



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2017 – 09:07 am GMT

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

This is a wwPDB 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28986

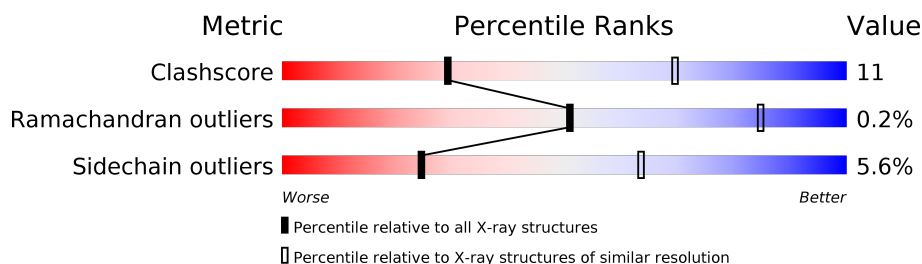
1 Overall quality at a glance

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))
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)


























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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AA	504	
1	AB	504	
1	AC	504	
1	AD	504	
1	AE	504	
1	AF	504	
1	AG	504	


























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Mol	Chain	Length	Quality of chain
1	AH	504	 78%19%.
1	AI	504	 79%18%.
1	AJ	504	 78%19%.
1	AK	504	 78%19%.
1	AL	504	 79%19%.
1	AM	504	 80%18%.
1	AN	504	 78%19%.
1	AO	504	 79%18%.
1	AP	504	 81%16%.
1	AQ	504	 79%19%.
1	AR	504	 81%17%.
1	AS	504	 82%16%.
1	AT	504	 80%18%.
1	BA	504	 80%18%.
1	BB	504	 82%16%.
1	BC	504	 80%17%.
1	BD	504	 81%17%.
1	BE	504	 81%17%.
1	BF	504	 79%19%.
1	BG	504	 80%18%.
1	BH	504	 81%17%.
1	BI	504	 82%16%.
1	BJ	504	 81%16%.
1	BK	504	 82%16%.
1	BL	504	 81%16%.




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Mol	Chain	Length	Quality of chain
1	BM	504	 81% 17% .
1	BN	504	 81% 16% .
1	BO	504	 80% 17% .
1	BP	504	 82% 15% .
1	BQ	504	 81% 17% .
1	BR	504	 81% 16% .
1	BS	504	 81% 17% .
1	BT	504	 79% 18% .
1	CA	504	 82% 16% .
1	CB	504	 80% 18% .
1	CC	504	 82% 16% .
1	CD	504	 81% 17% .
1	CE	504	 79% 18% .
1	CF	504	 81% 17% .
1	CG	504	 82% 16% .
1	CH	504	 79% 18% .
1	CI	504	 79% 18% .
1	CJ	504	 79% 18% .
1	CK	504	 80% 18% .
1	CL	504	 82% 16% .
1	CM	504	 80% 17% .
1	CN	504	 82% 16% .
1	CO	504	 80% 18% .
1	CP	504	 81% 16% .
1	CQ	504	 81% 17% .

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Mol	Chain	Length	Quality of chain	
1	CR	504		•
1	CS	504		•
1	CT	504		•

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 237060 atoms, of which 0 are 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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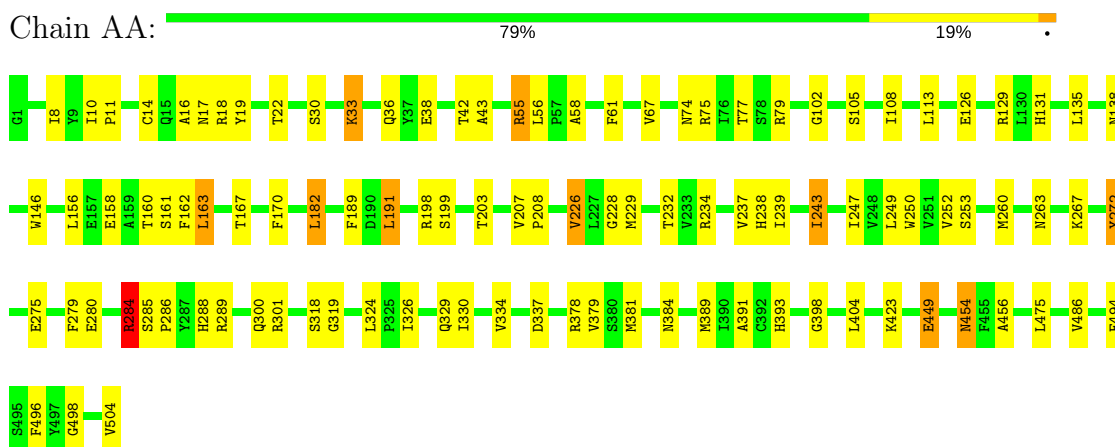
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CS	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			
1	CT	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			

3 Residue-property plots

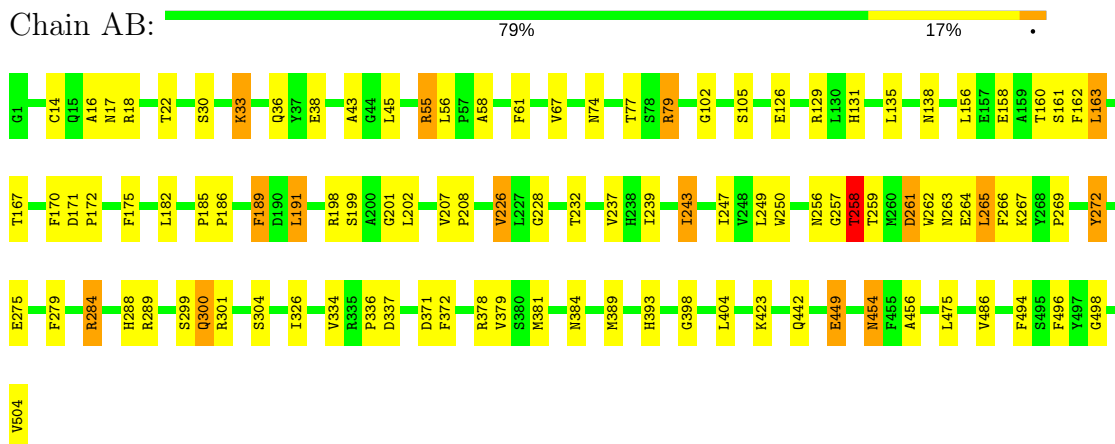
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS failed to run properly.

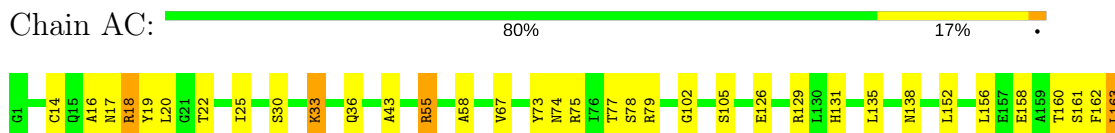
• Molecule 1: COAT PROTEIN

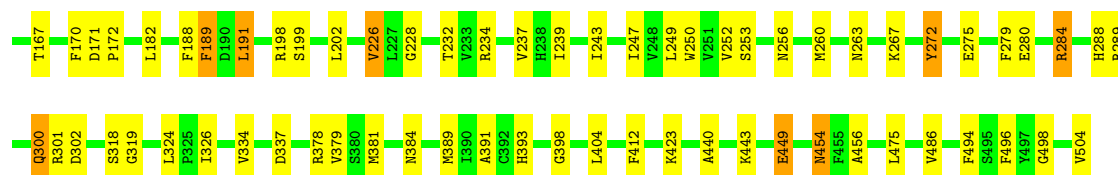


• Molecule 1: COAT PROTEIN



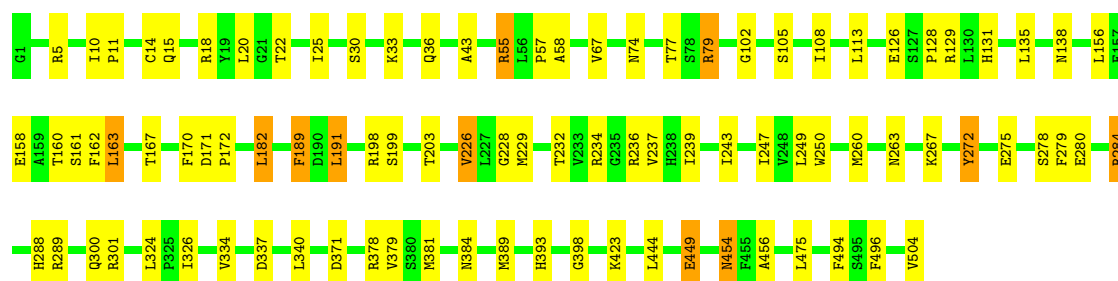
• Molecule 1: COAT PROTEIN





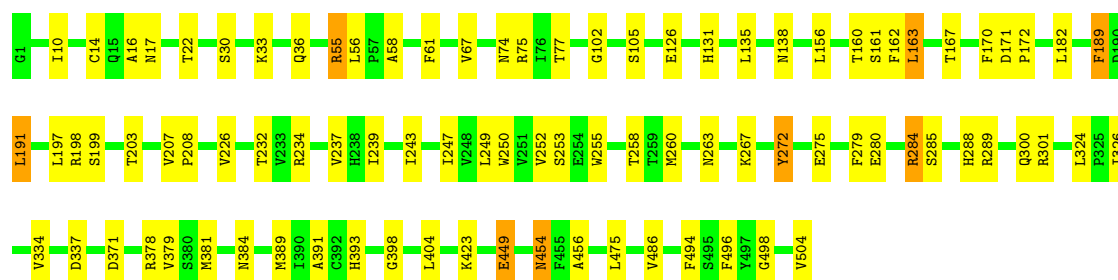
• Molecule 1: COAT PROTEIN

Chain AD: 82% 16%



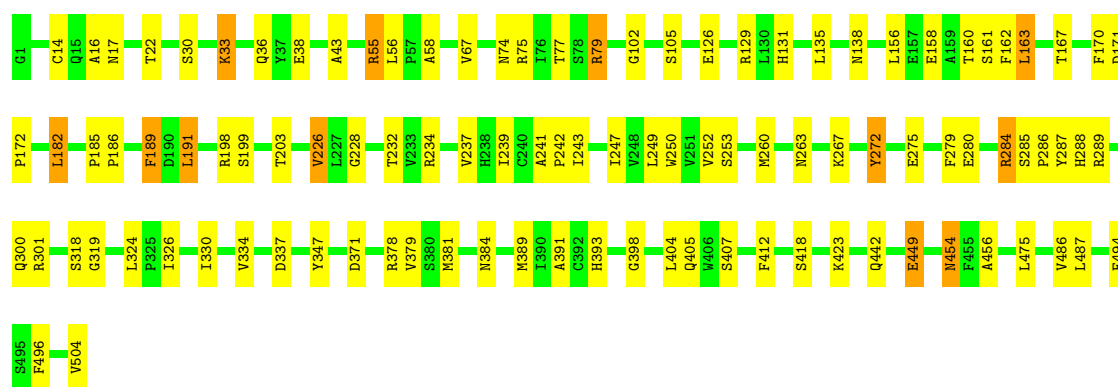
• Molecule 1: COAT PROTEIN

Chain AE: 82% 16%



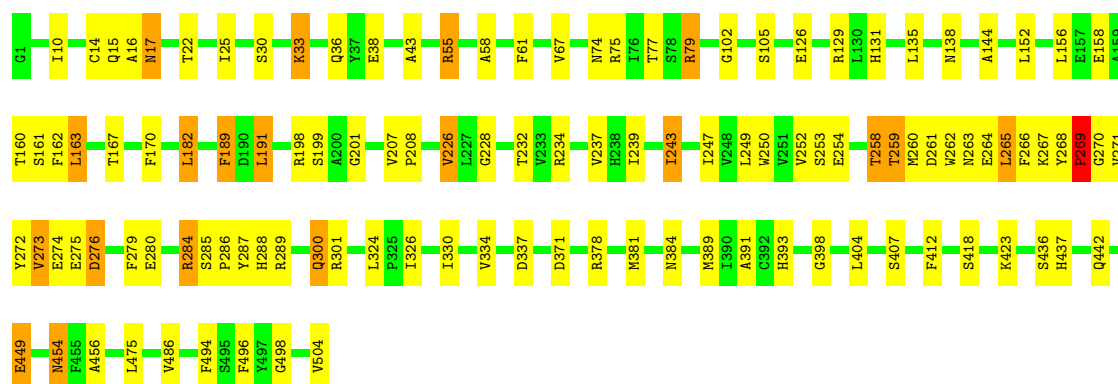
• Molecule 1: COAT PROTEIN

Chain AF: 79% 18%



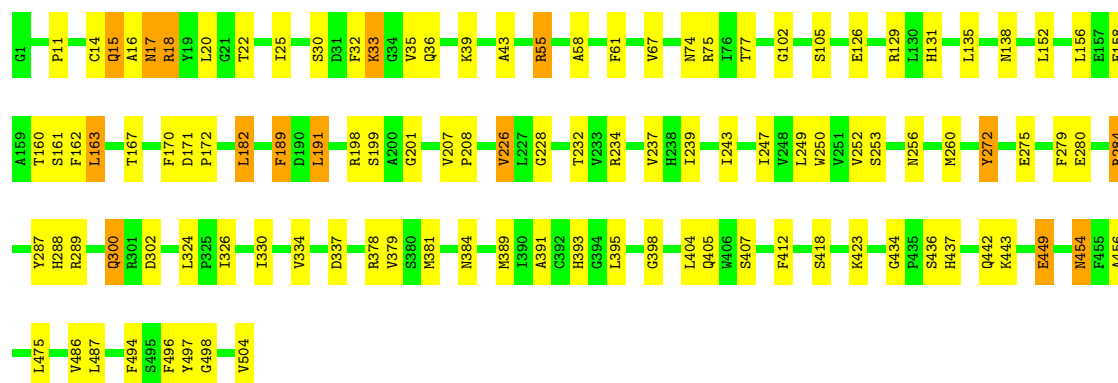
• Molecule 1: COAT PROTEIN

Chain AG: 77% 19%



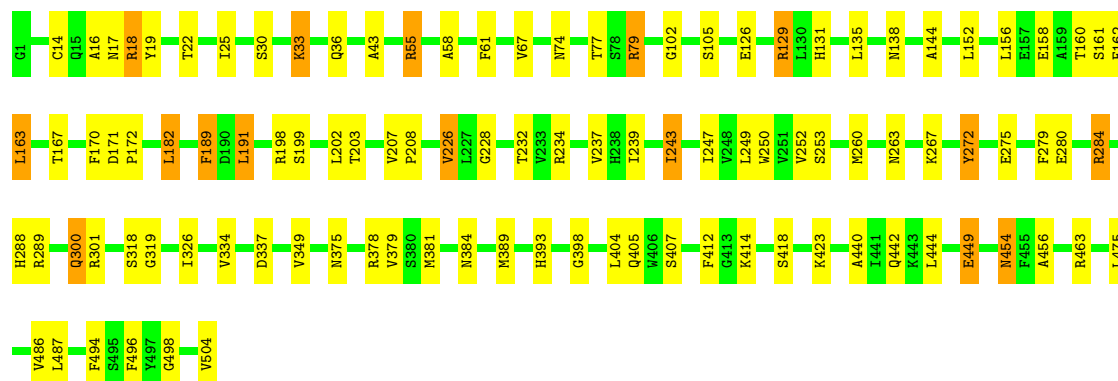
• Molecule 1: COAT PROTEIN

Chain AH: 78% 19% •



• Molecule 1: COAT PROTEIN

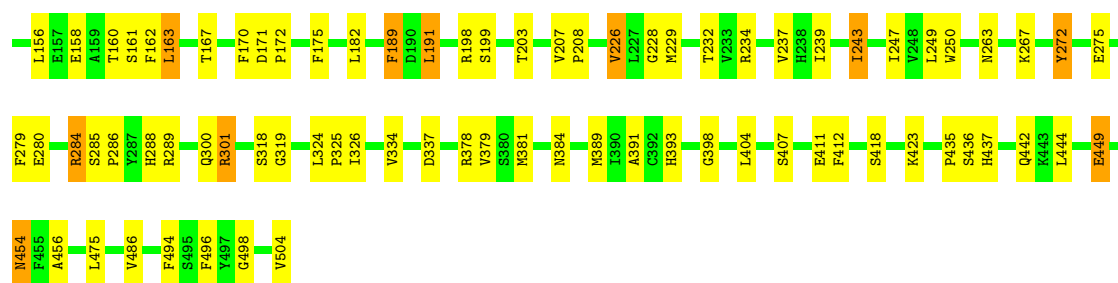
Chain AI: 79% 18% •



• Molecule 1: COAT PROTEIN

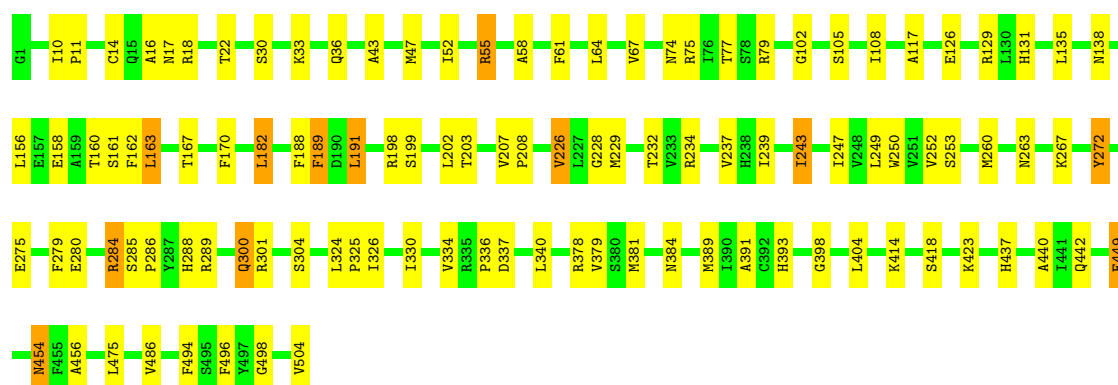
Chain AJ: 78% 19% •





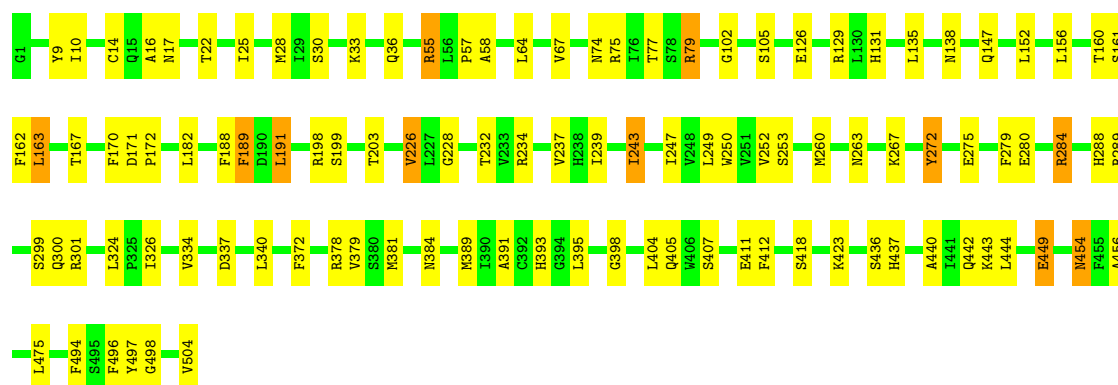
• Molecule 1: COAT PROTEIN

Chain AK: 78% 19%



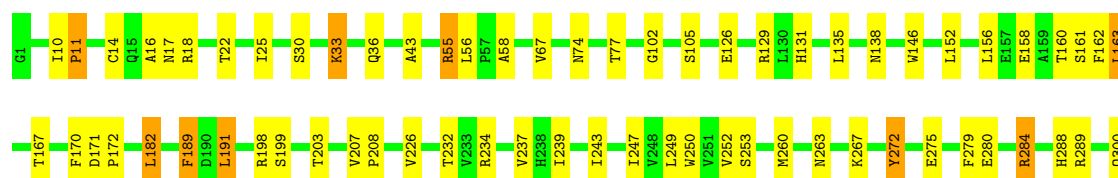
• Molecule 1: COAT PROTEIN

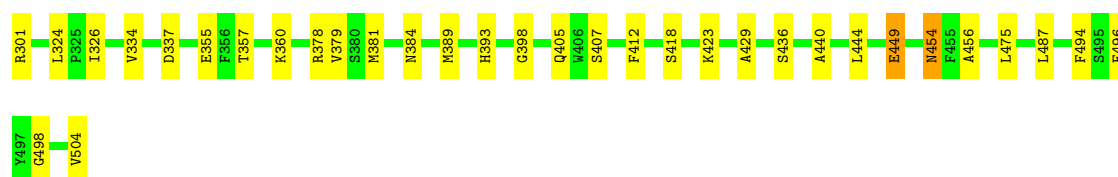
Chain AL: 79% 19%



• Molecule 1: COAT PROTEIN

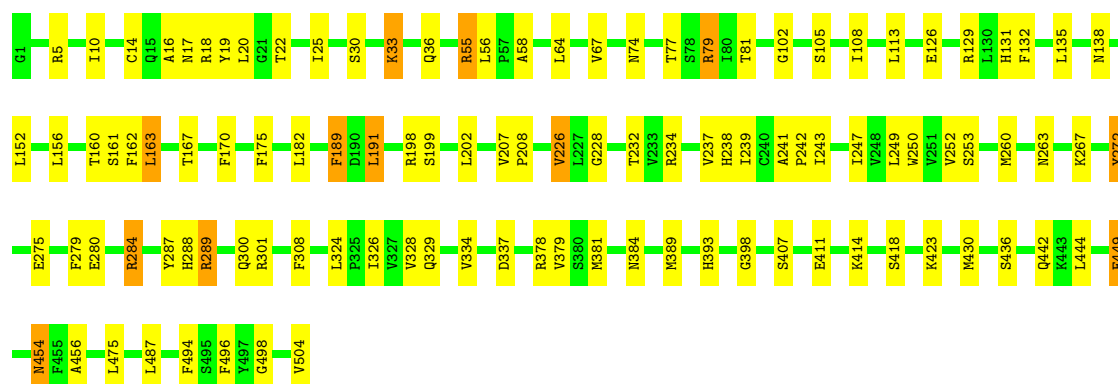
Chain AM: 80% 18%





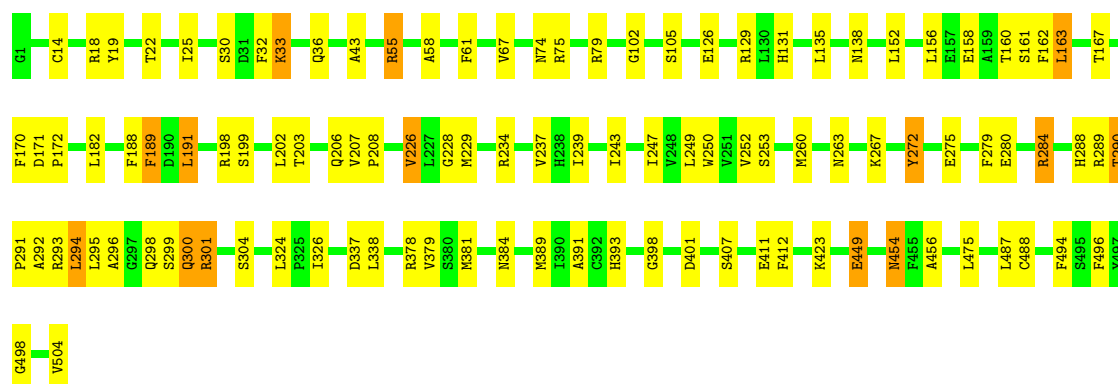
• Molecule 1: COAT PROTEIN

Chain AN: 78% 19% •



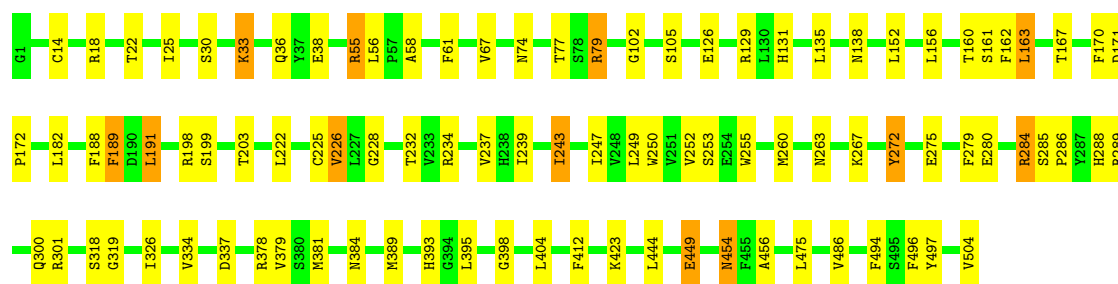
• Molecule 1: COAT PROTEIN

Chain AO: 79% 18% •




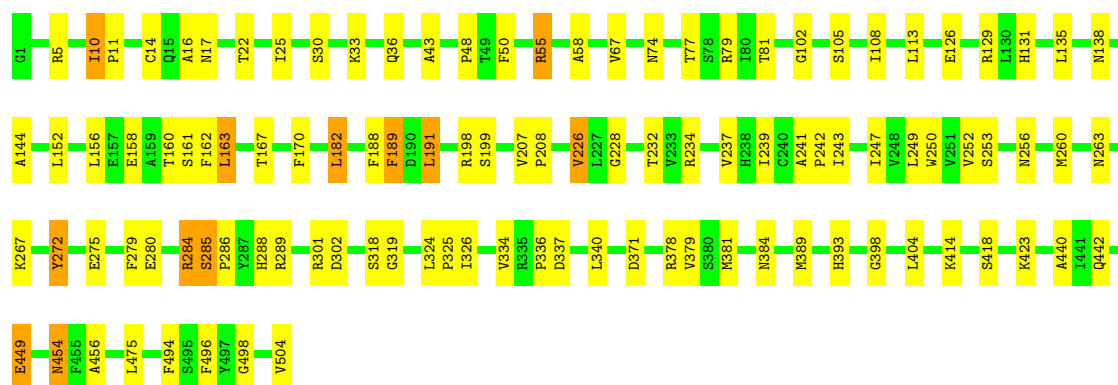
• Molecule 1: COAT PROTEIN

Chain AP: 81% 16% •




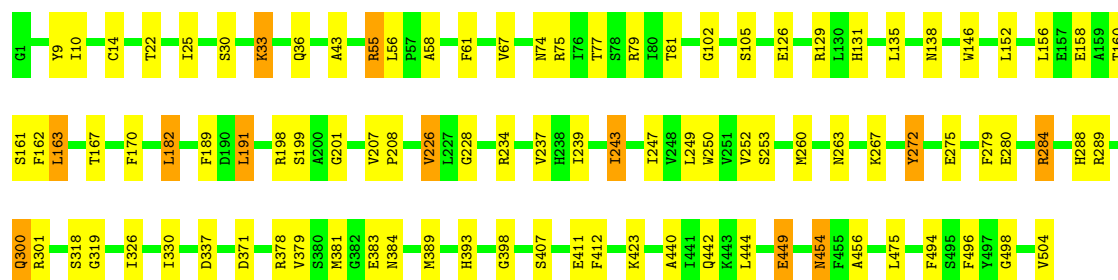
• Molecule 1: COAT PROTEIN

Chain AQ:  79% 19%




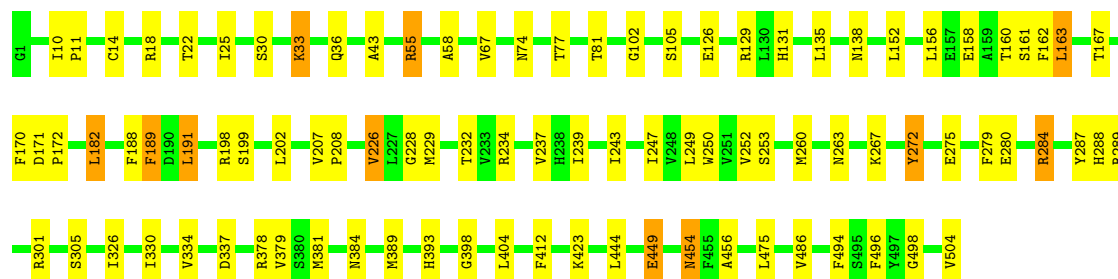
• Molecule 1: COAT PROTEIN

Chain AR:  81% 17%




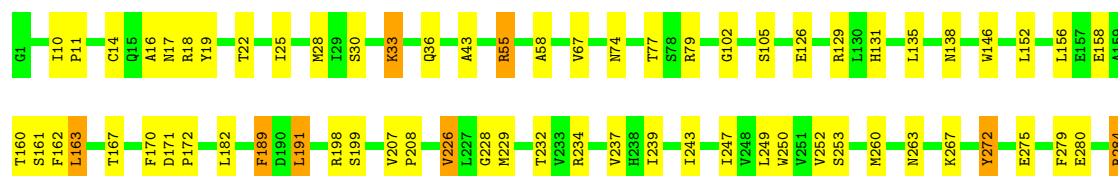
• Molecule 1: COAT PROTEIN

Chain AS:  82% 16%



• Molecule 1: COAT PROTEIN

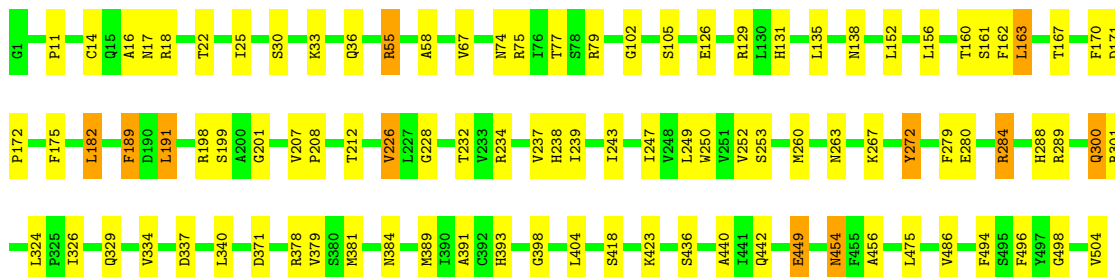
Chain AT:  80% 18%





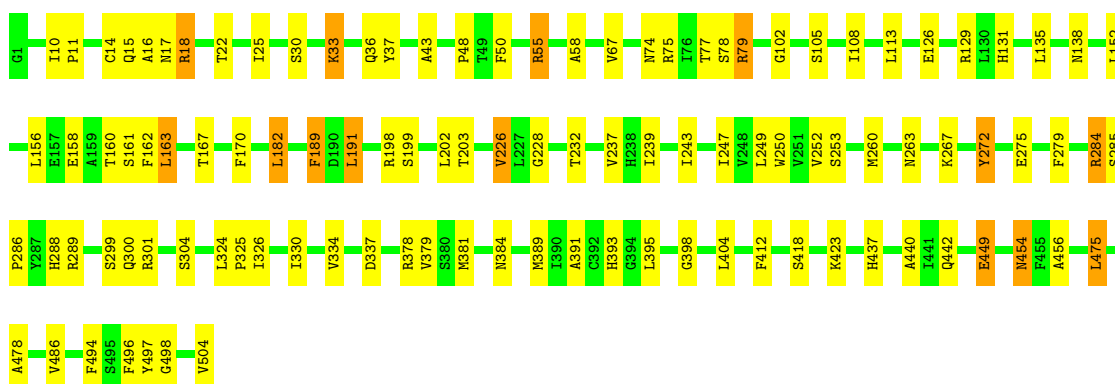
• Molecule 1: COAT PROTEIN

Chain BE: 81% 17%



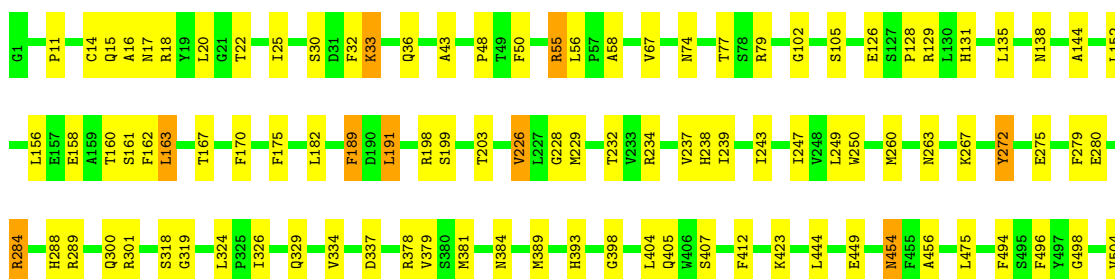
• Molecule 1: COAT PROTEIN

Chain BF: 79% 19%



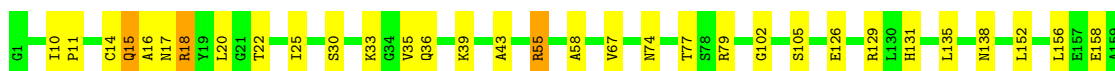
• Molecule 1: COAT PROTEIN

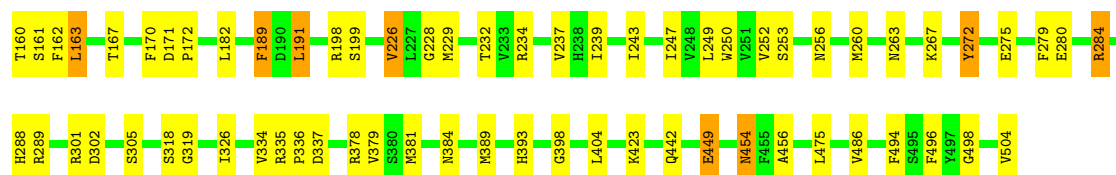
Chain BG: 80% 18%



• Molecule 1: COAT PROTEIN

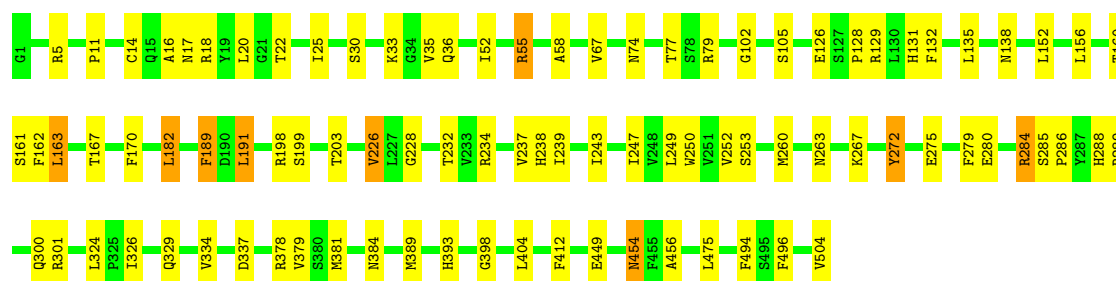
Chain BH: 81% 17%





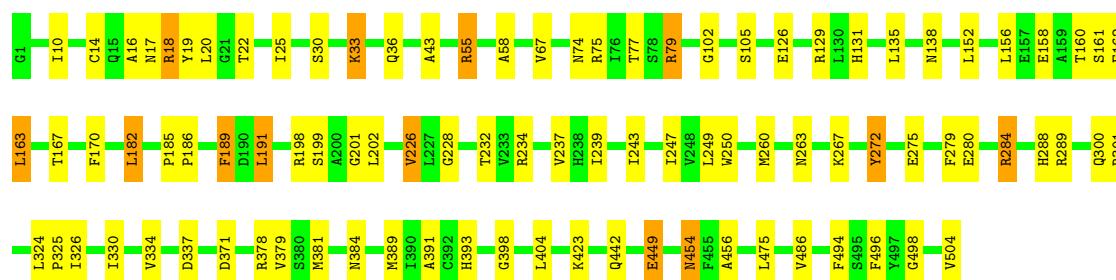
• Molecule 1: COAT PROTEIN

Chain BI: 82% 16%



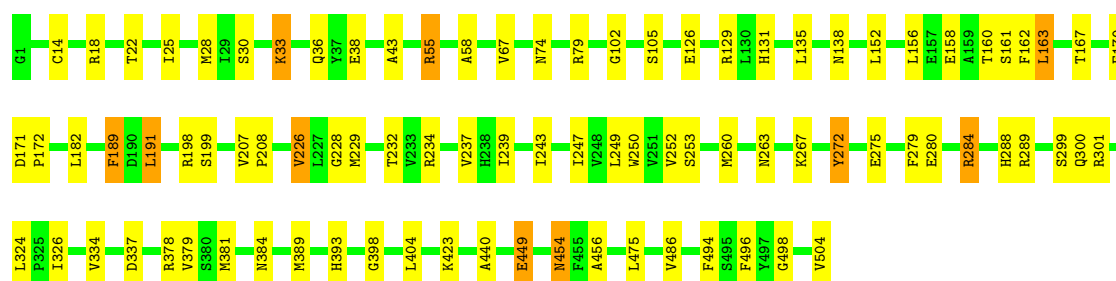
• Molecule 1: COAT PROTEIN

Chain BJ: 81% 16%



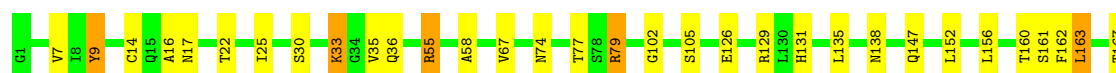
• Molecule 1: COAT PROTEIN

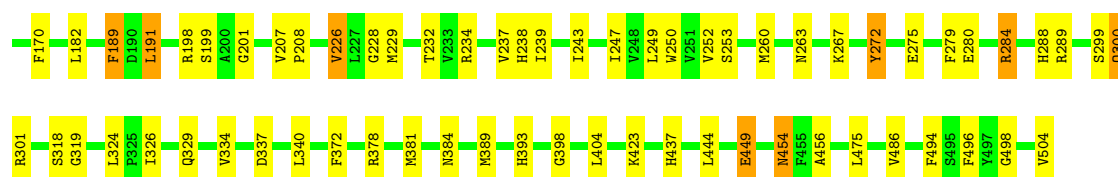
Chain BK: 82% 16%



• Molecule 1: COAT PROTEIN

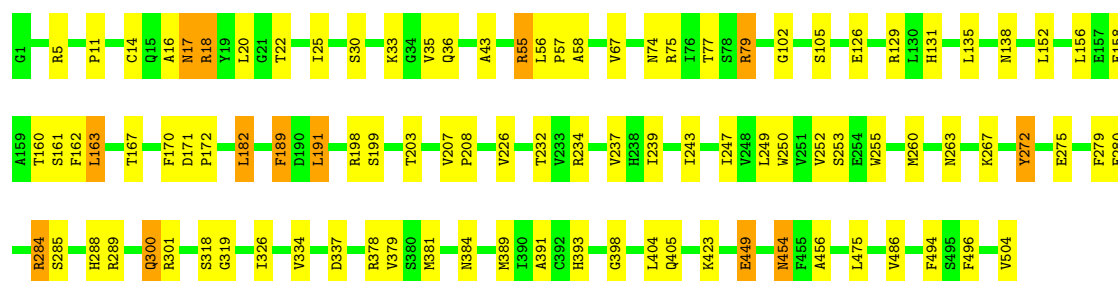
Chain BL: 81% 16%





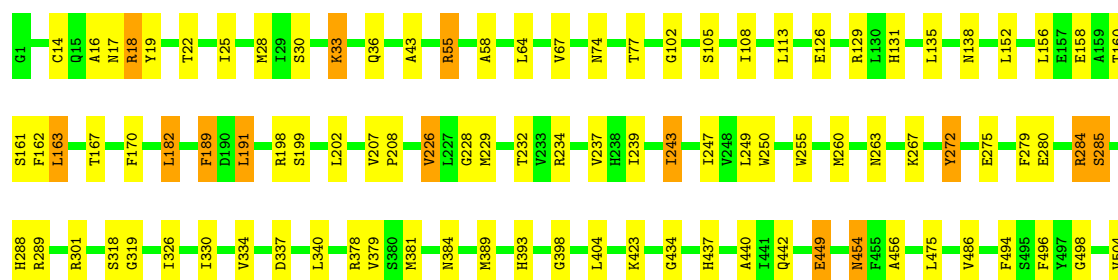
• Molecule 1: COAT PROTEIN

Chain BM: 81% 17%



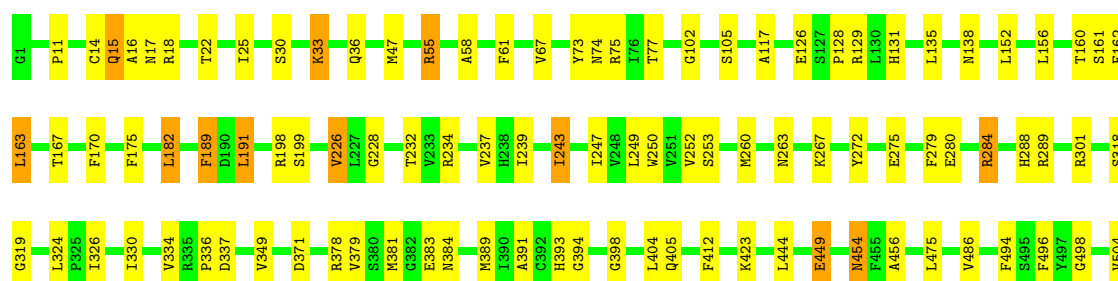
• Molecule 1: COAT PROTEIN

Chain BN: 81% 16%



• Molecule 1: COAT PROTEIN

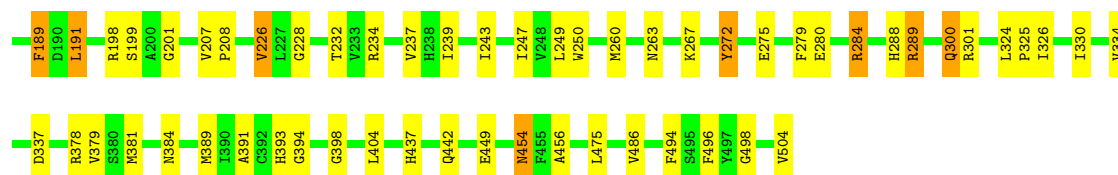
Chain BO: 80% 17%



• Molecule 1: COAT PROTEIN

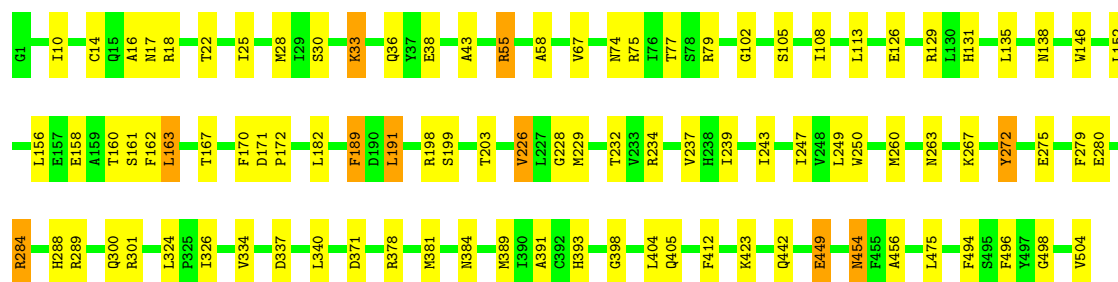
Chain BP: 82% 15%





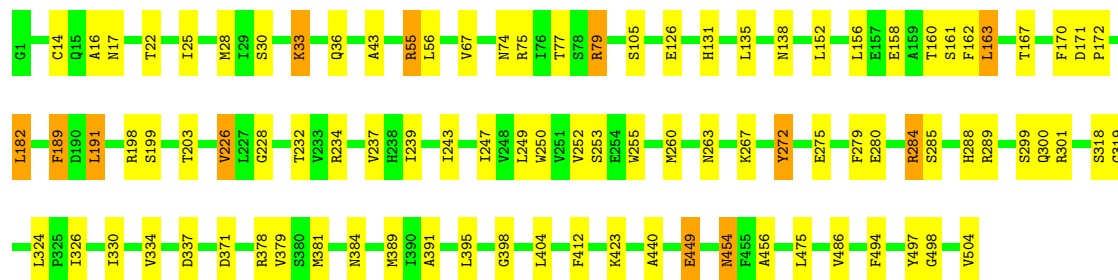
• Molecule 1: COAT PROTEIN

Chain BQ: 81% 17% •



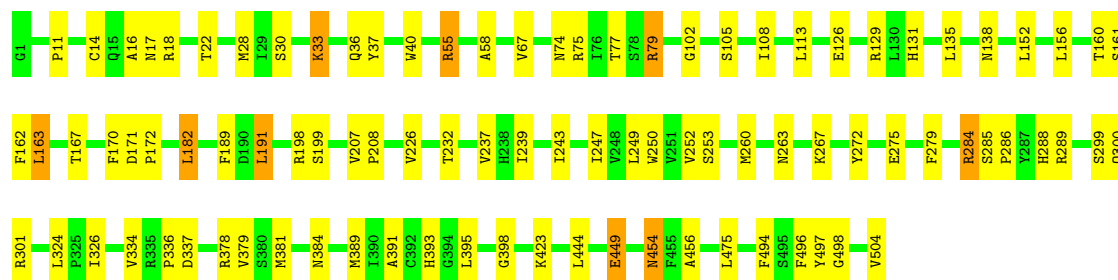
• Molecule 1: COAT PROTEIN

Chain BR: 81% 16% •



• Molecule 1: COAT PROTEIN

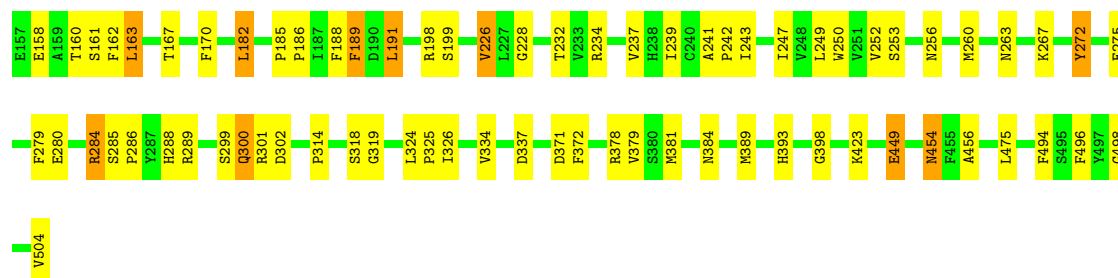
Chain BS: 81% 17% •



• Molecule 1: COAT PROTEIN

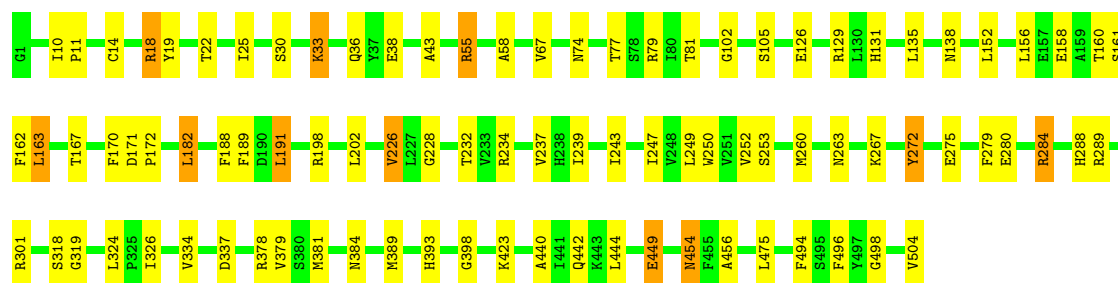
Chain BT: 79% 18% •





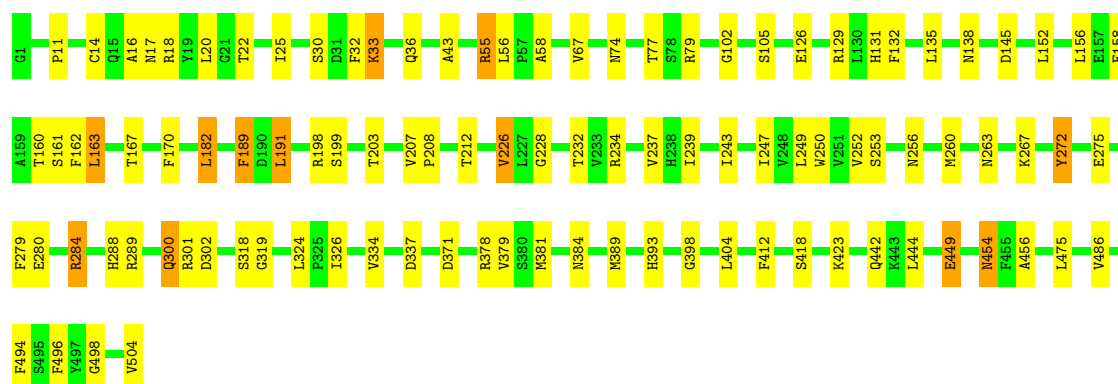
• Molecule 1: COAT PROTEIN

Chain CA: 82% 16%



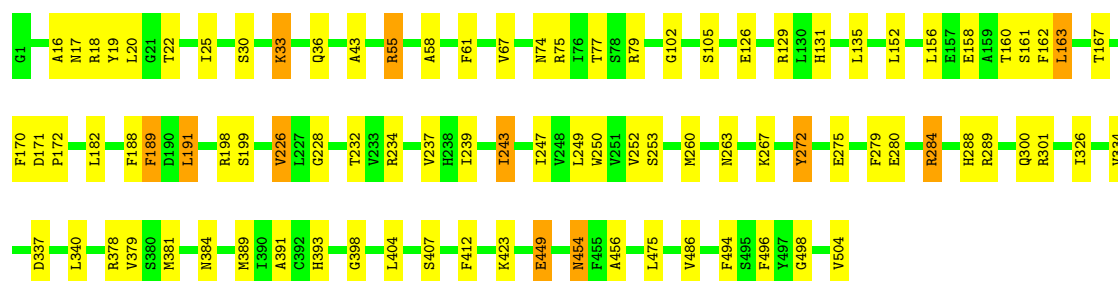
• Molecule 1: COAT PROTEIN

Chain CB: 80% 18%

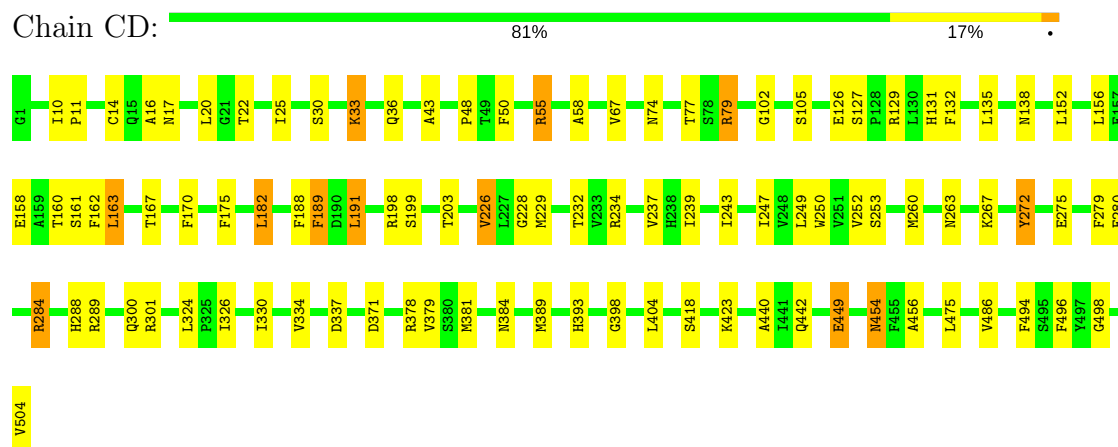


• Molecule 1: COAT PROTEIN

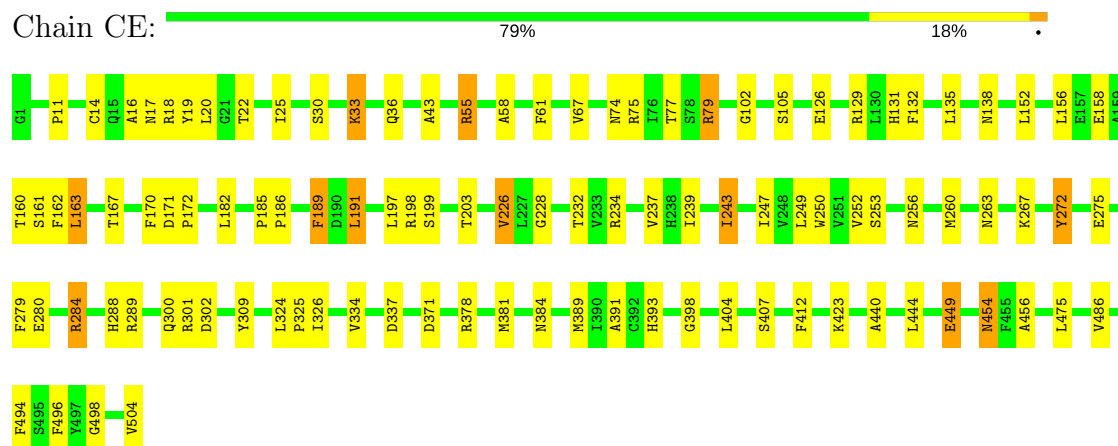
Chain CC: 82% 16%



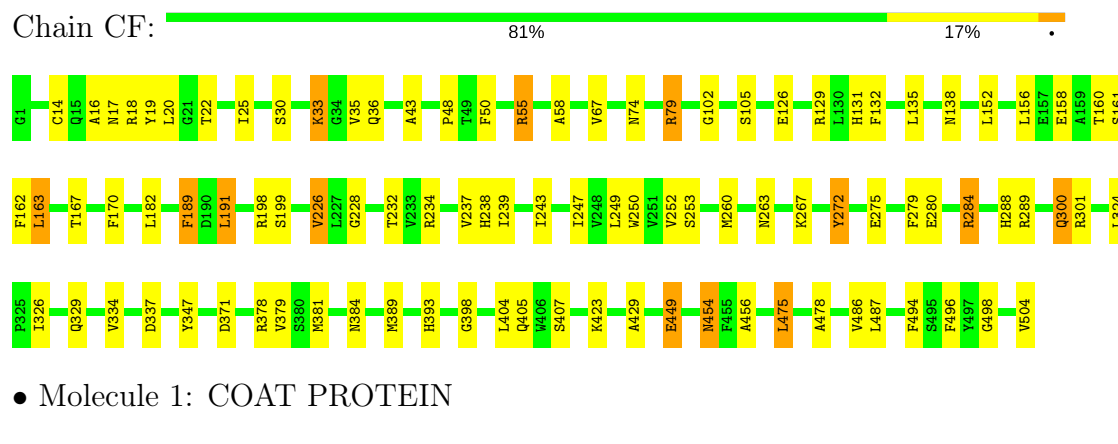
• Molecule 1: COAT PROTEIN



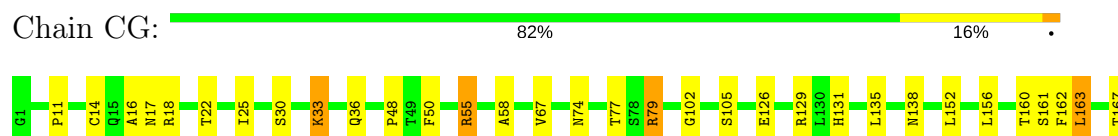
• Molecule 1: COAT PROTEIN

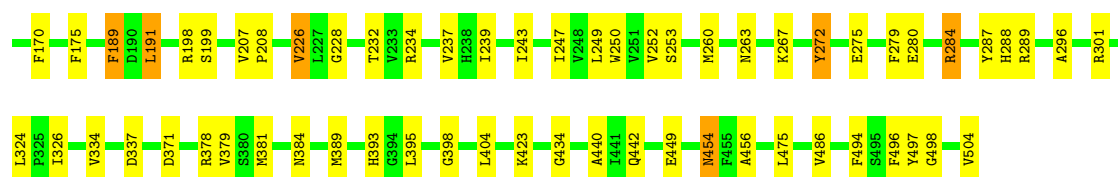


• Molecule 1: COAT PROTEIN



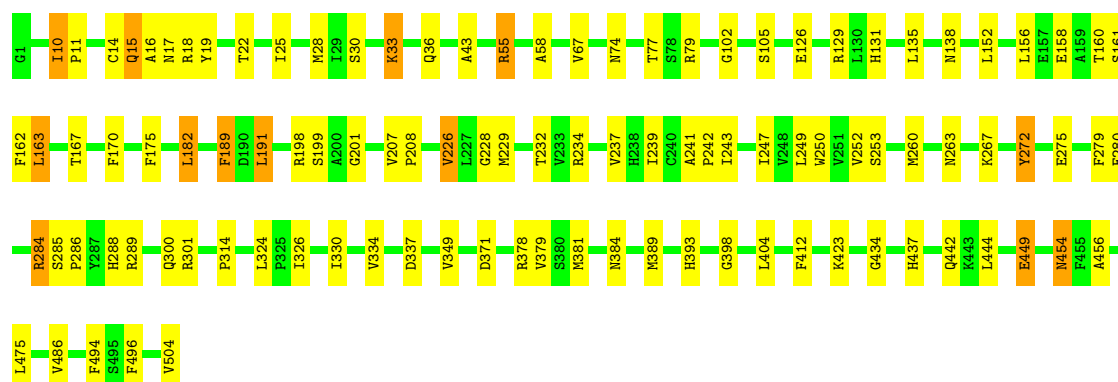
• Molecule 1: COAT PROTEIN





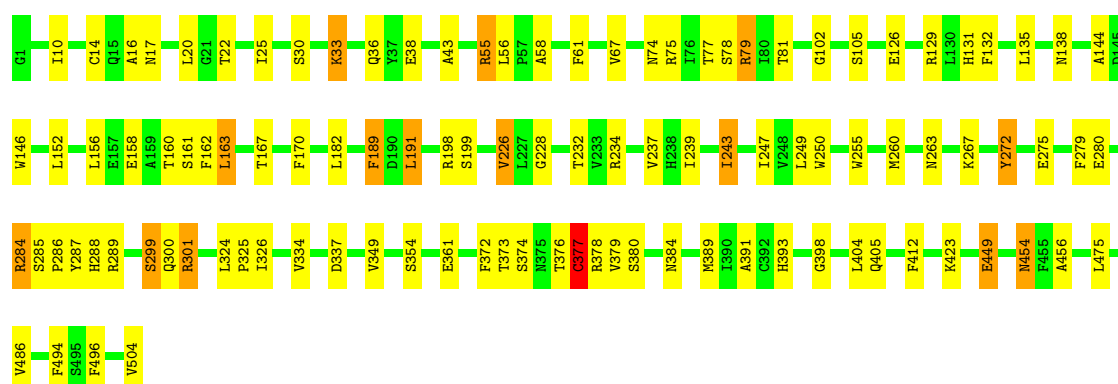
• Molecule 1: COAT PROTEIN

Chain CH: 79% 18%



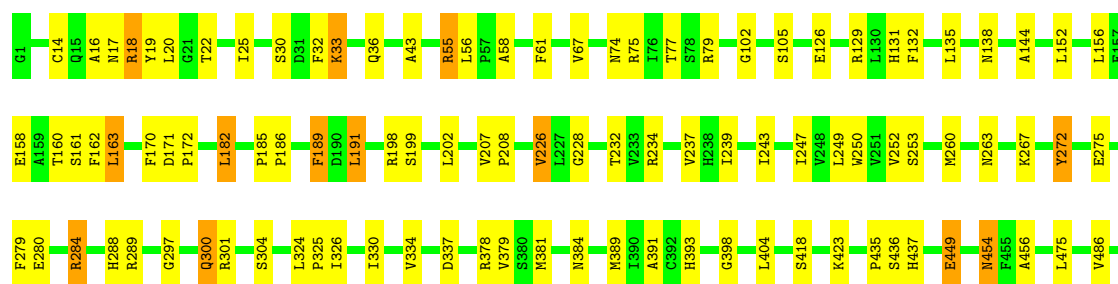
• Molecule 1: COAT PROTEIN

Chain CI: 79% 18%

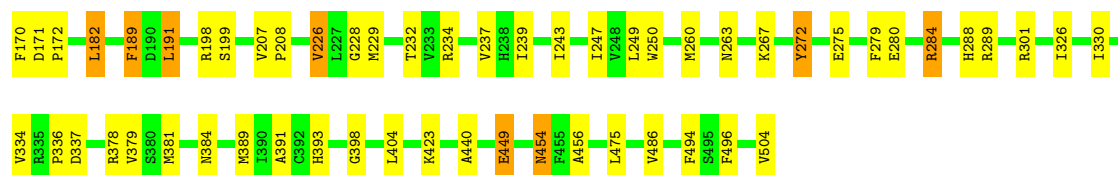


• Molecule 1: COAT PROTEIN

Chain CJ: 79% 18%

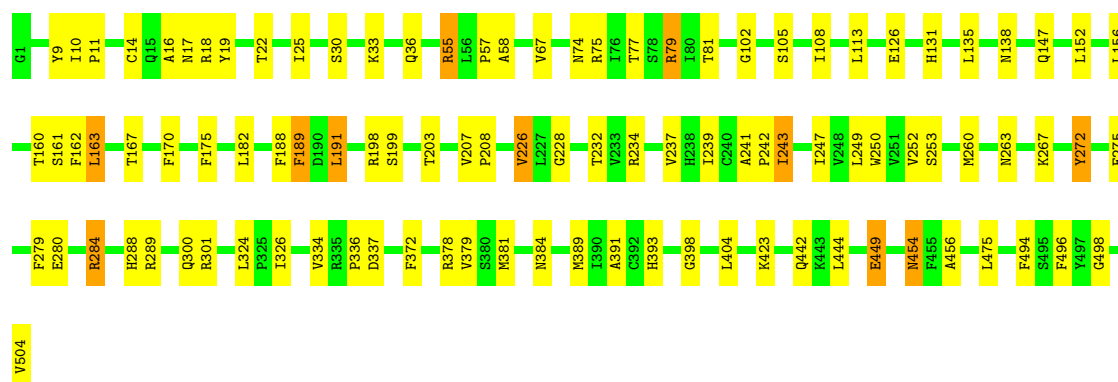






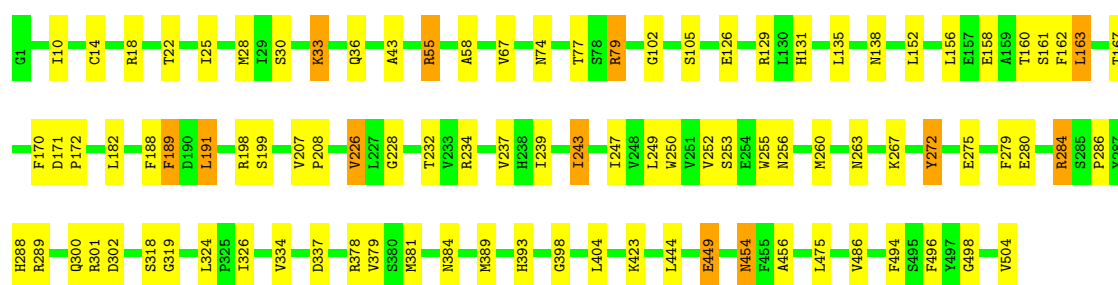
• Molecule 1: COAT PROTEIN

Chain CO: 80% 18%



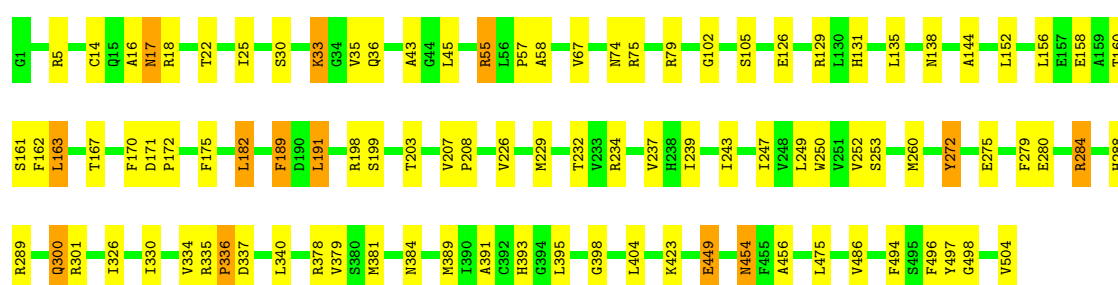
• Molecule 1: COAT PROTEIN

Chain CP: 81% 16%



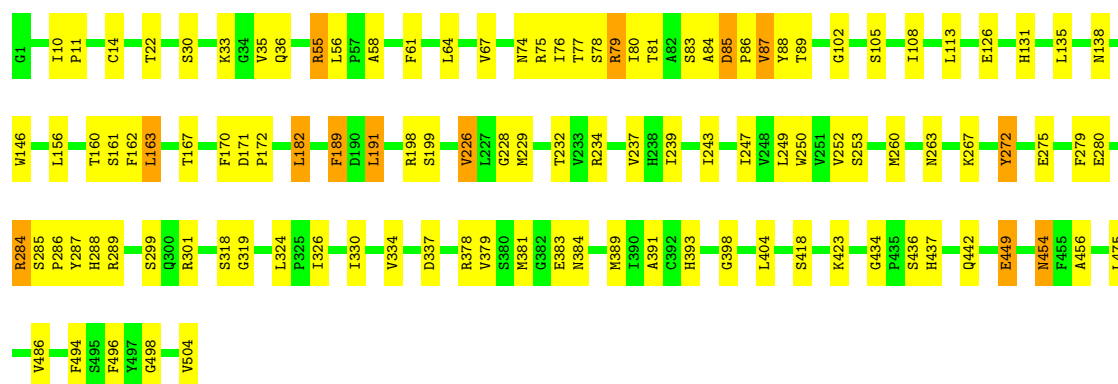
• Molecule 1: COAT PROTEIN

Chain CQ: 81% 17%



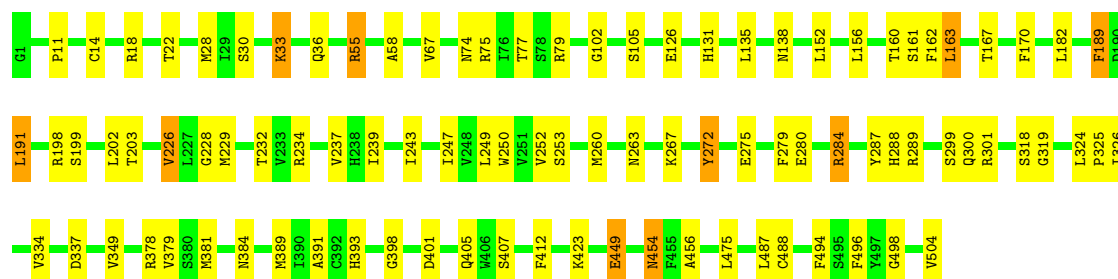
• Molecule 1: COAT PROTEIN

Chain CR: 78% 20%



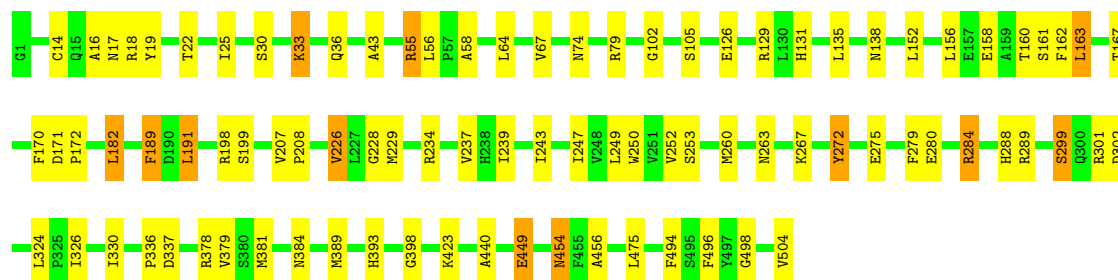
• Molecule 1: COAT PROTEIN

Chain CS: 81% 17% •



• Molecule 1: COAT PROTEIN

Chain CT: 82% 15% •



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

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	Depositor
% Data completeness (in resolution range)	99.0 (49.80-3.70)	Depositor
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	Depositor
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.406	Xtriage
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
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	0.50	0/4058	0.62	2/5517 (0.0%)
1	AB	0.56	2/4058 (0.0%)	0.64	2/5517 (0.0%)
1	AC	0.49	2/4058 (0.0%)	0.62	0/5517
1	AD	0.50	2/4058 (0.0%)	0.62	0/5517
1	AE	0.53	2/4058 (0.0%)	0.63	1/5517 (0.0%)
1	AF	0.49	1/4058 (0.0%)	0.62	1/5517 (0.0%)
1	AG	0.59	1/4058 (0.0%)	0.65	2/5517 (0.0%)
1	AH	0.51	2/4058 (0.0%)	0.62	0/5517
1	AI	0.50	2/4058 (0.0%)	0.62	0/5517
1	AJ	0.49	1/4058 (0.0%)	0.62	0/5517
1	AK	0.49	2/4058 (0.0%)	0.61	0/5517
1	AL	0.53	2/4058 (0.0%)	0.64	0/5517
1	AM	0.51	2/4058 (0.0%)	0.62	1/5517 (0.0%)
1	AN	0.50	1/4058 (0.0%)	0.63	1/5517 (0.0%)
1	AO	0.57	2/4058 (0.0%)	0.66	0/5517
1	AP	0.51	2/4058 (0.0%)	0.63	1/5517 (0.0%)
1	AQ	0.50	1/4058 (0.0%)	0.61	0/5517
1	AR	0.52	2/4058 (0.0%)	0.63	1/5517 (0.0%)
1	AS	0.51	1/4058 (0.0%)	0.62	0/5517
1	AT	0.49	1/4058 (0.0%)	0.61	0/5517
1	BA	0.49	1/4058 (0.0%)	0.63	0/5517
1	BB	0.52	2/4058 (0.0%)	0.63	1/5517 (0.0%)
1	BC	0.49	1/4058 (0.0%)	0.62	0/5517
1	BD	0.48	2/4058 (0.0%)	0.62	0/5517
1	BE	0.50	2/4058 (0.0%)	0.63	0/5517
1	BF	0.51	2/4058 (0.0%)	0.62	0/5517
1	BG	0.50	2/4058 (0.0%)	0.62	1/5517 (0.0%)
1	BH	0.49	2/4058 (0.0%)	0.62	0/5517
1	BI	0.51	1/4058 (0.0%)	0.63	0/5517
1	BJ	0.50	1/4058 (0.0%)	0.62	0/5517
1	BK	0.49	2/4058 (0.0%)	0.61	0/5517
1	BL	0.52	3/4058 (0.1%)	0.62	0/5517
1	BM	0.53	3/4058 (0.1%)	0.64	1/5517 (0.0%)
1	BN	0.51	2/4058 (0.0%)	0.63	0/5517

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

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

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

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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 95 bond length outliers are listed below:

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

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

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

There are no chirality outliers.

5 of 108 planarity outliers are listed below:

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

5.2 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	93	0
1	AB	3951	0	3909	116	0
1	AC	3951	0	3909	92	0
1	AD	3951	0	3909	89	0
1	AE	3951	0	3909	89	0
1	AF	3951	0	3909	99	0
1	AG	3951	0	3907	149	1
1	AH	3951	0	3909	108	0
1	AI	3951	0	3909	113	5
1	AJ	3951	0	3909	109	1
1	AK	3951	0	3909	106	0
1	AL	3951	0	3909	110	0
1	AM	3951	0	3909	94	5
1	AN	3951	0	3909	111	1
1	AO	3951	0	3909	129	0
1	AP	3951	0	3909	84	0
1	AQ	3951	0	3909	101	0
1	AR	3951	0	3909	96	0
1	AS	3951	0	3909	92	0
1	AT	3951	0	3909	96	0
1	BA	3951	0	3909	97	0
1	BB	3951	0	3909	87	0
1	BC	3951	0	3909	80	0
1	BD	3951	0	3909	86	2
1	BE	3951	0	3909	93	1
1	BF	3951	0	3909	101	0
1	BG	3951	0	3909	108	2
1	BH	3951	0	3909	90	0
1	BI	3951	0	3909	86	0
1	BJ	3951	0	3909	91	0
1	BK	3951	0	3909	72	0
1	BL	3951	0	3909	90	0
1	BM	3951	0	3909	90	0
1	BN	3951	0	3909	90	0
1	BO	3951	0	3909	100	0
1	BP	3951	0	3909	93	0
1	BQ	3951	0	3909	85	0

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

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 5081 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

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%)	51	85
1	AB	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	51	85
1	AC	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	38	77
1	AD	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AE	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	51	85
1	AF	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AG	502/504 (100%)	480 (96%)	18 (4%)	4 (1%)	22	66
1	AH	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	38	77
1	AI	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	AJ	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	51	85
1	AK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	AL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	AM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	51	85
1	AN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	AO	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	51	85
1	AP	502/504 (100%)	483 (96%)	19 (4%)	0	100	100
1	AQ	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	51	85
1	AR	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	51	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AS	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	51	85
1	AT	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	51	85
1	BA	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	51	85
1	BB	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	38	77
1	BC	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	BD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	BE	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	BF	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	38	77
1	BG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	51	85
1	BH	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	BI	502/504 (100%)	479 (95%)	23 (5%)	0	100	100
1	BJ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	BK	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	51	85
1	BL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	BM	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	BN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	BO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	BP	502/504 (100%)	479 (95%)	21 (4%)	2 (0%)	38	77
1	BQ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	BR	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	BS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	BT	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	51	85
1	CA	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	CB	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	51	85
1	CC	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	CD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	CE	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	51	85
1	CF	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	51	85
1	CG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	51	85
1	CH	502/504 (100%)	481 (96%)	21 (4%)	0	100	100
1	CI	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	38	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CJ	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	51	85
1	CK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	51	85
1	CL	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	CM	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	38	77
1	CN	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	CO	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	CP	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	51	85
1	CQ	502/504 (100%)	482 (96%)	18 (4%)	2 (0%)	38	77
1	CR	502/504 (100%)	479 (95%)	21 (4%)	2 (0%)	38	77
1	CS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	51	85
1	CT	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	51	85
All	All	30120/30240 (100%)	28873 (96%)	1181 (4%)	66 (0%)	51	85

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%)	26	65
1	AB	430/430 (100%)	402 (94%)	28 (6%)	20	59
1	AC	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	AD	430/430 (100%)	404 (94%)	26 (6%)	22	61
1	AE	430/430 (100%)	409 (95%)	21 (5%)	29	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AF	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	AG	430/430 (100%)	403 (94%)	27 (6%)	21	60
1	AH	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	AI	430/430 (100%)	405 (94%)	25 (6%)	23	62
1	AJ	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	AK	430/430 (100%)	404 (94%)	26 (6%)	22	61
1	AL	430/430 (100%)	404 (94%)	26 (6%)	22	61
1	AM	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	AN	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	AO	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	AP	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	AQ	430/430 (100%)	405 (94%)	25 (6%)	23	62
1	AR	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	AS	430/430 (100%)	405 (94%)	25 (6%)	23	62
1	AT	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	BA	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	BB	430/430 (100%)	405 (94%)	25 (6%)	23	62
1	BC	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	BD	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	BE	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	BF	430/430 (100%)	404 (94%)	26 (6%)	22	61
1	BG	430/430 (100%)	408 (95%)	22 (5%)	28	66
1	BH	430/430 (100%)	404 (94%)	26 (6%)	22	61
1	BI	430/430 (100%)	408 (95%)	22 (5%)	28	66
1	BJ	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	BK	430/430 (100%)	404 (94%)	26 (6%)	22	61
1	BL	430/430 (100%)	404 (94%)	26 (6%)	22	61
1	BM	430/430 (100%)	404 (94%)	26 (6%)	22	61
1	BN	430/430 (100%)	405 (94%)	25 (6%)	23	62
1	BO	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	BP	430/430 (100%)	407 (95%)	23 (5%)	26	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BQ	430/430 (100%)	405 (94%)	25 (6%)	23	62
1	BR	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	BS	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	BT	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	CA	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	CB	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	CC	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	CD	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	CE	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	CF	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	CG	430/430 (100%)	409 (95%)	21 (5%)	29	66
1	CH	430/430 (100%)	405 (94%)	25 (6%)	23	62
1	CI	430/430 (100%)	405 (94%)	25 (6%)	23	62
1	CJ	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	CK	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	CL	430/430 (100%)	406 (94%)	24 (6%)	25	63
1	CM	430/430 (100%)	403 (94%)	27 (6%)	21	60
1	CN	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	CO	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	CP	430/430 (100%)	405 (94%)	25 (6%)	23	62
1	CQ	430/430 (100%)	403 (94%)	27 (6%)	21	60
1	CR	430/430 (100%)	404 (94%)	26 (6%)	22	61
1	CS	430/430 (100%)	407 (95%)	23 (5%)	26	65
1	CT	430/430 (100%)	405 (94%)	25 (6%)	23	62
All	All	25800/25800 (100%)	24348 (94%)	1452 (6%)	25	63

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

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

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

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

5.3.3 RNA [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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.