wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2020 – 10:53 AM BST

PDB ID	:	6YFJ
Title	:	Virus-like particle of bacteriophage ESE001
Authors	:	Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on	:	2020-03-26
Resolution	:	3.23 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

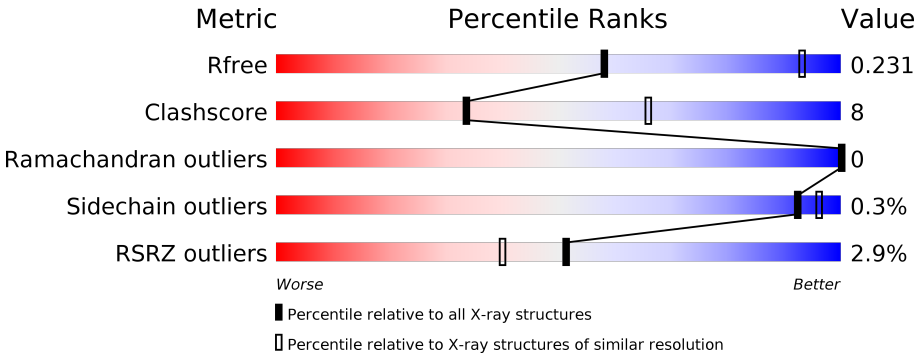
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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}	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	118	4% 73% 27%
1	AB	118	7% 80% 20%
1	AC	118	3% 80% 20%
1	AD	118	83% 17%
1	AE	118	4% 82% 18%
1	AF	118	% 85% 15%

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Mol	Chain	Length	Quality of chain
1	AG	118	77% 23%
1	AH	118	8% 73% 27%
1	AI	118	2% 82% 17%
1	AJ	118	3% 77% 23%
1	AK	118	9% 76% 24%
1	AL	118	3% 72% 28%
1	AM	118	% 75% 25%
1	AN	118	5% 79% 21%
1	AO	118	3% 89% 11%
1	AP	118	5% 75% 25%
1	AQ	118	4% 87% 13%
1	AR	118	3% 84% 16%
1	AS	118	2% 72% 28%
1	AT	118	3% 82% 18%
1	AU	118	% 86% 14%
1	AV	118	81% 19%
1	AW	118	3% 81% 19%
1	AX	118	3% 83% 17%
1	AY	118	3% 77% 23%
1	AZ	118	4% 74% 26%
1	BA	118	% 84% 16%
1	BB	118	69% 31%
1	BC	118	4% 87% 13%
1	BD	118	% 85% 15%
1	BE	118	% 72% 28%

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Mol	Chain	Length	Quality of chain
1	BF	118	6% 76% 24%
1	BG	118	% 79% 20%
1	BH	118	2% 75% 25%
1	BI	118	4% 76% 24%
1	BJ	118	% 84% 16%
1	BK	118	3% 81% 19%
1	BL	118	5% 77% 23%
1	BM	118	2% 84% 16%
1	BN	118	3% 77% 23%
1	BO	118	5% 86% 14%
1	BP	118	2% 75% 25%
1	BQ	118	81% 19%
1	BR	118	4% 80% 20%
1	BS	118	2% 85% 15%
1	BT	118	3% 80% 20%
1	BU	118	4% 78% 22%
1	BV	118	2% 85% 15%
1	BW	118	78% 22%
1	BX	118	4% 84% 16%
1	BY	118	2% 83% 16%
1	BZ	118	% 69% 31%
1	CA	118	7% 79% 21%
1	CB	118	% 90% 10%
1	CC	118	% 80% 20%
1	CD	118	7% 77% 23%

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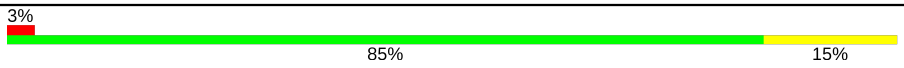
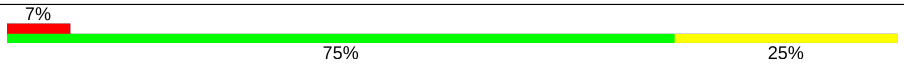
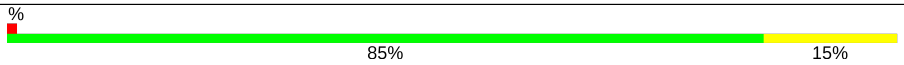
Mol	Chain	Length	Quality of chain
1	CE	118	
1	CF	118	
1	CG	118	
1	CH	118	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 52380 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	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AB	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AC	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AD	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AE	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AF	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AG	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AH	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AI	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AJ	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AK	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AL	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AM	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AN	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AO	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AP	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AR	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AS	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AT	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AU	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AV	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AW	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AX	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AY	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	AZ	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BA	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BB	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BC	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BD	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BE	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BF	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BG	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BH	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BI	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BJ	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BK	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BM	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BN	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BO	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BP	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BQ	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BR	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BS	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BT	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BU	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BV	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BW	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BX	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BY	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	BZ	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	CA	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	CB	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	CC	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	CD	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	CE	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	CF	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			

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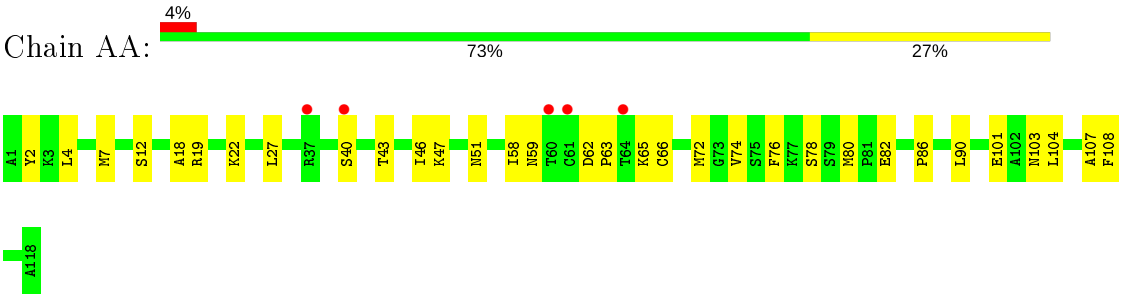
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			
1	CH	118	Total	C	N	O	S	0	0	0
			873	542	150	176	5			

3 Residue-property plots (i)

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

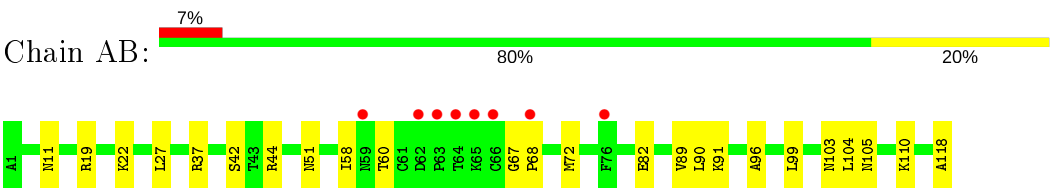
- Molecule 1: coat protein

Chain AA:



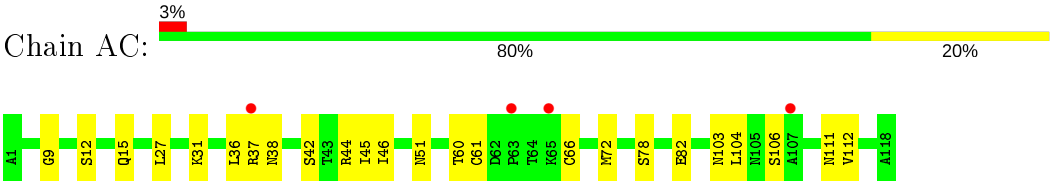
- Molecule 1: coat protein

Chain AB:



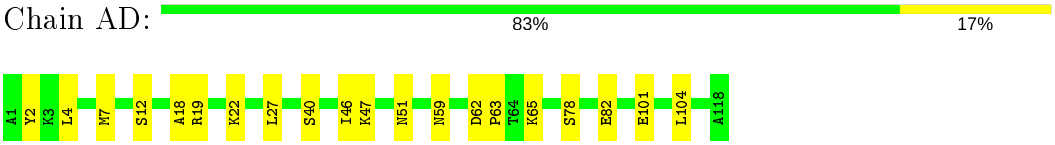
- Molecule 1: coat protein

Chain AC:



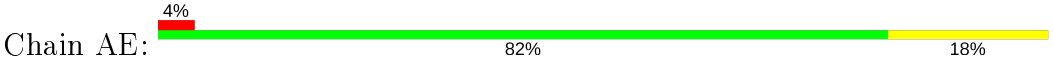
- Molecule 1: coat protein

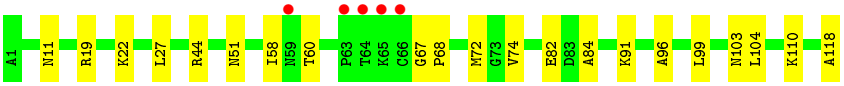
Chain AD:



- Molecule 1: coat protein

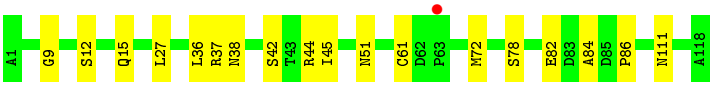
Chain AE:





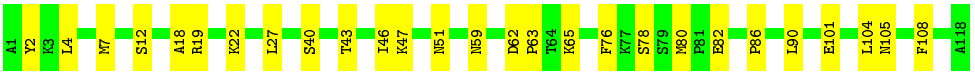
• Molecule 1: coat protein

Chain AF:



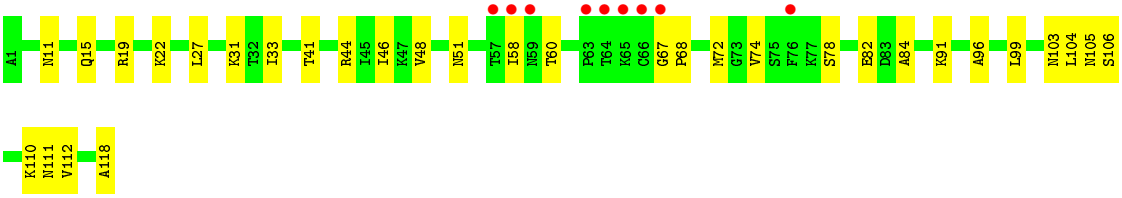
• Molecule 1: coat protein

Chain AG:



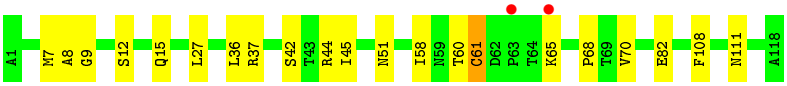
• Molecule 1: coat protein

Chain AH:



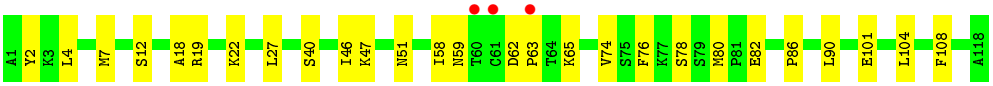
• Molecule 1: coat protein

Chain AI:



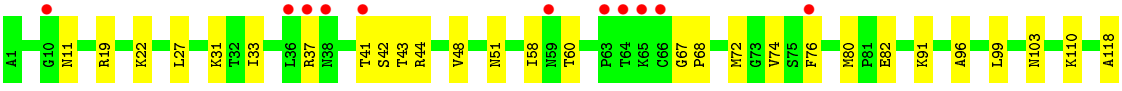
• Molecule 1: coat protein

Chain AJ:



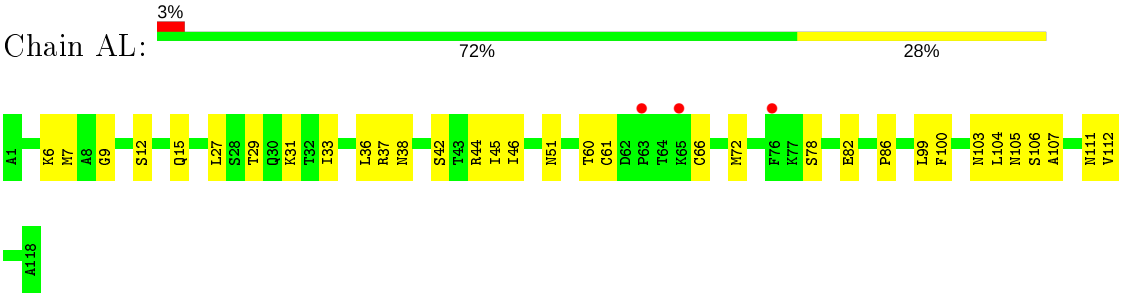
• Molecule 1: coat protein

Chain AK:



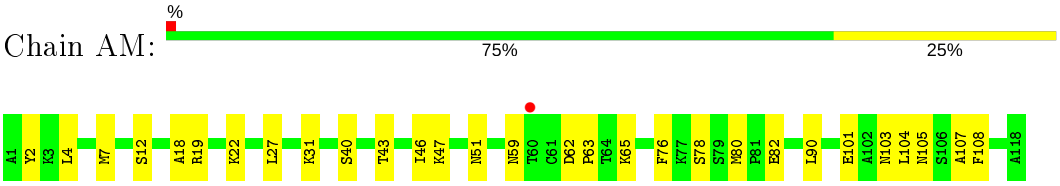
- Molecule 1: coat protein

Chain AL:



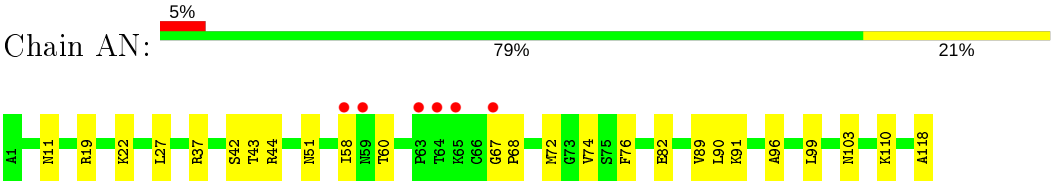
- Molecule 1: coat protein

Chain AM:



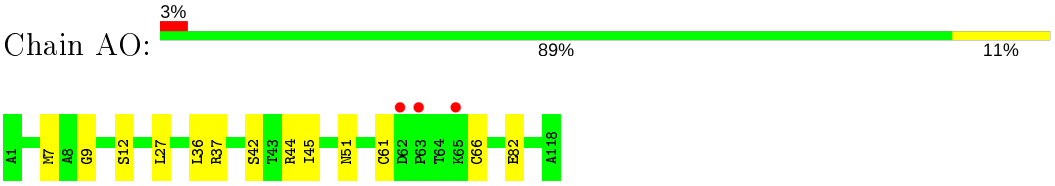
- Molecule 1: coat protein

Chain AN:



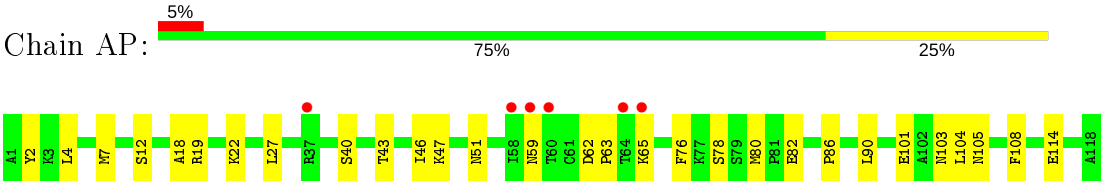
- Molecule 1: coat protein

Chain AO:



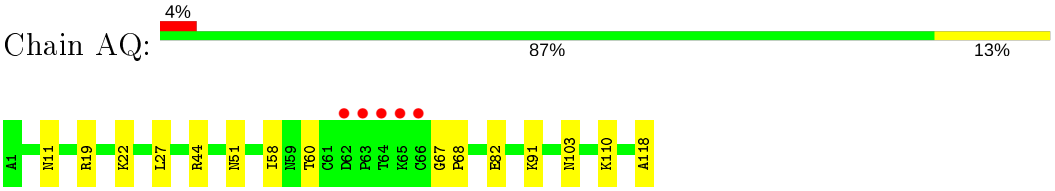
- Molecule 1: coat protein

Chain AP:



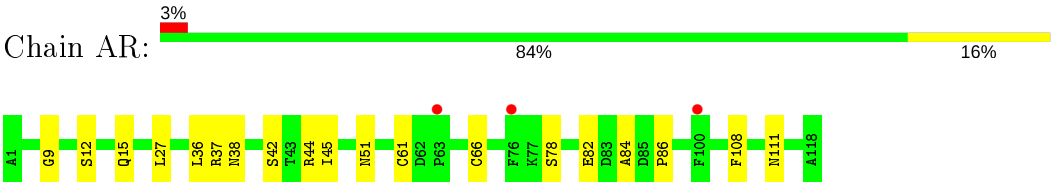
- Molecule 1: coat protein

Chain AQ:



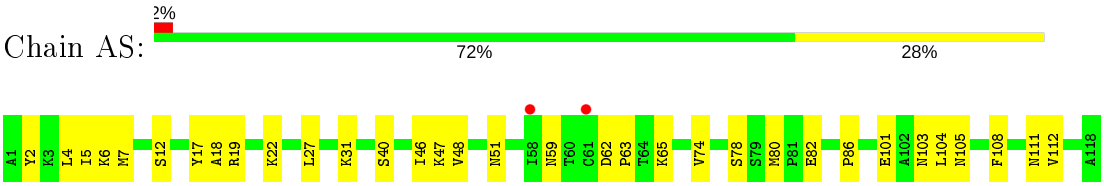
- Molecule 1: coat protein

Chain AR:



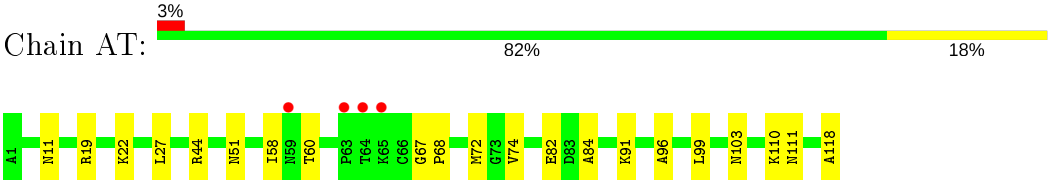
• Molecule 1: coat protein

Chain AS:



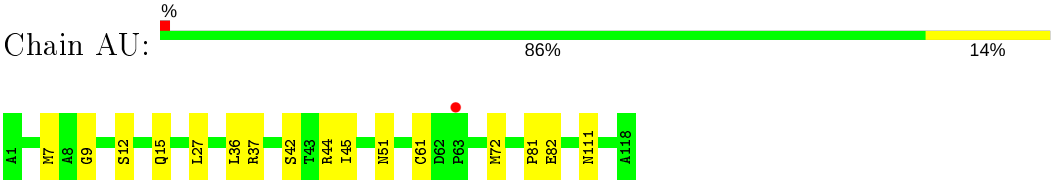
• Molecule 1: coat protein

Chain AT:



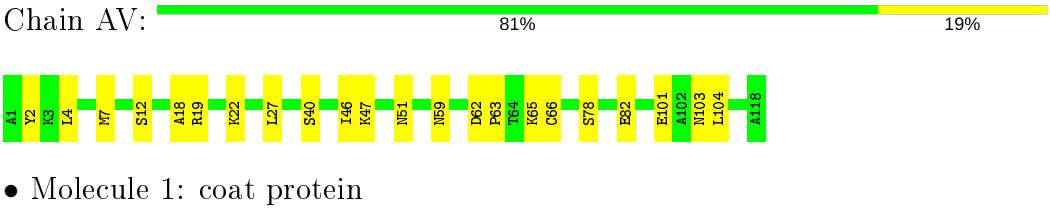
• Molecule 1: coat protein

Chain AU:



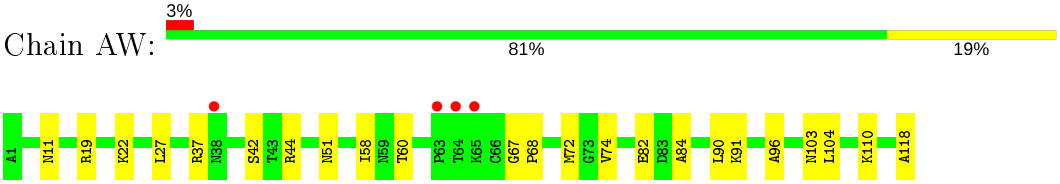
• Molecule 1: coat protein

Chain AV:



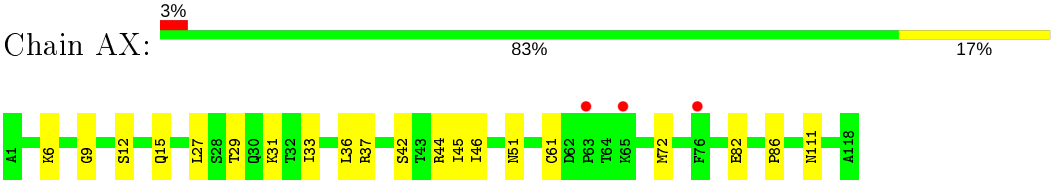
• Molecule 1: coat protein

Chain AW:



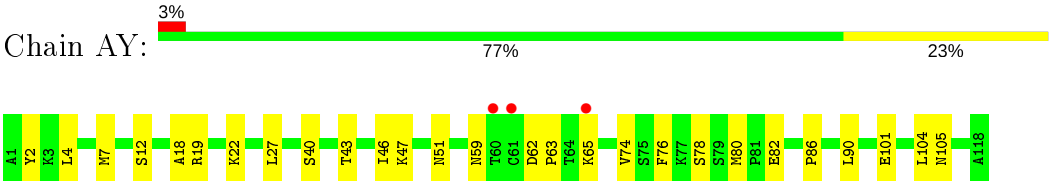
• Molecule 1: coat protein

Chain AX:



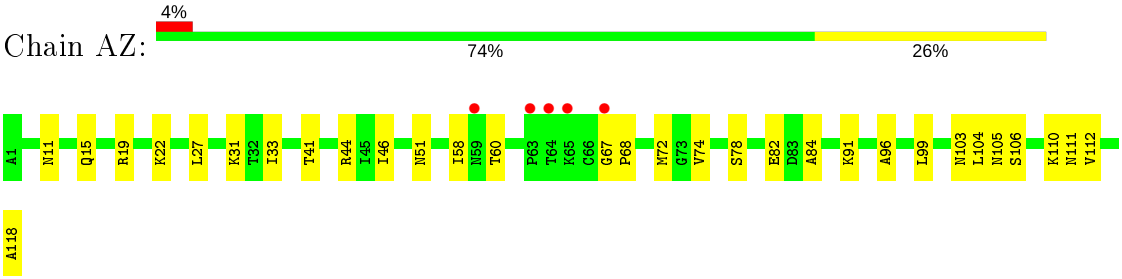
• Molecule 1: coat protein

Chain AY:



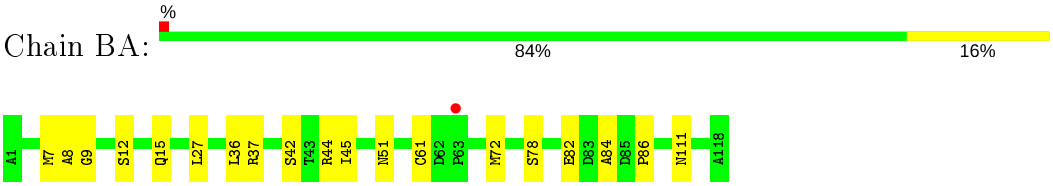
• Molecule 1: coat protein

Chain AZ:



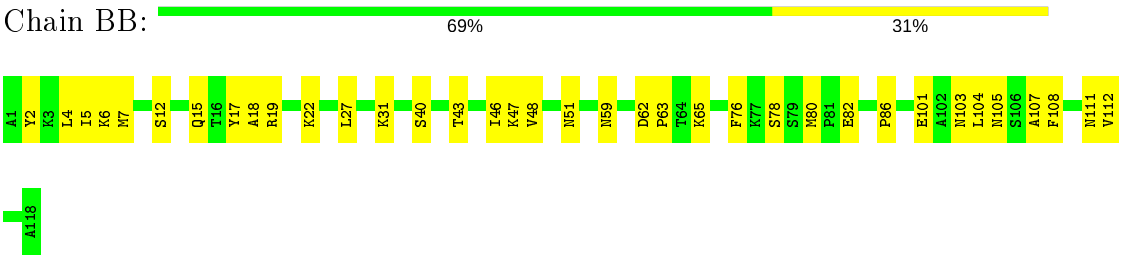
• Molecule 1: coat protein

Chain BA:



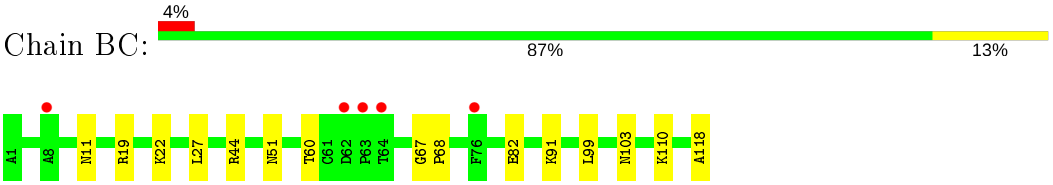
• Molecule 1: coat protein

Chain BB:



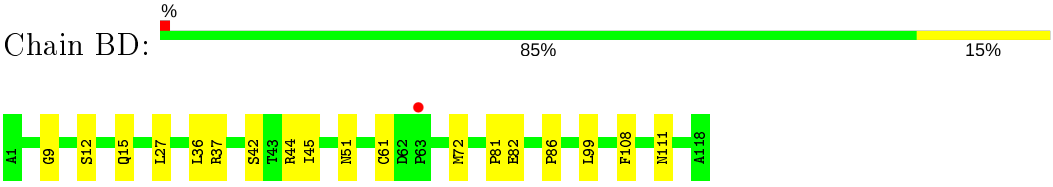
• Molecule 1: coat protein

Chain BC:



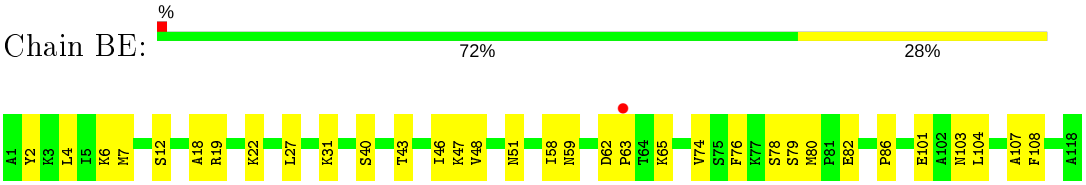
• Molecule 1: coat protein

Chain BD:



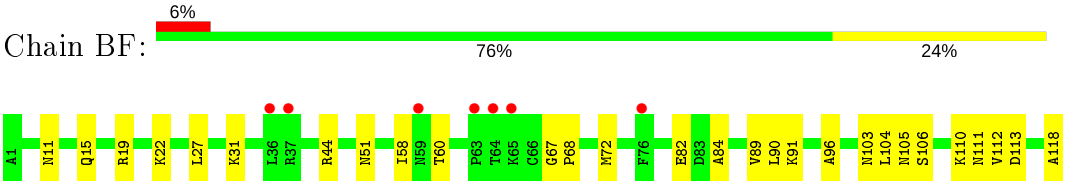
• Molecule 1: coat protein

Chain BE:



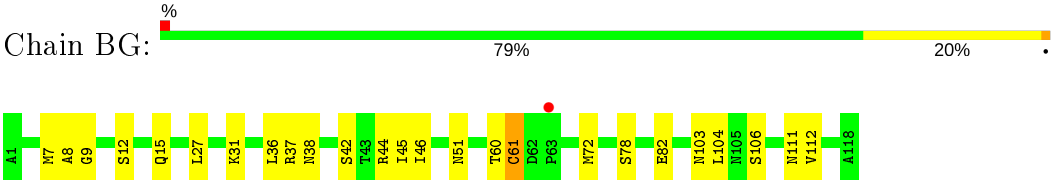
• Molecule 1: coat protein

Chain BF:



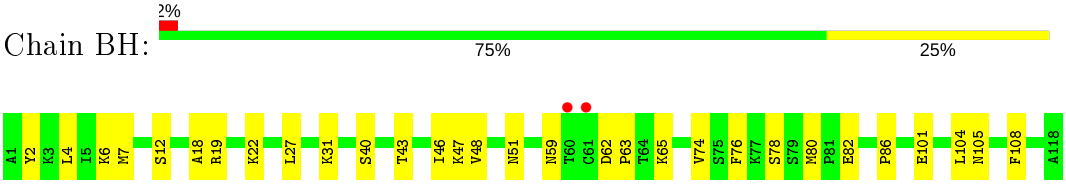
• Molecule 1: coat protein

Chain BG:



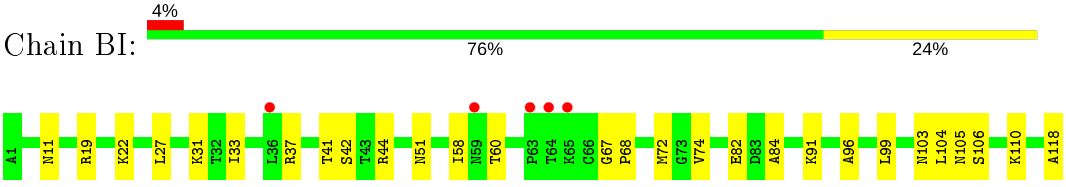
• Molecule 1: coat protein

Chain BH:



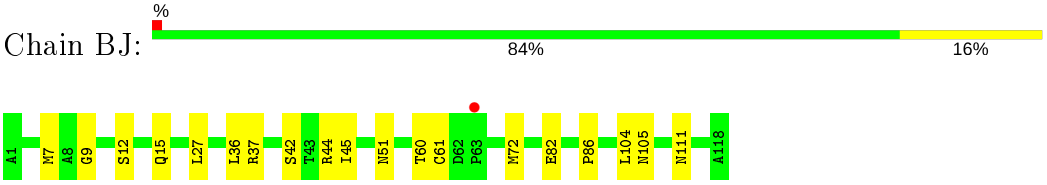
• Molecule 1: coat protein

Chain BI:



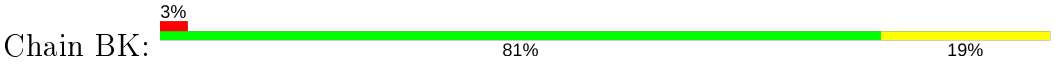
• Molecule 1: coat protein

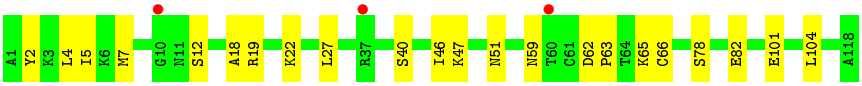
Chain BJ:



• Molecule 1: coat protein

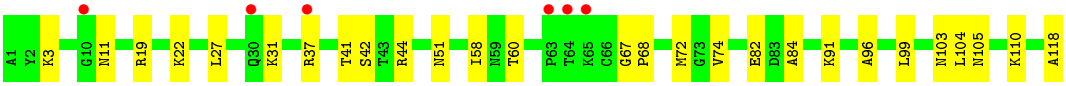
Chain BK:





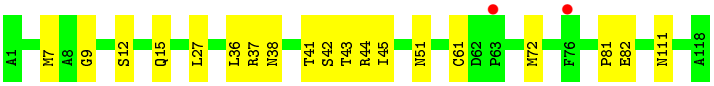
• Molecule 1: coat protein

Chain BL:



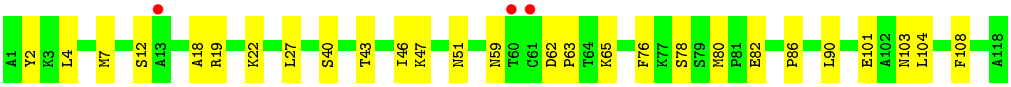
• Molecule 1: coat protein

Chain BM:



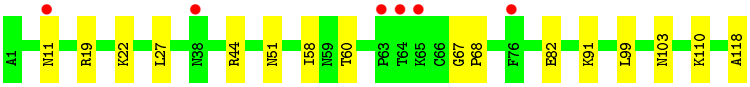
• Molecule 1: coat protein

Chain BN:



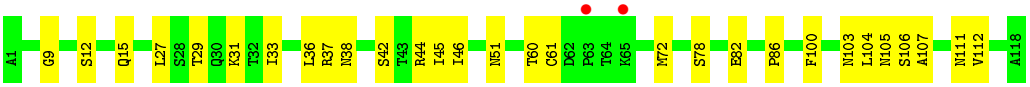
• Molecule 1: coat protein

Chain BO:



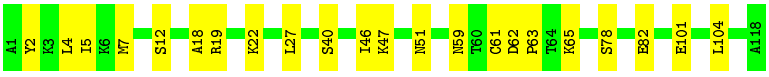
• Molecule 1: coat protein

Chain BP:



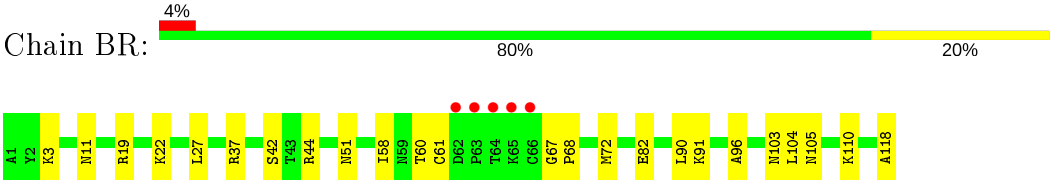
• Molecule 1: coat protein

Chain BQ:



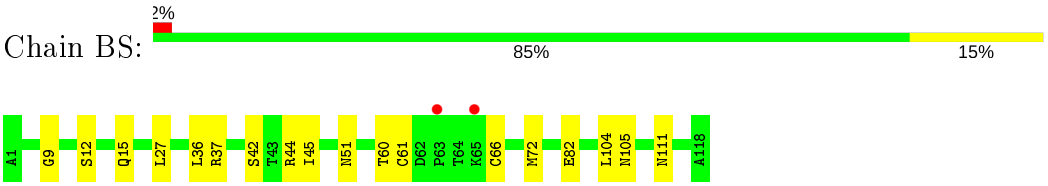
• Molecule 1: coat protein

Chain BR:



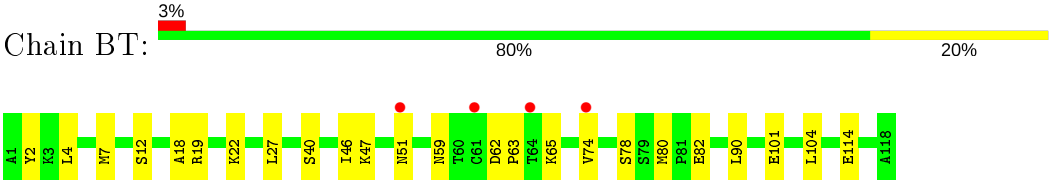
• Molecule 1: coat protein

Chain BS:



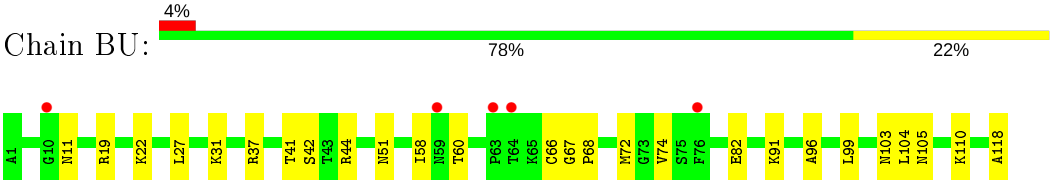
• Molecule 1: coat protein

Chain BT:



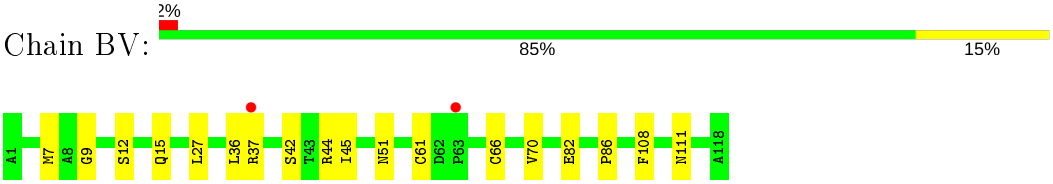
• Molecule 1: coat protein

Chain BU:



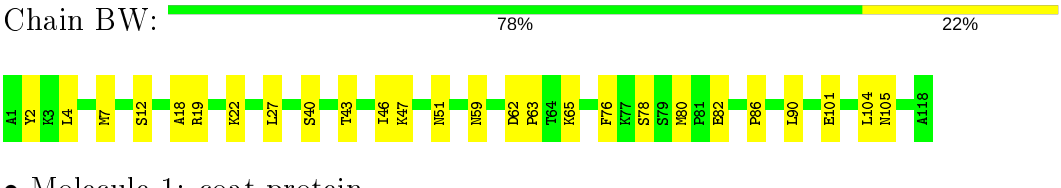
• Molecule 1: coat protein

Chain BV:



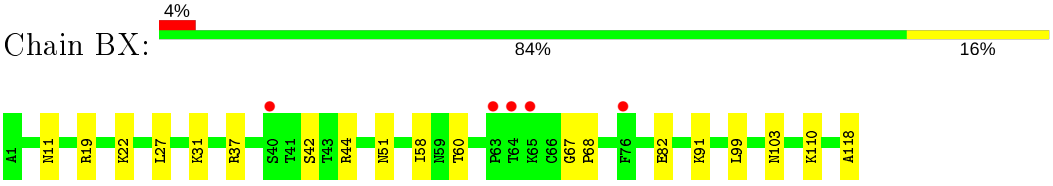
• Molecule 1: coat protein

Chain BW:



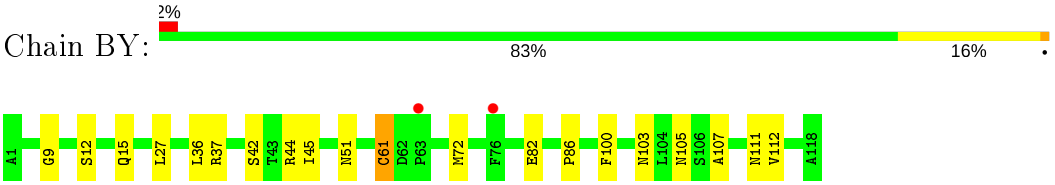
• Molecule 1: coat protein

Chain BX:



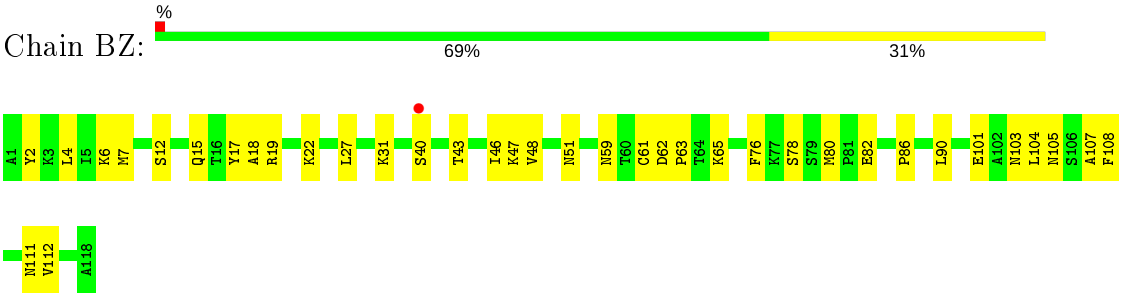
• Molecule 1: coat protein

Chain BY:



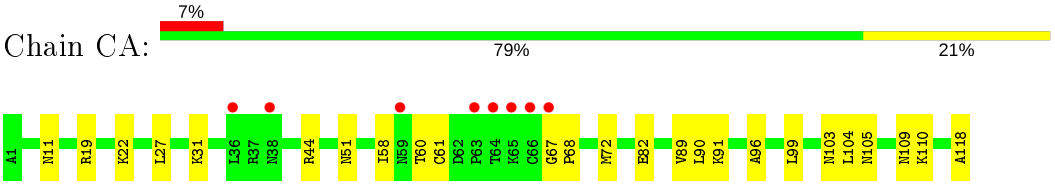
• Molecule 1: coat protein

Chain BZ:



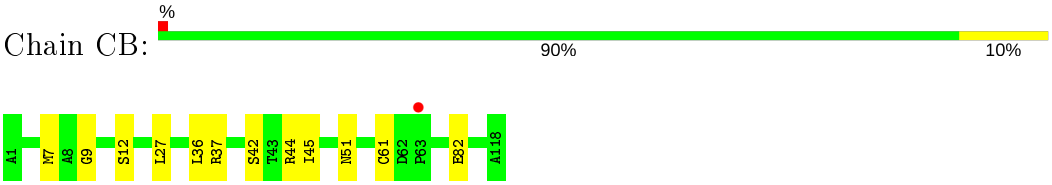
• Molecule 1: coat protein

Chain CA:



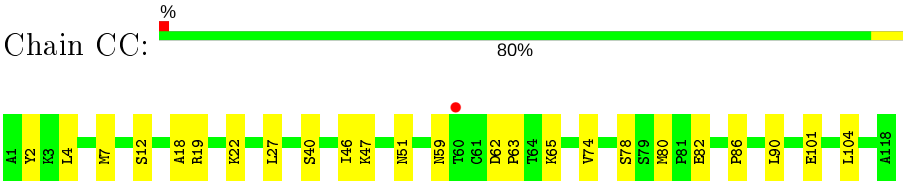
• Molecule 1: coat protein

Chain CB:



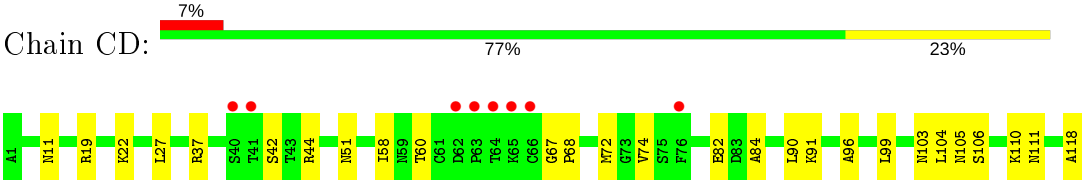
• Molecule 1: coat protein

Chain CC:



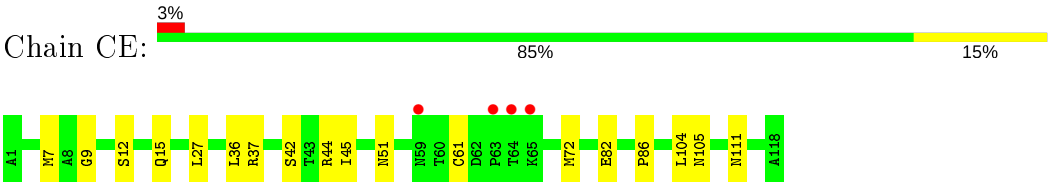
• Molecule 1: coat protein

Chain CD:



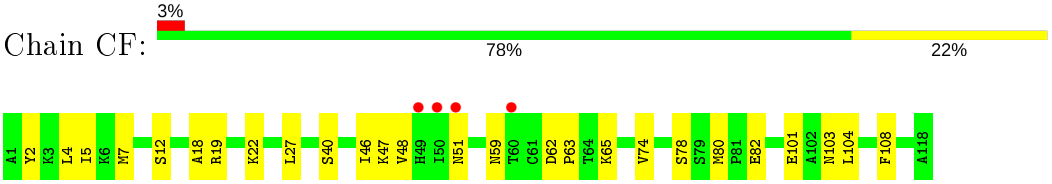
• Molecule 1: coat protein

Chain CE:



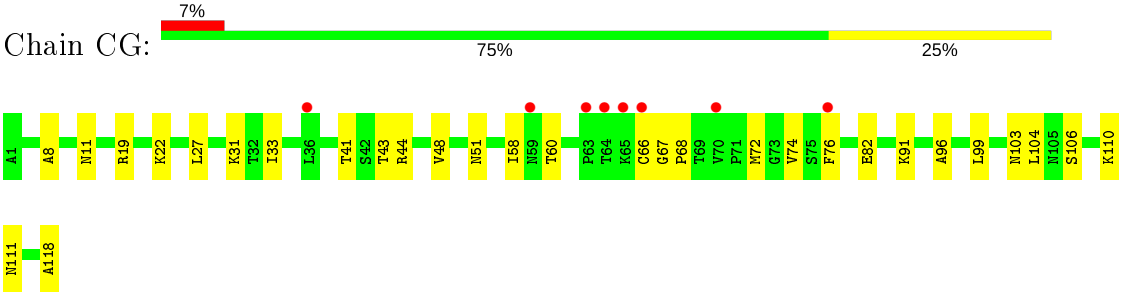
• Molecule 1: coat protein

Chain CF:



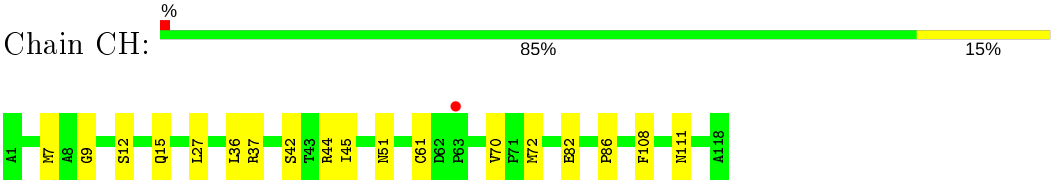
• Molecule 1: coat protein

Chain CG:



• Molecule 1: coat protein

Chain CH:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	283.35Å 283.35Å 666.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.94 – 3.23 48.94 – 3.23	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.94-3.23) 97.9 (48.94-3.23)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.232 , 0.232 0.230 , 0.231	Depositor DCC
R_{free} test set	10054 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å^2)	120.1	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 62.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.013 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.009 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.017 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.010 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.017 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.010 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.033 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	52380	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.31	0/884	0.53	0/1198
1	AB	0.31	0/884	0.53	0/1198
1	AC	0.31	0/884	0.54	0/1198
1	AD	0.31	0/884	0.53	0/1198
1	AE	0.31	0/884	0.53	0/1198
1	AF	0.32	0/884	0.54	0/1198
1	AG	0.31	0/884	0.53	0/1198
1	AH	0.32	0/884	0.53	0/1198
1	AI	0.32	0/884	0.54	0/1198
1	AJ	0.31	0/884	0.53	0/1198
1	AK	0.32	0/884	0.53	0/1198
1	AL	0.32	0/884	0.54	0/1198
1	AM	0.31	0/884	0.53	0/1198
1	AN	0.32	0/884	0.53	0/1198
1	AO	0.32	0/884	0.54	0/1198
1	AP	0.31	0/884	0.53	0/1198
1	AQ	0.32	0/884	0.53	0/1198
1	AR	0.32	0/884	0.54	0/1198
1	AS	0.31	0/884	0.53	0/1198
1	AT	0.31	0/884	0.53	0/1198
1	AU	0.31	0/884	0.54	0/1198
1	AV	0.31	0/884	0.53	0/1198
1	AW	0.32	0/884	0.53	0/1198
1	AX	0.32	0/884	0.54	0/1198
1	AY	0.31	0/884	0.53	0/1198
1	AZ	0.32	0/884	0.53	0/1198
1	BA	0.31	0/884	0.54	0/1198
1	BB	0.31	0/884	0.53	0/1198
1	BC	0.31	0/884	0.53	0/1198
1	BD	0.31	0/884	0.54	0/1198
1	BE	0.31	0/884	0.53	0/1198
1	BF	0.32	0/884	0.53	0/1198
1	BG	0.32	0/884	0.54	0/1198
1	BH	0.31	0/884	0.53	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	BI	0.31	0/884	0.53	0/1198
1	BJ	0.32	0/884	0.54	0/1198
1	BK	0.31	0/884	0.53	0/1198
1	BL	0.31	0/884	0.53	0/1198
1	BM	0.32	0/884	0.54	0/1198
1	BN	0.31	0/884	0.53	0/1198
1	BO	0.31	0/884	0.53	0/1198
1	BP	0.31	0/884	0.54	0/1198
1	BQ	0.31	0/884	0.53	0/1198
1	BR	0.31	0/884	0.53	0/1198
1	BS	0.32	0/884	0.54	0/1198
1	BT	0.31	0/884	0.53	0/1198
1	BU	0.31	0/884	0.53	0/1198
1	BV	0.32	0/884	0.54	0/1198
1	BW	0.31	0/884	0.53	0/1198
1	BX	0.31	0/884	0.53	0/1198
1	BY	0.32	0/884	0.54	0/1198
1	BZ	0.31	0/884	0.53	0/1198
1	CA	0.31	0/884	0.53	0/1198
1	CB	0.32	0/884	0.54	0/1198
1	CC	0.31	0/884	0.53	0/1198
1	CD	0.31	0/884	0.53	0/1198
1	CE	0.31	0/884	0.54	0/1198
1	CF	0.31	0/884	0.53	0/1198
1	CG	0.32	0/884	0.53	0/1198
1	CH	0.32	0/884	0.54	0/1198
All	All	0.31	0/53040	0.53	0/71880

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	873	0	895	32	0
1	AB	873	0	895	18	0
1	AC	873	0	895	22	0
1	AD	873	0	896	12	0
1	AE	873	0	896	19	0
1	AF	873	0	895	19	0
1	AG	873	0	895	24	0
1	AH	873	0	895	34	0
1	AI	873	0	895	21	0
1	AJ	873	0	896	24	0
1	AK	873	0	895	27	0
1	AL	873	0	895	41	0
1	AM	873	0	896	27	0
1	AN	873	0	895	22	0
1	AO	873	0	897	8	0
1	AP	873	0	895	25	0
1	AQ	873	0	896	10	0
1	AR	873	0	896	16	1
1	AS	873	0	895	31	0
1	AT	873	0	895	22	0
1	AU	873	0	895	13	0
1	AV	873	0	896	13	1
1	AW	873	0	896	19	0
1	AX	873	0	895	22	0
1	AY	873	0	895	22	0
1	AZ	873	0	895	33	0
1	BA	873	0	895	18	0
1	BB	873	0	895	38	0
1	BC	873	0	896	9	0
1	BD	873	0	896	15	0
1	BE	873	0	895	32	0
1	BF	873	0	895	25	0
1	BG	873	0	895	25	0
1	BH	873	0	895	26	0
1	BI	873	0	895	24	0
1	BJ	873	0	895	21	0
1	BK	873	0	896	15	0
1	BL	873	0	896	24	0
1	BM	873	0	895	16	0
1	BN	873	0	895	27	0
1	BO	873	0	896	11	0
1	BP	873	0	896	37	0
1	BQ	873	0	896	13	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	873	0	896	20	0
1	BS	873	0	895	17	0
1	BT	873	0	895	20	0
1	BU	873	0	895	24	0
1	BV	873	0	895	16	0
1	BW	873	0	895	20	0
1	BX	873	0	896	11	1
1	BY	873	0	896	22	0
1	BZ	873	0	896	43	0
1	CA	873	0	895	22	0
1	CB	873	0	896	8	0
1	CC	873	0	895	20	0
1	CD	873	0	895	23	0
1	CE	873	0	895	17	0
1	CF	873	0	895	24	0
1	CG	873	0	895	29	0
1	CH	873	0	895	17	0
All	All	52380	0	53722	899	2

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 8.

The worst 5 of 899 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:AI:7:MET:HG2	1:BZ:108:PHE:HE1	1.28	0.95
1:AI:7:MET:HG2	1:BZ:108:PHE:CE1	2.03	0.93
1:AL:15:GLN:HE22	1:BP:111:ASN:HA	1.38	0.89
1:AL:111:ASN:HA	1:BP:15:GLN:HE22	1.42	0.85
1:AS:27:LEU:HD21	1:BF:96:ALA:HB2	1.57	0.84

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:66:CYS:SG	1:BQ:61:CYS:SG[2_555]	1.80	0.40
1:AV:103:ASN:O	1:BX:31:LYS:NZ[2_555]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	AB	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	AC	116/118 (98%)	116 (100%)	0	0	100	100
1	AD	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	AE	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	AF	116/118 (98%)	116 (100%)	0	0	100	100
1	AG	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	AH	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	AI	116/118 (98%)	116 (100%)	0	0	100	100
1	AJ	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	AK	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	AL	116/118 (98%)	116 (100%)	0	0	100	100
1	AM	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	AN	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	AO	116/118 (98%)	116 (100%)	0	0	100	100
1	AP	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	AQ	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	AR	116/118 (98%)	116 (100%)	0	0	100	100
1	AS	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	AT	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	AU	116/118 (98%)	116 (100%)	0	0	100	100
1	AV	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	AW	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	AX	116/118 (98%)	116 (100%)	0	0	100	100
1	AY	116/118 (98%)	115 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AZ	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	BA	116/118 (98%)	116 (100%)	0	0	100	100
1	BB	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	BC	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	BD	116/118 (98%)	116 (100%)	0	0	100	100
1	BE	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	BF	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	BG	116/118 (98%)	116 (100%)	0	0	100	100
1	BH	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	BI	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	BJ	116/118 (98%)	116 (100%)	0	0	100	100
1	BK	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	BL	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	BM	116/118 (98%)	116 (100%)	0	0	100	100
1	BN	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	BO	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	BP	116/118 (98%)	116 (100%)	0	0	100	100
1	BQ	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	BR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	BS	116/118 (98%)	116 (100%)	0	0	100	100
1	BT	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	BU	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	BV	116/118 (98%)	116 (100%)	0	0	100	100
1	BW	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	BX	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	BY	116/118 (98%)	116 (100%)	0	0	100	100
1	BZ	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	CA	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	CB	116/118 (98%)	116 (100%)	0	0	100	100
1	CC	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	CD	116/118 (98%)	114 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CE	116/118 (98%)	116 (100%)	0	0	100	100
1	CF	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
1	CG	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	CH	116/118 (98%)	116 (100%)	0	0	100	100
All	All	6960/7080 (98%)	6900 (99%)	60 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	98/98 (100%)	98 (100%)	0	100	100
1	AB	98/98 (100%)	98 (100%)	0	100	100
1	AC	98/98 (100%)	97 (99%)	1 (1%)	76	88
1	AD	98/98 (100%)	98 (100%)	0	100	100
1	AE	98/98 (100%)	98 (100%)	0	100	100
1	AF	98/98 (100%)	97 (99%)	1 (1%)	76	88
1	AG	98/98 (100%)	98 (100%)	0	100	100
1	AH	98/98 (100%)	98 (100%)	0	100	100
1	AI	98/98 (100%)	97 (99%)	1 (1%)	76	88
1	AJ	98/98 (100%)	98 (100%)	0	100	100
1	AK	98/98 (100%)	98 (100%)	0	100	100
1	AL	98/98 (100%)	97 (99%)	1 (1%)	76	88
1	AM	98/98 (100%)	98 (100%)	0	100	100
1	AN	98/98 (100%)	98 (100%)	0	100	100
1	AO	98/98 (100%)	97 (99%)	1 (1%)	76	88
1	AP	98/98 (100%)	98 (100%)	0	100	100
1	AQ	98/98 (100%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AR	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	AS	98/98 (100%)	98 (100%)	0	100 100
1	AT	98/98 (100%)	98 (100%)	0	100 100
1	AU	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	AV	98/98 (100%)	98 (100%)	0	100 100
1	AW	98/98 (100%)	98 (100%)	0	100 100
1	AX	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	AY	98/98 (100%)	98 (100%)	0	100 100
1	AZ	98/98 (100%)	98 (100%)	0	100 100
1	BA	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	BB	98/98 (100%)	98 (100%)	0	100 100
1	BC	98/98 (100%)	98 (100%)	0	100 100
1	BD	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	BE	98/98 (100%)	98 (100%)	0	100 100
1	BF	98/98 (100%)	98 (100%)	0	100 100
1	BG	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	BH	98/98 (100%)	98 (100%)	0	100 100
1	BI	98/98 (100%)	98 (100%)	0	100 100
1	BJ	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	BK	98/98 (100%)	98 (100%)	0	100 100
1	BL	98/98 (100%)	98 (100%)	0	100 100
1	BM	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	BN	98/98 (100%)	98 (100%)	0	100 100
1	BO	98/98 (100%)	98 (100%)	0	100 100
1	BP	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	BQ	98/98 (100%)	98 (100%)	0	100 100
1	BR	98/98 (100%)	98 (100%)	0	100 100
1	BS	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	BT	98/98 (100%)	98 (100%)	0	100 100
1	BU	98/98 (100%)	98 (100%)	0	100 100
1	BV	98/98 (100%)	97 (99%)	1 (1%)	76 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	BW	98/98 (100%)	98 (100%)	0	100 100
1	BX	98/98 (100%)	98 (100%)	0	100 100
1	BY	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	BZ	98/98 (100%)	98 (100%)	0	100 100
1	CA	98/98 (100%)	98 (100%)	0	100 100
1	CB	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	CC	98/98 (100%)	98 (100%)	0	100 100
1	CD	98/98 (100%)	98 (100%)	0	100 100
1	CE	98/98 (100%)	97 (99%)	1 (1%)	76 88
1	CF	98/98 (100%)	98 (100%)	0	100 100
1	CG	98/98 (100%)	98 (100%)	0	100 100
1	CH	98/98 (100%)	97 (99%)	1 (1%)	76 88
All	All	5880/5880 (100%)	5860 (100%)	20 (0%)	92 96

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BD	61	CYS
1	BG	61	CYS
1	BY	61	CYS
1	AX	61	CYS
1	BA	61	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	BD	38	ASN
1	BI	15	GLN
1	CG	15	GLN
1	BD	111	ASN
1	BG	15	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	118/118 (100%)	0.26	5 (4%) 36 25	53, 84, 186, 256	0
1	AB	118/118 (100%)	0.55	8 (6%) 17 12	53, 85, 203, 280	0
1	AC	118/118 (100%)	0.19	4 (3%) 45 33	54, 83, 206, 294	0
1	AD	118/118 (100%)	0.09	0 100 100	53, 84, 186, 256	0
1	AE	118/118 (100%)	0.33	5 (4%) 36 25	53, 85, 203, 280	0
1	AF	118/118 (100%)	0.01	1 (0%) 86 80	54, 83, 206, 294	0
1	AG	118/118 (100%)	-0.00	0 100 100	53, 84, 186, 256	0
1	AH	118/118 (100%)	0.43	9 (7%) 13 9	53, 85, 203, 280	0
1	AI	118/118 (100%)	0.10	2 (1%) 70 60	54, 83, 206, 294	0
1	AJ	118/118 (100%)	0.17	3 (2%) 57 46	53, 84, 186, 256	0
1	AK	118/118 (100%)	0.43	11 (9%) 8 6	53, 85, 203, 280	0
1	AL	118/118 (100%)	0.05	3 (2%) 57 46	54, 83, 206, 294	0
1	AM	118/118 (100%)	0.13	1 (0%) 86 80	53, 84, 186, 256	0
1	AN	118/118 (100%)	0.40	6 (5%) 28 18	53, 85, 203, 280	0
1	AO	118/118 (100%)	0.27	3 (2%) 57 46	54, 83, 206, 294	0
1	AP	118/118 (100%)	0.26	6 (5%) 28 18	53, 84, 186, 256	0
1	AQ	118/118 (100%)	0.38	5 (4%) 36 25	53, 85, 203, 280	0
1	AR	118/118 (100%)	0.19	3 (2%) 57 46	54, 83, 206, 294	0
1	AS	118/118 (100%)	0.15	2 (1%) 70 60	53, 84, 186, 256	0
1	AT	118/118 (100%)	0.17	4 (3%) 45 33	53, 85, 203, 280	0
1	AU	118/118 (100%)	-0.04	1 (0%) 86 80	54, 83, 206, 294	0
1	AV	118/118 (100%)	0.19	0 100 100	53, 84, 186, 256	0
1	AW	118/118 (100%)	0.13	4 (3%) 45 33	53, 85, 203, 280	0
1	AX	118/118 (100%)	0.24	3 (2%) 57 46	54, 83, 206, 294	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AY	118/118 (100%)	0.29	3 (2%) 57 46	53, 84, 186, 256	0
1	AZ	118/118 (100%)	0.35	5 (4%) 36 25	53, 85, 203, 280	0
1	BA	118/118 (100%)	0.20	1 (0%) 86 80	54, 83, 206, 294	0
1	BB	118/118 (100%)	0.31	0 100 100	53, 84, 186, 256	0
1	BC	118/118 (100%)	0.37	5 (4%) 36 25	53, 85, 203, 280	0
1	BD	118/118 (100%)	0.16	1 (0%) 86 80	54, 83, 206, 294	0
1	BE	118/118 (100%)	0.12	1 (0%) 86 80	53, 84, 186, 256	0
1	BF	118/118 (100%)	0.44	7 (5%) 22 15	53, 85, 203, 280	0
1	BG	118/118 (100%)	0.11	1 (0%) 86 80	54, 83, 206, 294	0
1	BH	118/118 (100%)	0.03	2 (1%) 70 60	53, 84, 186, 256	0
1	BI	118/118 (100%)	0.17	5 (4%) 36 25	53, 85, 203, 280	0
1	BJ	118/118 (100%)	0.05	1 (0%) 86 80	54, 83, 206, 294	0
1	BK	118/118 (100%)	0.22	3 (2%) 57 46	53, 84, 186, 256	0
1	BL	118/118 (100%)	0.45	6 (5%) 28 18	53, 85, 203, 280	0
1	BM	118/118 (100%)	0.29	2 (1%) 70 60	54, 83, 206, 294	0
1	BN	118/118 (100%)	0.22	3 (2%) 57 46	53, 84, 186, 256	0
1	BO	118/118 (100%)	0.44	6 (5%) 28 18	53, 85, 203, 280	0
1	BP	118/118 (100%)	0.05	2 (1%) 70 60	54, 83, 206, 294	0
1	BQ	118/118 (100%)	0.14	0 100 100	53, 84, 186, 256	0
1	BR	118/118 (100%)	0.38	5 (4%) 36 25	53, 85, 203, 280	0
1	BS	118/118 (100%)	0.19	2 (1%) 70 60	54, 83, 206, 294	0
1	BT	118/118 (100%)	0.21	4 (3%) 45 33	53, 84, 186, 256	0
1	BU	118/118 (100%)	0.17	5 (4%) 36 25	53, 85, 203, 280	0
1	BV	118/118 (100%)	0.05	2 (1%) 70 60	54, 83, 206, 294	0
1	BW	118/118 (100%)	0.08	0 100 100	53, 84, 186, 256	0
1	BX	118/118 (100%)	0.42	5 (4%) 36 25	53, 85, 203, 280	0
1	BY	118/118 (100%)	0.22	2 (1%) 70 60	54, 83, 206, 294	0
1	BZ	118/118 (100%)	0.21	1 (0%) 86 80	53, 84, 186, 256	0
1	CA	118/118 (100%)	0.49	8 (6%) 17 12	53, 85, 203, 280	0
1	CB	118/118 (100%)	0.21	1 (0%) 86 80	54, 83, 206, 294	0
1	CC	118/118 (100%)	0.18	1 (0%) 86 80	53, 84, 186, 256	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	CD	118/118 (100%)	0.24	8 (6%) 17 12	53, 85, 203, 280	0
1	CE	118/118 (100%)	0.21	4 (3%) 45 33	54, 83, 206, 294	0
1	CF	118/118 (100%)	0.28	4 (3%) 45 33	53, 84, 186, 256	0
1	CG	118/118 (100%)	0.27	8 (6%) 17 12	53, 85, 203, 280	0
1	CH	118/118 (100%)	-0.06	1 (0%) 86 80	54, 83, 206, 294	0
All	All	7080/7080 (100%)	0.22	204 (2%) 51 40	53, 84, 203, 294	0

The worst 5 of 204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BM	63	PRO	15.0
1	BR	63	PRO	14.8
1	BR	64	THR	11.8
1	BL	63	PRO	11.0
1	BD	63	PRO	11.0

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 monosaccharides 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.