



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 5, 2019 – 10:58 AM EDT

PDB ID : 4V5T  
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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

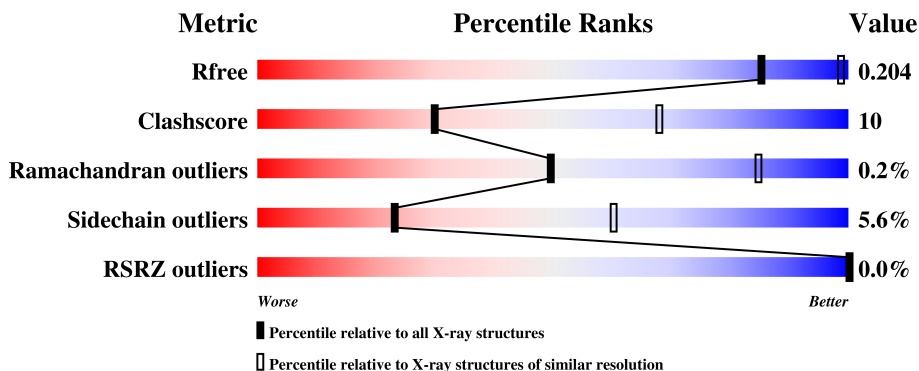
# 1 Overall quality at a glance

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))
$R_{free}$	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	AA	504	<div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	AB	504	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	AC	504	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	AD	504	<div> <div>80%</div> <div>17%</div> <div>.</div> </div>
1	AE	504	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>














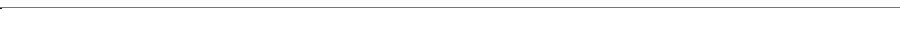


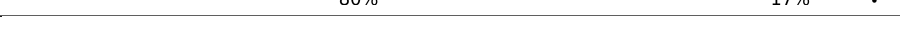
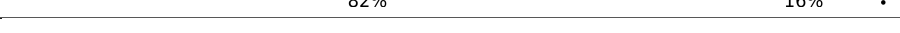







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Mol	Chain	Length	Quality of chain	
1	AF	504		•
1	AG	504		•
1	AH	504		•
1	AI	504		•
1	AJ	504		•
1	AK	504		•
1	AL	504		•
1	AM	504		•
1	AN	504		•
1	AO	504		•
1	AP	504		•
1	AQ	504		•
1	AR	504		•
1	AS	504		•
1	AT	504		•
1	BA	504		•
1	BB	504		•
1	BC	504		•
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	 81% 16% .
1	CQ	504	 82% 16% .
1	CR	504	 81% 17% .
1	CS	504	 81% 17% .
1	CT	504	 82% 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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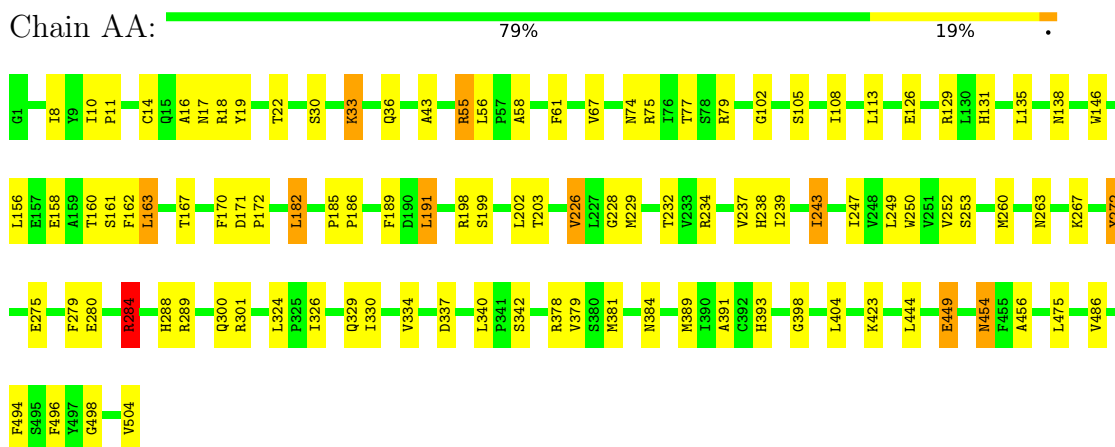
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CS	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			
1	CT	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			

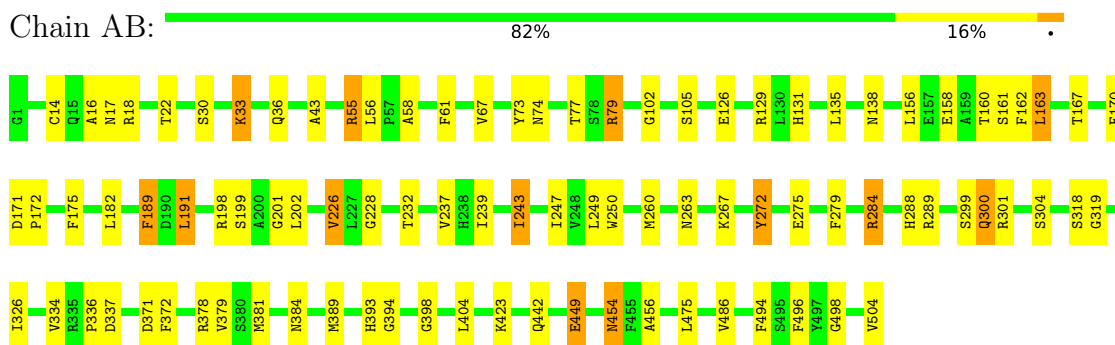
### 3 Residue-property plots

These plots are drawn for all protein, RNA 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.

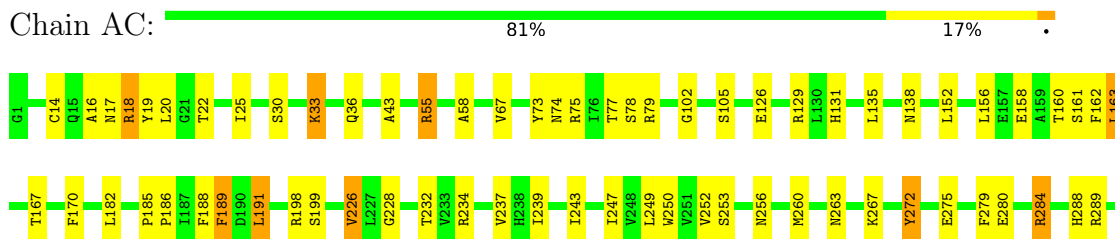
#### • Molecule 1: COAT PROTEIN



#### • Molecule 1: COAT PROTEIN

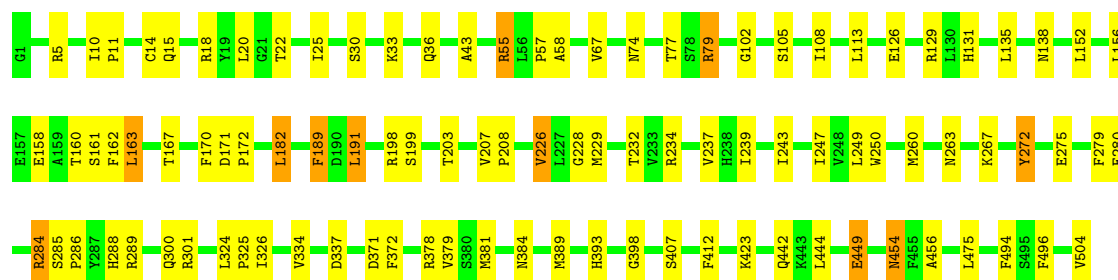


#### • Molecule 1: COAT PROTEIN

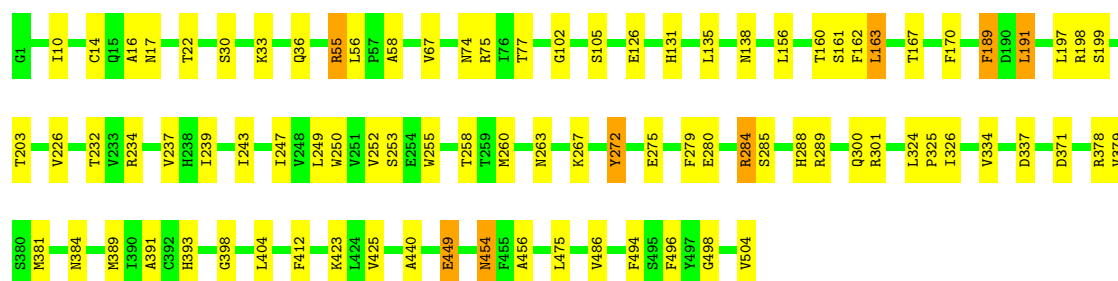




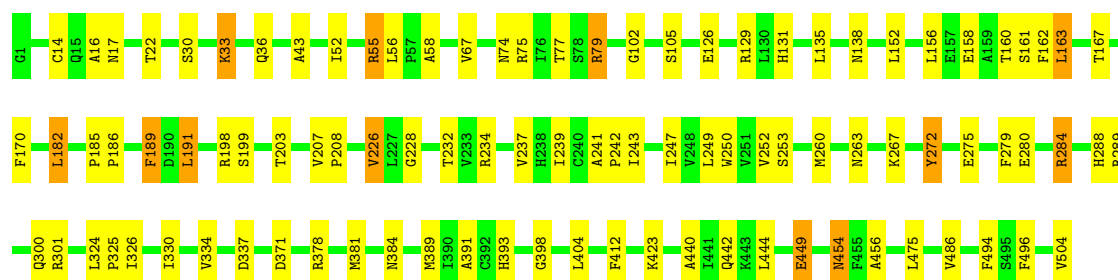
## ● Molecule 1: COAT PROTEIN

Chain AD:   
80% 17%

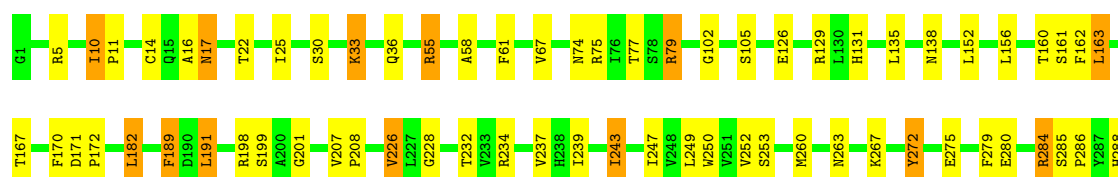
## ● Molecule 1: COAT PROTEIN

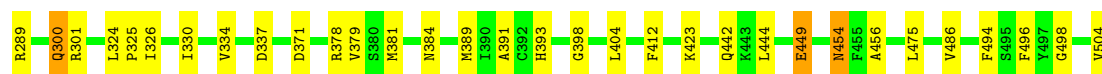
Chain AE:   
83% 16%

## ● Molecule 1: COAT PROTEIN

Chain AF:   
81% 17%

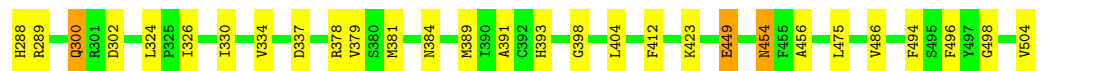
## ● Molecule 1: COAT PROTEIN

Chain AG:   
80% 16%



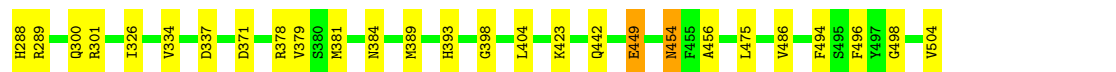
• Molecule 1: COAT PROTEIN

Chain AH: 81% 16% .



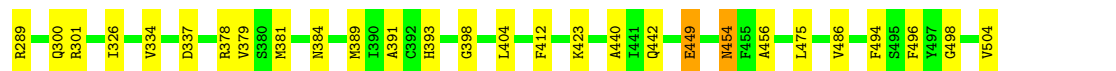
• Molecule 1: COAT PROTEIN

Chain AI: 81% 16% .



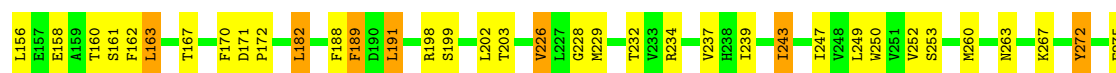
• Molecule 1: COAT PROTEIN

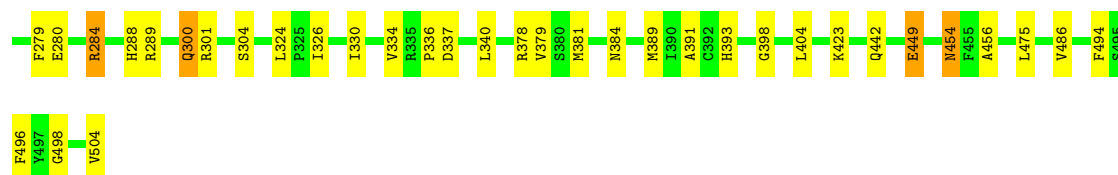
Chain AJ: 82% 16% .



• Molecule 1: COAT PROTEIN

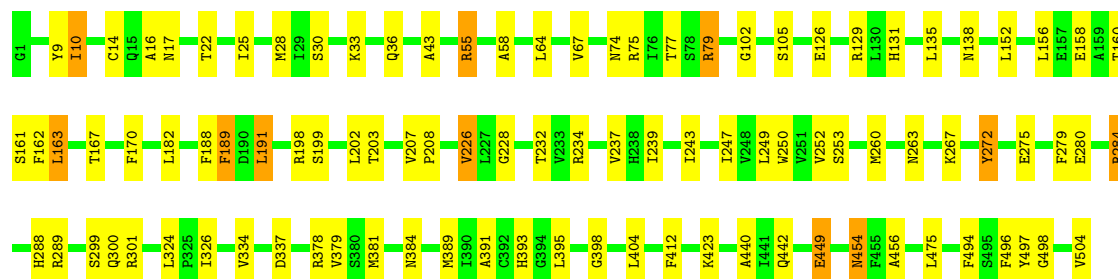
Chain AK: 80% 18% .





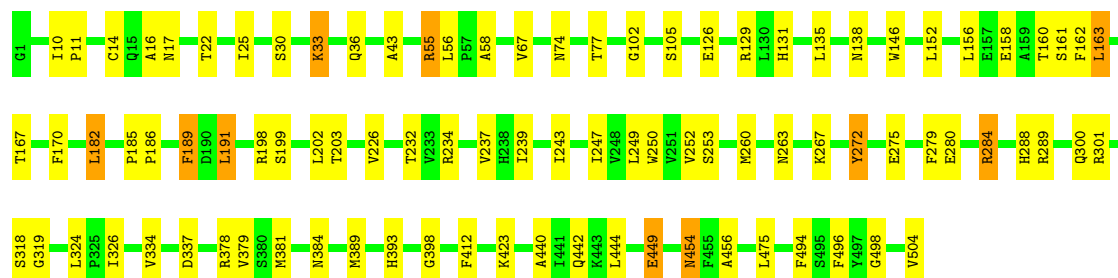
• Molecule 1: COAT PROTEIN

Chain AL: 81% 17% .



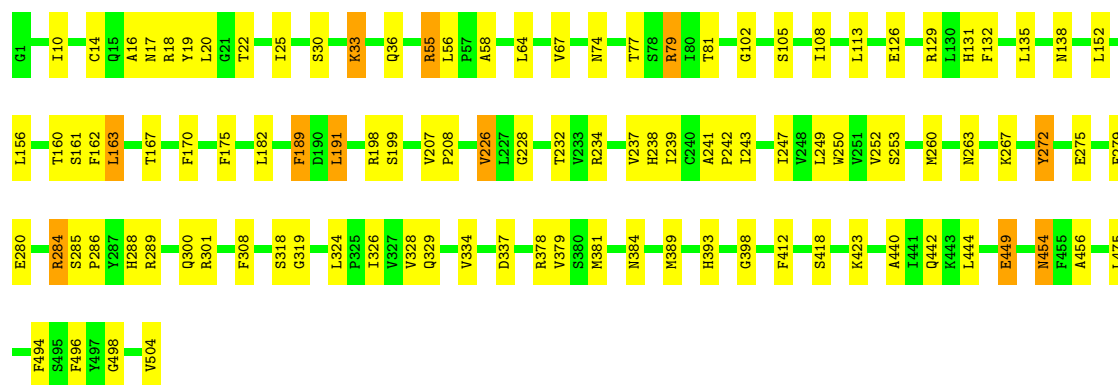
• Molecule 1: COAT PROTEIN

Chain AM: 82% 16% .



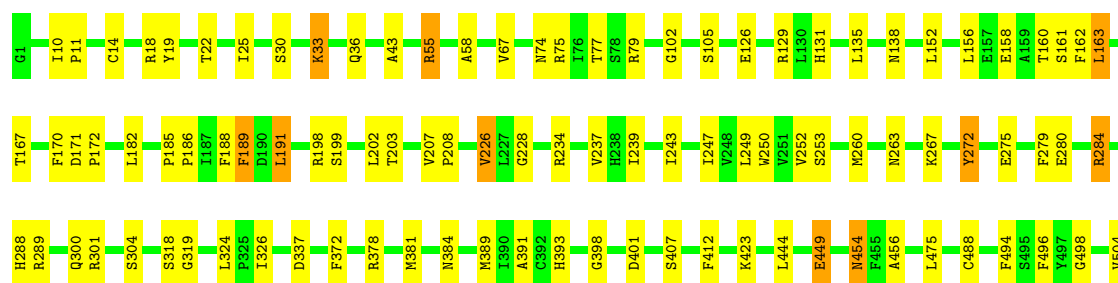
• Molecule 1: COAT PROTEIN

Chain AN: 79% 19% .



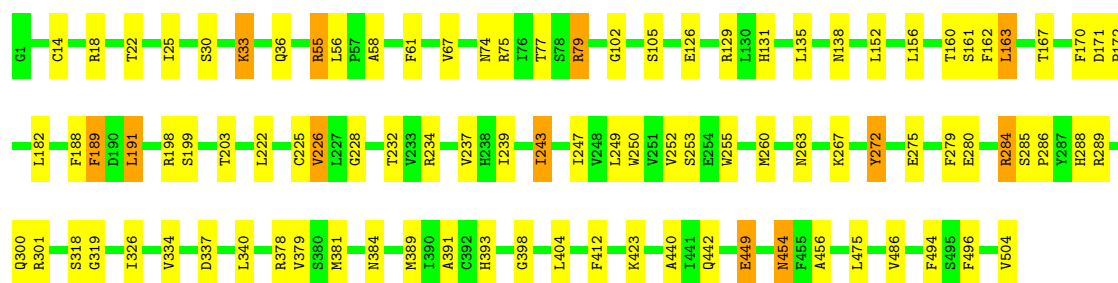
• Molecule 1: COAT PROTEIN

Chain AO: 80% 18% .



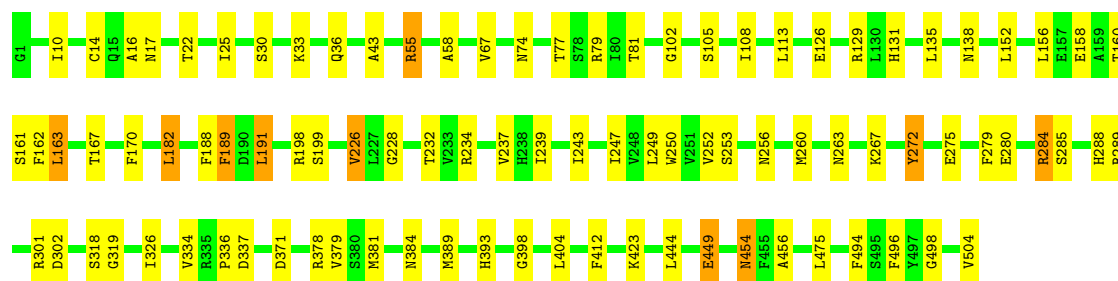
• Molecule 1: COAT PROTEIN

Chain AP: 81% 17% .



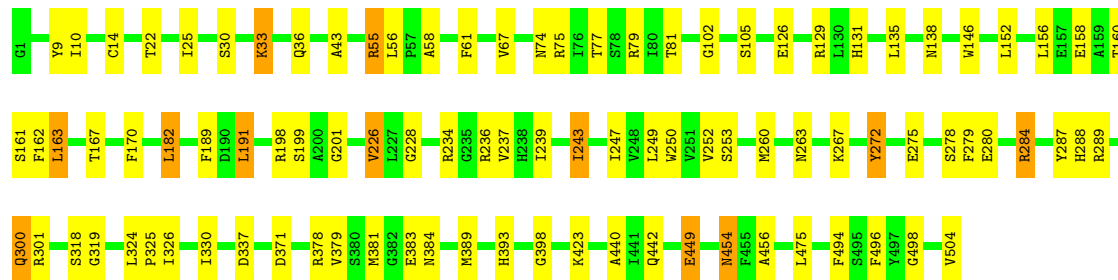
• Molecule 1: COAT PROTEIN

Chain AQ: 82% 16% .



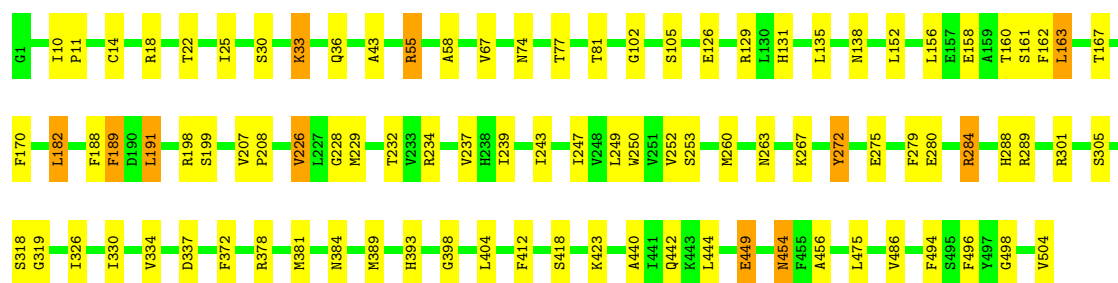
• Molecule 1: COAT PROTEIN

Chain AR: 81% 16% .



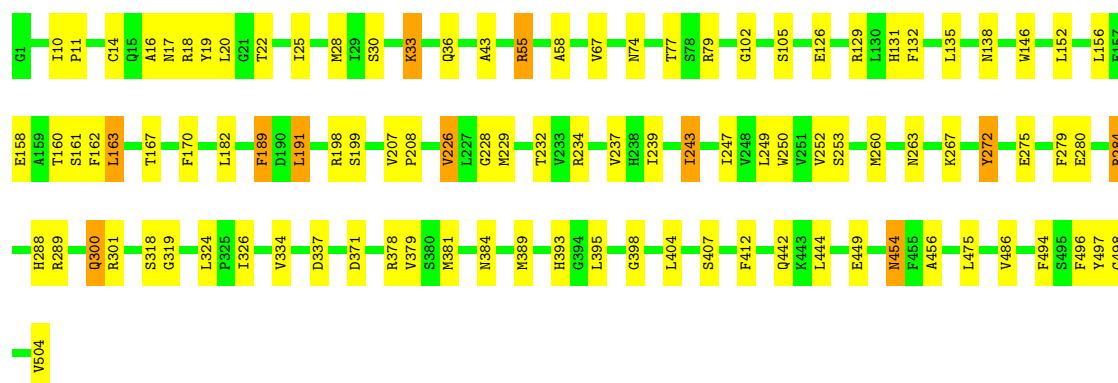
• Molecule 1: COAT PROTEIN

Chain AS: 81% 16% .



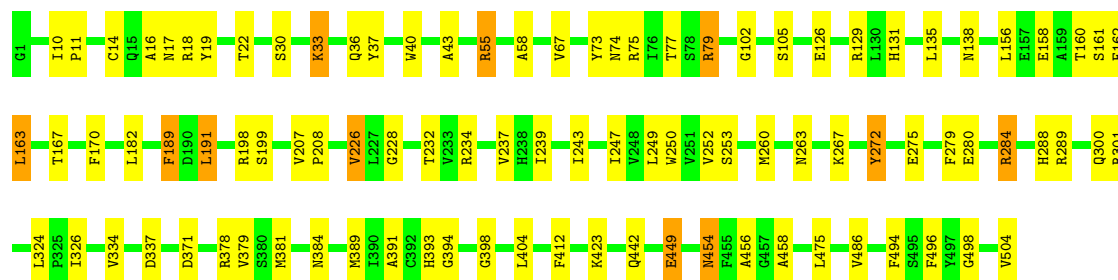
• Molecule 1: COAT PROTEIN

Chain AT: 80% 18% .



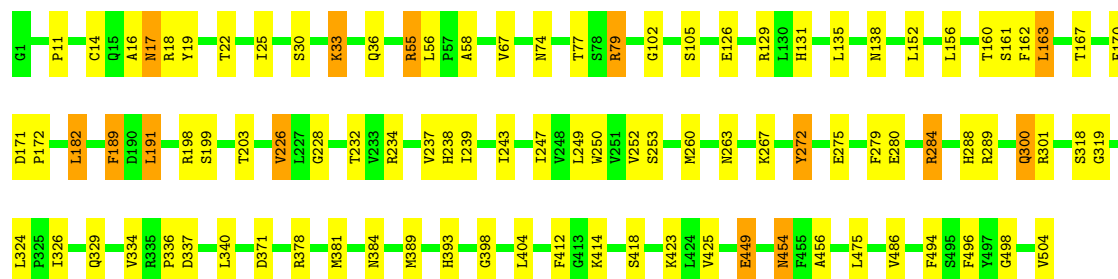
• Molecule 1: COAT PROTEIN

Chain BA: 81% 17% .

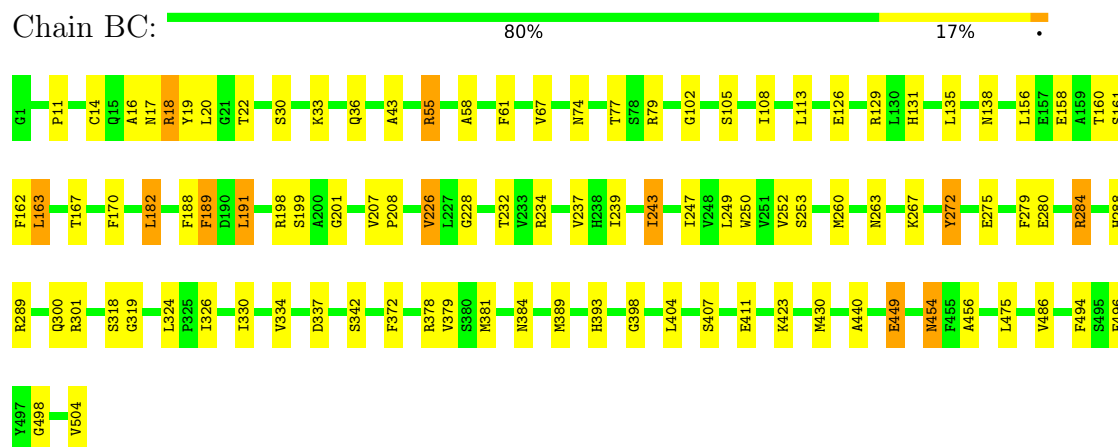


• Molecule 1: COAT PROTEIN

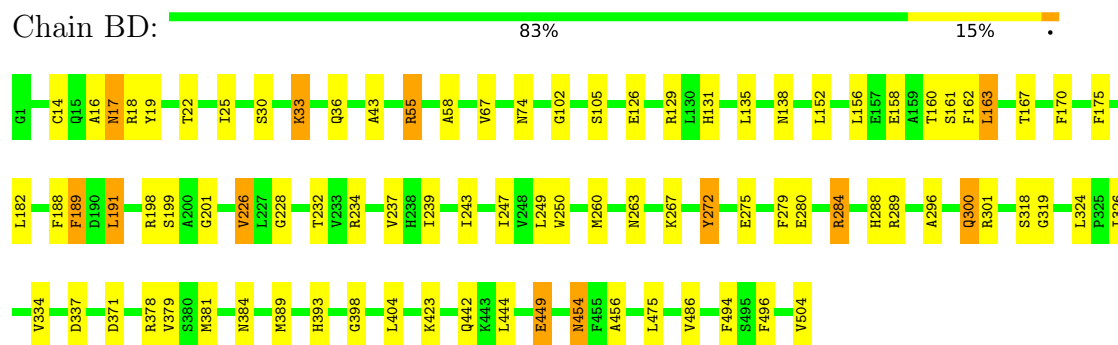
Chain BB: 81% 16% .



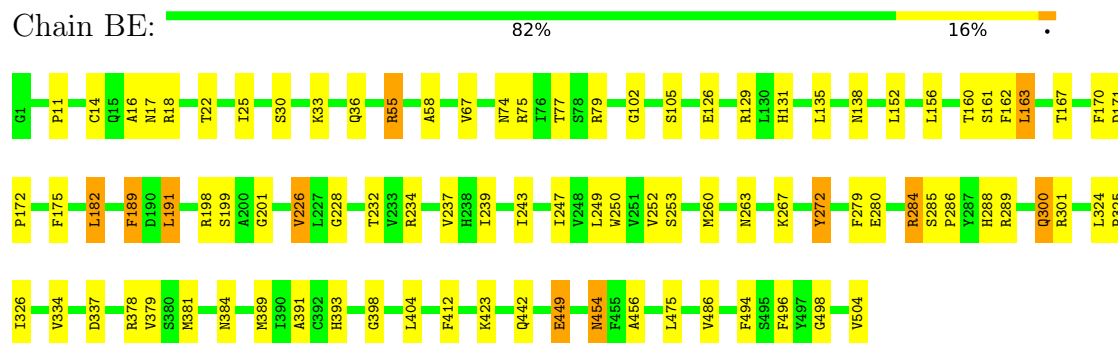
• Molecule 1: COAT PROTEIN



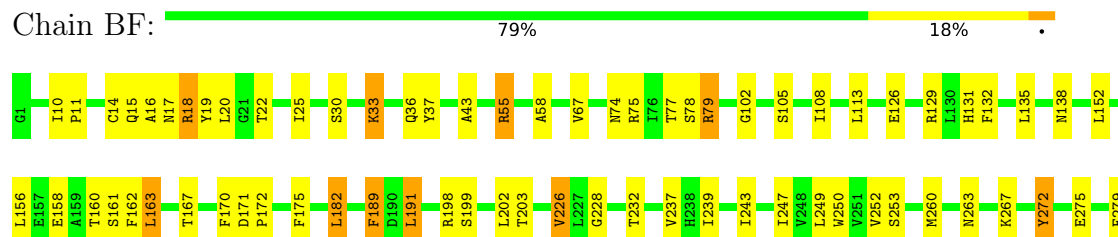
## • Molecule 1: COAT PROTEIN



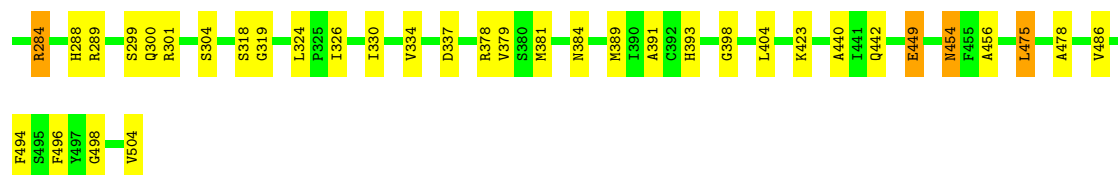
## • Molecule 1: COAT PROTEIN



## • Molecule 1: COAT PROTEIN

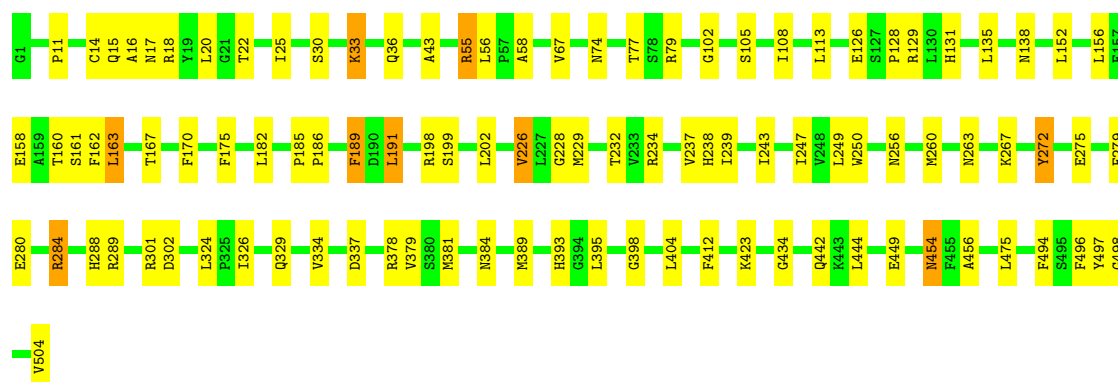






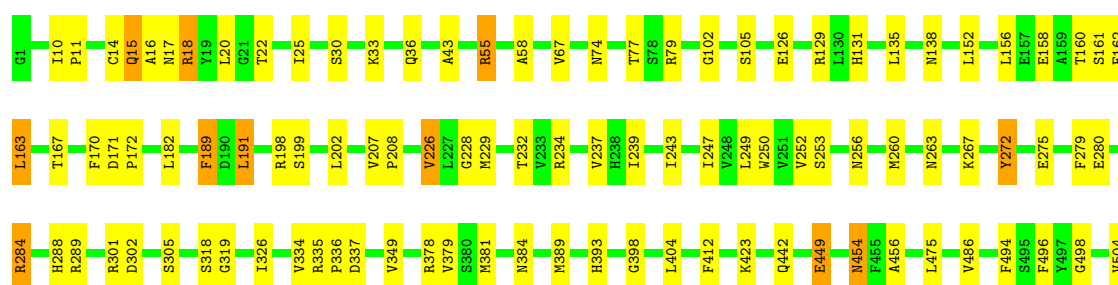
• Molecule 1: COAT PROTEIN

Chain BG: 80% 18%



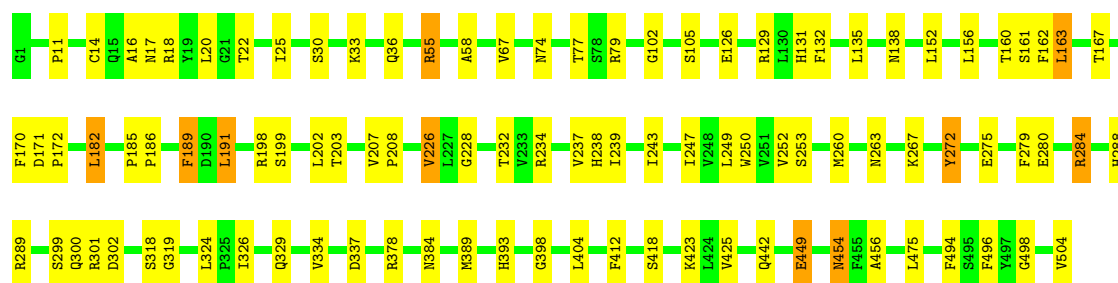
• Molecule 1: COAT PROTEIN

Chain BH: 80% 18%



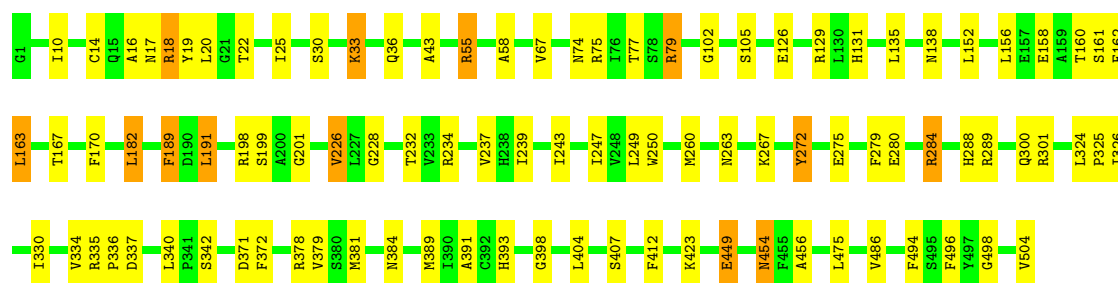
• Molecule 1: COAT PROTEIN

Chain BI: 80% 18%



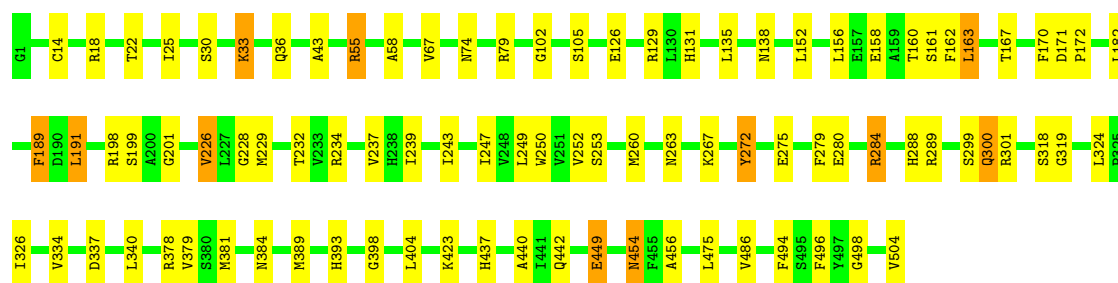
• Molecule 1: COAT PROTEIN

Chain BJ: 81% 17%



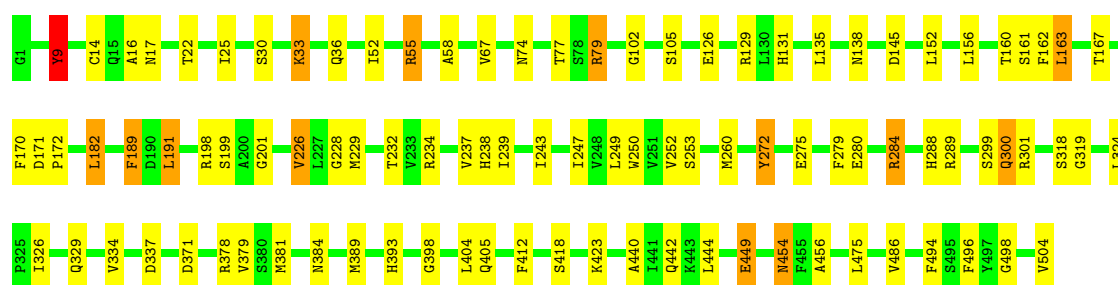
• Molecule 1: COAT PROTEIN

Chain BK: 82% 16% .



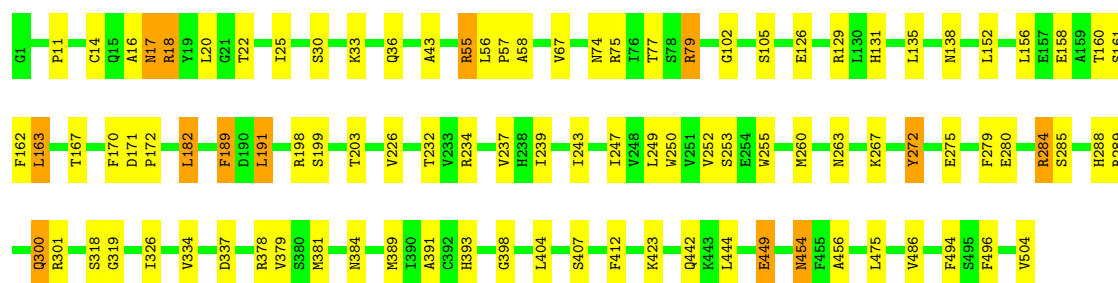
• Molecule 1: COAT PROTEIN

Chain BL: 81% 16% .



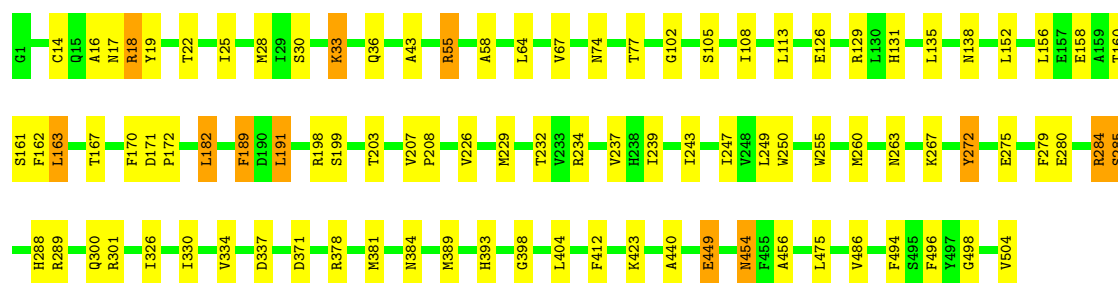
• Molecule 1: COAT PROTEIN

Chain BM: 81% 17% .



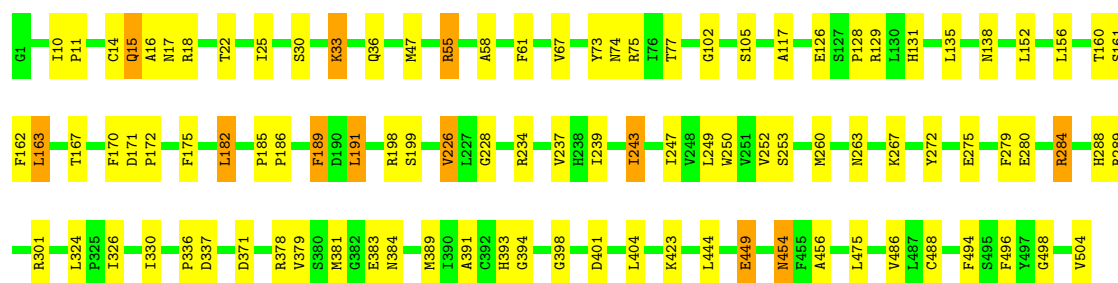
• Molecule 1: COAT PROTEIN

Chain BN: 81% 16% .



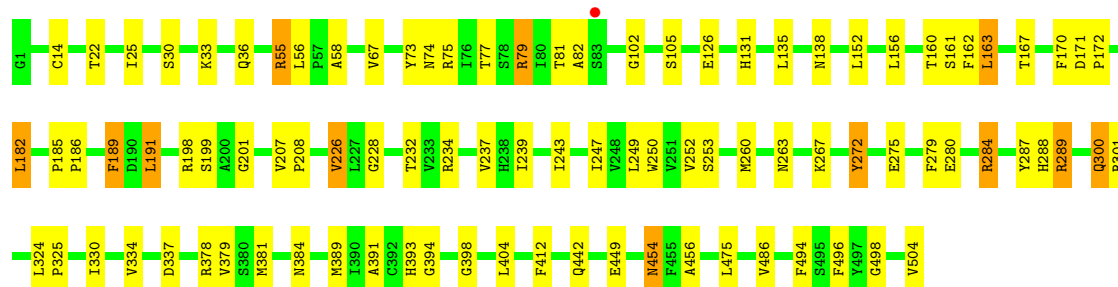
• Molecule 1: COAT PROTEIN

Chain BO: 80% 17% .



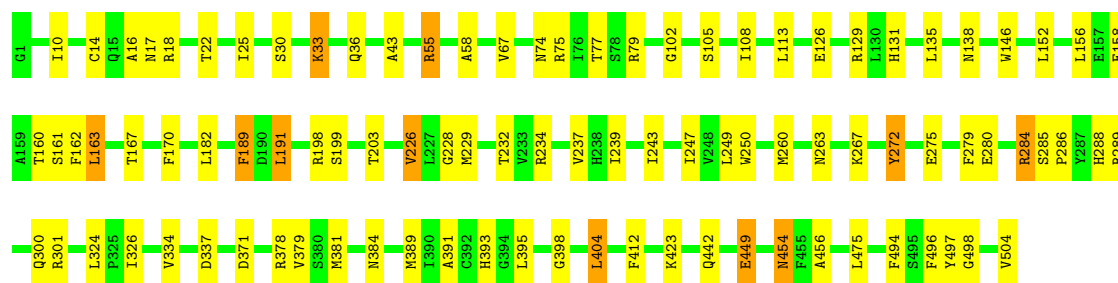
• Molecule 1: COAT PROTEIN

Chain BP: 81% 16% .



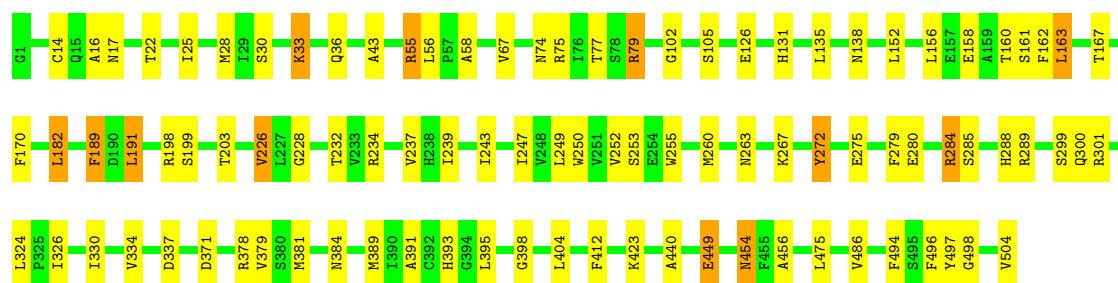
• Molecule 1: COAT PROTEIN

Chain BQ: 81% 17% .

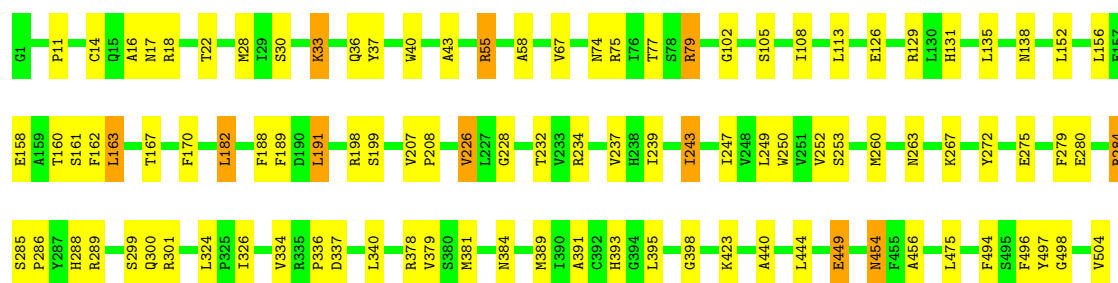
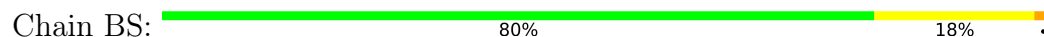


• Molecule 1: COAT PROTEIN

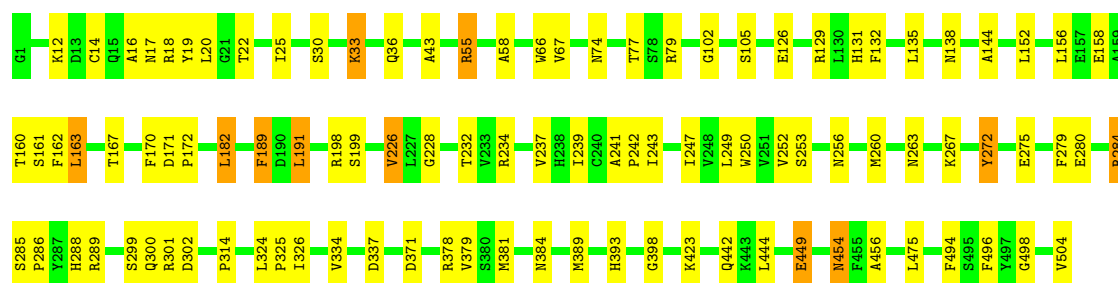
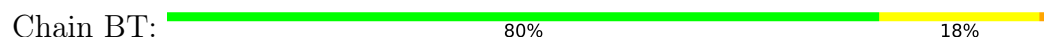
Chain BR: 81% 16% .



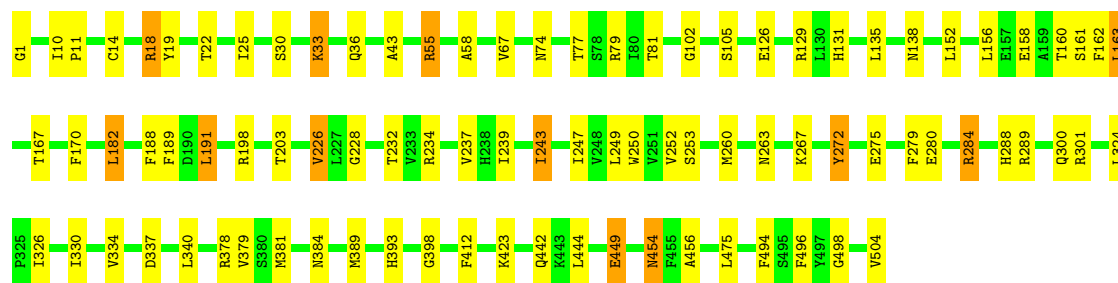
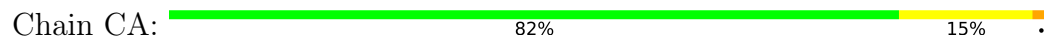
• Molecule 1: COAT PROTEIN



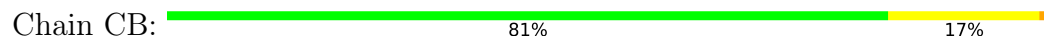
• Molecule 1: COAT PROTEIN

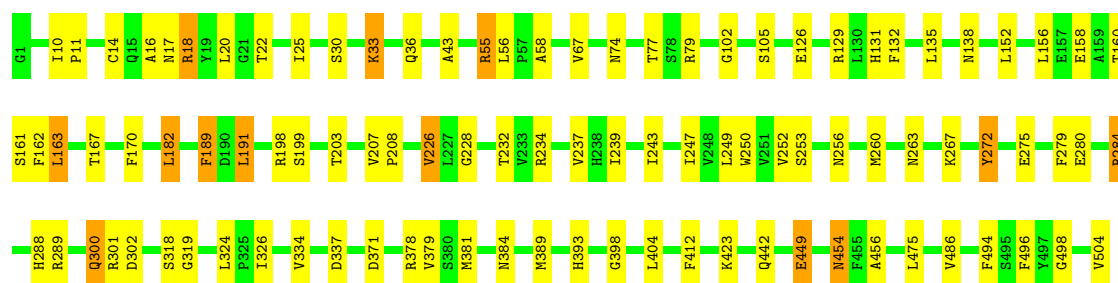


• Molecule 1: COAT PROTEIN



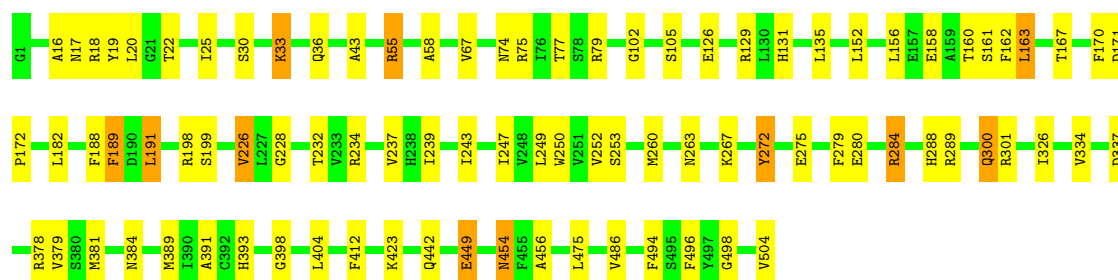
• Molecule 1: COAT PROTEIN





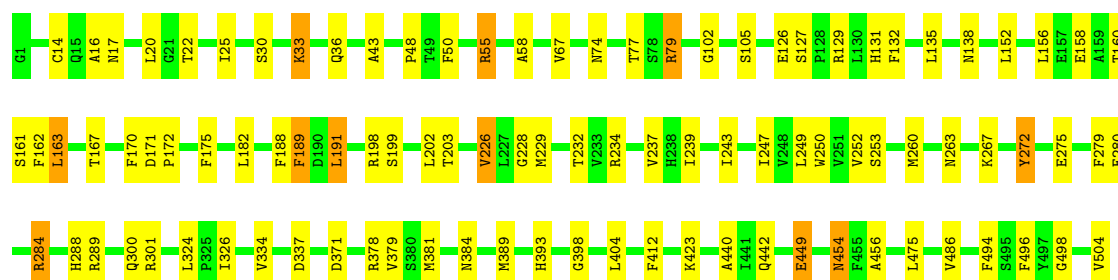
• Molecule 1: COAT PROTEIN

Chain CC: 82% 15% .



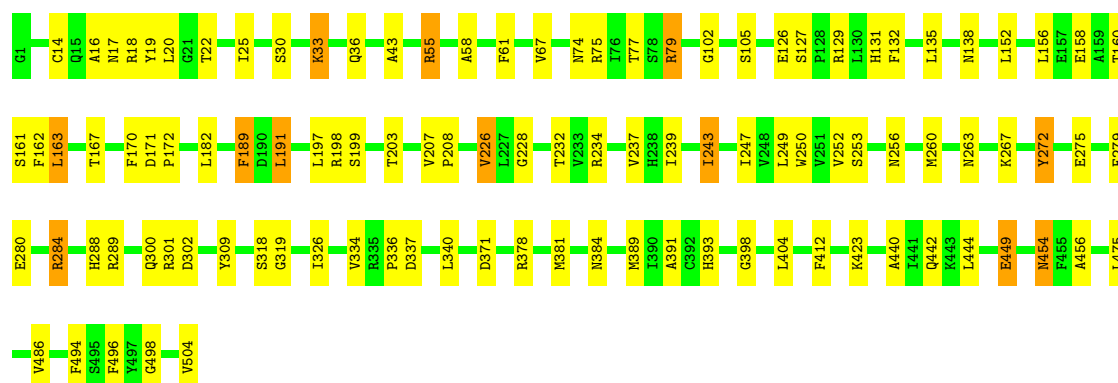
• Molecule 1: COAT PROTEIN

Chain CD: 81% 17% .

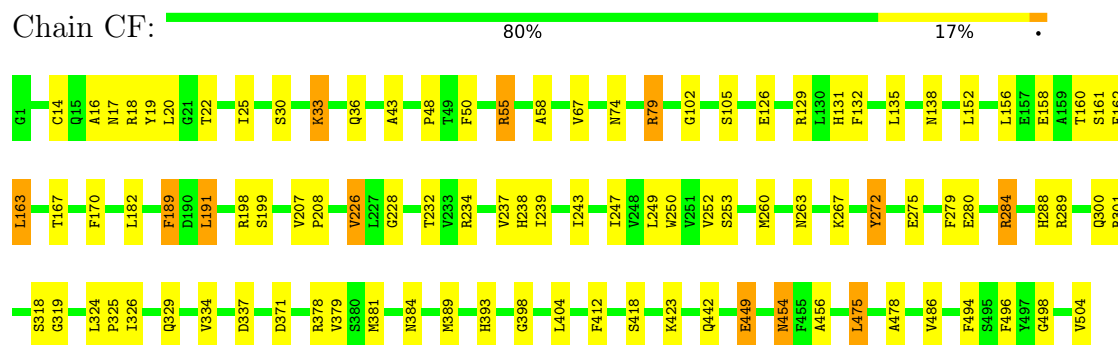


• Molecule 1: COAT PROTEIN

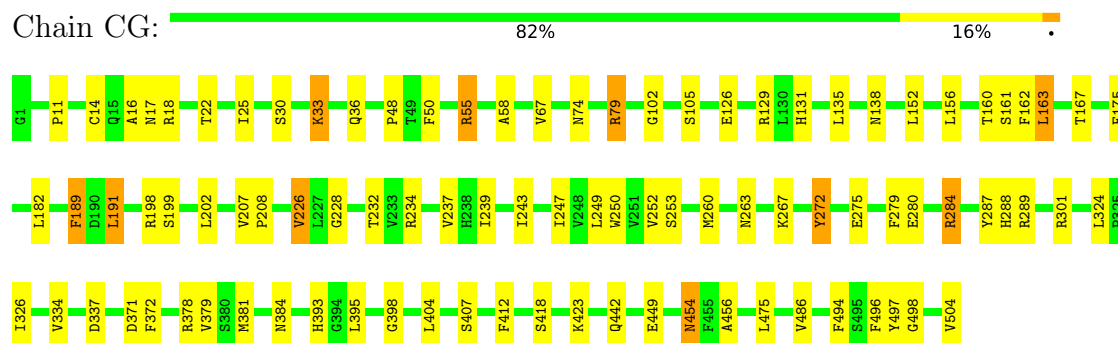
Chain CE: 79% 19% .



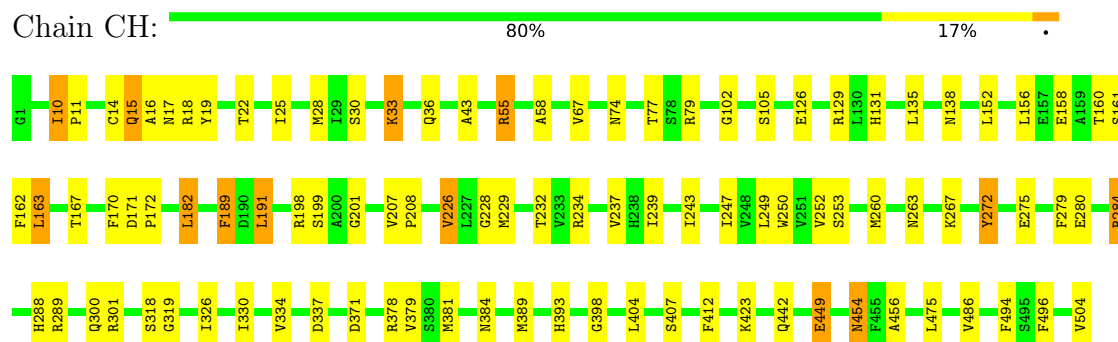
• Molecule 1: COAT PROTEIN



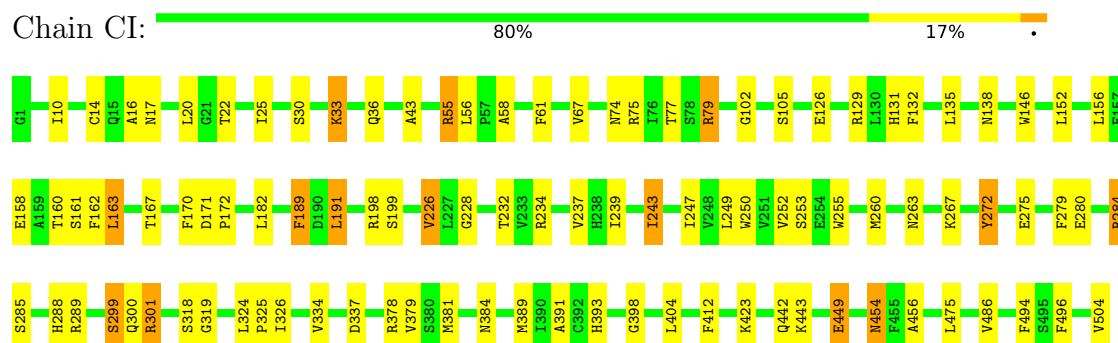
• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN



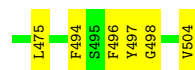
• Molecule 1: COAT PROTEIN

S318	G1
G319	C14
L324	G15
F325	A16
I326	N17
V334	R18
D337	Y19
F372	G21
R378	L20
V379	T22
S380	I25
M381	S30
N384	K33
M389	Q36
L390	A43
A391	R55
G392	L56
H393	P57
G398	A58
L404	V67
F412	N74
K423	R75
Q442	T77
E449	S78
M454	R79
F455	G102
A456	S105
L475	E126
V486	R129
F494	L130
S495	H131
F496	F132
Y497	L135
G498	N138
V504	L152
	L156
	E157
	A158
	A159
	T160
	S161
	F162
L163	
F170	
D171	
P172	
L182	
F189	
G190	
L191	
R198	
S199	
V207	
P208	
V226	
L227	
G228	
T232	
V233	
R234	
V237	
H238	
I239	
I243	
I247	
V248	
L249	
W250	
V251	
V252	
S253	
M260	
N263	
K267	
Y272	
E275	
F279	
E280	
R284	
H288	
R289	
Q300	
R301	

F279	L152	G1
E280	L156	Y9
R284	E157	I10
	E158	P11
H288	A159	K12
R289	T160	D13
	S161	C14
	F162	Q15
Q300	L163	A16
R301		N17
	T167	R18
I326	F170	T22
V334	D171	
	P172	I25
D337		
	F175	S30
R378	L182	K33
S380	F188	Q36
M381	F189	
N384	D190	A43
	L191	
M389	R198	R55
H393	S199	A58
G394		
L395	V226	V67
	L227	
G398	G228	N74
S407	T232	T77
	V233	S78
F412	R234	R79
K423	V237	G102
	H238	
Q442	I239	S105
K443		
L444	I243	I108
E449	I247	L113
	V248	
N454	T249	E126
F455	V250	
A456	V251	R129
	V252	L130
L475	S253	H131
F484	M260	L135
A485		
F486	N263	N138
Y487		
G488	K267	A144
V504	Y272	V146
		Q147
	F375	

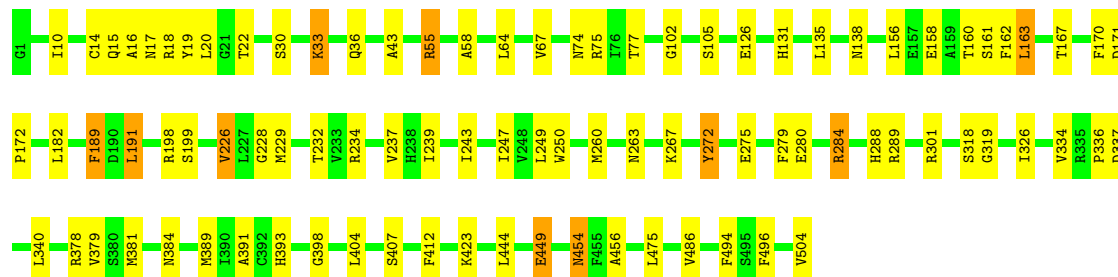
V334	L182	G1
D337	F188	Y9
	F189	I10
	D190	P11
R378	L191	C14
V379	R198	T22
S380	S199	
M381	L202	S30
N384	T203	R33
M389	V207	Q36
H393	P208	
	V226	A43
G398	L227	R55
L404	G228	L56
	M229	P57
F412	T232	A58
K423	V233	L64
	R234	
A440	V237	V67
I441	H238	
Q442	I239	N74
E449	T243	R79
M454	I247	G102
F455	V248	S105
A456	L249	
L475	H250	E126
	V251	R129
F494	S253	L130
S495	F259	H131
F496	M260	
Y497		L135
G498	Y272	N138
	E275	
V504		L156
	F279	E157
	E280	E158
	R284	A159
	H288	T160
	R289	S161
		F162
	S299	L163
	Q300	T167
	R301	
	L324	F170
	P325	L171
	T326	P172

R284	L163	G1
H288	T167	I10
R289	F170	C14
	D171	R15
S289	P172	A16
Q300		N17
R301	L182	R18
D302	F189	V19
	D190	L20
S318	L191	G21
G319		T22
L324	R198	S30
P325	S199	
I326	A200	K33
V334	G201	
D337	V207	Q36
	P208	R55
L340	V226	L56
R378	L227	P57
S380	G228	A58
M381		
N384	T232	V67
M389	V233	N74
A391	R234	R75
C392	V237	I76
H393	H238	S78
G394	L239	R79
L396	C240	I80
	A241	T81
	P242	
	I243	G102
	L247	S105
G398	V248	
L404	L249	I108
	W250	
	V251	L113
F412	V252	
	S253	E126
S418		
	N256	R129
K423	M260	L130
A440		H131
I441	N263	F132
K442		
K443	K267	L135
L444		
	Y272	N138
E449	E275	L156
N454		T160
F455	F279	E162
A556		



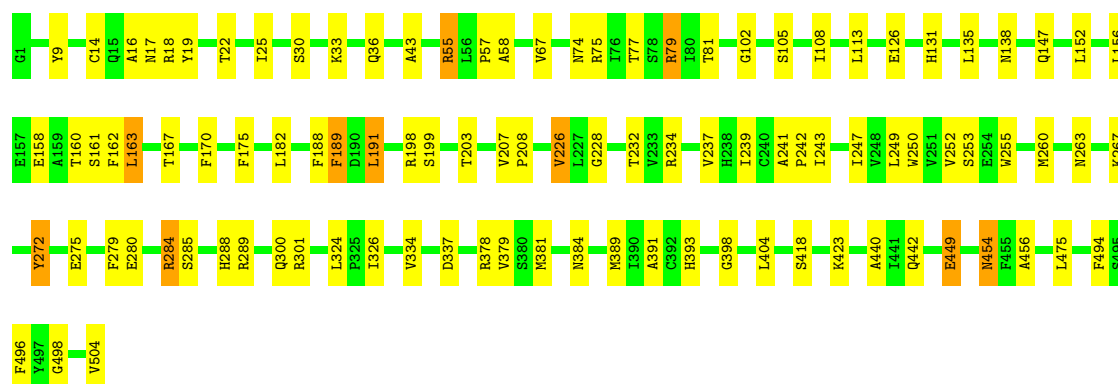
## • Molecule 1: COAT PROTEIN

Chain CN: 82% 16%



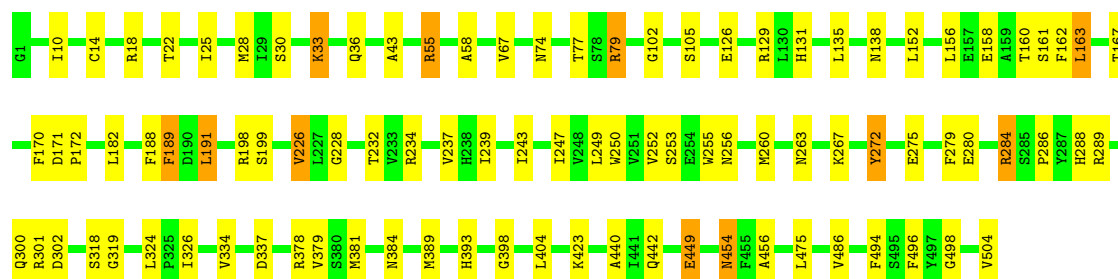
## • Molecule 1: COAT PROTEIN

Chain CO: 80% 18%



## • Molecule 1: COAT PROTEIN

Chain CP: 81% 16%

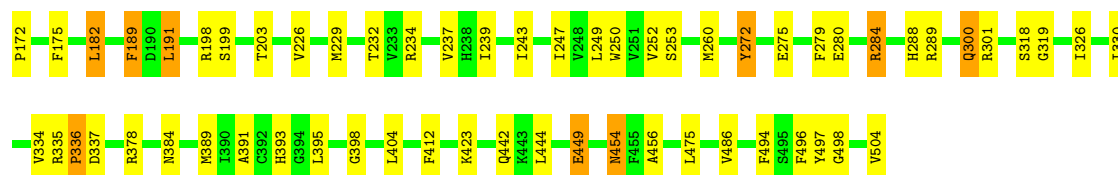


## • Molecule 1: COAT PROTEIN

Chain CQ: 82% 16%

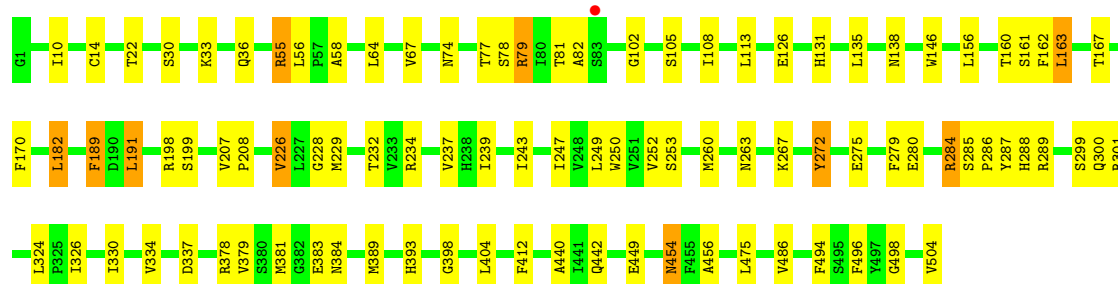






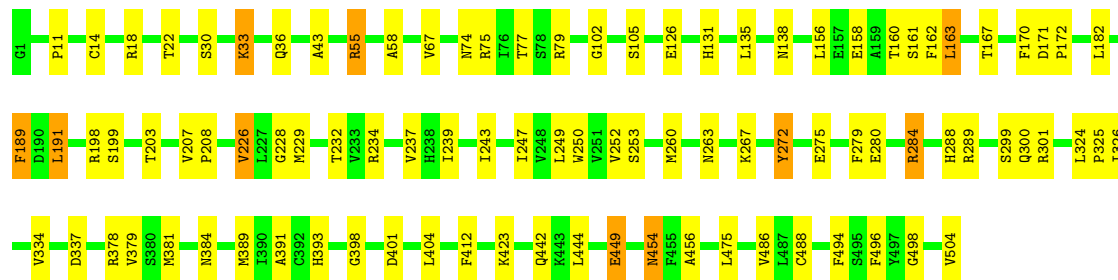
• Molecule 1: COAT PROTEIN

Chain CR: 81% 17% .



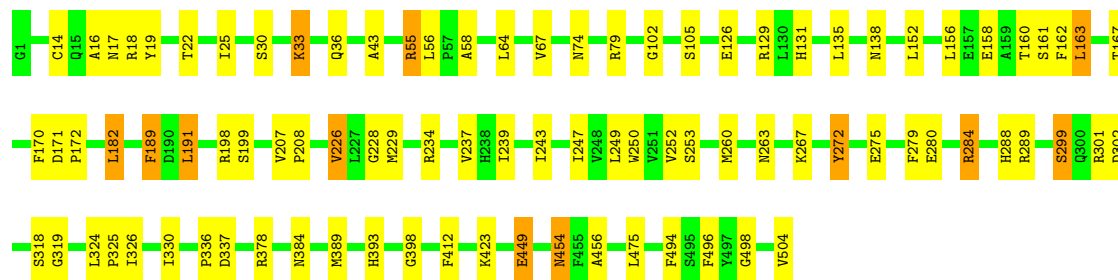
• Molecule 1: COAT PROTEIN

Chain CS: 81% 17% .



• Molecule 1: COAT PROTEIN

Chain CT: 82% 16% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.190 , 0.207 0.187 , 0.204	Depositor DCC
$R_{free}$ test set	66376 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.61	2/5517 (0.0%)
1	AB	0.50	2/4058 (0.0%)	0.62	1/5517 (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	0.49	1/4058 (0.0%)	0.61	0/5517
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	0.48	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	0.52	2/4058 (0.0%)	0.63	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	0.49	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%)	0.62	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	0.51	1/4058 (0.0%)	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	0.50	1/4058 (0.0%)	0.62	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	1/4058 (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	0.53	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	0.50	95/243480 (0.0%)	0.62	20/331020 (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	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

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	-6.84	1.24	1.37
1	AL	189	PHE	CE1-CZ	-6.45	1.25	1.37
1	CJ	189	PHE	CE1-CZ	-6.29	1.25	1.37
1	BL	189	PHE	CE1-CZ	-6.29	1.25	1.37
1	BN	189	PHE	CE1-CZ	-6.23	1.25	1.37

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	284	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	CJ	56	LEU	CA-CB-CG	5.46	127.86	115.30
1	AF	56	LEU	CA-CB-CG	5.34	127.57	115.30
1	CT	56	LEU	CA-CB-CG	5.29	127.46	115.30
1	AR	56	LEU	CA-CB-CG	5.25	127.36	115.30

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	91	0
1	AB	3951	0	3909	89	0
1	AC	3951	0	3909	87	0
1	AD	3951	0	3909	93	0
1	AE	3951	0	3909	86	0
1	AF	3951	0	3909	92	0
1	AG	3951	0	3909	91	0
1	AH	3951	0	3909	90	0
1	AI	3951	0	3909	88	0
1	AJ	3951	0	3909	86	0
1	AK	3951	0	3909	88	0
1	AL	3951	0	3909	87	0
1	AM	3951	0	3909	83	0
1	AN	3951	0	3909	104	0
1	AO	3951	0	3909	91	0
1	AP	3951	0	3909	87	0
1	AQ	3951	0	3909	85	0
1	AR	3951	0	3909	88	0
1	AS	3951	0	3909	89	0
1	AT	3951	0	3909	91	0
1	BA	3951	0	3909	93	0
1	BB	3951	0	3909	97	0
1	BC	3951	0	3909	85	0
1	BD	3951	0	3909	78	0
1	BE	3951	0	3909	86	0
1	BF	3951	0	3909	92	0
1	BG	3951	0	3909	92	0
1	BH	3951	0	3909	97	0
1	BI	3951	0	3909	89	0
1	BJ	3951	0	3909	93	0
1	BK	3951	0	3909	81	0
1	BL	3951	0	3909	89	0
1	BM	3951	0	3909	89	0
1	BN	3951	0	3909	80	0
1	BO	3951	0	3909	93	0
1	BP	3951	0	3909	93	0
1	BQ	3951	0	3909	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	3951	0	3909	90	0
1	BS	3951	0	3909	87	0
1	BT	3951	0	3909	87	0
1	CA	3951	0	3909	81	0
1	CB	3951	0	3909	87	0
1	CC	3951	0	3909	84	0
1	CD	3951	0	3909	89	0
1	CE	3951	0	3909	97	0
1	CF	3951	0	3909	94	0
1	CG	3951	0	3909	92	0
1	CH	3951	0	3909	91	0
1	CI	3951	0	3909	92	0
1	CJ	3951	0	3909	94	0
1	CK	3951	0	3909	84	0
1	CL	3951	0	3909	81	0
1	CM	3951	0	3909	93	0
1	CN	3951	0	3909	81	0
1	CO	3951	0	3909	96	0
1	CP	3951	0	3909	85	0
1	CQ	3951	0	3909	85	0
1	CR	3951	0	3909	86	0
1	CS	3951	0	3909	86	0
1	CT	3951	0	3909	76	0
All	All	237060	0	234540	4775	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 10.

The worst 5 of 4775 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:HG3	1:CF:79:ARG:HH11	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%)	49	85
1	AB	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	AC	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	36	76
1	AD	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AE	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85
1	AF	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AG	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	36	76
1	AH	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	36	76
1	AI	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	AJ	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85
1	AK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	AL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	AM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85
1	AN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85
1	AO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	AP	502/504 (100%)	483 (96%)	19 (4%)	0	100	100
1	AQ	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	AR	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	49	85
1	AS	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85
1	AT	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	49	85
1	BA	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85
1	BB	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	36	76
1	BC	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85
1	BD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	BE	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BF	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	36	76
1	BG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85
1	BH	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	49	85
1	BI	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	49	85
1	BJ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85
1	BK	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	49	85
1	BL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	BM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85
1	BN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85
1	BO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	BP	502/504 (100%)	479 (95%)	21 (4%)	2 (0%)	36	76
1	BQ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85
1	BR	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85
1	BS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85
1	BT	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	CA	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	CB	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	CC	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85
1	CD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	CE	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	49	85
1	CF	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85
1	CG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85
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%)	49	85
1	CK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	49	85
1	CL	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85
1	CM	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	36	76
1	CN	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	CO	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85
1	CP	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	49	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CQ	502/504 (100%)	482 (96%)	18 (4%)	2 (0%)	36	76
1	CR	502/504 (100%)	478 (95%)	22 (4%)	2 (0%)	36	76
1	CS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	49	85
1	CT	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	49	85
All	All	30120/30240 (100%)	28870 (96%)	1187 (4%)	63 (0%)	49	85

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%)	25	62
1	AB	430/430 (100%)	404 (94%)	26 (6%)	21	57
1	AC	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	AD	430/430 (100%)	404 (94%)	26 (6%)	21	57
1	AE	430/430 (100%)	409 (95%)	21 (5%)	27	66
1	AF	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	AG	430/430 (100%)	405 (94%)	25 (6%)	22	59
1	AH	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	AI	430/430 (100%)	404 (94%)	26 (6%)	21	57
1	AJ	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	AK	430/430 (100%)	404 (94%)	26 (6%)	21	57
1	AL	430/430 (100%)	404 (94%)	26 (6%)	21	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AM	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	AN	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	AO	430/430 (100%)	408 (95%)	22 (5%)	26	64
1	AP	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	AQ	430/430 (100%)	405 (94%)	25 (6%)	22	59
1	AR	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	AS	430/430 (100%)	405 (94%)	25 (6%)	22	59
1	AT	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	BA	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	BB	430/430 (100%)	405 (94%)	25 (6%)	22	59
1	BC	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	BD	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	BE	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	BF	430/430 (100%)	404 (94%)	26 (6%)	21	57
1	BG	430/430 (100%)	408 (95%)	22 (5%)	26	64
1	BH	430/430 (100%)	404 (94%)	26 (6%)	21	57
1	BI	430/430 (100%)	408 (95%)	22 (5%)	26	64
1	BJ	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	BK	430/430 (100%)	404 (94%)	26 (6%)	21	57
1	BL	430/430 (100%)	403 (94%)	27 (6%)	20	55
1	BM	430/430 (100%)	404 (94%)	26 (6%)	21	57
1	BN	430/430 (100%)	405 (94%)	25 (6%)	22	59
1	BO	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	BP	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	BQ	430/430 (100%)	405 (94%)	25 (6%)	22	59
1	BR	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	BS	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	BT	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	CA	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	CB	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	CC	430/430 (100%)	407 (95%)	23 (5%)	25	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	CE	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	CF	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	CG	430/430 (100%)	408 (95%)	22 (5%)	26	64
1	CH	430/430 (100%)	405 (94%)	25 (6%)	22	59
1	CI	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	CJ	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	CK	430/430 (100%)	406 (94%)	24 (6%)	23	60
1	CL	430/430 (100%)	405 (94%)	25 (6%)	22	59
1	CM	430/430 (100%)	403 (94%)	27 (6%)	20	55
1	CN	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	CO	430/430 (100%)	408 (95%)	22 (5%)	26	64
1	CP	430/430 (100%)	405 (94%)	25 (6%)	22	59
1	CQ	430/430 (100%)	404 (94%)	26 (6%)	21	57
1	CR	430/430 (100%)	405 (94%)	25 (6%)	22	59
1	CS	430/430 (100%)	407 (95%)	23 (5%)	25	62
1	CT	430/430 (100%)	405 (94%)	25 (6%)	22	59
All	All	25800/25800 (100%)	24352 (94%)	1448 (6%)	23	60

5 of 1448 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BH	163	LEU
1	BN	226	VAL
1	CP	272	TYR
1	BH	504	VAL
1	BK	272	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 662 such sidechains are listed below:

Mol	Chain	Res	Type
1	BG	288	HIS
1	BN	74	ASN
1	CP	256	ASN
1	BH	238	HIS

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Mol	Chain	Res	Type
1	BK	74	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 ⓘ

### 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, 95<sup>th</sup> 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(Å²)	Q<0.9	
1	AA	504/504 (100%)	-0.59	0	100	100	23, 33, 53, 78	0
1	AB	504/504 (100%)	-0.62	0	100	100	22, 34, 54, 78	0
1	AC	504/504 (100%)	-0.58	0	100	100	23, 34, 54, 78	0
1	AD	504/504 (100%)	-0.59	0	100	100	22, 33, 52, 78	0
1	AE	504/504 (100%)	-0.53	0	100	100	17, 31, 52, 77	0
1	AF	504/504 (100%)	-0.63	0	100	100	24, 34, 54, 80	0
1	AG	504/504 (100%)	-0.62	0	100	100	23, 34, 55, 80	0
1	AH	504/504 (100%)	-0.62	0	100	100	24, 35, 56, 79	0
1	AI	504/504 (100%)	-0.61	0	100	100	23, 34, 55, 80	0
1	AJ	504/504 (100%)	-0.57	0	100	100	22, 34, 54, 80	0
1	AK	504/504 (100%)	-0.61	0	100	100	23, 34, 55, 79	0
1	AL	504/504 (100%)	-0.57	0	100	100	23, 33, 54, 77	0
1	AM	504/504 (100%)	-0.58	0	100	100	21, 32, 52, 77	0
1	AN	504/504 (100%)	-0.55	0	100	100	22, 33, 54, 78	0
1	AO	504/504 (100%)	-0.53	0	100	100	21, 33, 54, 80	0
1	AP	504/504 (100%)	-0.55	0	100	100	19, 32, 53, 79	0
1	AQ	504/504 (100%)	-0.61	0	100	100	23, 33, 54, 77	0
1	AR	504/504 (100%)	-0.57	0	100	100	21, 32, 52, 77	0
1	AS	504/504 (100%)	-0.59	0	100	100	23, 33, 54, 80	0
1	AT	504/504 (100%)	-0.55	0	100	100	22, 33, 54, 77	0
1	BA	504/504 (100%)	-0.59	0	100	100	23, 33, 54, 79	0
1	BB	504/504 (100%)	-0.59	0	100	100	23, 34, 55, 77	0
1	BC	504/504 (100%)	-0.60	0	100	100	23, 34, 54, 78	0
1	BD	504/504 (100%)	-0.57	0	100	100	23, 34, 54, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	BE	504/504 (100%)	-0.58	0	100	100	23, 33, 54, 77	0
1	BF	504/504 (100%)	-0.54	0	100	100	22, 35, 56, 80	0
1	BG	504/504 (100%)	-0.62	0	100	100	22, 34, 54, 79	0
1	BH	504/504 (100%)	-0.61	0	100	100	21, 33, 54, 75	0
1	BI	504/504 (100%)	-0.53	0	100	100	22, 32, 54, 78	0
1	BJ	504/504 (100%)	-0.60	0	100	100	22, 34, 54, 79	0
1	BK	504/504 (100%)	-0.61	0	100	100	22, 33, 53, 77	0
1	BL	504/504 (100%)	-0.57	0	100	100	21, 32, 52, 75	0
1	BM	504/504 (100%)	-0.51	0	100	100	21, 32, 52, 77	0
1	BN	504/504 (100%)	-0.57	0	100	100	20, 33, 53, 76	0
1	BO	504/504 (100%)	-0.58	0	100	100	22, 33, 53, 80	0
1	BP	504/504 (100%)	-0.50	1 (0%)	94	86	21, 32, 53, 76	0
1	BQ	504/504 (100%)	-0.57	0	100	100	22, 33, 54, 80	0
1	BR	504/504 (100%)	-0.60	0	100	100	22, 33, 54, 79	0
1	BS	504/504 (100%)	-0.57	0	100	100	22, 33, 54, 80	0
1	BT	504/504 (100%)	-0.61	0	100	100	22, 34, 53, 77	0
1	CA	504/504 (100%)	-0.61	0	100	100	23, 35, 56, 80	0
1	CB	504/504 (100%)	-0.64	0	100	100	23, 34, 54, 77	0
1	CC	504/504 (100%)	-0.61	0	100	100	23, 34, 54, 81	0
1	CD	504/504 (100%)	-0.60	0	100	100	23, 34, 54, 79	0
1	CE	504/504 (100%)	-0.61	0	100	100	23, 33, 54, 78	0
1	CF	504/504 (100%)	-0.61	0	100	100	23, 34, 55, 80	0
1	CG	504/504 (100%)	-0.58	0	100	100	24, 34, 55, 81	0
1	CH	504/504 (100%)	-0.60	0	100	100	24, 34, 55, 79	0
1	CI	504/504 (100%)	-0.59	0	100	100	23, 33, 53, 79	0
1	CJ	504/504 (100%)	-0.57	0	100	100	24, 33, 54, 79	0
1	CK	504/504 (100%)	-0.54	0	100	100	21, 34, 54, 79	0
1	CL	504/504 (100%)	-0.61	0	100	100	22, 33, 54, 77	0
1	CM	504/504 (100%)	-0.57	0	100	100	22, 32, 53, 79	0
1	CN	504/504 (100%)	-0.57	0	100	100	22, 32, 54, 79	0
1	CO	504/504 (100%)	-0.56	0	100	100	23, 32, 54, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	CP	504/504 (100%)	-0.55	0 100 100	21, 31, 53, 78	0
1	CQ	504/504 (100%)	-0.56	0 100 100	21, 32, 53, 79	0
1	CR	504/504 (100%)	-0.47	1 (0%) 94 86	17, 31, 53, 75	0
1	CS	504/504 (100%)	-0.58	0 100 100	22, 32, 53, 78	0
1	CT	504/504 (100%)	-0.60	0 100 100	21, 32, 52, 77	0
All	All	30240/30240 (100%)	-0.58	2 (0%) 100 100	17, 33, 54, 81	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CR	83	SER	2.5
1	BP	83	SER	2.0

## 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 carbohydrates 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.