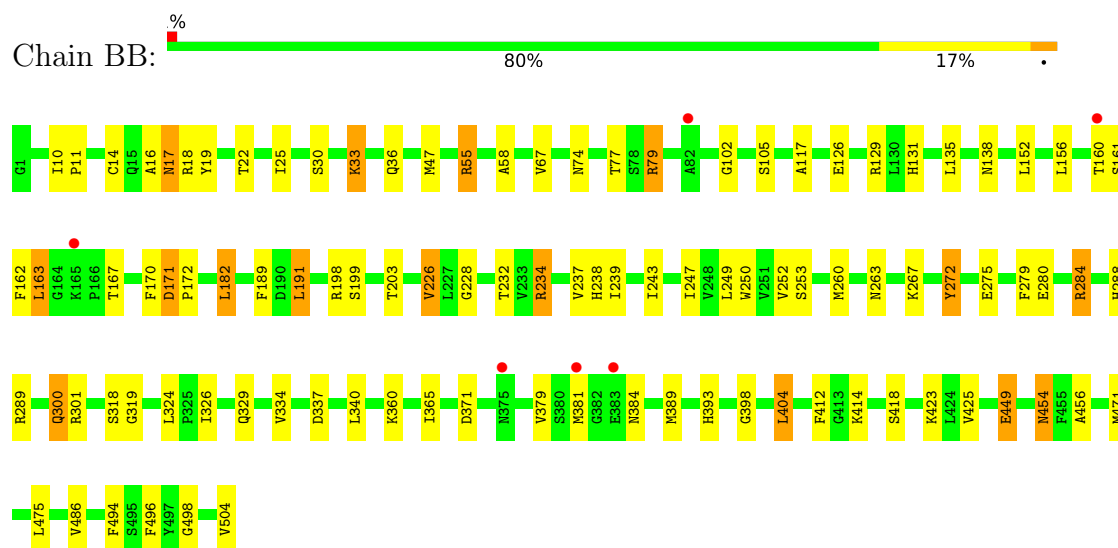
• Molecule 1: COAT PROTEIN



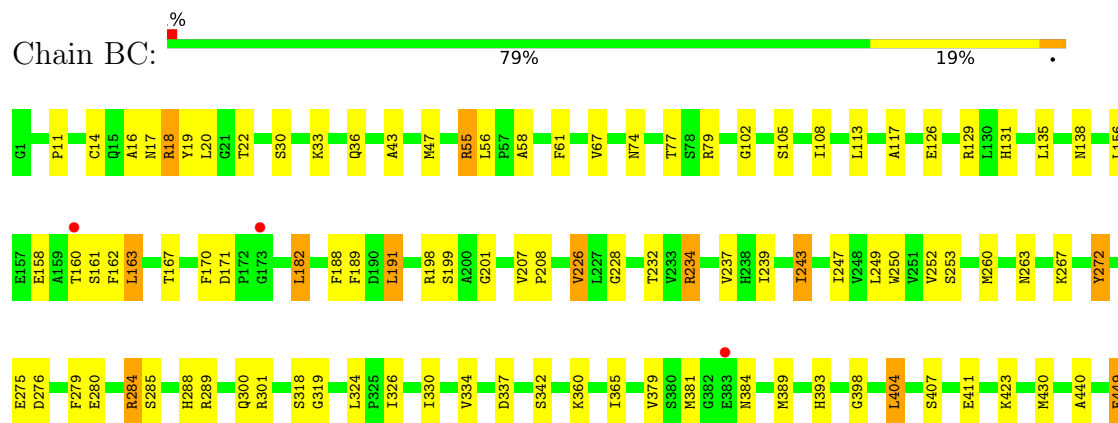
• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN

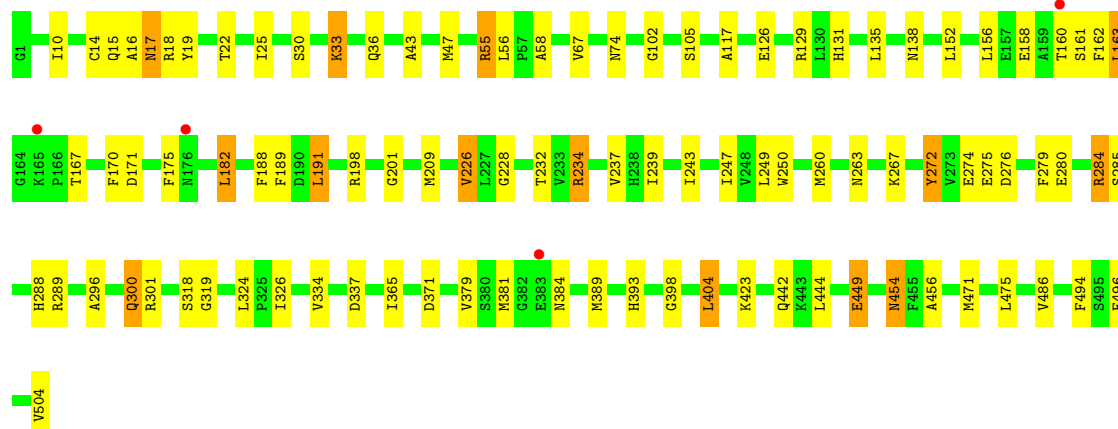
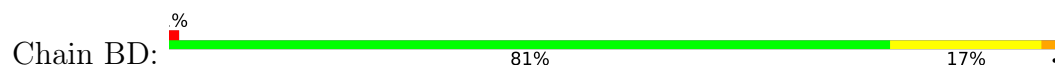


• Molecule 1: COAT PROTEIN

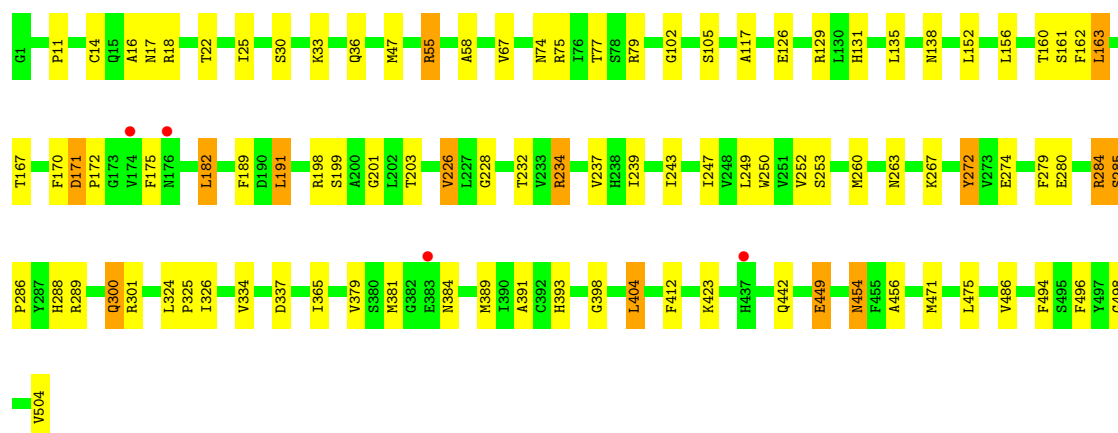
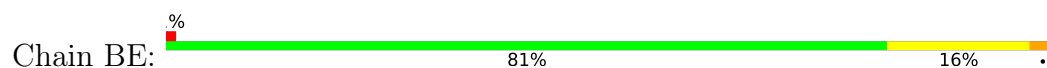




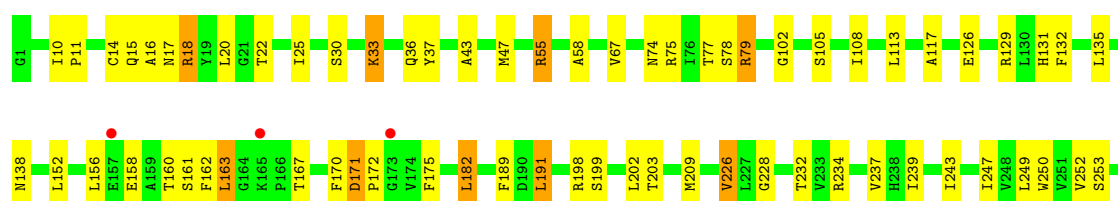
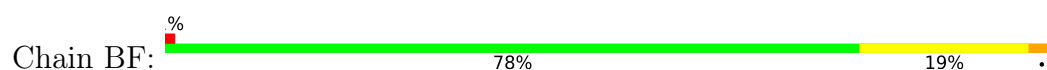
• Molecule 1: COAT PROTEIN

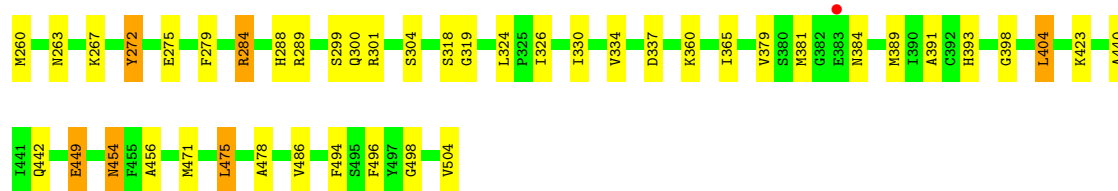


• Molecule 1: COAT PROTEIN

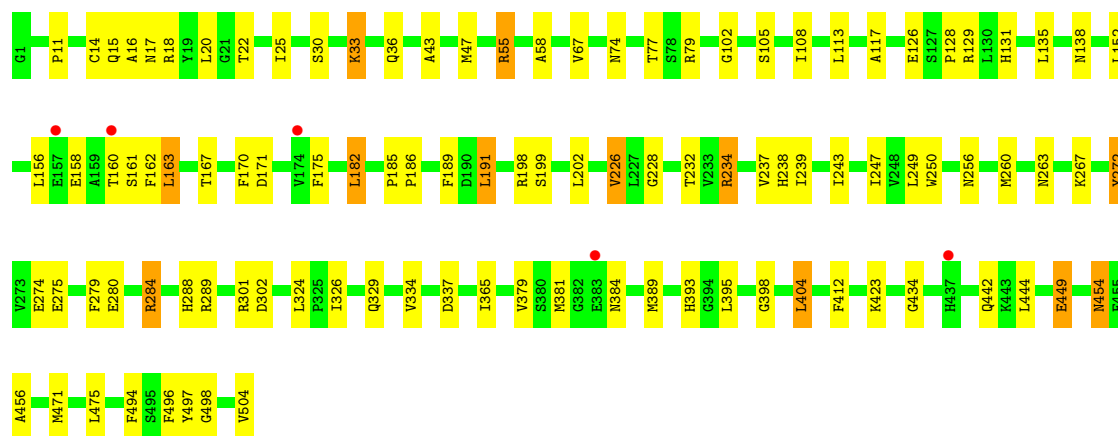
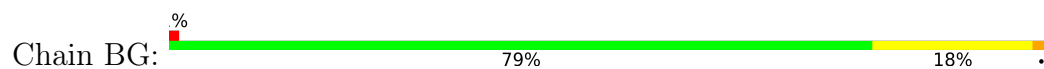


• Molecule 1: COAT PROTEIN

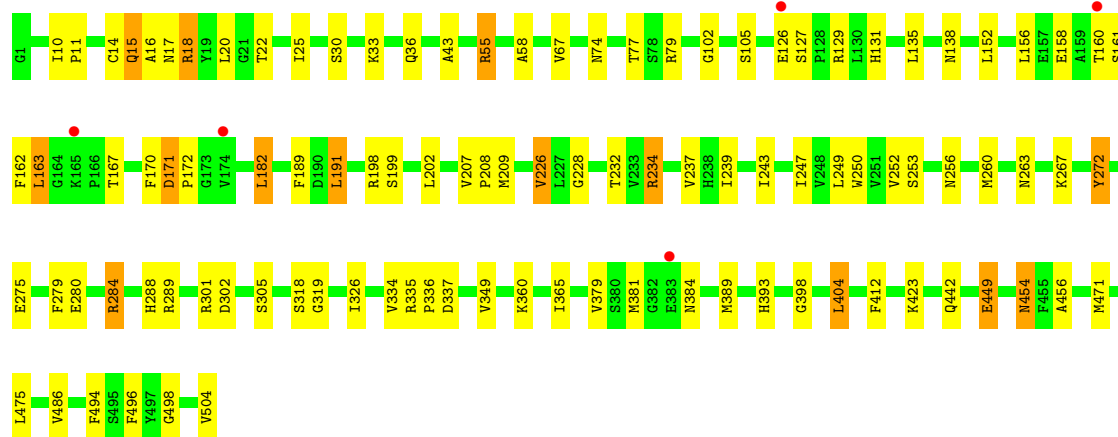
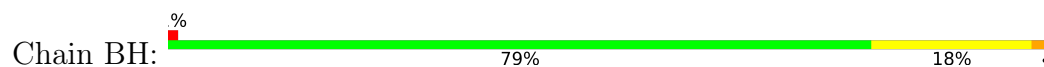




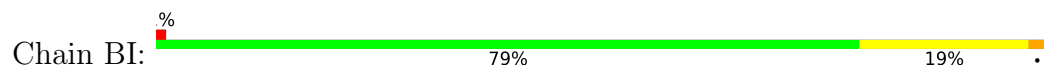
• Molecule 1: COAT PROTEIN

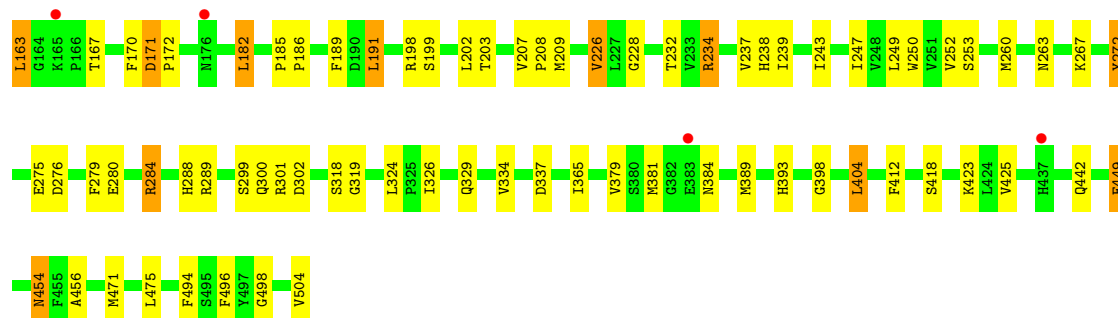


• Molecule 1: COAT PROTEIN



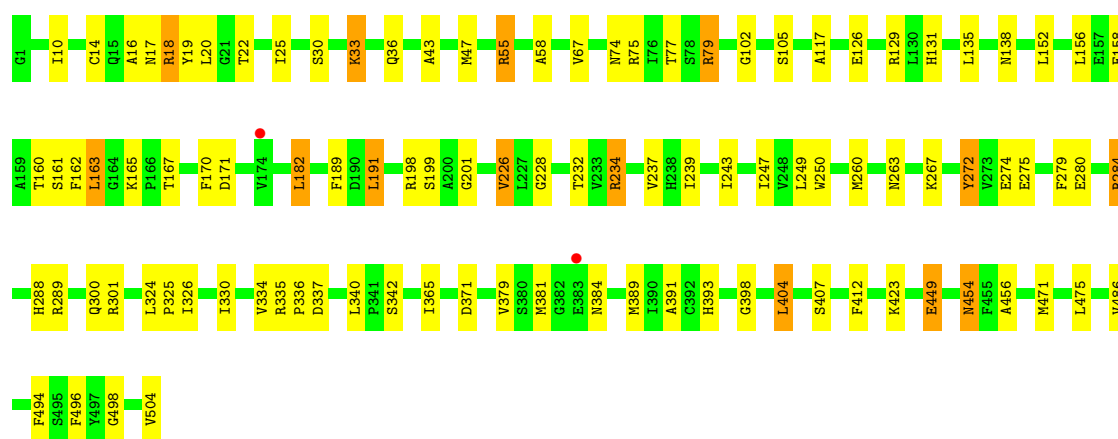
• Molecule 1: COAT PROTEIN





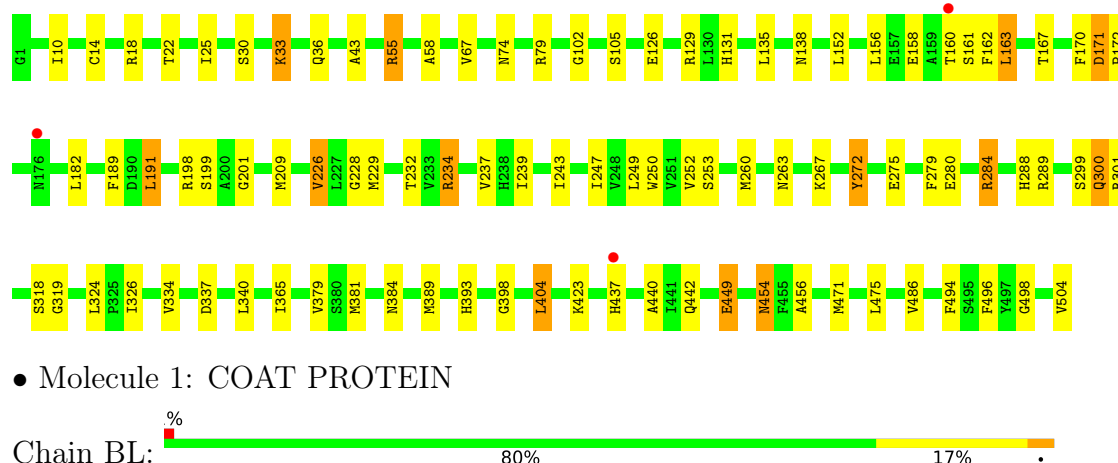
• Molecule 1: COAT PROTEIN

Chain BJ: 80% 17% .



• Molecule 1: COAT PROTEIN

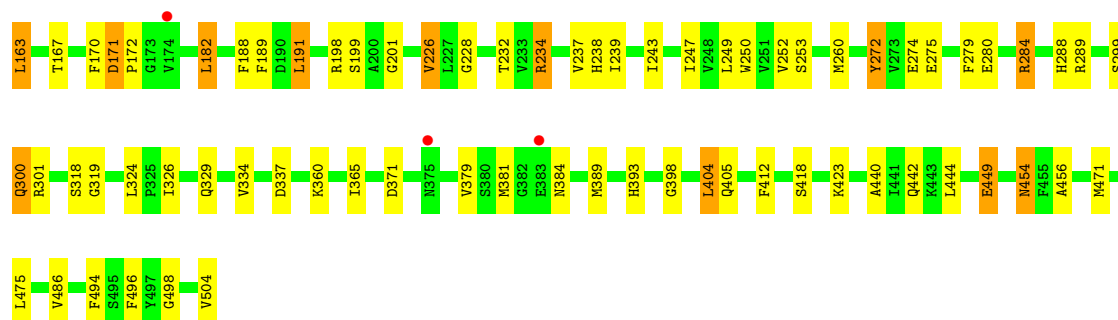
Chain BK: 81% 16% .



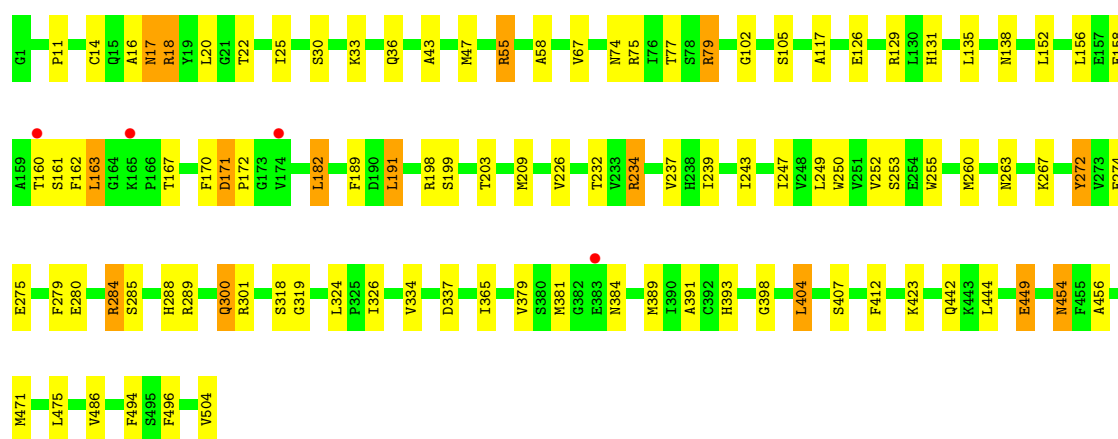
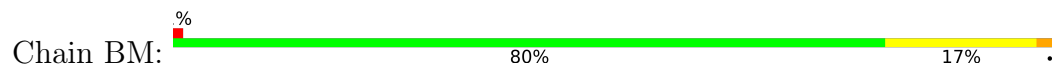
• Molecule 1: COAT PROTEIN

Chain BL: 80% 17% .

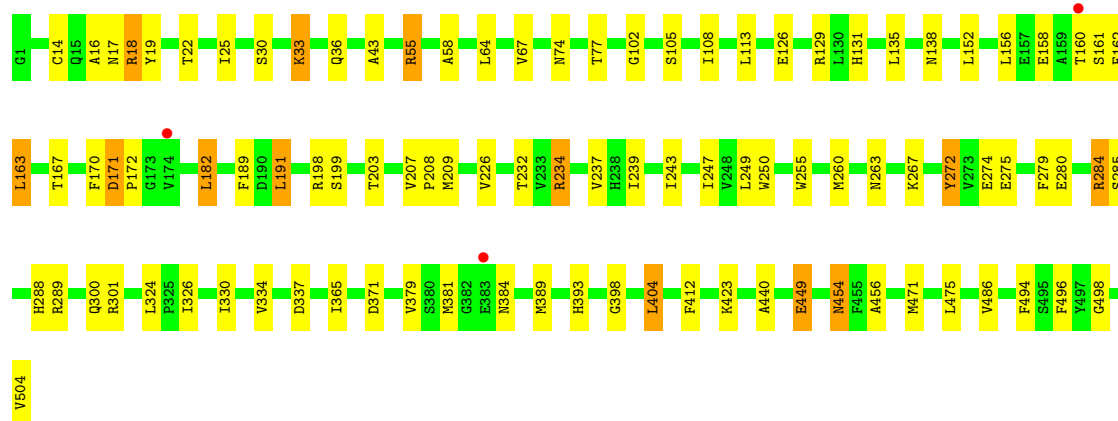
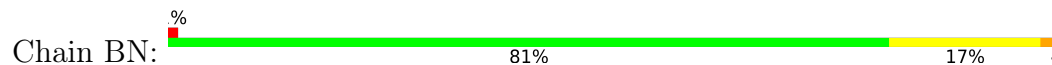




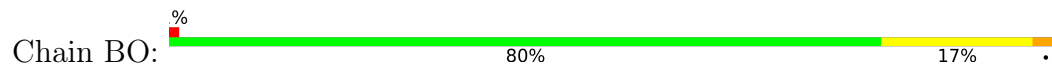
• Molecule 1: COAT PROTEIN

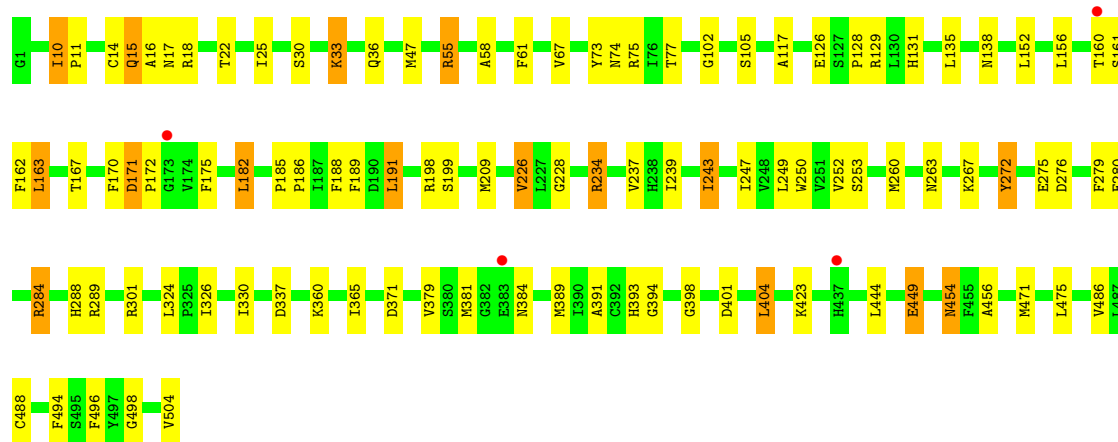


• Molecule 1: COAT PROTEIN

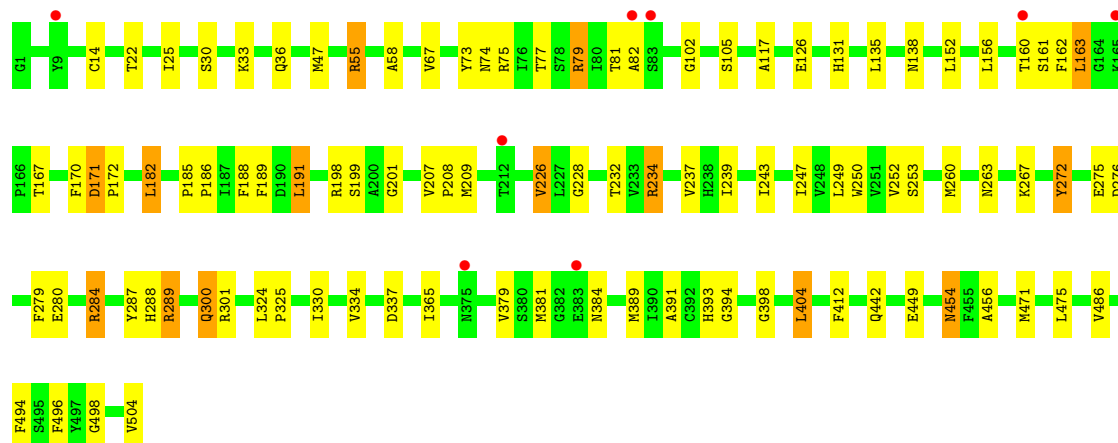
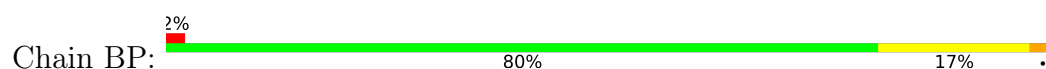


• Molecule 1: COAT PROTEIN

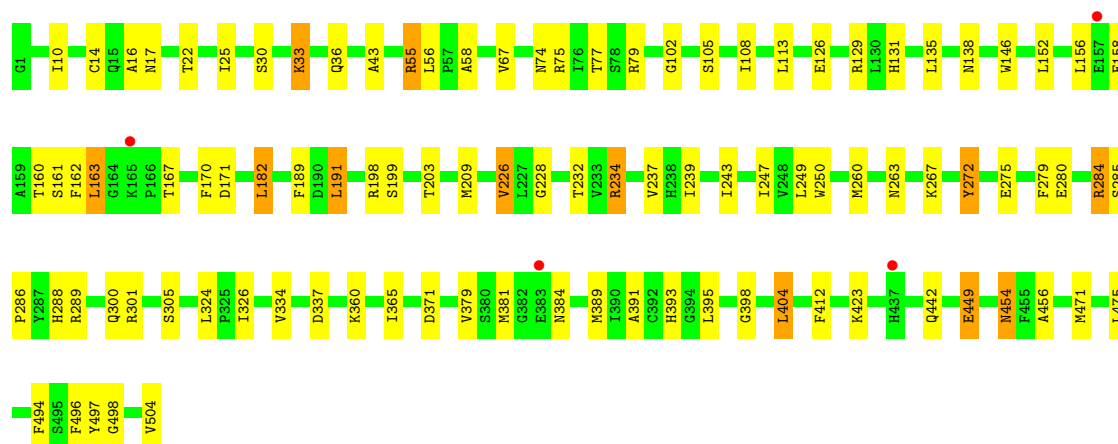
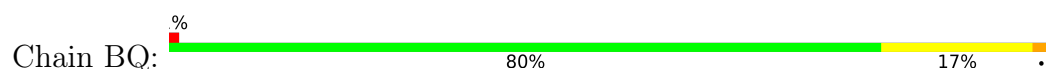




• Molecule 1: COAT PROTEIN

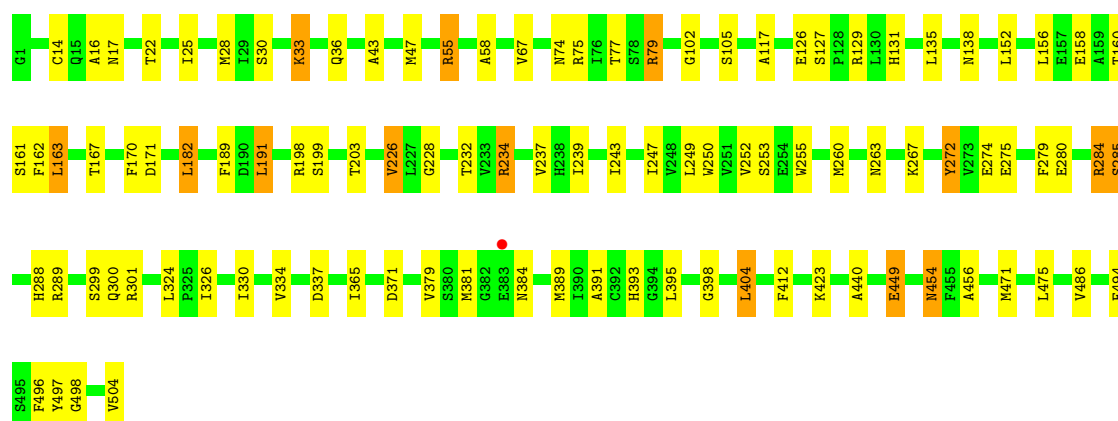


• Molecule 1: COAT PROTEIN



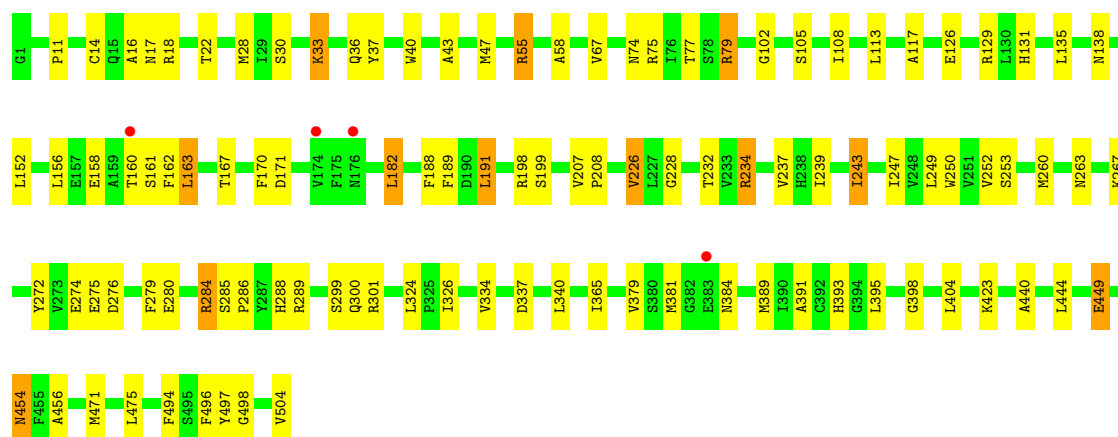
• Molecule 1: COAT PROTEIN

Chain BR:  80% 17% .



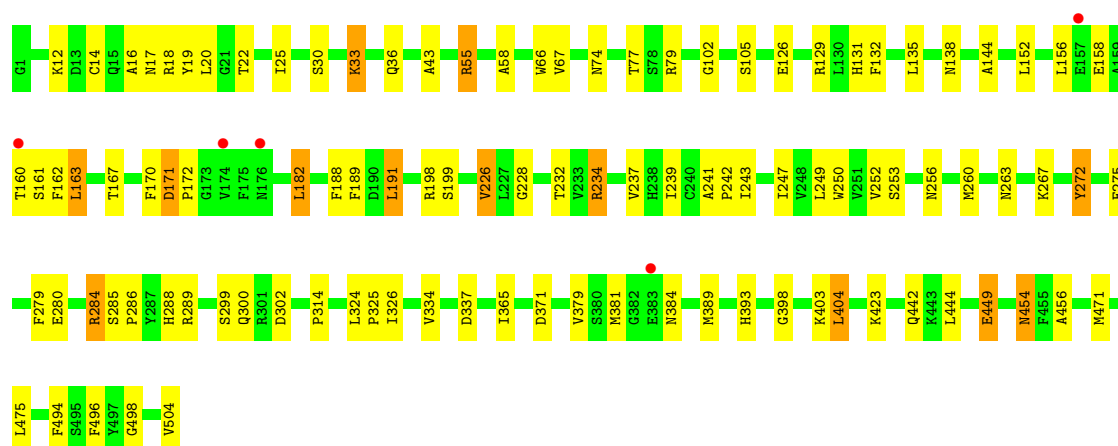
• Molecule 1: COAT PROTEIN

Chain BS:  79% 19% .

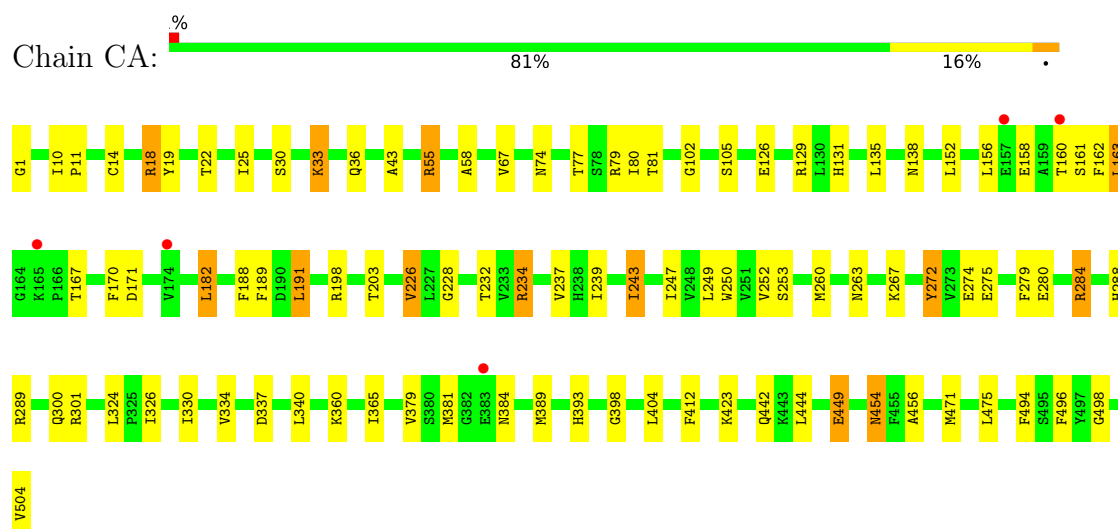


• Molecule 1: COAT PROTEIN

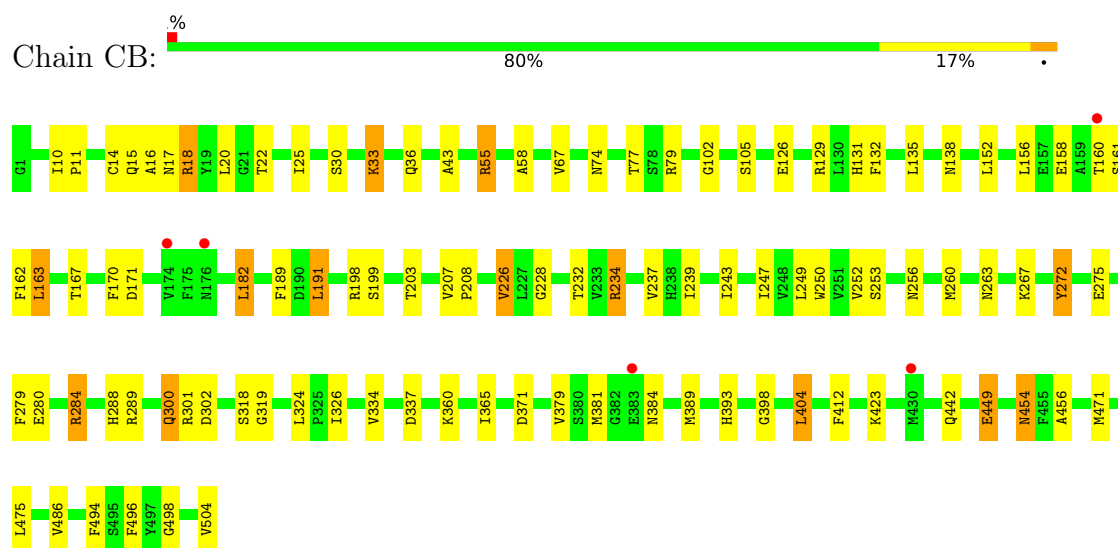
Chain BT:  79% 18% .



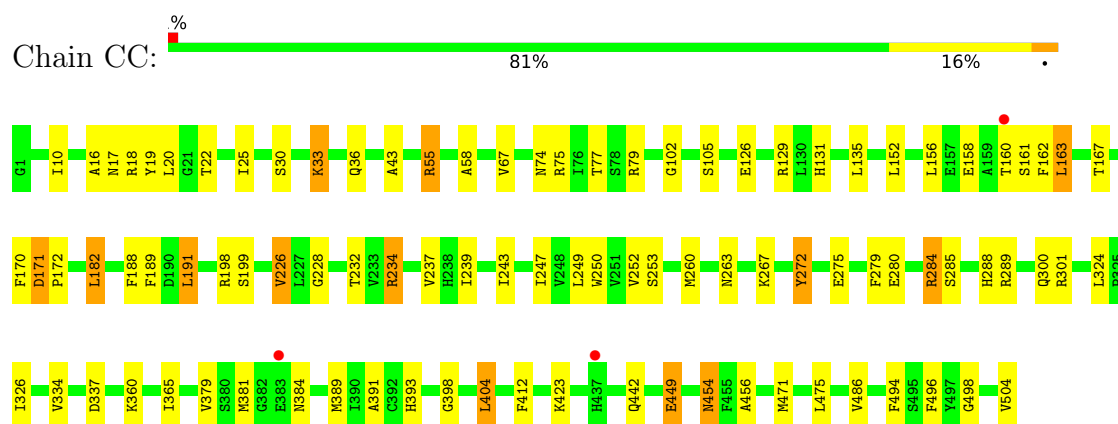
• Molecule 1: COAT PROTEIN



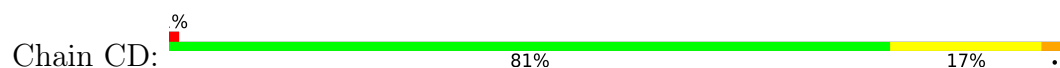
● Molecule 1: COAT PROTEIN

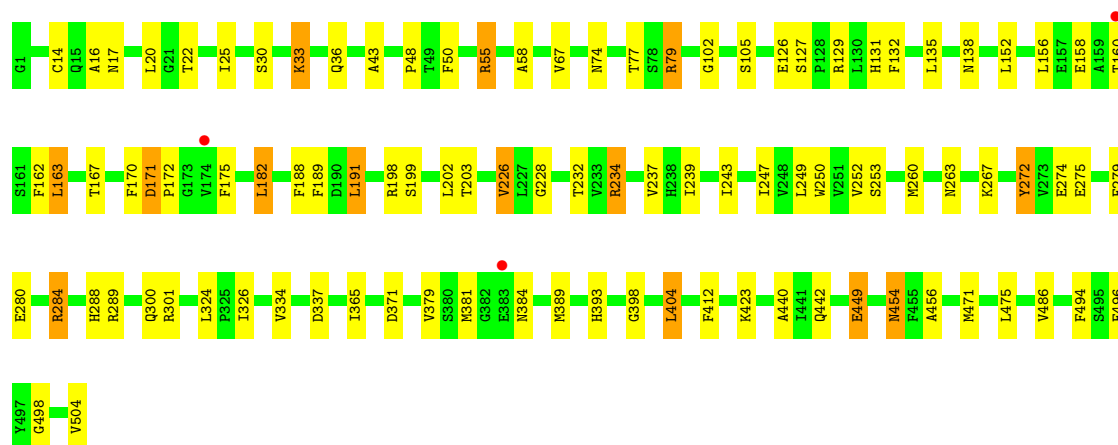


● Molecule 1: COAT PROTEIN



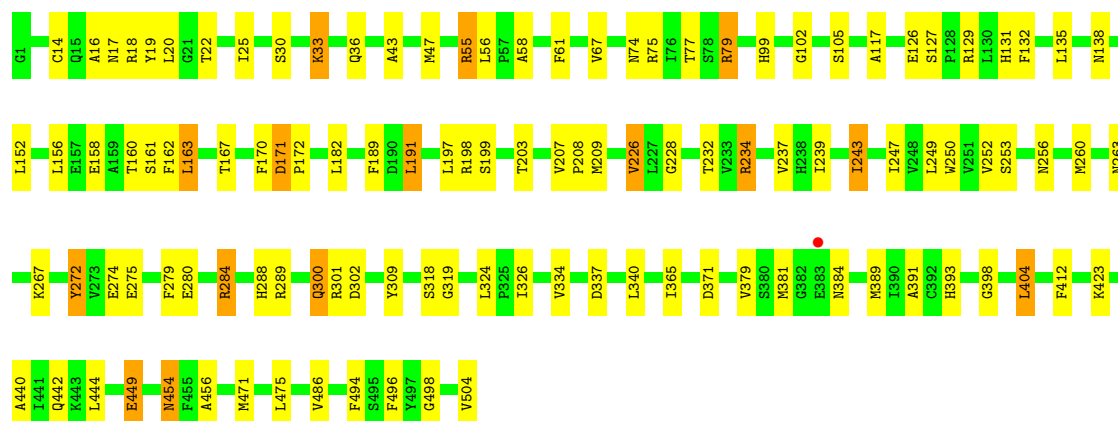
● Molecule 1: COAT PROTEIN





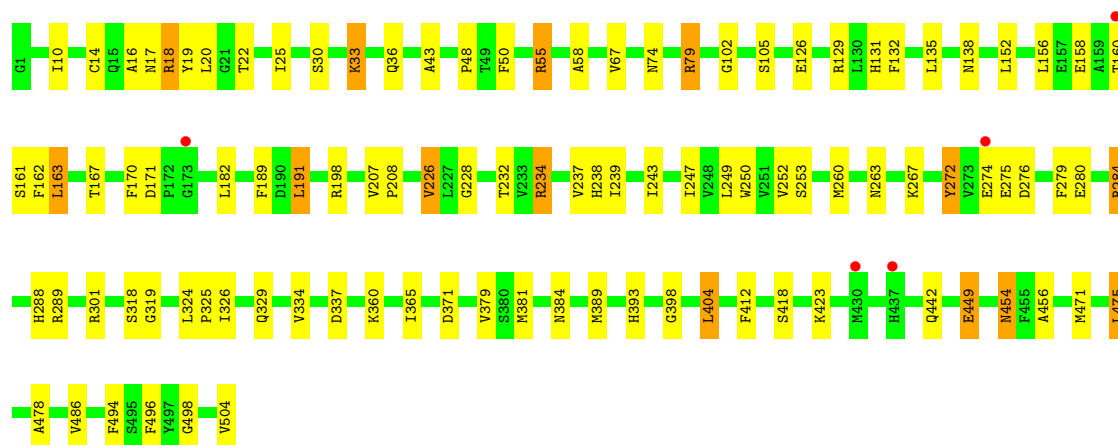
• Molecule 1: COAT PROTEIN

Chain CE: 77% 20% .

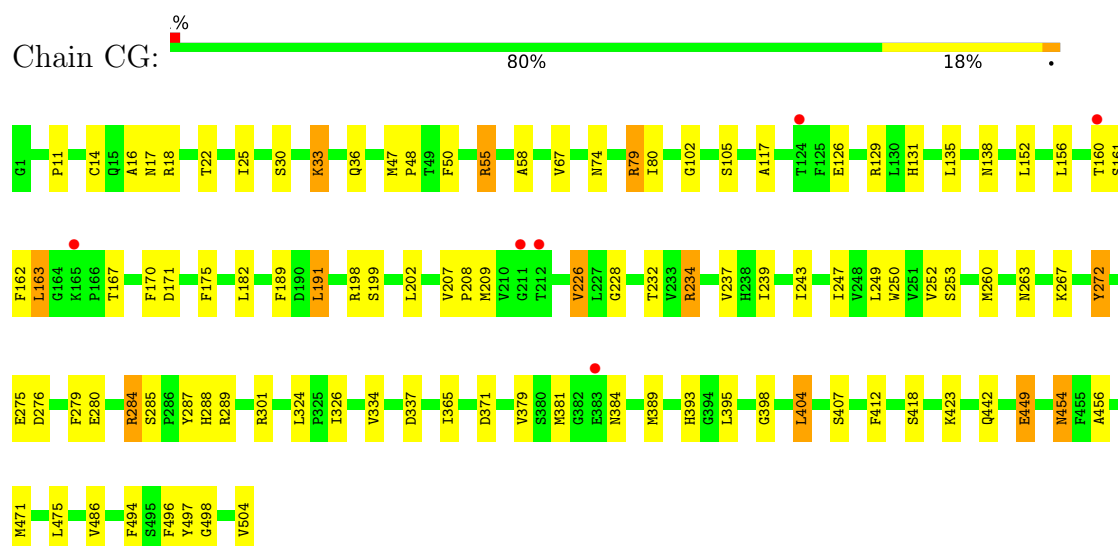


• Molecule 1: COAT PROTEIN

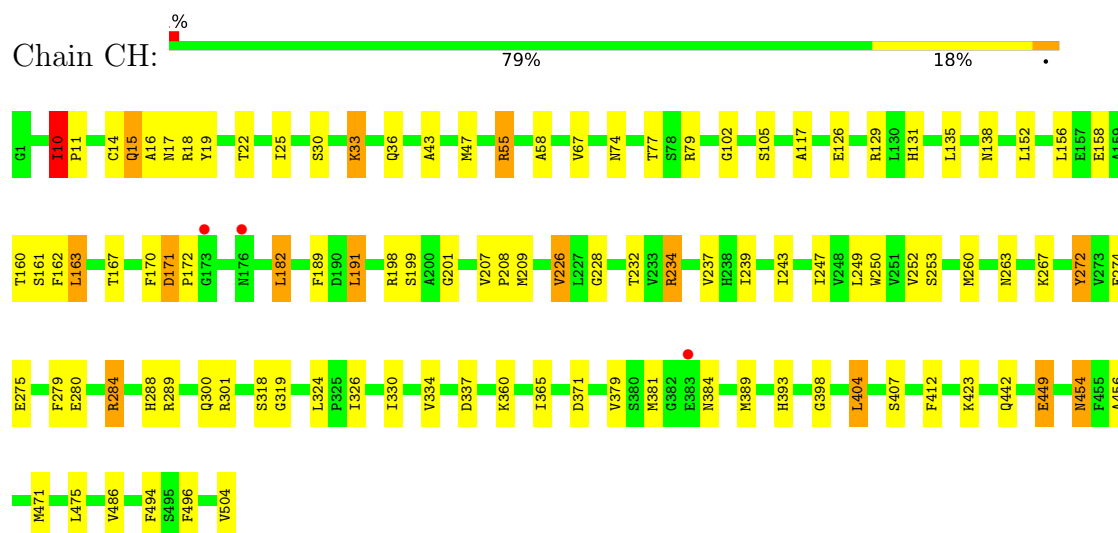
Chain CF: 80% 18% .



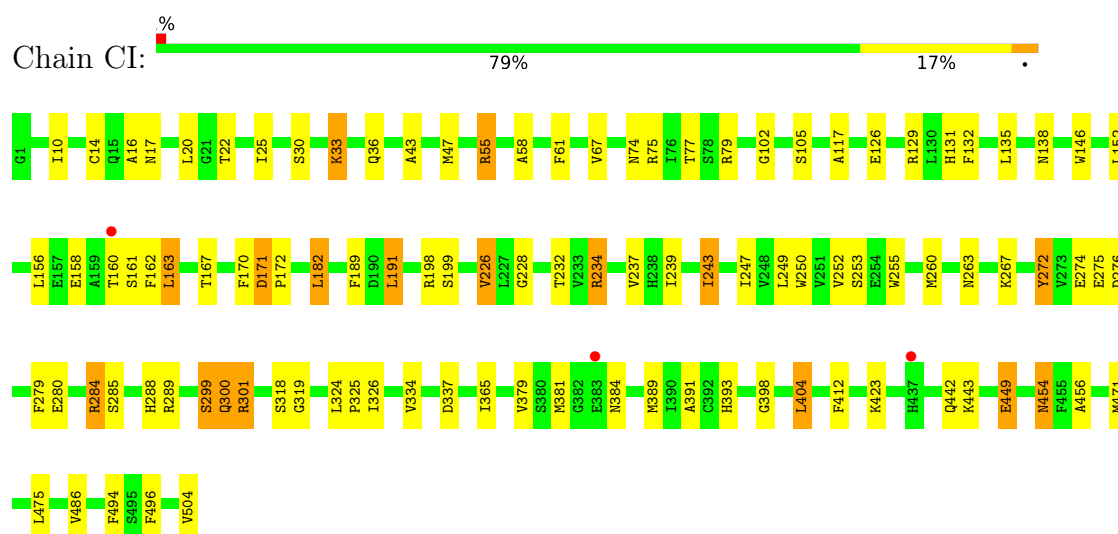
• Molecule 1: COAT PROTEIN



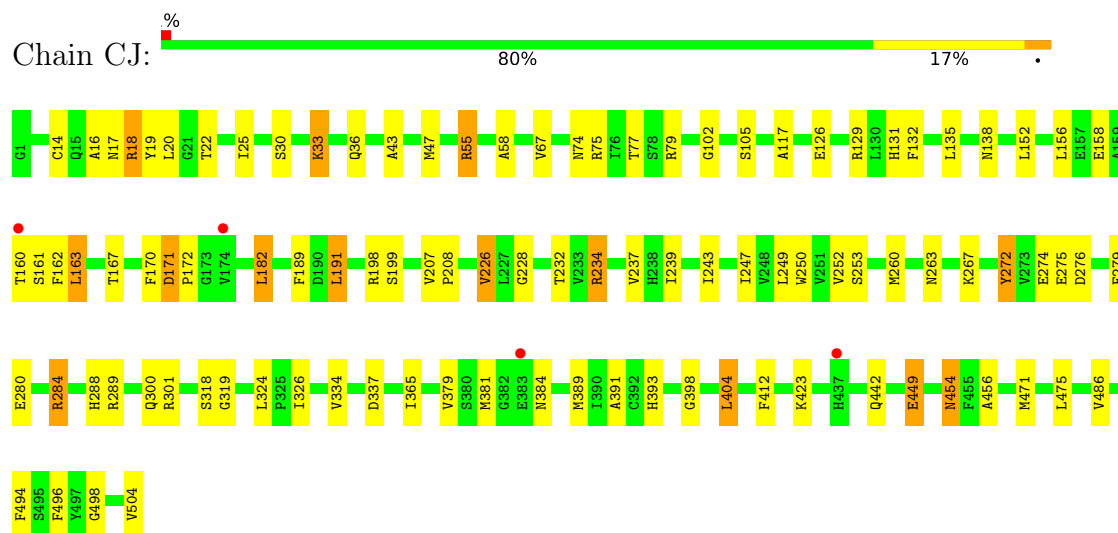
• Molecule 1: COAT PROTEIN



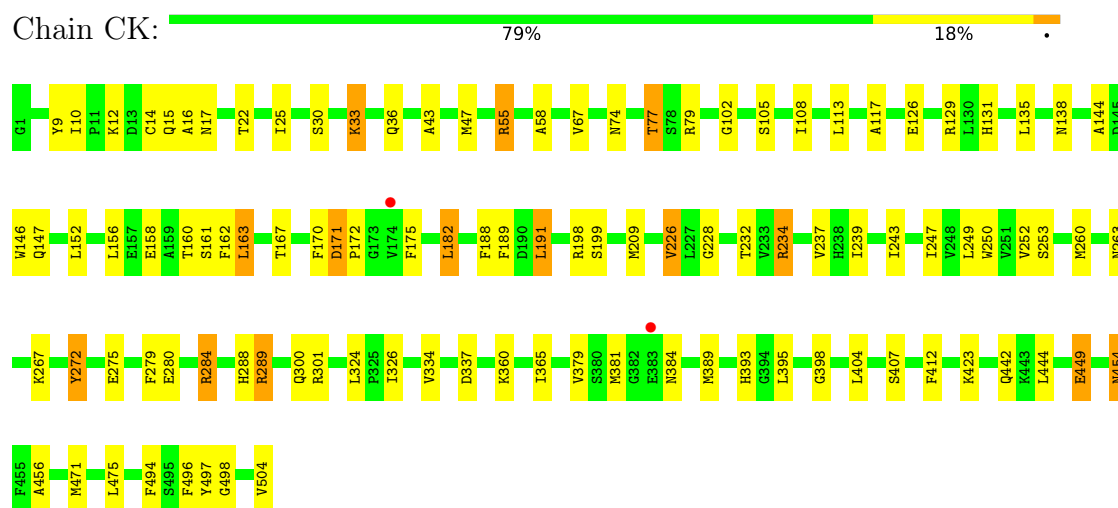
• Molecule 1: COAT PROTEIN



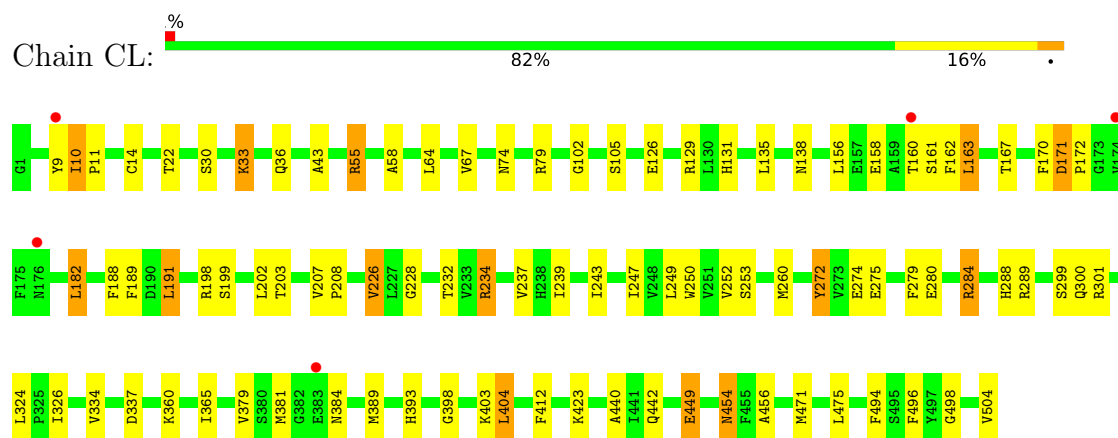
- Molecule 1: COAT PROTEIN



- Molecule 1: COAT PROTEIN

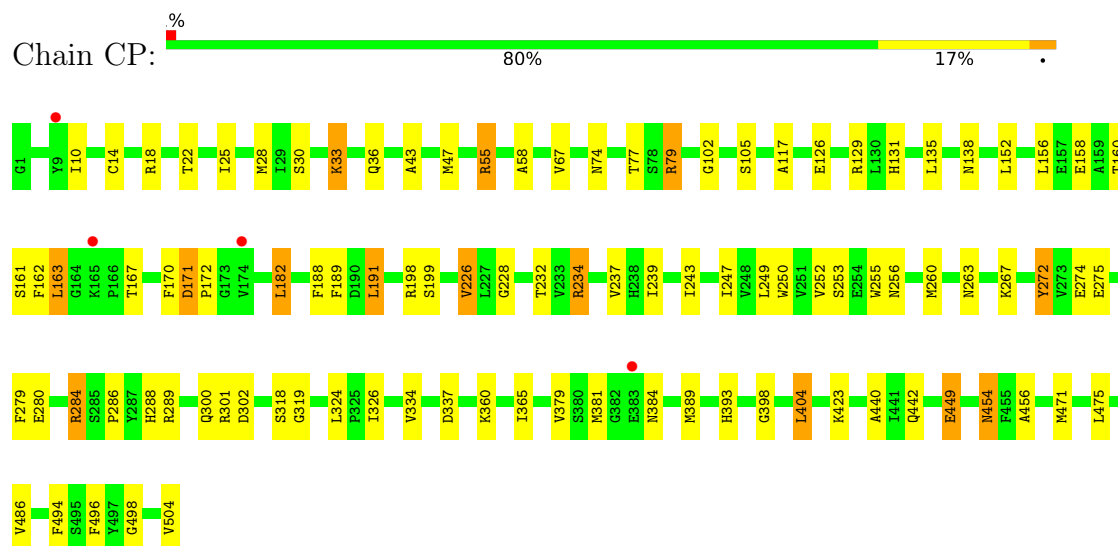


- Molecule 1: COAT PROTEIN

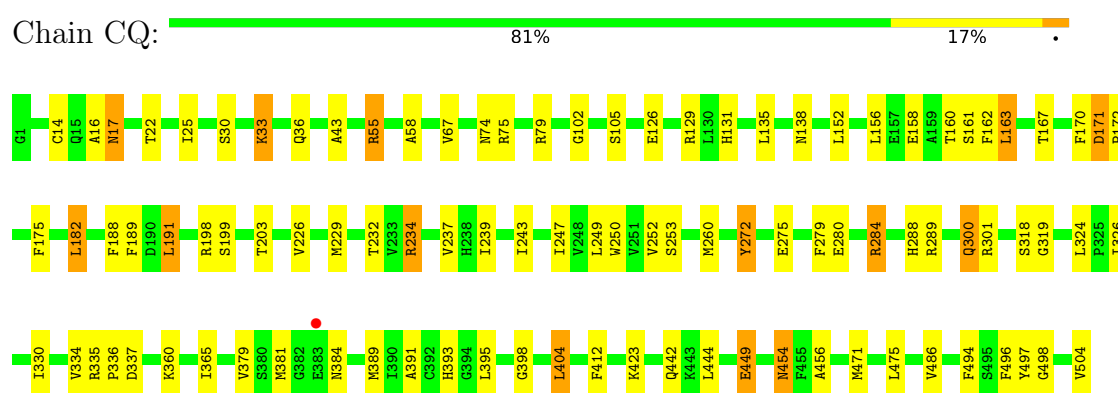


- Molecule 1: COAT PROTEIN

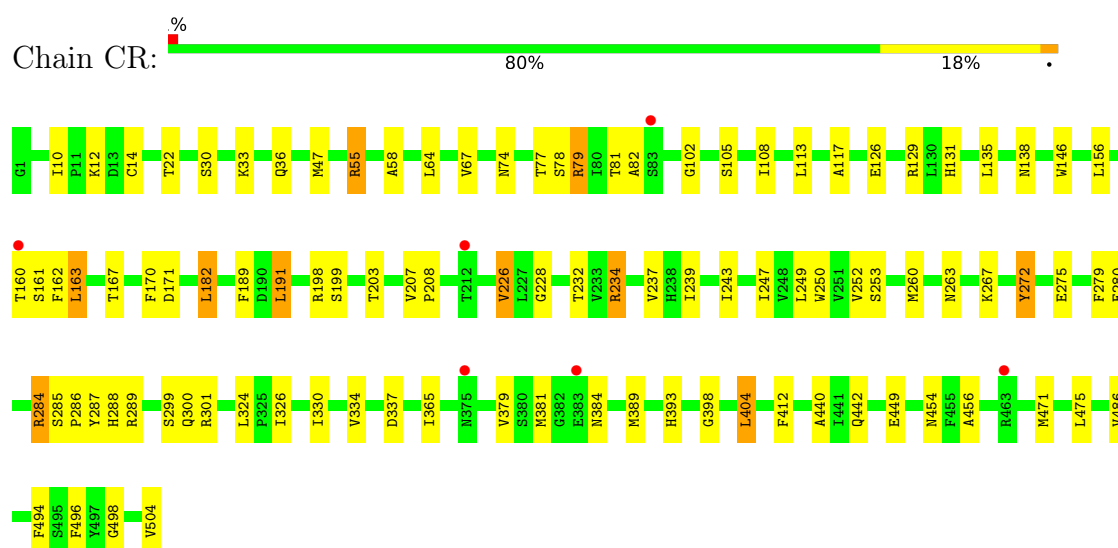
- Molecule 1: COAT PROTEIN



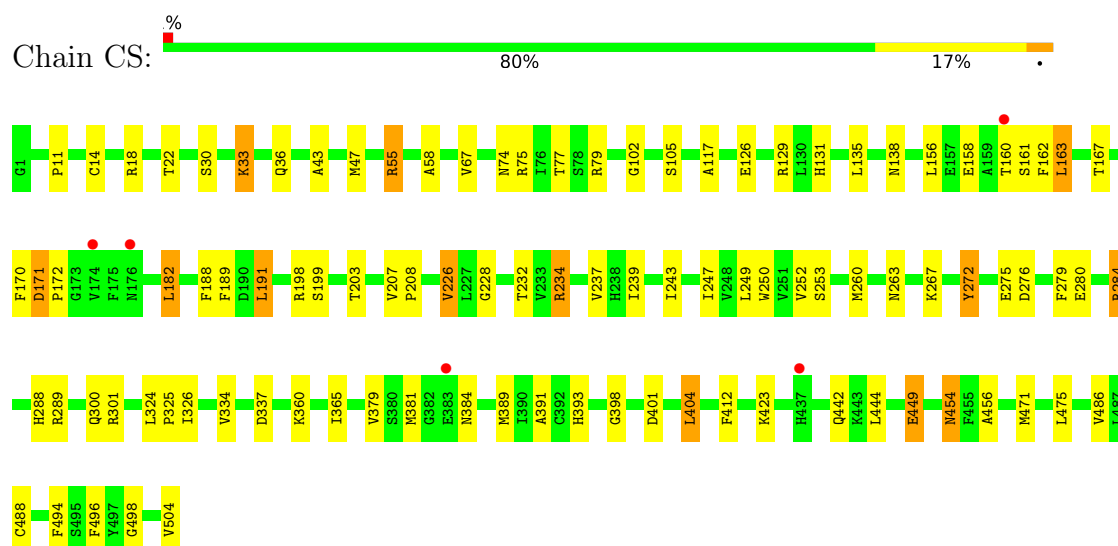
- Molecule 1: COAT PROTEIN



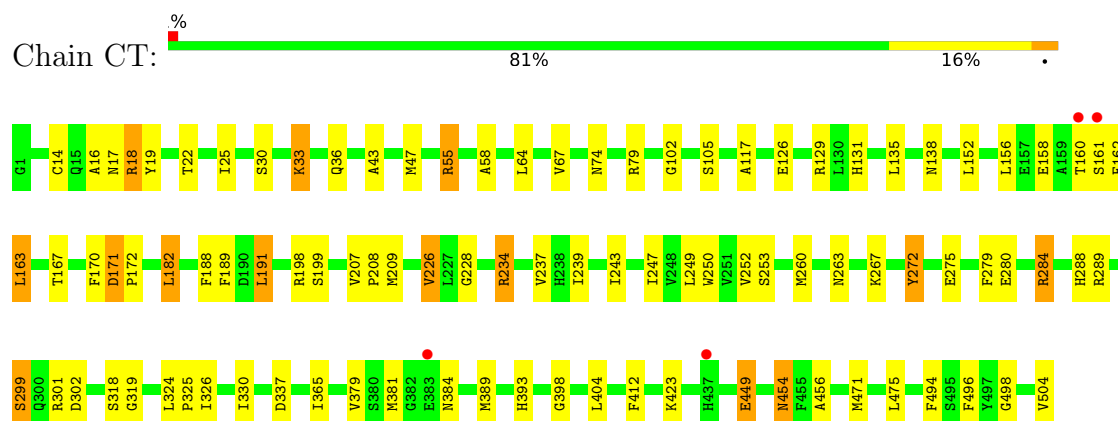
- Molecule 1: COAT PROTEIN



- Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	279.40Å 279.60Å 293.30Å 102.40° 116.40° 108.20°	Depositor
Resolution (Å)	135.43 – 3.00 135.43 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.3 (135.43-3.00) 96.3 (135.43-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.190 , 0.207 0.186 , 0.203	Depositor DCC
R_{free} test set	66376 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	237060	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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	0.56	0/4058	0.87	2/5517 (0.0%)
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	0.62	0/4058	0.90	4/5517 (0.1%)
1	AF	0.57	0/4058	0.89	2/5517 (0.0%)
1	AG	0.56	0/4058	0.87	4/5517 (0.1%)
1	AH	0.57	0/4058	0.89	3/5517 (0.1%)
1	AI	0.57	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	0.87	2/5517 (0.0%)
1	AL	0.58	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	0.61	0/4058	0.89	2/5517 (0.0%)
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	0.55	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	0.88	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	6/5517 (0.1%)
1	BS	0.57	0/4058	0.89	2/5517 (0.0%)
1	BT	0.55	0/4058	0.87	2/5517 (0.0%)
1	CA	0.56	1/4058 (0.0%)	0.88	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	0.57	1/4058 (0.0%)	0.88	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	0.57	0/4058	0.89	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	0.60	0/4058	0.89	2/5517 (0.0%)
1	CQ	0.58	0/4058	0.89	2/5517 (0.0%)
1	CR	0.63	0/4058	0.90	2/5517 (0.0%)
1	CS	0.58	0/4058	0.88	2/5517 (0.0%)
1	CT	0.58	0/4058	0.87	2/5517 (0.0%)
All	All	0.58	2/243480 (0.0%)	0.88	179/331020 (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	2
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	107

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CA	1	GLY	N-CA	-5.38	1.36	1.45
1	CE	99	HIS	ND1-CE1	-5.02	1.27	1.32

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CN	171	ASP	CA-C-N	7.04	126.87	119.05
1	CN	171	ASP	C-N-CA	7.04	126.87	119.05
1	CS	171	ASP	CA-C-N	7.04	126.86	119.05
1	CS	171	ASP	C-N-CA	7.04	126.86	119.05
1	AE	171	ASP	CA-C-N	7.03	126.86	119.05

There are no chirality outliers.

5 of 107 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	100	0
1	AB	3951	0	3909	97	0
1	AC	3951	0	3909	95	0
1	AD	3951	0	3909	98	0
1	AE	3951	0	3909	94	0
1	AF	3951	0	3909	99	0
1	AG	3951	0	3909	99	0
1	AH	3951	0	3909	95	0
1	AI	3951	0	3909	95	0
1	AJ	3951	0	3909	93	0
1	AK	3951	0	3909	95	0
1	AL	3951	0	3909	93	0
1	AM	3951	0	3909	88	0
1	AN	3951	0	3909	111	0
1	AO	3951	0	3909	98	0
1	AP	3951	0	3909	95	0
1	AQ	3951	0	3909	93	0
1	AR	3951	0	3909	96	0
1	AS	3951	0	3909	93	0
1	AT	3951	0	3909	95	0
1	BA	3951	0	3909	101	0
1	BB	3951	0	3909	102	0
1	BC	3951	0	3909	93	0
1	BD	3951	0	3909	86	0
1	BE	3951	0	3909	92	0
1	BF	3951	0	3909	98	0
1	BG	3951	0	3909	98	0
1	BH	3951	0	3909	101	0
1	BI	3951	0	3909	97	0
1	BJ	3951	0	3909	97	0
1	BK	3951	0	3909	86	0
1	BL	3951	0	3909	95	0
1	BM	3951	0	3909	95	0
1	BN	3951	0	3909	86	0
1	BO	3951	0	3909	101	0
1	BP	3951	0	3909	101	0
1	BQ	3951	0	3909	89	0
1	BR	3951	0	3909	94	0
1	BS	3951	0	3909	93	0
1	BT	3951	0	3909	95	0
1	CA	3951	0	3909	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CB	3951	0	3909	91	0
1	CC	3951	0	3909	90	0
1	CD	3951	0	3909	95	0
1	CE	3951	0	3909	106	0
1	CF	3951	0	3909	100	0
1	CG	3951	0	3909	97	0
1	CH	3951	0	3909	99	0
1	CI	3951	0	3909	98	0
1	CJ	3951	0	3909	99	0
1	CK	3951	0	3909	92	0
1	CL	3951	0	3909	88	0
1	CM	3951	0	3909	97	0
1	CN	3951	0	3909	92	0
1	CO	3951	0	3909	103	0
1	CP	3951	0	3909	90	0
1	CQ	3951	0	3909	92	0
1	CR	3951	0	3909	94	0
1	CS	3951	0	3909	94	0
1	CT	3951	0	3909	85	0
All	All	237060	0	234540	5171	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 5171 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:CF:79:ARG:HH11	1:CF:79:ARG:HG3	1.18	1.07
1:CC:250:TRP:CZ3	1:CC:272:TYR:HE1	1.77	1.02
1:BO:250:TRP:CZ3	1:BO:272:TYR:HE1	1.83	0.97
1:BS:79:ARG:HG3	1:BS:79:ARG:HH11	1.31	0.96
1:BJ:250:TRP:CZ3	1:BJ:272:TYR:HE1	1.85	0.94

There are no symmetry-related clashes.

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%)	43	76
1	AB	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	AC	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	30	65
1	AD	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AE	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76
1	AF	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AG	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	30	65
1	AH	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	30	65
1	AI	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	AJ	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76
1	AK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	AL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	AM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76
1	AN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76
1	AO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	AP	502/504 (100%)	483 (96%)	19 (4%)	0	100	100
1	AQ	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	AR	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	76
1	AS	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76
1	AT	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	43	76
1	BA	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76
1	BB	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	30	65
1	BC	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76
1	BD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	BE	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BF	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	30	65
1	BG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76
1	BH	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	76
1	BI	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	43	76
1	BJ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76
1	BK	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	76
1	BL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	BM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76
1	BN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76
1	BO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	BP	502/504 (100%)	479 (95%)	21 (4%)	2 (0%)	30	65
1	BQ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76
1	BR	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76
1	BS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76
1	BT	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	CA	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	CB	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	CC	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76
1	CD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	CE	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	43	76
1	CF	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76
1	CG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76
1	CH	502/504 (100%)	481 (96%)	21 (4%)	0	100	100
1	CI	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	CJ	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	43	76
1	CK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	43	76
1	CL	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76
1	CM	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	30	65
1	CN	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	CO	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76
1	CP	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	43	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CQ	502/504 (100%)	482 (96%)	18 (4%)	2 (0%)	30	65
1	CR	502/504 (100%)	478 (95%)	22 (4%)	2 (0%)	30	65
1	CS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	43	76
1	CT	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	43	76
All	All	30120/30240 (100%)	28870 (96%)	1187 (4%)	63 (0%)	43	76

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BP	82	ALA
1	CR	82	ALA
1	BM	17	ASN
1	AC	78	SER
1	BB	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	54
1	AB	430/430 (100%)	401 (93%)	29 (7%)	15	46
1	AC	430/430 (100%)	402 (94%)	28 (6%)	15	47
1	AD	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	AE	430/430 (100%)	407 (95%)	23 (5%)	20	54
1	AF	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	AG	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	AH	430/430 (100%)	401 (93%)	29 (7%)	15	46
1	AI	430/430 (100%)	403 (94%)	27 (6%)	16	48
1	AJ	430/430 (100%)	407 (95%)	23 (5%)	20	54
1	AK	430/430 (100%)	407 (95%)	23 (5%)	20	54
1	AL	430/430 (100%)	403 (94%)	27 (6%)	16	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AM	430/430 (100%)	406 (94%)	24 (6%)	19	52
1	AN	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	AO	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	AP	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	AQ	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	AR	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	AS	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	AT	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	BA	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	BB	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	BC	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	BD	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	BE	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	BF	430/430 (100%)	402 (94%)	28 (6%)	15	47
1	BG	430/430 (100%)	406 (94%)	24 (6%)	19	52
1	BH	430/430 (100%)	403 (94%)	27 (6%)	16	48
1	BI	430/430 (100%)	407 (95%)	23 (5%)	20	54
1	BJ	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	BK	430/430 (100%)	403 (94%)	27 (6%)	16	48
1	BL	430/430 (100%)	401 (93%)	29 (7%)	15	46
1	BM	430/430 (100%)	403 (94%)	27 (6%)	16	48
1	BN	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	BO	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	BP	430/430 (100%)	406 (94%)	24 (6%)	19	52
1	BQ	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	BR	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	BS	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	BT	430/430 (100%)	406 (94%)	24 (6%)	19	52
1	CA	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	CB	430/430 (100%)	403 (94%)	27 (6%)	16	48
1	CC	430/430 (100%)	405 (94%)	25 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	430/430 (100%)	406 (94%)	24 (6%)	19	52
1	CE	430/430 (100%)	403 (94%)	27 (6%)	16	48
1	CF	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	CG	430/430 (100%)	406 (94%)	24 (6%)	19	52
1	CH	430/430 (100%)	403 (94%)	27 (6%)	16	48
1	CI	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	CJ	430/430 (100%)	405 (94%)	25 (6%)	18	51
1	CK	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	CL	430/430 (100%)	403 (94%)	27 (6%)	16	48
1	CM	430/430 (100%)	402 (94%)	28 (6%)	15	47
1	CN	430/430 (100%)	407 (95%)	23 (5%)	20	54
1	CO	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	CP	430/430 (100%)	402 (94%)	28 (6%)	15	47
1	CQ	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	CR	430/430 (100%)	404 (94%)	26 (6%)	17	50
1	CS	430/430 (100%)	406 (94%)	24 (6%)	19	52
1	CT	430/430 (100%)	405 (94%)	25 (6%)	18	51
All	All	25800/25800 (100%)	24260 (94%)	1540 (6%)	17	50

5 of 1540 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BQ	160	THR
1	CE	301	ARG
1	BR	161	SER
1	BQ	129	ARG
1	CA	284	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 750 such sidechains are listed below:

Mol	Chain	Res	Type
1	BQ	288	HIS
1	CF	437	HIS
1	BR	288	HIS
1	BQ	263	ASN

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Mol	Chain	Res	Type
1	CB	98	HIS

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%)	-0.46	5 (0%) 79 59	23, 33, 53, 78	0
1	AB	504/504 (100%)	-0.46	4 (0%) 82 64	22, 34, 54, 78	0
1	AC	504/504 (100%)	-0.45	2 (0%) 88 76	23, 34, 54, 78	0
1	AD	504/504 (100%)	-0.48	4 (0%) 82 64	22, 33, 52, 78	0
1	AE	504/504 (100%)	-0.41	5 (0%) 79 59	17, 31, 52, 77	0
1	AF	504/504 (100%)	-0.47	1 (0%) 91 83	24, 34, 54, 80	0
1	AG	504/504 (100%)	-0.44	3 (0%) 85 69	23, 34, 55, 80	0
1	AH	504/504 (100%)	-0.31	5 (0%) 79 59	24, 35, 56, 79	0
1	AI	504/504 (100%)	-0.39	4 (0%) 82 64	23, 34, 55, 80	0
1	AJ	504/504 (100%)	-0.46	4 (0%) 82 64	22, 34, 54, 80	0
1	AK	504/504 (100%)	-0.44	4 (0%) 82 64	23, 34, 54, 79	0
1	AL	504/504 (100%)	-0.41	5 (0%) 79 59	23, 33, 54, 77	0
1	AM	504/504 (100%)	-0.47	4 (0%) 82 64	21, 32, 52, 77	0
1	AN	504/504 (100%)	-0.42	4 (0%) 82 64	22, 33, 54, 78	0
1	AO	504/504 (100%)	-0.28	7 (1%) 73 51	21, 33, 54, 80	0
1	AP	504/504 (100%)	-0.42	2 (0%) 88 76	19, 32, 53, 79	0
1	AQ	504/504 (100%)	-0.45	6 (1%) 76 55	23, 33, 54, 77	0
1	AR	504/504 (100%)	-0.41	5 (0%) 79 59	21, 32, 52, 77	0
1	AS	504/504 (100%)	-0.46	2 (0%) 88 76	23, 33, 54, 80	0
1	AT	504/504 (100%)	-0.48	4 (0%) 82 64	22, 33, 54, 77	0
1	BA	504/504 (100%)	-0.45	4 (0%) 82 64	23, 33, 54, 79	0
1	BB	504/504 (100%)	-0.27	6 (1%) 76 55	23, 34, 55, 77	0
1	BC	504/504 (100%)	-0.46	3 (0%) 85 69	23, 34, 54, 78	0
1	BD	504/504 (100%)	-0.45	4 (0%) 82 64	23, 34, 54, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	BE	504/504 (100%)	-0.46	4 (0%)	82 64	23, 33, 54, 77	0
1	BF	504/504 (100%)	-0.30	4 (0%)	82 64	22, 35, 56, 80	0
1	BG	504/504 (100%)	-0.39	5 (0%)	79 59	22, 34, 54, 79	0
1	BH	504/504 (100%)	-0.47	5 (0%)	79 59	21, 33, 54, 75	0
1	BI	504/504 (100%)	-0.35	4 (0%)	82 64	22, 32, 54, 78	0
1	BJ	504/504 (100%)	-0.45	2 (0%)	88 76	22, 34, 54, 79	0
1	BK	504/504 (100%)	-0.49	3 (0%)	85 69	22, 33, 53, 77	0
1	BL	504/504 (100%)	-0.43	5 (0%)	79 59	21, 32, 52, 75	0
1	BM	504/504 (100%)	-0.36	4 (0%)	82 64	21, 32, 52, 77	0
1	BN	504/504 (100%)	-0.44	3 (0%)	85 69	20, 33, 53, 76	0
1	BO	504/504 (100%)	-0.42	4 (0%)	82 64	22, 33, 53, 80	0
1	BP	504/504 (100%)	-0.32	8 (1%)	70 47	21, 32, 53, 76	0
1	BQ	504/504 (100%)	-0.40	4 (0%)	82 64	22, 33, 54, 80	0
1	BR	504/504 (100%)	-0.44	1 (0%)	91 83	22, 33, 54, 79	0
1	BS	504/504 (100%)	-0.42	4 (0%)	82 64	22, 33, 54, 80	0
1	BT	504/504 (100%)	-0.46	5 (0%)	79 59	22, 34, 53, 77	0
1	CA	504/504 (100%)	-0.37	5 (0%)	79 59	23, 35, 56, 80	0
1	CB	504/504 (100%)	-0.41	5 (0%)	79 59	23, 34, 54, 77	0
1	CC	504/504 (100%)	-0.46	3 (0%)	85 69	23, 34, 54, 81	0
1	CD	504/504 (100%)	-0.46	3 (0%)	85 69	23, 34, 54, 79	0
1	CE	504/504 (100%)	-0.47	1 (0%)	91 83	23, 33, 54, 78	0
1	CF	504/504 (100%)	-0.42	5 (0%)	79 59	23, 34, 55, 80	0
1	CG	504/504 (100%)	-0.25	6 (1%)	76 55	24, 34, 55, 81	0
1	CH	504/504 (100%)	-0.37	3 (0%)	85 69	24, 34, 55, 79	0
1	CI	504/504 (100%)	-0.45	3 (0%)	85 69	23, 33, 53, 79	0
1	CJ	504/504 (100%)	-0.45	4 (0%)	82 64	24, 33, 54, 79	0
1	CK	504/504 (100%)	-0.48	2 (0%)	88 76	21, 34, 54, 79	0
1	CL	504/504 (100%)	-0.48	5 (0%)	79 59	22, 33, 54, 77	0
1	CM	504/504 (100%)	-0.40	5 (0%)	79 59	22, 32, 53, 79	0
1	CN	504/504 (100%)	-0.47	3 (0%)	85 69	22, 32, 54, 79	0
1	CO	504/504 (100%)	-0.39	6 (1%)	76 55	23, 32, 54, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	CP	504/504 (100%)	-0.44	4 (0%) 82 64	21, 31, 53, 78	0
1	CQ	504/504 (100%)	-0.47	1 (0%) 91 83	21, 32, 53, 79	0
1	CR	504/504 (100%)	-0.33	6 (1%) 76 55	17, 31, 53, 75	0
1	CS	504/504 (100%)	-0.48	5 (0%) 79 59	22, 32, 53, 78	0
1	CT	504/504 (100%)	-0.45	4 (0%) 82 64	21, 32, 52, 77	0
All	All	30240/30240 (100%)	-0.42	241 (0%) 82 64	17, 33, 54, 81	0

The worst 5 of 241 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CR	83	SER	5.3
1	BP	83	SER	4.8
1	AB	160	THR	4.3
1	CM	160	THR	4.2
1	BM	160	THR	4.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.