



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 01:31 PM EDT

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

<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 : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

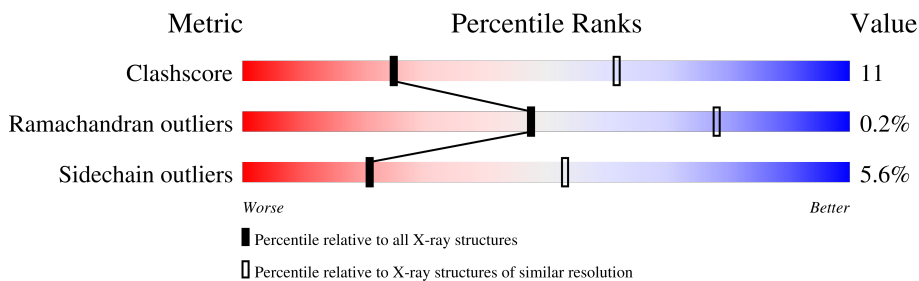
1 Overall quality at a glance

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	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)

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 $\leq 5\%$.

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	
1	AH	504	

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Mol	Chain	Length	Quality of chain	
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%
1	BM	504	81%	17%



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Mol	Chain	Length	Quality of chain	
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%
1	CR	504	78%	20%

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Mol	Chain	Length	Quality of chain
1	CS	504	 81% 17% •
1	CT	504	 82% 15% •

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

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

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

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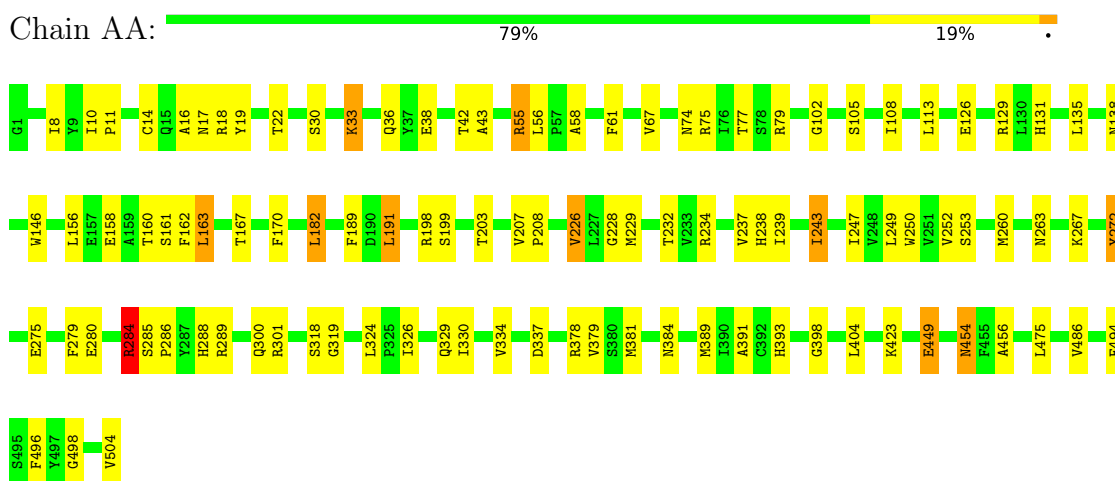
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	CS	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			
1	CT	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			

3 Residue-property plots [i](#)

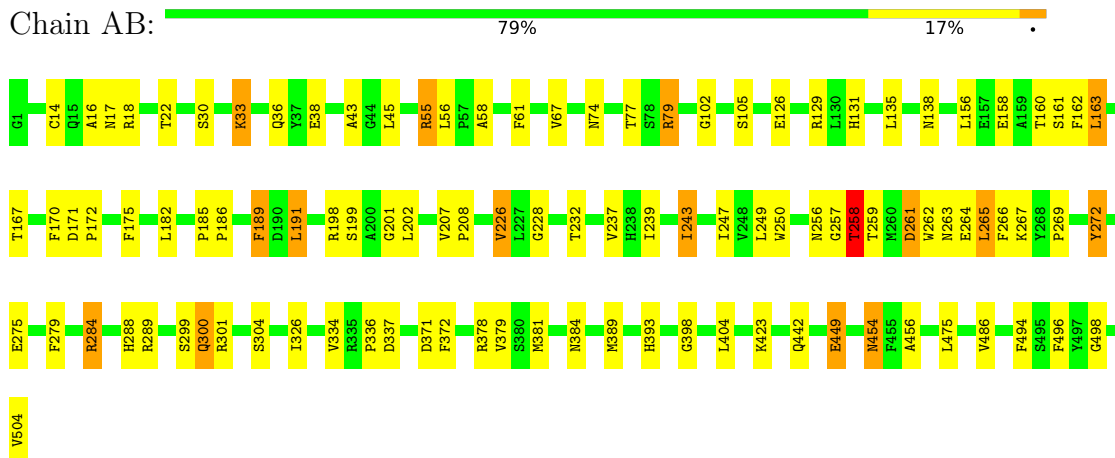
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

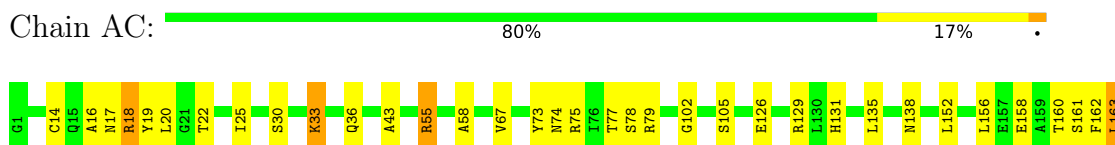
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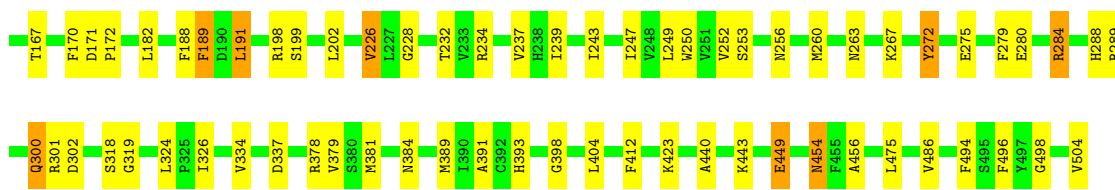


- Molecule 1: COAT PROTEIN



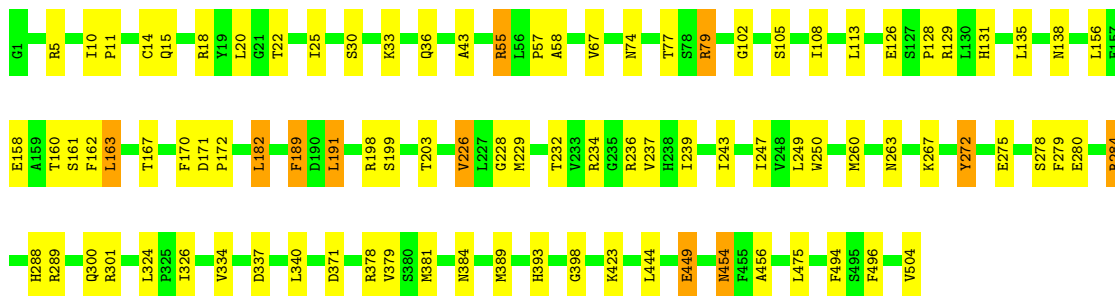
- Molecule 1: COAT PROTEIN





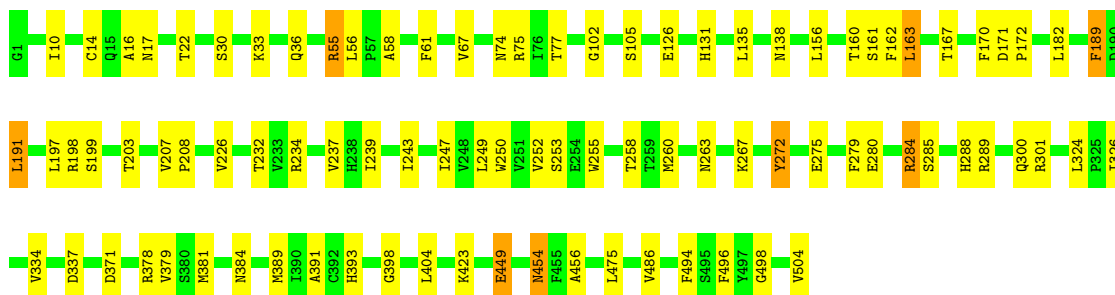
- Molecule 1: COAT PROTEIN

Chain AD: 82% 16%



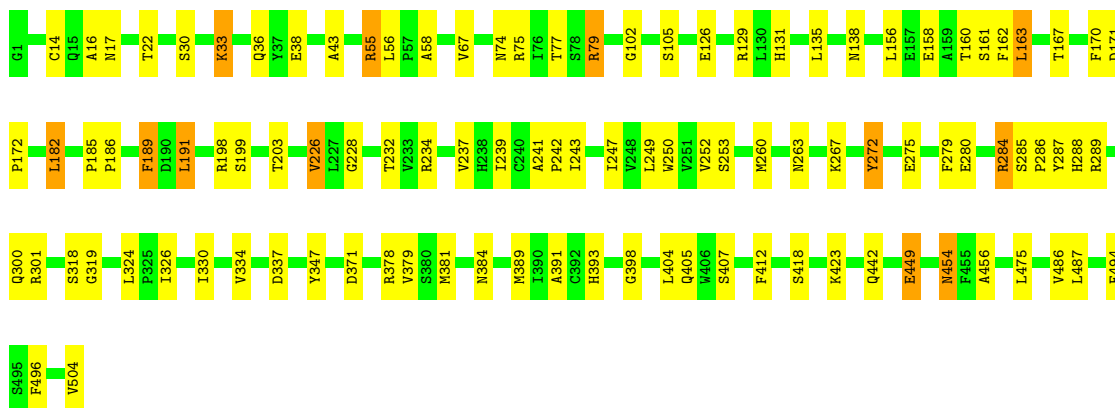
- Molecule 1: COAT PROTEIN

Chain AE: 82% 16%



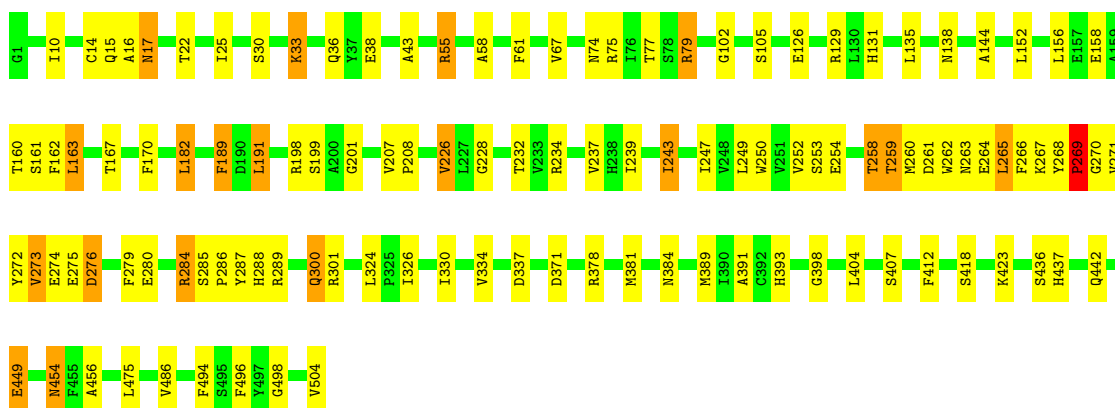
- Molecule 1: COAT PROTEIN

Chain AF: 79% 18%



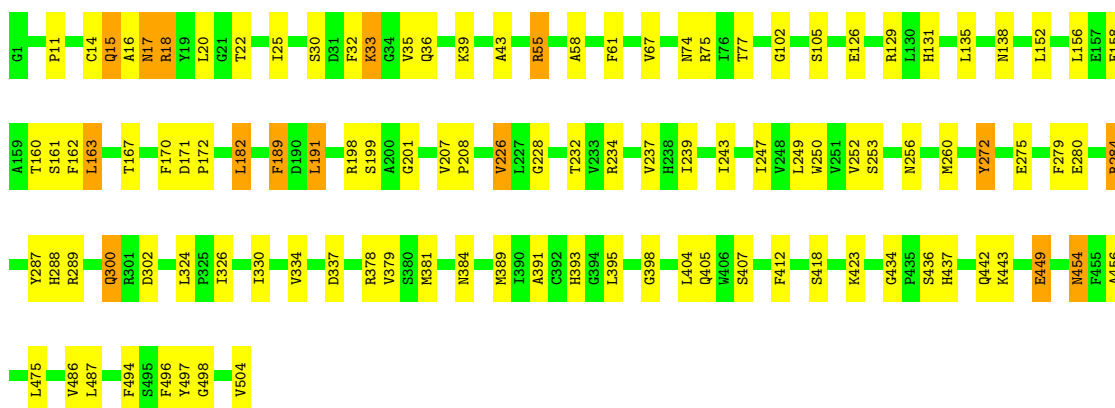
- Molecule 1: COAT PROTEIN

Chain AG: 77% 19%



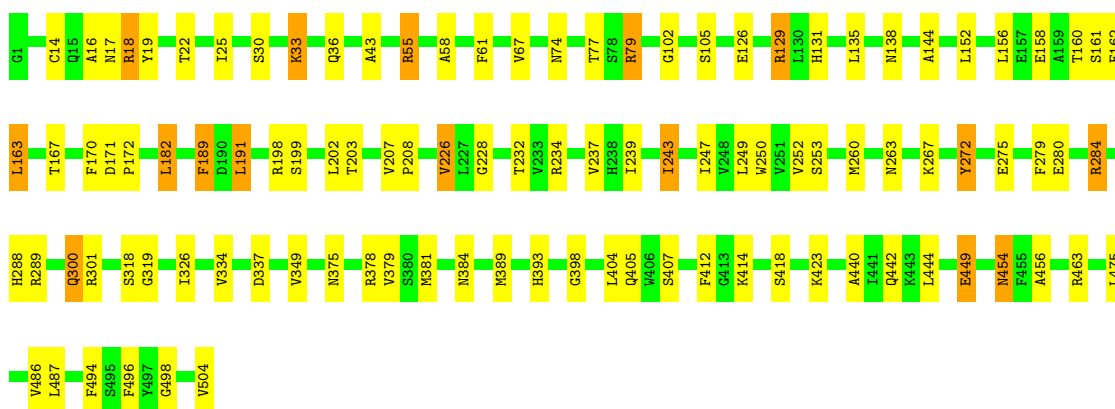
• Molecule 1: COAT PROTEIN

Chain AH: 78% 19%



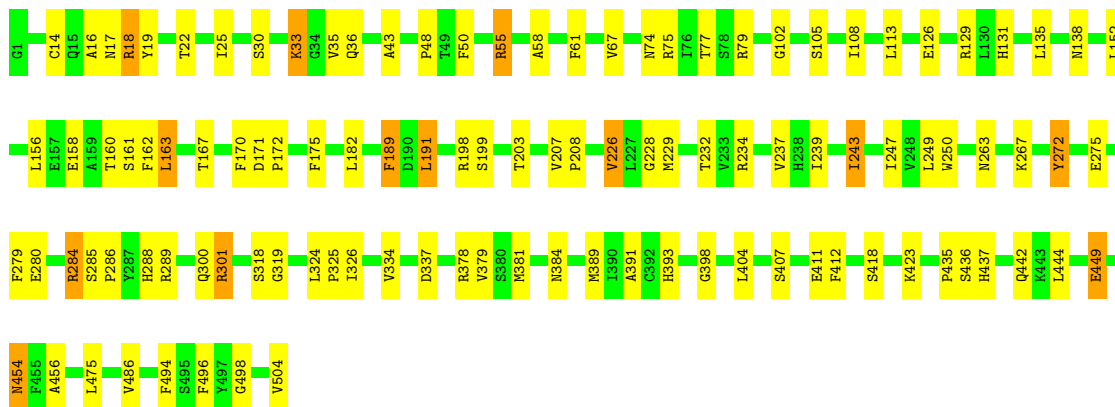
• Molecule 1: COAT PROTEIN

Chain AI: 79% 18%

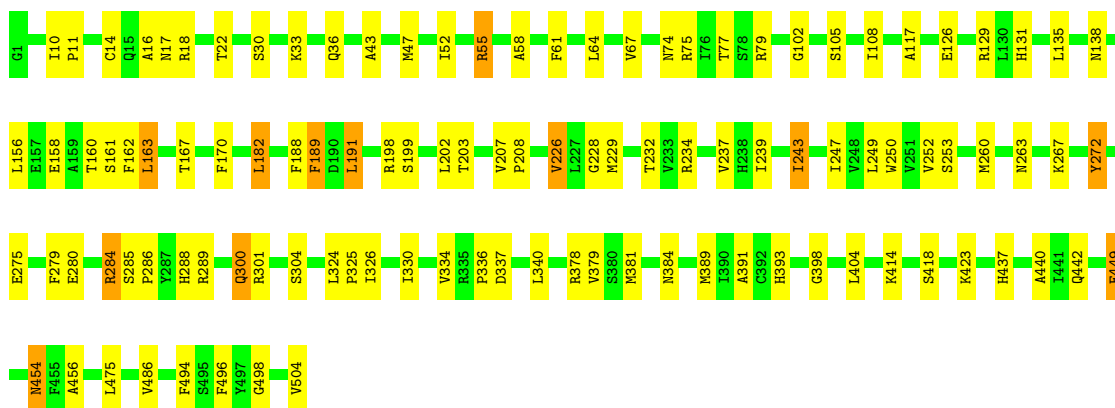
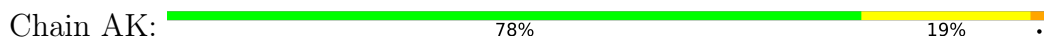


• Molecule 1: COAT PROTEIN

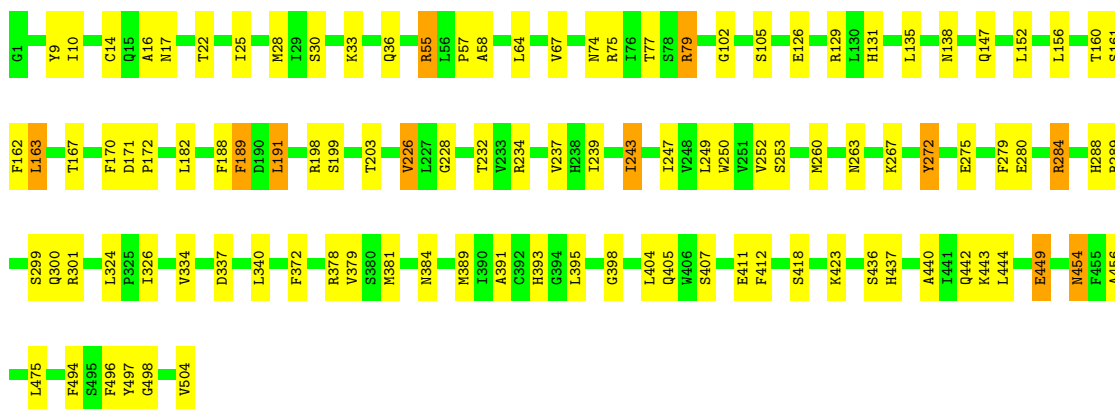
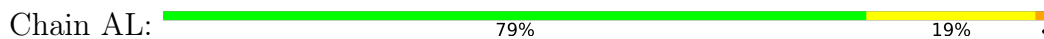
Chain AJ: 78% 19%



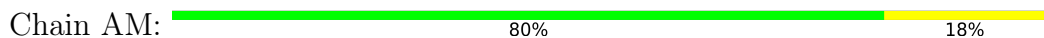
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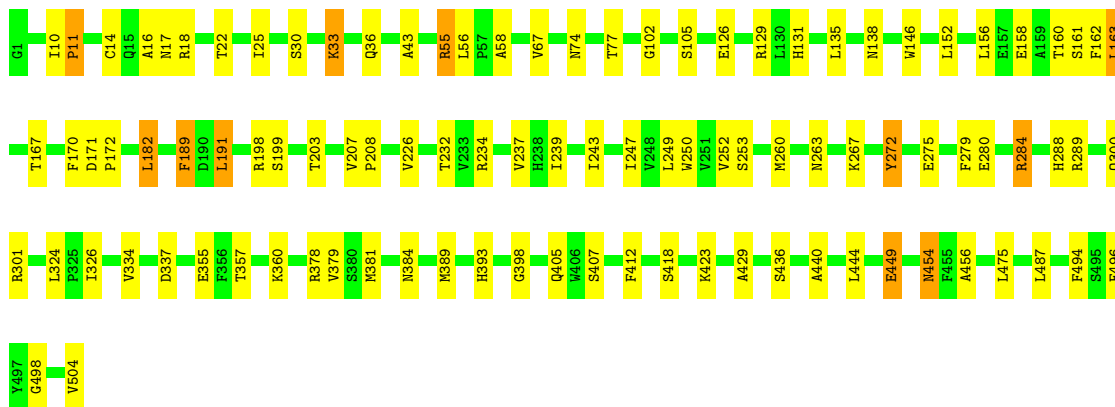


● Molecule 1: COAT PROTEIN

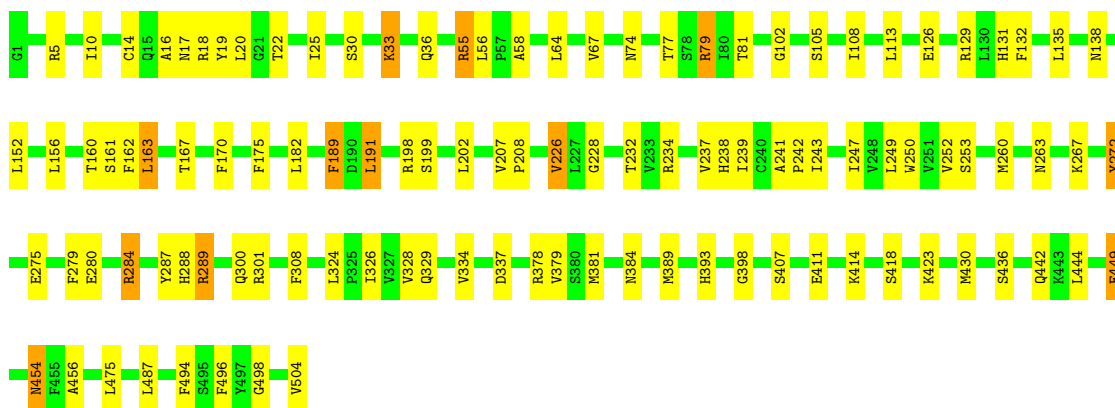
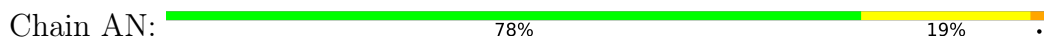


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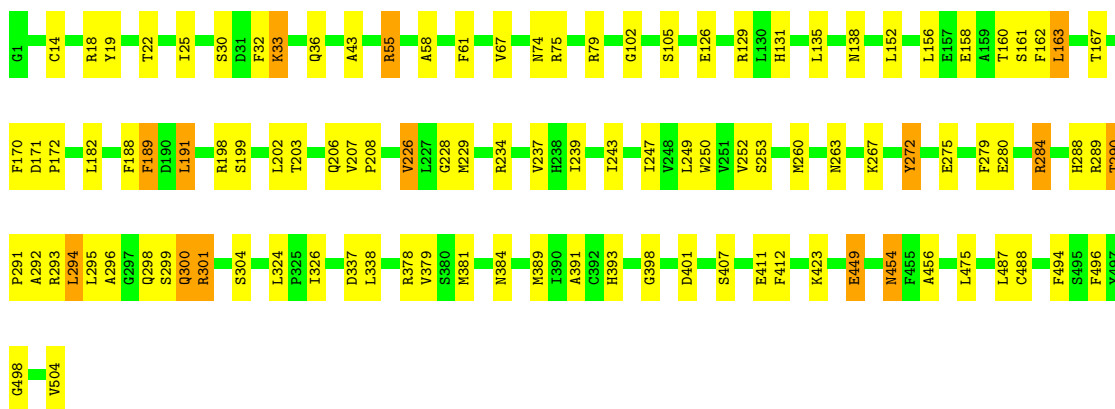
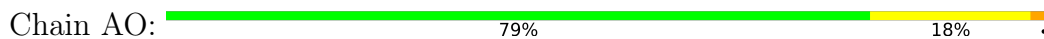




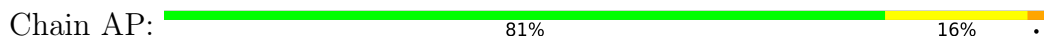
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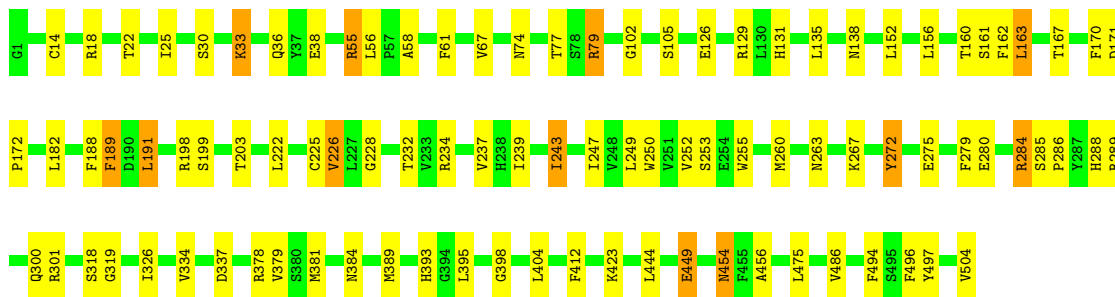


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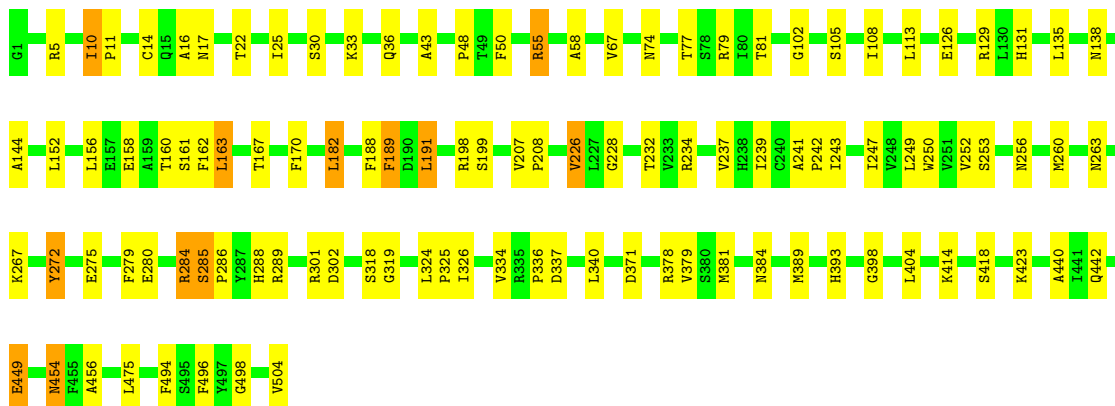
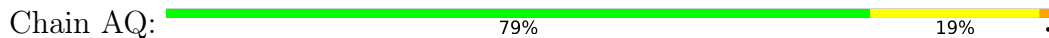


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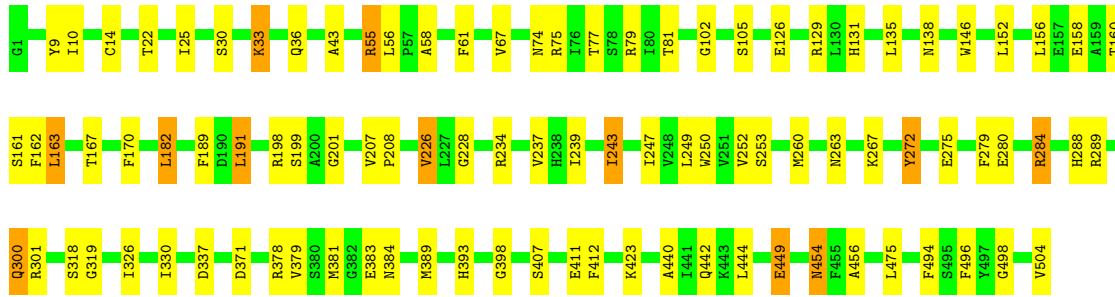
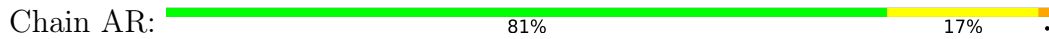




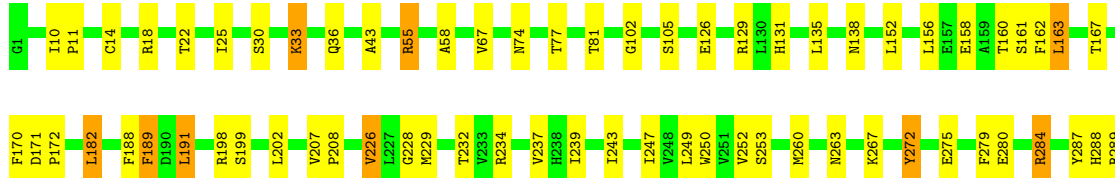
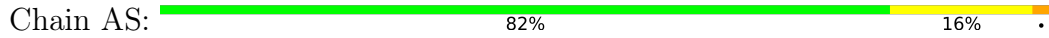
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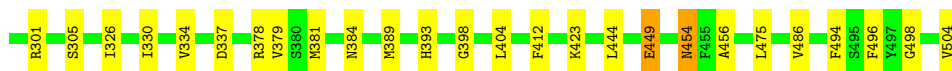


• Molecule 1: COAT PROTEIN

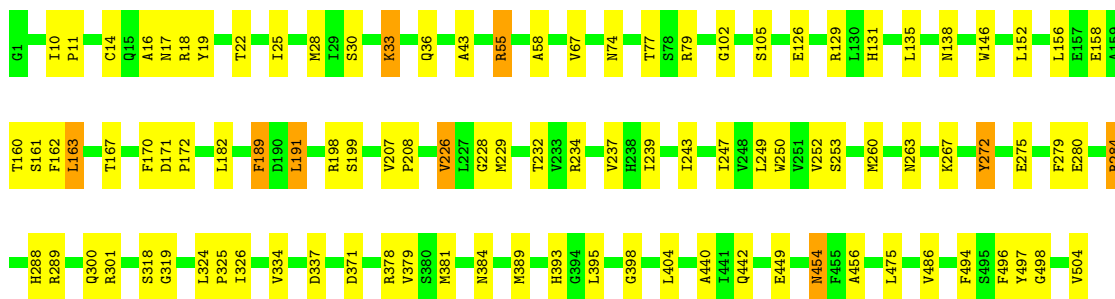
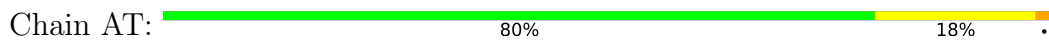


• Molecule 1: COAT PROTEIN

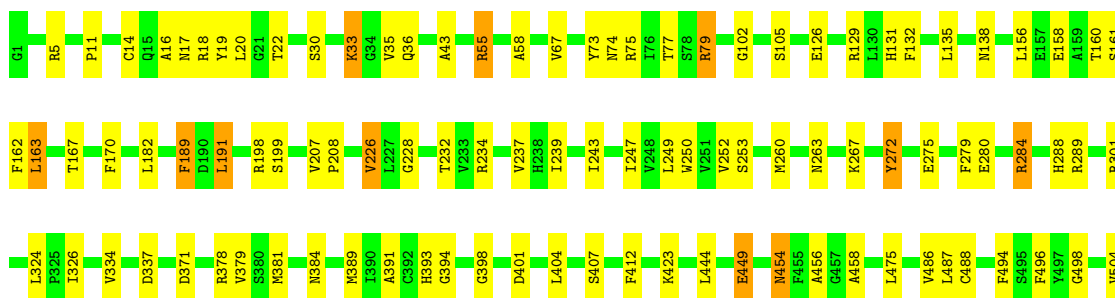
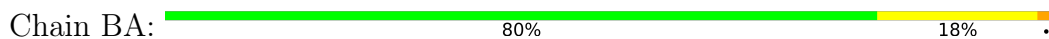




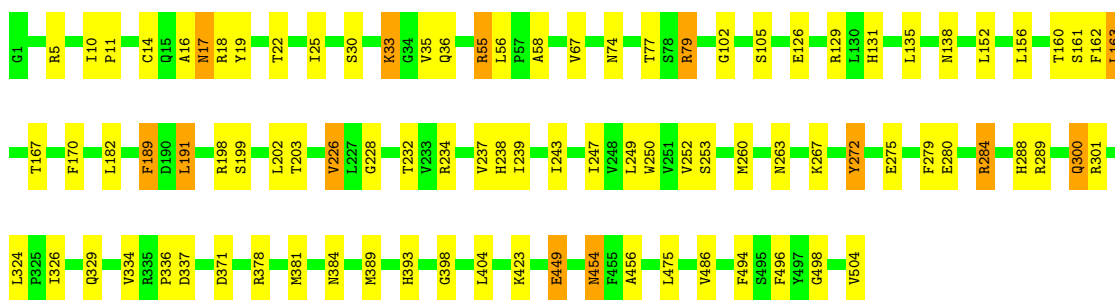
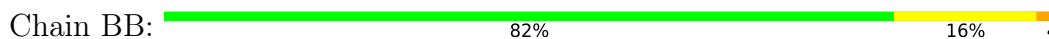
Molecule 1: COAT PROTEIN



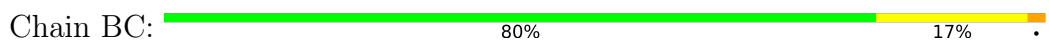
Molecule 1: COAT PROTEIN

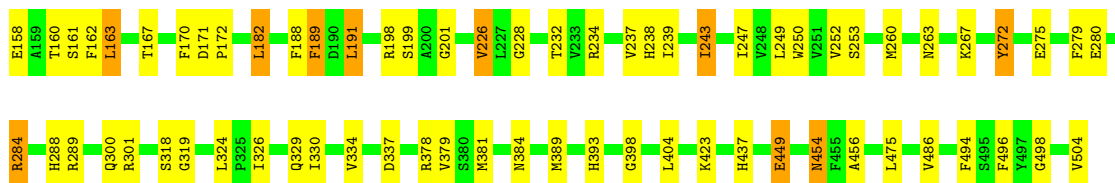


Molecule 1: COAT PROTEIN

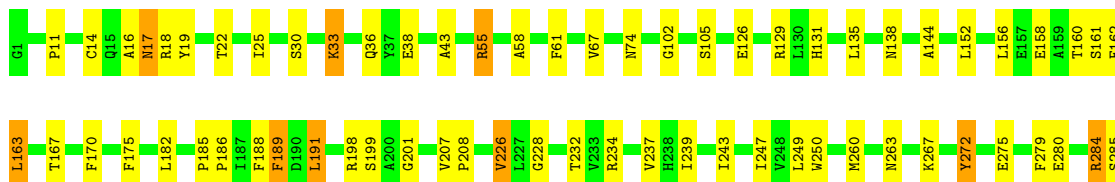
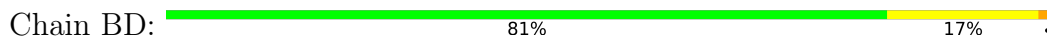


Molecule 1: COAT PROTEIN

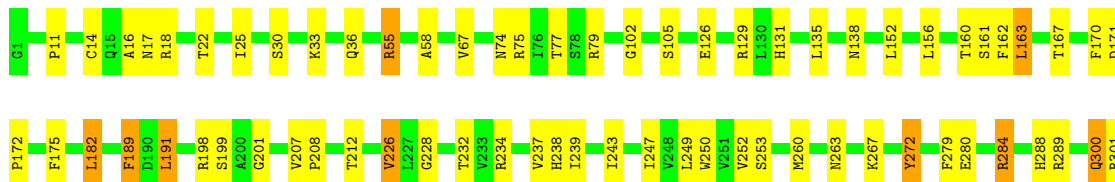
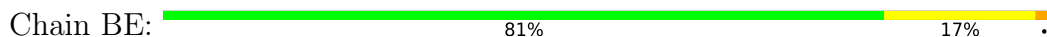




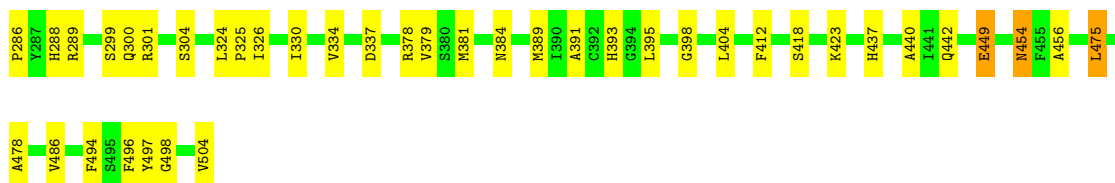
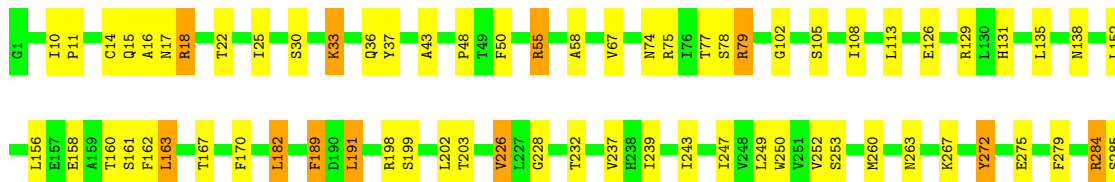
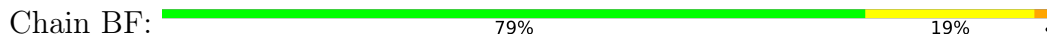
- Molecule 1: COAT PROTEIN




- Molecule 1: COAT PROTEIN

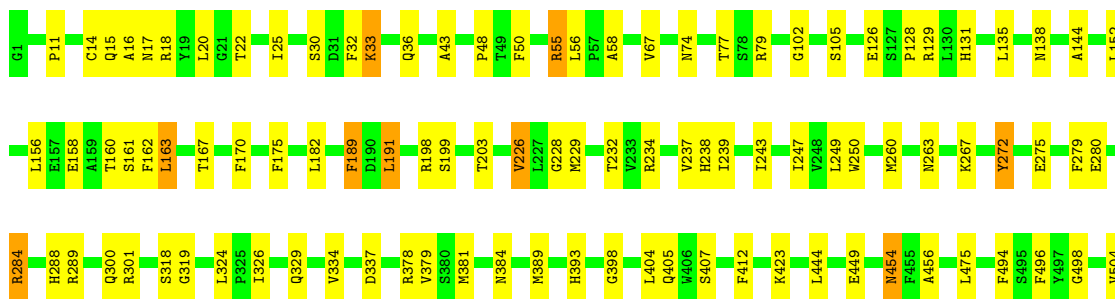


- Molecule 1: COAT PROTEIN




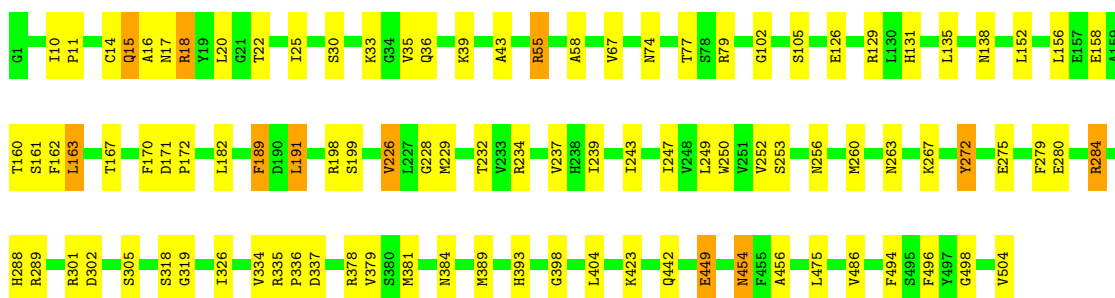
- Molecule 1: COAT PROTEIN

Chain BG:  80% 18%




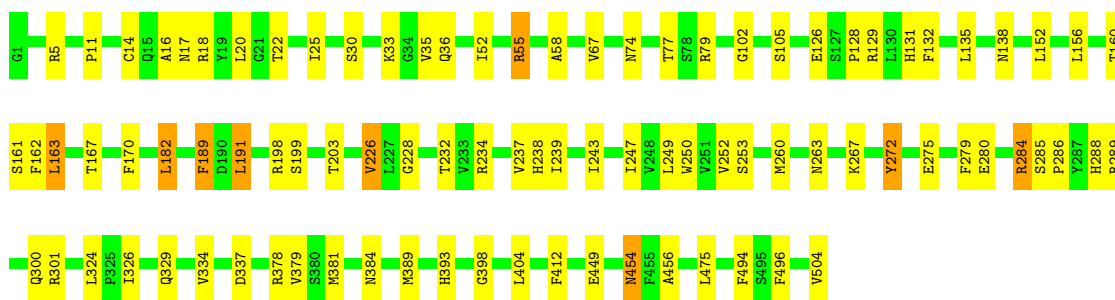
• Molecule 1: COAT PROTEIN

Chain BH:  81% 17%




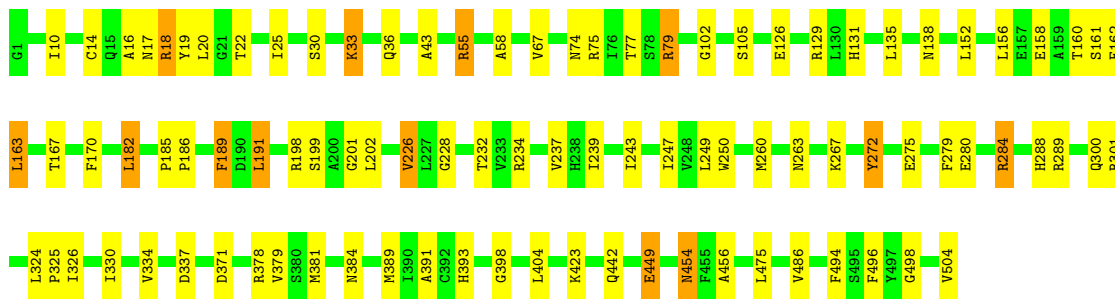
• Molecule 1: COAT PROTEIN

Chain BI:  82% 16%


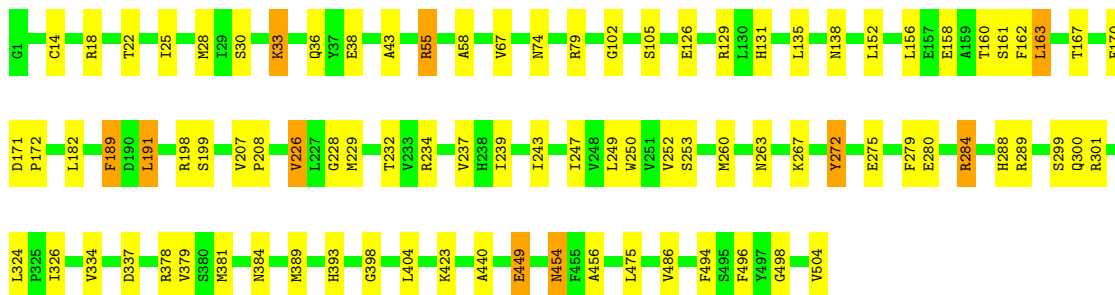


• Molecule 1: COAT PROTEIN


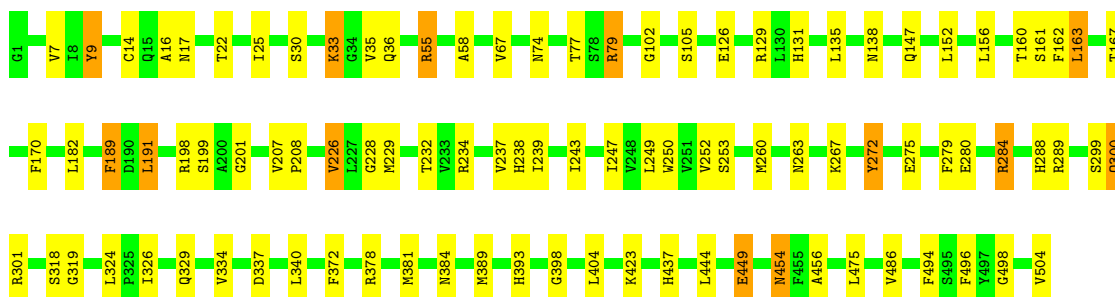
Chain BJ:  81% 16%




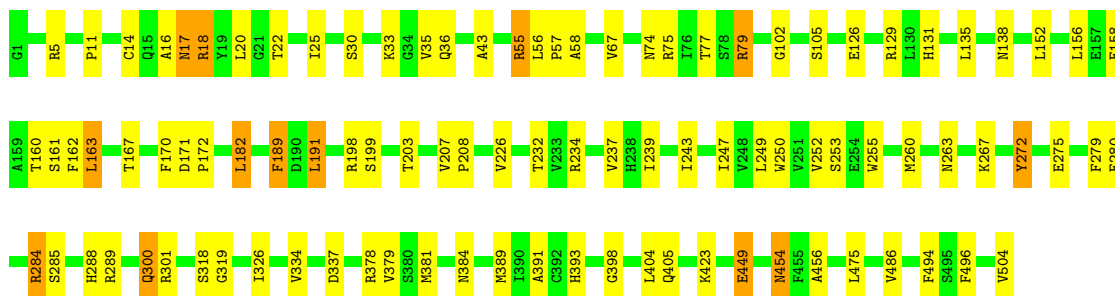
- Molecule 1: COAT PROTEIN

Chain BK:  82% 16%


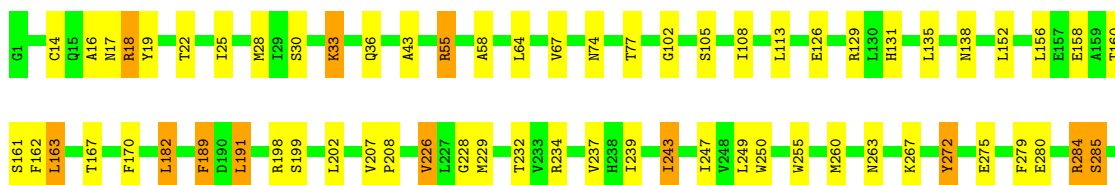
- Molecule 1: COAT PROTEIN

Chain BL:  81% 16%

- Molecule 1: COAT PROTEIN

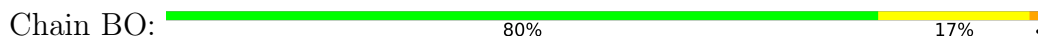
Chain BM:  81% 17%

- Molecule 1: COAT PROTEIN

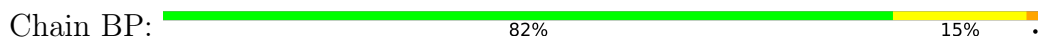
Chain BN:  81% 16%



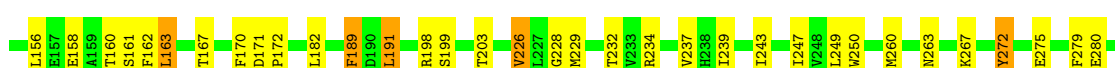
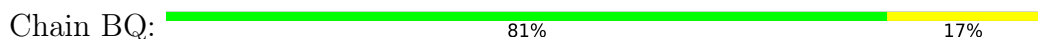
● Molecule 1: COAT PROTEIN



● Molecule 1: COAT PROTEIN

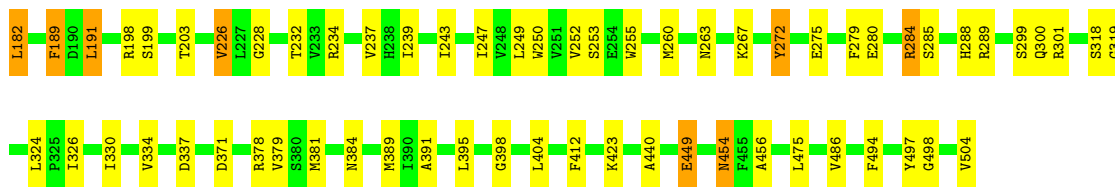


● Molecule 1: COAT PROTEIN

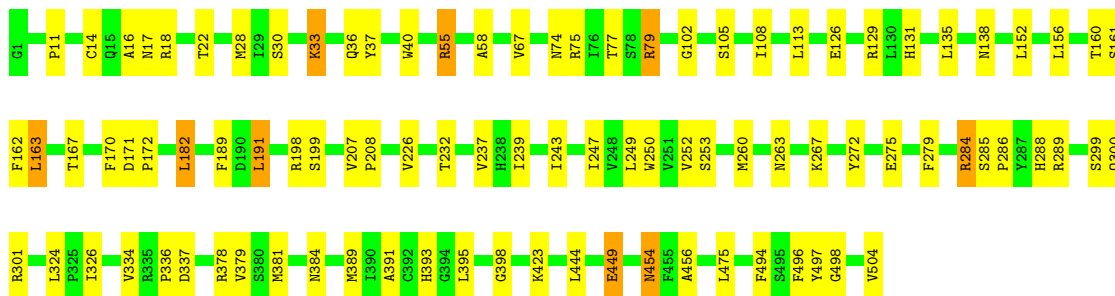
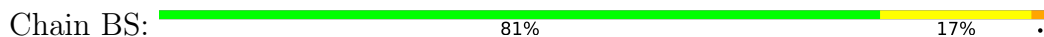


● Molecule 1: COAT PROTEIN

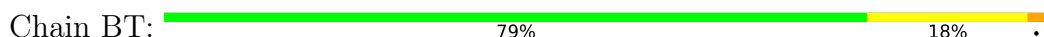




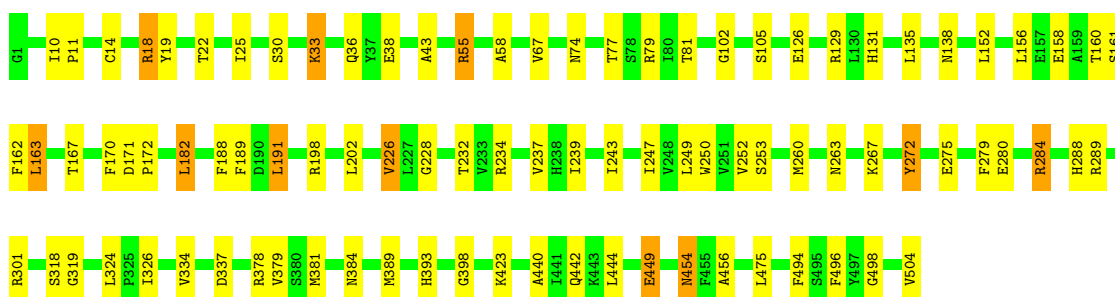
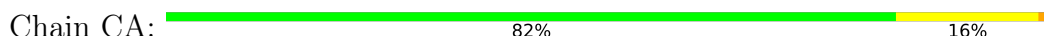
• Molecule 1: COAT PROTEIN




• Molecule 1: COAT PROTEIN

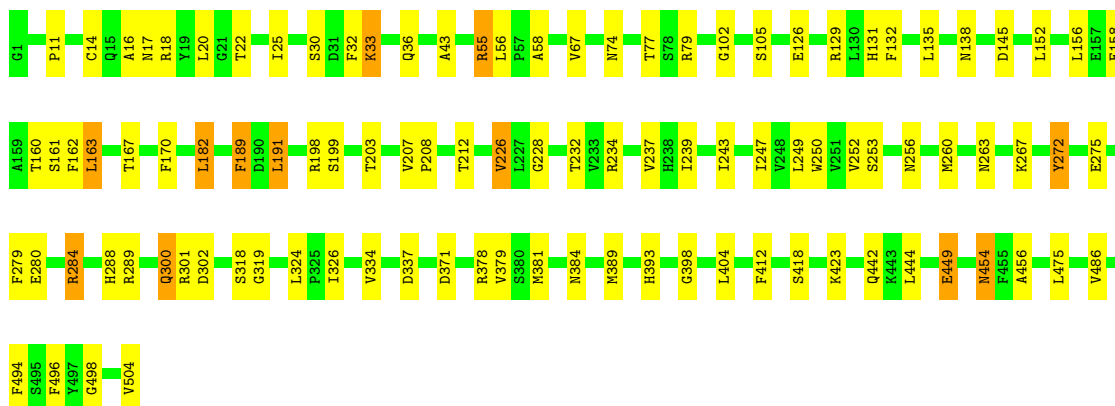


• Molecule 1: COAT PROTEIN




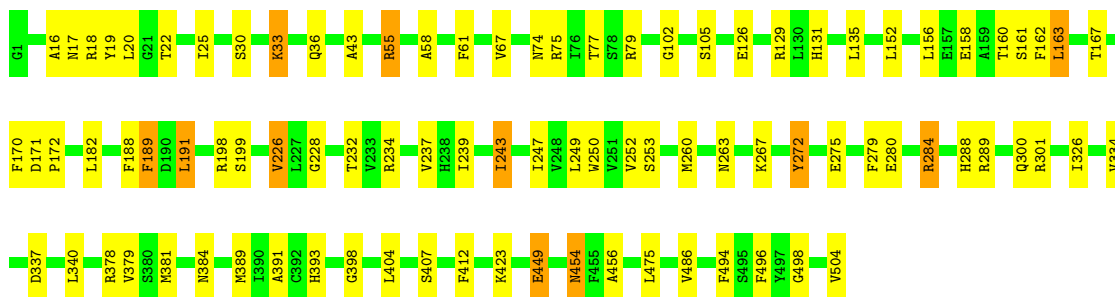
• Molecule 1: COAT PROTEIN

Chain CB:  80% 18%




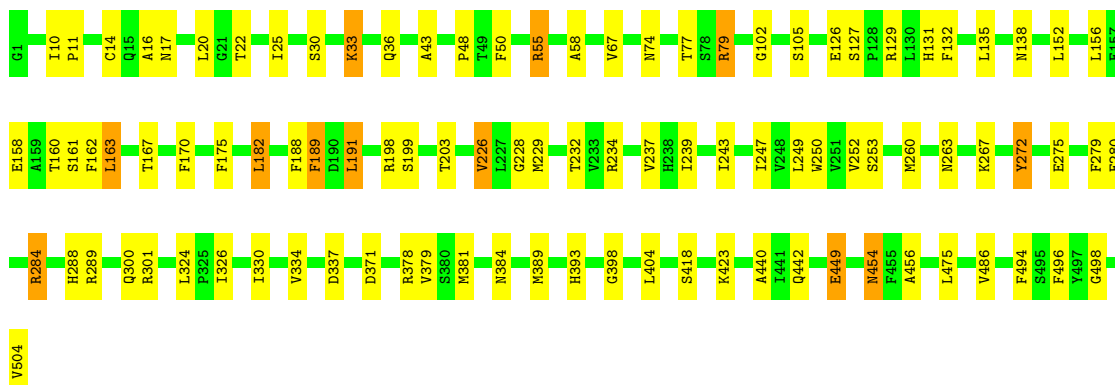
• Molecule 1: COAT PROTEIN

Chain CC:  82% 16%




• Molecule 1: COAT PROTEIN

Chain CD:  81% 17%



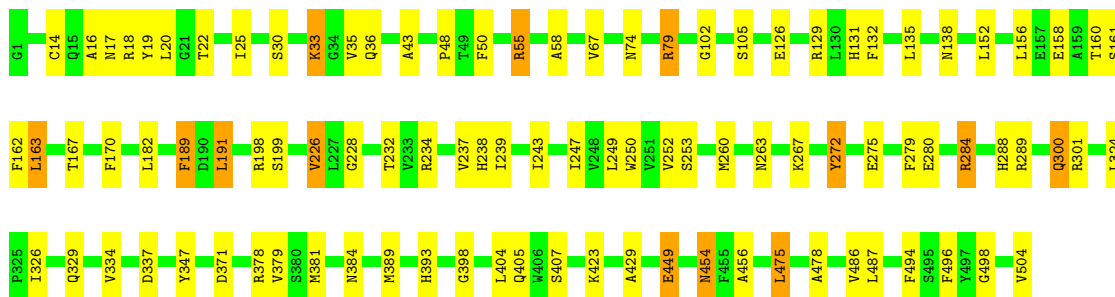
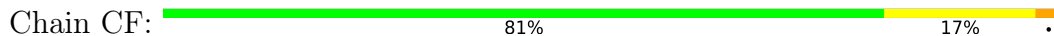
• Molecule 1: COAT PROTEIN

Chain CE:  79% 18%

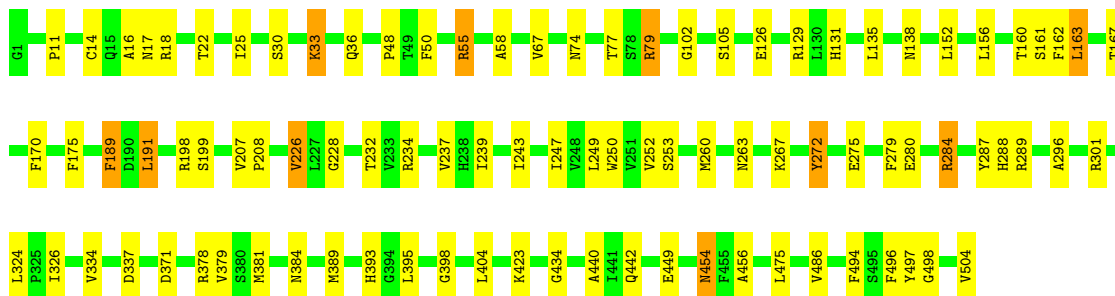
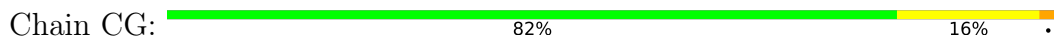




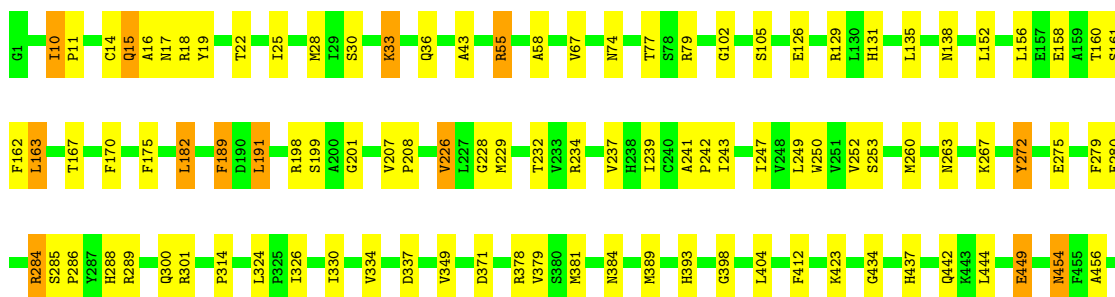
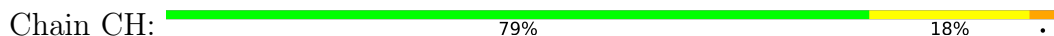
● Molecule 1: COAT PROTEIN



● Molecule 1: COAT PROTEIN




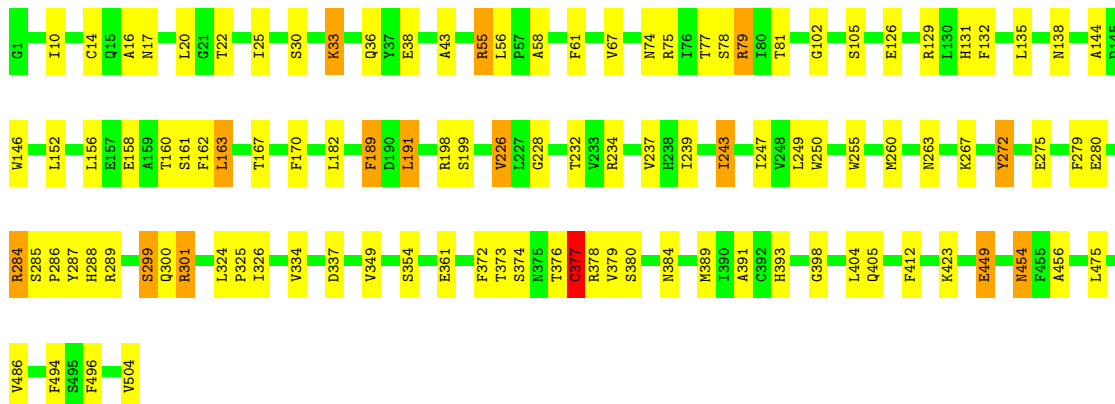
● Molecule 1: COAT PROTEIN




L475
W496
F494
S495
F496
V504

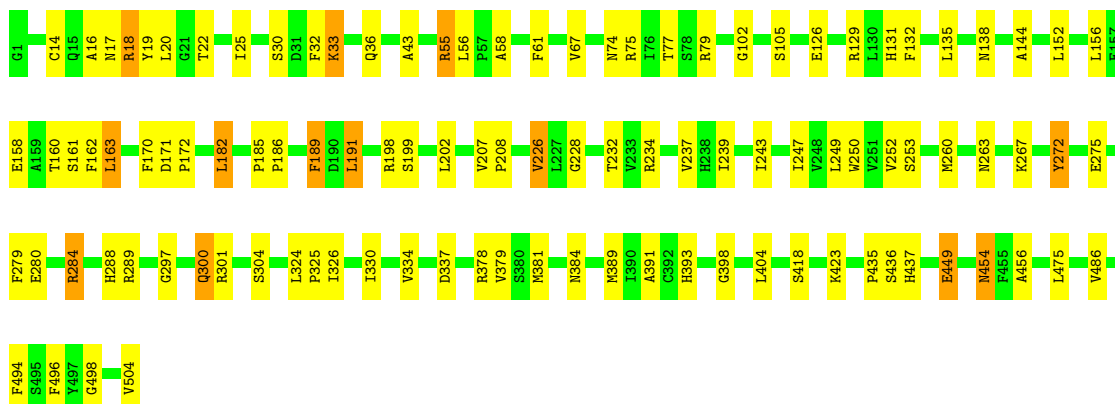
• Molecule 1: COAT PROTEIN

Chain CI:  79% 18%




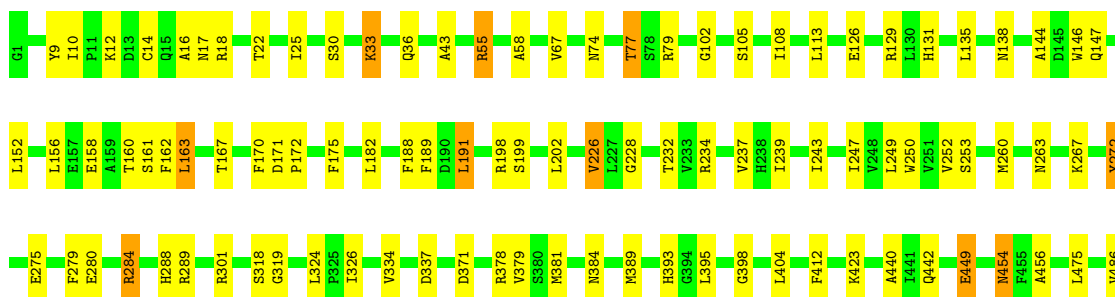
• Molecule 1: COAT PROTEIN

Chain CJ:  79% 18%



• Molecule 1: COAT PROTEIN

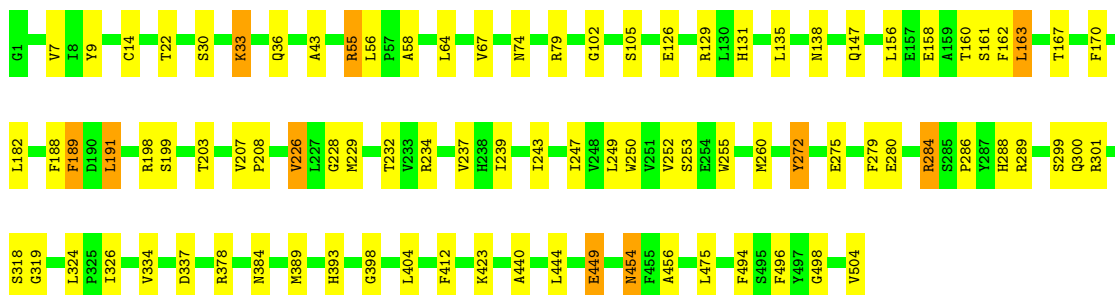
Chain CK:  80% 18%





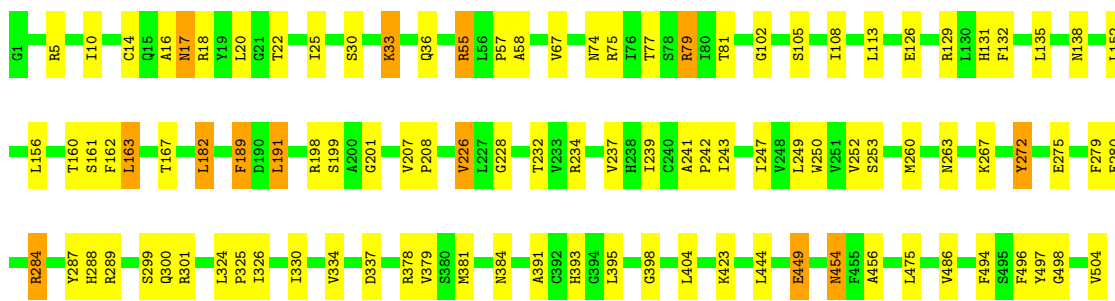
- Molecule 1: COAT PROTEIN

Chain CL: 82% 16%



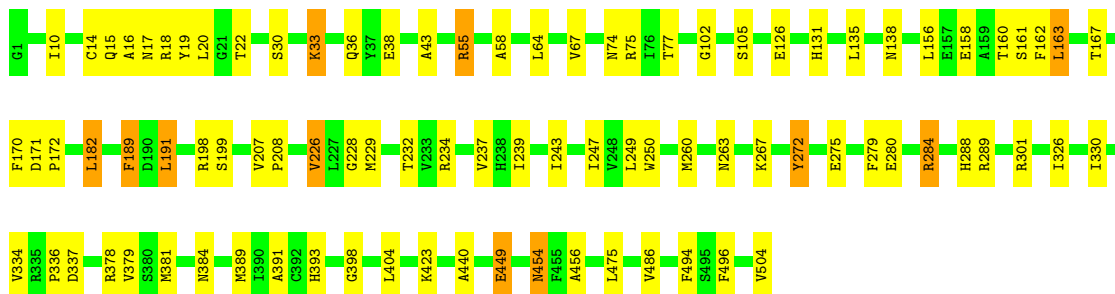
- Molecule 1: COAT PROTEIN

Chain CM: 80% 17%



- Molecule 1: COAT PROTEIN

Chain CN: 82% 16%



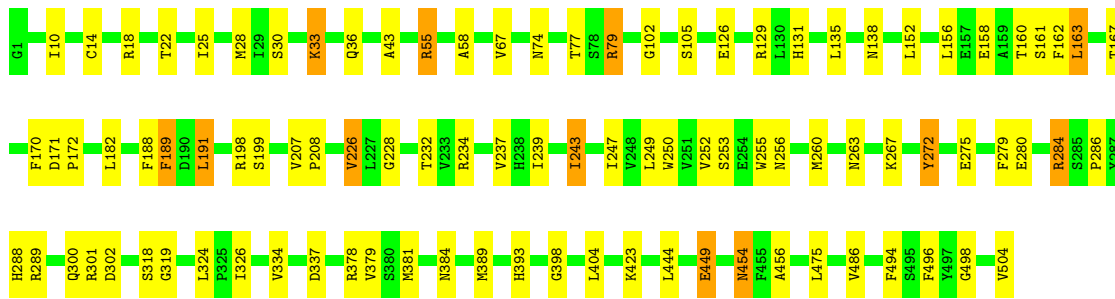
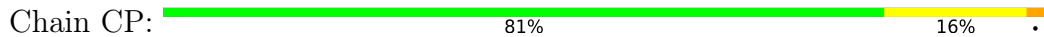
- Molecule 1: COAT PROTEIN

Chain CO: 80% 18%

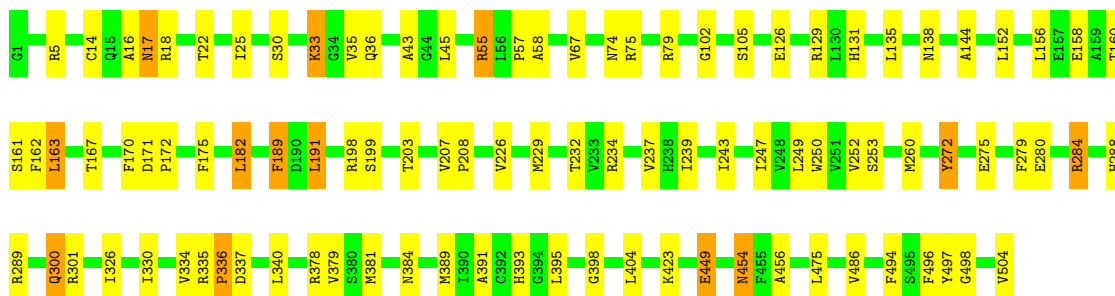
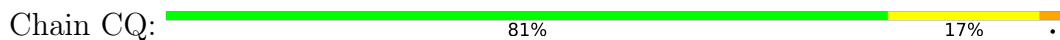




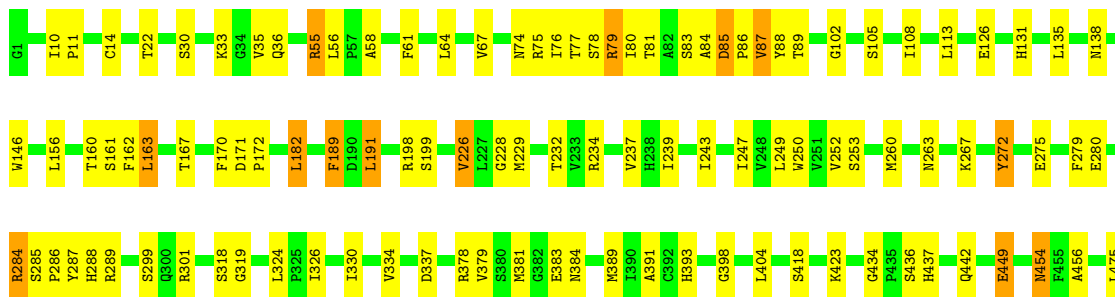
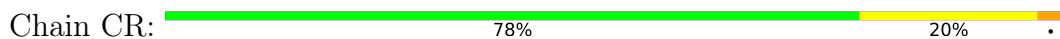
• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN



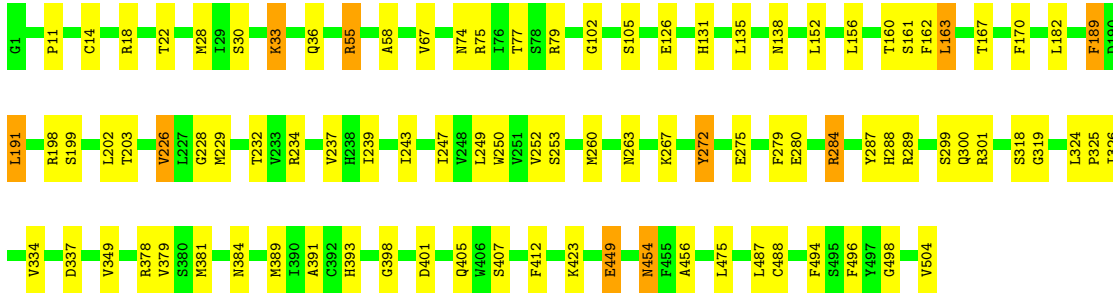
• Molecule 1: COAT PROTEIN





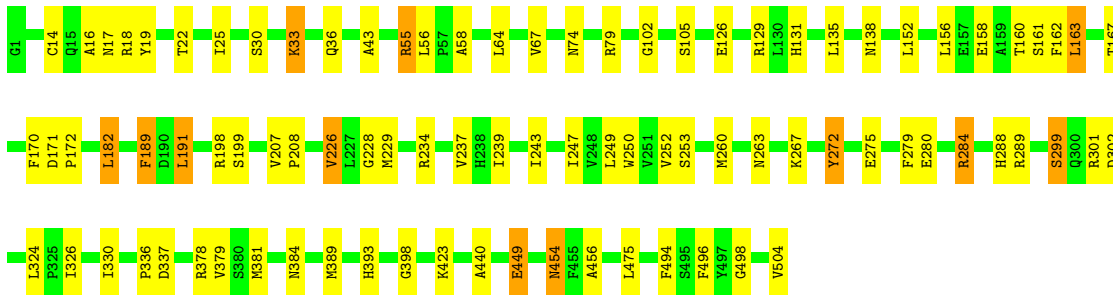
- Molecule 1: COAT PROTEIN

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)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.232 , 0.247	Depositor
Wilson B-factor (Å ²)	66.2	Xtrriage
Anisotropy	0.406	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.088 for -k,-h,-l 0.087 for k,h,-l 0.089 for h,-k,-l	Xtrriage
Total number of atoms	237060	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage'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 [i](#)

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 [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%)	47	78
1	AB	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	78
1	AC	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	34	69
1	AD	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AE	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	78
1	AF	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AG	502/504 (100%)	480 (96%)	18 (4%)	4 (1%)	19	56
1	AH	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	34	69
1	AI	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	AJ	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	78
1	AK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	AL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	AM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	78
1	AN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	AO	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	78
1	AP	502/504 (100%)	483 (96%)	19 (4%)	0	100	100
1	AQ	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	78
1	AR	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AS	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	78
1	AT	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	47	78
1	BA	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	78
1	BB	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	34	69
1	BC	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	BD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	BE	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	BF	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	34	69
1	BG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	78
1	BH	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	BI	502/504 (100%)	479 (95%)	23 (5%)	0	100	100
1	BJ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	BK	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	78
1	BL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	BM	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	BN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	BO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	BP	502/504 (100%)	479 (95%)	21 (4%)	2 (0%)	34	69
1	BQ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	BR	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	BS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	BT	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	78
1	CA	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	CB	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	78
1	CC	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	CD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	CE	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	47	78
1	CF	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	78
1	CG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	78
1	CH	502/504 (100%)	481 (96%)	21 (4%)	0	100	100
1	CI	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	34	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CJ	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	47	78
1	CK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	47	78
1	CL	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	CM	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	34	69
1	CN	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	CO	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	CP	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	47	78
1	CQ	502/504 (100%)	482 (96%)	18 (4%)	2 (0%)	34	69
1	CR	502/504 (100%)	479 (95%)	21 (4%)	2 (0%)	34	69
1	CS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	47	78
1	CT	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	47	78
All	All	30120/30240 (100%)	28873 (96%)	1181 (4%)	66 (0%)	47	78

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 [i](#)

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%)	22	54
1	AB	430/430 (100%)	402 (94%)	28 (6%)	17	48
1	AC	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	AD	430/430 (100%)	404 (94%)	26 (6%)	19	50
1	AE	430/430 (100%)	409 (95%)	21 (5%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AF	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	AG	430/430 (100%)	403 (94%)	27 (6%)	18	49
1	AH	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	AI	430/430 (100%)	405 (94%)	25 (6%)	20	52
1	AJ	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	AK	430/430 (100%)	404 (94%)	26 (6%)	19	50
1	AL	430/430 (100%)	404 (94%)	26 (6%)	19	50
1	AM	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	AN	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	AO	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	AP	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	AQ	430/430 (100%)	405 (94%)	25 (6%)	20	52
1	AR	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	AS	430/430 (100%)	405 (94%)	25 (6%)	20	52
1	AT	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	BA	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	BB	430/430 (100%)	405 (94%)	25 (6%)	20	52
1	BC	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	BD	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	BE	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	BF	430/430 (100%)	404 (94%)	26 (6%)	19	50
1	BG	430/430 (100%)	408 (95%)	22 (5%)	24	55
1	BH	430/430 (100%)	404 (94%)	26 (6%)	19	50
1	BI	430/430 (100%)	408 (95%)	22 (5%)	24	55
1	BJ	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	BK	430/430 (100%)	404 (94%)	26 (6%)	19	50
1	BL	430/430 (100%)	404 (94%)	26 (6%)	19	50
1	BM	430/430 (100%)	404 (94%)	26 (6%)	19	50
1	BN	430/430 (100%)	405 (94%)	25 (6%)	20	52
1	BO	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	BP	430/430 (100%)	407 (95%)	23 (5%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BQ	430/430 (100%)	405 (94%)	25 (6%)	20	52
1	BR	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	BS	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	BT	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	CA	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	CB	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	CC	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	CD	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	CE	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	CF	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	CG	430/430 (100%)	409 (95%)	21 (5%)	25	56
1	CH	430/430 (100%)	405 (94%)	25 (6%)	20	52
1	CI	430/430 (100%)	405 (94%)	25 (6%)	20	52
1	CJ	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	CK	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	CL	430/430 (100%)	406 (94%)	24 (6%)	21	53
1	CM	430/430 (100%)	403 (94%)	27 (6%)	18	49
1	CN	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	CO	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	CP	430/430 (100%)	405 (94%)	25 (6%)	20	52
1	CQ	430/430 (100%)	403 (94%)	27 (6%)	18	49
1	CR	430/430 (100%)	404 (94%)	26 (6%)	19	50
1	CS	430/430 (100%)	407 (95%)	23 (5%)	22	54
1	CT	430/430 (100%)	405 (94%)	25 (6%)	20	52
All	All	25800/25800 (100%)	24348 (94%)	1452 (6%)	21	53

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

Mol	Chain	Res	Type
1	BS	160	THR
1	CH	260	MET
1	BT	182	LEU
1	BS	129	ARG
1	CD	79	ARG

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

Mol	Chain	Res	Type
1	CC	147	GLN
1	CM	454	ASN
1	CD	256	ASN
1	CC	131	HIS
1	CH	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 monosaccharides 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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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