wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 06:25 PM EDT

PDB ID	:	6YFC
Title	:	Virus-like particle of bacteriophage AVE019
Authors	:	Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on	:	2020-03-26
Resolution	:	3.25 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

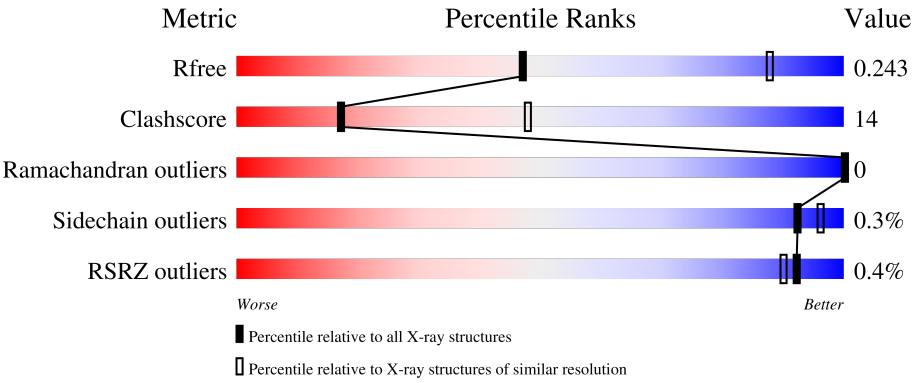
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.25 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	124	69% 31%
1	AB	124	2% 60% 34% 6%
1	AC	124	70% 30%
1	AD	124	% 69% 31%
1	AE	124	2% 57% 36% • 6%

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Mol	Chain	Length	Quality of chain
1	AF	124	69% 31%
1	AG	124	70% 30%
1	AH	124	% 65% 28% • 6%
1	AI	124	69% 31%
1	AJ	124	67% 33%
1	AK	124	% 60% 34% 6%
1	AL	124	69% 31%
1	AM	124	62% 38%
1	AN	124	60% 34% • 6%
1	AO	124	70% 30%
1	AP	124	67% 33%
1	AQ	124	% 64% 30% • 6%
1	AR	124	65% 35%
1	AS	124	65% 35%
1	AT	124	% 69% 26% 6%
1	AU	124	70% 30%
1	AV	124	% 68% 32%
1	AW	124	?% 62% 32% 6%
1	AX	124	65% 35%
1	AY	124	65% 35%
1	AZ	124	% 66% 27% • 6%
1	BA	124	70% 30%
1	BB	124	71% 29%
1	BC	124	65% 29% 6%
1	BD	124	67% 33%

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Mol	Chain	Length	Quality of chain
1	BE	124	71% 29%
1	BF	124	% 65% 29% 6%
1	BG	124	71% 29%
1	BH	124	70% 30%
1	BI	124	% 63% 31% 6%
1	BJ	124	71% 29%
1	BK	124	2% 65% 35%
1	BL	124	% 64% 30% 6%
1	BM	124	68% 32%
1	BN	124	% 65% 35%
1	BO	124	% 64% 30% 6%
1	BP	124	73% 27%
1	BQ	124	72% 28%
1	BR	124	% 68% 26% 6%
1	BS	124	72% 28%
1	BT	124	63% 37%
1	BU	124	63% 31% 6%
1	BV	124	72% 28%
1	BW	124	70% 30%
1	BX	124	% 62% 32% 6%
1	BY	124	69% 31%
1	BZ	124	67% 33%
1	CA	124	% 61% 32% 6%
1	CB	124	62% 38%
1	CC	124	65% 35%

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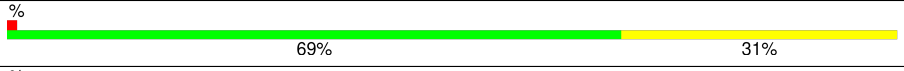
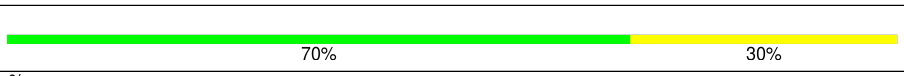
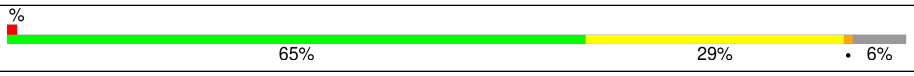
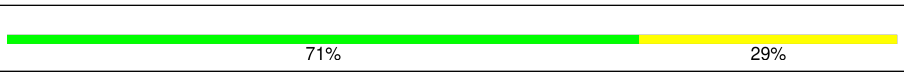
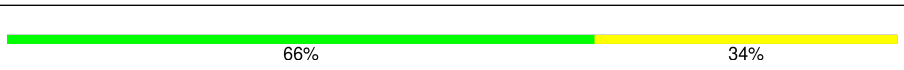
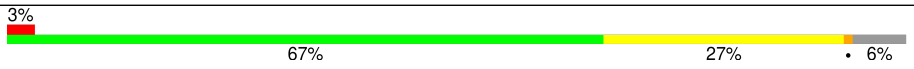
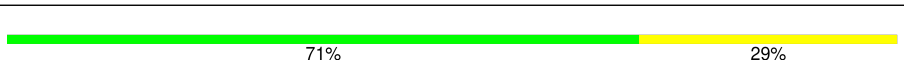
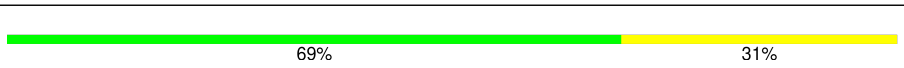
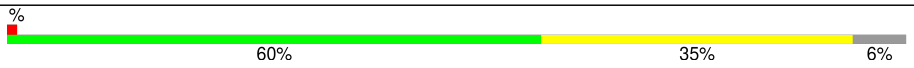
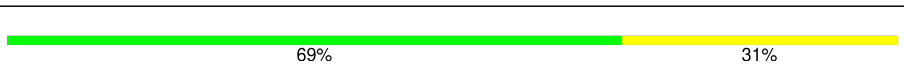
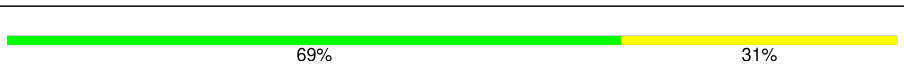
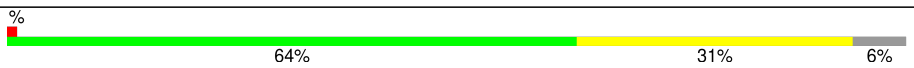
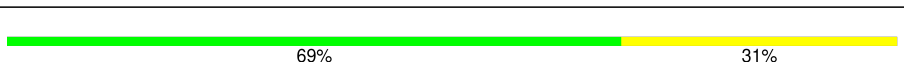
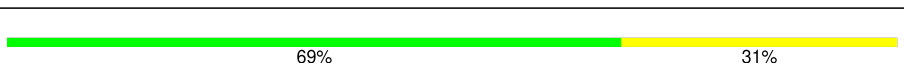
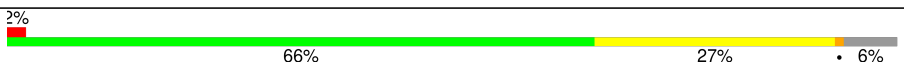
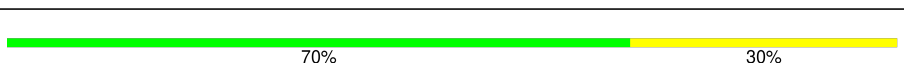
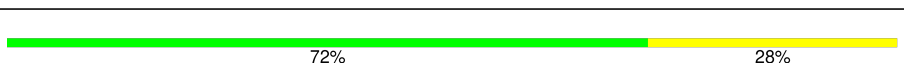
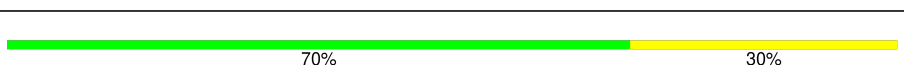
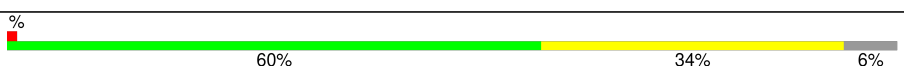
Mol	Chain	Length	Quality of chain
1	CD	124	
1	CE	124	
1	CF	124	
1	CG	124	
1	CH	124	
1	CI	124	
1	CJ	124	
1	CK	124	
1	CL	124	
1	CM	124	
1	CN	124	
1	CO	124	
1	CP	124	
1	CQ	124	
1	CR	124	
1	CS	124	
1	CT	124	
1	CU	124	
1	CV	124	
1	CW	124	
1	CX	124	
1	CY	124	
1	CZ	124	
1	DA	124	
1	DB	124	

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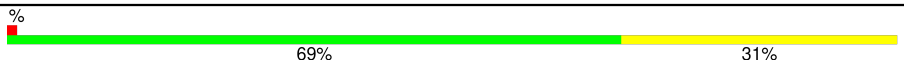
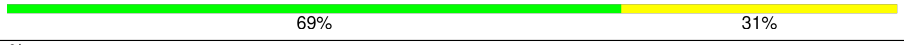
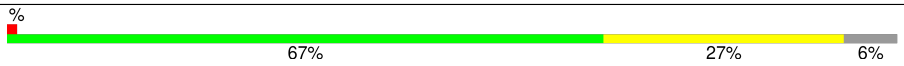
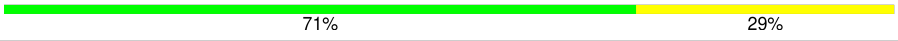
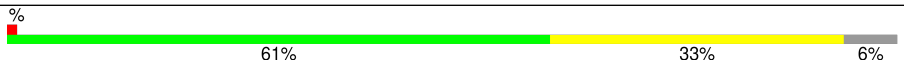
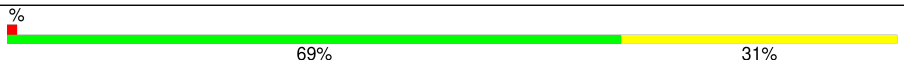
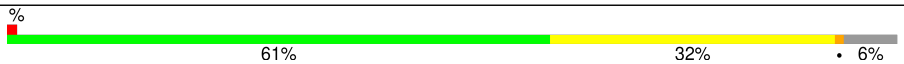
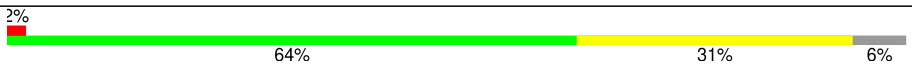
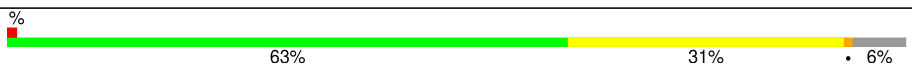
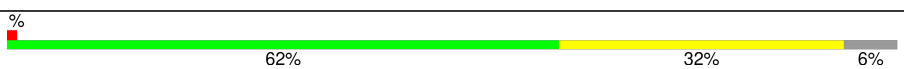
Mol	Chain	Length	Quality of chain
1	DC	124	
1	DD	124	
1	DE	124	
1	DF	124	
1	DG	124	
1	DH	124	
1	DI	124	
1	DJ	124	
1	DK	124	
1	DL	124	
1	DM	124	
1	DN	124	
1	DO	124	
1	DP	124	
1	DQ	124	
1	DR	124	
1	DS	124	
1	DT	124	
1	DU	124	
1	DV	124	
1	DW	124	
1	DX	124	
1	DY	124	
1	DZ	124	
1	EA	124	

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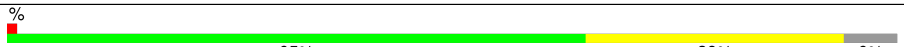
Mol	Chain	Length	Quality of chain
1	EB	124	
1	EC	124	
1	ED	124	
1	EE	124	
1	EF	124	
1	EG	124	
1	EH	124	
1	EI	124	
1	EJ	124	
1	EK	124	
1	EL	124	
1	EM	124	
1	EN	124	
1	EO	124	
1	EP	124	
1	EQ	124	
1	ER	124	
1	ES	124	
1	ET	124	
1	EU	124	
1	EV	124	
1	EW	124	
1	EX	124	
1	EY	124	
1	EZ	124	

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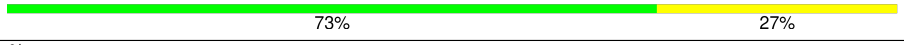
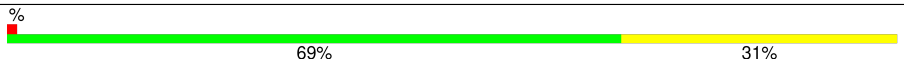
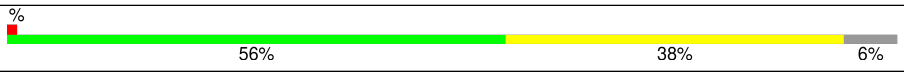
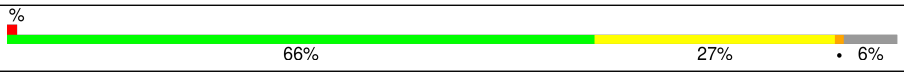
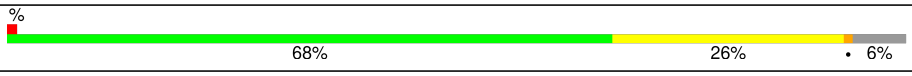
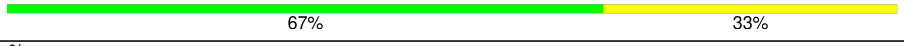
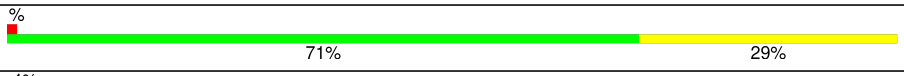
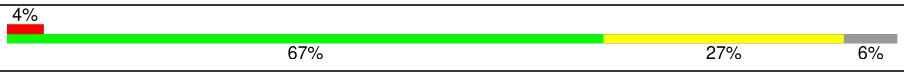
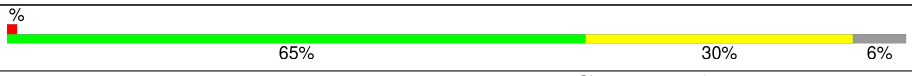
Mol	Chain	Length	Quality of chain
1	FA	124	
1	FB	124	
1	FC	124	
1	FD	124	
1	FE	124	
1	FF	124	
1	FG	124	
1	FH	124	
1	FI	124	
1	FJ	124	
1	FK	124	
1	FL	124	
1	FM	124	
1	FN	124	
1	FO	124	
1	FP	124	
1	FQ	124	
1	FR	124	
1	FS	124	
1	FT	124	
1	FU	124	
1	FV	124	
1	FW	124	
1	FX	124	
1	FY	124	

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Mol	Chain	Length	Quality of chain
1	FZ	124	71% 29%
1	GA	124	62% 38%
1	GB	124	64% 30% • 6%
1	GC	124	70% 30%
1	GD	124	69% 31%
1	GE	124	% 59% 35% • 6%
1	GF	124	68% 32%
1	GG	124	66% 34%
1	GH	124	4% 65% 30% 6%
1	GI	124	69% 31%
1	GJ	124	68% 32%
1	GK	124	57% 36% • 6%
1	GL	124	68% 32%
1	GM	124	% 65% 35%
1	GN	124	64% 30% • 6%
1	GO	124	67% 33%
1	GP	124	70% 30%
1	GQ	124	2% 64% 31% 6%
1	GR	124	71% 29%
1	GS	124	71% 29%
1	GT	124	% 65% 29% • 6%
1	GU	124	69% 31%
1	GV	124	69% 31%
1	GW	124	65% 29% 6%
1	GX	124	72% 28%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 169260 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	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AB	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AC	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AD	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AE	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AF	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AG	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AH	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AI	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AJ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AK	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AL	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AM	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AN	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AO	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AP	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AR	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AS	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AT	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AU	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AV	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AW	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AX	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AY	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AZ	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	BA	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BB	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BC	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	BD	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BE	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BF	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	BG	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BH	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BI	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	BJ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BK	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	BM	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BN	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BO	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	BP	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BQ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BR	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	BS	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BT	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BU	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	BV	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BW	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BX	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	BY	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	BZ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CA	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	CB	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CC	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CD	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	CE	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CF	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	CH	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CI	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CJ	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	CK	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CL	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CM	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	CN	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CO	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CP	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	CQ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CR	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CS	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	CT	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CU	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CV	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	CW	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CX	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	CY	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	CZ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DA	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DB	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	DC	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DD	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DE	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	DF	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DG	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DH	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	DI	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DJ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DK	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	DL	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DM	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DN	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	DO	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DP	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DQ	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	DR	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DS	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DT	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	DU	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DV	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DW	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	DX	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DY	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	DZ	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	EA	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EB	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EC	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	ED	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EE	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EF	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	EG	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EH	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EI	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	EJ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EK	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EL	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	EM	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EN	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EO	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	EP	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EQ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	ER	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	ES	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	ET	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EU	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	EV	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EW	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EX	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	EY	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	EZ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FA	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	FB	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FC	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FD	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	FE	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FF	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FG	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	FH	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FI	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FJ	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	FK	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FL	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	FM	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	FN	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FO	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FP	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	FQ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FR	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FS	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	FT	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FU	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FV	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	FW	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FX	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	FY	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	FZ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GA	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GB	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	GC	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GD	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GE	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	GF	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GG	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	GH	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	GI	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GJ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GK	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	GL	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GM	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GN	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	GO	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GP	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GQ	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	GR	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GS	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GT	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	GU	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GV	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	GW	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	GX	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AA	1	Total	Ca	0	0
			1	1		
2	AD	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AG	1	Total Ca 1 1	0	0
2	AJ	1	Total Ca 1 1	0	0
2	AM	1	Total Ca 1 1	0	0
2	AP	1	Total Ca 1 1	0	0
2	AS	1	Total Ca 1 1	0	0
2	AV	1	Total Ca 1 1	0	0
2	AY	1	Total Ca 1 1	0	0
2	BB	1	Total Ca 1 1	0	0
2	BE	1	Total Ca 1 1	0	0
2	BH	1	Total Ca 1 1	0	0
2	BK	1	Total Ca 1 1	0	0
2	BN	1	Total Ca 1 1	0	0
2	BQ	1	Total Ca 1 1	0	0
2	BT	1	Total Ca 1 1	0	0
2	BW	1	Total Ca 1 1	0	0
2	BZ	1	Total Ca 1 1	0	0
2	CC	1	Total Ca 1 1	0	0
2	CF	1	Total Ca 1 1	0	0
2	CI	1	Total Ca 1 1	0	0
2	CL	1	Total Ca 1 1	0	0
2	CO	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	CR	1	Total Ca 1 1	0	0
2	CU	1	Total Ca 1 1	0	0
2	CX	1	Total Ca 1 1	0	0
2	DA	1	Total Ca 1 1	0	0
2	DD	1	Total Ca 1 1	0	0
2	DG	1	Total Ca 1 1	0	0
2	DJ	1	Total Ca 1 1	0	0
2	DM	1	Total Ca 1 1	0	0
2	DP	1	Total Ca 1 1	0	0
2	DS	1	Total Ca 1 1	0	0
2	DV	1	Total Ca 1 1	0	0
2	DY	1	Total Ca 1 1	0	0
2	EB	1	Total Ca 1 1	0	0
2	EE	1	Total Ca 1 1	0	0
2	EH	1	Total Ca 1 1	0	0
2	EK	1	Total Ca 1 1	0	0
2	EN	1	Total Ca 1 1	0	0
2	EQ	1	Total Ca 1 1	0	0
2	ET	1	Total Ca 1 1	0	0
2	EW	1	Total Ca 1 1	0	0
2	EZ	1	Total Ca 1 1	0	0

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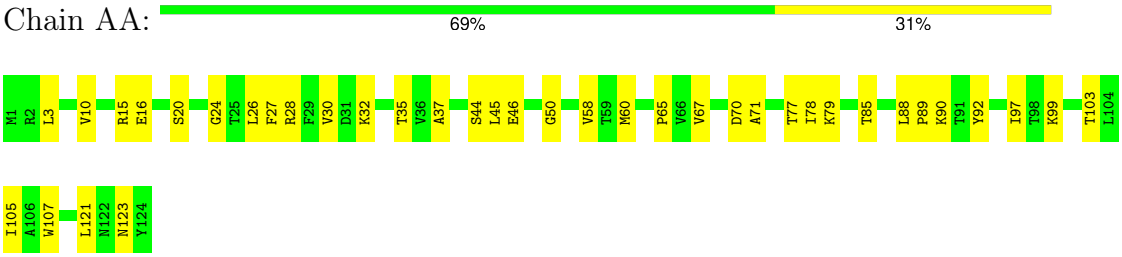
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	FC	1	Total Ca 1 1	0	0
2	FF	1	Total Ca 1 1	0	0
2	FI	1	Total Ca 1 1	0	0
2	FL	1	Total Ca 1 1	0	0
2	FO	1	Total Ca 1 1	0	0
2	FR	1	Total Ca 1 1	0	0
2	FU	1	Total Ca 1 1	0	0
2	FX	1	Total Ca 1 1	0	0
2	GA	1	Total Ca 1 1	0	0
2	GD	1	Total Ca 1 1	0	0
2	GG	1	Total Ca 1 1	0	0
2	GJ	1	Total Ca 1 1	0	0
2	GM	1	Total Ca 1 1	0	0
2	GP	1	Total Ca 1 1	0	0
2	GS	1	Total Ca 1 1	0	0
2	GV	1	Total Ca 1 1	0	0

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.

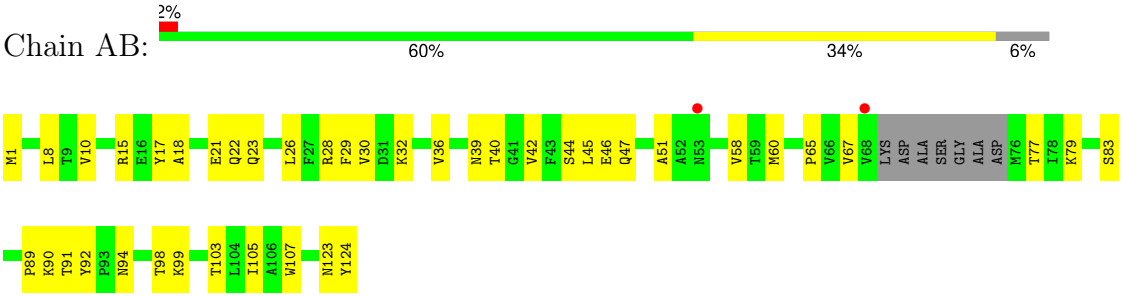
• Molecule 1: coat protein

Chain AA:



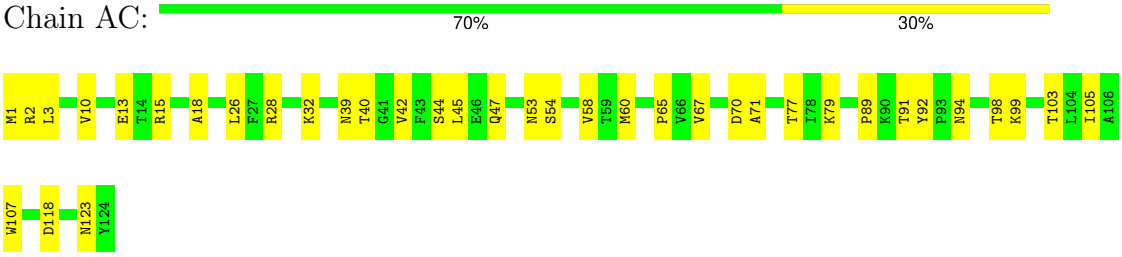
• Molecule 1: coat protein

Chain AB:



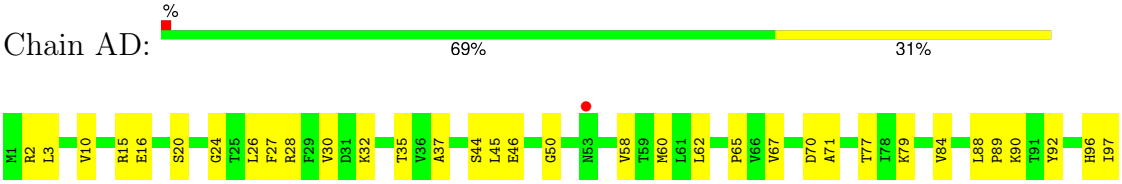
• Molecule 1: coat protein

Chain AC:



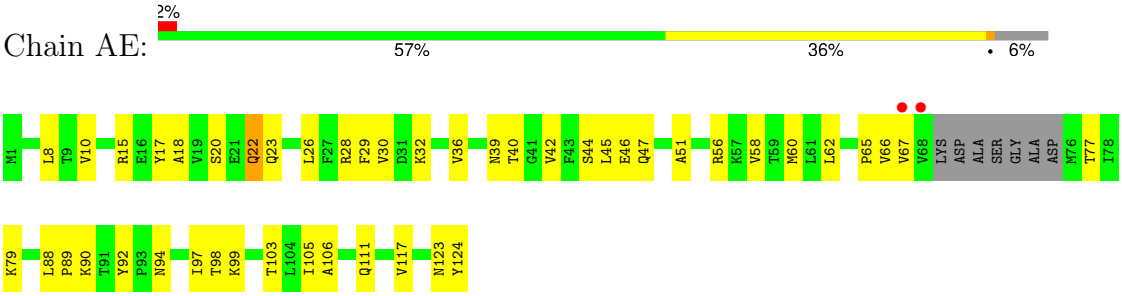
• Molecule 1: coat protein

Chain AD:



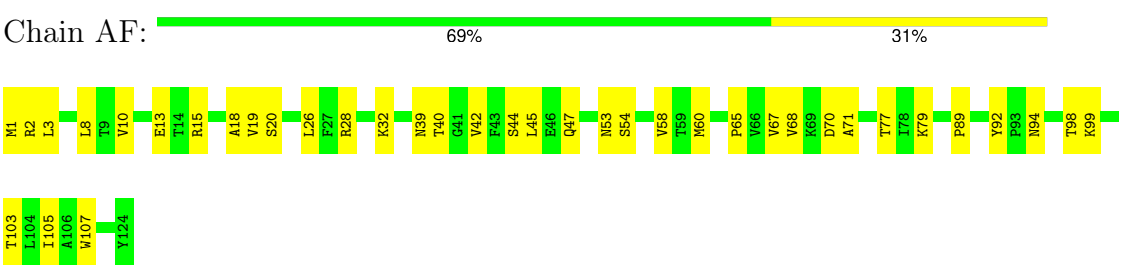
• Molecule 1: coat protein

Chain AE:



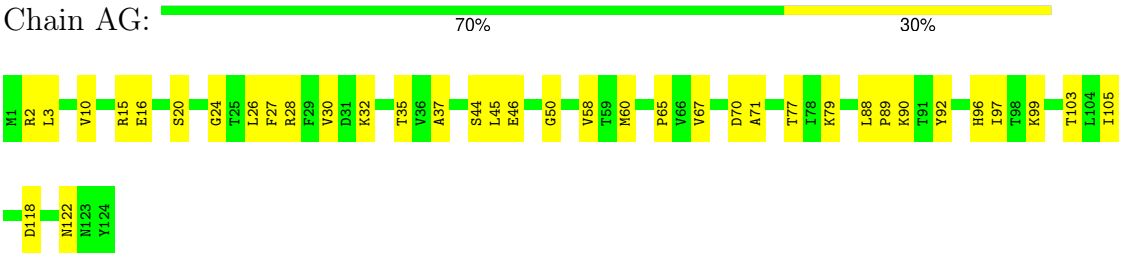
• Molecule 1: coat protein

Chain AF:



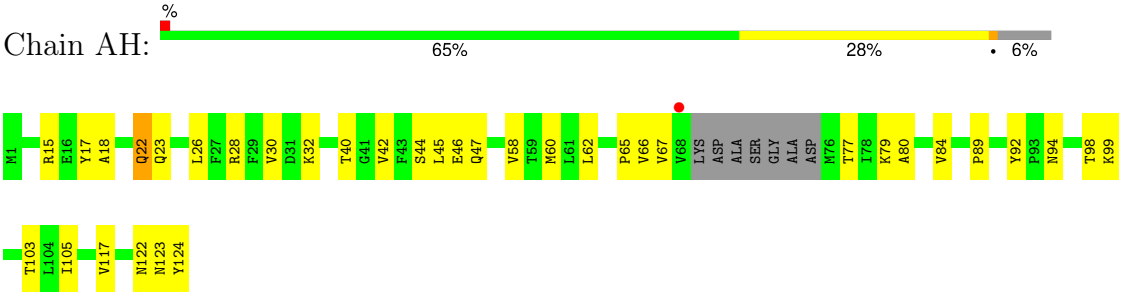
• Molecule 1: coat protein

Chain AG:



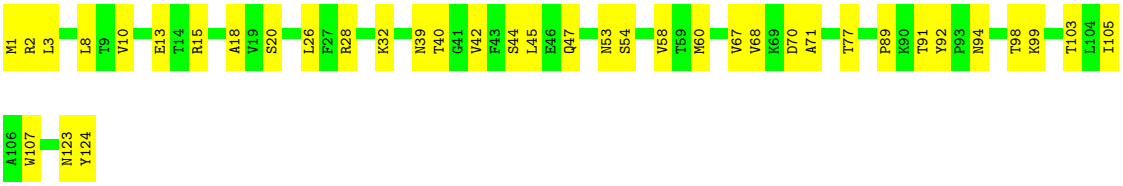
• Molecule 1: coat protein

Chain AH:



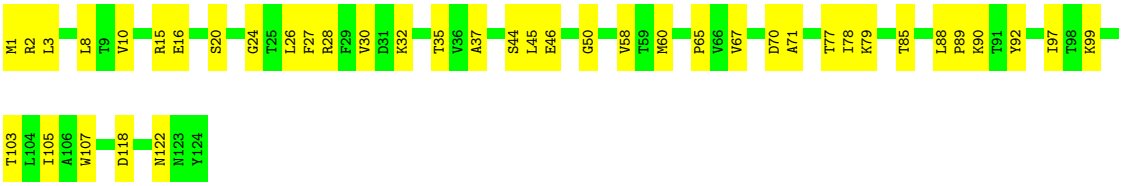
• Molecule 1: coat protein

Chain AI:



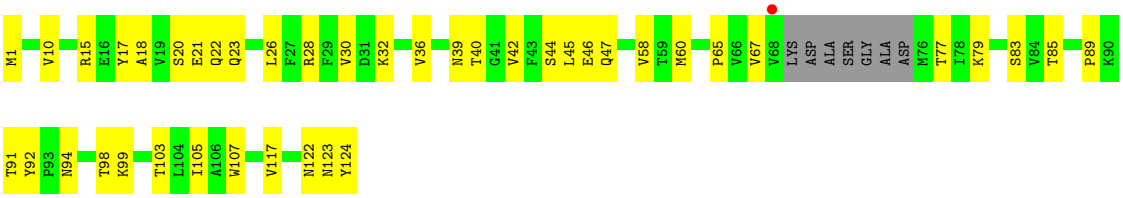
• Molecule 1: coat protein

Chain AJ:



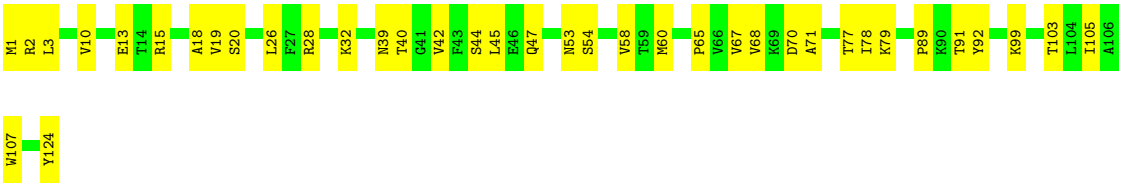
• Molecule 1: coat protein

Chain AK:



• Molecule 1: coat protein

Chain AL:

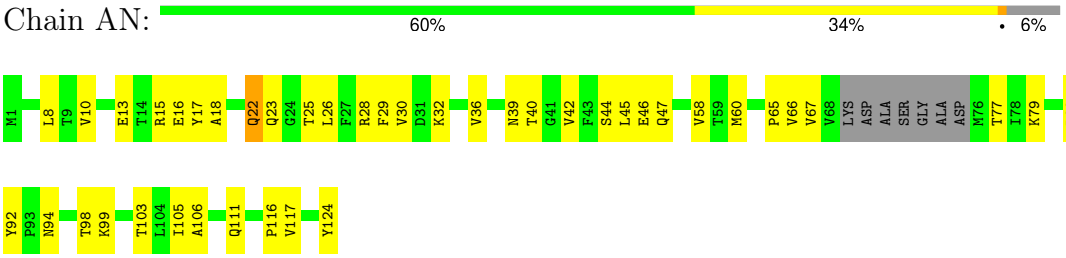


• Molecule 1: coat protein

Chain AM:

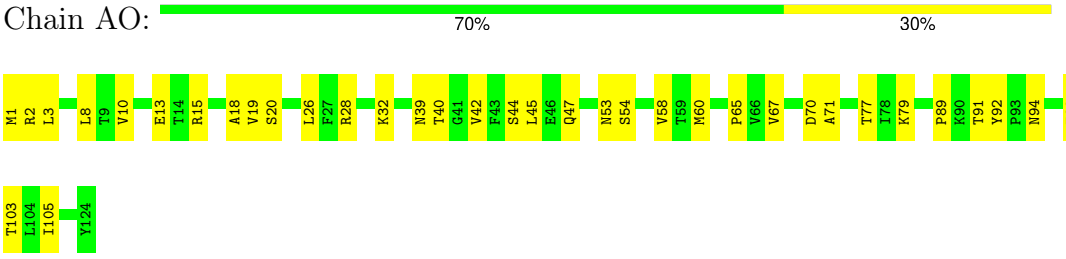
• Molecule 1: coat protein

Chain AN:



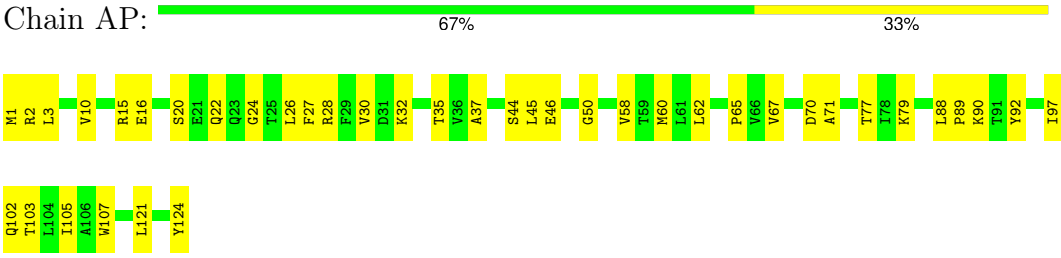
• Molecule 1: coat protein

Chain AO:



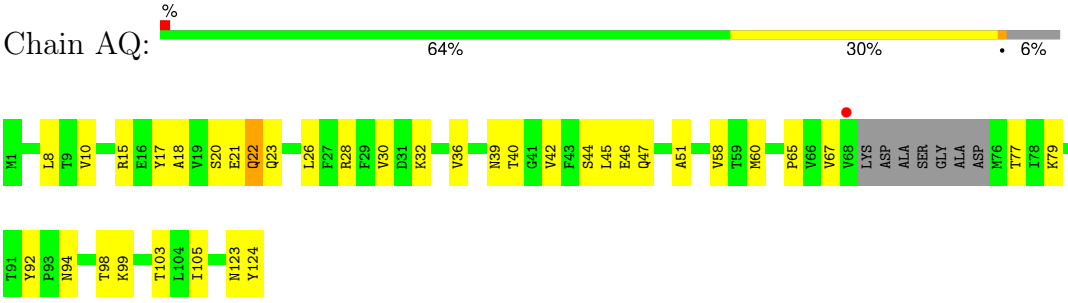
• Molecule 1: coat protein

Chain AP:



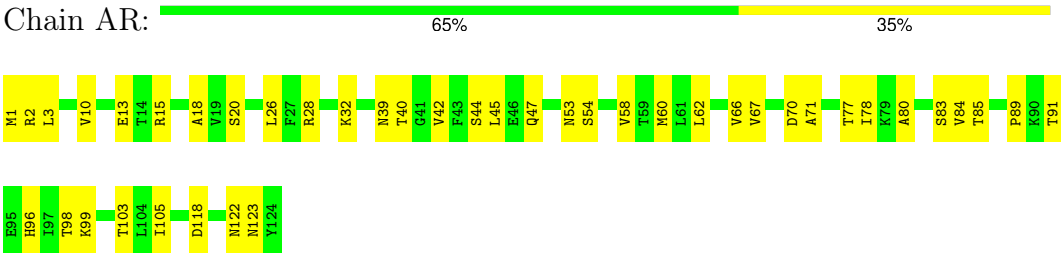
• Molecule 1: coat protein

Chain AQ:



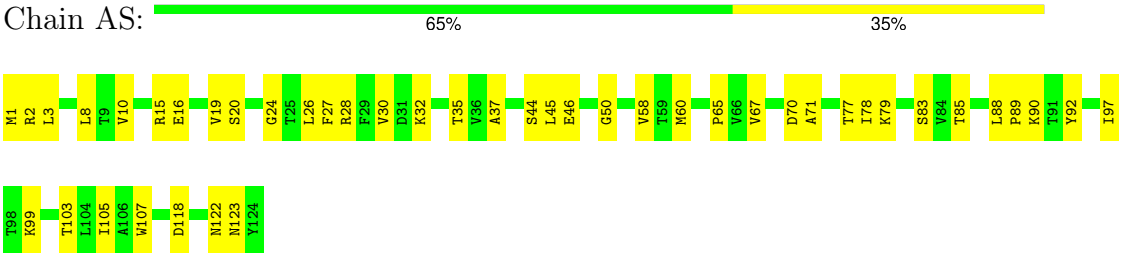
• Molecule 1: coat protein

Chain AR:



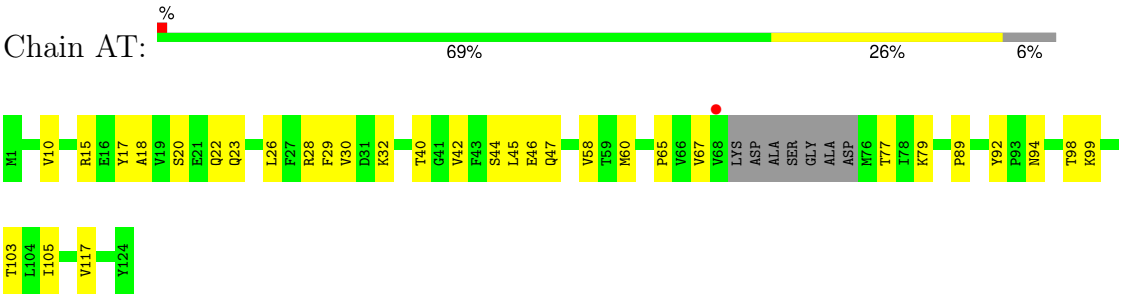
• Molecule 1: coat protein

Chain AS:



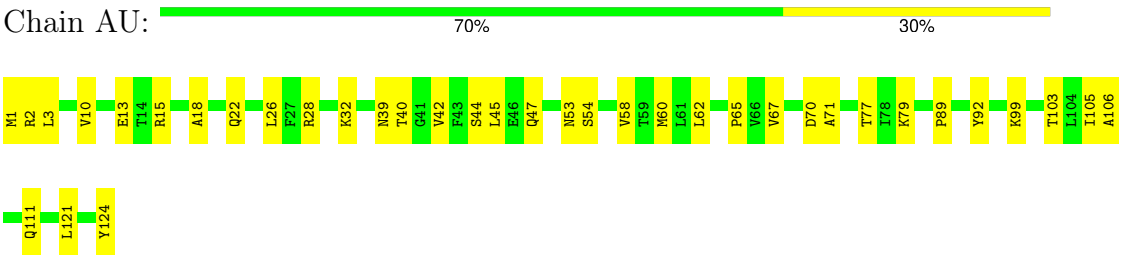
• Molecule 1: coat protein

Chain AT:



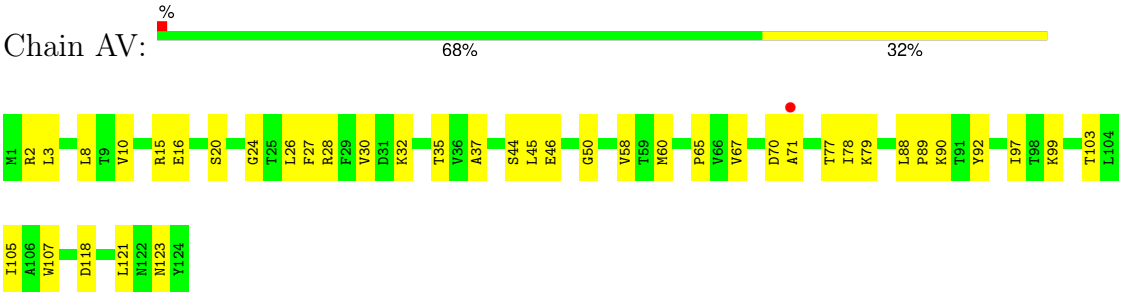
• Molecule 1: coat protein

Chain AU:



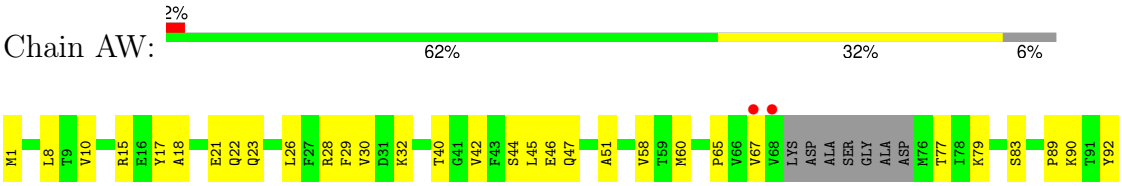
• Molecule 1: coat protein

Chain AV:



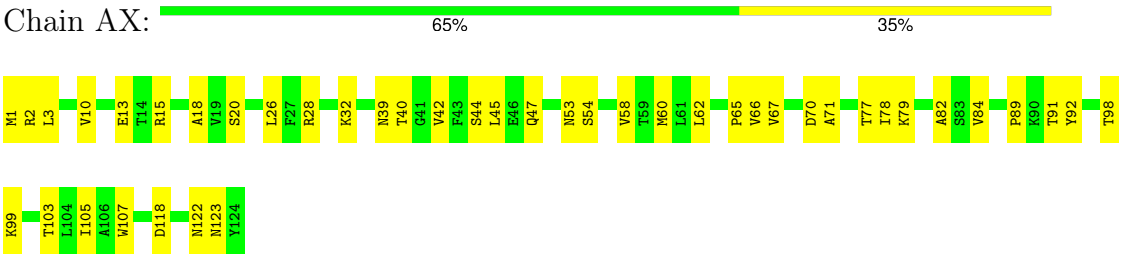
• Molecule 1: coat protein

Chain AW:



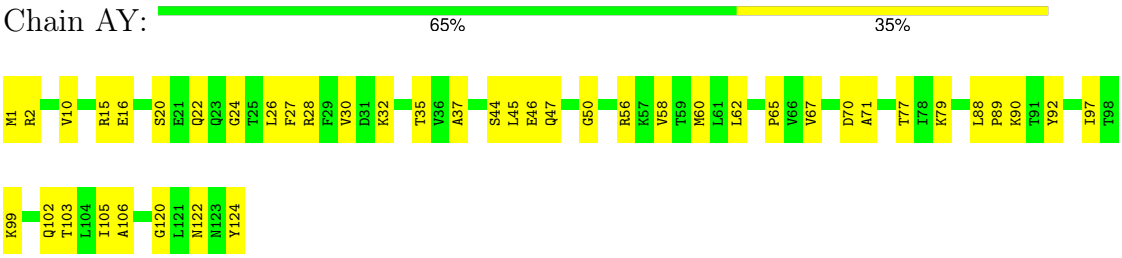
• Molecule 1: coat protein

Chain AX:



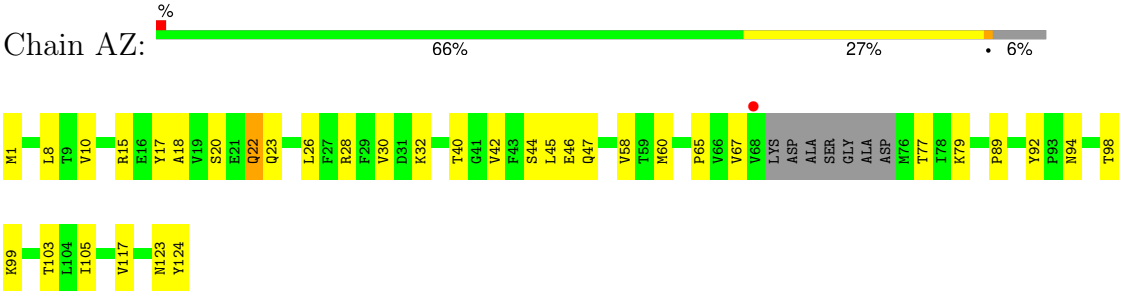
• Molecule 1: coat protein

Chain AY:



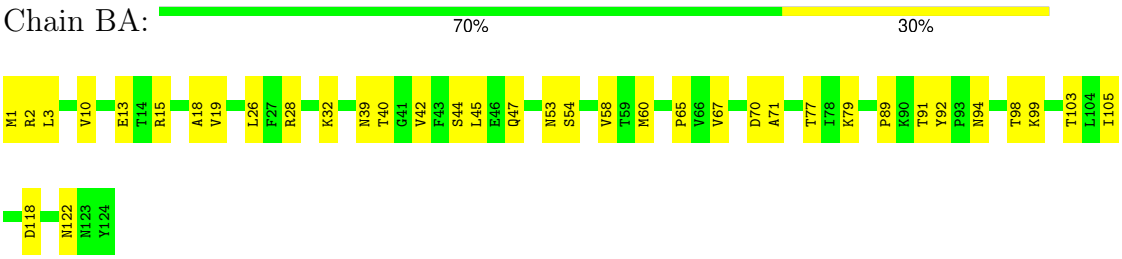
• Molecule 1: coat protein

Chain AZ:



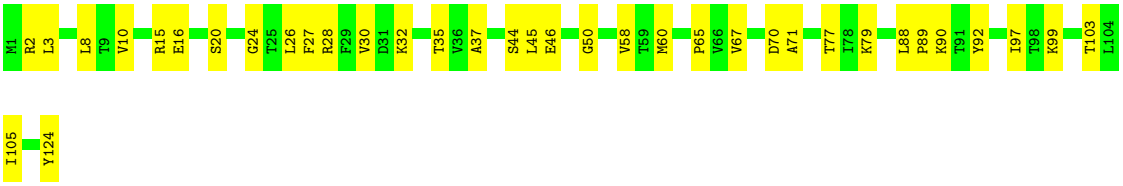
• Molecule 1: coat protein

Chain BA:



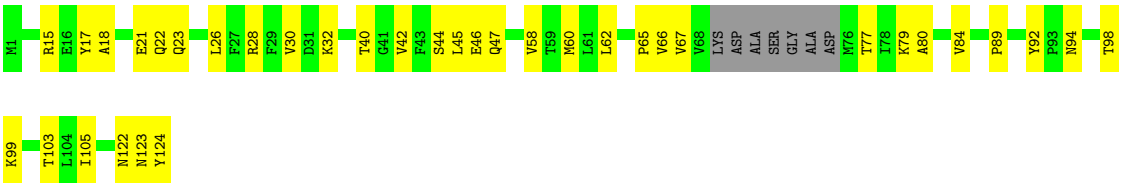
• Molecule 1: coat protein

Chain BB:



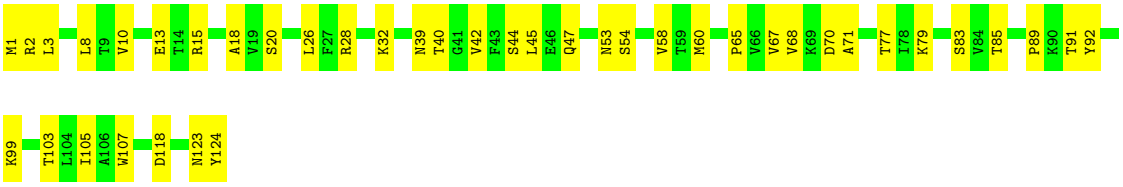
• Molecule 1: coat protein

Chain BC:



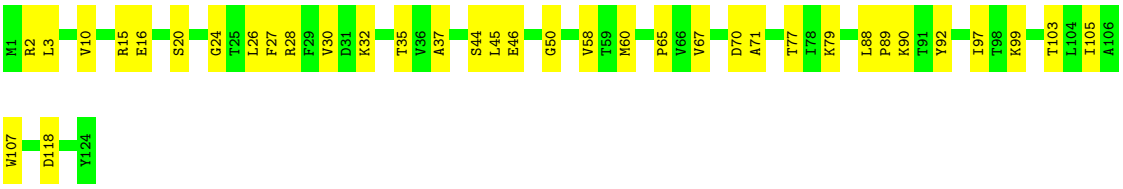
• Molecule 1: coat protein

Chain BD:



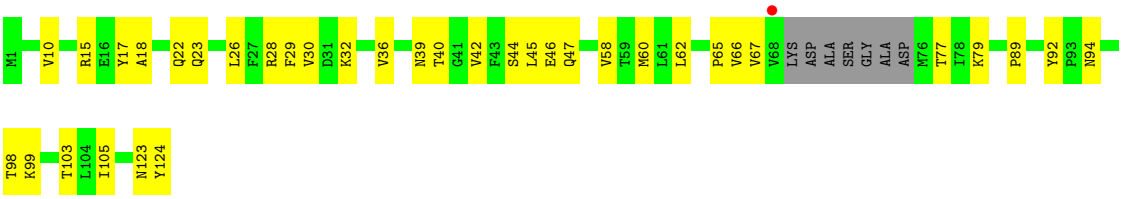
• Molecule 1: coat protein

Chain BE:



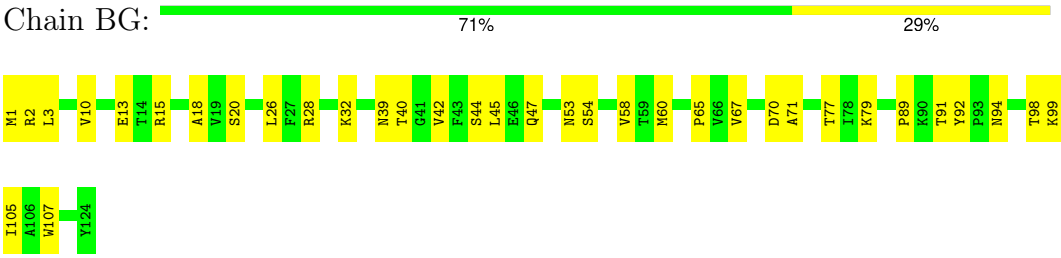
• Molecule 1: coat protein

Chain BF:



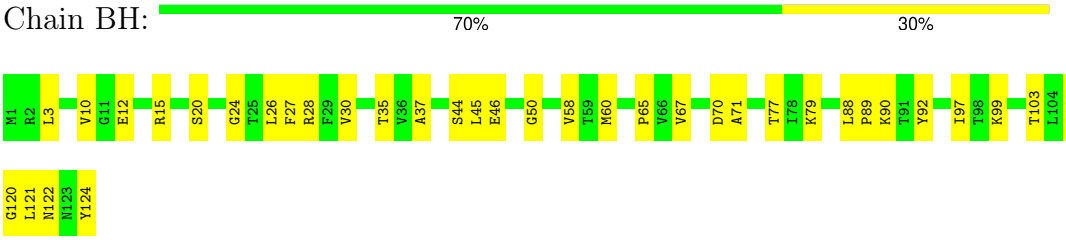
• Molecule 1: coat protein

Chain BG:



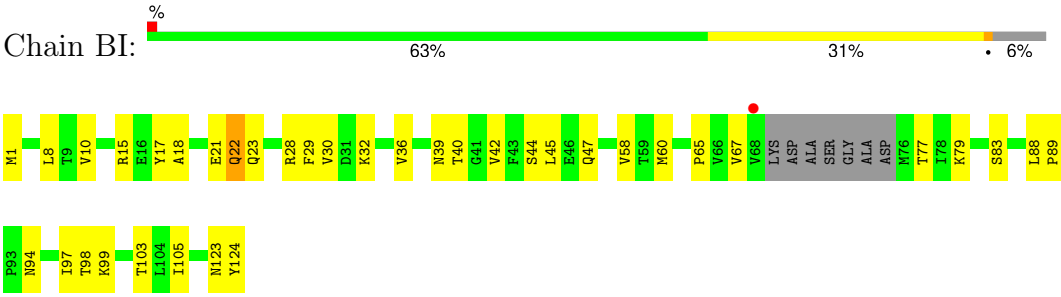
• Molecule 1: coat protein

Chain BH:



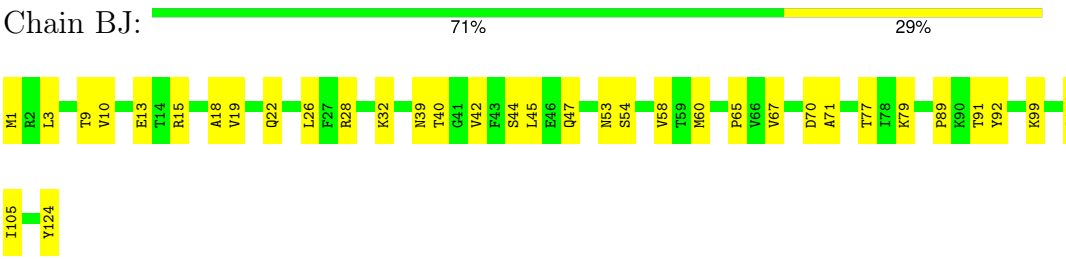
• Molecule 1: coat protein

Chain BI:



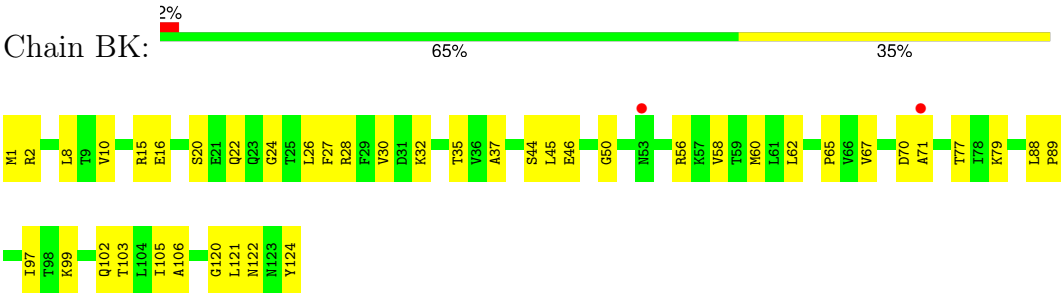
• Molecule 1: coat protein

Chain BJ:



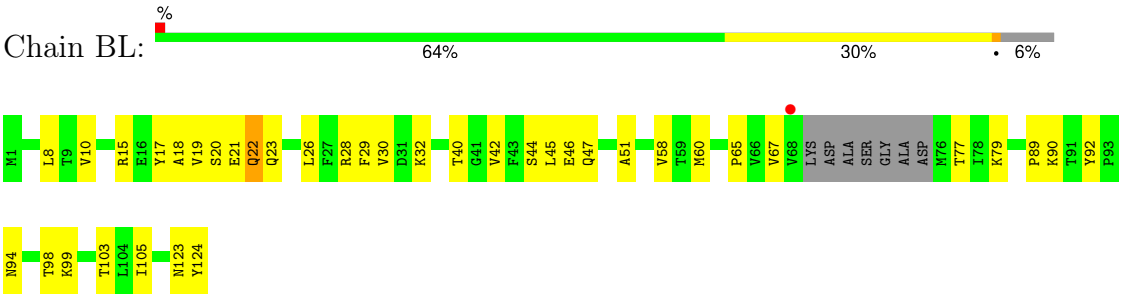
• Molecule 1: coat protein

Chain BK:



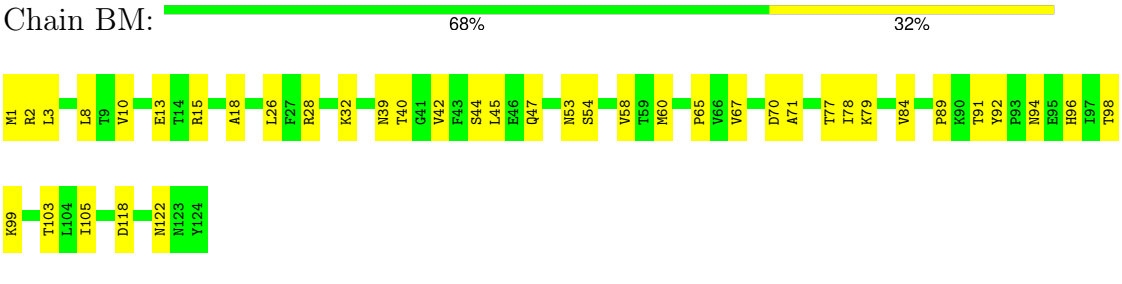
• Molecule 1: coat protein

Chain BL:



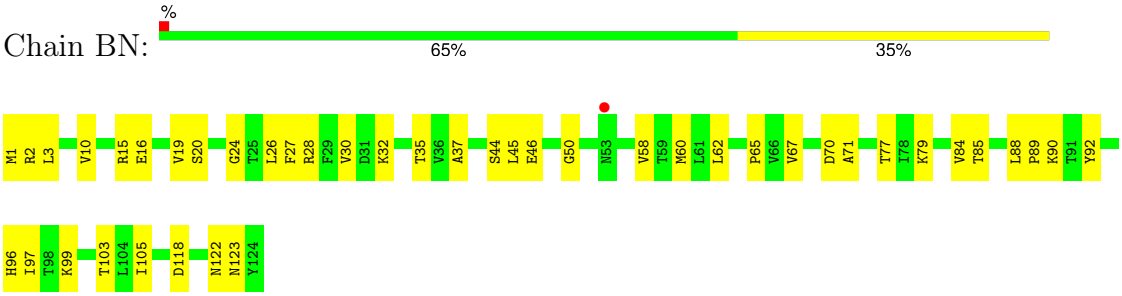
• Molecule 1: coat protein

Chain BM:



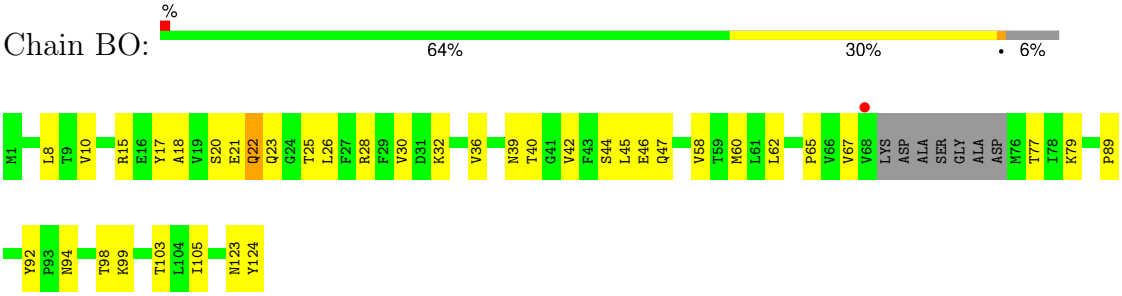
• Molecule 1: coat protein

Chain BN:



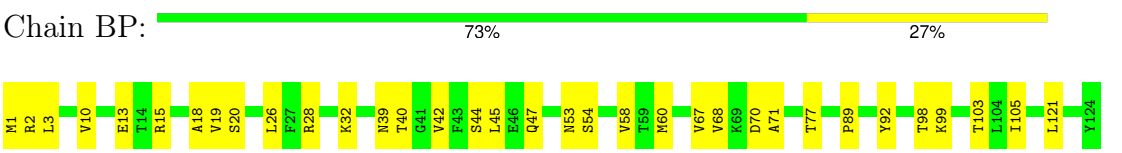
• Molecule 1: coat protein

Chain BO:



• Molecule 1: coat protein

Chain BP:



• Molecule 1: coat protein

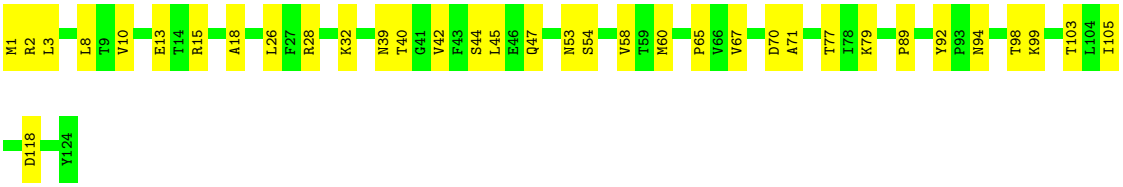
Chain BQ:

• Molecule 1: coat protein

Chain BR:

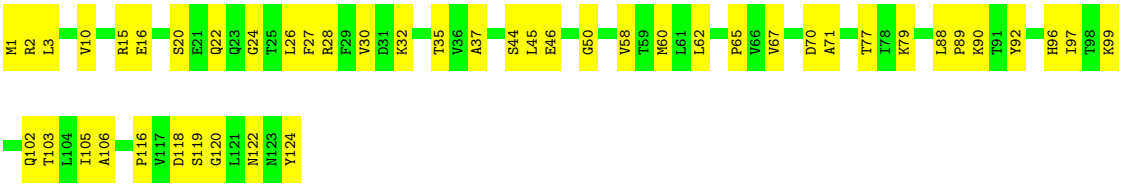
• Molecule 1: coat protein

Chain BS:



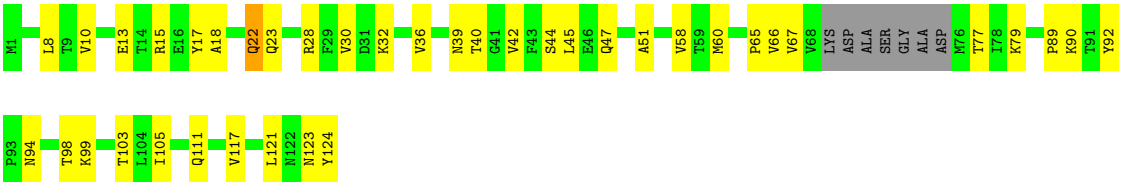
• Molecule 1: coat protein

Chain BT:



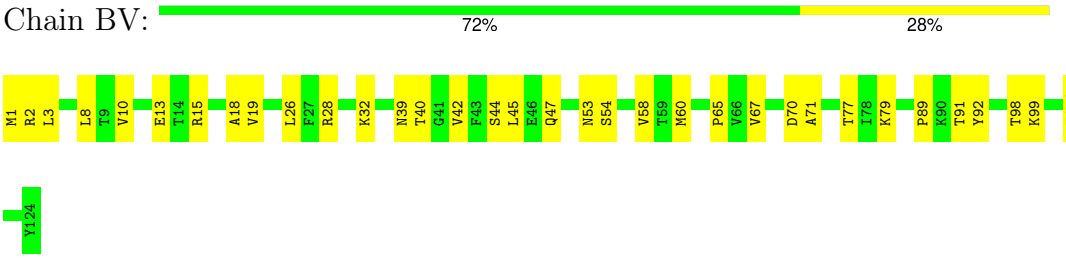
• Molecule 1: coat protein

Chain BU:



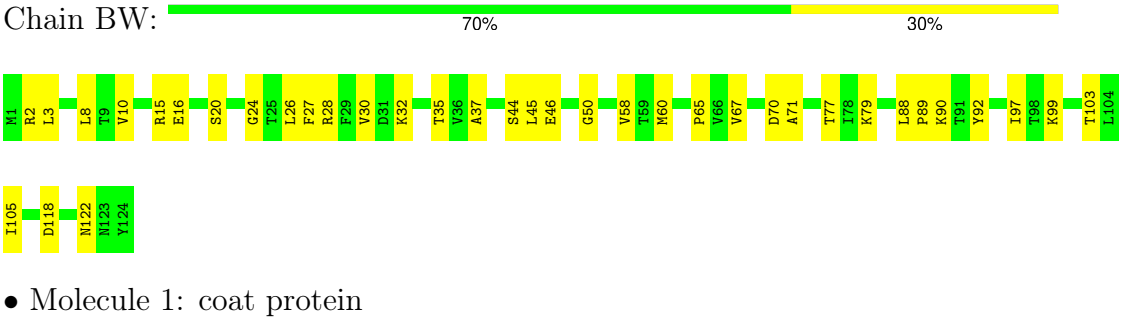
• Molecule 1: coat protein

Chain BV:



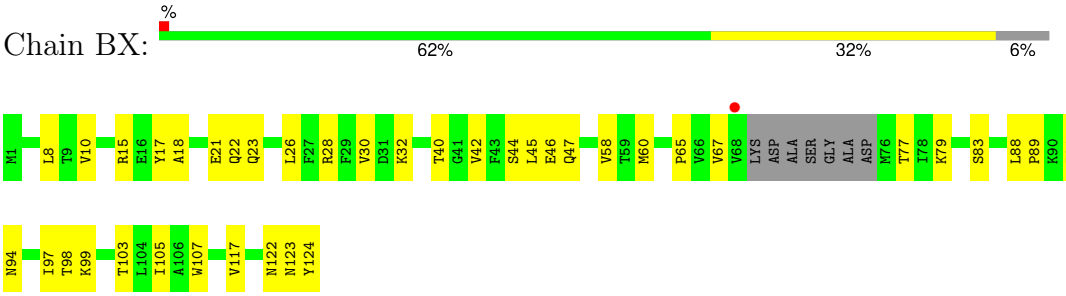
• Molecule 1: coat protein

Chain BW:



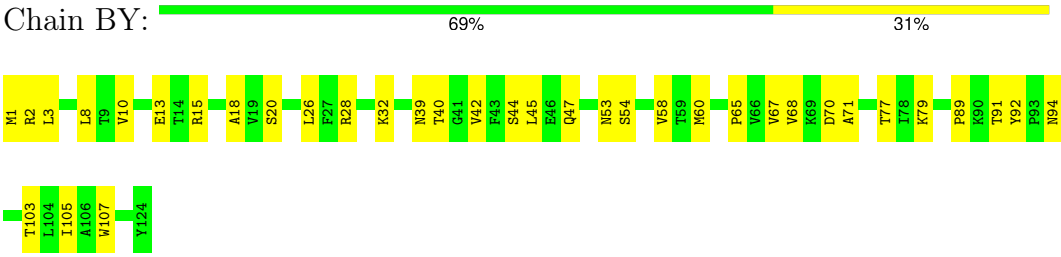
• Molecule 1: coat protein

Chain BX:



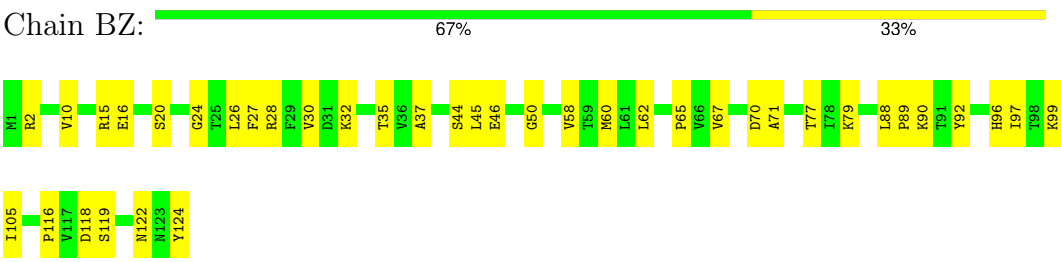
• Molecule 1: coat protein

Chain BY:



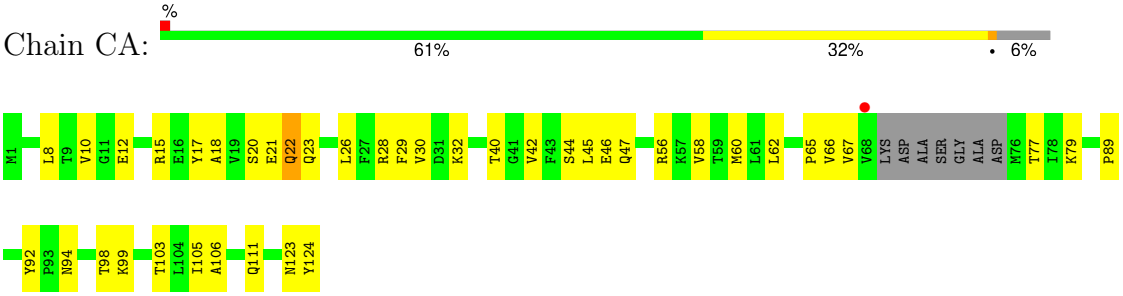
• Molecule 1: coat protein

Chain BZ:



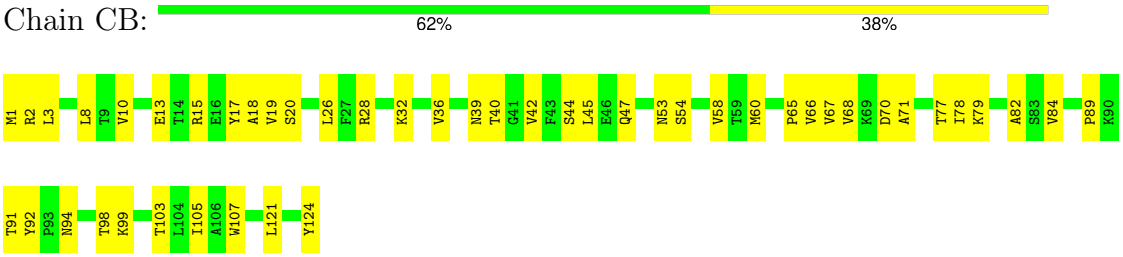
• Molecule 1: coat protein

Chain CA:



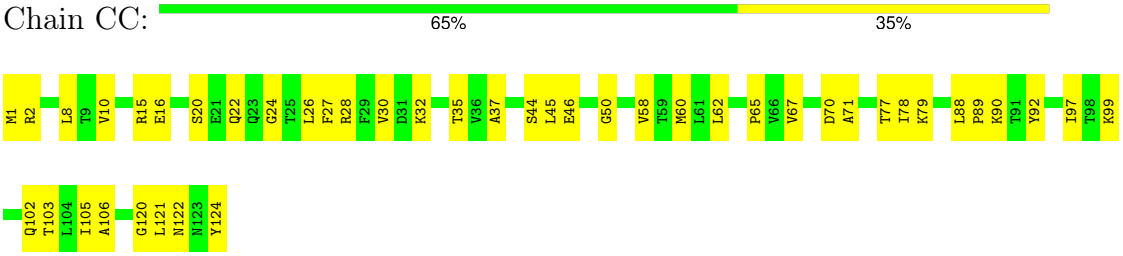
• Molecule 1: coat protein

Chain CB:



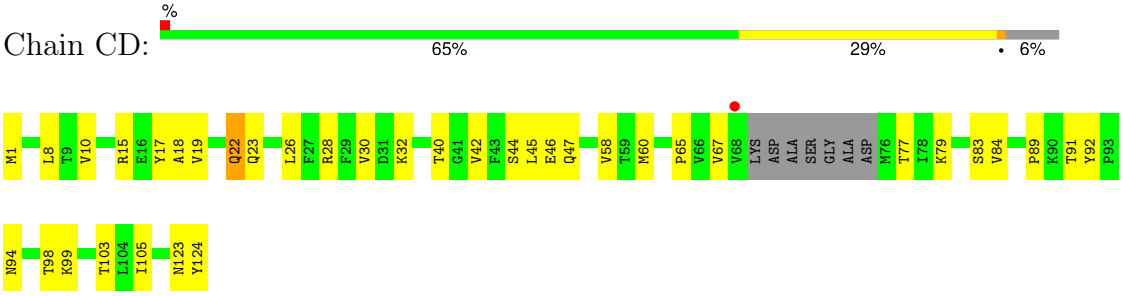
• Molecule 1: coat protein

Chain CC:



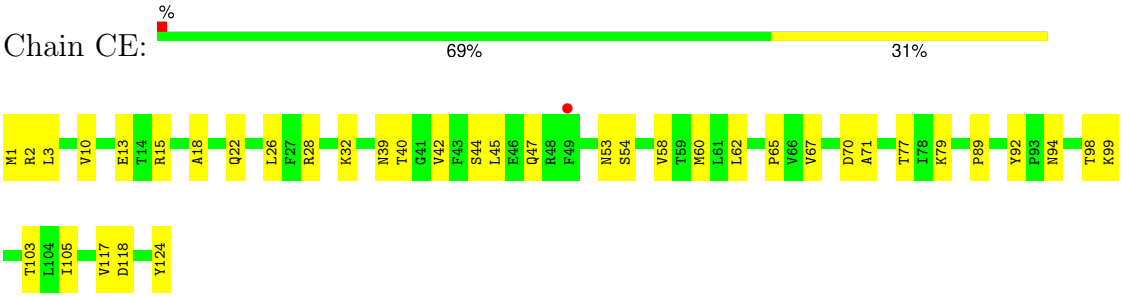
• Molecule 1: coat protein

Chain CD:



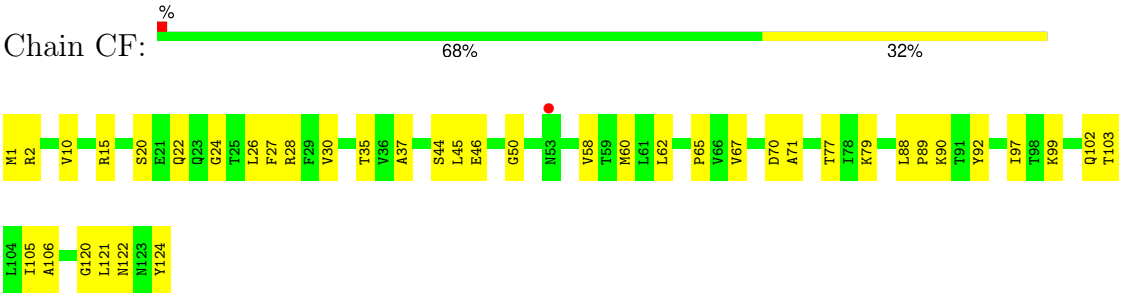
• Molecule 1: coat protein

Chain CE:



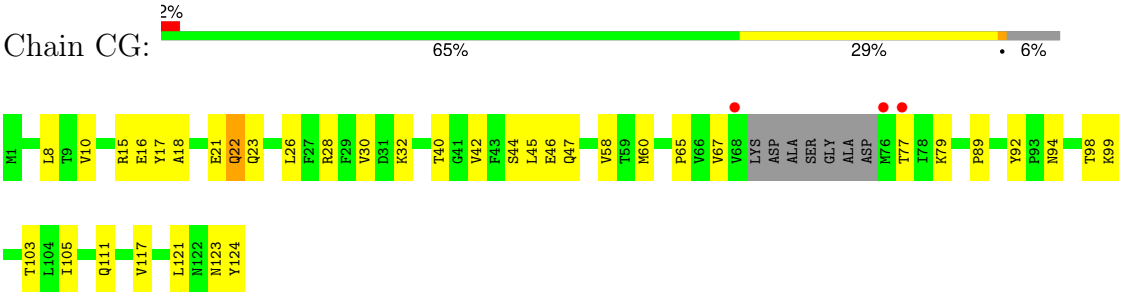
• Molecule 1: coat protein

Chain CF:



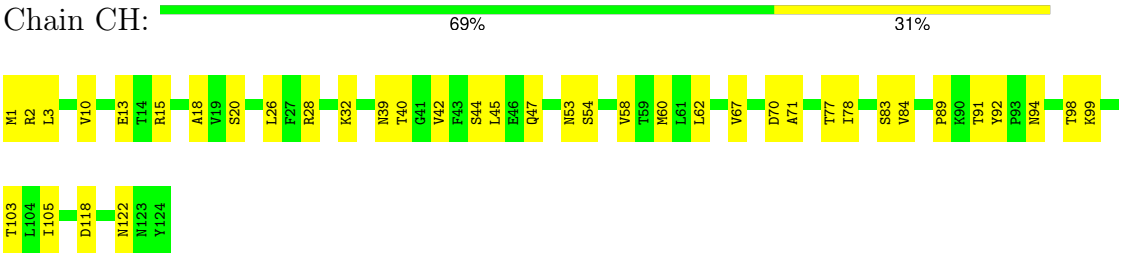
• Molecule 1: coat protein

Chain CG:



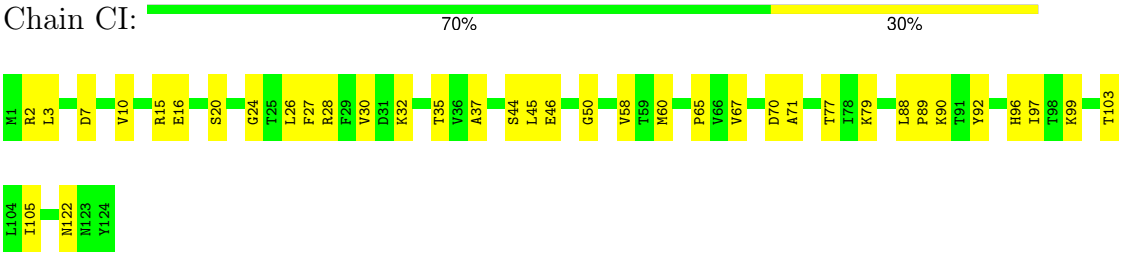
• Molecule 1: coat protein

Chain CH:



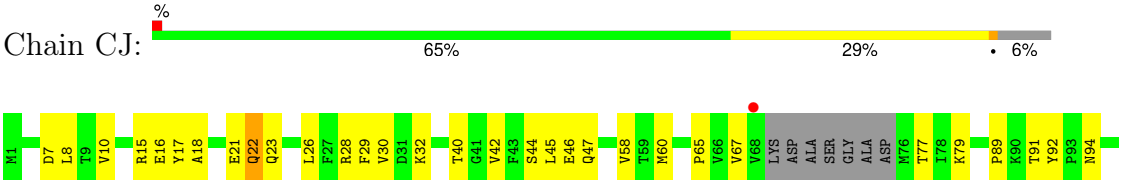
• Molecule 1: coat protein

Chain CI:



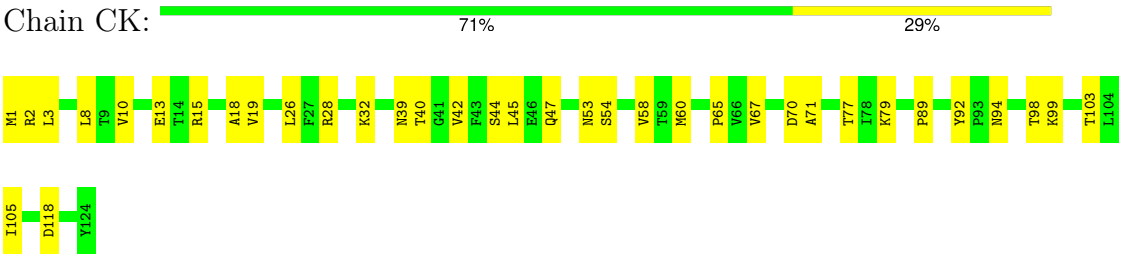
• Molecule 1: coat protein

Chain CJ:



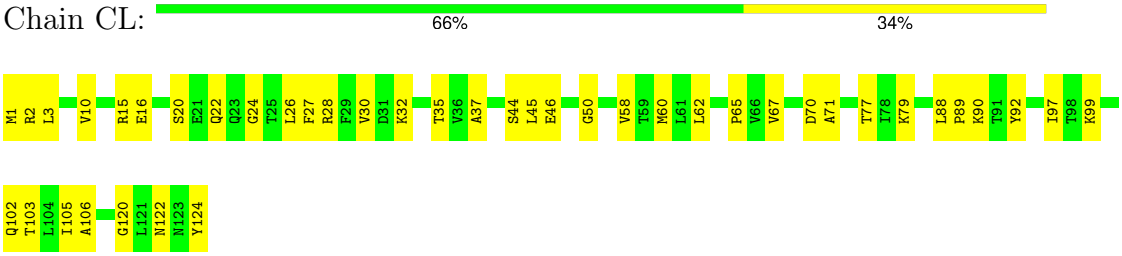
• Molecule 1: coat protein

Chain CK:



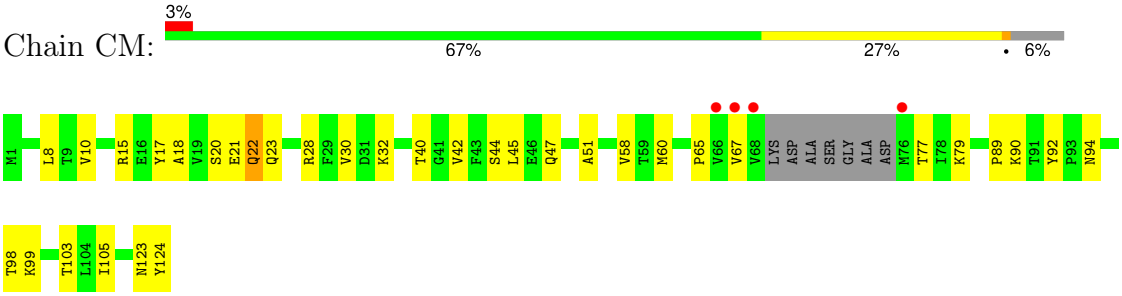
• Molecule 1: coat protein

Chain CL:



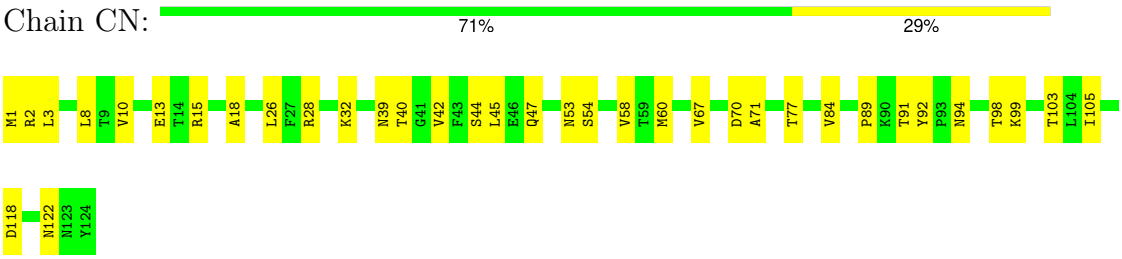
• Molecule 1: coat protein

Chain CM:



• Molecule 1: coat protein

Chain CN:

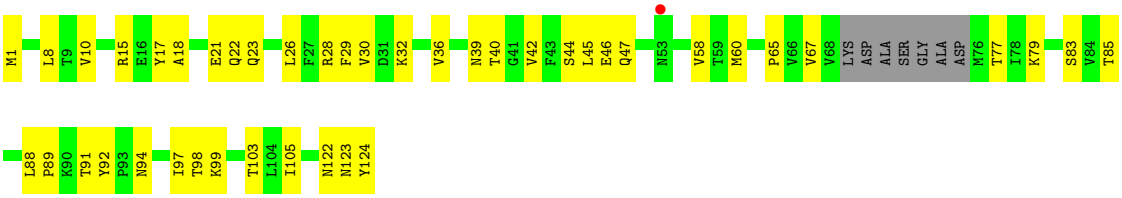


• Molecule 1: coat protein

Chain CO:

• Molecule 1: coat protein

Chain CP:

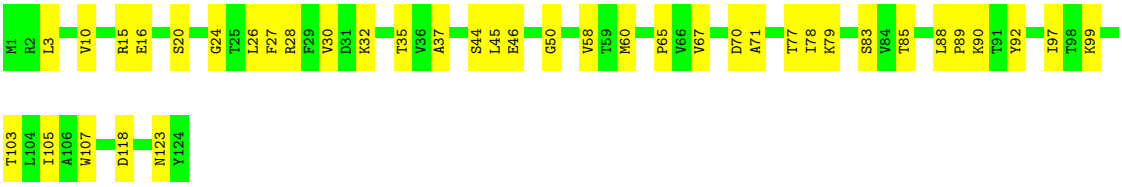


• Molecule 1: coat protein

Chain CQ:

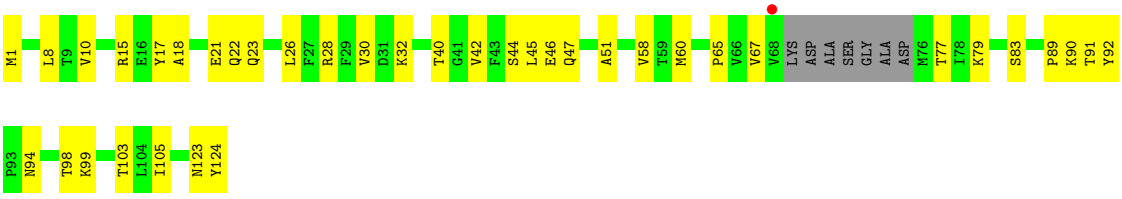
• Molecule 1: coat protein

Chain CR:



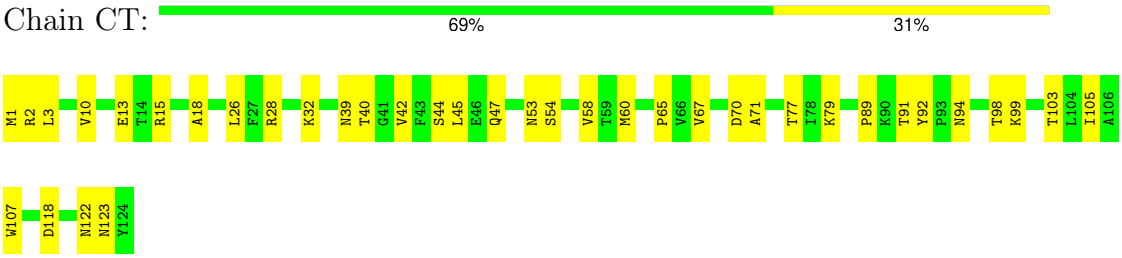
• Molecule 1: coat protein

Chain CS:



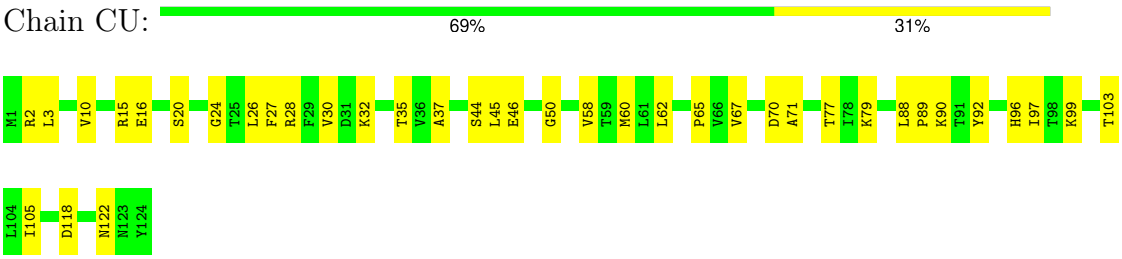
• Molecule 1: coat protein

Chain CT:



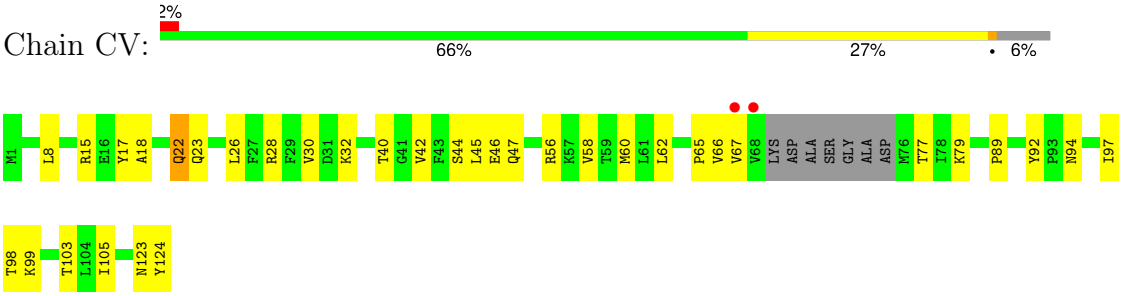
• Molecule 1: coat protein

Chain CU:



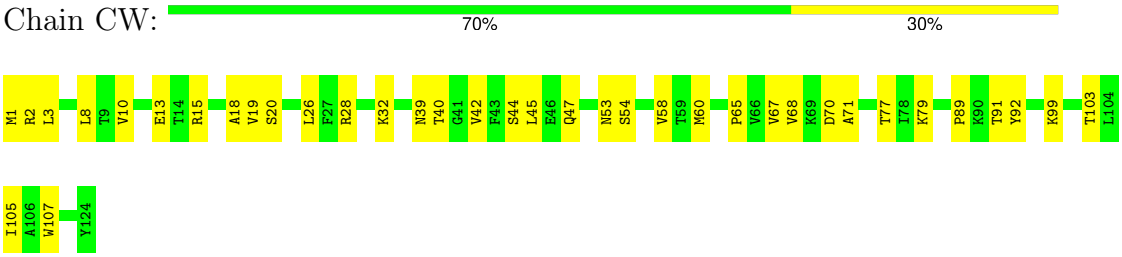
• Molecule 1: coat protein

Chain CV:



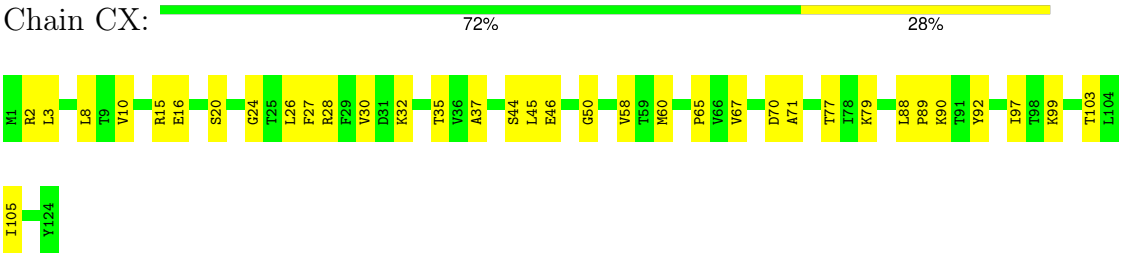
• Molecule 1: coat protein

Chain CW:



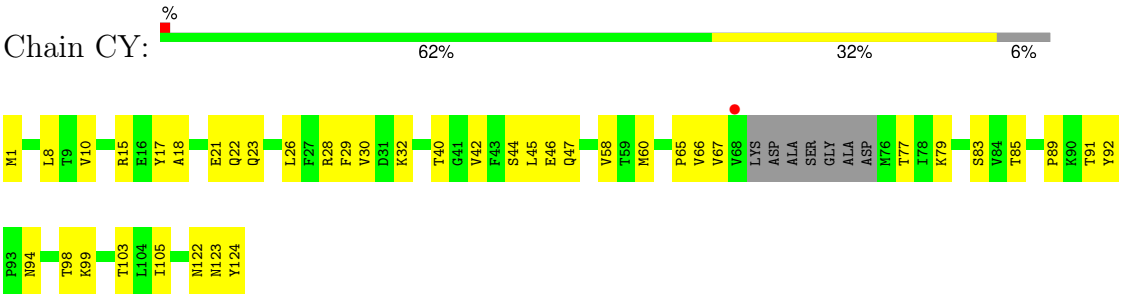
• Molecule 1: coat protein

Chain CX:



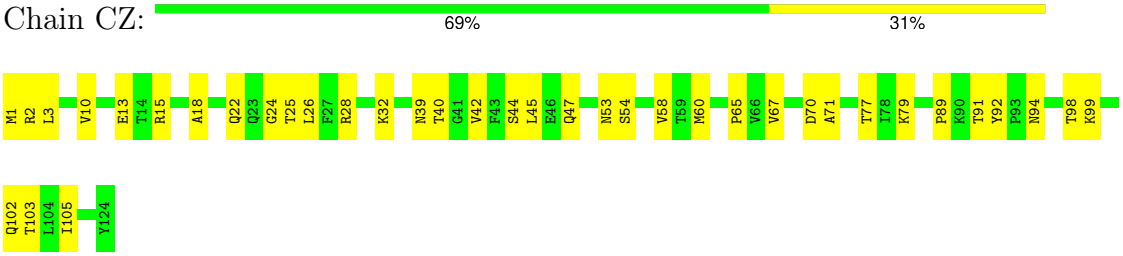
• Molecule 1: coat protein

Chain CY:



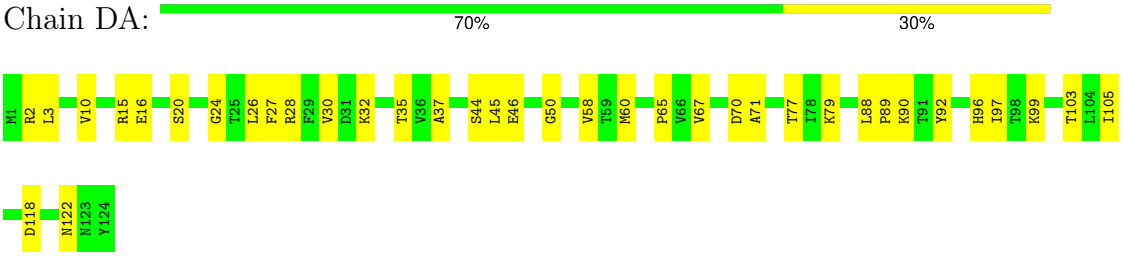
• Molecule 1: coat protein

Chain CZ:



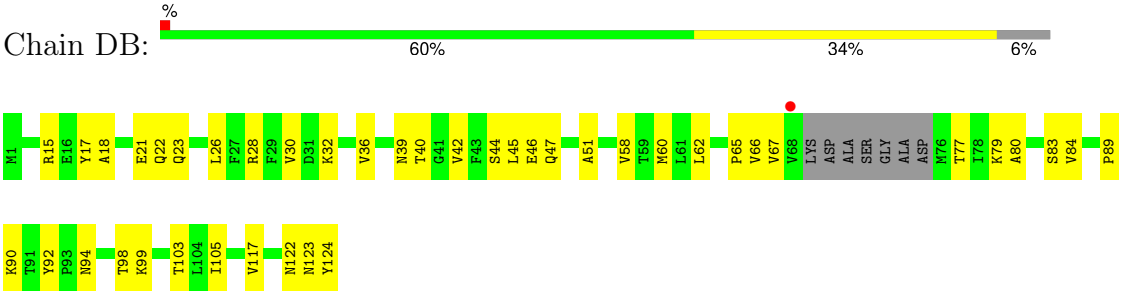
• Molecule 1: coat protein

Chain DA:



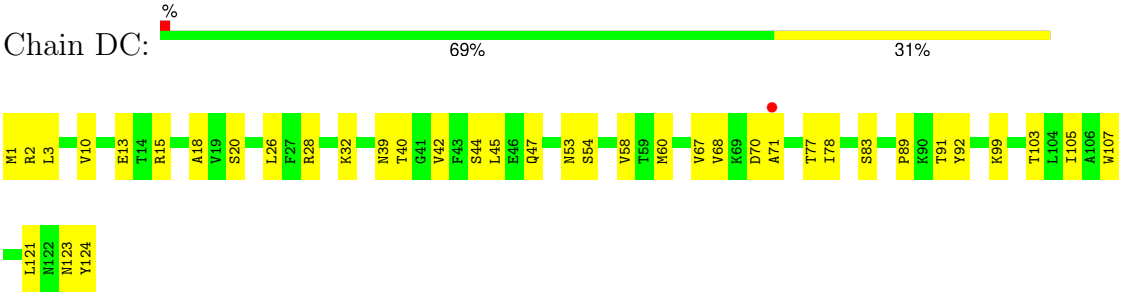
• Molecule 1: coat protein

Chain DB:



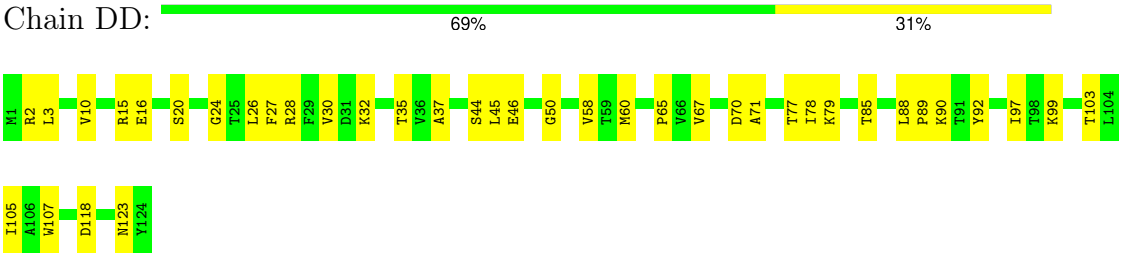
• Molecule 1: coat protein

Chain DC:



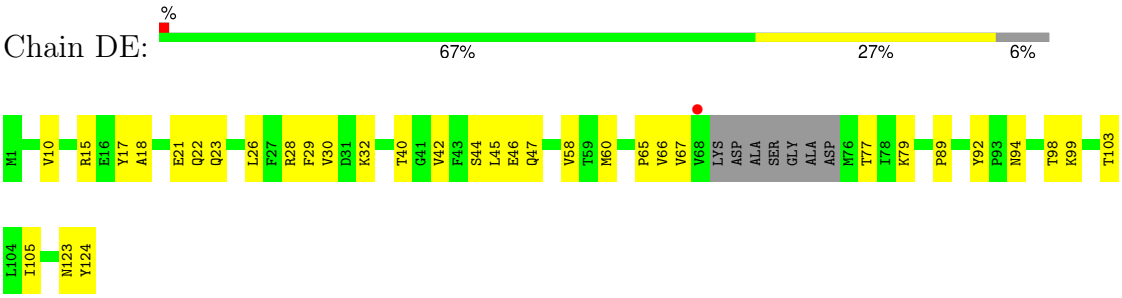
• Molecule 1: coat protein

Chain DD:



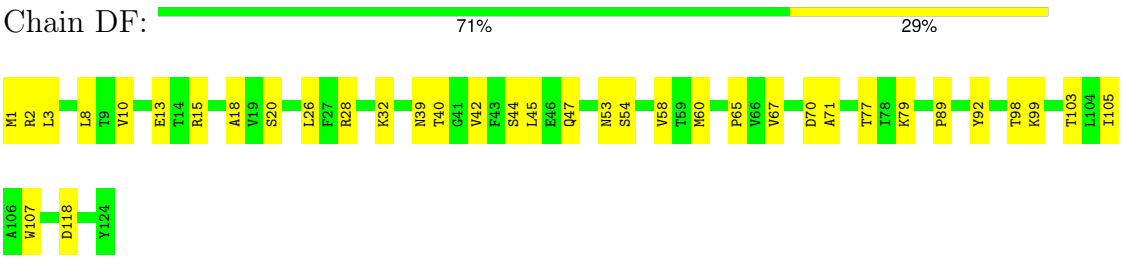
• Molecule 1: coat protein

Chain DE:



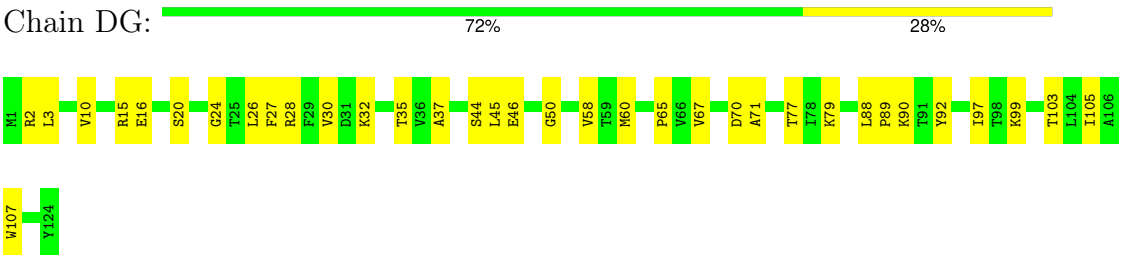
• Molecule 1: coat protein

Chain DF:



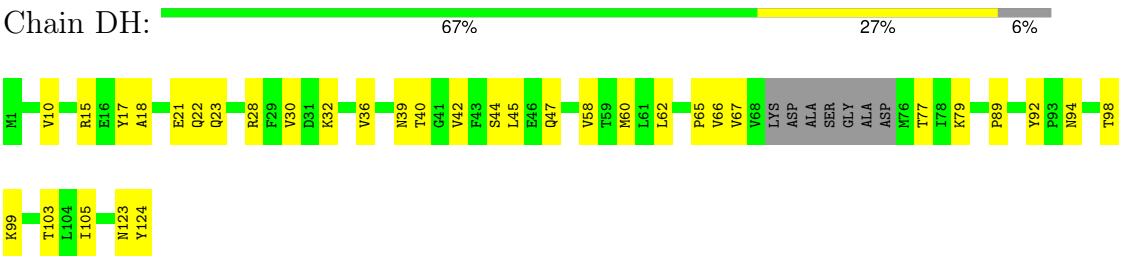
• Molecule 1: coat protein

Chain DG:



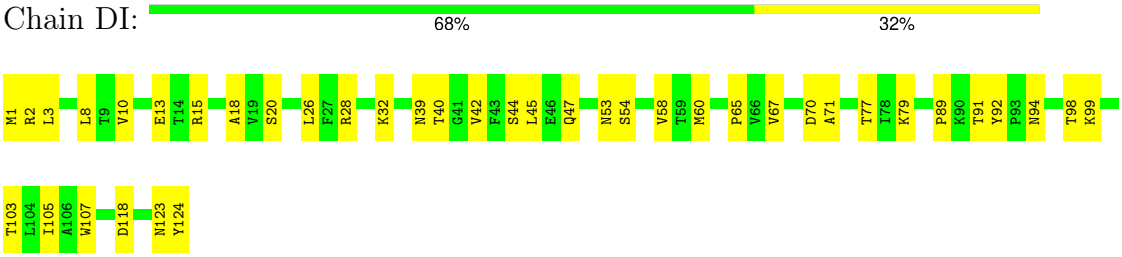
• Molecule 1: coat protein

Chain DH:



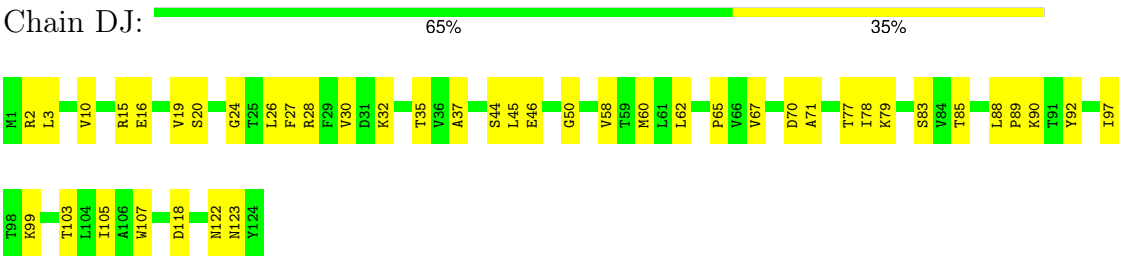
• Molecule 1: coat protein

Chain DI:



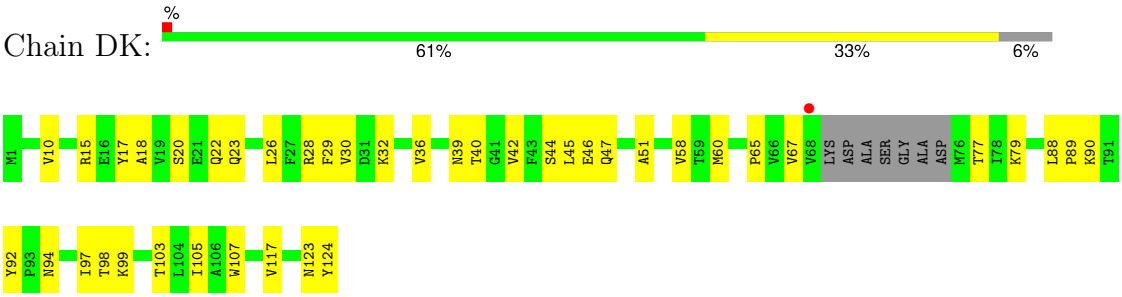
• Molecule 1: coat protein

Chain DJ:



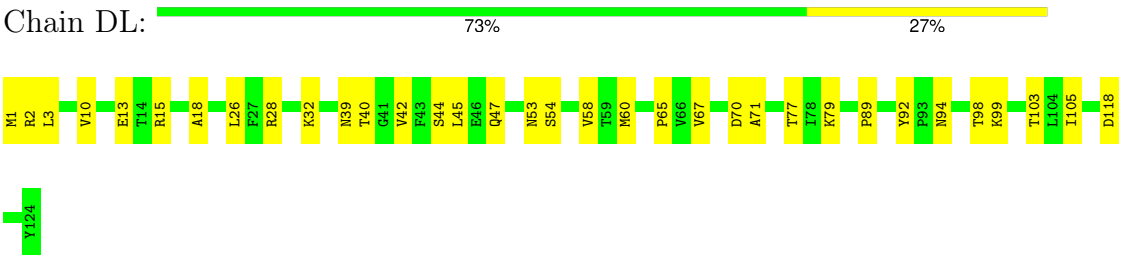
• Molecule 1: coat protein

Chain DK:



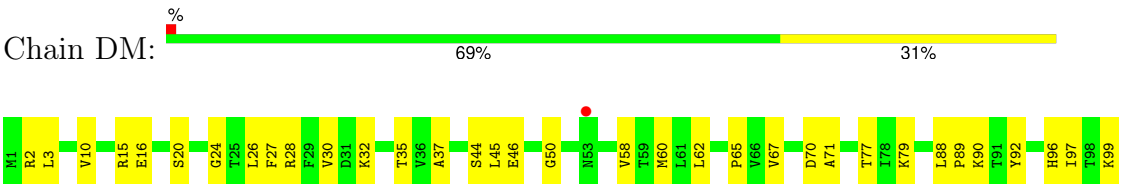
• Molecule 1: coat protein

Chain DL:



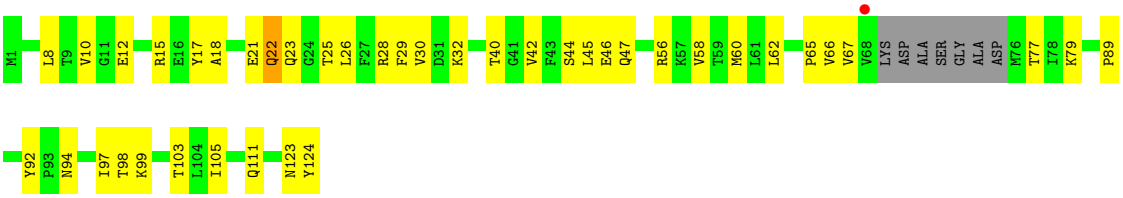
• Molecule 1: coat protein

Chain DM:



• Molecule 1: coat protein

Chain DN:

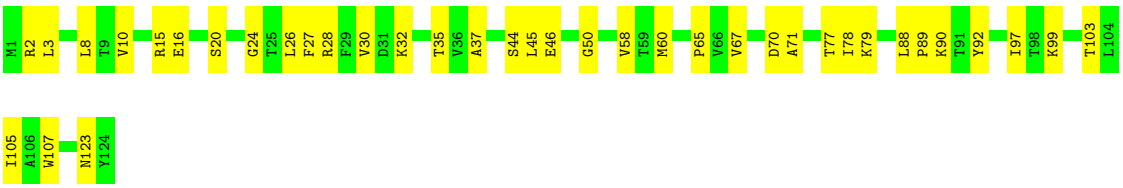


• Molecule 1: coat protein

Chain DO:

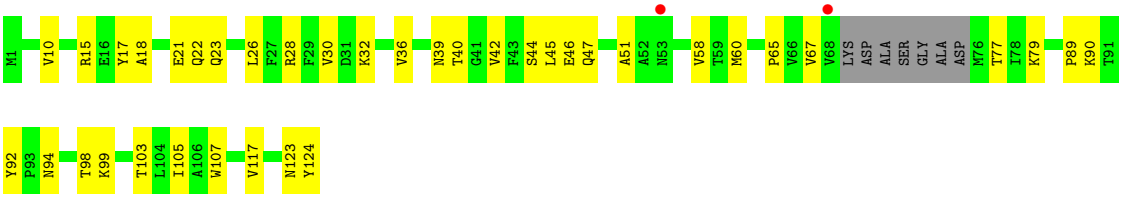
• Molecule 1: coat protein

Chain DP:



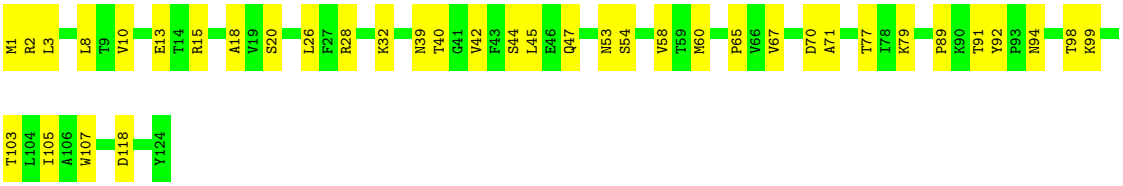
• Molecule 1: coat protein

Chain DQ:



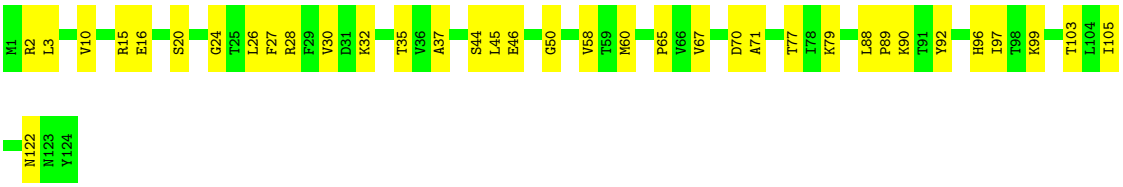
• Molecule 1: coat protein

Chain DR:



• Molecule 1: coat protein

Chain DS:

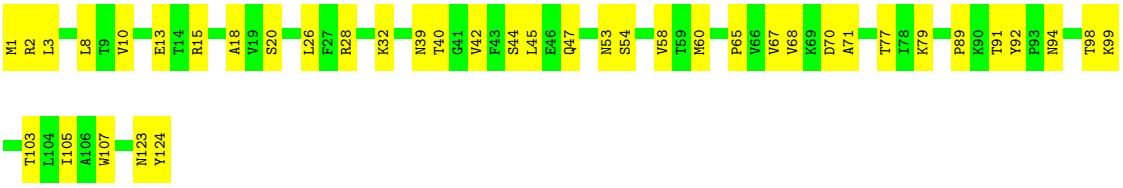


• Molecule 1: coat protein

Chain DT:

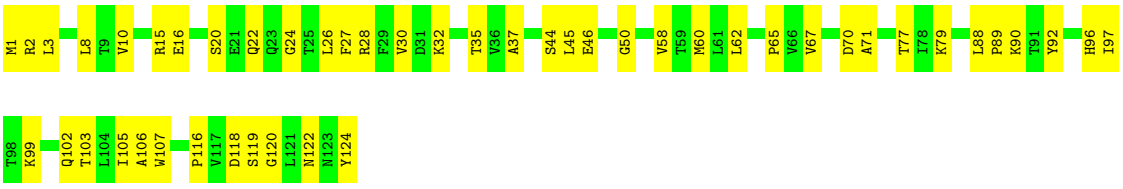
• Molecule 1: coat protein

Chain DU:



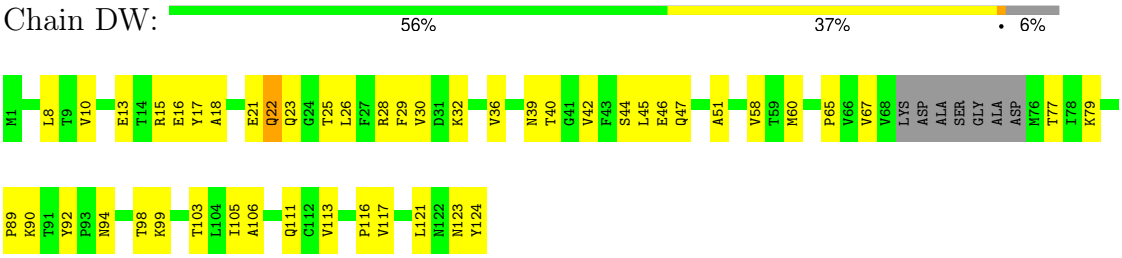
• Molecule 1: coat protein

Chain DV:



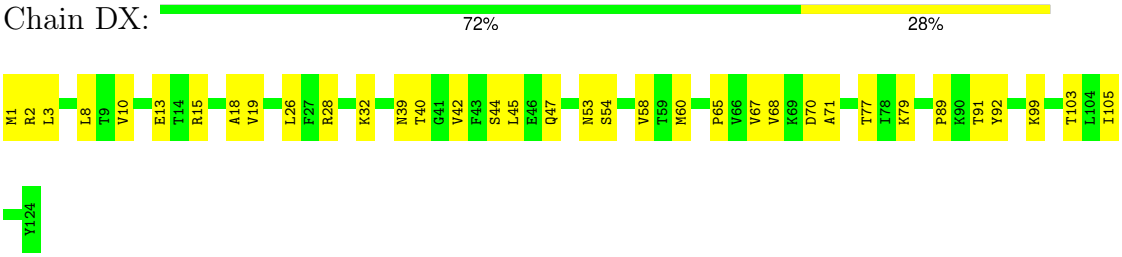
• Molecule 1: coat protein

Chain DW:



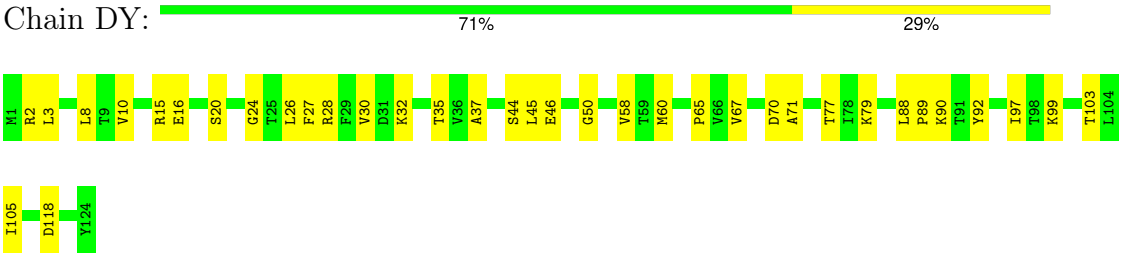
• Molecule 1: coat protein

Chain DX:



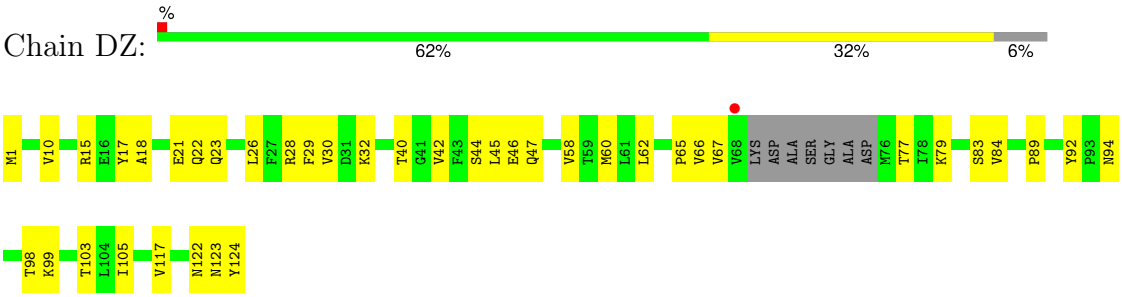
• Molecule 1: coat protein

Chain DY:



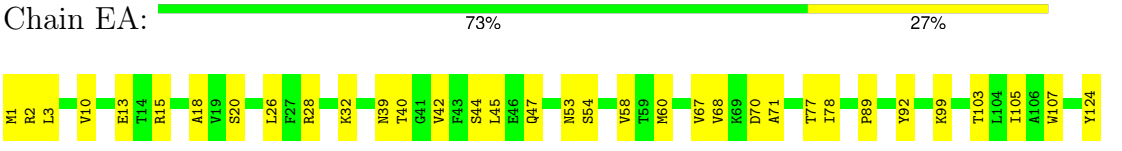
• Molecule 1: coat protein

Chain DZ:



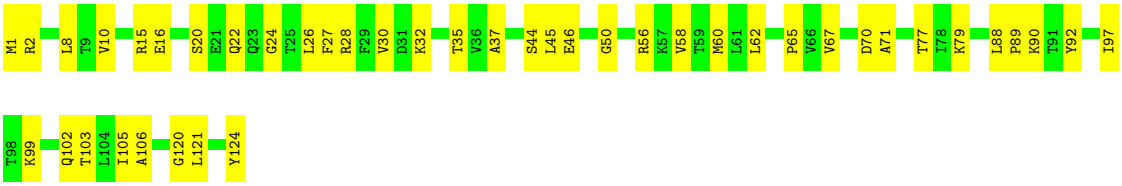
• Molecule 1: coat protein

Chain EA:



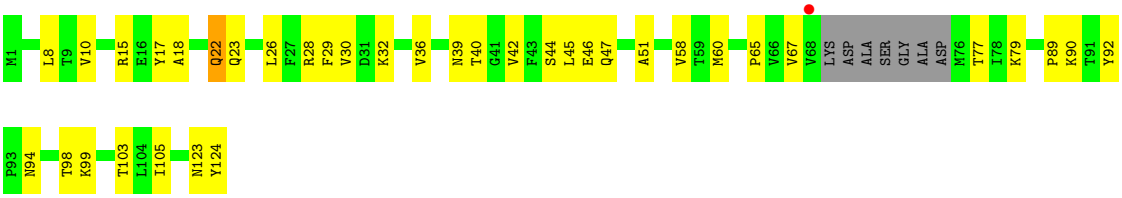
• Molecule 1: coat protein

Chain EB:



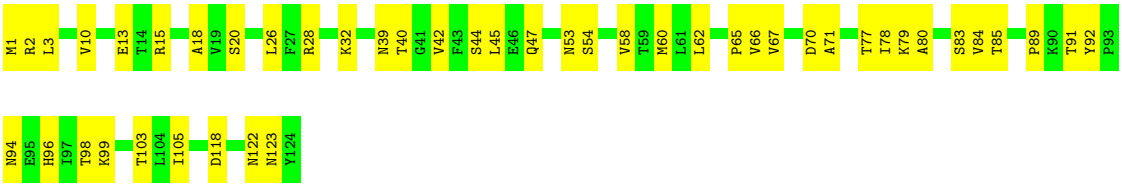
• Molecule 1: coat protein

Chain EC:



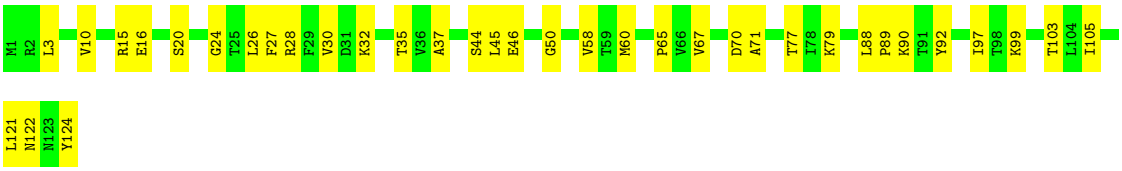
• Molecule 1: coat protein

Chain ED:



• Molecule 1: coat protein

Chain EE:

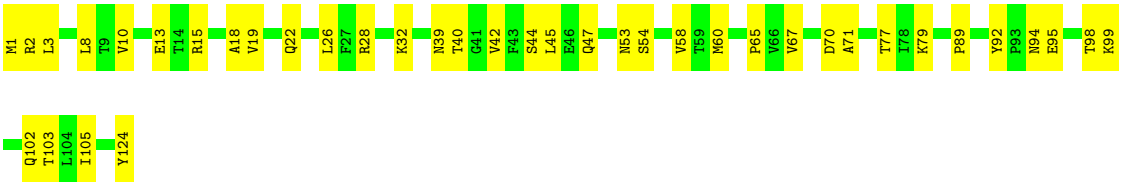


• Molecule 1: coat protein

Chain EF:

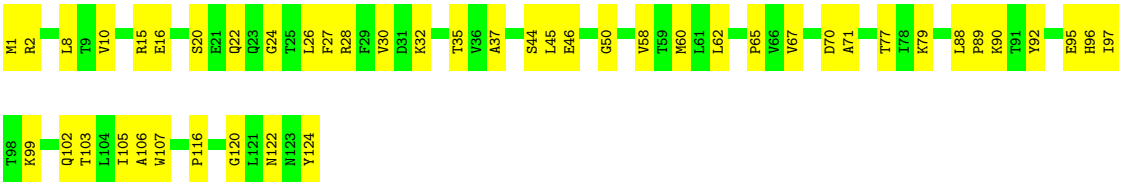
• Molecule 1: coat protein

Chain EG:



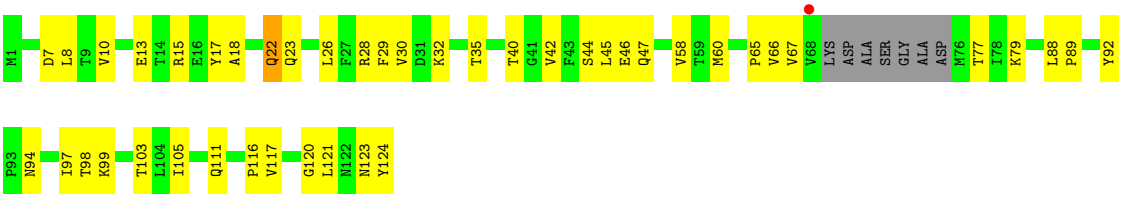
• Molecule 1: coat protein

Chain EH:



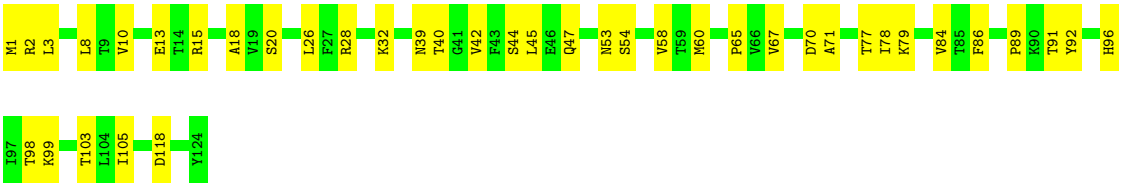
• Molecule 1: coat protein

Chain EI:



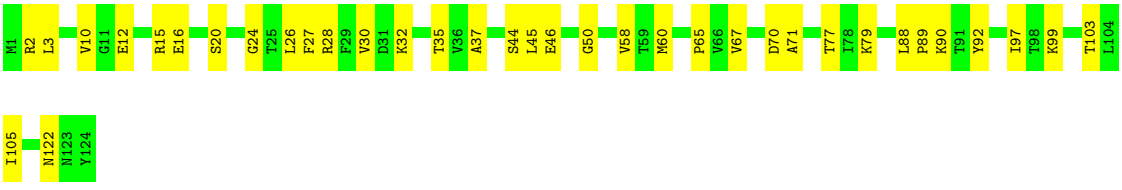
• Molecule 1: coat protein

Chain EJ:



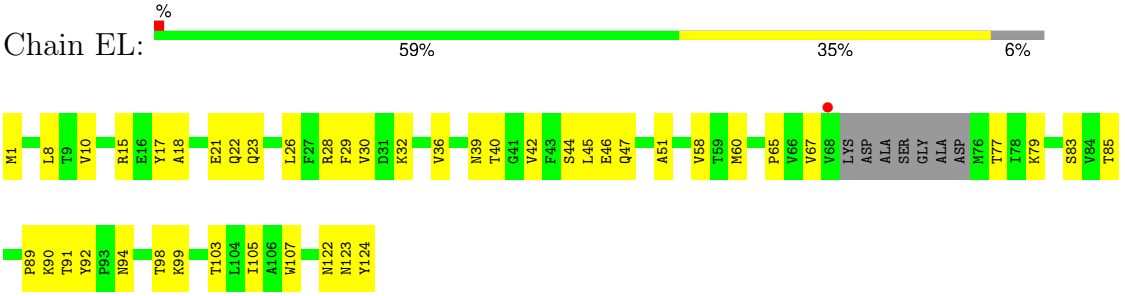
• Molecule 1: coat protein

Chain EK:



• Molecule 1: coat protein

Chain EL:

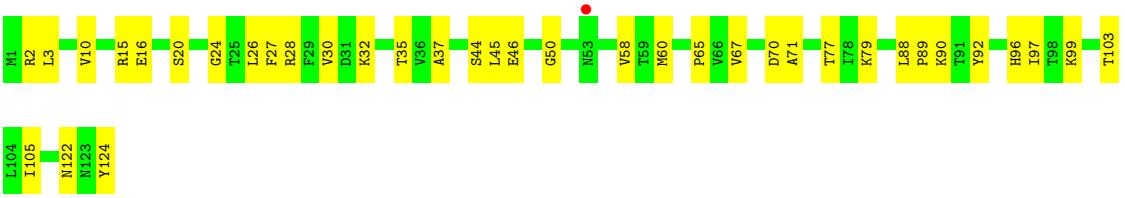


• Molecule 1: coat protein

Chain EM:

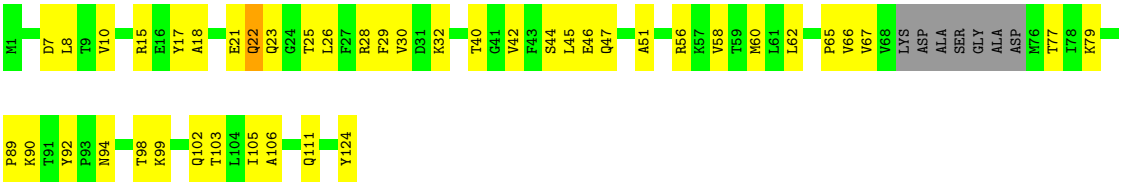
• Molecule 1: coat protein

Chain EN:



• Molecule 1: coat protein

Chain EO:

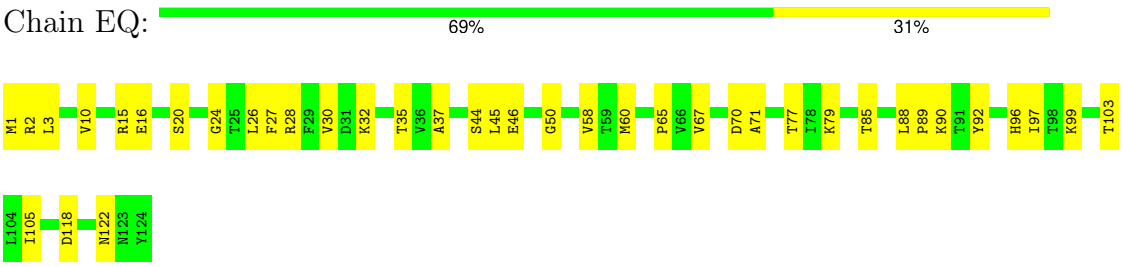


• Molecule 1: coat protein

Chain EP:

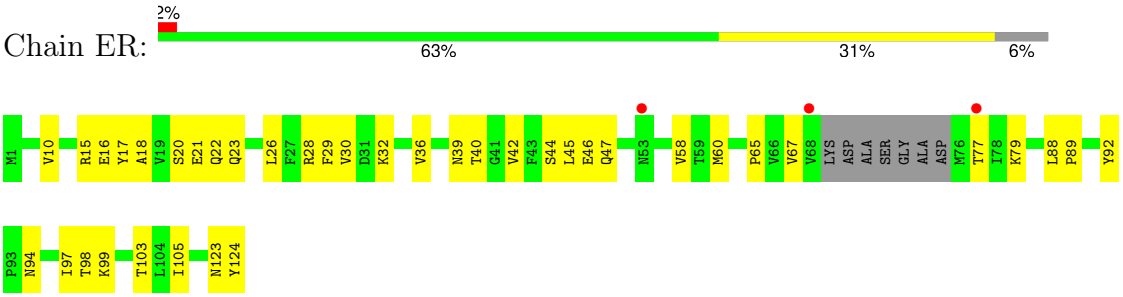
• Molecule 1: coat protein

Chain EQ:



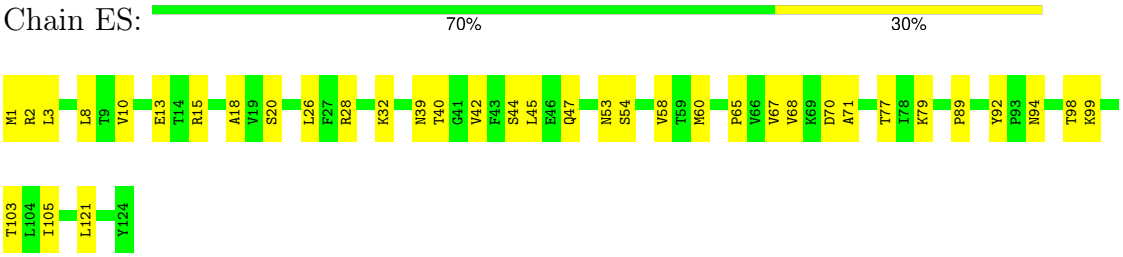
• Molecule 1: coat protein

Chain ER:



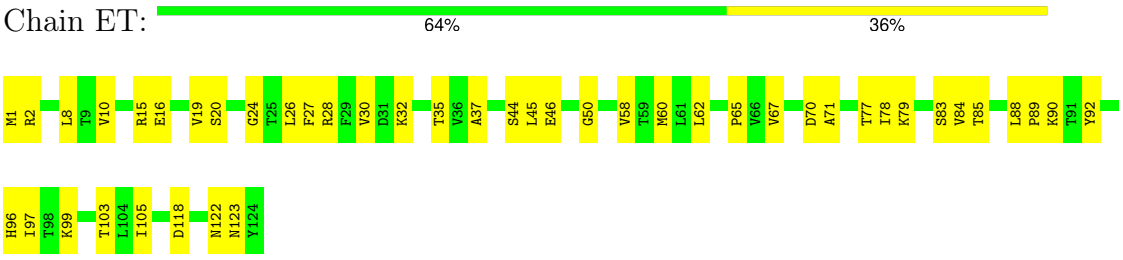
• Molecule 1: coat protein

Chain ES:



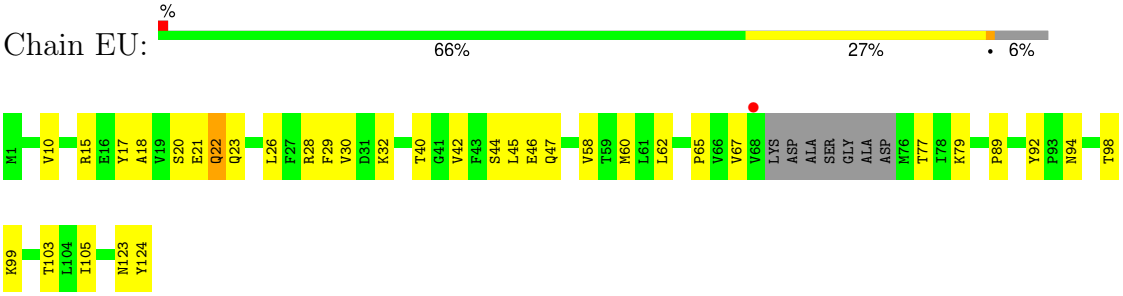
• Molecule 1: coat protein

Chain ET:



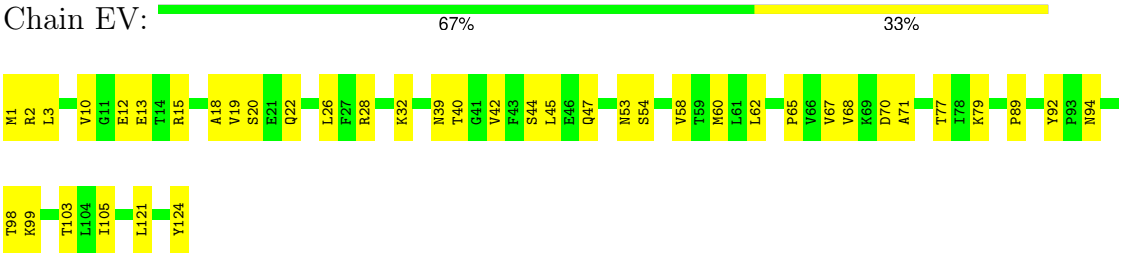
• Molecule 1: coat protein

Chain EU:



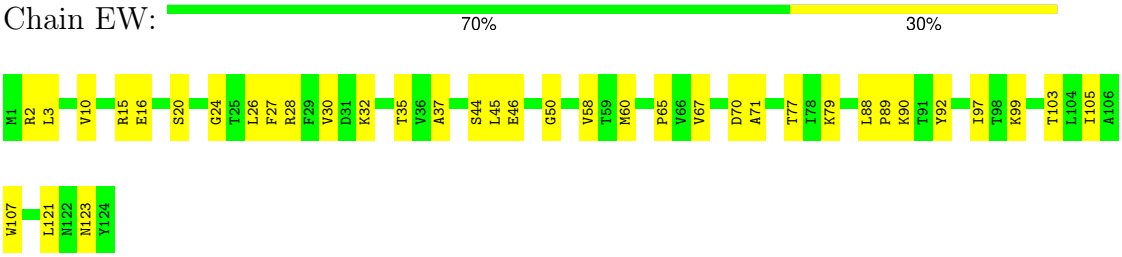
• Molecule 1: coat protein

Chain EV:



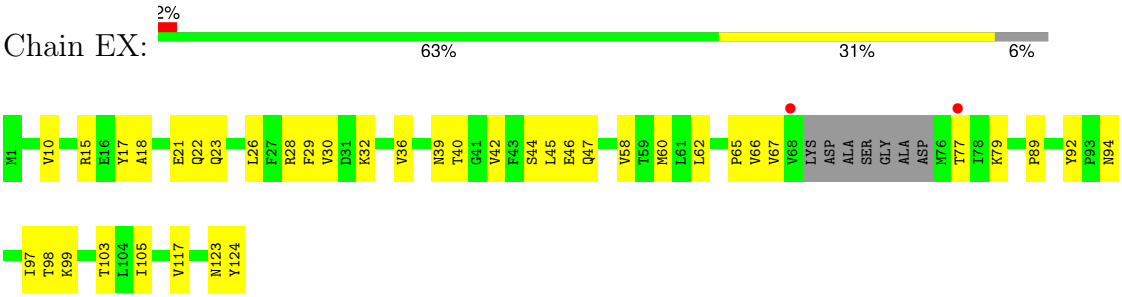
• Molecule 1: coat protein

Chain EW:



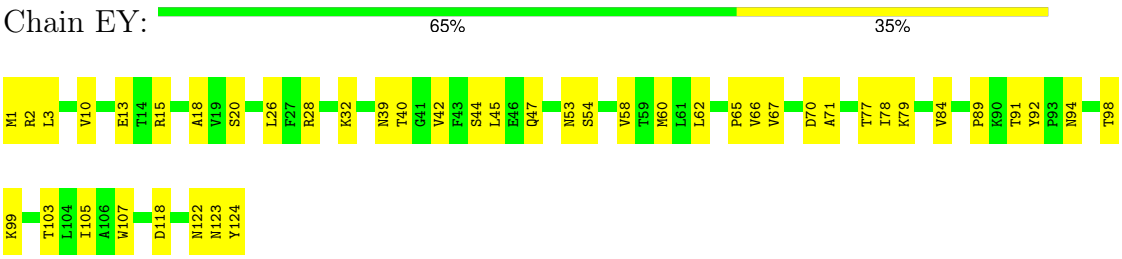
• Molecule 1: coat protein

Chain EX:



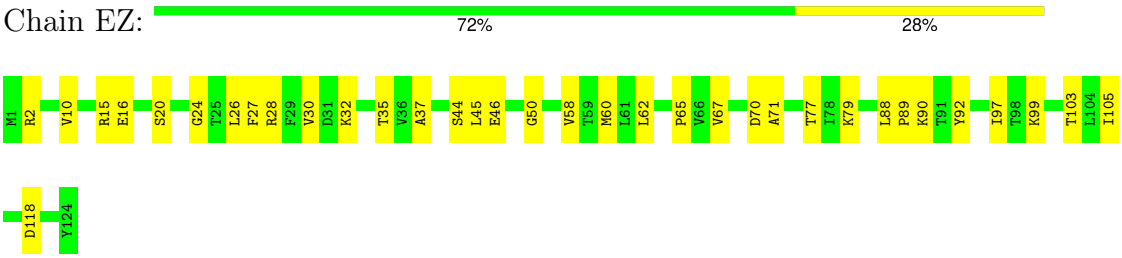
• Molecule 1: coat protein

Chain EY:



• Molecule 1: coat protein

Chain EZ:



• Molecule 1: coat protein

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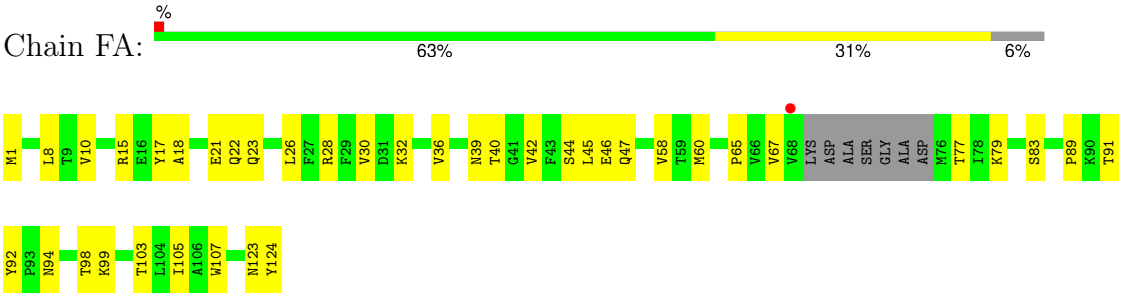
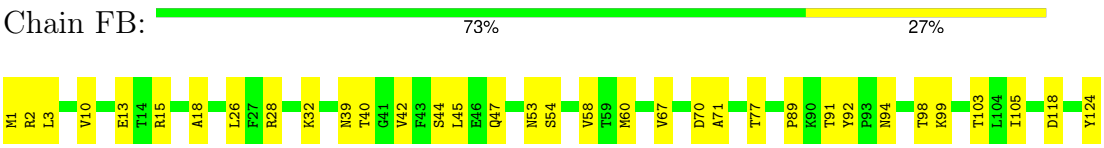


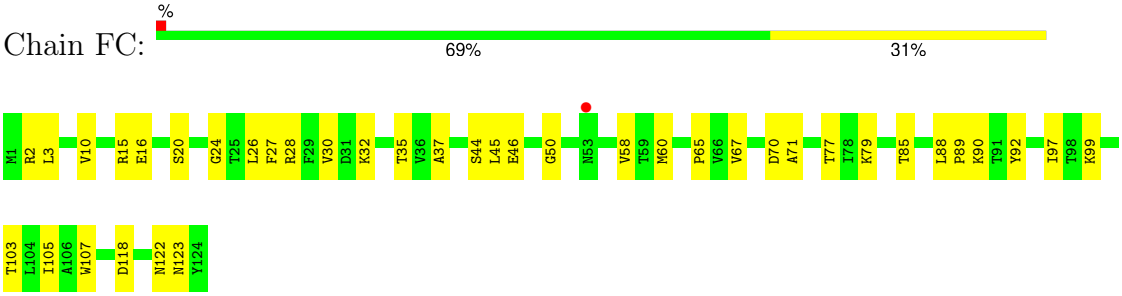
• Molecule 1: coat protein

Chain FB:



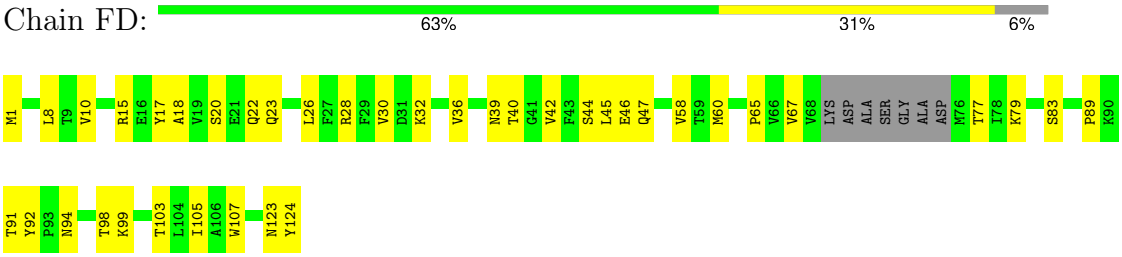
• Molecule 1: coat protein

Chain FC:



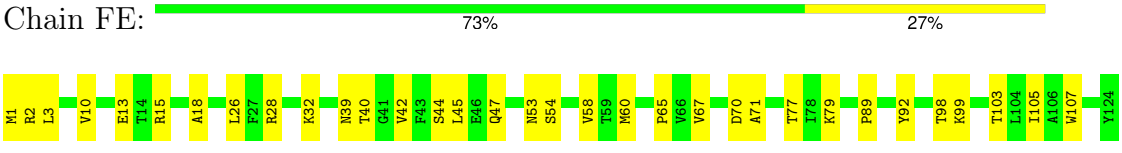
• Molecule 1: coat protein

Chain FD:



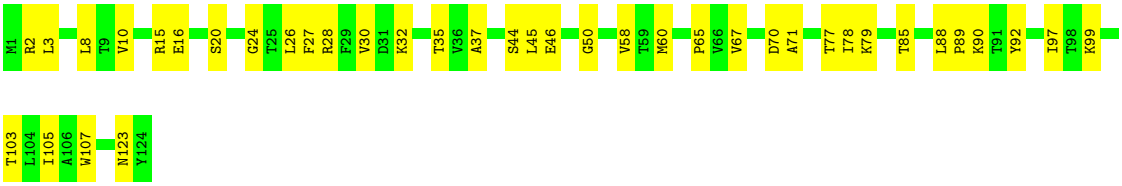
• Molecule 1: coat protein

Chain FE:



• Molecule 1: coat protein

Chain FF:

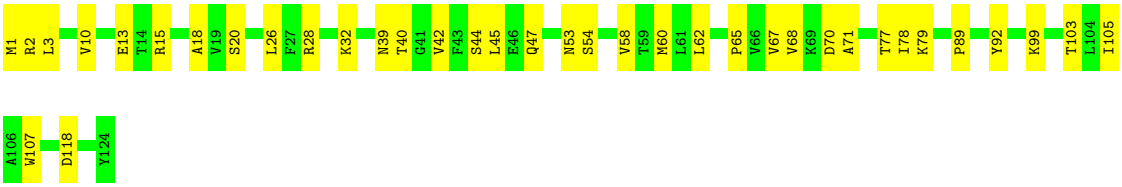


• Molecule 1: coat protein

Chain FG:

• Molecule 1: coat protein

Chain FH:

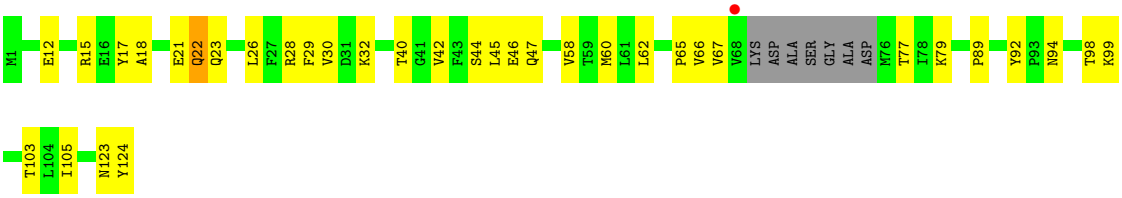


• Molecule 1: coat protein

Chain FI:

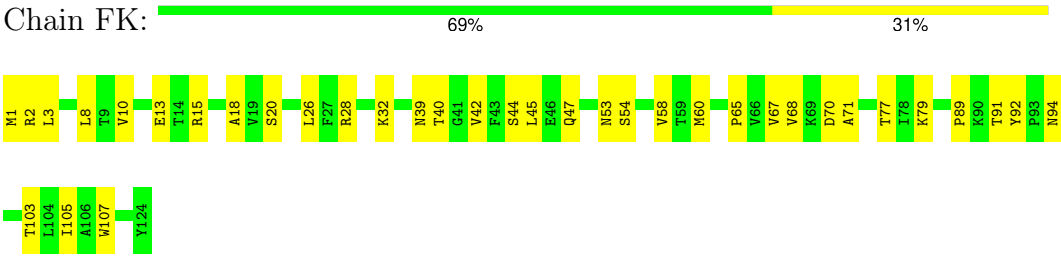
• Molecule 1: coat protein

Chain FJ:



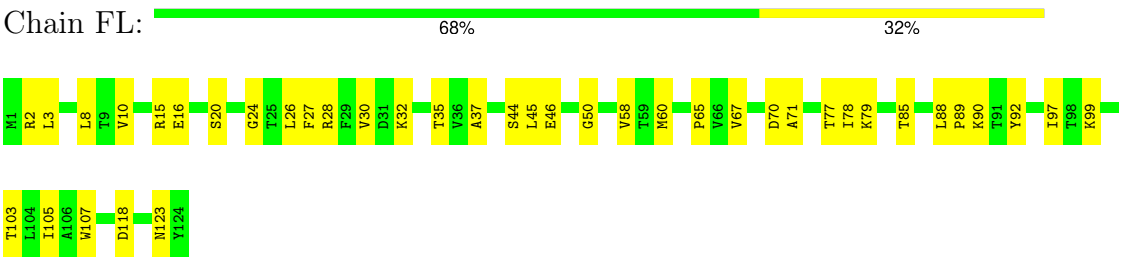
• Molecule 1: coat protein

Chain FK:



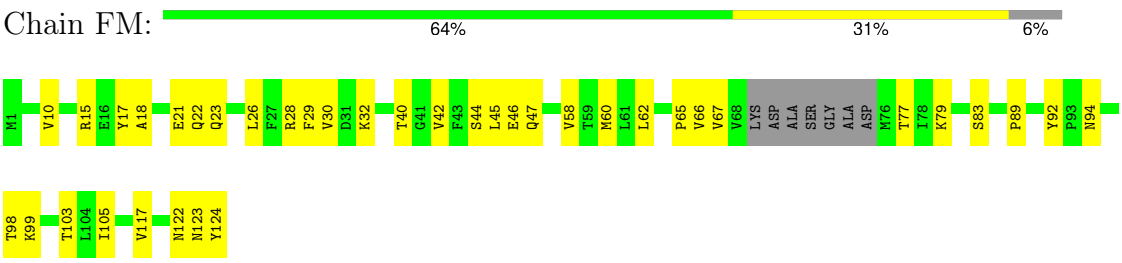
• Molecule 1: coat protein

Chain FL:



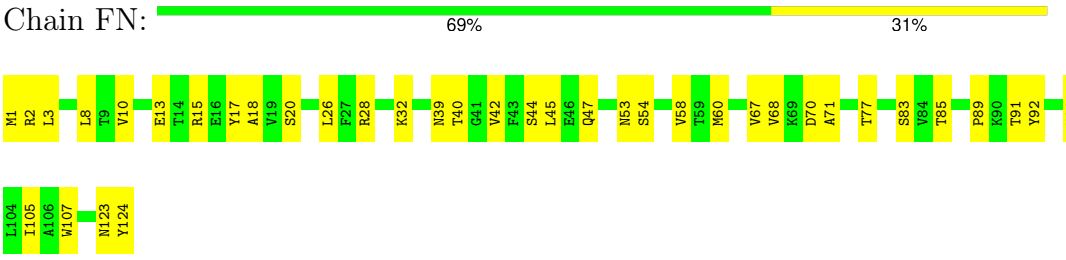
• Molecule 1: coat protein

Chain FM:



• Molecule 1: coat protein

Chain FN:



• Molecule 1: coat protein

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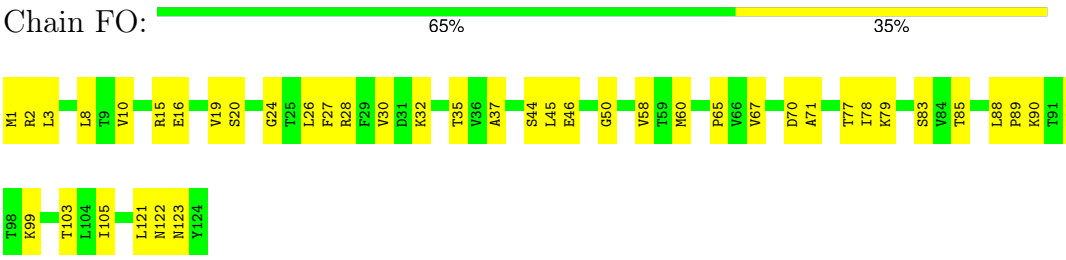

• Molecule 1: coat protein

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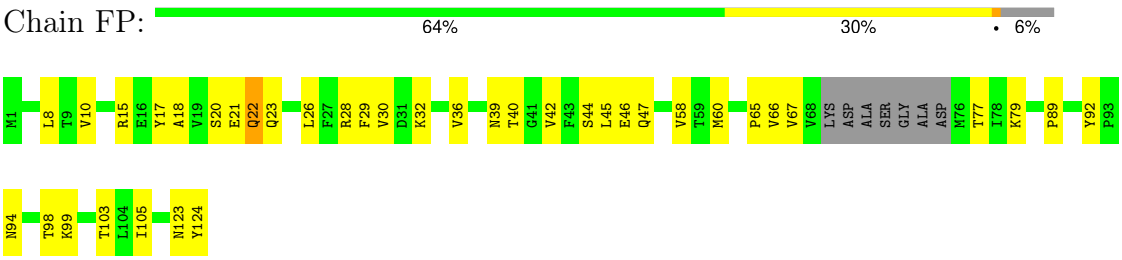
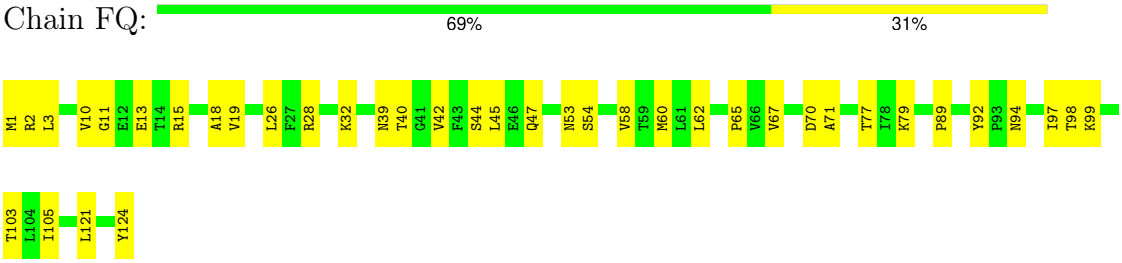


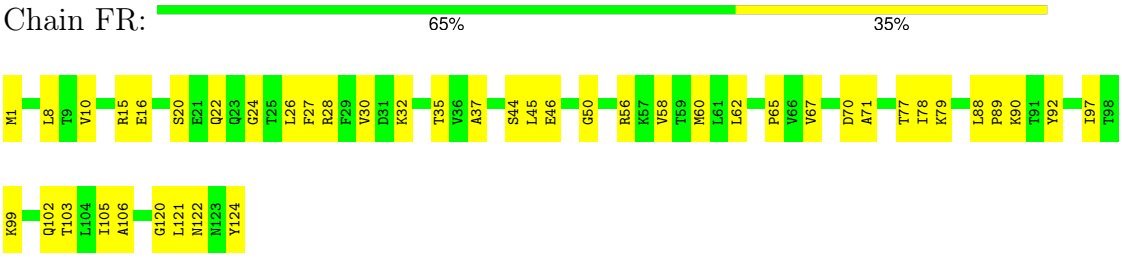
• Molecule 1: coat protein

Chain FQ:



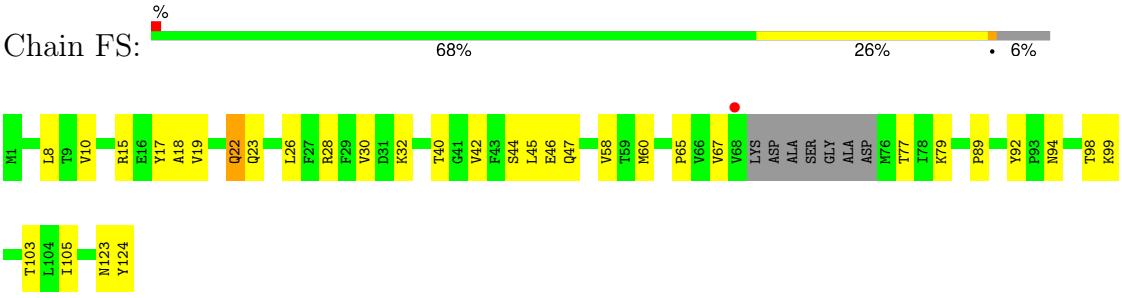
• Molecule 1: coat protein

Chain FR:



• Molecule 1: coat protein

Chain FS:



• Molecule 1: coat protein

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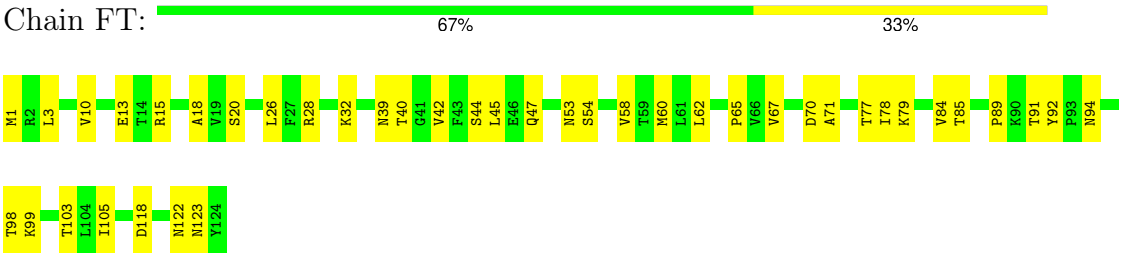
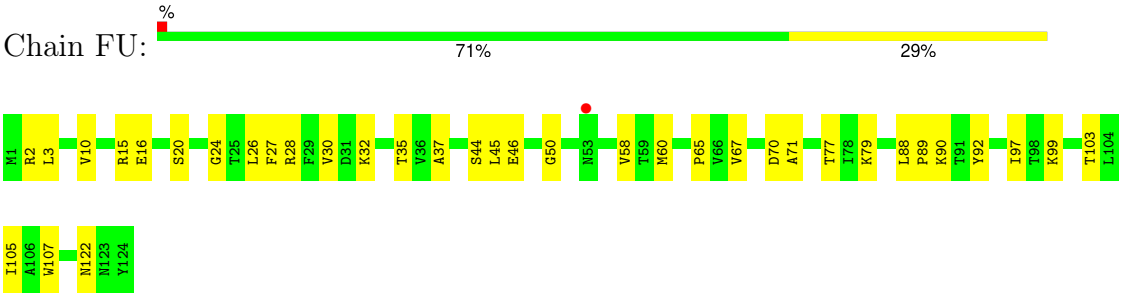


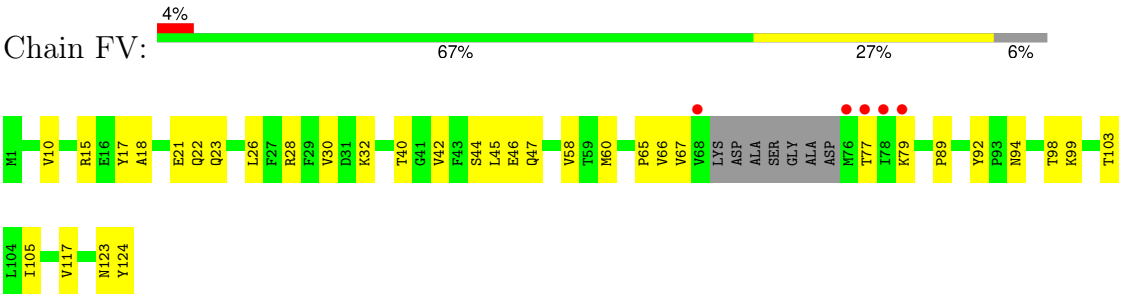
• Molecule 1: coat protein

Chain FU:



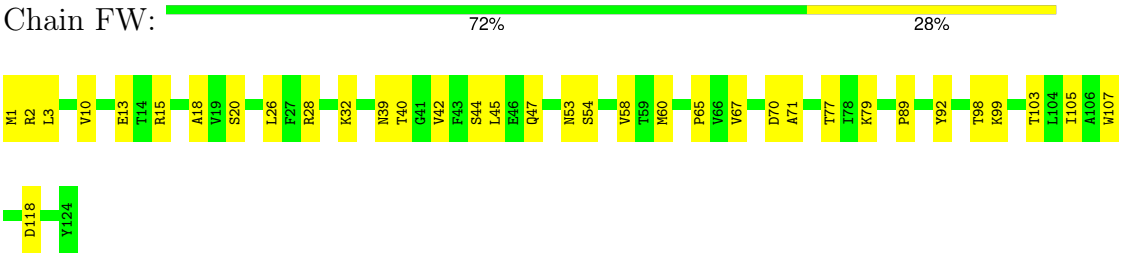
• Molecule 1: coat protein

Chain FV:



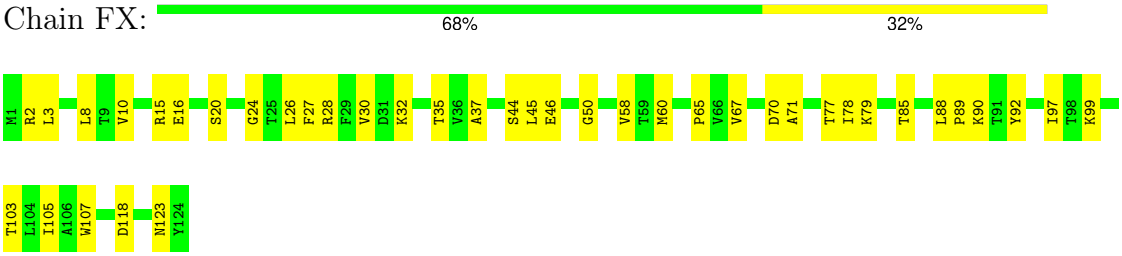
• Molecule 1: coat protein

Chain FW:



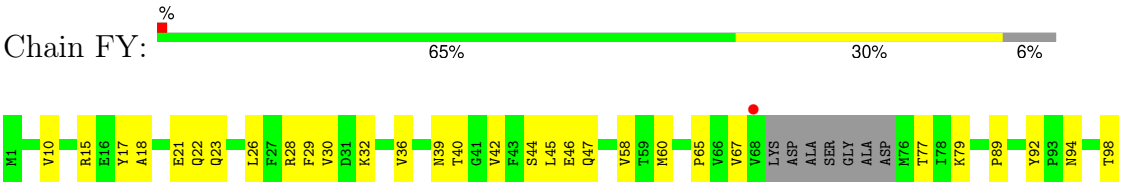
• Molecule 1: coat protein

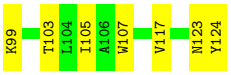
Chain FX:



• Molecule 1: coat protein

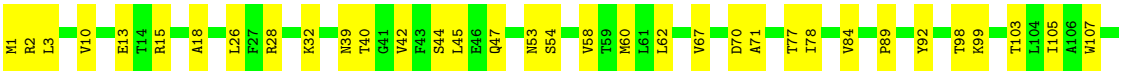
Chain FY:





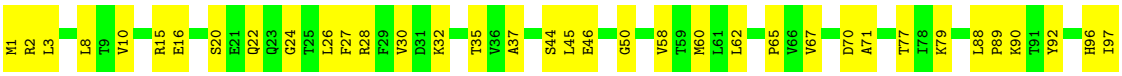
• Molecule 1: coat protein

Chain FZ:



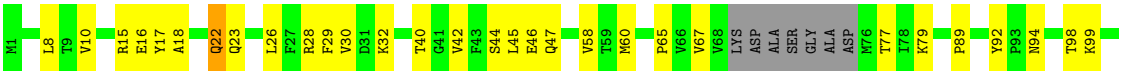
• Molecule 1: coat protein

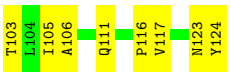
Chain GA:



• Molecule 1: coat protein

Chain GB:



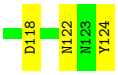


• Molecule 1: coat protein

Chain GC:

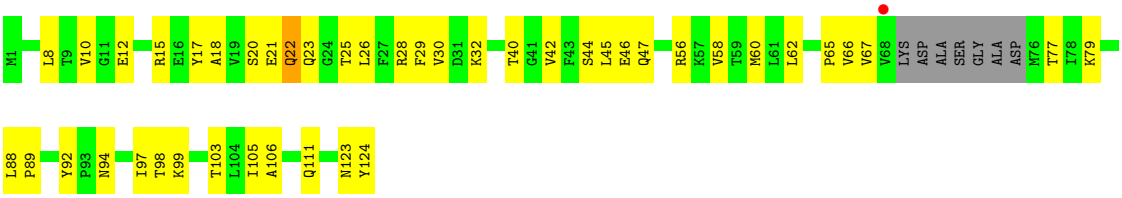
• Molecule 1: coat protein

Chain GD:



• Molecule 1: coat protein

Chain GE:



• Molecule 1: coat protein

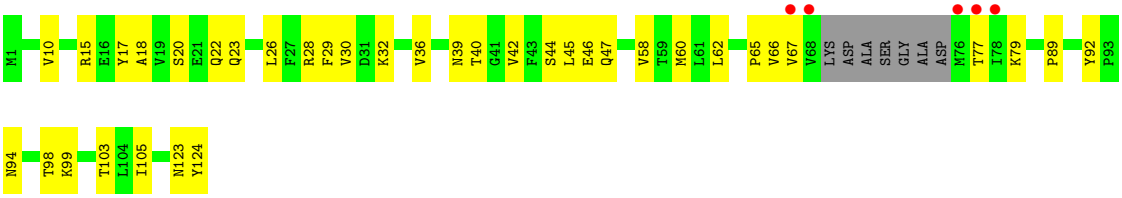
Chain GF:

• Molecule 1: coat protein

Chain GG:

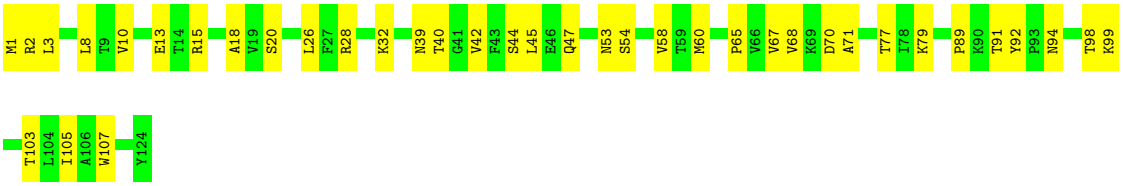
• Molecule 1: coat protein

Chain GH:



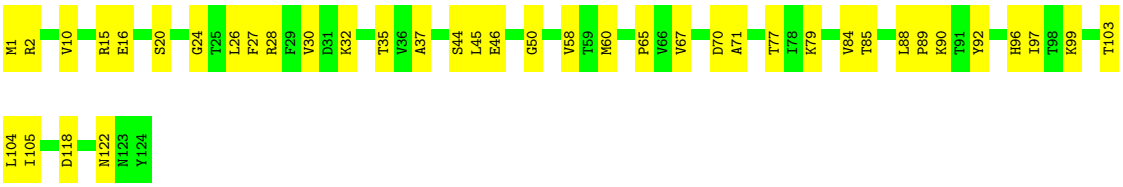
• Molecule 1: coat protein

Chain GI:



• Molecule 1: coat protein

Chain GJ:

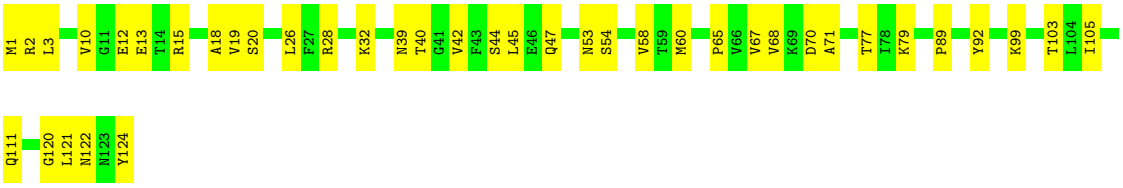


• Molecule 1: coat protein

Chain GK:

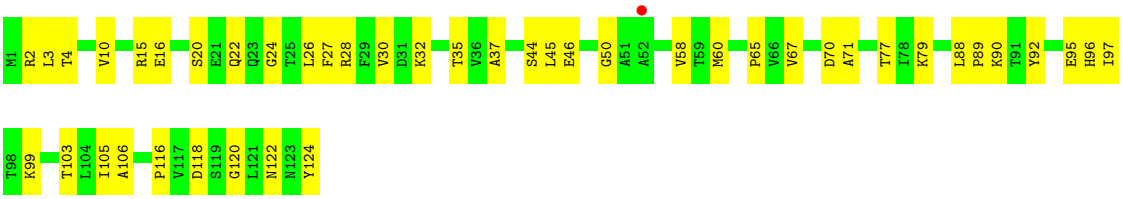
• Molecule 1: coat protein

Chain GL:



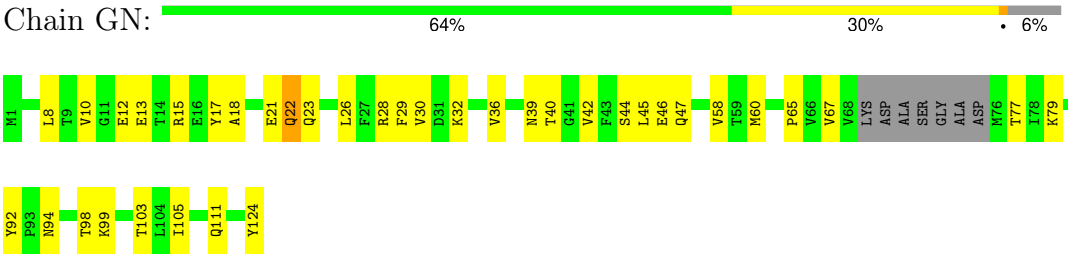
• Molecule 1: coat protein

Chain GM:



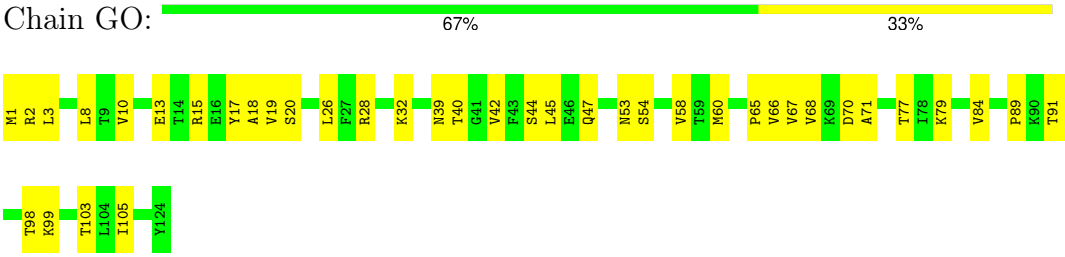
• Molecule 1: coat protein

Chain GN:



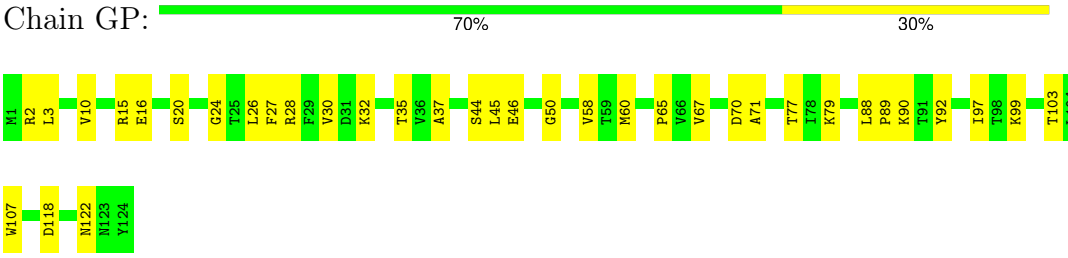
• Molecule 1: coat protein

Chain GO:



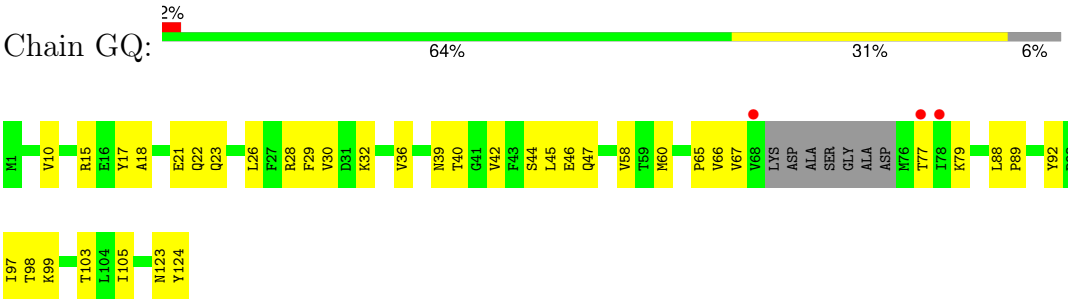
• Molecule 1: coat protein

Chain GP:



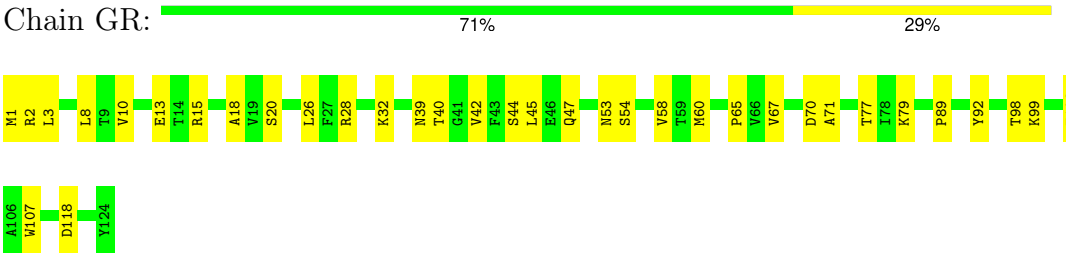
• Molecule 1: coat protein

Chain GQ:



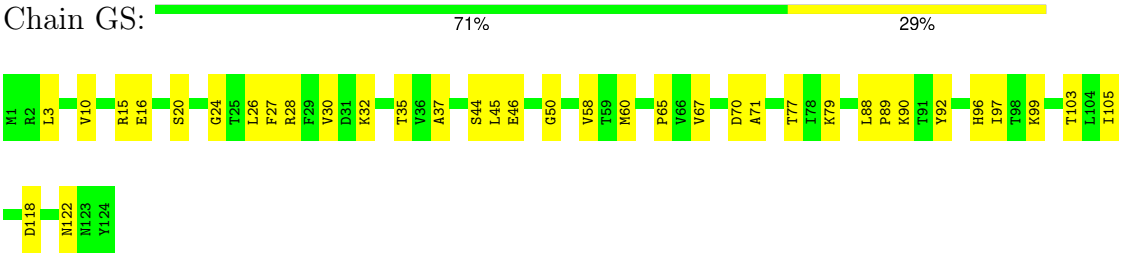
• Molecule 1: coat protein

Chain GR:



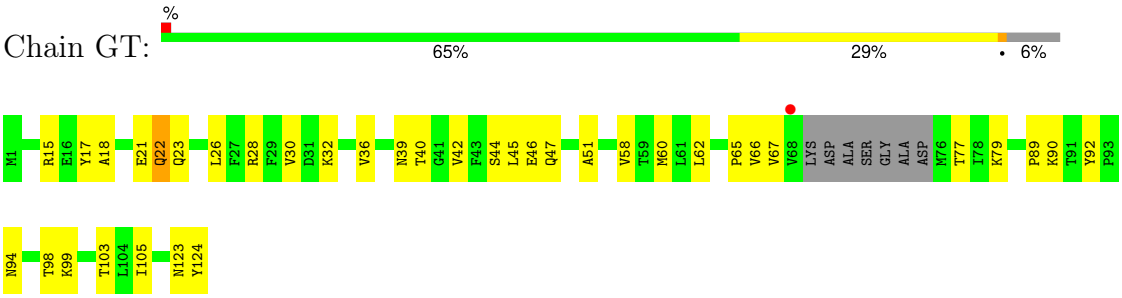
• Molecule 1: coat protein

Chain GS:



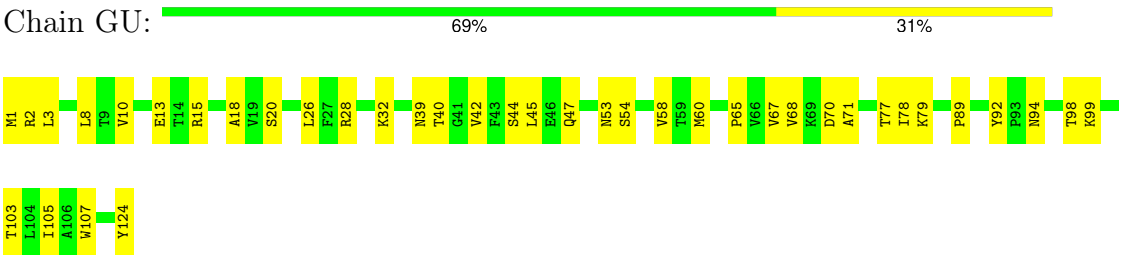
• Molecule 1: coat protein

Chain GT:



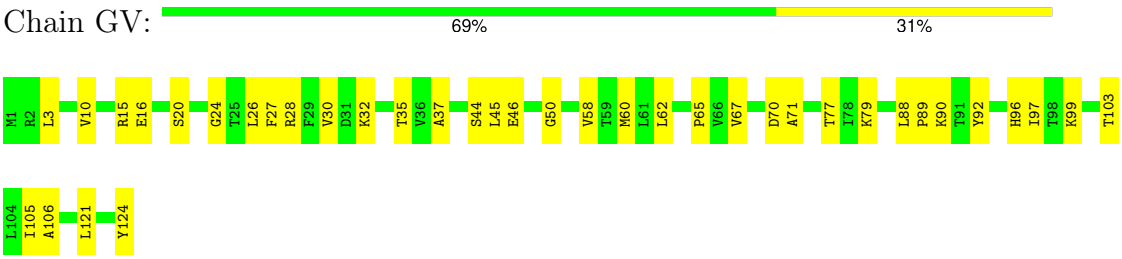
• Molecule 1: coat protein

Chain GU:



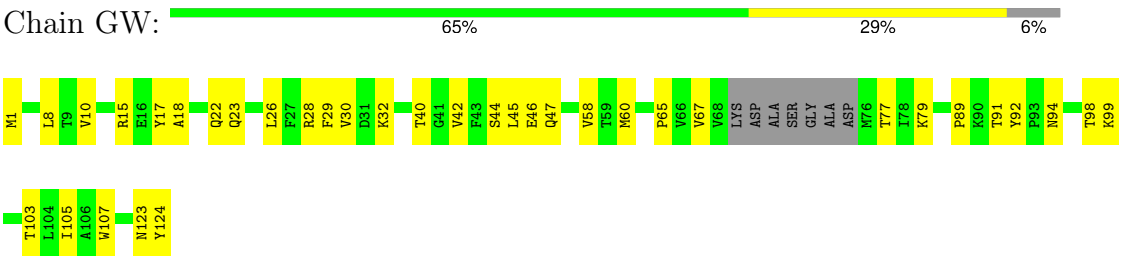
• Molecule 1: coat protein

Chain GV:



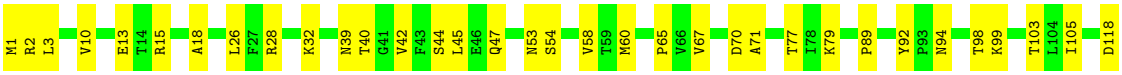
• Molecule 1: coat protein

Chain GW:



• Molecule 1: coat protein

Chain GX:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	269.42Å 277.20Å 277.44Å 103.91° 117.39° 106.96°	Depositor
Resolution (Å)	49.27 – 3.25 49.26 – 3.25	Depositor EDS
% Data completeness (in resolution range)	92.9 (49.27-3.25) 94.2 (49.26-3.25)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.241 , 0.239 0.244 , 0.243	Depositor DCC
R_{free} test set	10021 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å^2)	89.3	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.026 for k,h,-h-k-l 0.026 for l,-h-k-l,h 0.026 for -h-k-l,l,k	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	169260	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 2.26% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.33	0/969	0.56	0/1314
1	AB	0.33	0/923	0.55	0/1251
1	AC	0.32	0/969	0.55	0/1314
1	AD	0.33	0/969	0.56	0/1314
1	AE	0.33	0/923	0.55	0/1251
1	AF	0.33	0/969	0.55	0/1314
1	AG	0.33	0/969	0.56	0/1314
1	AH	0.33	0/923	0.55	0/1251
1	AI	0.33	0/969	0.55	0/1314
1	AJ	0.33	0/969	0.56	0/1314
1	AK	0.33	0/923	0.55	0/1251
1	AL	0.33	0/969	0.55	0/1314
1	AM	0.33	0/969	0.56	0/1314
1	AN	0.33	0/923	0.55	0/1251
1	AO	0.32	0/969	0.55	0/1314
1	AP	0.33	0/969	0.56	0/1314
1	AQ	0.33	0/923	0.55	0/1251
1	AR	0.33	0/969	0.55	0/1314
1	AS	0.33	0/969	0.56	0/1314
1	AT	0.33	0/923	0.55	0/1251
1	AU	0.32	0/969	0.55	0/1314
1	AV	0.33	0/969	0.56	0/1314
1	AW	0.33	0/923	0.55	0/1251
1	AX	0.32	0/969	0.55	0/1314
1	AY	0.33	0/969	0.56	0/1314
1	AZ	0.33	0/923	0.55	0/1251
1	BA	0.32	0/969	0.55	0/1314
1	BB	0.33	0/969	0.56	0/1314
1	BC	0.33	0/923	0.55	0/1251
1	BD	0.33	0/969	0.55	0/1314
1	BE	0.33	0/969	0.56	0/1314
1	BF	0.33	0/923	0.55	0/1251

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	BG	0.32	0/969	0.55	0/1314
1	BH	0.33	0/969	0.56	0/1314
1	BI	0.33	0/923	0.55	0/1251
1	BJ	0.33	0/969	0.55	0/1314
1	BK	0.33	0/969	0.56	0/1314
1	BL	0.33	0/923	0.55	0/1251
1	BM	0.32	0/969	0.55	0/1314
1	BN	0.33	0/969	0.56	0/1314
1	BO	0.33	0/923	0.55	0/1251
1	BP	0.32	0/969	0.55	0/1314
1	BQ	0.33	0/969	0.56	0/1314
1	BR	0.33	0/923	0.55	0/1251
1	BS	0.32	0/969	0.55	0/1314
1	BT	0.33	0/969	0.56	0/1314
1	BU	0.33	0/923	0.55	0/1251
1	BV	0.32	0/969	0.55	0/1314
1	BW	0.33	0/969	0.56	0/1314
1	BX	0.33	0/923	0.55	0/1251
1	BY	0.32	0/969	0.55	0/1314
1	BZ	0.33	0/969	0.56	0/1314
1	CA	0.33	0/923	0.55	0/1251
1	CB	0.32	0/969	0.55	0/1314
1	CC	0.33	0/969	0.56	0/1314
1	CD	0.33	0/923	0.55	0/1251
1	CE	0.32	0/969	0.55	0/1314
1	CF	0.33	0/969	0.56	0/1314
1	CG	0.33	0/923	0.55	0/1251
1	CH	0.32	0/969	0.55	0/1314
1	CI	0.33	0/969	0.56	0/1314
1	CJ	0.33	0/923	0.55	0/1251
1	CK	0.32	0/969	0.55	0/1314
1	CL	0.33	0/969	0.56	0/1314
1	CM	0.33	0/923	0.55	0/1251
1	CN	0.32	0/969	0.55	0/1314
1	CO	0.33	0/969	0.55	0/1314
1	CP	0.33	0/923	0.55	0/1251
1	CQ	0.32	0/969	0.55	0/1314
1	CR	0.33	0/969	0.56	0/1314
1	CS	0.33	0/923	0.55	0/1251
1	CT	0.32	0/969	0.55	0/1314
1	CU	0.33	0/969	0.56	0/1314
1	CV	0.33	0/923	0.55	0/1251
1	CW	0.33	0/969	0.55	0/1314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	CX	0.33	0/969	0.56	0/1314
1	CY	0.33	0/923	0.55	0/1251
1	CZ	0.32	0/969	0.55	0/1314
1	DA	0.33	0/969	0.56	0/1314
1	DB	0.33	0/923	0.55	0/1251
1	DC	0.32	0/969	0.55	0/1314
1	DD	0.33	0/969	0.56	0/1314
1	DE	0.33	0/923	0.55	0/1251
1	DF	0.32	0/969	0.55	0/1314
1	DG	0.33	0/969	0.56	0/1314
1	DH	0.33	0/923	0.55	0/1251
1	DI	0.33	0/969	0.55	0/1314
1	DJ	0.33	0/969	0.56	0/1314
1	DK	0.33	0/923	0.55	0/1251
1	DL	0.32	0/969	0.55	0/1314
1	DM	0.33	0/969	0.56	0/1314
1	DN	0.33	0/923	0.55	0/1251
1	DO	0.32	0/969	0.55	0/1314
1	DP	0.33	0/969	0.56	0/1314
1	DQ	0.33	0/923	0.55	0/1251
1	DR	0.33	0/969	0.55	0/1314
1	DS	0.33	0/969	0.56	0/1314
1	DT	0.33	0/923	0.55	0/1251
1	DU	0.32	0/969	0.55	0/1314
1	DV	0.33	0/969	0.56	0/1314
1	DW	0.33	0/923	0.55	0/1251
1	DX	0.33	0/969	0.55	0/1314
1	DY	0.33	0/969	0.56	0/1314
1	DZ	0.33	0/923	0.55	0/1251
1	EA	0.33	0/969	0.55	0/1314
1	EB	0.33	0/969	0.56	0/1314
1	EC	0.33	0/923	0.55	0/1251
1	ED	0.32	0/969	0.55	0/1314
1	EE	0.33	0/969	0.56	0/1314
1	EF	0.33	0/923	0.55	0/1251
1	EG	0.32	0/969	0.55	0/1314
1	EH	0.33	0/969	0.56	0/1314
1	EI	0.33	0/923	0.55	0/1251
1	EJ	0.33	0/969	0.55	0/1314
1	EK	0.33	0/969	0.56	0/1314
1	EL	0.33	0/923	0.55	0/1251
1	EM	0.32	0/969	0.55	0/1314
1	EN	0.33	0/969	0.56	0/1314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	EO	0.33	0/923	0.55	0/1251
1	EP	0.32	0/969	0.55	0/1314
1	EQ	0.33	0/969	0.56	0/1314
1	ER	0.33	0/923	0.55	0/1251
1	ES	0.32	0/969	0.55	0/1314
1	ET	0.33	0/969	0.56	0/1314
1	EU	0.33	0/923	0.55	0/1251
1	EV	0.33	0/969	0.55	0/1314
1	EW	0.33	0/969	0.56	0/1314
1	EX	0.33	0/923	0.55	0/1251
1	EY	0.32	0/969	0.55	0/1314
1	EZ	0.33	0/969	0.56	0/1314
1	FA	0.33	0/923	0.55	0/1251
1	FB	0.32	0/969	0.55	0/1314
1	FC	0.33	0/969	0.56	0/1314
1	FD	0.33	0/923	0.55	0/1251
1	FE	0.32	0/969	0.55	0/1314
1	FF	0.33	0/969	0.56	0/1314
1	FG	0.33	0/923	0.55	0/1251
1	FH	0.32	0/969	0.55	0/1314
1	FI	0.33	0/969	0.56	0/1314
1	FJ	0.33	0/923	0.55	0/1251
1	FK	0.32	0/969	0.55	0/1314
1	FL	0.33	0/969	0.56	0/1314
1	FM	0.33	0/923	0.55	0/1251
1	FN	0.32	0/969	0.55	0/1314
1	FO	0.33	0/969	0.56	0/1314
1	FP	0.33	0/923	0.55	0/1251
1	FQ	0.33	0/969	0.55	0/1314
1	FR	0.33	0/969	0.56	0/1314
1	FS	0.33	0/923	0.55	0/1251
1	FT	0.32	0/969	0.55	0/1314
1	FU	0.33	0/969	0.56	0/1314
1	FV	0.33	0/923	0.55	0/1251
1	FW	0.32	0/969	0.55	0/1314
1	FX	0.33	0/969	0.56	0/1314
1	FY	0.33	0/923	0.55	0/1251
1	FZ	0.33	0/969	0.55	0/1314
1	GA	0.33	0/969	0.56	0/1314
1	GB	0.33	0/923	0.55	0/1251
1	GC	0.32	0/969	0.55	0/1314
1	GD	0.33	0/969	0.56	0/1314
1	GE	0.33	0/923	0.55	0/1251

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	GF	0.32	0/969	0.55	0/1314
1	GG	0.33	0/969	0.56	0/1314
1	GH	0.33	0/923	0.55	0/1251
1	GI	0.32	0/969	0.55	0/1314
1	GJ	0.33	0/969	0.56	0/1314
1	GK	0.33	0/923	0.55	0/1251
1	GL	0.33	0/969	0.55	0/1314
1	GM	0.33	0/969	0.56	0/1314
1	GN	0.33	0/923	0.55	0/1251
1	GO	0.33	0/969	0.55	0/1314
1	GP	0.33	0/969	0.56	0/1314
1	GQ	0.33	0/923	0.55	0/1251
1	GR	0.32	0/969	0.55	0/1314
1	GS	0.33	0/969	0.56	0/1314
1	GT	0.33	0/923	0.55	0/1251
1	GU	0.32	0/969	0.55	0/1314
1	GV	0.33	0/969	0.56	0/1314
1	GW	0.33	0/923	0.55	0/1251
1	GX	0.32	0/969	0.55	0/1314
All	All	0.33	0/171660	0.55	0/232740

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	955	0	947	31	0
1	AB	910	0	907	37	0
1	AC	955	0	947	36	0
1	AD	955	0	947	33	0
1	AE	910	0	907	48	0
1	AF	955	0	947	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AG	955	0	947	32	0
1	AH	910	0	907	36	0
1	AI	955	0	947	37	0
1	AJ	955	0	947	35	0
1	AK	910	0	907	37	0
1	AL	955	0	947	32	0
1	AM	955	0	947	46	0
1	AN	910	0	907	51	2
1	AO	955	0	947	30	0
1	AP	955	0	947	40	0
1	AQ	910	0	907	34	0
1	AR	955	0	947	45	0
1	AS	955	0	947	37	0
1	AT	910	0	907	27	0
1	AU	955	0	947	33	0
1	AV	955	0	947	37	0
1	AW	910	0	907	34	0
1	AX	955	0	947	39	0
1	AY	955	0	947	44	0
1	AZ	910	0	907	31	0
1	BA	955	0	947	33	0
1	BB	955	0	947	29	0
1	BC	910	0	907	33	0
1	BD	955	0	947	40	0
1	BE	955	0	947	30	0
1	BF	910	0	907	32	0
1	BG	955	0	947	29	0
1	BH	955	0	947	37	2
1	BI	910	0	907	33	0
1	BJ	955	0	947	30	1
1	BK	955	0	947	48	0
1	BL	910	0	907	35	0
1	BM	955	0	947	41	0
1	BN	955	0	947	42	0
1	BO	910	0	907	37	0
1	BP	955	0	947	29	0
1	BQ	955	0	947	30	0
1	BR	910	0	907	28	0
1	BS	955	0	947	29	0
1	BT	955	0	947	47	1
1	BU	910	0	907	41	1
1	BV	955	0	947	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BW	955	0	947	31	0
1	BX	910	0	907	36	0
1	BY	955	0	947	31	0
1	BZ	955	0	947	39	0
1	CA	910	0	907	45	1
1	CB	955	0	947	44	0
1	CC	955	0	947	44	0
1	CD	910	0	907	37	0
1	CE	955	0	947	30	0
1	CF	955	0	947	39	0
1	CG	910	0	907	42	1
1	CH	955	0	947	37	0
1	CI	955	0	947	30	1
1	CJ	910	0	907	30	3
1	CK	955	0	947	30	0
1	CL	955	0	947	41	0
1	CM	910	0	907	31	0
1	CN	955	0	947	33	0
1	CO	955	0	947	31	0
1	CP	910	0	907	38	0
1	CQ	955	0	947	35	0
1	CR	955	0	947	36	0
1	CS	910	0	907	32	0
1	CT	955	0	947	36	0
1	CU	955	0	947	33	0
1	CV	910	0	907	35	0
1	CW	955	0	947	32	0
1	CX	955	0	947	30	0
1	CY	910	0	907	36	0
1	CZ	955	0	947	37	0
1	DA	955	0	947	29	0
1	DB	910	0	907	40	0
1	DC	955	0	947	43	0
1	DD	955	0	947	31	0
1	DE	910	0	907	29	0
1	DF	955	0	947	31	0
1	DG	955	0	947	28	0
1	DH	910	0	907	32	0
1	DI	955	0	947	39	0
1	DJ	955	0	947	35	0
1	DK	910	0	907	33	0
1	DL	955	0	947	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DM	955	0	947	33	0
1	DN	910	0	907	45	1
1	DO	955	0	947	41	0
1	DP	955	0	947	31	0
1	DQ	910	0	907	32	0
1	DR	955	0	947	34	0
1	DS	955	0	947	29	0
1	DT	910	0	907	39	0
1	DU	955	0	947	38	0
1	DV	955	0	947	50	1
1	DW	910	0	907	53	1
1	DX	955	0	947	29	0
1	DY	955	0	947	29	0
1	DZ	910	0	907	42	0
1	EA	955	0	947	29	0
1	EB	955	0	947	44	0
1	EC	910	0	907	34	0
1	ED	955	0	947	46	0
1	EE	955	0	947	33	0
1	EF	910	0	907	36	0
1	EG	955	0	947	33	3
1	EH	955	0	947	50	1
1	EI	910	0	907	47	3
1	EJ	955	0	947	36	0
1	EK	955	0	947	28	3
1	EL	910	0	907	39	0
1	EM	955	0	947	31	0
1	EN	955	0	947	32	0
1	EO	910	0	907	48	1
1	EP	955	0	947	43	0
1	EQ	955	0	947	36	0
1	ER	910	0	907	29	1
1	ES	955	0	947	30	0
1	ET	955	0	947	46	0
1	EU	910	0	907	32	0
1	EV	955	0	947	35	1
1	EW	955	0	947	31	0
1	EX	910	0	907	37	0
1	EY	955	0	947	44	0
1	EZ	955	0	947	29	0
1	FA	910	0	907	34	0
1	FB	955	0	947	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FC	955	0	947	32	0
1	FD	910	0	907	32	0
1	FE	955	0	947	28	0
1	FF	955	0	947	31	0
1	FG	910	0	907	48	0
1	FH	955	0	947	31	0
1	FI	955	0	947	36	0
1	FJ	910	0	907	32	2
1	FK	955	0	947	31	0
1	FL	955	0	947	34	0
1	FM	910	0	907	37	0
1	FN	955	0	947	40	0
1	FO	955	0	947	37	0
1	FP	910	0	907	32	0
1	FQ	955	0	947	33	3
1	FR	955	0	947	48	0
1	FS	910	0	907	33	0
1	FT	955	0	947	37	0
1	FU	955	0	947	30	0
1	FV	910	0	907	30	0
1	FW	955	0	947	29	0
1	FX	955	0	947	35	0
1	FY	910	0	907	31	0
1	FZ	955	0	947	33	0
1	GA	955	0	947	47	1
1	GB	910	0	907	44	2
1	GC	955	0	947	34	0
1	GD	955	0	947	38	0
1	GE	910	0	907	50	1
1	GF	955	0	947	40	0
1	GG	955	0	947	34	0
1	GH	910	0	907	31	0
1	GI	955	0	947	32	0
1	GJ	955	0	947	38	0
1	GK	910	0	907	46	2
1	GL	955	0	947	39	2
1	GM	955	0	947	40	3
1	GN	910	0	907	38	3
1	GO	955	0	947	44	0
1	GP	955	0	947	31	0
1	GQ	910	0	907	31	0
1	GR	955	0	947	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GS	955	0	947	30	0
1	GT	910	0	907	34	0
1	GU	955	0	947	38	0
1	GV	955	0	947	30	0
1	GW	910	0	907	31	0
1	GX	955	0	947	28	0
2	AA	1	0	0	0	0
2	AD	1	0	0	0	0
2	AG	1	0	0	0	0
2	AJ	1	0	0	0	0
2	AM	1	0	0	0	0
2	AP	1	0	0	0	0
2	AS	1	0	0	0	0
2	AV	1	0	0	0	0
2	AY	1	0	0	0	0
2	BB	1	0	0	0	0
2	BE	1	0	0	0	0
2	BH	1	0	0	0	0
2	BK	1	0	0	0	0
2	BN	1	0	0	0	0
2	BQ	1	0	0	0	0
2	BT	1	0	0	0	0
2	BW	1	0	0	0	0
2	BZ	1	0	0	0	0
2	CC	1	0	0	0	0
2	CF	1	0	0	0	0
2	CI	1	0	0	0	0
2	CL	1	0	0	0	0
2	CO	1	0	0	0	0
2	CR	1	0	0	0	0
2	CU	1	0	0	0	0
2	CX	1	0	0	0	0
2	DA	1	0	0	0	0
2	DD	1	0	0	0	0
2	DG	1	0	0	0	0
2	DJ	1	0	0	0	0
2	DM	1	0	0	0	0
2	DP	1	0	0	0	0
2	DS	1	0	0	0	0
2	DV	1	0	0	0	0
2	DY	1	0	0	0	0
2	EB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	EE	1	0	0	0	0
2	EH	1	0	0	0	0
2	EK	1	0	0	0	0
2	EN	1	0	0	0	0
2	EQ	1	0	0	0	0
2	ET	1	0	0	0	0
2	EW	1	0	0	0	0
2	EZ	1	0	0	0	0
2	FC	1	0	0	0	0
2	FF	1	0	0	0	0
2	FI	1	0	0	0	0
2	FL	1	0	0	0	0
2	FO	1	0	0	0	0
2	FR	1	0	0	0	0
2	FU	1	0	0	0	0
2	FX	1	0	0	0	0
2	GA	1	0	0	0	0
2	GD	1	0	0	0	0
2	GG	1	0	0	0	0
2	GJ	1	0	0	0	0
2	GM	1	0	0	0	0
2	GP	1	0	0	0	0
2	GS	1	0	0	0	0
2	GV	1	0	0	0	0
All	All	169260	0	168060	4697	24

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 14.

The worst 5 of 4697 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:BK:15:ARG:HH11	1:DW:103:THR:HG21	1.14	1.12
1:EB:15:ARG:HH11	1:GB:103:THR:HG21	1.17	1.08
1:FP:103:THR:HG21	1:GV:15:ARG:HH11	1.16	1.07
1:CG:103:THR:HG21	1:CL:15:ARG:HH11	1.19	1.05
1:AE:103:THR:HG21	1:GA:15:ARG:HH11	1.23	1.03

The worst 5 of 24 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:AN:32:LYS:NZ	1:GB:16:GLU:OE2[1_666]	1.39	0.81
1:BU:32:LYS:NZ	1:DW:16:GLU:OE2[1_554]	1.50	0.70
1:BH:12:GLU:O	1:GK:5:ASP:O[1_655]	1.55	0.65
1:EI:35:THR:CG2	1:GN:12:GLU:OE1[1_545]	1.55	0.65
1:BH:12:GLU:OE1	1:GK:7:ASP:OD1[1_655]	1.57	0.63

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	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	AB	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	AC	122/124 (98%)	122 (100%)	0	0	100	100
1	AD	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	AE	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	AF	122/124 (98%)	122 (100%)	0	0	100	100
1	AG	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	AH	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	AI	122/124 (98%)	122 (100%)	0	0	100	100
1	AJ	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	AK	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	AL	122/124 (98%)	122 (100%)	0	0	100	100
1	AM	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	AN	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	AO	122/124 (98%)	122 (100%)	0	0	100	100
1	AP	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	AQ	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	AR	122/124 (98%)	122 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AS	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	AT	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	AU	122/124 (98%)	122 (100%)	0	0	100	100
1	AV	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	AW	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	AX	122/124 (98%)	122 (100%)	0	0	100	100
1	AY	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	AZ	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	BA	122/124 (98%)	122 (100%)	0	0	100	100
1	BB	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	BC	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	BD	122/124 (98%)	122 (100%)	0	0	100	100
1	BE	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	BF	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	BG	122/124 (98%)	122 (100%)	0	0	100	100
1	BH	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	BI	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	BJ	122/124 (98%)	122 (100%)	0	0	100	100
1	BK	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	BL	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	BM	122/124 (98%)	122 (100%)	0	0	100	100
1	BN	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	BO	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	BP	122/124 (98%)	122 (100%)	0	0	100	100
1	BQ	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	BR	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	BS	122/124 (98%)	122 (100%)	0	0	100	100
1	BT	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	BU	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	BV	122/124 (98%)	122 (100%)	0	0	100	100
1	BW	122/124 (98%)	121 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BX	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	BY	122/124 (98%)	122 (100%)	0	0	100	100
1	BZ	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	CA	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	CB	122/124 (98%)	122 (100%)	0	0	100	100
1	CC	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	CD	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	CE	122/124 (98%)	122 (100%)	0	0	100	100
1	CF	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	CG	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	CH	122/124 (98%)	122 (100%)	0	0	100	100
1	CI	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	CJ	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	CK	122/124 (98%)	122 (100%)	0	0	100	100
1	CL	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	CM	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	CN	122/124 (98%)	122 (100%)	0	0	100	100
1	CO	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	CP	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	CQ	122/124 (98%)	122 (100%)	0	0	100	100
1	CR	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	CS	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	CT	122/124 (98%)	122 (100%)	0	0	100	100
1	CU	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	CV	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	CW	122/124 (98%)	122 (100%)	0	0	100	100
1	CX	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	CY	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	CZ	122/124 (98%)	122 (100%)	0	0	100	100
1	DA	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	DB	113/124 (91%)	110 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DC	122/124 (98%)	122 (100%)	0	0	100	100
1	DD	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	DE	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	DF	122/124 (98%)	122 (100%)	0	0	100	100
1	DG	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	DH	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	DI	122/124 (98%)	122 (100%)	0	0	100	100
1	DJ	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	DK	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	DL	122/124 (98%)	122 (100%)	0	0	100	100
1	DM	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	DN	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	DO	122/124 (98%)	122 (100%)	0	0	100	100
1	DP	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	DQ	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	DR	122/124 (98%)	122 (100%)	0	0	100	100
1	DS	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	DT	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	DU	122/124 (98%)	122 (100%)	0	0	100	100
1	DV	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	DW	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	DX	122/124 (98%)	122 (100%)	0	0	100	100
1	DY	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	DZ	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	EA	122/124 (98%)	122 (100%)	0	0	100	100
1	EB	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	EC	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	ED	122/124 (98%)	122 (100%)	0	0	100	100
1	EE	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	EF	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	EG	122/124 (98%)	122 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EH	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	EI	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	EJ	122/124 (98%)	122 (100%)	0	0	100	100
1	EK	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	EL	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	EM	122/124 (98%)	122 (100%)	0	0	100	100
1	EN	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	EO	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	EP	122/124 (98%)	122 (100%)	0	0	100	100
1	EQ	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	ER	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	ES	122/124 (98%)	122 (100%)	0	0	100	100
1	ET	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	EU	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	EV	122/124 (98%)	122 (100%)	0	0	100	100
1	EW	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	EX	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	EY	122/124 (98%)	122 (100%)	0	0	100	100
1	EZ	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	FA	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	FB	122/124 (98%)	122 (100%)	0	0	100	100
1	FC	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	FD	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	FE	122/124 (98%)	122 (100%)	0	0	100	100
1	FF	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	FG	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	FH	122/124 (98%)	122 (100%)	0	0	100	100
1	FI	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	FJ	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	FK	122/124 (98%)	122 (100%)	0	0	100	100
1	FL	122/124 (98%)	121 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	FM	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	FN	122/124 (98%)	122 (100%)	0	0	100	100
1	FO	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	FP	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	FQ	122/124 (98%)	122 (100%)	0	0	100	100
1	FR	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	FS	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	FT	122/124 (98%)	122 (100%)	0	0	100	100
1	FU	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	FV	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	FW	122/124 (98%)	122 (100%)	0	0	100	100
1	FX	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	FY	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	FZ	122/124 (98%)	122 (100%)	0	0	100	100
1	GA	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	GB	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	GC	122/124 (98%)	122 (100%)	0	0	100	100
1	GD	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	GE	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	GF	122/124 (98%)	122 (100%)	0	0	100	100
1	GG	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	GH	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	GI	122/124 (98%)	122 (100%)	0	0	100	100
1	GJ	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	GK	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	GL	122/124 (98%)	122 (100%)	0	0	100	100
1	GM	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	GN	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	GO	122/124 (98%)	122 (100%)	0	0	100	100
1	GP	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	GQ	113/124 (91%)	110 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GR	122/124 (98%)	122 (100%)	0	0	100	100
1	GS	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	GT	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	GU	122/124 (98%)	122 (100%)	0	0	100	100
1	GV	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	GW	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	GX	122/124 (98%)	122 (100%)	0	0	100	100
All	All	21420/22320 (96%)	21180 (99%)	240 (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	107/107 (100%)	107 (100%)	0	100	100
1	AB	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	AC	107/107 (100%)	107 (100%)	0	100	100
1	AD	107/107 (100%)	107 (100%)	0	100	100
1	AE	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	AF	107/107 (100%)	107 (100%)	0	100	100
1	AG	107/107 (100%)	107 (100%)	0	100	100
1	AH	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	AI	107/107 (100%)	107 (100%)	0	100	100
1	AJ	107/107 (100%)	107 (100%)	0	100	100
1	AK	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	AL	107/107 (100%)	107 (100%)	0	100	100
1	AM	107/107 (100%)	107 (100%)	0	100	100
1	AN	103/107 (96%)	102 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AO	107/107 (100%)	107 (100%)	0	100	100
1	AP	107/107 (100%)	107 (100%)	0	100	100
1	AQ	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	AR	107/107 (100%)	107 (100%)	0	100	100
1	AS	107/107 (100%)	107 (100%)	0	100	100
1	AT	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	AU	107/107 (100%)	107 (100%)	0	100	100
1	AV	107/107 (100%)	107 (100%)	0	100	100
1	AW	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	AX	107/107 (100%)	107 (100%)	0	100	100
1	AY	107/107 (100%)	107 (100%)	0	100	100
1	AZ	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	BA	107/107 (100%)	107 (100%)	0	100	100
1	BB	107/107 (100%)	107 (100%)	0	100	100
1	BC	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	BD	107/107 (100%)	107 (100%)	0	100	100
1	BE	107/107 (100%)	107 (100%)	0	100	100
1	BF	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	BG	107/107 (100%)	107 (100%)	0	100	100
1	BH	107/107 (100%)	107 (100%)	0	100	100
1	BI	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	BJ	107/107 (100%)	107 (100%)	0	100	100
1	BK	107/107 (100%)	107 (100%)	0	100	100
1	BL	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	BM	107/107 (100%)	107 (100%)	0	100	100
1	BN	107/107 (100%)	107 (100%)	0	100	100
1	BO	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	BP	107/107 (100%)	107 (100%)	0	100	100
1	BQ	107/107 (100%)	107 (100%)	0	100	100
1	BR	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	BS	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BT	107/107 (100%)	107 (100%)	0	100	100
1	BU	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	BV	107/107 (100%)	107 (100%)	0	100	100
1	BW	107/107 (100%)	107 (100%)	0	100	100
1	BX	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	BY	107/107 (100%)	107 (100%)	0	100	100
1	BZ	107/107 (100%)	107 (100%)	0	100	100
1	CA	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	CB	107/107 (100%)	107 (100%)	0	100	100
1	CC	107/107 (100%)	107 (100%)	0	100	100
1	CD	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	CE	107/107 (100%)	107 (100%)	0	100	100
1	CF	107/107 (100%)	107 (100%)	0	100	100
1	CG	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	CH	107/107 (100%)	107 (100%)	0	100	100
1	CI	107/107 (100%)	107 (100%)	0	100	100
1	CJ	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	CK	107/107 (100%)	107 (100%)	0	100	100
1	CL	107/107 (100%)	107 (100%)	0	100	100
1	CM	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	CN	107/107 (100%)	107 (100%)	0	100	100
1	CO	107/107 (100%)	107 (100%)	0	100	100
1	CP	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	CQ	107/107 (100%)	107 (100%)	0	100	100
1	CR	107/107 (100%)	107 (100%)	0	100	100
1	CS	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	CT	107/107 (100%)	107 (100%)	0	100	100
1	CU	107/107 (100%)	107 (100%)	0	100	100
1	CV	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	CW	107/107 (100%)	107 (100%)	0	100	100
1	CX	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CY	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	CZ	107/107 (100%)	107 (100%)	0	100 100
1	DA	107/107 (100%)	107 (100%)	0	100 100
1	DB	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	DC	107/107 (100%)	107 (100%)	0	100 100
1	DD	107/107 (100%)	107 (100%)	0	100 100
1	DE	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	DF	107/107 (100%)	107 (100%)	0	100 100
1	DG	107/107 (100%)	107 (100%)	0	100 100
1	DH	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	DI	107/107 (100%)	107 (100%)	0	100 100
1	DJ	107/107 (100%)	107 (100%)	0	100 100
1	DK	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	DL	107/107 (100%)	107 (100%)	0	100 100
1	DM	107/107 (100%)	107 (100%)	0	100 100
1	DN	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	DO	107/107 (100%)	107 (100%)	0	100 100
1	DP	107/107 (100%)	107 (100%)	0	100 100
1	DQ	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	DR	107/107 (100%)	107 (100%)	0	100 100
1	DS	107/107 (100%)	107 (100%)	0	100 100
1	DT	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	DU	107/107 (100%)	107 (100%)	0	100 100
1	DV	107/107 (100%)	107 (100%)	0	100 100
1	DW	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	DX	107/107 (100%)	107 (100%)	0	100 100
1	DY	107/107 (100%)	107 (100%)	0	100 100
1	DZ	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	EA	107/107 (100%)	107 (100%)	0	100 100
1	EB	107/107 (100%)	107 (100%)	0	100 100
1	EC	103/107 (96%)	102 (99%)	1 (1%)	76 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ED	107/107 (100%)	107 (100%)	0	100	100
1	EE	107/107 (100%)	107 (100%)	0	100	100
1	EF	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	EG	107/107 (100%)	107 (100%)	0	100	100
1	EH	107/107 (100%)	107 (100%)	0	100	100
1	EI	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	EJ	107/107 (100%)	107 (100%)	0	100	100
1	EK	107/107 (100%)	107 (100%)	0	100	100
1	EL	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	EM	107/107 (100%)	107 (100%)	0	100	100
1	EN	107/107 (100%)	107 (100%)	0	100	100
1	EO	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	EP	107/107 (100%)	107 (100%)	0	100	100
1	EQ	107/107 (100%)	107 (100%)	0	100	100
1	ER	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	ES	107/107 (100%)	107 (100%)	0	100	100
1	ET	107/107 (100%)	107 (100%)	0	100	100
1	EU	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	EV	107/107 (100%)	107 (100%)	0	100	100
1	EW	107/107 (100%)	107 (100%)	0	100	100
1	EX	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	EY	107/107 (100%)	107 (100%)	0	100	100
1	EZ	107/107 (100%)	107 (100%)	0	100	100
1	FA	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	FB	107/107 (100%)	107 (100%)	0	100	100
1	FC	107/107 (100%)	107 (100%)	0	100	100
1	FD	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	FE	107/107 (100%)	107 (100%)	0	100	100
1	FF	107/107 (100%)	107 (100%)	0	100	100
1	FG	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	FH	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FI	107/107 (100%)	107 (100%)	0	100	100
1	FJ	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	FK	107/107 (100%)	107 (100%)	0	100	100
1	FL	107/107 (100%)	107 (100%)	0	100	100
1	FM	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	FN	107/107 (100%)	107 (100%)	0	100	100
1	FO	107/107 (100%)	107 (100%)	0	100	100
1	FP	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	FQ	107/107 (100%)	107 (100%)	0	100	100
1	FR	107/107 (100%)	107 (100%)	0	100	100
1	FS	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	FT	107/107 (100%)	107 (100%)	0	100	100
1	FU	107/107 (100%)	107 (100%)	0	100	100
1	FV	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	FW	107/107 (100%)	107 (100%)	0	100	100
1	FX	107/107 (100%)	107 (100%)	0	100	100
1	FY	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	FZ	107/107 (100%)	107 (100%)	0	100	100
1	GA	107/107 (100%)	107 (100%)	0	100	100
1	GB	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	GC	107/107 (100%)	107 (100%)	0	100	100
1	GD	107/107 (100%)	107 (100%)	0	100	100
1	GE	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	GF	107/107 (100%)	107 (100%)	0	100	100
1	GG	107/107 (100%)	107 (100%)	0	100	100
1	GH	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	GI	107/107 (100%)	107 (100%)	0	100	100
1	GJ	107/107 (100%)	107 (100%)	0	100	100
1	GK	103/107 (96%)	102 (99%)	1 (1%)	76	88
1	GL	107/107 (100%)	107 (100%)	0	100	100
1	GM	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	GN	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	GO	107/107 (100%)	107 (100%)	0	100 100
1	GP	107/107 (100%)	107 (100%)	0	100 100
1	GQ	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	GR	107/107 (100%)	107 (100%)	0	100 100
1	GS	107/107 (100%)	107 (100%)	0	100 100
1	GT	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	GU	107/107 (100%)	107 (100%)	0	100 100
1	GV	107/107 (100%)	107 (100%)	0	100 100
1	GW	103/107 (96%)	102 (99%)	1 (1%)	76 88
1	GX	107/107 (100%)	107 (100%)	0	100 100
All	All	19020/19260 (99%)	18960 (100%)	60 (0%)	92 96

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DH	22	GLN
1	GK	22	GLN
1	EC	22	GLN
1	GH	22	GLN
1	GW	22	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	FY	47	GLN
1	GW	47	GLN
1	GB	47	GLN
1	GK	22	GLN
1	CJ	47	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 60 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	124/124 (100%)	-0.42	0 100 100	66, 92, 154, 183	0
1	AB	117/124 (94%)	-0.41	2 (1%) 70 60	67, 92, 140, 186	0
1	AC	124/124 (100%)	-0.49	0 100 100	63, 92, 150, 173	0
1	AD	124/124 (100%)	-0.45	1 (0%) 86 80	66, 92, 154, 183	0
1	AE	117/124 (94%)	-0.31	2 (1%) 70 60	67, 92, 140, 186	0
1	AF	124/124 (100%)	-0.43	0 100 100	63, 92, 150, 173	0
1	AG	124/124 (100%)	-0.41	0 100 100	66, 92, 154, 183	0
1	AH	117/124 (94%)	-0.30	1 (0%) 84 78	67, 92, 140, 186	0
1	AI	124/124 (100%)	-0.56	0 100 100	63, 92, 150, 173	0
1	AJ	124/124 (100%)	-0.61	0 100 100	66, 92, 154, 183	0
1	AK	117/124 (94%)	-0.43	1 (0%) 84 78	67, 92, 140, 186	0
1	AL	124/124 (100%)	-0.53	0 100 100	63, 92, 150, 173	0
1	AM	124/124 (100%)	-0.36	0 100 100	66, 92, 154, 183	0
1	AN	117/124 (94%)	-0.27	0 100 100	67, 92, 140, 186	0
1	AO	124/124 (100%)	-0.40	0 100 100	63, 92, 150, 173	0
1	AP	124/124 (100%)	-0.41	0 100 100	66, 92, 154, 183	0
1	AQ	117/124 (94%)	-0.39	1 (0%) 84 78	67, 92, 140, 186	0
1	AR	124/124 (100%)	-0.47	0 100 100	63, 92, 150, 173	0
1	AS	124/124 (100%)	-0.40	0 100 100	66, 92, 154, 183	0
1	AT	117/124 (94%)	-0.41	1 (0%) 84 78	67, 92, 140, 186	0
1	AU	124/124 (100%)	-0.40	0 100 100	63, 92, 150, 173	0
1	AV	124/124 (100%)	-0.34	1 (0%) 86 80	66, 92, 154, 183	0
1	AW	117/124 (94%)	-0.34	2 (1%) 70 60	67, 92, 140, 186	0
1	AX	124/124 (100%)	-0.36	0 100 100	63, 92, 150, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AY	124/124 (100%)	-0.33	0 100 100	66, 92, 154, 183	0
1	AZ	117/124 (94%)	-0.24	1 (0%) 84 78	67, 92, 140, 186	0
1	BA	124/124 (100%)	-0.45	0 100 100	63, 92, 150, 173	0
1	BB	124/124 (100%)	-0.54	0 100 100	66, 92, 154, 183	0
1	BC	117/124 (94%)	-0.36	0 100 100	67, 92, 140, 186	0
1	BD	124/124 (100%)	-0.52	0 100 100	63, 92, 150, 173	0
1	BE	124/124 (100%)	-0.50	0 100 100	66, 92, 154, 183	0
1	BF	117/124 (94%)	-0.32	1 (0%) 84 78	67, 92, 140, 186	0
1	BG	124/124 (100%)	-0.44	0 100 100	63, 92, 150, 173	0
1	BH	124/124 (100%)	-0.36	0 100 100	66, 92, 154, 183	0
1	BI	117/124 (94%)	-0.35	1 (0%) 84 78	67, 92, 140, 186	0
1	BJ	124/124 (100%)	-0.40	0 100 100	63, 92, 150, 173	0
1	BK	124/124 (100%)	-0.34	2 (1%) 72 63	66, 92, 154, 183	0
1	BL	117/124 (94%)	-0.29	1 (0%) 84 78	67, 92, 140, 186	0
1	BM	124/124 (100%)	-0.49	0 100 100	63, 92, 150, 173	0
1	BN	124/124 (100%)	-0.56	1 (0%) 86 80	66, 92, 154, 183	0
1	BO	117/124 (94%)	-0.33	1 (0%) 84 78	67, 92, 140, 186	0
1	BP	124/124 (100%)	-0.44	0 100 100	63, 92, 150, 173	0
1	BQ	124/124 (100%)	-0.58	0 100 100	66, 92, 154, 183	0
1	BR	117/124 (94%)	-0.40	1 (0%) 84 78	67, 92, 140, 186	0
1	BS	124/124 (100%)	-0.52	0 100 100	63, 92, 150, 173	0
1	BT	124/124 (100%)	-0.28	0 100 100	66, 92, 154, 183	0
1	BU	117/124 (94%)	-0.23	0 100 100	67, 92, 140, 186	0
1	BV	124/124 (100%)	-0.36	0 100 100	63, 92, 150, 173	0
1	BW	124/124 (100%)	-0.54	0 100 100	66, 92, 154, 183	0
1	BX	117/124 (94%)	-0.29	1 (0%) 84 78	67, 92, 140, 186	0
1	BY	124/124 (100%)	-0.61	0 100 100	63, 92, 150, 173	0
1	BZ	124/124 (100%)	-0.38	0 100 100	66, 92, 154, 183	0
1	CA	117/124 (94%)	-0.28	1 (0%) 84 78	67, 92, 140, 186	0
1	CB	124/124 (100%)	-0.37	0 100 100	63, 92, 150, 173	0
1	CC	124/124 (100%)	-0.42	0 100 100	66, 92, 154, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	CD	117/124 (94%)	-0.36	1 (0%) 84 78	67, 92, 140, 186	0
1	CE	124/124 (100%)	-0.39	1 (0%) 86 80	63, 92, 150, 173	0
1	CF	124/124 (100%)	-0.39	1 (0%) 86 80	66, 92, 154, 183	0
1	CG	117/124 (94%)	-0.28	3 (2%) 56 44	67, 92, 140, 186	0
1	CH	124/124 (100%)	-0.48	0 100 100	63, 92, 150, 173	0
1	CI	124/124 (100%)	-0.31	0 100 100	66, 92, 154, 183	0
1	CJ	117/124 (94%)	-0.27	1 (0%) 84 78	67, 92, 140, 186	0
1	CK	124/124 (100%)	-0.37	0 100 100	63, 92, 150, 173	0
1	CL	124/124 (100%)	-0.45	0 100 100	66, 92, 154, 183	0
1	CM	117/124 (94%)	-0.41	4 (3%) 45 33	67, 92, 140, 186	0
1	CN	124/124 (100%)	-0.53	0 100 100	63, 92, 150, 173	0
1	CO	124/124 (100%)	-0.50	0 100 100	66, 92, 154, 183	0
1	CP	117/124 (94%)	-0.43	1 (0%) 84 78	67, 92, 140, 186	0
1	CQ	124/124 (100%)	-0.54	0 100 100	63, 92, 150, 173	0
1	CR	124/124 (100%)	-0.37	0 100 100	66, 92, 154, 183	0
1	CS	117/124 (94%)	-0.42	1 (0%) 84 78	67, 92, 140, 186	0
1	CT	124/124 (100%)	-0.44	0 100 100	63, 92, 150, 173	0
1	CU	124/124 (100%)	-0.41	0 100 100	66, 92, 154, 183	0
1	CV	117/124 (94%)	-0.28	2 (1%) 70 60	67, 92, 140, 186	0
1	CW	124/124 (100%)	-0.54	0 100 100	63, 92, 150, 173	0
1	CX	124/124 (100%)	-0.47	0 100 100	66, 92, 154, 183	0
1	CY	117/124 (94%)	-0.38	1 (0%) 84 78	67, 92, 140, 186	0
1	CZ	124/124 (100%)	-0.36	0 100 100	63, 92, 150, 173	0
1	DA	124/124 (100%)	-0.45	0 100 100	66, 92, 154, 183	0
1	DB	117/124 (94%)	-0.32	1 (0%) 84 78	67, 92, 140, 186	0
1	DC	124/124 (100%)	-0.40	1 (0%) 86 80	63, 92, 150, 173	0
1	DD	124/124 (100%)	-0.48	0 100 100	66, 92, 154, 183	0
1	DE	117/124 (94%)	-0.38	1 (0%) 84 78	67, 92, 140, 186	0
1	DF	124/124 (100%)	-0.52	0 100 100	63, 92, 150, 173	0
1	DG	124/124 (100%)	-0.49	0 100 100	66, 92, 154, 183	0
1	DH	117/124 (94%)	-0.36	0 100 100	67, 92, 140, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	DI	124/124 (100%)	-0.50	0 100 100	63, 92, 150, 173	0
1	DJ	124/124 (100%)	-0.52	0 100 100	66, 92, 154, 183	0
1	DK	117/124 (94%)	-0.42	1 (0%) 84 78	67, 92, 140, 186	0
1	DL	124/124 (100%)	-0.57	0 100 100	63, 92, 150, 173	0
1	DM	124/124 (100%)	-0.38	1 (0%) 86 80	66, 92, 154, 183	0
1	DN	117/124 (94%)	-0.25	1 (0%) 84 78	67, 92, 140, 186	0
1	DO	124/124 (100%)	-0.49	0 100 100	63, 92, 150, 173	0
1	DP	124/124 (100%)	-0.44	0 100 100	66, 92, 154, 183	0
1	DQ	117/124 (94%)	-0.52	2 (1%) 70 60	67, 92, 140, 186	0
1	DR	124/124 (100%)	-0.48	0 100 100	63, 92, 150, 173	0
1	DS	124/124 (100%)	-0.48	0 100 100	66, 92, 154, 183	0
1	DT	117/124 (94%)	-0.26	1 (0%) 84 78	67, 92, 140, 186	0
1	DU	124/124 (100%)	-0.56	0 100 100	63, 92, 150, 173	0
1	DV	124/124 (100%)	-0.32	0 100 100	66, 92, 154, 183	0
1	DW	117/124 (94%)	-0.17	0 100 100	67, 92, 140, 186	0
1	DX	124/124 (100%)	-0.34	0 100 100	63, 92, 150, 173	0
1	DY	124/124 (100%)	-0.60	0 100 100	66, 92, 154, 183	0
1	DZ	117/124 (94%)	-0.37	1 (0%) 84 78	67, 92, 140, 186	0
1	EA	124/124 (100%)	-0.46	0 100 100	63, 92, 150, 173	0
1	EB	124/124 (100%)	-0.41	0 100 100	66, 92, 154, 183	0
1	EC	117/124 (94%)	-0.38	1 (0%) 84 78	67, 92, 140, 186	0
1	ED	124/124 (100%)	-0.53	0 100 100	63, 92, 150, 173	0
1	EE	124/124 (100%)	-0.33	0 100 100	66, 92, 154, 183	0
1	EF	117/124 (94%)	-0.35	1 (0%) 84 78	67, 92, 140, 186	0
1	EG	124/124 (100%)	-0.28	0 100 100	63, 92, 150, 173	0
1	EH	124/124 (100%)	-0.41	0 100 100	66, 92, 154, 183	0
1	EI	117/124 (94%)	-0.15	1 (0%) 84 78	67, 92, 140, 186	0
1	EJ	124/124 (100%)	-0.46	0 100 100	63, 92, 150, 173	0
1	EK	124/124 (100%)	-0.38	0 100 100	66, 92, 154, 183	0
1	EL	117/124 (94%)	-0.35	1 (0%) 84 78	67, 92, 140, 186	0
1	EM	124/124 (100%)	-0.50	0 100 100	63, 92, 150, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	EN	124/124 (100%)	-0.32	1 (0%) 86 80	66, 92, 154, 183	0
1	EO	117/124 (94%)	-0.34	0 100 100	67, 92, 140, 186	0
1	EP	124/124 (100%)	-0.54	0 100 100	63, 92, 150, 173	0
1	EQ	124/124 (100%)	-0.46	0 100 100	66, 92, 154, 183	0
1	ER	117/124 (94%)	-0.11	3 (2%) 56 44	67, 92, 140, 186	0
1	ES	124/124 (100%)	-0.32	0 100 100	63, 92, 150, 173	0
1	ET	124/124 (100%)	-0.38	0 100 100	66, 92, 154, 183	0
1	EU	117/124 (94%)	-0.30	1 (0%) 84 78	67, 92, 140, 186	0
1	EV	124/124 (100%)	-0.37	0 100 100	63, 92, 150, 173	0
1	EW	124/124 (100%)	-0.44	0 100 100	66, 92, 154, 183	0
1	EX	117/124 (94%)	-0.44	2 (1%) 70 60	67, 92, 140, 186	0
1	EY	124/124 (100%)	-0.48	0 100 100	63, 92, 150, 173	0
1	EZ	124/124 (100%)	-0.48	0 100 100	66, 92, 154, 183	0
1	FA	117/124 (94%)	-0.37	1 (0%) 84 78	67, 92, 140, 186	0
1	FB	124/124 (100%)	-0.47	0 100 100	63, 92, 150, 173	0
1	FC	124/124 (100%)	-0.49	1 (0%) 86 80	66, 92, 154, 183	0
1	FD	117/124 (94%)	-0.34	0 100 100	67, 92, 140, 186	0
1	FE	124/124 (100%)	-0.53	0 100 100	63, 92, 150, 173	0
1	FF	124/124 (100%)	-0.51	0 100 100	66, 92, 154, 183	0
1	FG	117/124 (94%)	-0.32	1 (0%) 84 78	67, 92, 140, 186	0
1	FH	124/124 (100%)	-0.46	0 100 100	63, 92, 150, 173	0
1	FI	124/124 (100%)	-0.51	0 100 100	66, 92, 154, 183	0
1	FJ	117/124 (94%)	-0.36	1 (0%) 84 78	67, 92, 140, 186	0
1	FK	124/124 (100%)	-0.56	0 100 100	63, 92, 150, 173	0
1	FL	124/124 (100%)	-0.50	0 100 100	66, 92, 154, 183	0
1	FM	117/124 (94%)	-0.40	0 100 100	67, 92, 140, 186	0
1	FN	124/124 (100%)	-0.51	0 100 100	63, 92, 150, 173	0
1	FO	124/124 (100%)	-0.48	0 100 100	66, 92, 154, 183	0
1	FP	117/124 (94%)	-0.39	0 100 100	67, 92, 140, 186	0
1	FQ	124/124 (100%)	-0.29	0 100 100	63, 92, 150, 173	0
1	FR	124/124 (100%)	-0.38	0 100 100	66, 92, 154, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	FS	117/124 (94%)	-0.49	1 (0%) 84 78	67, 92, 140, 186	0
1	FT	124/124 (100%)	-0.52	0 100 100	63, 92, 150, 173	0
1	FU	124/124 (100%)	-0.47	1 (0%) 86 80	66, 92, 154, 183	0
1	FV	117/124 (94%)	-0.34	5 (4%) 35 25	67, 92, 140, 186	0
1	FW	124/124 (100%)	-0.50	0 100 100	63, 92, 150, 173	0
1	FX	124/124 (100%)	-0.52	0 100 100	66, 92, 154, 183	0
1	FY	117/124 (94%)	-0.45	1 (0%) 84 78	67, 92, 140, 186	0
1	FZ	124/124 (100%)	-0.55	0 100 100	63, 92, 150, 173	0
1	GA	124/124 (100%)	-0.31	0 100 100	66, 92, 154, 183	0
1	GB	117/124 (94%)	-0.29	0 100 100	67, 92, 140, 186	0
1	GC	124/124 (100%)	-0.40	0 100 100	63, 92, 150, 173	0
1	GD	124/124 (100%)	-0.39	0 100 100	66, 92, 154, 183	0
1	GE	117/124 (94%)	-0.22	1 (0%) 84 78	67, 92, 140, 186	0
1	GF	124/124 (100%)	-0.38	0 100 100	63, 92, 150, 173	0
1	GG	124/124 (100%)	-0.49	0 100 100	66, 92, 154, 183	0
1	GH	117/124 (94%)	-0.14	5 (4%) 35 25	67, 92, 140, 186	0
1	GI	124/124 (100%)	-0.51	0 100 100	63, 92, 150, 173	0
1	GJ	124/124 (100%)	-0.40	0 100 100	66, 92, 154, 183	0
1	GK	117/124 (94%)	-0.40	0 100 100	67, 92, 140, 186	0
1	GL	124/124 (100%)	-0.26	0 100 100	63, 92, 150, 173	0
1	GM	124/124 (100%)	-0.30	1 (0%) 86 80	66, 92, 154, 183	0
1	GN	117/124 (94%)	-0.29	0 100 100	67, 92, 140, 186	0
1	GO	124/124 (100%)	-0.46	0 100 100	63, 92, 150, 173	0
1	GP	124/124 (100%)	-0.52	0 100 100	66, 92, 154, 183	0
1	GQ	117/124 (94%)	-0.34	3 (2%) 56 44	67, 92, 140, 186	0
1	GR	124/124 (100%)	-0.50	0 100 100	63, 92, 150, 173	0
1	GS	124/124 (100%)	-0.41	0 100 100	66, 92, 154, 183	0
1	GT	117/124 (94%)	-0.23	1 (0%) 84 78	67, 92, 140, 186	0
1	GU	124/124 (100%)	-0.38	0 100 100	63, 92, 150, 173	0
1	GV	124/124 (100%)	-0.45	0 100 100	66, 92, 154, 183	0
1	GW	117/124 (94%)	-0.46	0 100 100	67, 92, 140, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	GX	124/124 (100%)	-0.50	0 100 100	63, 92, 150, 173	0
All	All	21900/22320 (98%)	-0.41	83 (0%) 92 90	63, 92, 152, 186	0

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FG	68	VAL	6.2
1	AE	68	VAL	5.3
1	GQ	68	VAL	5.3
1	GH	68	VAL	5.2
1	EF	68	VAL	5.1

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	GA	201	1/1	0.71	0.14	64,64,64,64	0
2	CA	BT	201	1/1	0.81	0.13	64,64,64,64	0
2	CA	BE	201	1/1	0.86	0.14	64,64,64,64	0
2	CA	EH	201	1/1	0.87	0.10	64,64,64,64	0
2	CA	EN	201	1/1	0.88	0.09	64,64,64,64	0
2	CA	DG	201	1/1	0.88	0.17	64,64,64,64	0
2	CA	BK	201	1/1	0.90	0.07	64,64,64,64	0
2	CA	AG	201	1/1	0.90	0.18	64,64,64,64	0
2	CA	FO	201	1/1	0.91	0.14	64,64,64,64	0
2	CA	DM	201	1/1	0.91	0.15	64,64,64,64	0
2	CA	EQ	201	1/1	0.92	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	AV	201	1/1	0.92	0.20	64,64,64,64	0
2	CA	AD	201	1/1	0.92	0.11	64,64,64,64	0
2	CA	GM	201	1/1	0.92	0.06	64,64,64,64	0
2	CA	FX	201	1/1	0.93	0.18	64,64,64,64	0
2	CA	DJ	201	1/1	0.93	0.12	64,64,64,64	0
2	CA	GD	201	1/1	0.93	0.18	64,64,64,64	0
2	CA	EE	201	1/1	0.93	0.09	64,64,64,64	0
2	CA	CI	201	1/1	0.94	0.15	64,64,64,64	0
2	CA	DD	201	1/1	0.94	0.16	64,64,64,64	0
2	CA	AY	201	1/1	0.94	0.12	64,64,64,64	0
2	CA	FC	201	1/1	0.94	0.18	64,64,64,64	0
2	CA	FI	201	1/1	0.94	0.10	64,64,64,64	0
2	CA	ET	201	1/1	0.95	0.12	64,64,64,64	0
2	CA	AP	201	1/1	0.95	0.09	64,64,64,64	0
2	CA	BZ	201	1/1	0.95	0.14	64,64,64,64	0
2	CA	BH	201	1/1	0.95	0.10	64,64,64,64	0
2	CA	CL	201	1/1	0.95	0.14	64,64,64,64	0
2	CA	EK	201	1/1	0.95	0.11	64,64,64,64	0
2	CA	AS	201	1/1	0.95	0.15	64,64,64,64	0
2	CA	GG	201	1/1	0.95	0.13	64,64,64,64	0
2	CA	BN	201	1/1	0.95	0.14	64,64,64,64	0
2	CA	GS	201	1/1	0.95	0.15	64,64,64,64	0
2	CA	DY	201	1/1	0.96	0.15	64,64,64,64	0
2	CA	CO	201	1/1	0.96	0.12	64,64,64,64	0
2	CA	CX	201	1/1	0.96	0.13	64,64,64,64	0
2	CA	DS	201	1/1	0.96	0.15	64,64,64,64	0
2	CA	FR	201	1/1	0.97	0.11	64,64,64,64	0
2	CA	AJ	201	1/1	0.97	0.17	64,64,64,64	0
2	CA	EW	201	1/1	0.97	0.10	64,64,64,64	0
2	CA	EZ	201	1/1	0.97	0.12	64,64,64,64	0
2	CA	BW	201	1/1	0.97	0.08	64,64,64,64	0
2	CA	GJ	201	1/1	0.97	0.11	64,64,64,64	0
2	CA	AM	201	1/1	0.97	0.07	64,64,64,64	0
2	CA	CR	201	1/1	0.97	0.20	64,64,64,64	0
2	CA	GV	201	1/1	0.97	0.13	64,64,64,64	0
2	CA	FU	201	1/1	0.98	0.14	64,64,64,64	0
2	CA	BB	201	1/1	0.98	0.12	64,64,64,64	0
2	CA	DA	201	1/1	0.98	0.20	64,64,64,64	0
2	CA	DP	201	1/1	0.98	0.14	64,64,64,64	0
2	CA	FF	201	1/1	0.98	0.21	64,64,64,64	0
2	CA	CC	201	1/1	0.98	0.11	64,64,64,64	0
2	CA	FL	201	1/1	0.98	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CA	GP	201	1/1	0.98	0.14	64,64,64,64	0
2	CA	DV	201	1/1	0.98	0.11	64,64,64,64	0
2	CA	BQ	201	1/1	0.98	0.12	64,64,64,64	0
2	CA	CF	201	1/1	0.99	0.05	64,64,64,64	0
2	CA	CU	201	1/1	0.99	0.14	64,64,64,64	0
2	CA	AA	201	1/1	0.99	0.11	64,64,64,64	0
2	CA	EB	201	1/1	0.99	0.10	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.