



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:32 PM GMT

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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

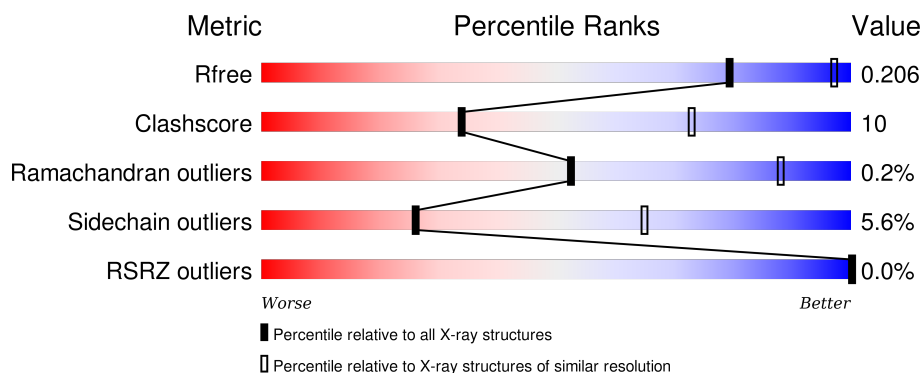
# 1 Overall quality at a glance ⓘ

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.













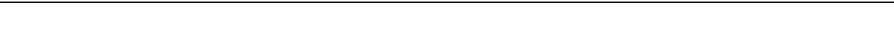

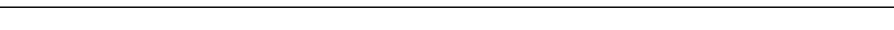
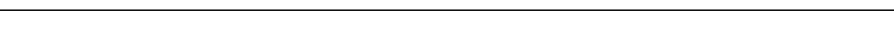











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	 81% 17% .
1	AG	504	 80% 16% .
1	AH	504	 81% 16% .
1	AI	504	 81% 16% .
1	AJ	504	 82% 16% .
1	AK	504	 80% 18% .
1	AL	504	 81% 17% .
1	AM	504	 82% 16% .
1	AN	504	 79% 19% .
1	AO	504	 80% 18% .
1	AP	504	 81% 17% .
1	AQ	504	 82% 16% .
1	AR	504	 81% 16% .
1	AS	504	 81% 16% .
1	AT	504	 80% 18% .
1	BA	504	 81% 17% .
1	BB	504	 81% 16% .
1	BC	504	 80% 17% .
1	BD	504	 83% 15% .
1	BE	504	 82% 16% .
1	BF	504	 79% 18% .
1	BG	504	 80% 18% .
1	BH	504	 80% 18% .
1	BI	504	 80% 18% .
1	BJ	504	 81% 17% .






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Mol	Chain	Length	Quality of chain
1	BK	504	 82% 16% .
1	BL	504	 81% 16% .
1	BM	504	 81% 17% .
1	BN	504	 81% 16% .
1	BO	504	 80% 17% .
1	BP	504	 81% 16% .
1	BQ	504	 81% 17% .
1	BR	504	 81% 16% .
1	BS	504	 80% 18% .
1	BT	504	 80% 18% .
1	CA	504	 82% 15% .
1	CB	504	 81% 17% .
1	CC	504	 82% 15% .
1	CD	504	 81% 17% .
1	CE	504	 79% 19% .
1	CF	504	 80% 17% .
1	CG	504	 82% 16% .
1	CH	504	 80% 17% .
1	CI	504	 80% 17% .
1	CJ	504	 81% 17% .
1	CK	504	 81% 17% .
1	CL	504	 82% 16% .
1	CM	504	 79% 19% .
1	CN	504	 82% 16% .
1	CO	504	 80% 18% .

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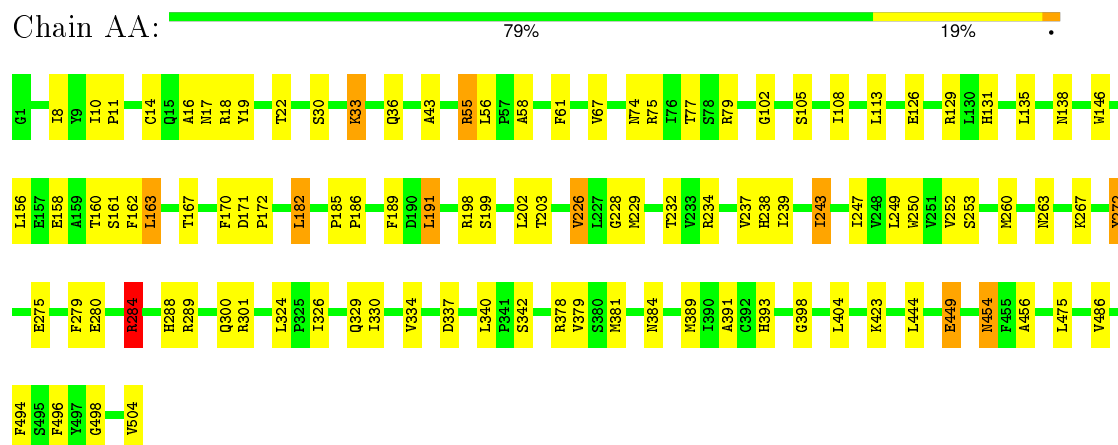
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CS	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			
1	CT	504	Total	C	N	O	S	0	0	0
			3951	2555	653	721	22			

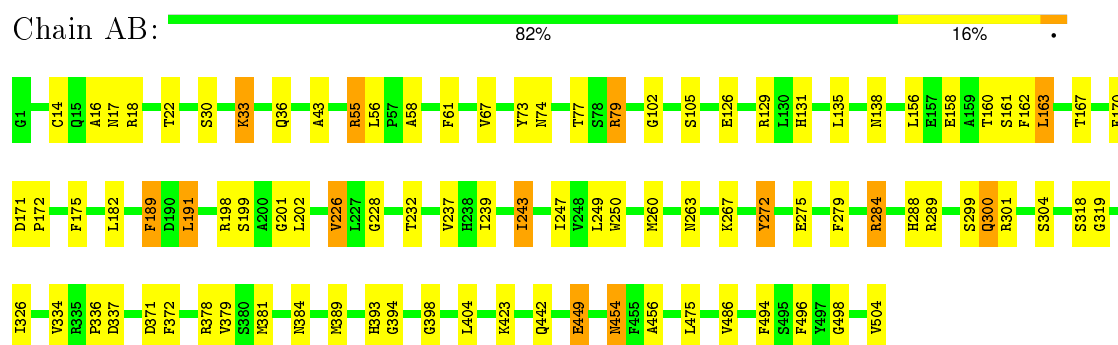
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

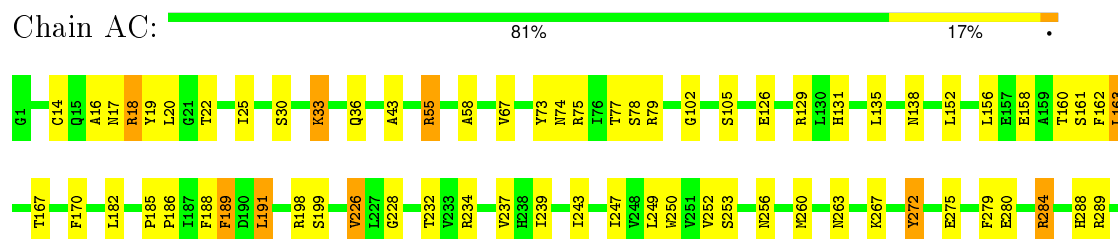
#### • Molecule 1: COAT PROTEIN



#### • Molecule 1: COAT PROTEIN



#### • Molecule 1: COAT PROTEIN

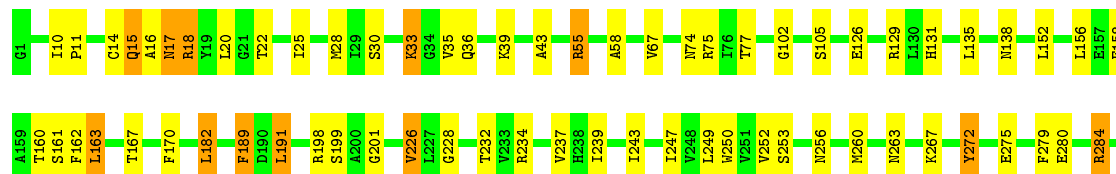






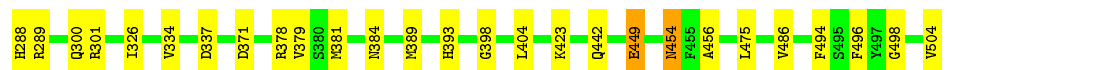
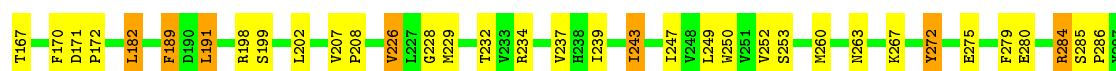
• Molecule 1: COAT PROTEIN

Chain AH: 81% 16% •



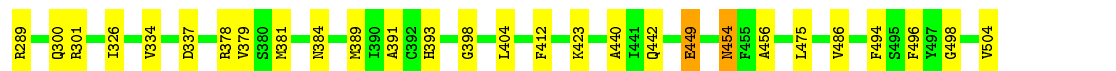
• Molecule 1: COAT PROTEIN

Chain AI: 81% 16% •



• Molecule 1: COAT PROTEIN

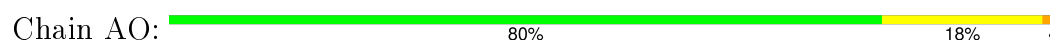
Chain AJ: 82% 16% •

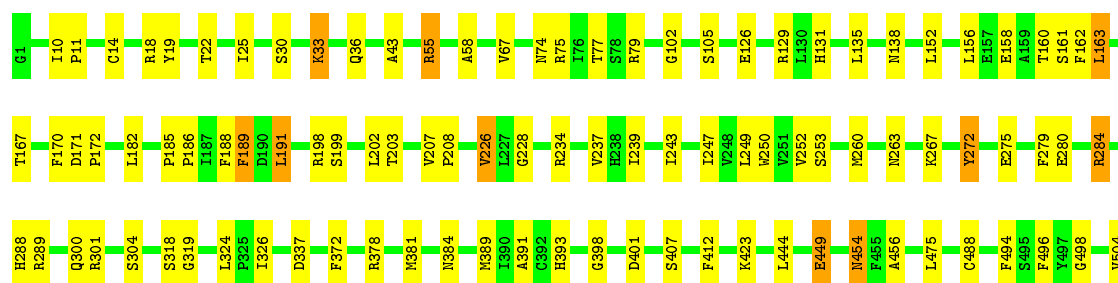


• Molecule 1: COAT PROTEIN

Chain AK: 80% 18% •

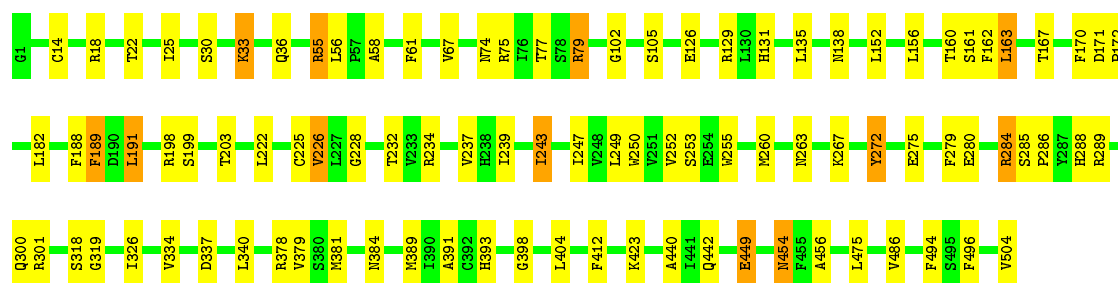






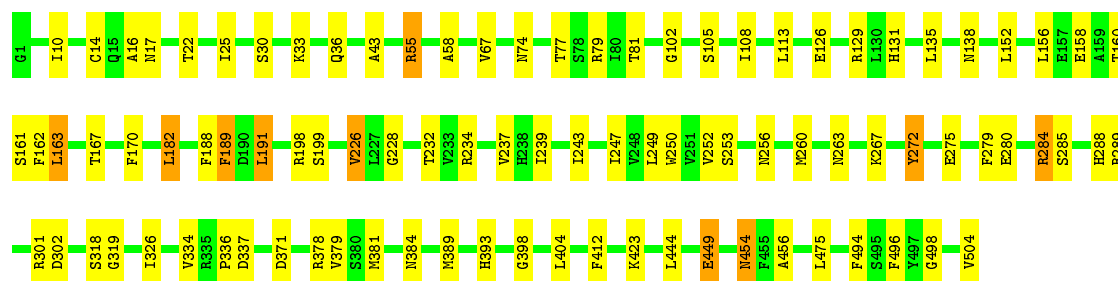
• Molecule 1: COAT PROTEIN

Chain AP: 81% 17% .



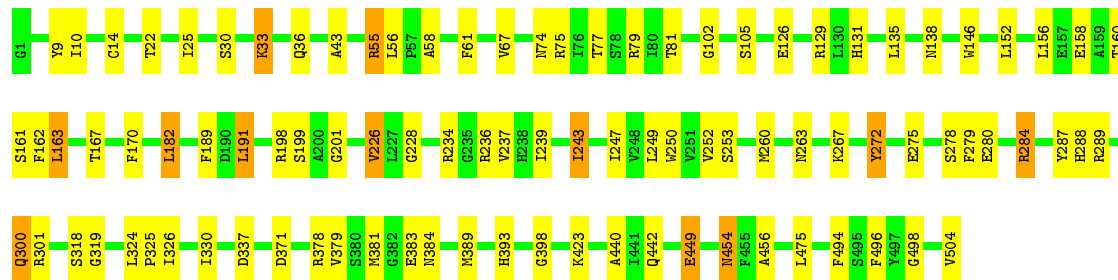
• Molecule 1: COAT PROTEIN

Chain AQ: 82% 16% .



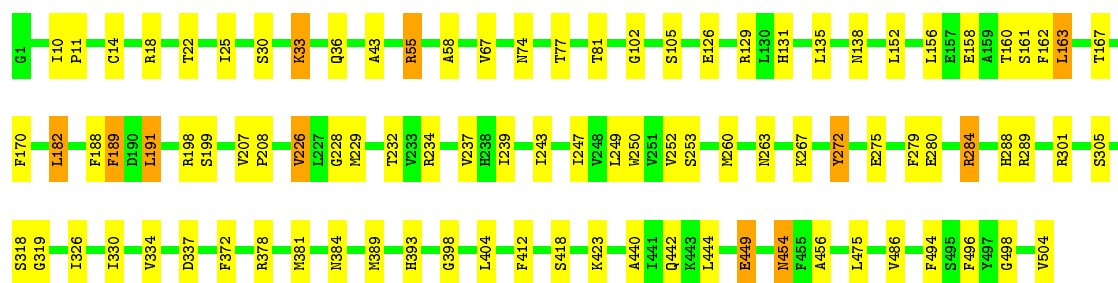
• Molecule 1: COAT PROTEIN

Chain AR: 81% 16% .



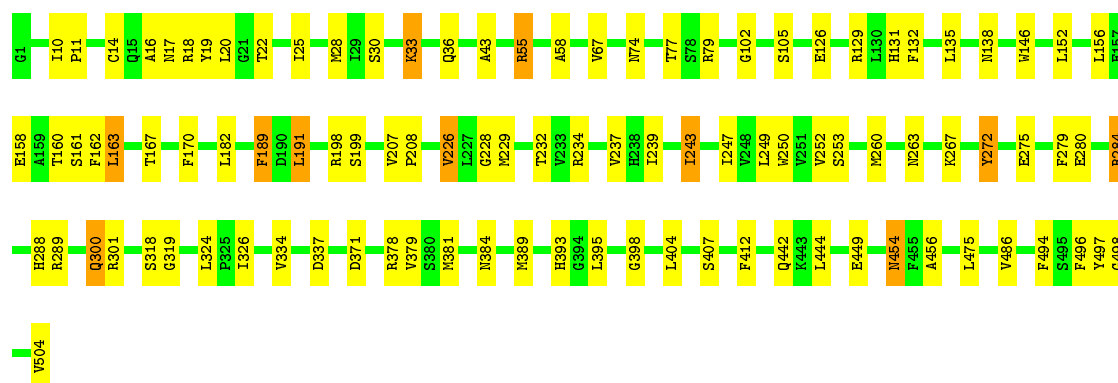
• Molecule 1: COAT PROTEIN

Chain AS: 81% 16% .



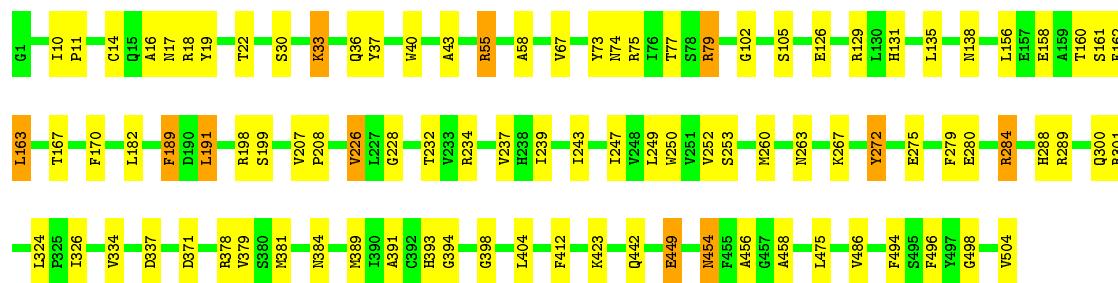
• Molecule 1: COAT PROTEIN

Chain AT: 80% 18% .



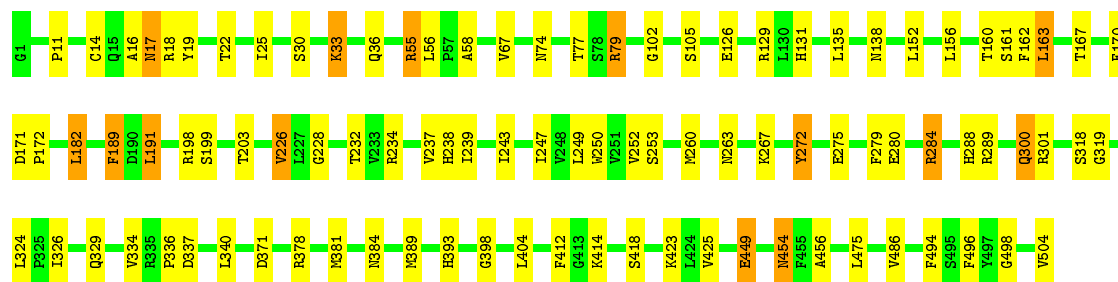
• Molecule 1: COAT PROTEIN

Chain BA: 81% 17% .



• Molecule 1: COAT PROTEIN

Chain BB: 81% 16% .



• Molecule 1: COAT PROTEIN

Response	Percentage
Doing a good job	80%
Not doing a good job	17%



Response	Percentage
Yes, it is a crisis	83%
No, it is not a crisis	15%



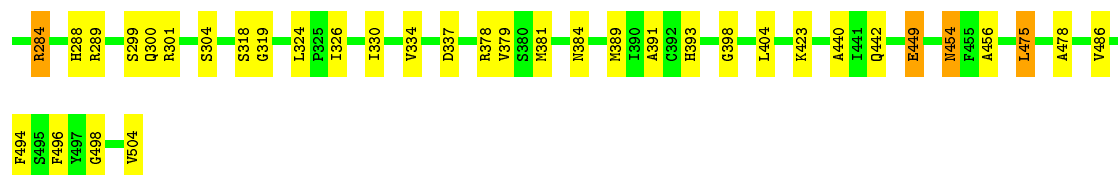
Response	Percentage
Yes, it is a crisis	82%
No, it is not a crisis	16%



Response	Percentage
Doing a good job	79%
Doing a bad job	18%

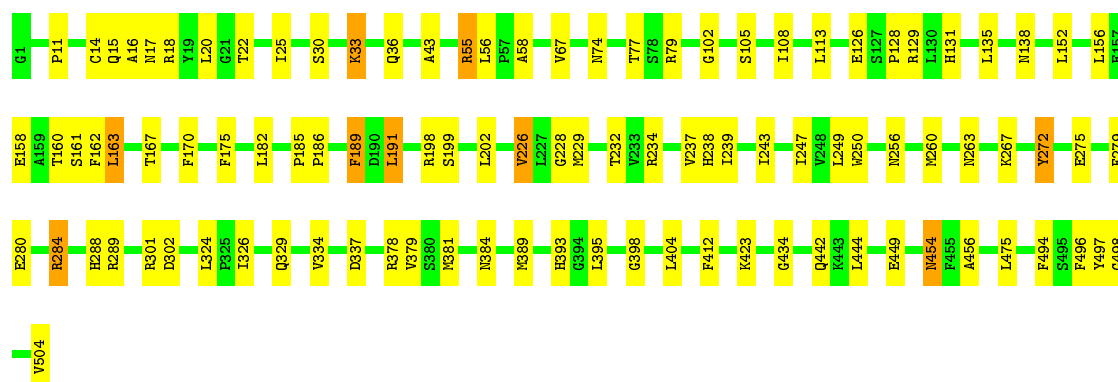






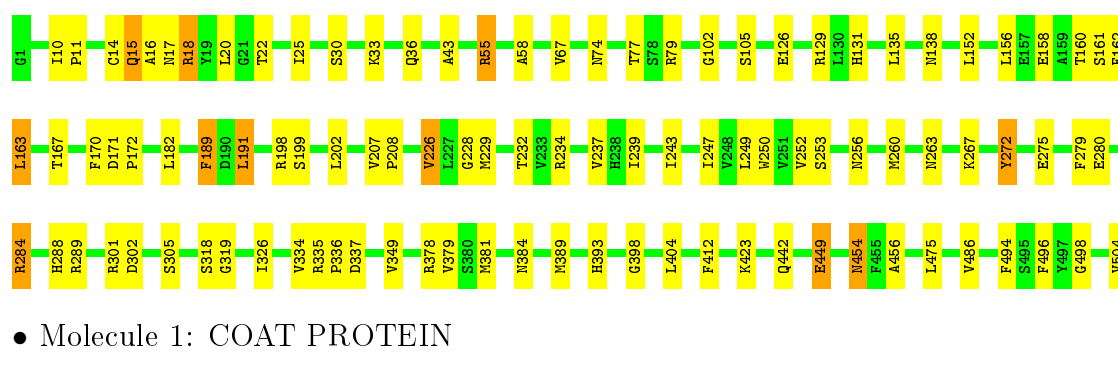
• Molecule 1: COAT PROTEIN

Chain BG: 80% 18%



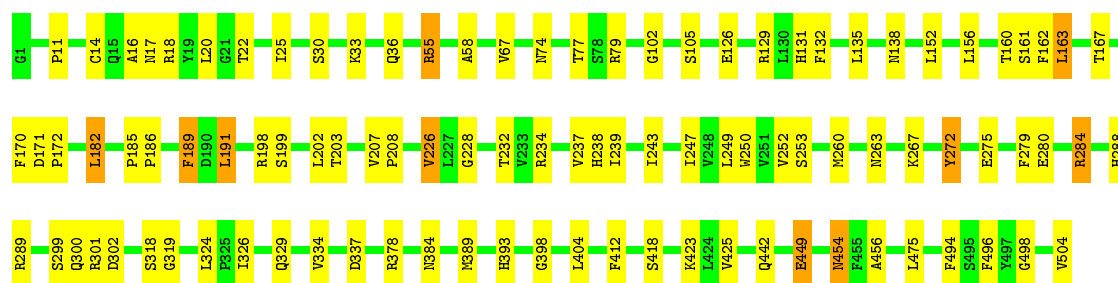
• Molecule 1: COAT PROTEIN

Chain BH: 80% 18%



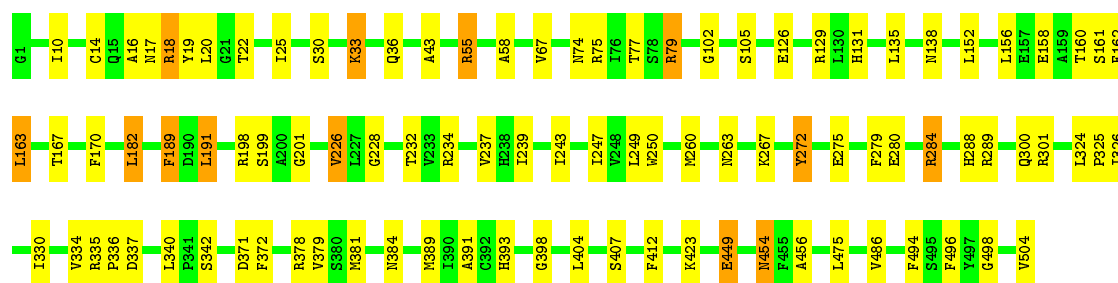
• Molecule 1: COAT PROTEIN

Chain BI: 80% 18%



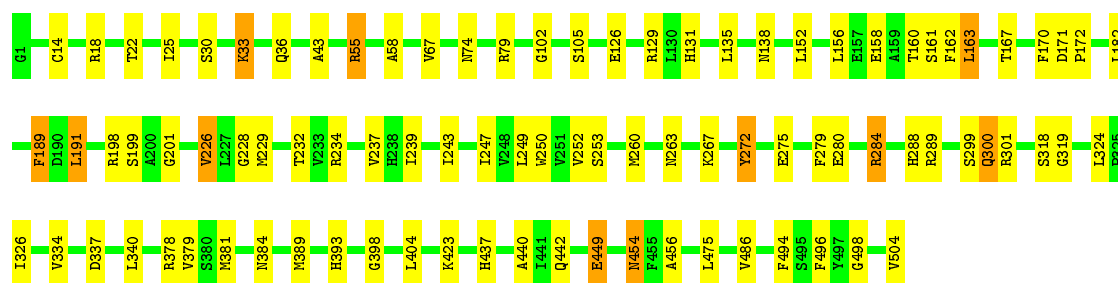
• Molecule 1: COAT PROTEIN

Chain BJ: 81% 17%



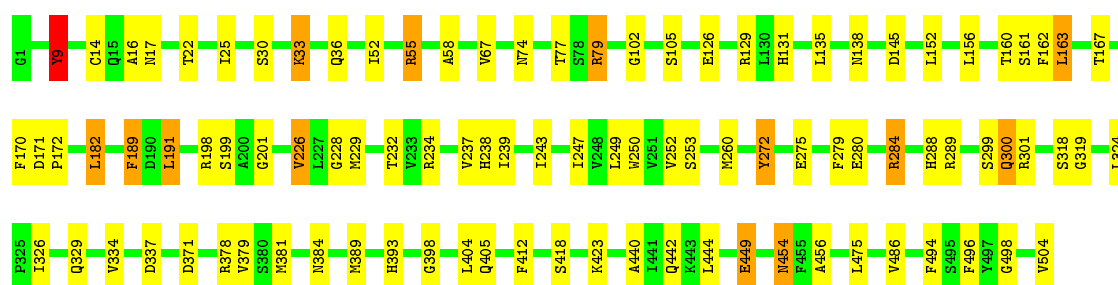
• Molecule 1: COAT PROTEIN

Chain BK: 82% 16%



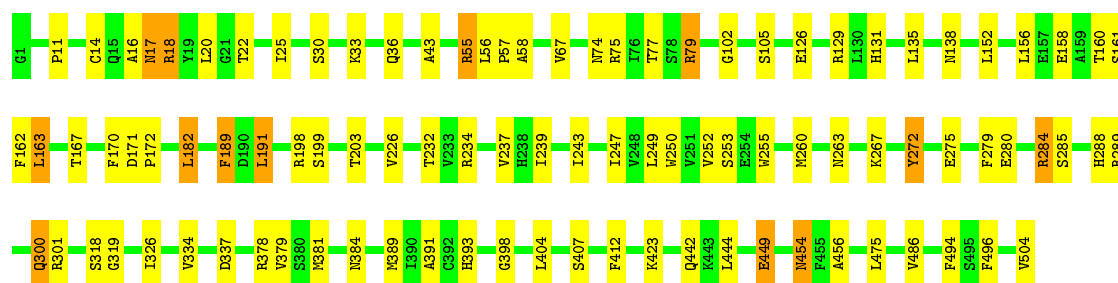
• Molecule 1: COAT PROTEIN

Chain BL: 81% 16%



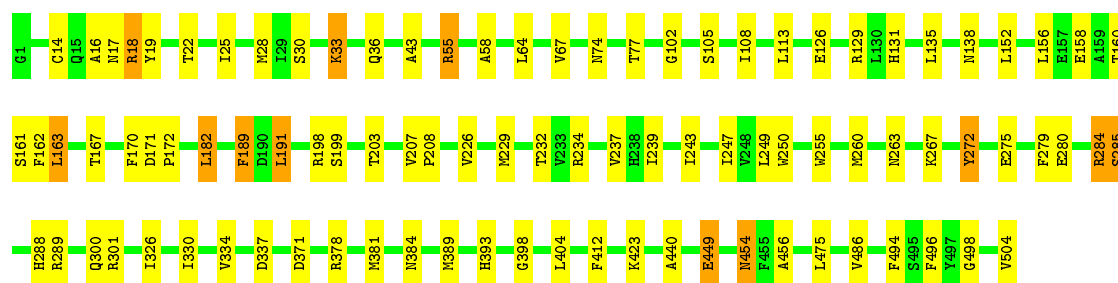
• Molecule 1: COAT PROTEIN

Chain BM: 81% 17%



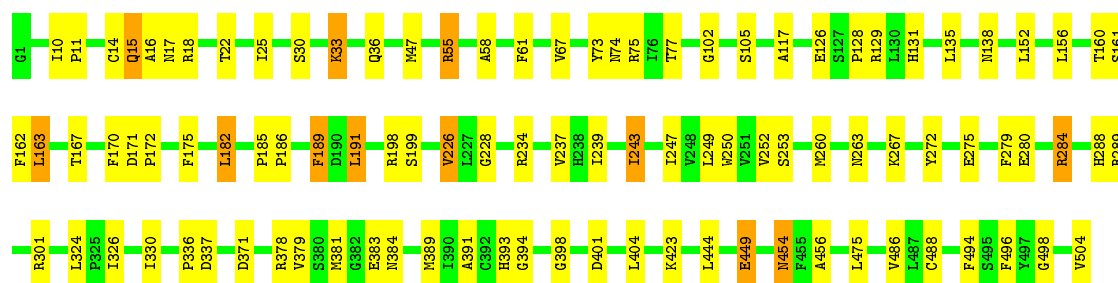
• Molecule 1: COAT PROTEIN

Chain BN: 81% 16%



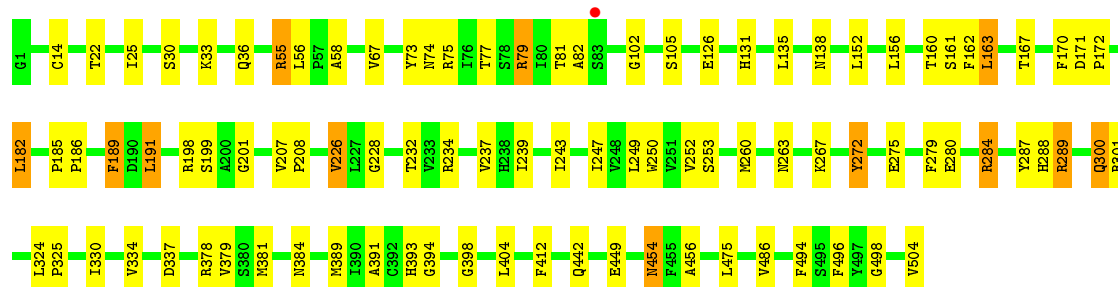
• Molecule 1: COAT PROTEIN

Chain BO: 80% 17% .



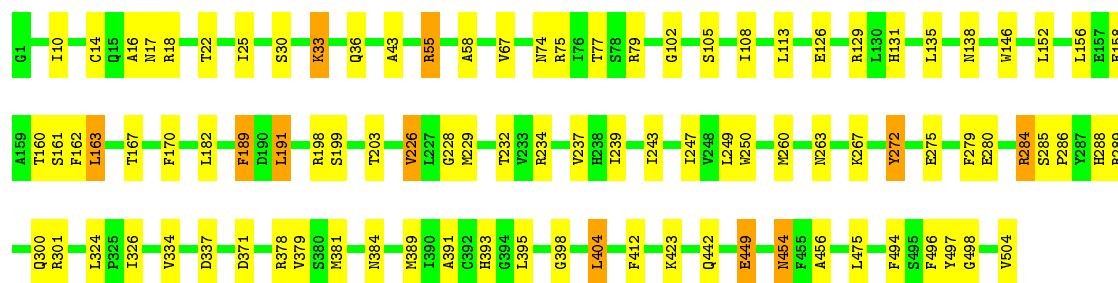
• Molecule 1: COAT PROTEIN

Chain BP: 81% 16% .



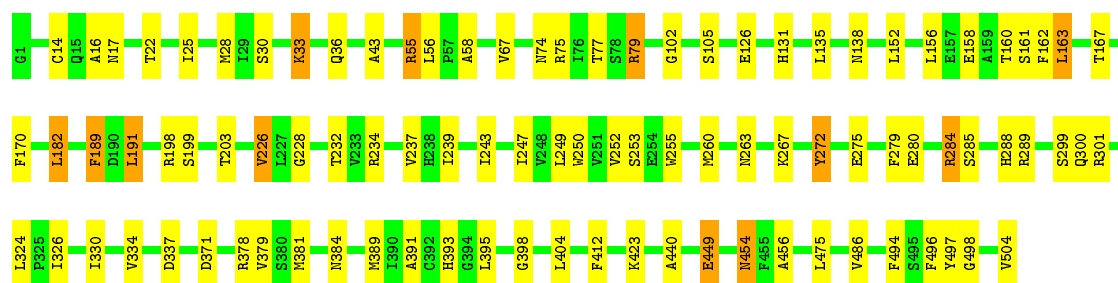
• Molecule 1: COAT PROTEIN

Chain BQ: 81% 17% .



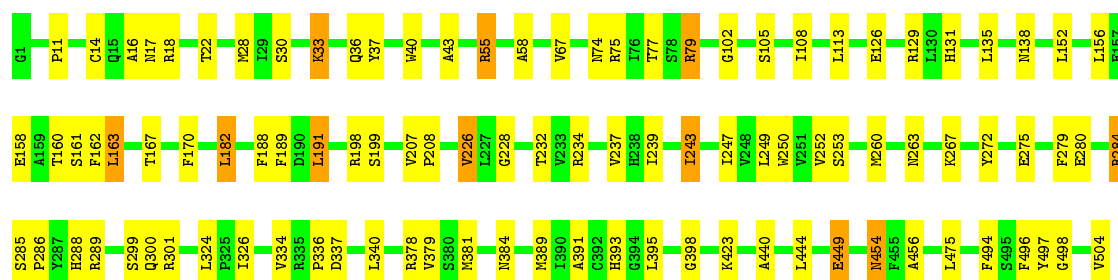
• Molecule 1: COAT PROTEIN

Chain BR: 81% 16% .



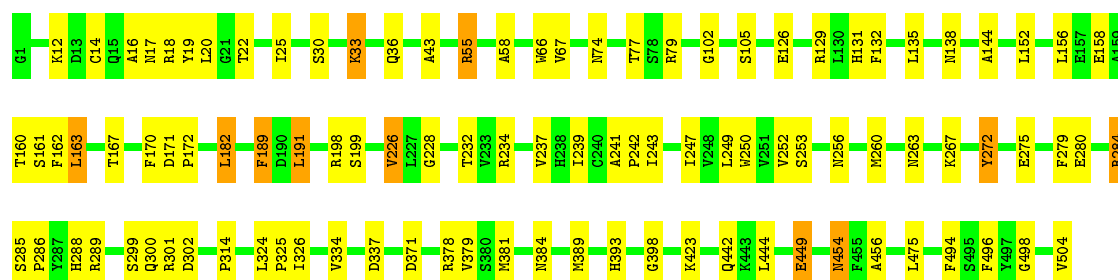
• Molecule 1: COAT PROTEIN

Chain BS: 80% 18% .



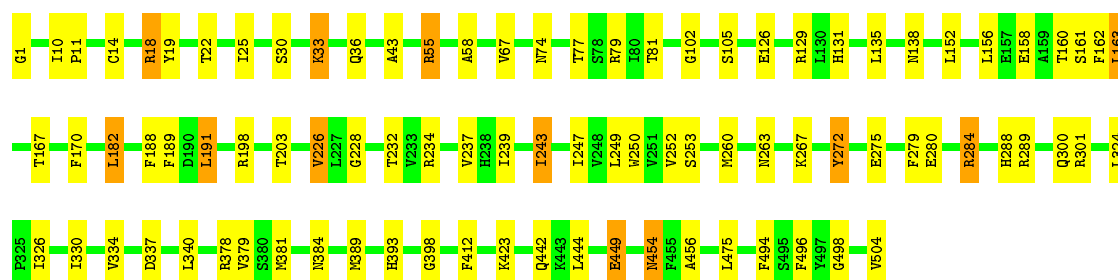
• Molecule 1: COAT PROTEIN

Chain BT: 80% 18% .



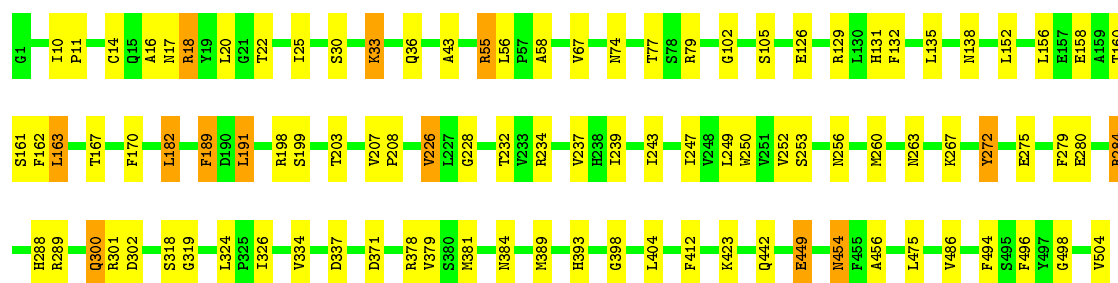
• Molecule 1: COAT PROTEIN

Chain CA: 82% 15% .



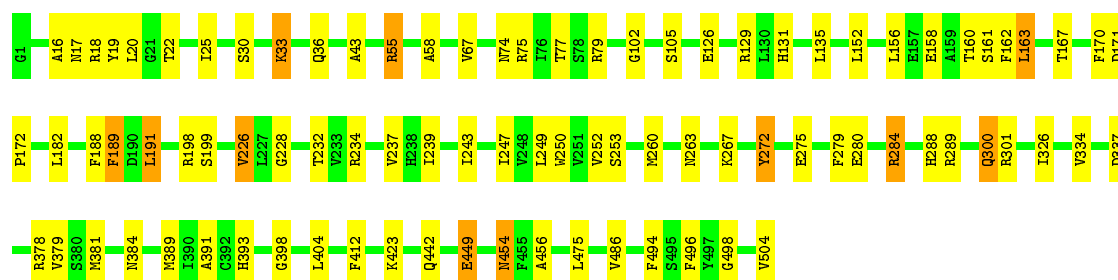
• Molecule 1: COAT PROTEIN

Chain CB: 81% 17% .



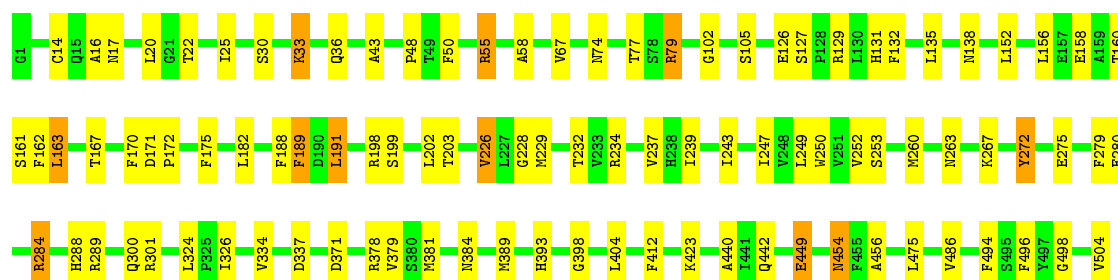
• Molecule 1: COAT PROTEIN

Chain CC: 82% 15% .



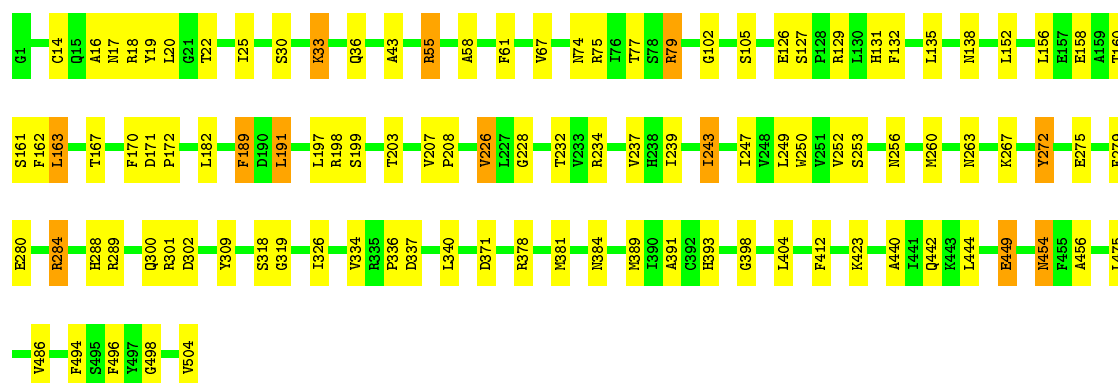
• Molecule 1: COAT PROTEIN

Chain CD: 81% 17% .

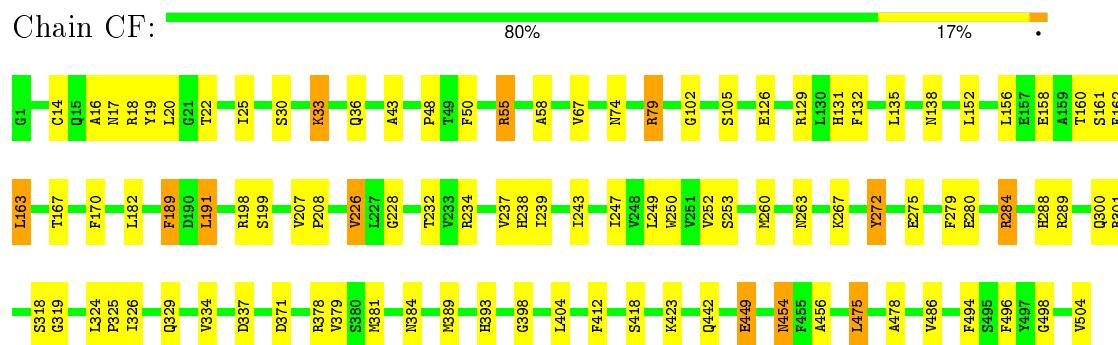


• Molecule 1: COAT PROTEIN

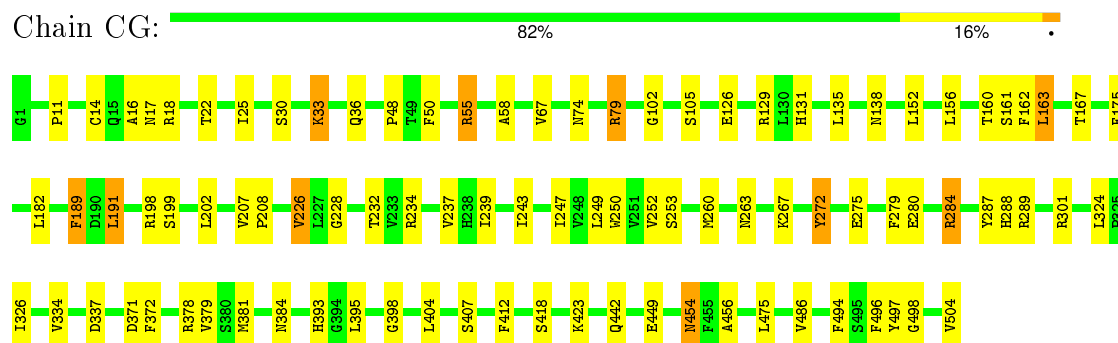
Chain CE: 79% 19% .



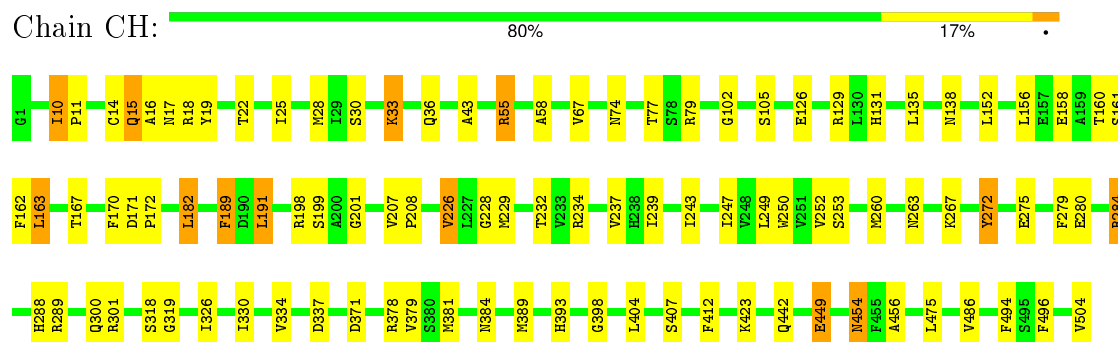
• Molecule 1: COAT PROTEIN



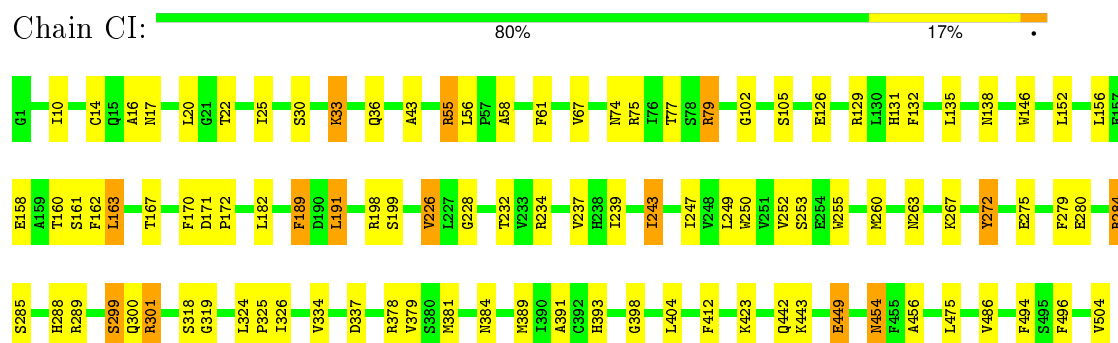
- Molecule 1: COAT PROTEIN



- Molecule 1: COAT PROTEIN

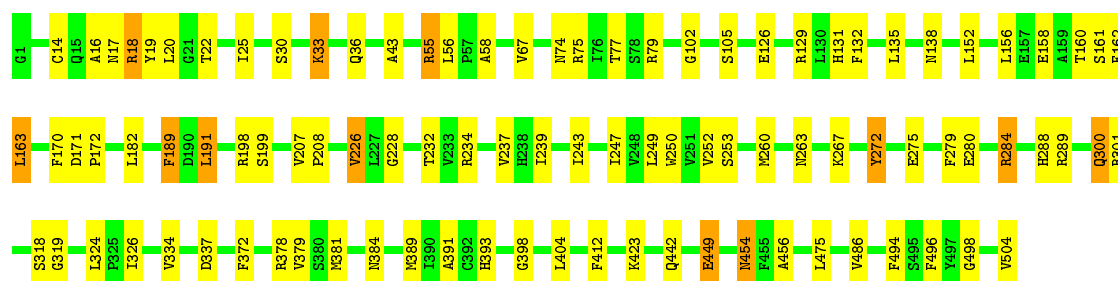


- Molecule 1: COAT PROTEIN



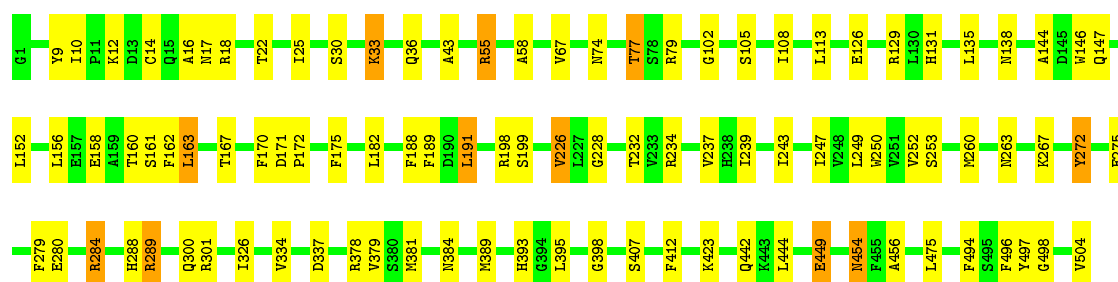
- Molecule 1: COAT PROTEIN

Chain CJ:  81% 17% .




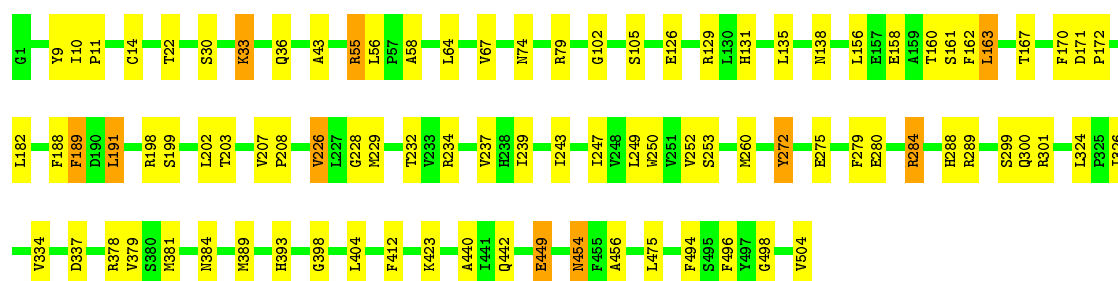
• Molecule 1: COAT PROTEIN

Chain CK:  81% 17% .



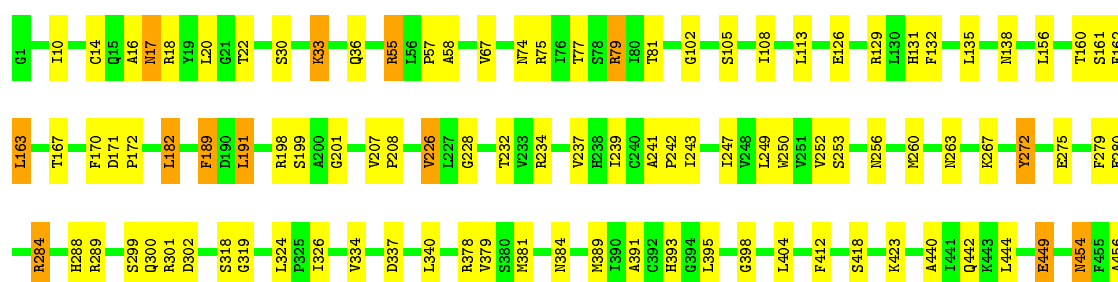
• Molecule 1: COAT PROTEIN

Chain CL:  82% 16% .



• Molecule 1: COAT PROTEIN

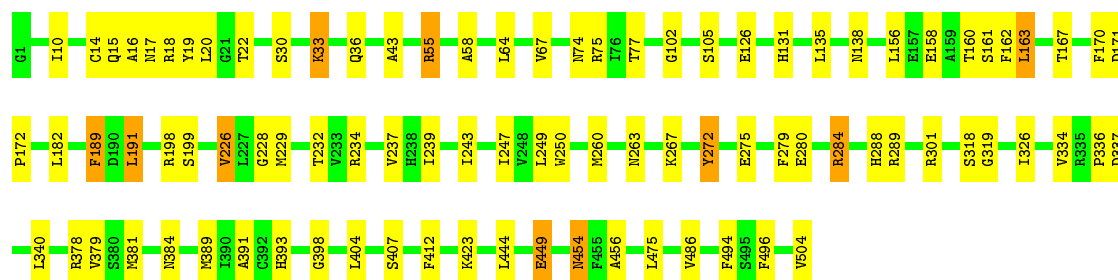
Chain CM:  79% 19% .





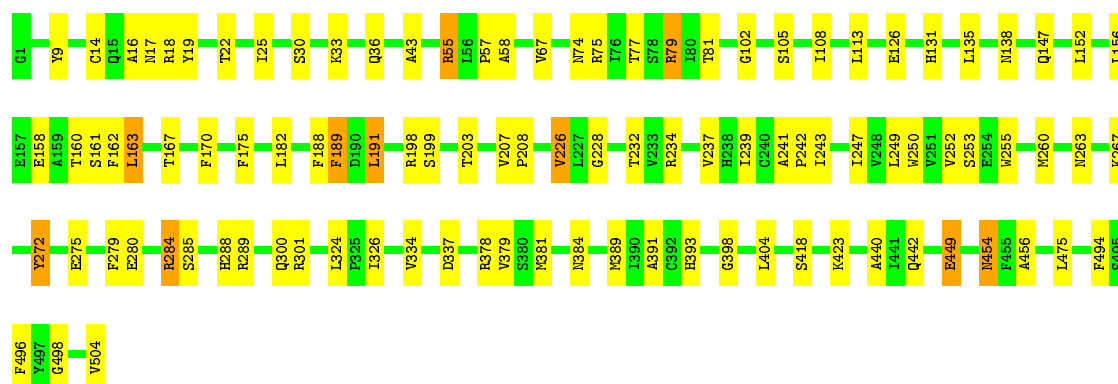
## • Molecule 1: COAT PROTEIN

Chain CN: 82% 16%



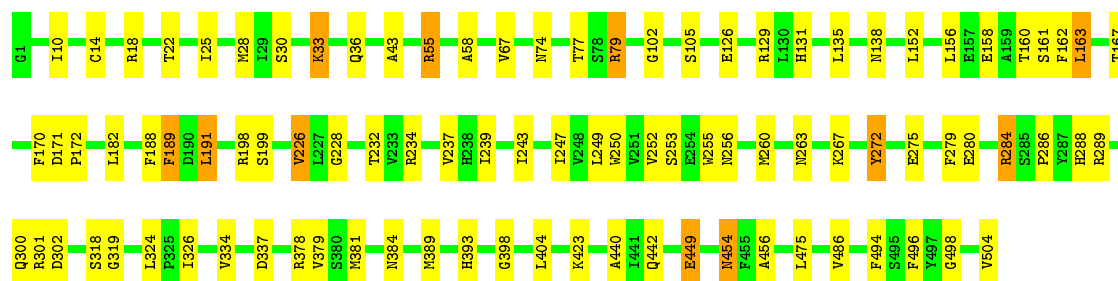
## • Molecule 1: COAT PROTEIN

Chain CO: 80% 18%



## • Molecule 1: COAT PROTEIN

Chain CP: 81% 16%

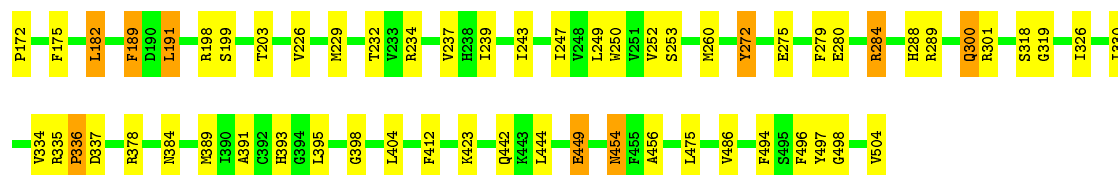


## • Molecule 1: COAT PROTEIN

Chain CQ: 82% 16%

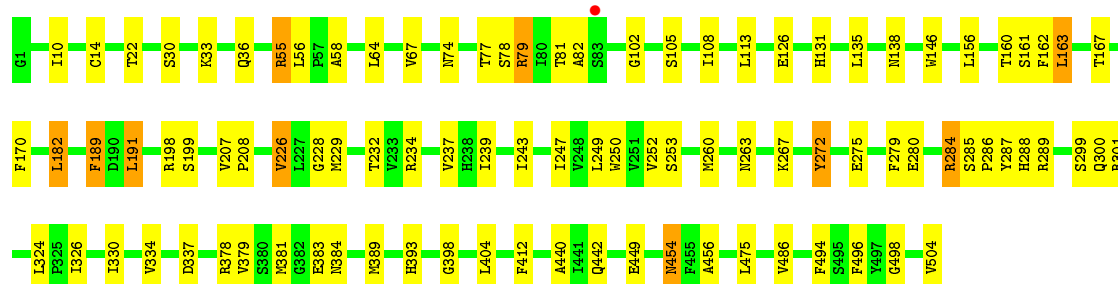






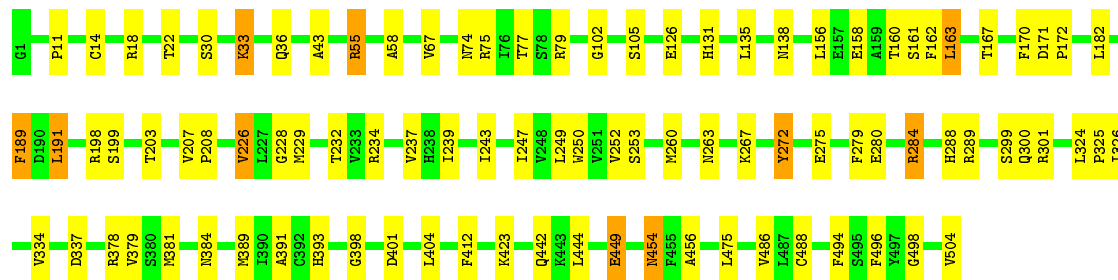
• Molecule 1: COAT PROTEIN

Chain CR: 81% 17%



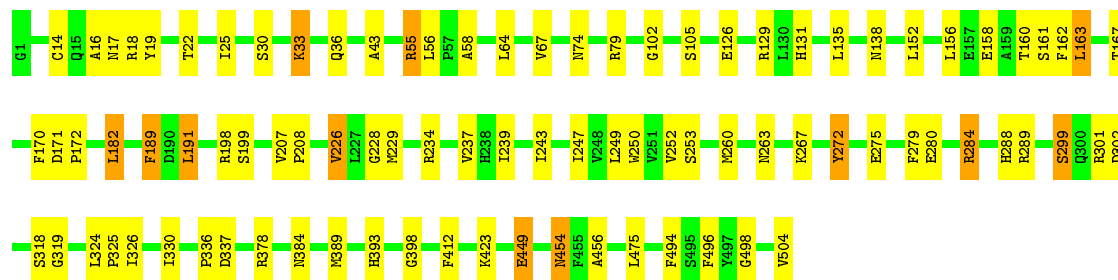
• Molecule 1: COAT PROTEIN

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) 82.0 (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 0.192 , 0.206	Depositor DCC
$R_{free}$ test set	66376 reflections (5.28%)	DCC
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> )	0.33 , 35.3	EDS
Estimated twinning fraction	0.000 for k,h,-h-k-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 1324087 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:CC:250:TRP:CZ3	1:CC:272:TYR:CE1	2.54	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%)	52	88
1	AB	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	AC	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	39	80
1	AD	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AE	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88
1	AF	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	AG	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	39	80
1	AH	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	39	80
1	AI	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	AJ	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88
1	AK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	AL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	AM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88
1	AN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88
1	AO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	AP	502/504 (100%)	483 (96%)	19 (4%)	0	100	100
1	AQ	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	AR	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	52	88
1	AS	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88
1	AT	502/504 (100%)	484 (96%)	17 (3%)	1 (0%)	52	88
1	BA	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88
1	BB	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	39	80
1	BC	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88
1	BD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	BE	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BF	502/504 (100%)	481 (96%)	19 (4%)	2 (0%)	39	80
1	BG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88
1	BH	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	52	88
1	BI	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	52	88
1	BJ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88
1	BK	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	52	88
1	BL	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	BM	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88
1	BN	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88
1	BO	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	BP	502/504 (100%)	479 (95%)	21 (4%)	2 (0%)	39	80
1	BQ	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88
1	BR	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88
1	BS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88
1	BT	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	CA	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	CB	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	CC	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88
1	CD	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	CE	502/504 (100%)	483 (96%)	18 (4%)	1 (0%)	52	88
1	CF	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88
1	CG	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88
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%)	52	88
1	CK	502/504 (100%)	482 (96%)	19 (4%)	1 (0%)	52	88
1	CL	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88
1	CM	502/504 (100%)	480 (96%)	20 (4%)	2 (0%)	39	80
1	CN	502/504 (100%)	482 (96%)	20 (4%)	0	100	100
1	CO	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88
1	CP	502/504 (100%)	480 (96%)	21 (4%)	1 (0%)	52	88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CQ	502/504 (100%)	482 (96%)	18 (4%)	2 (0%)	39	80
1	CR	502/504 (100%)	478 (95%)	22 (4%)	2 (0%)	39	80
1	CS	502/504 (100%)	481 (96%)	20 (4%)	1 (0%)	52	88
1	CT	502/504 (100%)	479 (95%)	22 (4%)	1 (0%)	52	88
All	All	30120/30240 (100%)	28870 (96%)	1187 (4%)	63 (0%)	52	88

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%)	28	67
1	AB	430/430 (100%)	404 (94%)	26 (6%)	24	62
1	AC	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	AD	430/430 (100%)	404 (94%)	26 (6%)	24	62
1	AE	430/430 (100%)	409 (95%)	21 (5%)	31	71
1	AF	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	AG	430/430 (100%)	405 (94%)	25 (6%)	25	63
1	AH	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	AI	430/430 (100%)	404 (94%)	26 (6%)	24	62
1	AJ	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	AK	430/430 (100%)	404 (94%)	26 (6%)	24	62
1	AL	430/430 (100%)	404 (94%)	26 (6%)	24	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AM	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	AN	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	AO	430/430 (100%)	408 (95%)	22 (5%)	29	69
1	AP	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	AQ	430/430 (100%)	405 (94%)	25 (6%)	25	63
1	AR	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	AS	430/430 (100%)	405 (94%)	25 (6%)	25	63
1	AT	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	BA	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	BB	430/430 (100%)	405 (94%)	25 (6%)	25	63
1	BC	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	BD	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	BE	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	BF	430/430 (100%)	404 (94%)	26 (6%)	24	62
1	BG	430/430 (100%)	408 (95%)	22 (5%)	29	69
1	BH	430/430 (100%)	404 (94%)	26 (6%)	24	62
1	BI	430/430 (100%)	408 (95%)	22 (5%)	29	69
1	BJ	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	BK	430/430 (100%)	404 (94%)	26 (6%)	24	62
1	BL	430/430 (100%)	403 (94%)	27 (6%)	22	60
1	BM	430/430 (100%)	404 (94%)	26 (6%)	24	62
1	BN	430/430 (100%)	405 (94%)	25 (6%)	25	63
1	BO	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	BP	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	BQ	430/430 (100%)	405 (94%)	25 (6%)	25	63
1	BR	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	BS	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	BT	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	CA	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	CB	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	CC	430/430 (100%)	407 (95%)	23 (5%)	28	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CD	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	CE	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	CF	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	CG	430/430 (100%)	408 (95%)	22 (5%)	29	69
1	CH	430/430 (100%)	405 (94%)	25 (6%)	25	63
1	CI	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	CJ	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	CK	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	CL	430/430 (100%)	405 (94%)	25 (6%)	25	63
1	CM	430/430 (100%)	403 (94%)	27 (6%)	22	60
1	CN	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	CO	430/430 (100%)	408 (95%)	22 (5%)	29	69
1	CP	430/430 (100%)	405 (94%)	25 (6%)	25	63
1	CQ	430/430 (100%)	404 (94%)	26 (6%)	24	62
1	CR	430/430 (100%)	405 (94%)	25 (6%)	25	63
1	CS	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	CT	430/430 (100%)	405 (94%)	25 (6%)	25	63
All	All	25800/25800 (100%)	24352 (94%)	1448 (6%)	26	65

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 [i](#)

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

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(Å <sup>2</sup> )	Q<0.9
1	AA	504/504 (100%)	-0.55	0	100 100	23, 33, 53, 78	0
1	AB	504/504 (100%)	-0.57	0	100 100	22, 34, 54, 78	0
1	AC	504/504 (100%)	-0.52	0	100 100	23, 34, 54, 78	0
1	AD	504/504 (100%)	-0.54	0	100 100	22, 33, 52, 78	0
1	AE	504/504 (100%)	-0.49	0	100 100	17, 31, 52, 77	0
1	AF	504/504 (100%)	-0.59	0	100 100	24, 34, 54, 80	0
1	AG	504/504 (100%)	-0.58	0	100 100	23, 34, 55, 80	0
1	AH	504/504 (100%)	-0.57	0	100 100	24, 35, 56, 79	0
1	AI	504/504 (100%)	-0.56	0	100 100	23, 34, 55, 80	0
1	AJ	504/504 (100%)	-0.53	0	100 100	22, 34, 54, 80	0
1	AK	504/504 (100%)	-0.57	0	100 100	23, 34, 55, 79	0
1	AL	504/504 (100%)	-0.51	0	100 100	23, 33, 54, 77	0
1	AM	504/504 (100%)	-0.53	0	100 100	21, 32, 52, 77	0
1	AN	504/504 (100%)	-0.50	0	100 100	22, 33, 54, 78	0
1	AO	504/504 (100%)	-0.50	0	100 100	21, 33, 54, 80	0
1	AP	504/504 (100%)	-0.52	0	100 100	19, 32, 53, 79	0
1	AQ	504/504 (100%)	-0.57	0	100 100	23, 33, 54, 77	0
1	AR	504/504 (100%)	-0.54	0	100 100	21, 32, 52, 77	0
1	AS	504/504 (100%)	-0.54	0	100 100	23, 33, 54, 80	0
1	AT	504/504 (100%)	-0.50	0	100 100	22, 33, 54, 77	0
1	BA	504/504 (100%)	-0.55	0	100 100	23, 33, 54, 79	0
1	BB	504/504 (100%)	-0.55	0	100 100	23, 34, 55, 77	0
1	BC	504/504 (100%)	-0.56	0	100 100	23, 34, 54, 78	0
1	BD	504/504 (100%)	-0.51	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%)	-0.54	0	100	100	23, 33, 54, 77	0
1	BF	504/504 (100%)	-0.49	0	100	100	22, 35, 56, 80	0
1	BG	504/504 (100%)	-0.58	0	100	100	22, 34, 54, 79	0
1	BH	504/504 (100%)	-0.56	0	100	100	21, 33, 54, 75	0
1	BI	504/504 (100%)	-0.50	0	100	100	22, 32, 54, 78	0
1	BJ	504/504 (100%)	-0.55	0	100	100	22, 34, 54, 79	0
1	BK	504/504 (100%)	-0.57	0	100	100	22, 33, 53, 77	0
1	BL	504/504 (100%)	-0.53	0	100	100	21, 32, 52, 75	0
1	BM	504/504 (100%)	-0.46	0	100	100	21, 32, 52, 77	0
1	BN	504/504 (100%)	-0.52	0	100	100	20, 33, 53, 76	0
1	BO	504/504 (100%)	-0.53	0	100	100	22, 33, 53, 80	0
1	BP	504/504 (100%)	-0.46	1 (0%)	95	87	21, 32, 53, 76	0
1	BQ	504/504 (100%)	-0.53	0	100	100	22, 33, 54, 80	0
1	BR	504/504 (100%)	-0.55	0	100	100	22, 33, 54, 79	0
1	BS	504/504 (100%)	-0.52	0	100	100	22, 33, 54, 80	0
1	BT	504/504 (100%)	-0.57	0	100	100	22, 34, 53, 77	0
1	CA	504/504 (100%)	-0.56	0	100	100	23, 35, 56, 80	0
1	CB	504/504 (100%)	-0.60	0	100	100	23, 34, 54, 77	0
1	CC	504/504 (100%)	-0.57	0	100	100	23, 34, 54, 81	0
1	CD	504/504 (100%)	-0.56	0	100	100	23, 34, 54, 79	0
1	CE	504/504 (100%)	-0.57	0	100	100	23, 33, 54, 78	0
1	CF	504/504 (100%)	-0.56	0	100	100	23, 34, 55, 80	0
1	CG	504/504 (100%)	-0.55	0	100	100	24, 34, 55, 81	0
1	CH	504/504 (100%)	-0.55	0	100	100	24, 34, 55, 79	0
1	CI	504/504 (100%)	-0.55	0	100	100	23, 33, 53, 79	0
1	CJ	504/504 (100%)	-0.53	0	100	100	24, 33, 54, 79	0
1	CK	504/504 (100%)	-0.48	0	100	100	21, 34, 54, 79	0
1	CL	504/504 (100%)	-0.57	0	100	100	22, 33, 54, 77	0
1	CM	504/504 (100%)	-0.53	0	100	100	22, 32, 53, 79	0
1	CN	504/504 (100%)	-0.53	0	100	100	22, 32, 54, 79	0
1	CO	504/504 (100%)	-0.53	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%)	-0.51	0 100 100	21, 31, 53, 78	0
1	CQ	504/504 (100%)	-0.50	0 100 100	21, 32, 53, 79	0
1	CR	504/504 (100%)	-0.44	1 (0%) 95 87	17, 31, 53, 75	0
1	CS	504/504 (100%)	-0.54	0 100 100	22, 32, 53, 78	0
1	CT	504/504 (100%)	-0.56	0 100 100	21, 32, 52, 77	0
All	All	30240/30240 (100%)	-0.54	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	2.6
1	BP	83	SER	2.2

## 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.