



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 12:44 PM BST

PDB ID : 6YF9
Title : Virus-like particle of bacteriophage AVE002
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on : 2020-03-26
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

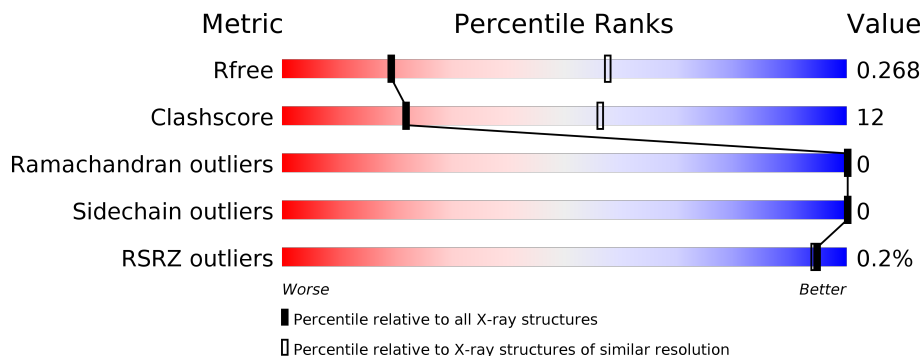
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.






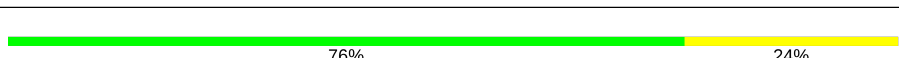
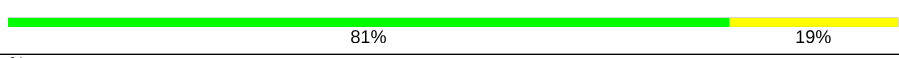

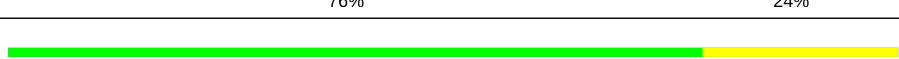



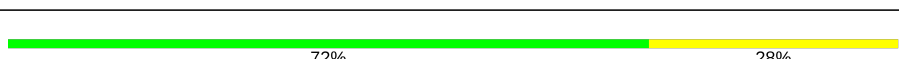



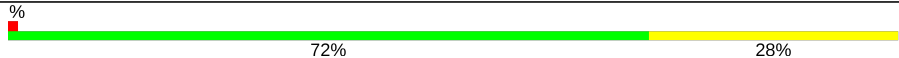

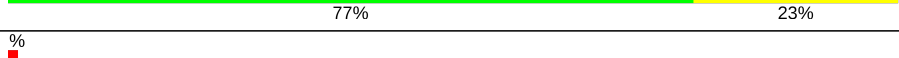






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	140	
1	AB	140	
1	AC	140	
1	AD	140	
1	AE	140	
1	AF	140	

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Mol	Chain	Length	Quality of chain	
1	AG	140		%
1	AH	140		%
1	AI	140		%
1	AJ	140		%
1	AK	140		%
1	AL	140		%
1	AM	140		%
1	AN	140		%
1	AO	140		%
1	AP	140		%
1	AQ	140		%
1	AR	140		%
1	AS	140		%
1	AT	140		%
1	AU	140		%
1	AV	140		%
1	AW	140		%
1	AX	140		%
1	AY	140		%
1	AZ	140		%
1	BA	140		%
1	BB	140		%
1	BC	140		%
1	BD	140		%
1	BE	140		%







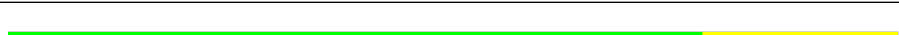
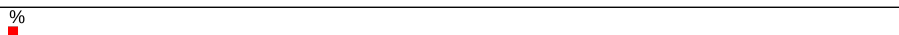
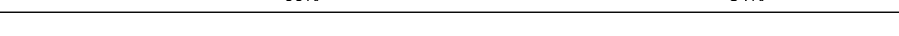


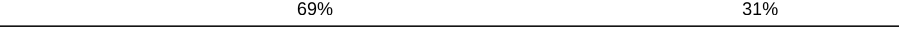









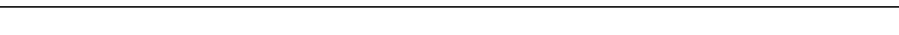
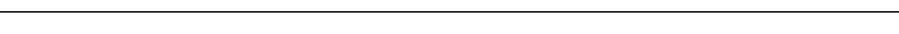
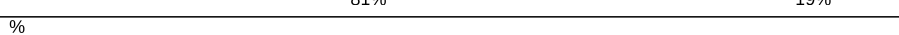
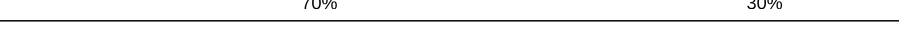
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Mol	Chain	Length	Quality of chain	
1	BF	140	75%	25%
1	BG	140	79%	21%
1	BH	140	71%	29%
1	BI	140	79%	21%
1	BJ	140	69%	31%
1	BK	140	72%	28%
1	BL	140	76%	24%
1	BM	140	80%	20%
1	BN	140	72%	28%
1	BO	140	76%	24%
1	BP	140	75%	25%
1	BQ	140	73%	27%
1	BR	140	76%	24%
1	BS	140	81%	19%
1	BT	140	73%	27%
1	BU	140	71%	29%
1	BV	140	77%	23%
1	BW	140	71%	29%
1	BX	140	75%	25%
1	BY	140	75%	25%
1	BZ	140	70%	30%
1	CA	140	72%	28%
1	CB	140	69%	31%
1	CC	140	71%	29%
1	CD	140	74%	26%








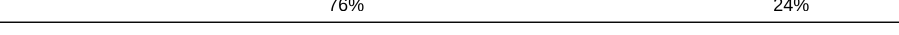
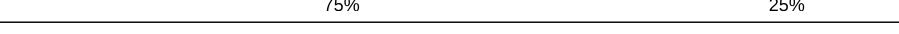
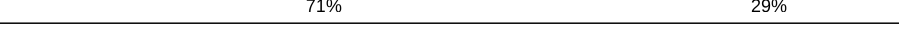
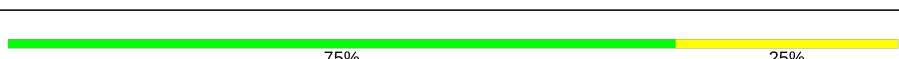








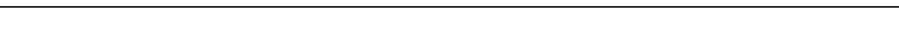
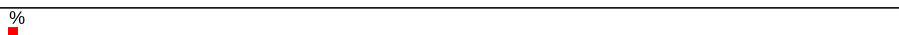
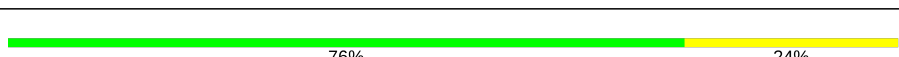



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Mol	Chain	Length	Quality of chain
1	CE	140	 77% 23%
1	CF	140	%  71% 29%
1	CG	140	 71% 29%
1	CH	140	 74% 26%
1	CI	140	 71% 29%
1	CJ	140	 73% 27%
1	CK	140	 78% 22%
1	CL	140	%  66% 34%
1	CM	140	 74% 26%
1	CN	140	 79% 21%
1	CO	140	 69% 31%
1	CP	140	 76% 24%
1	CQ	140	 72% 28%
1	CR	140	 71% 29%
1	CS	140	 69% 31%
1	CT	140	 73% 27%
1	CU	140	%  66% 34%
1	CV	140	 76% 24%
1	CW	140	 78% 22%
1	CX	140	 74% 26%
1	CY	140	 75% 25%
1	CZ	140	 81% 19%
1	DA	140	%  70% 30%
1	DB	140	 79% 21%
1	DC	140	 75% 25%

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Mol	Chain	Length	Quality of chain
1	DD	140	% 
1	DE	140	
1	DF	140	
1	DG	140	
1	DH	140	
1	DI	140	
1	DJ	140	% 
1	DK	140	
1	DL	140	
1	DM	140	
1	DN	140	
1	DO	140	
1	DP	140	% 
1	DQ	140	
1	DR	140	
1	DS	140	
1	DT	140	
1	DU	140	
1	DV	140	
1	DW	140	
1	DX	140	
1	DY	140	% 
1	DZ	140	
1	EA	140	
1	EB	140	

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Mol	Chain	Length	Quality of chain
1	EC	140	77% 23%
1	ED	140	% 72% 28%
1	EE	140	64% 36%
1	EF	140	75% 25%
1	EG	140	76% 24%
1	EH	140	% 71% 29%
1	EI	140	77% 23%
1	EJ	140	77% 23%
1	EK	140	% 73% 27%
1	EL	140	74% 26%
1	EM	140	77% 23%
1	EN	140	% 66% 34%
1	EO	140	76% 24%
1	EP	140	77% 23%
1	EQ	140	71% 29%
1	ER	140	76% 24%
1	ES	140	79% 21%
1	ET	140	71% 29%
1	EU	140	67% 33%
1	EV	140	71% 29%
1	EW	140	71% 29%
1	EX	140	76% 24%
1	EY	140	77% 23%
1	EZ	140	% 69% 31%
1	FA	140	73% 27%

























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Mol	Chain	Length	Quality of chain	
1	FB	140	74%	26%
1	FC	140	72%	28%
1	FD	140	73%	27%
1	FE	140	81%	19%
1	FF	140	70%	30%
1	FG	140	72%	28%
1	FH	140	75%	25%
1	FI	140	74%	26%
1	FJ	140	69%	31%
1	FK	140	78%	22%
1	FL	140	69%	31%
1	FM	140	73%	27%
1	FN	140	69%	31%
1	FO	140	72%	28%
1	FP	140	75%	25%
1	FQ	140	74%	26%
1	FR	140	72%	28%
1	FS	140	76%	24%
1	FT	140	76%	24%
1	FU	140	71%	29%
1	FV	140	75%	25%
1	FW	140	79%	21%
1	FX	140	74%	26%
1	FY	140	75%	25%
1	FZ	140	76%	24%

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Mol	Chain	Length	Quality of chain
1	GA	140	% 
1	GB	140	
1	GC	140	
1	GD	140	% 
1	GE	140	
1	GF	140	
1	GG	140	
1	GH	140	
1	GI	140	
1	GJ	140	% 
1	GK	140	
1	GL	140	
1	GM	140	% 
1	GN	140	
1	GO	140	
1	GP	140	
1	GQ	140	
1	GR	140	
1	GS	140	
1	GT	140	
1	GU	140	
1	GV	140	% 
1	GW	140	
1	GX	140	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 184320 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AA	140	1024	639	177	205	3	0	0	0
1	AB	140	1024	639	177	205	3	0	0	0
1	AC	140	1024	639	177	205	3	0	0	0
1	AD	140	1024	639	177	205	3	0	0	0
1	AE	140	1024	639	177	205	3	0	0	0
1	AF	140	1024	639	177	205	3	0	0	0
1	AG	140	1024	639	177	205	3	0	0	0
1	AH	140	1024	639	177	205	3	0	0	0
1	AI	140	1024	639	177	205	3	0	0	0
1	AJ	140	1024	639	177	205	3	0	0	0
1	AK	140	1024	639	177	205	3	0	0	0
1	AL	140	1024	639	177	205	3	0	0	0
1	AM	140	1024	639	177	205	3	0	0	0
1	AN	140	1024	639	177	205	3	0	0	0
1	AO	140	1024	639	177	205	3	0	0	0
1	AP	140	1024	639	177	205	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AQ	140	1024	639	177	205	3	0	0	0
1	AR	140	1024	639	177	205	3	0	0	0
1	AS	140	1024	639	177	205	3	0	0	0
1	AT	140	1024	639	177	205	3	0	0	0
1	AU	140	1024	639	177	205	3	0	0	0
1	AV	140	1024	639	177	205	3	0	0	0
1	AW	140	1024	639	177	205	3	0	0	0
1	AX	140	1024	639	177	205	3	0	0	0
1	AY	140	1024	639	177	205	3	0	0	0
1	AZ	140	1024	639	177	205	3	0	0	0
1	BA	140	1024	639	177	205	3	0	0	0
1	BB	140	1024	639	177	205	3	0	0	0
1	BC	140	1024	639	177	205	3	0	0	0
1	BD	140	1024	639	177	205	3	0	0	0
1	BE	140	1024	639	177	205	3	0	0	0
1	BF	140	1024	639	177	205	3	0	0	0
1	BG	140	1024	639	177	205	3	0	0	0
1	BH	140	1024	639	177	205	3	0	0	0
1	BI	140	1024	639	177	205	3	0	0	0
1	BJ	140	1024	639	177	205	3	0	0	0
1	BK	140	1024	639	177	205	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	BL	140	1024	639	177	205	3	0	0	0
1	BM	140	1024	639	177	205	3	0	0	0
1	BN	140	1024	639	177	205	3	0	0	0
1	BO	140	1024	639	177	205	3	0	0	0
1	BP	140	1024	639	177	205	3	0	0	0
1	BQ	140	1024	639	177	205	3	0	0	0
1	BR	140	1024	639	177	205	3	0	0	0
1	BS	140	1024	639	177	205	3	0	0	0
1	BT	140	1024	639	177	205	3	0	0	0
1	BU	140	1024	639	177	205	3	0	0	0
1	BV	140	1024	639	177	205	3	0	0	0
1	BW	140	1024	639	177	205	3	0	0	0
1	BX	140	1024	639	177	205	3	0	0	0
1	BY	140	1024	639	177	205	3	0	0	0
1	BZ	140	1024	639	177	205	3	0	0	0
1	CA	140	1024	639	177	205	3	0	0	0
1	CB	140	1024	639	177	205	3	0	0	0
1	CC	140	1024	639	177	205	3	0	0	0
1	CD	140	1024	639	177	205	3	0	0	0
1	CE	140	1024	639	177	205	3	0	0	0
1	CF	140	1024	639	177	205	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	CG	140	1024	639	177	205	3	0	0	0
1	CH	140	1024	639	177	205	3	0	0	0
1	CI	140	1024	639	177	205	3	0	0	0
1	CJ	140	1024	639	177	205	3	0	0	0
1	CK	140	1024	639	177	205	3	0	0	0
1	CL	140	1024	639	177	205	3	0	0	0
1	CM	140	1024	639	177	205	3	0	0	0
1	CN	140	1024	639	177	205	3	0	0	0
1	CO	140	1024	639	177	205	3	0	0	0
1	CP	140	1024	639	177	205	3	0	0	0
1	CQ	140	1024	639	177	205	3	0	0	0
1	CR	140	1024	639	177	205	3	0	0	0
1	CS	140	1024	639	177	205	3	0	0	0
1	CT	140	1024	639	177	205	3	0	0	0
1	CU	140	1024	639	177	205	3	0	0	0
1	CV	140	1024	639	177	205	3	0	0	0
1	CW	140	1024	639	177	205	3	0	0	0
1	CX	140	1024	639	177	205	3	0	0	0
1	CY	140	1024	639	177	205	3	0	0	0
1	CZ	140	1024	639	177	205	3	0	0	0
1	DA	140	1024	639	177	205	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	DB	140	1024	639	177	205	3	0	0	0
1	DC	140	1024	639	177	205	3	0	0	0
1	DD	140	1024	639	177	205	3	0	0	0
1	DE	140	1024	639	177	205	3	0	0	0
1	DF	140	1024	639	177	205	3	0	0	0
1	DG	140	1024	639	177	205	3	0	0	0
1	DH	140	1024	639	177	205	3	0	0	0
1	DI	140	1024	639	177	205	3	0	0	0
1	DJ	140	1024	639	177	205	3	0	0	0
1	DK	140	1024	639	177	205	3	0	0	0
1	DL	140	1024	639	177	205	3	0	0	0
1	DM	140	1024	639	177	205	3	0	0	0
1	DN	140	1024	639	177	205	3	0	0	0
1	DO	140	1024	639	177	205	3	0	0	0
1	DP	140	1024	639	177	205	3	0	0	0
1	DQ	140	1024	639	177	205	3	0	0	0
1	DR	140	1024	639	177	205	3	0	0	0
1	DS	140	1024	639	177	205	3	0	0	0
1	DT	140	1024	639	177	205	3	0	0	0
1	DU	140	1024	639	177	205	3	0	0	0
1	DV	140	1024	639	177	205	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	DW	140	1024	639	177	205	3	0	0	0
1	DX	140	1024	639	177	205	3	0	0	0
1	DY	140	1024	639	177	205	3	0	0	0
1	DZ	140	1024	639	177	205	3	0	0	0
1	EA	140	1024	639	177	205	3	0	0	0
1	EB	140	1024	639	177	205	3	0	0	0
1	EC	140	1024	639	177	205	3	0	0	0
1	ED	140	1024	639	177	205	3	0	0	0
1	EE	140	1024	639	177	205	3	0	0	0
1	EF	140	1024	639	177	205	3	0	0	0
1	EG	140	1024	639	177	205	3	0	0	0
1	EH	140	1024	639	177	205	3	0	0	0
1	EI	140	1024	639	177	205	3	0	0	0
1	EJ	140	1024	639	177	205	3	0	0	0
1	EK	140	1024	639	177	205	3	0	0	0
1	EL	140	1024	639	177	205	3	0	0	0
1	EM	140	1024	639	177	205	3	0	0	0
1	EN	140	1024	639	177	205	3	0	0	0
1	EO	140	1024	639	177	205	3	0	0	0
1	EP	140	1024	639	177	205	3	0	0	0
1	EQ	140	1024	639	177	205	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	ER	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	ES	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	ET	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	EU	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	EV	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	EW	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	EX	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	EY	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	EZ	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FA	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FB	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FC	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FD	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FE	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FF	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FG	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FH	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FI	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FJ	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FK	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			
1	FL	140	Total	C	N	O	S	0	0	0
			1024	639	177	205	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	FM	140	1024	639	177	205	3	0	0	0
1	FN	140	1024	639	177	205	3	0	0	0
1	FO	140	1024	639	177	205	3	0	0	0
1	FP	140	1024	639	177	205	3	0	0	0
1	FQ	140	1024	639	177	205	3	0	0	0
1	FR	140	1024	639	177	205	3	0	0	0
1	FS	140	1024	639	177	205	3	0	0	0
1	FT	140	1024	639	177	205	3	0	0	0
1	FU	140	1024	639	177	205	3	0	0	0
1	FV	140	1024	639	177	205	3	0	0	0
1	FW	140	1024	639	177	205	3	0	0	0
1	FX	140	1024	639	177	205	3	0	0	0
1	FY	140	1024	639	177	205	3	0	0	0
1	FZ	140	1024	639	177	205	3	0	0	0
1	GA	140	1024	639	177	205	3	0	0	0
1	GB	140	1024	639	177	205	3	0	0	0
1	GC	140	1024	639	177	205	3	0	0	0
1	GD	140	1024	639	177	205	3	0	0	0
1	GE	140	1024	639	177	205	3	0	0	0
1	GF	140	1024	639	177	205	3	0	0	0
1	GG	140	1024	639	177	205	3	0	0	0

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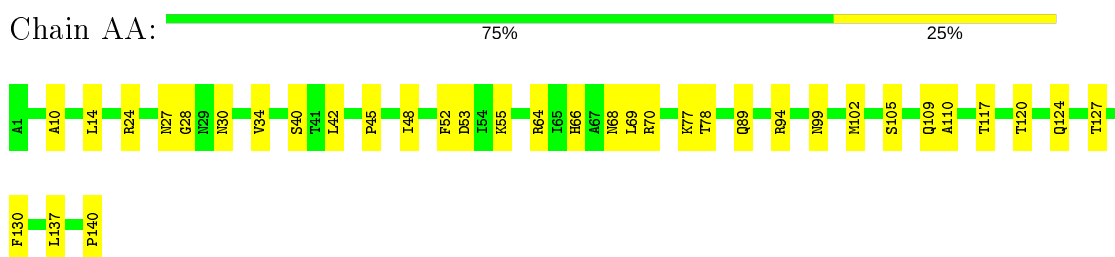
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	GH	140	1024	639	177	205	3	0	0	0
1	GI	140	1024	639	177	205	3	0	0	0
1	GJ	140	1024	639	177	205	3	0	0	0
1	GK	140	1024	639	177	205	3	0	0	0
1	GL	140	1024	639	177	205	3	0	0	0
1	GM	140	1024	639	177	205	3	0	0	0
1	GN	140	1024	639	177	205	3	0	0	0
1	GO	140	1024	639	177	205	3	0	0	0
1	GP	140	1024	639	177	205	3	0	0	0
1	GQ	140	1024	639	177	205	3	0	0	0
1	GR	140	1024	639	177	205	3	0	0	0
1	GS	140	1024	639	177	205	3	0	0	0
1	GT	140	1024	639	177	205	3	0	0	0
1	GU	140	1024	639	177	205	3	0	0	0
1	GV	140	1024	639	177	205	3	0	0	0
1	GW	140	1024	639	177	205	3	0	0	0
1	GX	140	1024	639	177	205	3	0	0	0

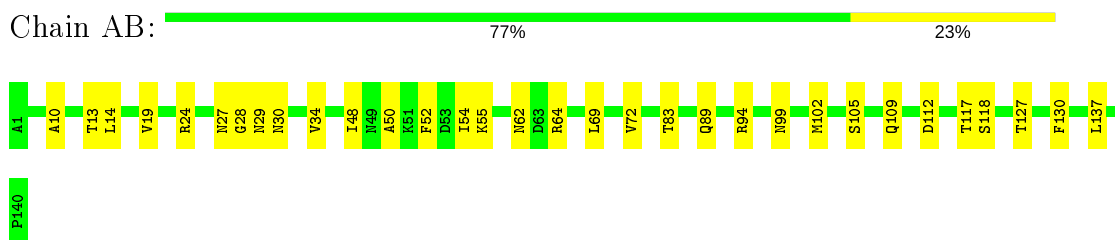
3 Residue-property plots [i](#)

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.

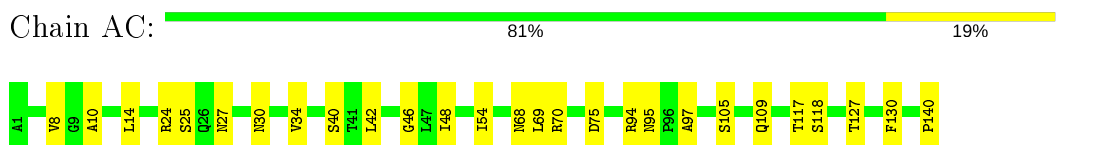
- Molecule 1: coat protein



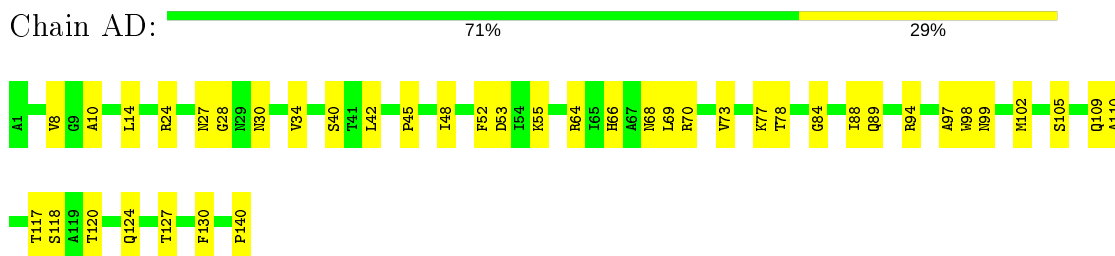
- Molecule 1: coat protein



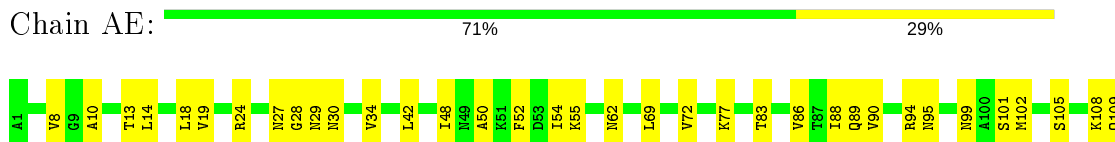
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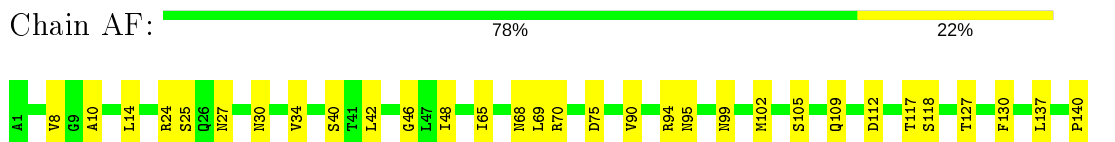
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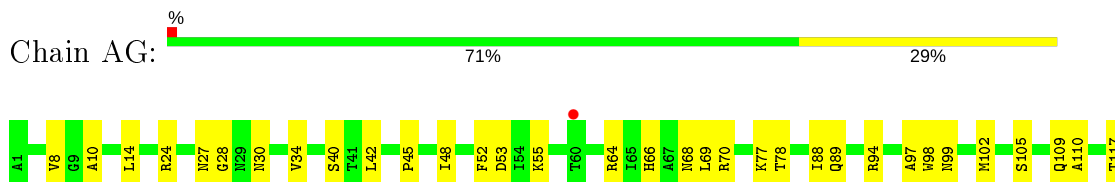
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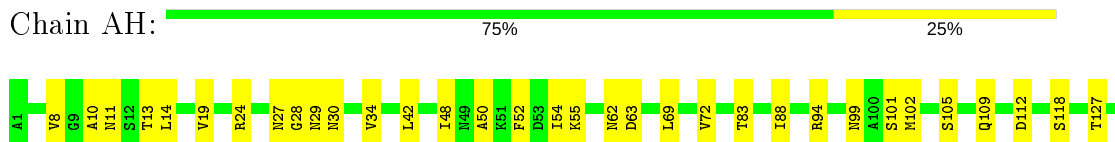
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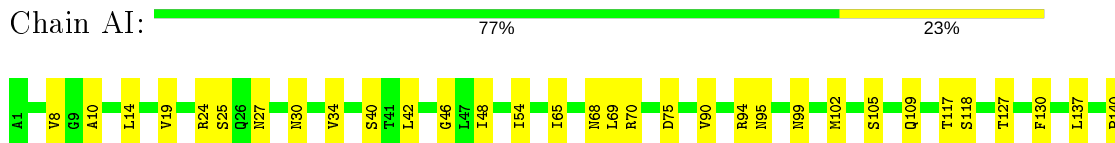
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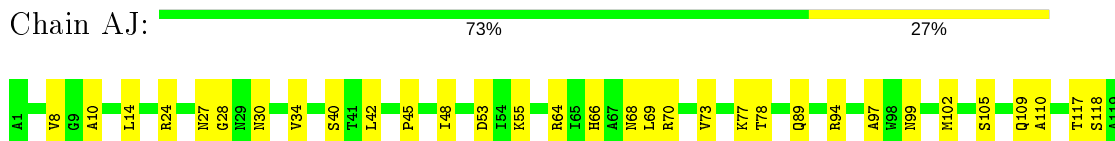
- Molecule 1: coat protein



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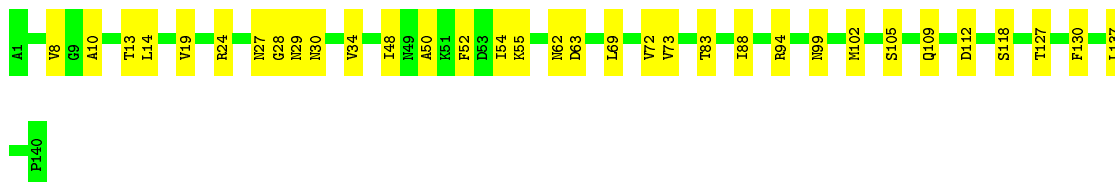
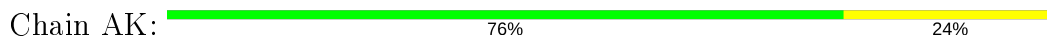


- Molecule 1: coat protein

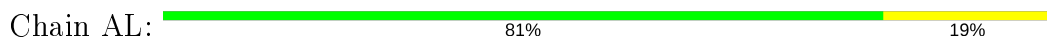




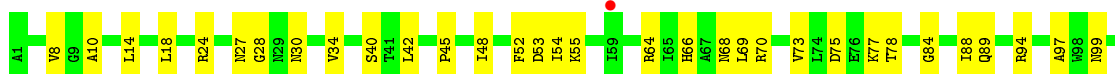
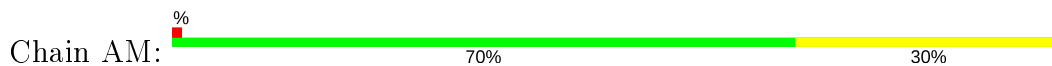
- Molecule 1: coat protein



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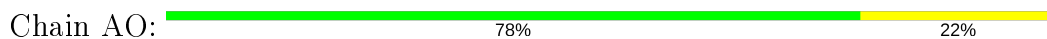
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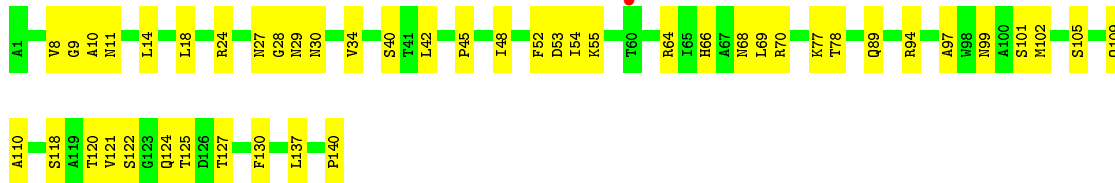
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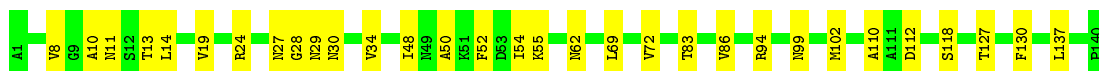
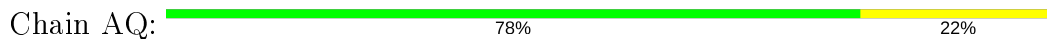
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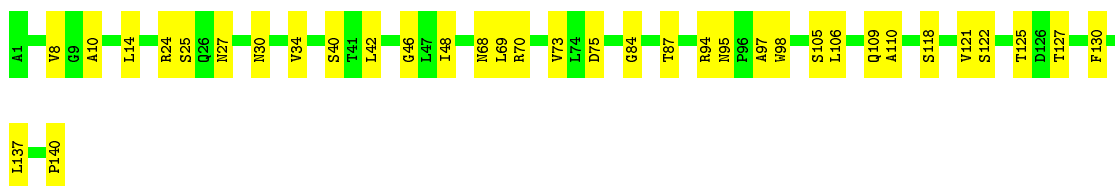
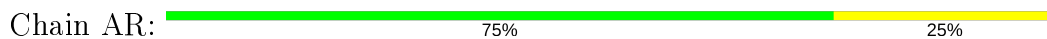
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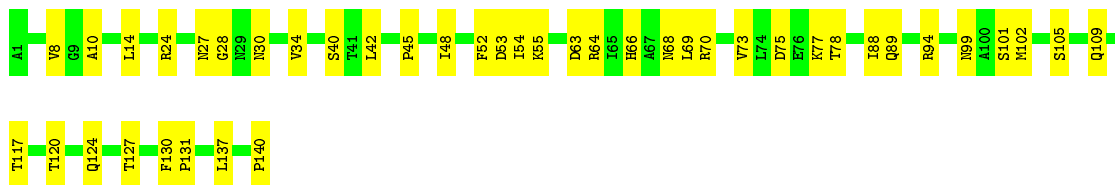
- Molecule 1: coat protein



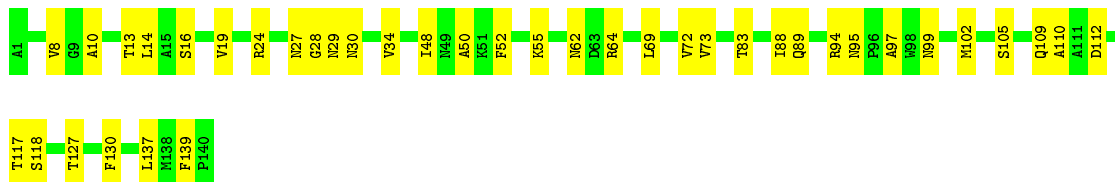
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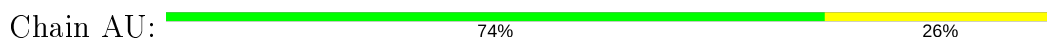
- Molecule 1: coat protein

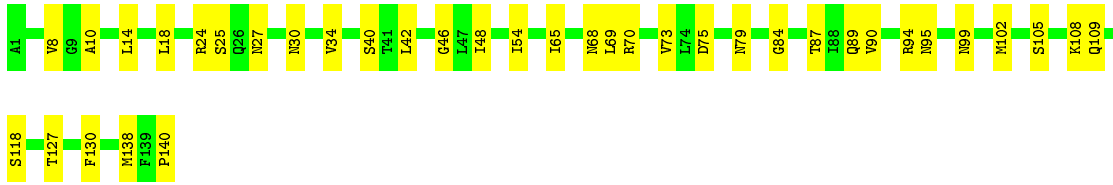


- Molecule 1: coat protein

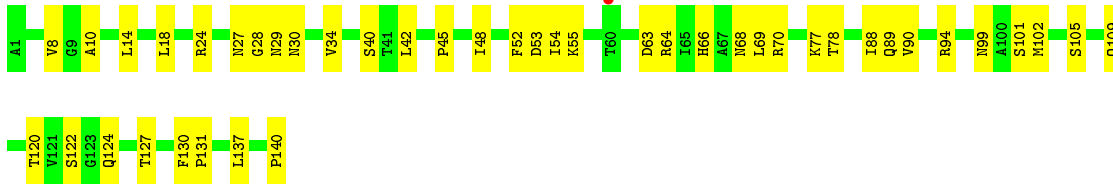


- Molecule 1: coat protein

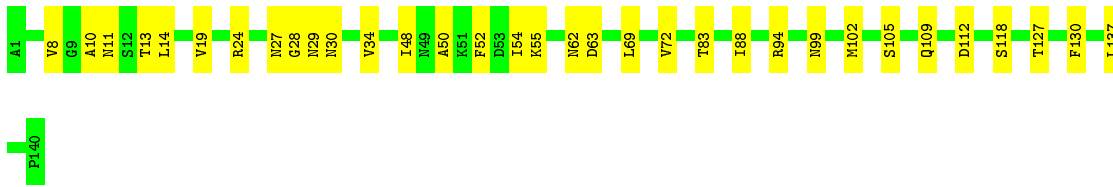
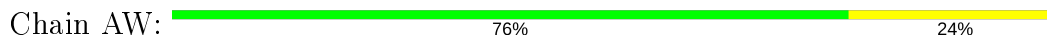




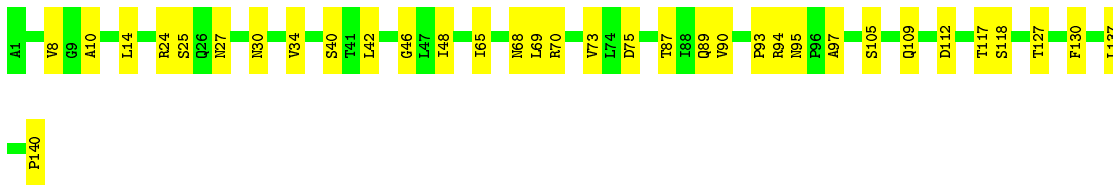
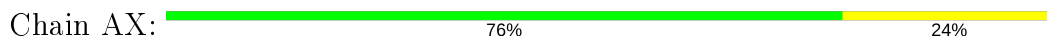
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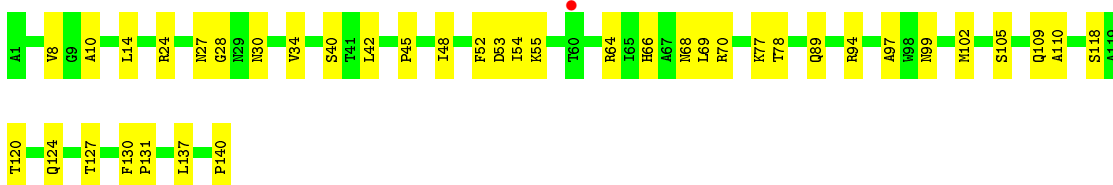
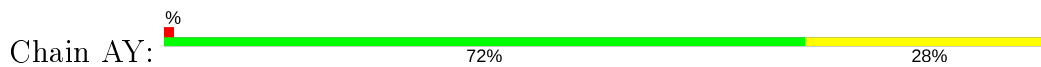
- Molecule 1: coat protein



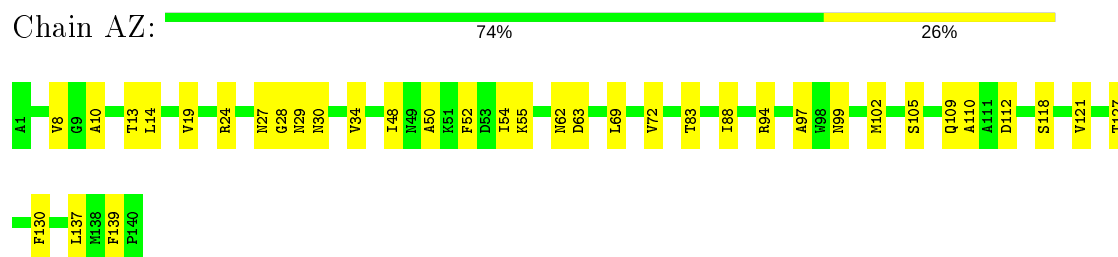
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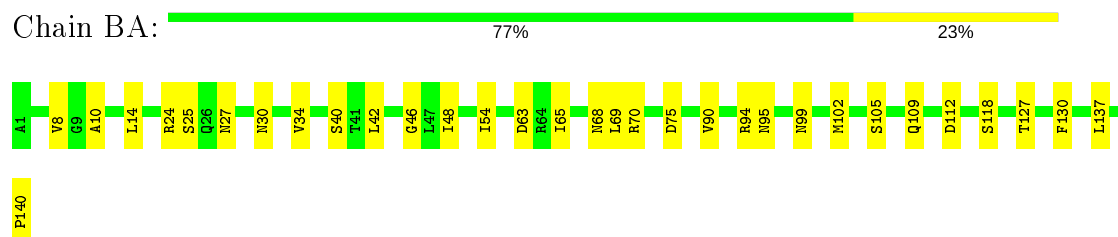
- Molecule 1: coat protein



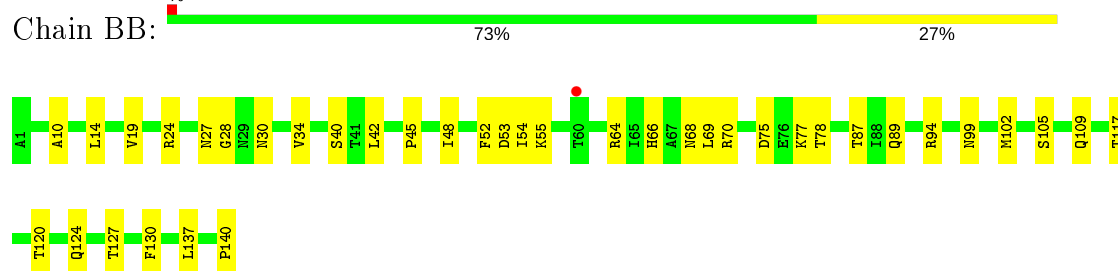
- Molecule 1: coat protein



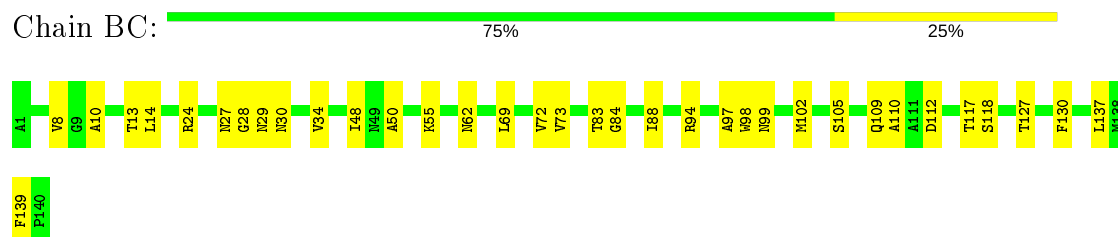
- Molecule 1: coat protein



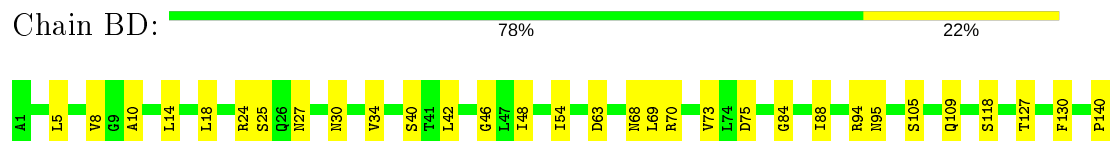
- Molecule 1: coat protein



- Molecule 1: coat protein

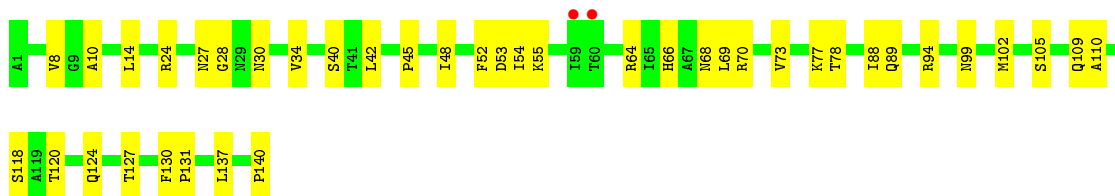


- Molecule 1: coat protein

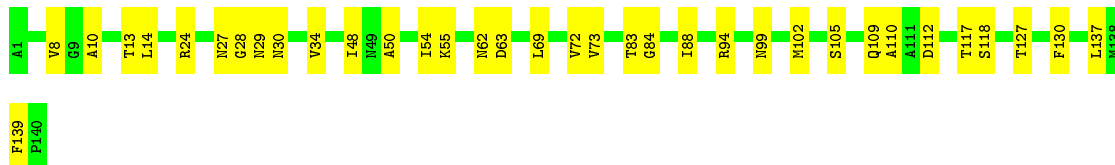
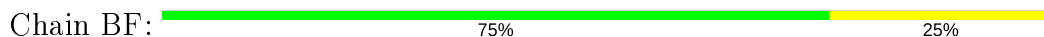


- Molecule 1: coat protein

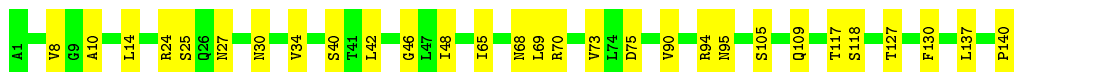
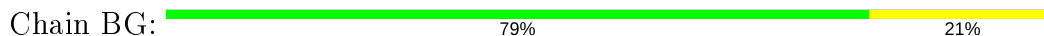




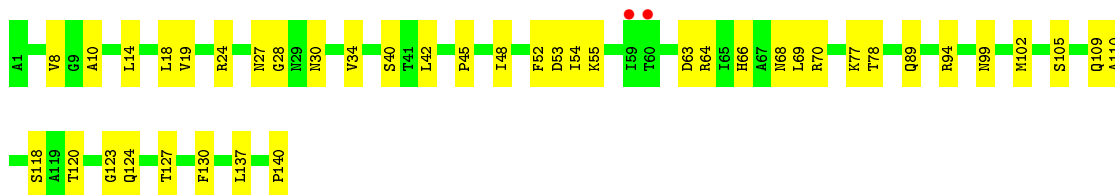
• Molecule 1: coat protein



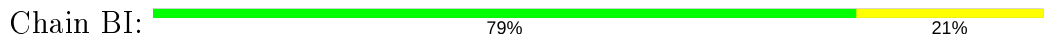
• Molecule 1: coat protein



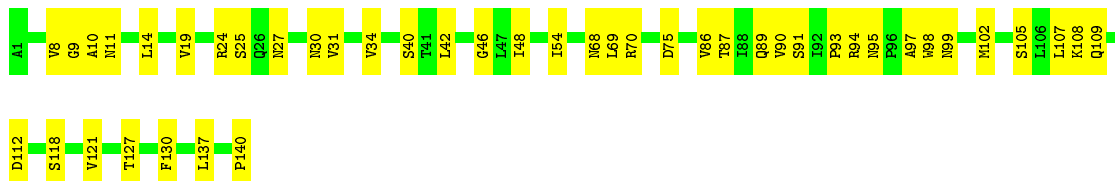
• Molecule 1: coat protein



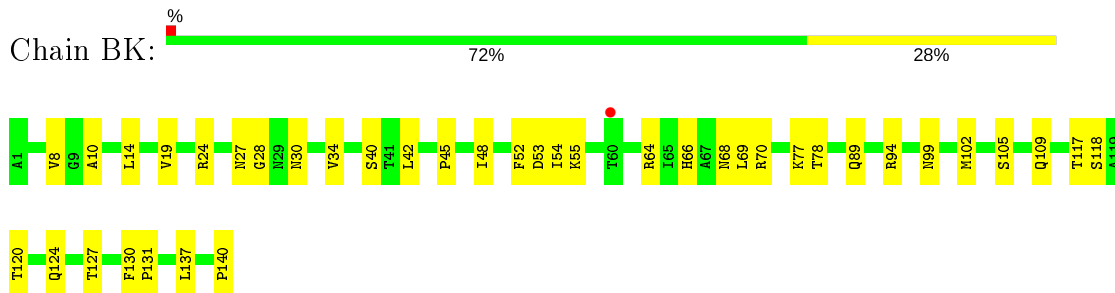
• Molecule 1: coat protein



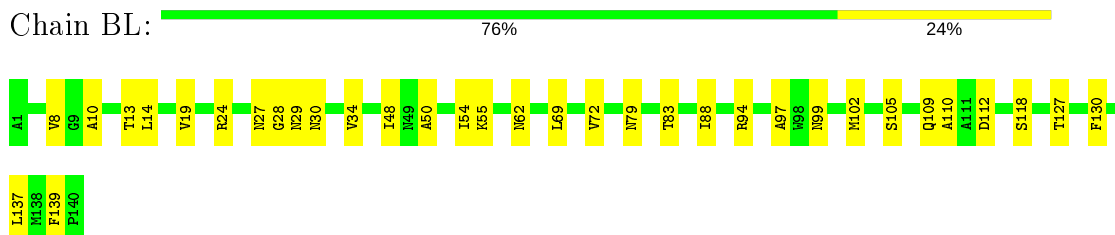
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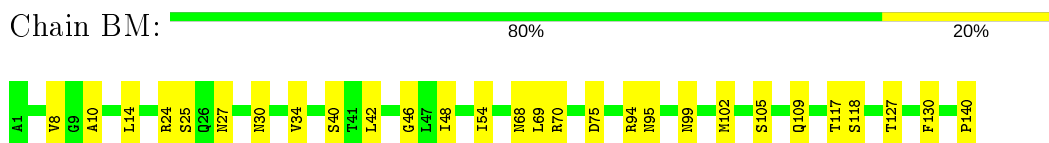
- Molecule 1: coat protein



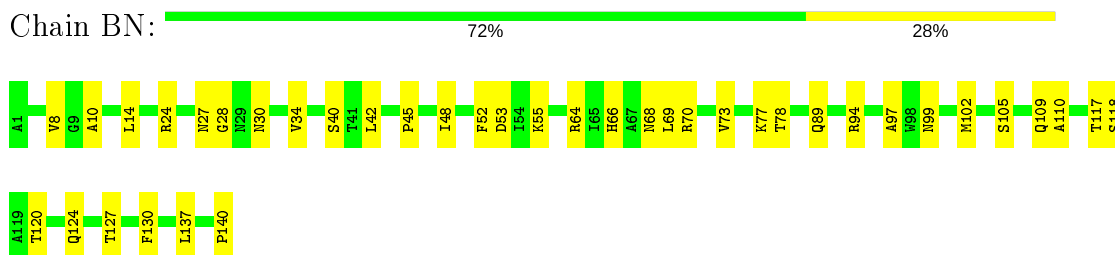
- Molecule 1: coat protein



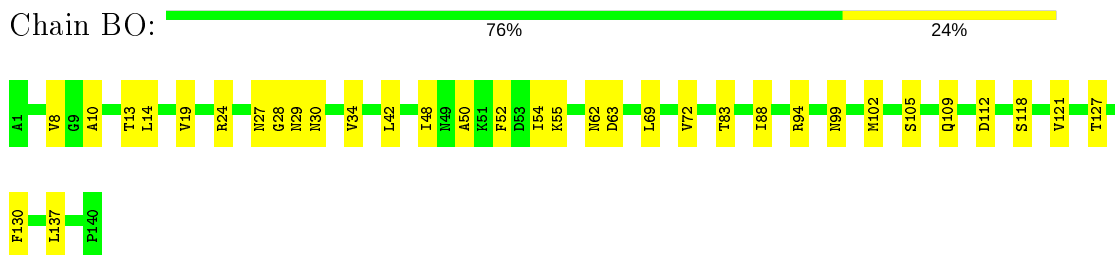
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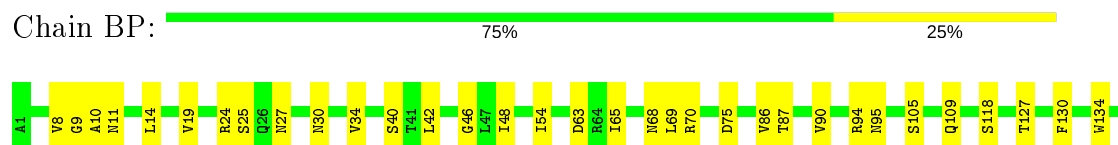
- Molecule 1: coat protein



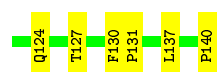
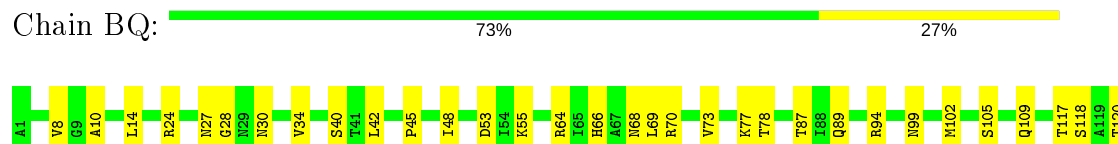
- Molecule 1: coat protein



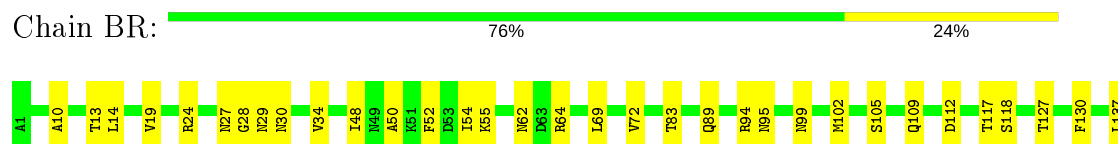
- Molecule 1: coat protein



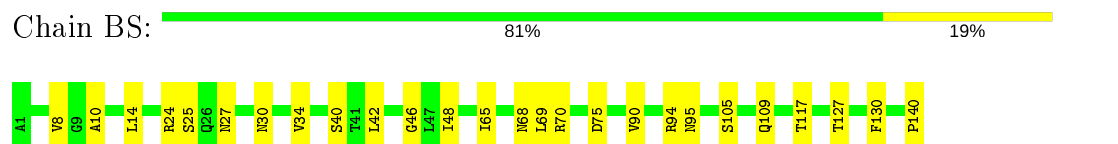
- Molecule 1: coat protein



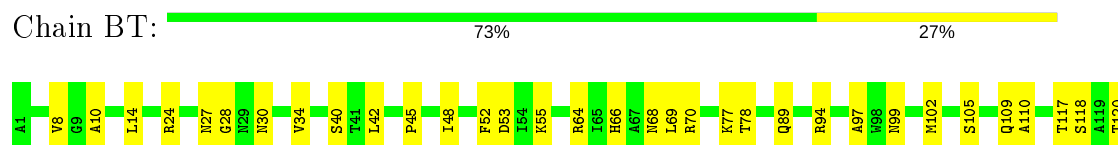
- Molecule 1: coat protein



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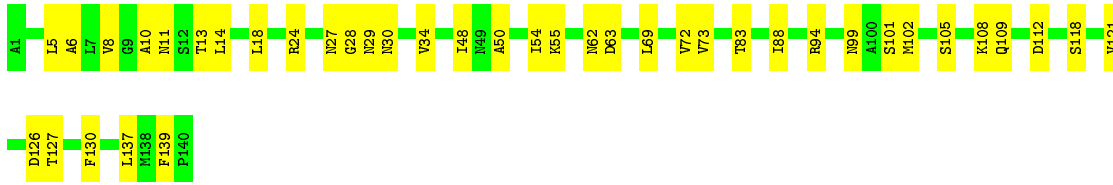


- Molecule 1: coat protein

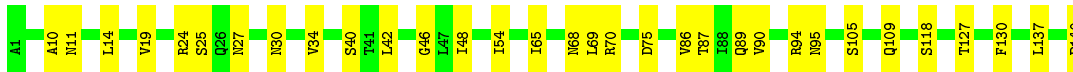
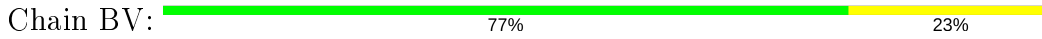


- Molecule 1: coat protein

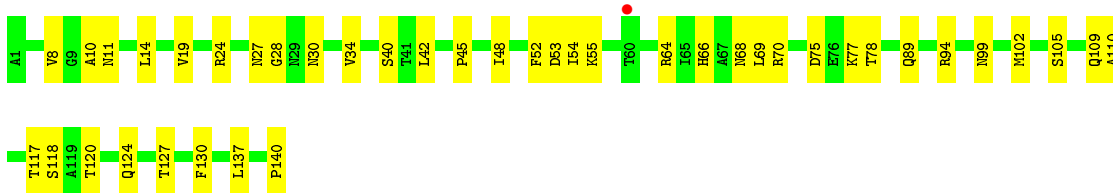
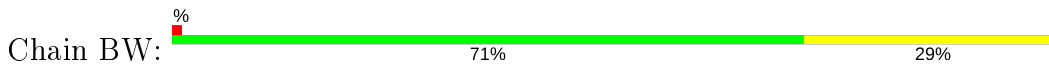




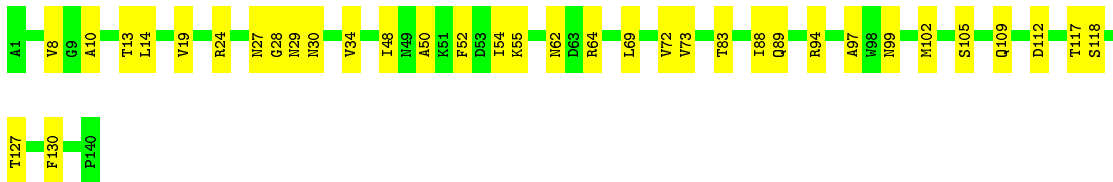
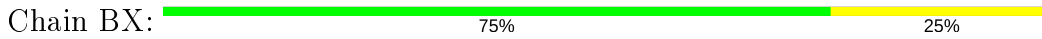
• Molecule 1: coat protein



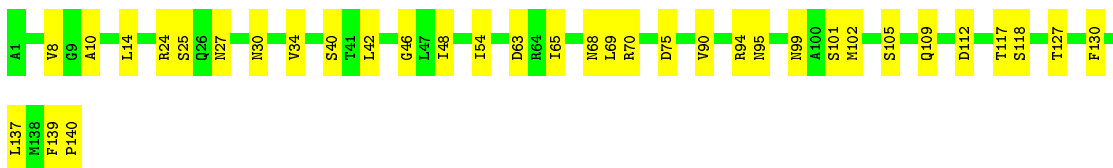
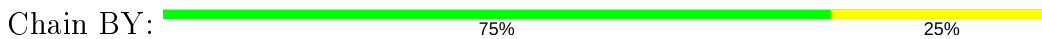
• Molecule 1: coat protein



• Molecule 1: coat protein



• Molecule 1: coat protein



• Molecule 1: coat protein

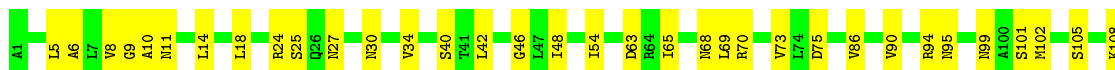




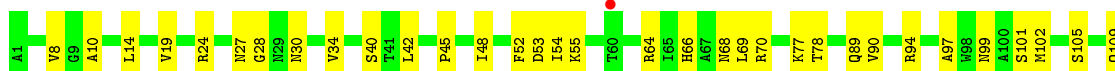
- Molecule 1: coat protein



- Molecule 1: coat protein



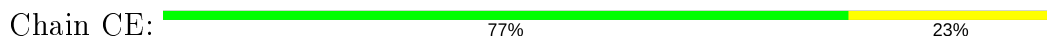
- Molecule 1: coat protein

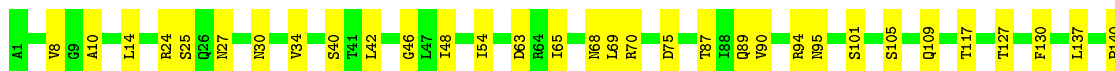


- Molecule 1: coat protein

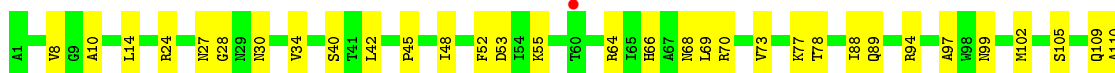
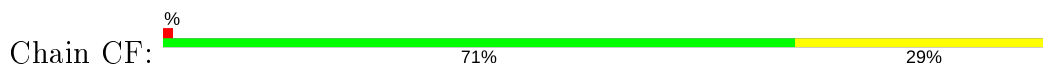


- Molecule 1: coat protein





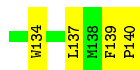
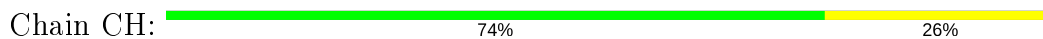
- Molecule 1: coat protein



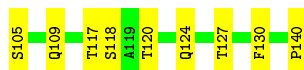
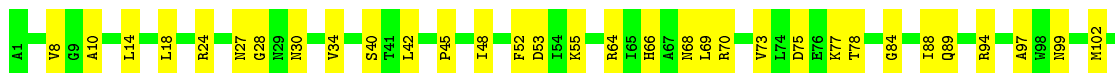
- Molecule 1: coat protein



- Molecule 1: coat protein

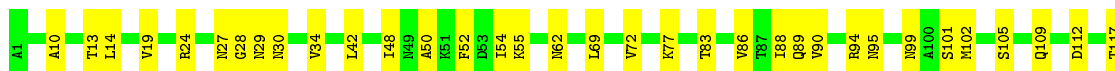


- Molecule 1: coat protein

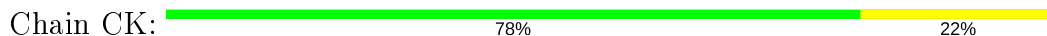


- Molecule 1: coat protein

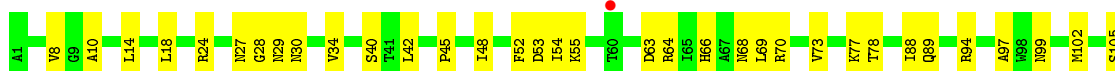




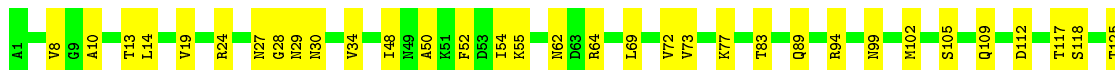
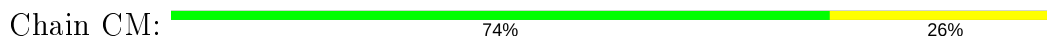
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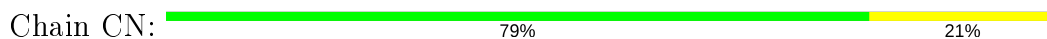
- Molecule 1: coat protein



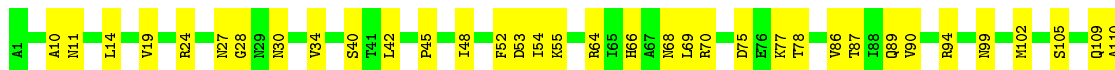
- Molecule 1: coat protein



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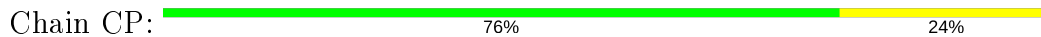


- Molecule 1: coat protein

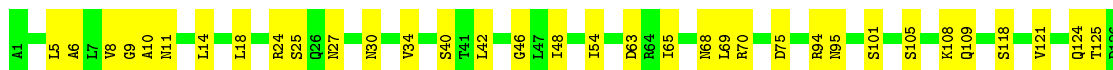




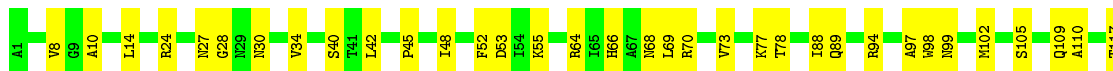
- Molecule 1: coat protein



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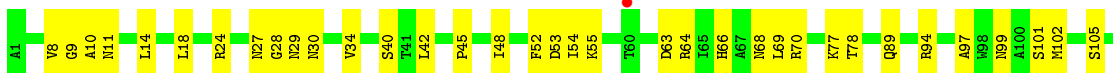


- Molecule 1: coat protein

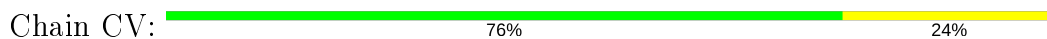




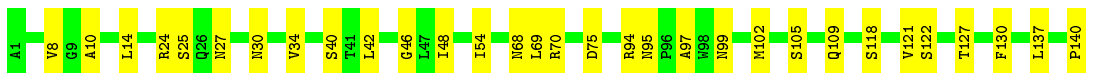
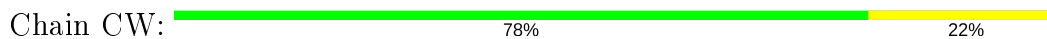
- Molecule 1: coat protein



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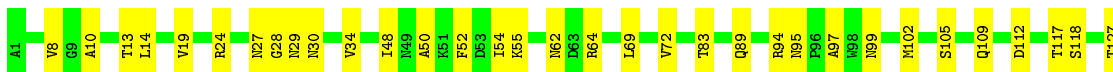
- Molecule 1: coat protein



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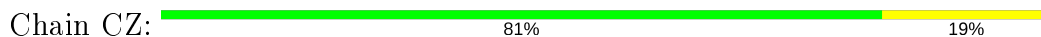


- Molecule 1: coat protein

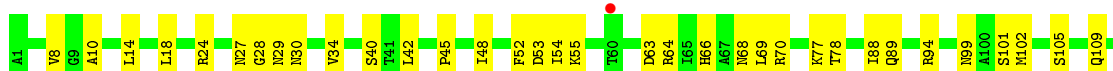
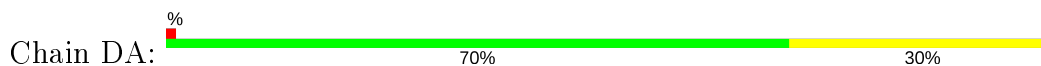




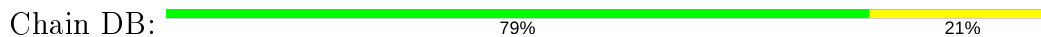
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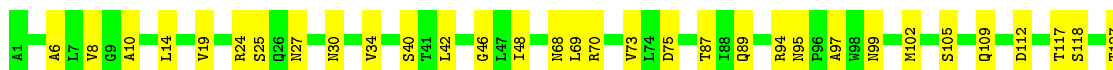
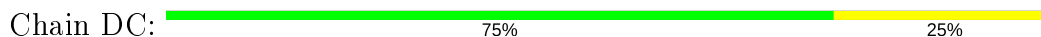
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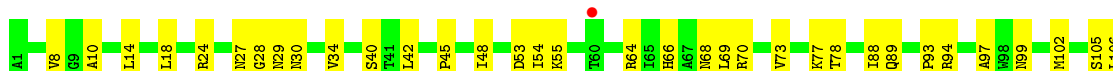
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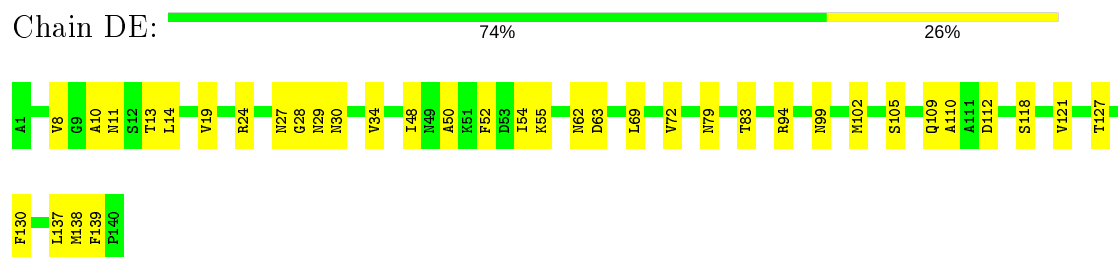
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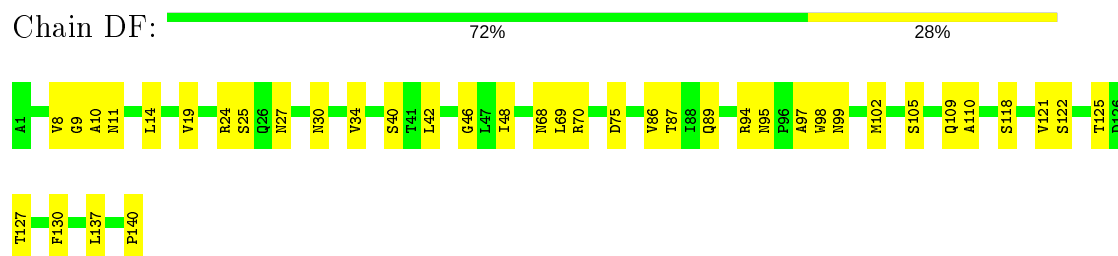
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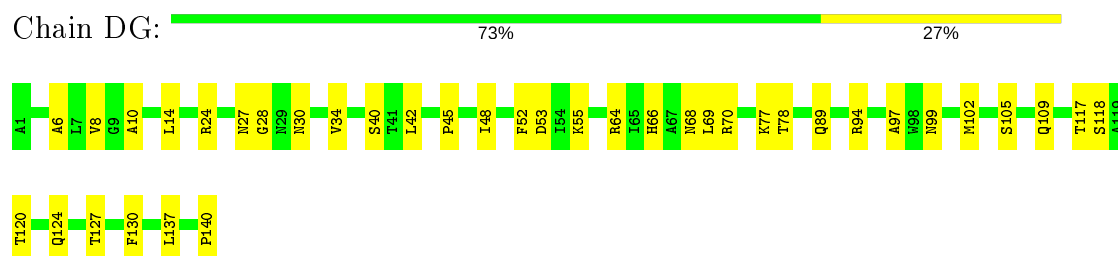
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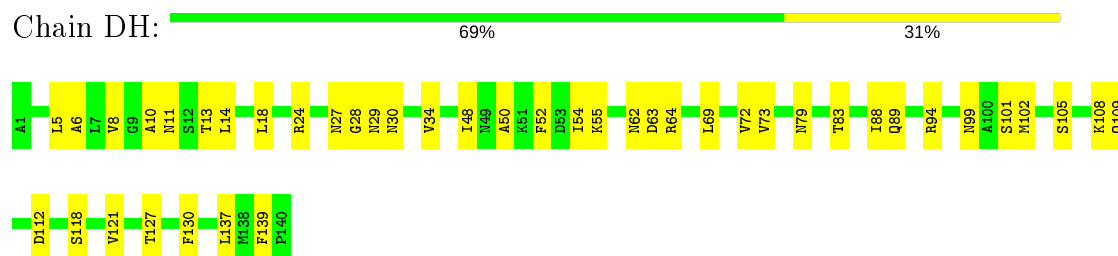
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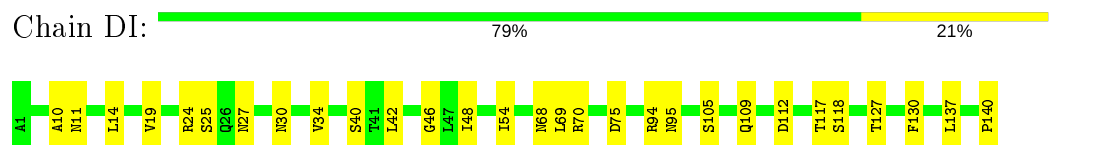
- Molecule 1: coat protein



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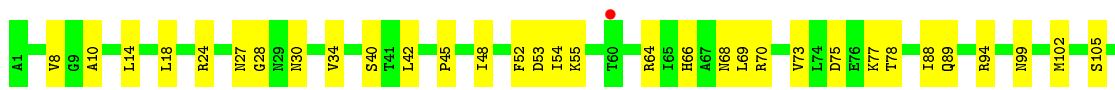


- Molecule 1: coat protein

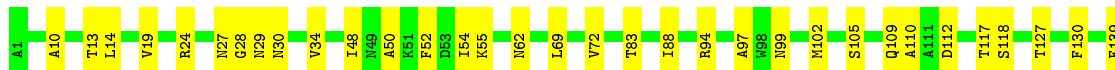
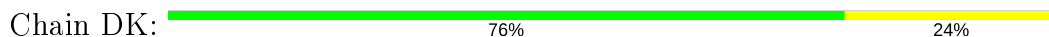


- Molecule 1: coat protein





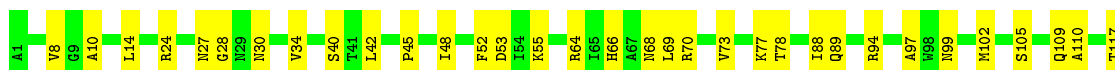
● Molecule 1: coat protein



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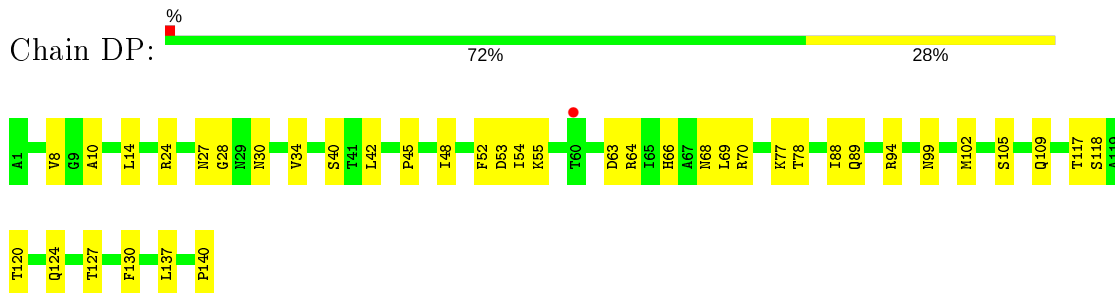
● Molecule 1: coat protein



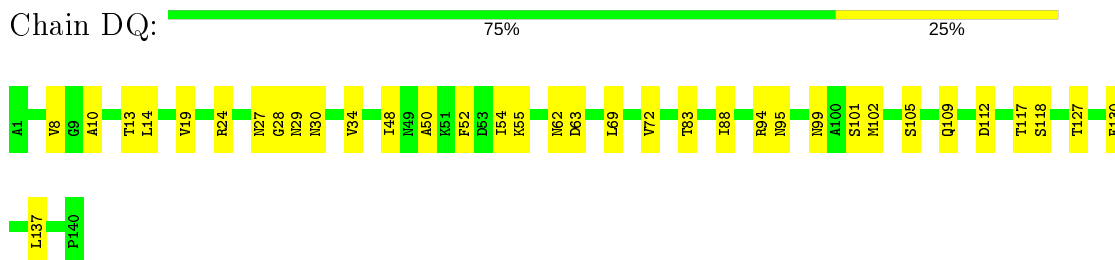
● Molecule 1: coat protein



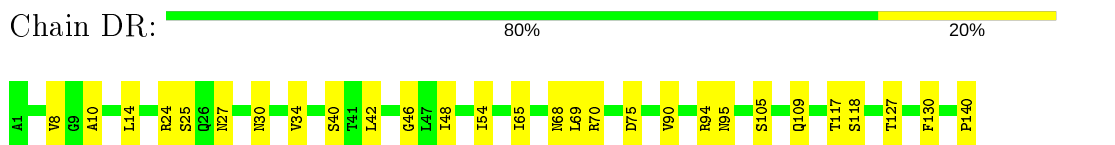
- Molecule 1: coat protein



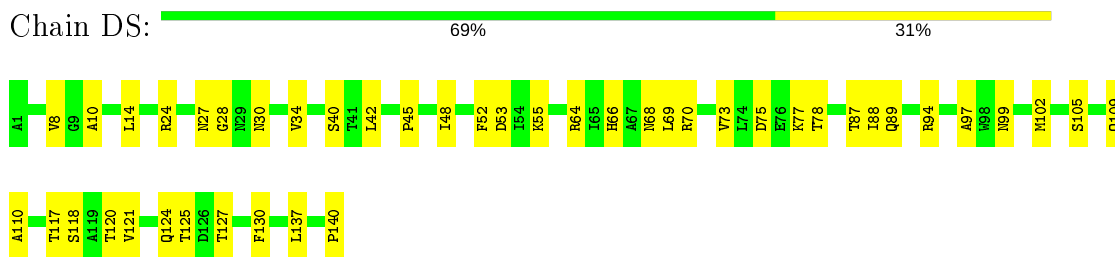
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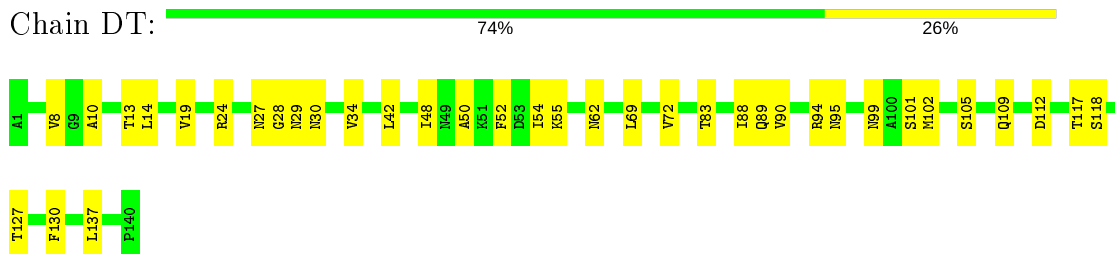
- Molecule 1: coat protein




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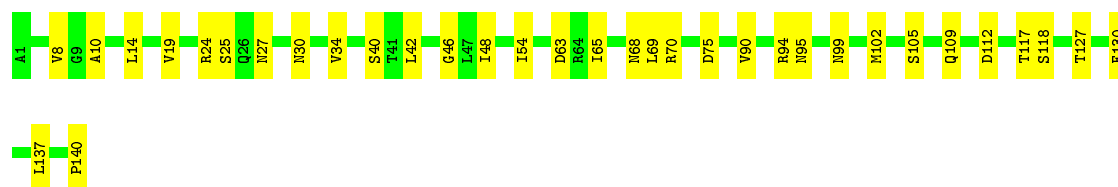


- Molecule 1: coat protein



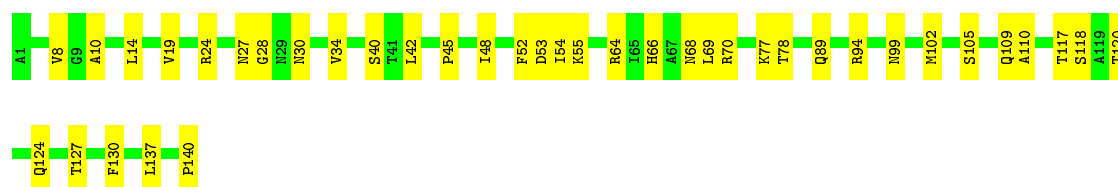
- Molecule 1: coat protein

Chain DU:  76% 24%




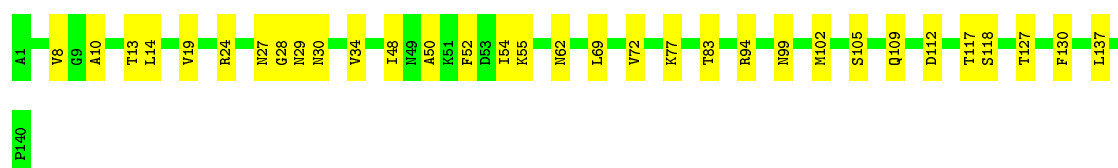
- Molecule 1: coat protein

Chain DV:  72% 28%




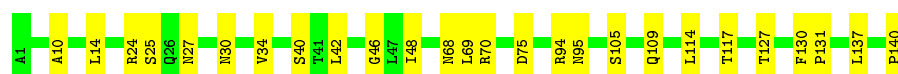
- Molecule 1: coat protein

Chain DW:  77% 23%




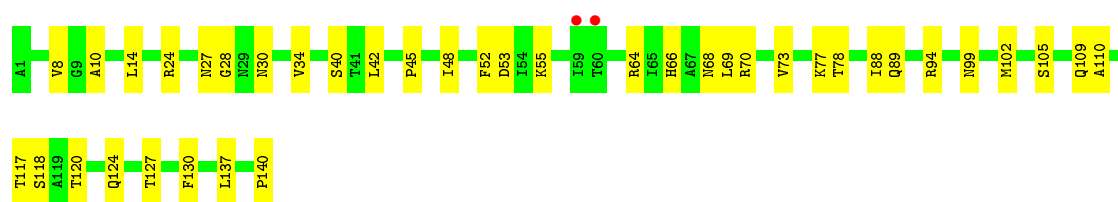
- Molecule 1: coat protein

Chain DX:  81% 19%




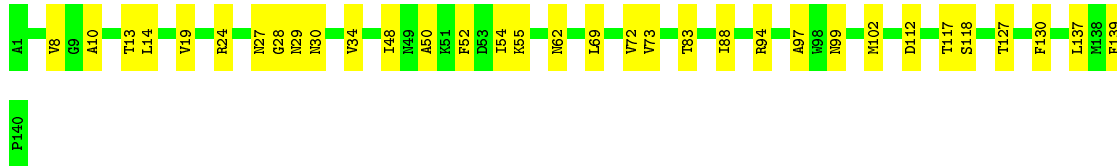
- Molecule 1: coat protein

Chain DY:  72% 28%

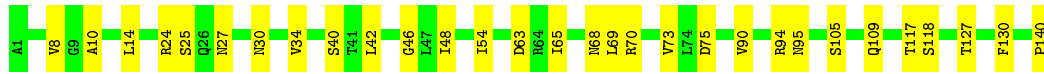
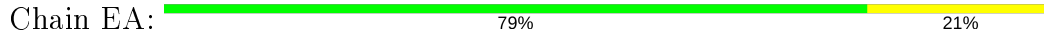


- Molecule 1: coat protein

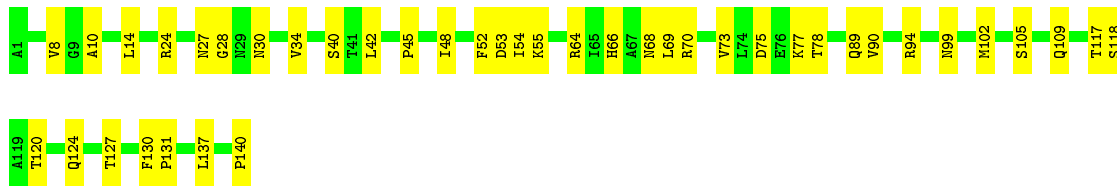
Chain DZ:  76% 24%



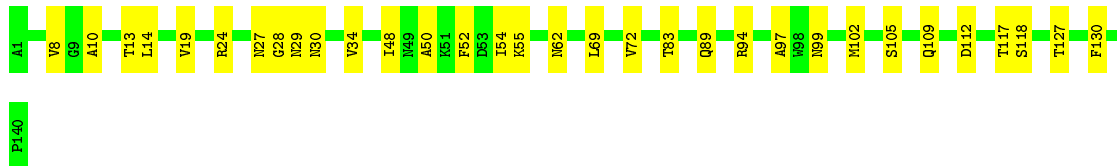
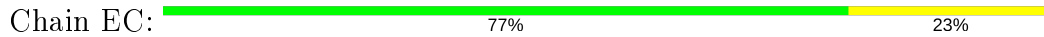
• Molecule 1: coat protein



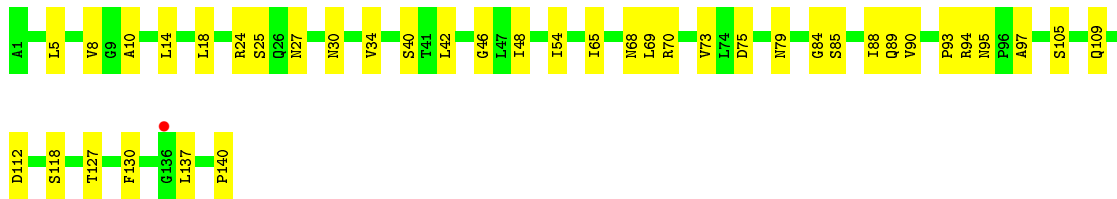
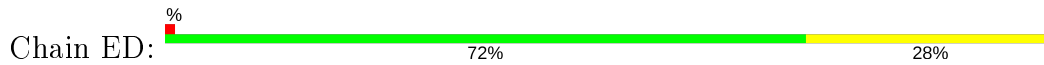
• Molecule 1: coat protein



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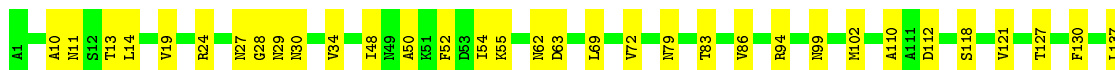


• Molecule 1: coat protein

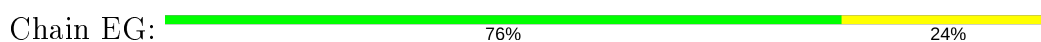




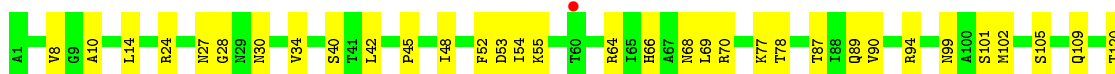
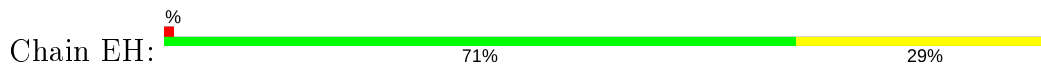
- Molecule 1: coat protein



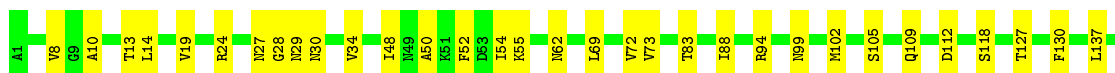
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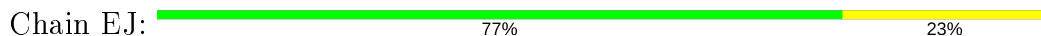
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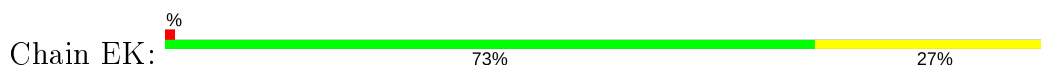
- Molecule 1: coat protein

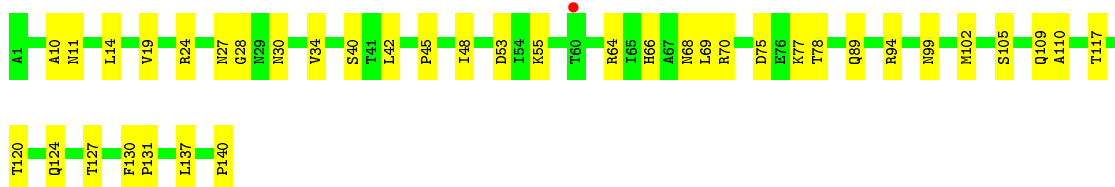


- Molecule 1: coat protein

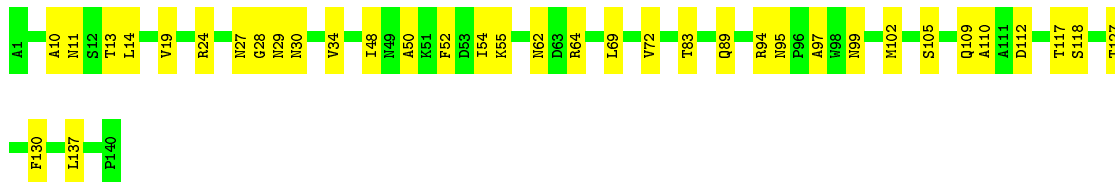
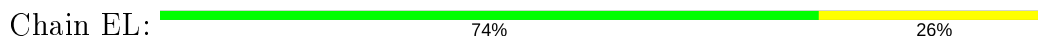


- Molecule 1: coat protein

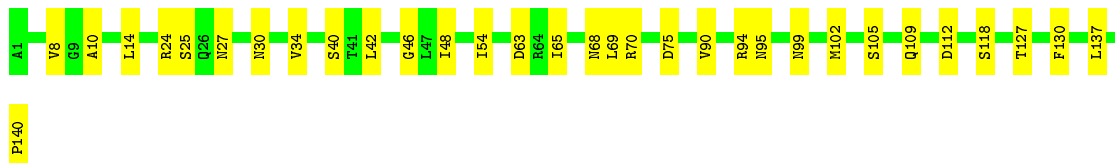
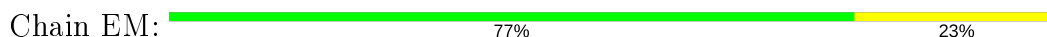




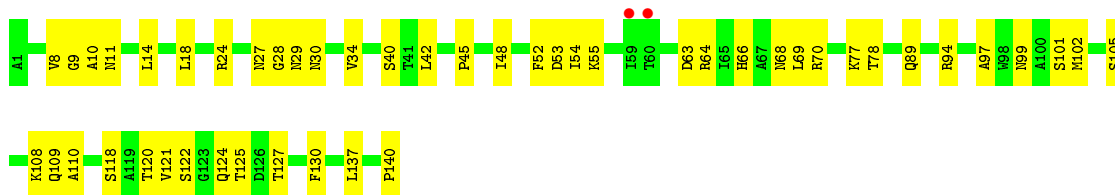
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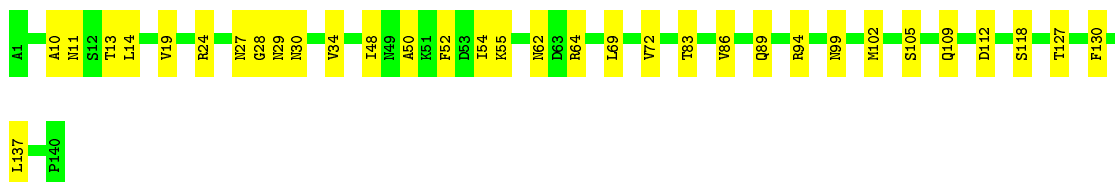
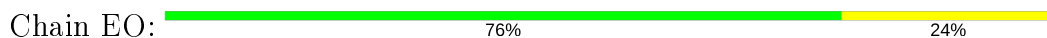
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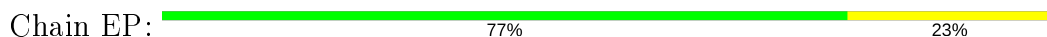
• Molecule 1: coat protein



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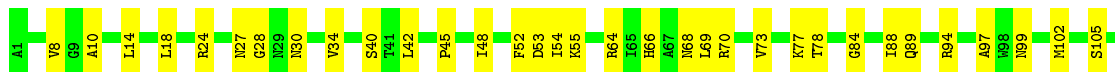


• Molecule 1: coat protein

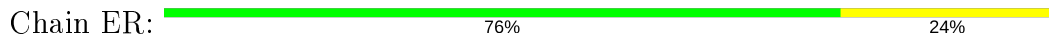




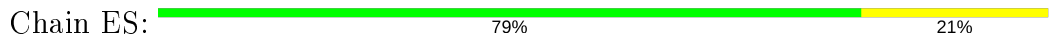
• Molecule 1: coat protein



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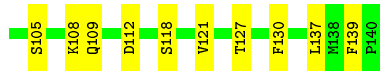
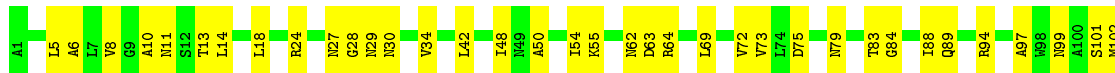
• Molecule 1: coat protein



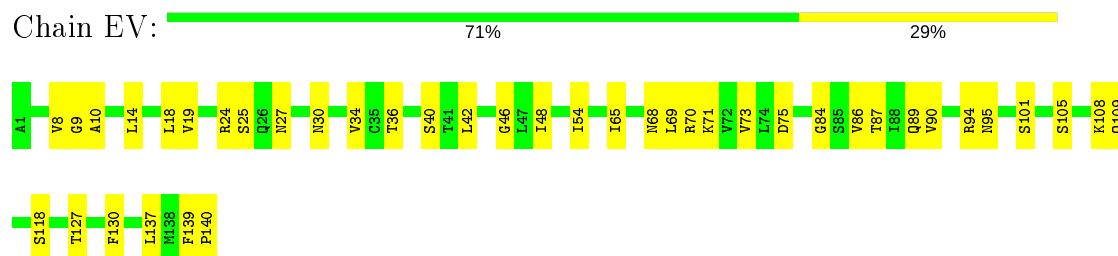
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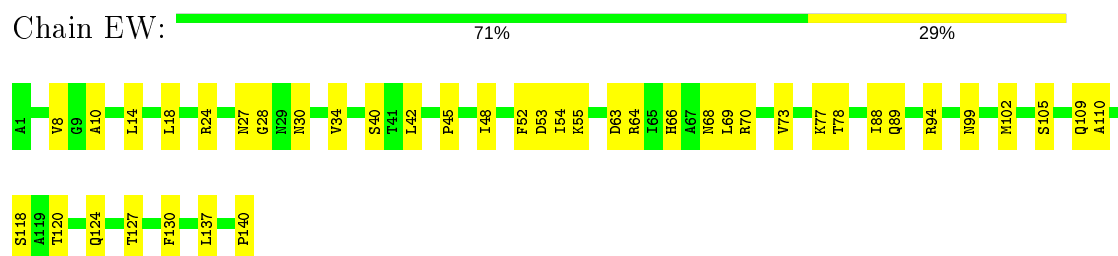
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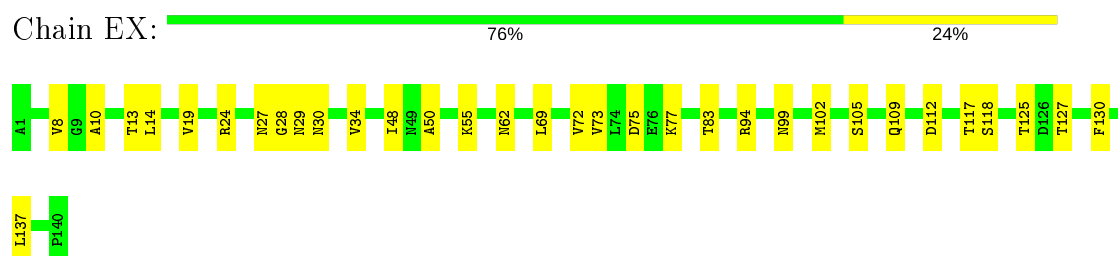
- Molecule 1: coat protein



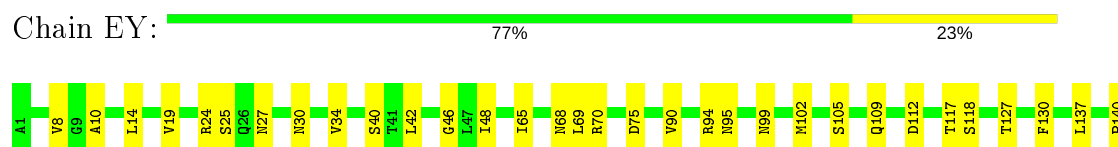
- Molecule 1: coat protein



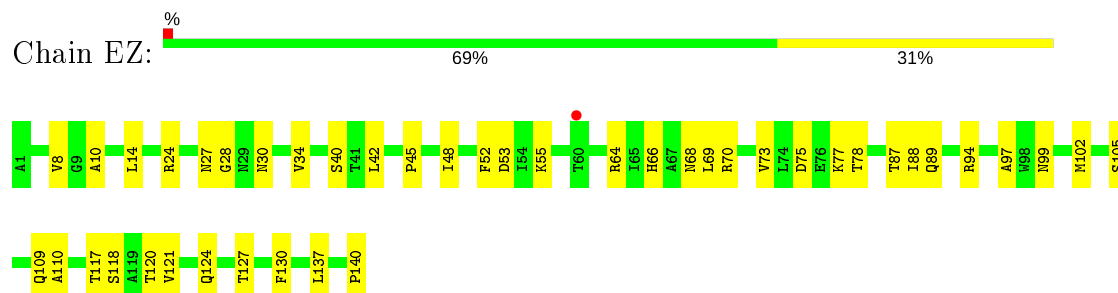
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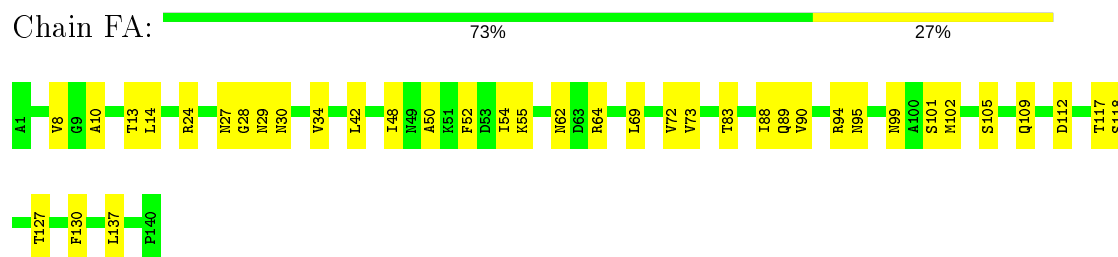
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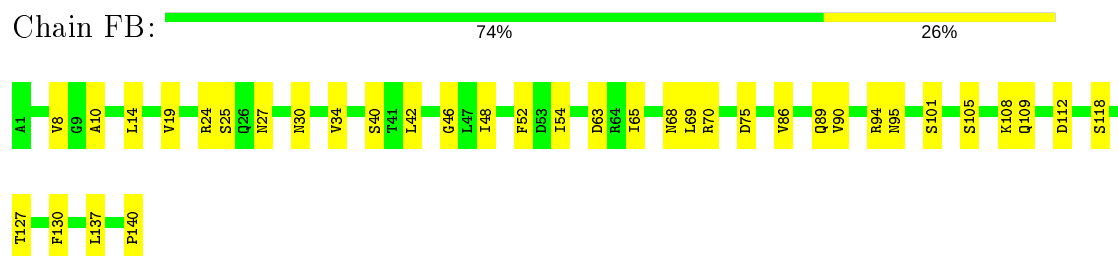
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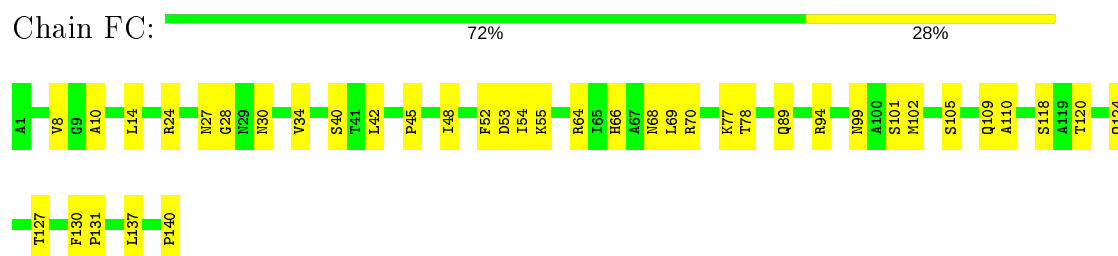
- Molecule 1: coat protein



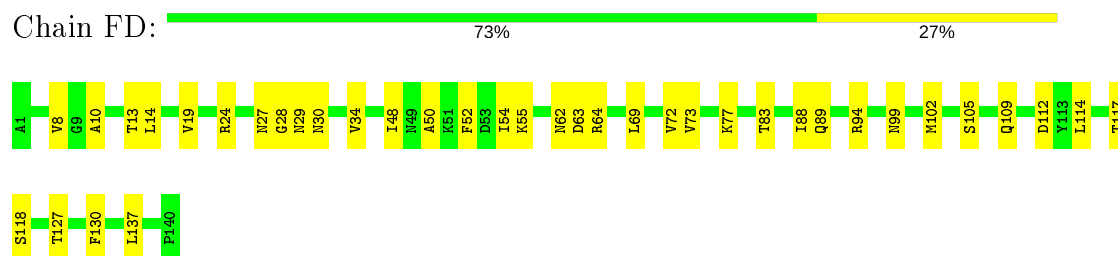
- Molecule 1: coat protein



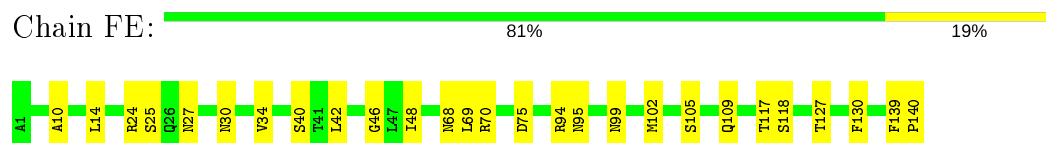
- Molecule 1: coat protein



- Molecule 1: coat protein

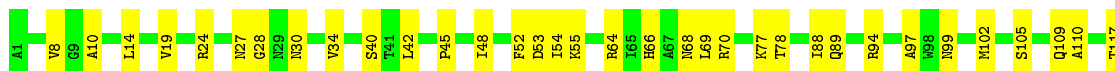


- Molecule 1: coat protein

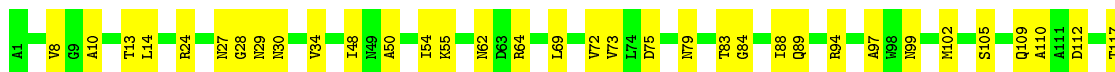


- Molecule 1: coat protein

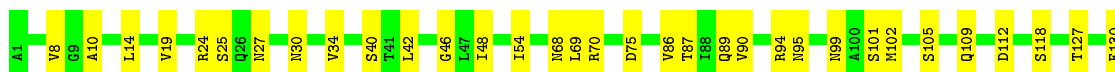




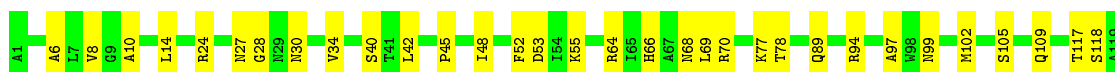
• Molecule 1: coat protein



• Molecule 1: coat protein



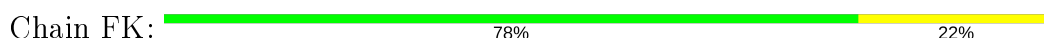
• Molecule 1: coat protein



• Molecule 1: coat protein

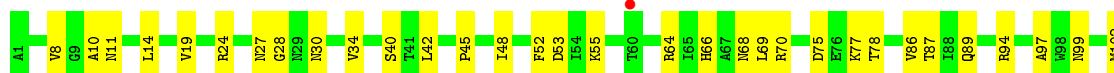


• Molecule 1: coat protein

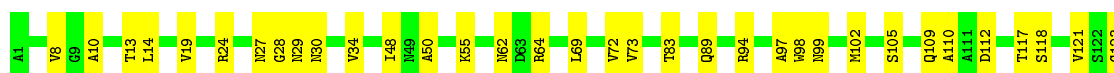
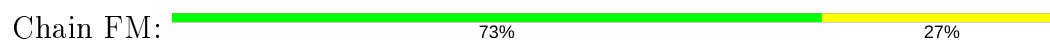




- Molecule 1: coat protein



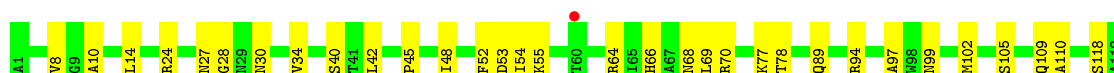
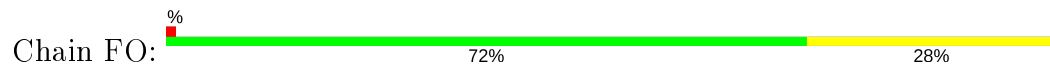
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

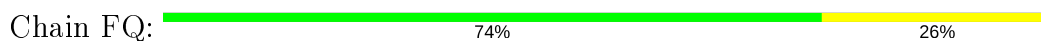


- Molecule 1: coat protein

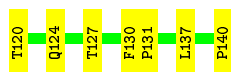
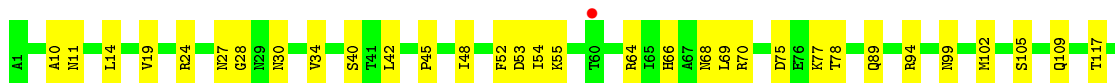
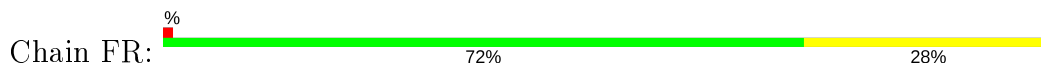




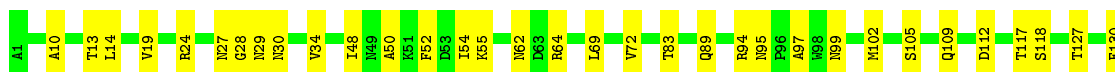
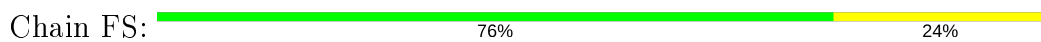
- Molecule 1: coat protein



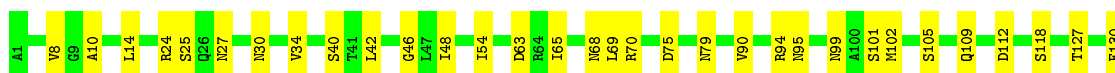
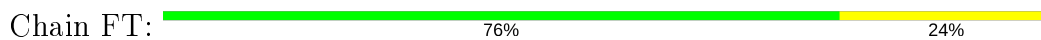
- Molecule 1: coat protein



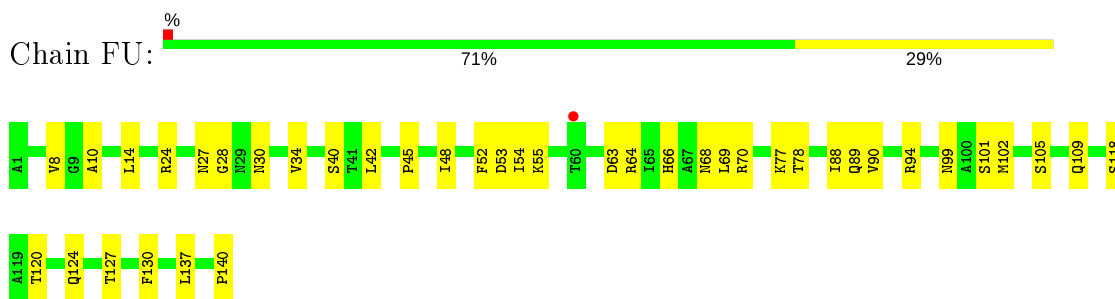
- Molecule 1: coat protein



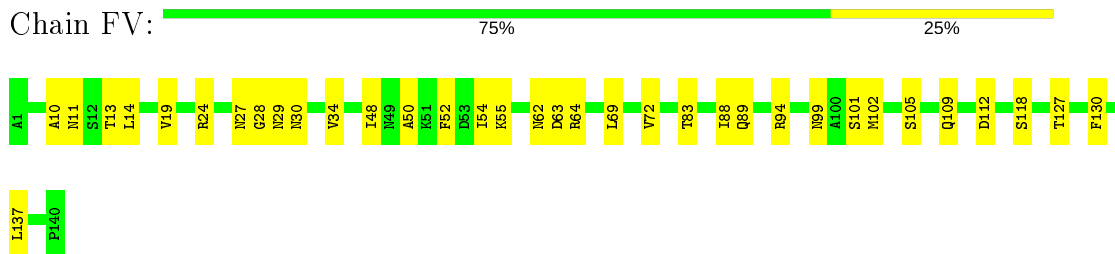
- Molecule 1: coat protein



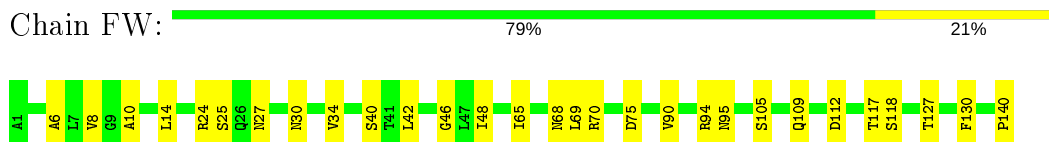
- Molecule 1: coat protein



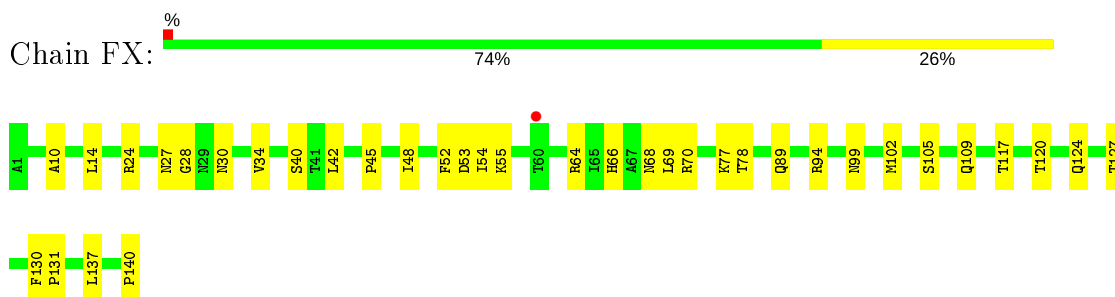
- Molecule 1: coat protein



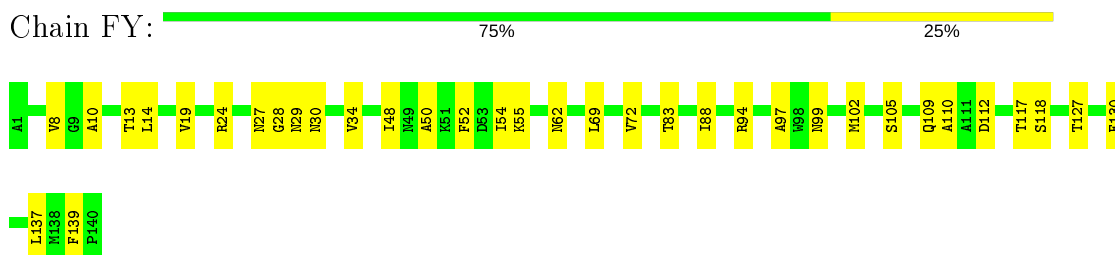
- Molecule 1: coat protein



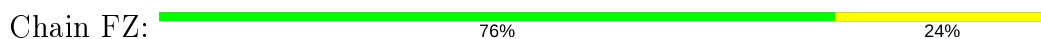
- Molecule 1: coat protein

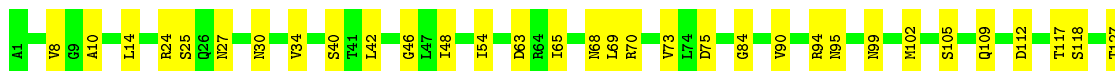


- Molecule 1: coat protein

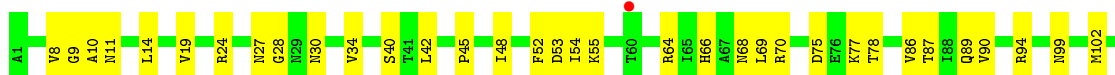


- Molecule 1: coat protein

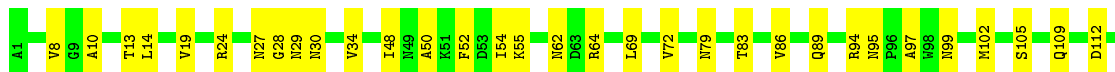
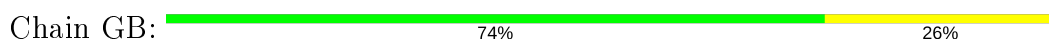




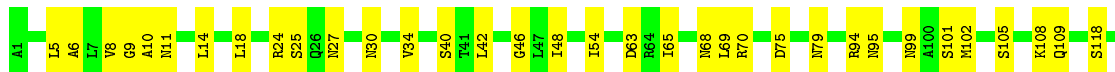
• Molecule 1: coat protein



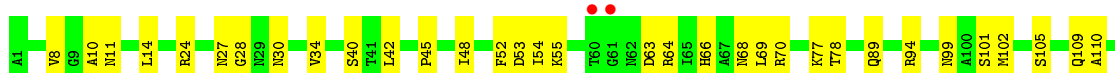
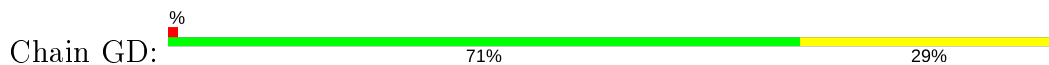
• Molecule 1: coat protein



• Molecule 1: coat protein

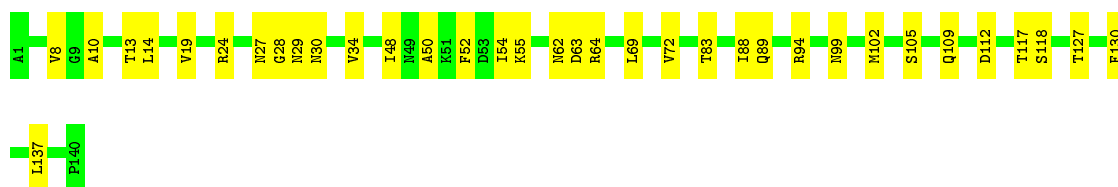


• Molecule 1: coat protein




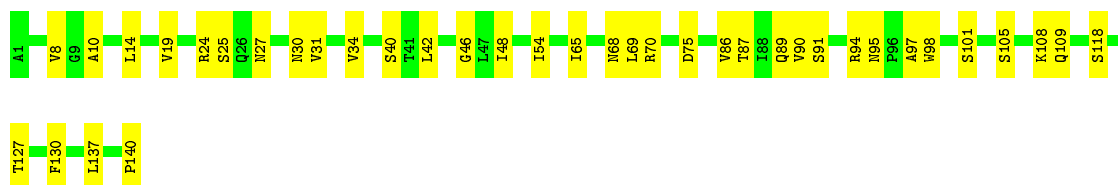
• Molecule 1: coat protein

Chain GE:  75% 25%



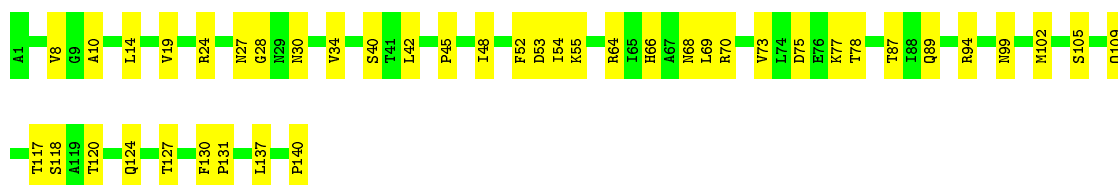
- Molecule 1: coat protein

Chain GF:  73% 27%



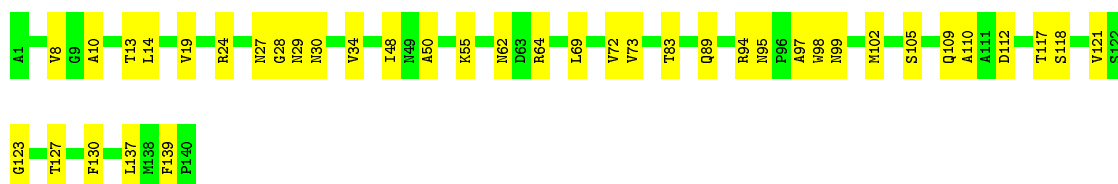
- Molecule 1: coat protein

Chain GG:  70% 30%




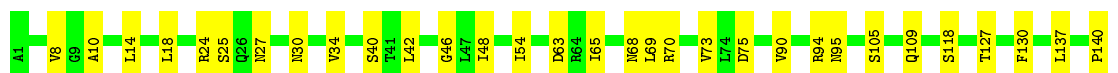
- Molecule 1: coat protein

Chain GH:  72% 28%




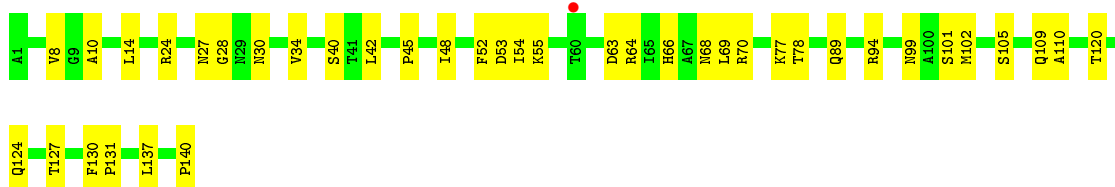
- Molecule 1: coat protein

Chain GI:  78% 22%

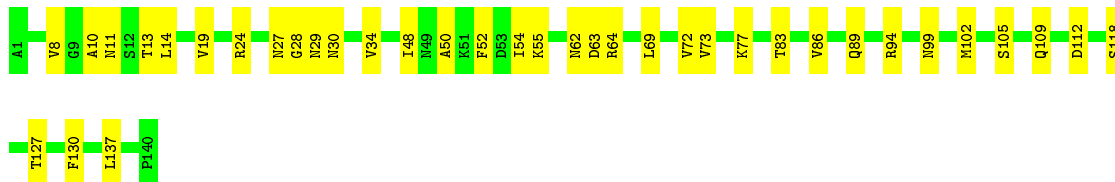
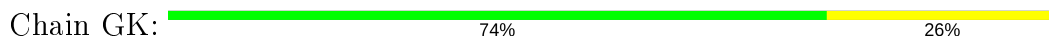


- Molecule 1: coat protein

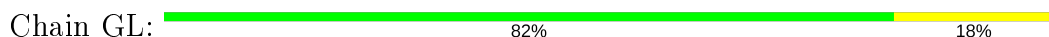
Chain GJ:  72% 28%



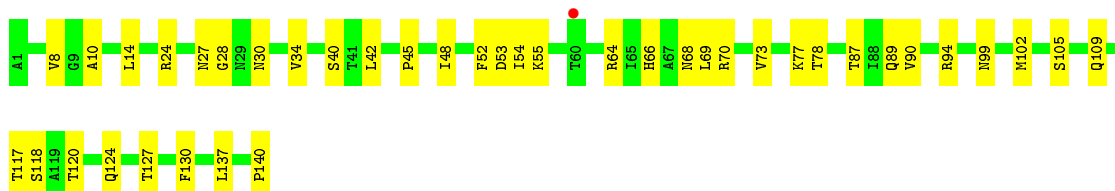
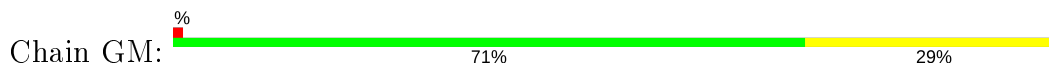
• Molecule 1: coat protein



• Molecule 1: coat protein



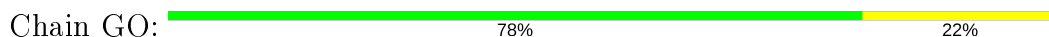
• Molecule 1: coat protein

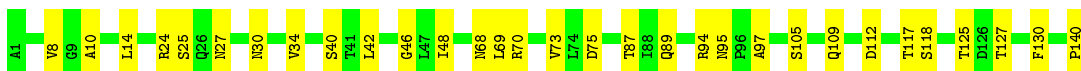


• Molecule 1: coat protein

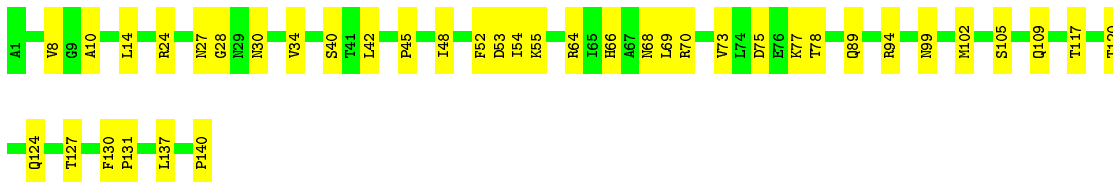


• Molecule 1: coat protein

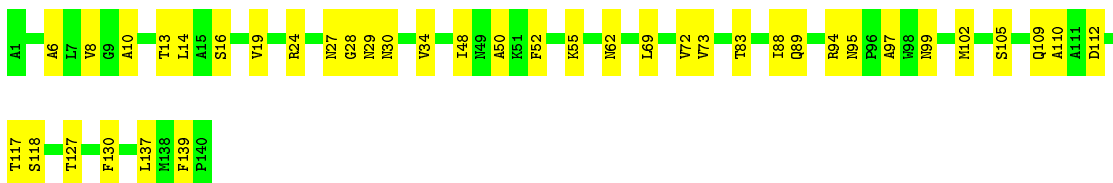




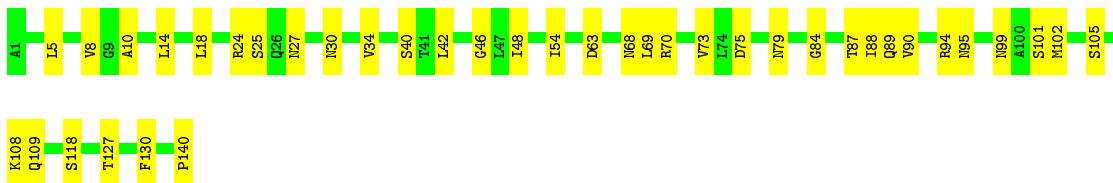
- Molecule 1: coat protein



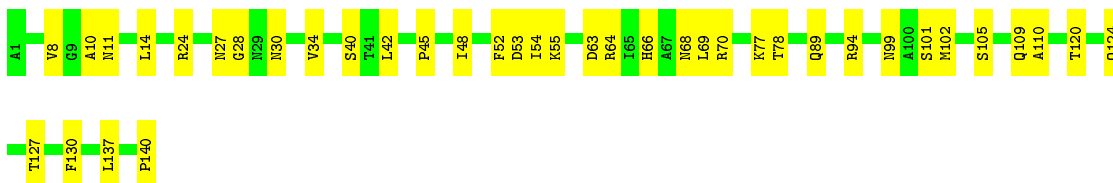
- Molecule 1: coat protein



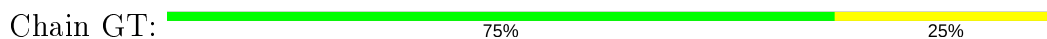
- Molecule 1: coat protein



- Molecule 1: coat protein

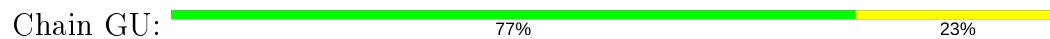


- Molecule 1: coat protein

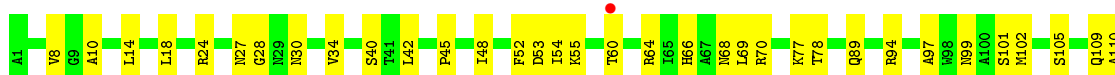
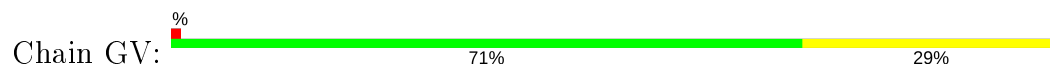




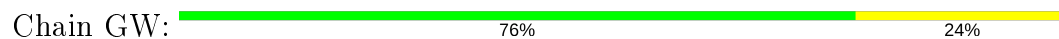
- Molecule 1: coat protein



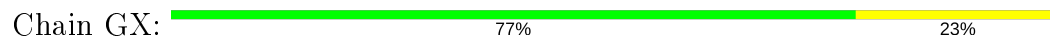
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	278.09Å 390.21Å 554.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.20 – 3.20 62.20 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (62.20-3.20) 98.7 (62.20-3.20)	Depositor EDS
R_{merge}	0.67	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.261 , 0.266 0.262 , 0.268	Depositor DCC
R_{free} test set	6526 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtrriage
Anisotropy	0.294	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 11.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	184320	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0/1043	0.54	0/1426
1	AB	0.31	0/1043	0.55	0/1426
1	AC	0.30	0/1043	0.54	0/1426
1	AD	0.33	0/1043	0.54	0/1426
1	AE	0.31	0/1043	0.55	0/1426
1	AF	0.31	0/1043	0.54	0/1426
1	AG	0.33	0/1043	0.54	0/1426
1	AH	0.31	0/1043	0.55	0/1426
1	AI	0.30	0/1043	0.54	0/1426
1	AJ	0.33	0/1043	0.54	0/1426
1	AK	0.31	0/1043	0.55	0/1426
1	AL	0.31	0/1043	0.54	0/1426
1	AM	0.33	0/1043	0.54	0/1426
1	AN	0.31	0/1043	0.55	0/1426
1	AO	0.31	0/1043	0.54	0/1426
1	AP	0.33	0/1043	0.54	0/1426
1	AQ	0.31	0/1043	0.55	0/1426
1	AR	0.30	0/1043	0.54	0/1426
1	AS	0.33	0/1043	0.54	0/1426
1	AT	0.31	0/1043	0.55	0/1426
1	AU	0.30	0/1043	0.54	0/1426
1	AV	0.33	0/1043	0.54	0/1426
1	AW	0.31	0/1043	0.55	0/1426
1	AX	0.31	0/1043	0.54	0/1426
1	AY	0.33	0/1043	0.54	0/1426
1	AZ	0.31	0/1043	0.55	0/1426
1	BA	0.31	0/1043	0.54	0/1426
1	BB	0.33	0/1043	0.54	0/1426
1	BC	0.31	0/1043	0.55	0/1426
1	BD	0.30	0/1043	0.54	0/1426
1	BE	0.33	0/1043	0.54	0/1426
1	BF	0.31	0/1043	0.55	0/1426
1	BG	0.31	0/1043	0.54	0/1426
1	BH	0.33	0/1043	0.54	0/1426

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BI	0.31	0/1043	0.55	0/1426
1	BJ	0.30	0/1043	0.54	0/1426
1	BK	0.33	0/1043	0.54	0/1426
1	BL	0.31	0/1043	0.55	0/1426
1	BM	0.31	0/1043	0.54	0/1426
1	BN	0.33	0/1043	0.54	0/1426
1	BO	0.31	0/1043	0.55	0/1426
1	BP	0.31	0/1043	0.54	0/1426
1	BQ	0.33	0/1043	0.54	0/1426
1	BR	0.31	0/1043	0.55	0/1426
1	BS	0.30	0/1043	0.54	0/1426
1	BT	0.33	0/1043	0.54	0/1426
1	BU	0.31	0/1043	0.55	0/1426
1	BV	0.31	0/1043	0.54	0/1426
1	BW	0.33	0/1043	0.54	0/1426
1	BX	0.31	0/1043	0.55	0/1426
1	BY	0.31	0/1043	0.54	0/1426
1	BZ	0.33	0/1043	0.54	0/1426
1	CA	0.31	0/1043	0.55	0/1426
1	CB	0.30	0/1043	0.54	0/1426
1	CC	0.33	0/1043	0.54	0/1426
1	CD	0.31	0/1043	0.55	0/1426
1	CE	0.31	0/1043	0.54	0/1426
1	CF	0.33	0/1043	0.54	0/1426
1	CG	0.31	0/1043	0.55	0/1426
1	CH	0.30	0/1043	0.54	0/1426
1	CI	0.33	0/1043	0.54	0/1426
1	CJ	0.31	0/1043	0.55	0/1426
1	CK	0.30	0/1043	0.54	0/1426
1	CL	0.33	0/1043	0.54	0/1426
1	CM	0.31	0/1043	0.55	0/1426
1	CN	0.30	0/1043	0.54	0/1426
1	CO	0.33	0/1043	0.54	0/1426
1	CP	0.31	0/1043	0.55	0/1426
1	CQ	0.30	0/1043	0.54	0/1426
1	CR	0.33	0/1043	0.54	0/1426
1	CS	0.31	0/1043	0.55	0/1426
1	CT	0.30	0/1043	0.54	0/1426
1	CU	0.33	0/1043	0.54	0/1426
1	CV	0.31	0/1043	0.55	0/1426
1	CW	0.30	0/1043	0.54	0/1426
1	CX	0.33	0/1043	0.54	0/1426
1	CY	0.31	0/1043	0.55	0/1426

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CZ	0.31	0/1043	0.54	0/1426
1	DA	0.33	0/1043	0.54	0/1426
1	DB	0.31	0/1043	0.55	0/1426
1	DC	0.30	0/1043	0.54	0/1426
1	DD	0.33	0/1043	0.54	0/1426
1	DE	0.31	0/1043	0.55	0/1426
1	DF	0.31	0/1043	0.54	0/1426
1	DG	0.33	0/1043	0.54	0/1426
1	DH	0.31	0/1043	0.55	0/1426
1	DI	0.31	0/1043	0.54	0/1426
1	DJ	0.33	0/1043	0.54	0/1426
1	DK	0.31	0/1043	0.55	0/1426
1	DL	0.30	0/1043	0.54	0/1426
1	DM	0.33	0/1043	0.54	0/1426
1	DN	0.31	0/1043	0.55	0/1426
1	DO	0.31	0/1043	0.54	0/1426
1	DP	0.33	0/1043	0.54	0/1426
1	DQ	0.31	0/1043	0.55	0/1426
1	DR	0.31	0/1043	0.54	0/1426
1	DS	0.33	0/1043	0.54	0/1426
1	DT	0.31	0/1043	0.55	0/1426
1	DU	0.30	0/1043	0.54	0/1426
1	DV	0.33	0/1043	0.54	0/1426
1	DW	0.31	0/1043	0.55	0/1426
1	DX	0.30	0/1043	0.54	0/1426
1	DY	0.33	0/1043	0.54	0/1426
1	DZ	0.31	0/1043	0.55	0/1426
1	EA	0.30	0/1043	0.54	0/1426
1	EB	0.33	0/1043	0.54	0/1426
1	EC	0.31	0/1043	0.55	0/1426
1	ED	0.31	0/1043	0.54	0/1426
1	EE	0.33	0/1043	0.54	0/1426
1	EF	0.31	0/1043	0.55	0/1426
1	EG	0.30	0/1043	0.54	0/1426
1	EH	0.33	0/1043	0.54	0/1426
1	EI	0.31	0/1043	0.55	0/1426
1	EJ	0.31	0/1043	0.54	0/1426
1	EK	0.33	0/1043	0.54	0/1426
1	EL	0.31	0/1043	0.55	0/1426
1	EM	0.30	0/1043	0.54	0/1426
1	EN	0.33	0/1043	0.54	0/1426
1	EO	0.31	0/1043	0.55	0/1426
1	EP	0.31	0/1043	0.54	0/1426

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	EQ	0.33	0/1043	0.54	0/1426
1	ER	0.31	0/1043	0.55	0/1426
1	ES	0.30	0/1043	0.54	0/1426
1	ET	0.33	0/1043	0.54	0/1426
1	EU	0.31	0/1043	0.55	0/1426
1	EV	0.31	0/1043	0.54	0/1426
1	EW	0.33	0/1043	0.54	0/1426
1	EX	0.31	0/1043	0.55	0/1426
1	EY	0.31	0/1043	0.54	0/1426
1	EZ	0.33	0/1043	0.54	0/1426
1	FA	0.31	0/1043	0.55	0/1426
1	FB	0.31	0/1043	0.54	0/1426
1	FC	0.33	0/1043	0.54	0/1426
1	FD	0.31	0/1043	0.55	0/1426
1	FE	0.30	0/1043	0.54	0/1426
1	FF	0.33	0/1043	0.54	0/1426
1	FG	0.31	0/1043	0.55	0/1426
1	FH	0.31	0/1043	0.54	0/1426
1	FI	0.33	0/1043	0.54	0/1426
1	FJ	0.31	0/1043	0.55	0/1426
1	FK	0.30	0/1043	0.54	0/1426
1	FL	0.33	0/1043	0.54	0/1426
1	FM	0.31	0/1043	0.55	0/1426
1	FN	0.31	0/1043	0.54	0/1426
1	FO	0.33	0/1043	0.54	0/1426
1	FP	0.31	0/1043	0.55	0/1426
1	FQ	0.30	0/1043	0.54	0/1426
1	FR	0.33	0/1043	0.54	0/1426
1	FS	0.31	0/1043	0.55	0/1426
1	FT	0.30	0/1043	0.54	0/1426
1	FU	0.33	0/1043	0.54	0/1426
1	FV	0.31	0/1043	0.55	0/1426
1	FW	0.30	0/1043	0.54	0/1426
1	FX	0.33	0/1043	0.54	0/1426
1	FY	0.31	0/1043	0.55	0/1426
1	FZ	0.31	0/1043	0.54	0/1426
1	GA	0.33	0/1043	0.54	0/1426
1	GB	0.31	0/1043	0.55	0/1426
1	GC	0.31	0/1043	0.54	0/1426
1	GD	0.33	0/1043	0.54	0/1426
1	GE	0.31	0/1043	0.55	0/1426
1	GF	0.30	0/1043	0.54	0/1426
1	GG	0.33	0/1043	0.54	0/1426

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GH	0.31	0/1043	0.55	0/1426
1	GI	0.31	0/1043	0.54	0/1426
1	GJ	0.33	0/1043	0.54	0/1426
1	GK	0.31	0/1043	0.55	0/1426
1	GL	0.31	0/1043	0.54	0/1426
1	GM	0.33	0/1043	0.54	0/1426
1	GN	0.31	0/1043	0.55	0/1426
1	GO	0.30	0/1043	0.54	0/1426
1	GP	0.33	0/1043	0.54	0/1426
1	GQ	0.31	0/1043	0.55	0/1426
1	GR	0.30	0/1043	0.54	0/1426
1	GS	0.33	0/1043	0.54	0/1426
1	GT	0.31	0/1043	0.55	0/1426
1	GU	0.31	0/1043	0.54	0/1426
1	GV	0.33	0/1043	0.54	0/1426
1	GW	0.31	0/1043	0.55	0/1426
1	GX	0.30	0/1043	0.54	0/1426
All	All	0.32	0/187740	0.54	0/256680

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	1024	0	1026	23	0
1	AB	1024	0	1026	30	0
1	AC	1024	0	1026	22	0
1	AD	1024	0	1026	34	0
1	AE	1024	0	1026	45	0
1	AF	1024	0	1026	23	0
1	AG	1024	0	1026	29	0
1	AH	1024	0	1026	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AI	1024	0	1026	29	0
1	AJ	1024	0	1026	29	0
1	AK	1024	0	1026	36	0
1	AL	1024	0	1026	21	0
1	AM	1024	0	1026	37	0
1	AN	1024	0	1026	38	0
1	AO	1024	0	1026	25	0
1	AP	1024	0	1026	41	0
1	AQ	1024	0	1026	36	0
1	AR	1024	0	1026	35	0
1	AS	1024	0	1026	35	0
1	AT	1024	0	1026	39	0
1	AU	1024	0	1026	38	0
1	AV	1024	0	1026	39	1
1	AW	1024	0	1026	34	0
1	AX	1024	0	1026	32	0
1	AY	1024	0	1026	31	0
1	AZ	1024	0	1026	37	0
1	BA	1024	0	1026	25	0
1	BB	1024	0	1026	27	0
1	BC	1024	0	1026	38	0
1	BD	1024	0	1026	30	0
1	BE	1024	0	1026	29	0
1	BF	1024	0	1026	32	0
1	BG	1024	0	1026	23	0
1	BH	1024	0	1026	35	1
1	BI	1024	0	1026	26	0
1	BJ	1024	0	1026	47	0
1	BK	1024	0	1026	31	0
1	BL	1024	0	1026	31	0
1	BM	1024	0	1026	23	0
1	BN	1024	0	1026	29	0
1	BO	1024	0	1026	37	0
1	BP	1024	0	1026	36	0
1	BQ	1024	0	1026	29	0
1	BR	1024	0	1026	31	0
1	BS	1024	0	1026	20	0
1	BT	1024	0	1026	28	0
1	BU	1024	0	1026	40	1
1	BV	1024	0	1026	33	0
1	BW	1024	0	1026	36	0
1	BX	1024	0	1026	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BY	1024	0	1026	35	0
1	BZ	1024	0	1026	36	0
1	CA	1024	0	1026	42	0
1	CB	1024	0	1026	43	0
1	CC	1024	0	1026	33	0
1	CD	1024	0	1026	35	0
1	CE	1024	0	1026	32	0
1	CF	1024	0	1026	28	0
1	CG	1024	0	1026	44	0
1	CH	1024	0	1026	30	0
1	CI	1024	0	1026	36	0
1	CJ	1024	0	1026	42	0
1	CK	1024	0	1026	24	0
1	CL	1024	0	1026	43	1
1	CM	1024	0	1026	33	0
1	CN	1024	0	1026	25	0
1	CO	1024	0	1026	37	0
1	CP	1024	0	1026	33	0
1	CQ	1024	0	1026	40	0
1	CR	1024	0	1026	30	0
1	CS	1024	0	1026	53	1
1	CT	1024	0	1026	40	0
1	CU	1024	0	1026	44	0
1	CV	1024	0	1026	34	0
1	CW	1024	0	1026	27	0
1	CX	1024	0	1026	27	0
1	CY	1024	0	1026	35	0
1	CZ	1024	0	1026	20	0
1	DA	1024	0	1026	38	2
1	DB	1024	0	1026	34	0
1	DC	1024	0	1026	34	0
1	DD	1024	0	1026	47	0
1	DE	1024	0	1026	46	0
1	DF	1024	0	1026	41	0
1	DG	1024	0	1026	29	0
1	DH	1024	0	1026	49	0
1	DI	1024	0	1026	26	0
1	DJ	1024	0	1026	33	0
1	DK	1024	0	1026	31	0
1	DL	1024	0	1026	34	0
1	DM	1024	0	1026	28	0
1	DN	1024	0	1026	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DO	1024	0	1026	23	0
1	DP	1024	0	1026	33	0
1	DQ	1024	0	1026	39	0
1	DR	1024	0	1026	21	0
1	DS	1024	0	1026	37	0
1	DT	1024	0	1026	39	0
1	DU	1024	0	1026	30	0
1	DV	1024	0	1026	30	0
1	DW	1024	0	1026	35	0
1	DX	1024	0	1026	21	0
1	DY	1024	0	1026	31	0
1	DZ	1024	0	1026	32	0
1	EA	1024	0	1026	24	0
1	EB	1024	0	1026	38	0
1	EC	1024	0	1026	30	0
1	ED	1024	0	1026	39	0
1	EE	1024	0	1026	52	0
1	EF	1024	0	1026	42	0
1	EG	1024	0	1026	33	0
1	EH	1024	0	1026	32	1
1	EI	1024	0	1026	33	0
1	EJ	1024	0	1026	31	0
1	EK	1024	0	1026	29	0
1	EL	1024	0	1026	38	0
1	EM	1024	0	1026	25	0
1	EN	1024	0	1026	49	0
1	EO	1024	0	1026	36	0
1	EP	1024	0	1026	30	0
1	EQ	1024	0	1026	32	0
1	ER	1024	0	1026	31	0
1	ES	1024	0	1026	24	0
1	ET	1024	0	1026	30	0
1	EU	1024	0	1026	58	2
1	EV	1024	0	1026	48	0
1	EW	1024	0	1026	34	0
1	EX	1024	0	1026	30	0
1	EY	1024	0	1026	25	0
1	EZ	1024	0	1026	35	0
1	FA	1024	0	1026	39	0
1	FB	1024	0	1026	37	0
1	FC	1024	0	1026	32	0
1	FD	1024	0	1026	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FE	1024	0	1026	21	0
1	FF	1024	0	1026	35	0
1	FG	1024	0	1026	37	0
1	FH	1024	0	1026	34	0
1	FI	1024	0	1026	26	0
1	FJ	1024	0	1026	56	1
1	FK	1024	0	1026	31	0
1	FL	1024	0	1026	37	0
1	FM	1024	0	1026	37	0
1	FN	1024	0	1026	42	0
1	FO	1024	0	1026	33	0
1	FP	1024	0	1026	36	0
1	FQ	1024	0	1026	34	0
1	FR	1024	0	1026	34	0
1	FS	1024	0	1026	35	0
1	FT	1024	0	1026	31	0
1	FU	1024	0	1026	33	1
1	FV	1024	0	1026	36	0
1	FW	1024	0	1026	23	0
1	FX	1024	0	1026	27	0
1	FY	1024	0	1026	33	0
1	FZ	1024	0	1026	27	0
1	GA	1024	0	1026	40	0
1	GB	1024	0	1026	38	0
1	GC	1024	0	1026	43	0
1	GD	1024	0	1026	34	0
1	GE	1024	0	1026	34	0
1	GF	1024	0	1026	39	0
1	GG	1024	0	1026	31	0
1	GH	1024	0	1026	41	0
1	GI	1024	0	1026	27	0
1	GJ	1024	0	1026	32	0
1	GK	1024	0	1026	39	0
1	GL	1024	0	1026	19	0
1	GM	1024	0	1026	33	0
1	GN	1024	0	1026	30	0
1	GO	1024	0	1026	32	0
1	GP	1024	0	1026	33	0
1	GQ	1024	0	1026	39	0
1	GR	1024	0	1026	42	0
1	GS	1024	0	1026	32	0
1	GT	1024	0	1026	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GU	1024	0	1026	27	0
1	GV	1024	0	1026	36	0
1	GW	1024	0	1026	37	0
1	GX	1024	0	1026	31	0
All	All	184320	0	184680	4335	6

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 12.

The worst 5 of 4335 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:AE:54:ILE:HG12	1:GA:137:LEU:HD13	1.36	1.06
1:CU:137:LEU:HD13	1:DH:54:ILE:HG12	1.40	1.04
1:FA:54:ILE:HG12	1:FL:137:LEU:HD13	1.42	1.02
1:BJ:95:ASN:HD21	1:EV:75:ASP:HA	1.24	0.99
1:EN:137:LEU:HD13	1:FJ:54:ILE:HG12	1.45	0.99

The worst 5 of 6 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:DA:122:SER:OG	1:EU:13:THR:O[1_455]	1.10	1.10
1:EH:122:SER:OG	1:FU:120:THR:OG1[3_645]	1.39	0.81
1:AV:122:SER:OG	1:CS:13:THR:O[1_655]	2.13	0.07
1:DA:120:THR:O	1:EU:11:ASN:ND2[1_455]	2.17	0.03
1:BH:123:GLY:CA	1:CL:124:GLN:NE2[4_556]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AB	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AC	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	AD	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AE	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AF	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	AG	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AH	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AI	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	AJ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AK	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AL	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	AM	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AO	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	AP	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AQ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AR	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	AS	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AT	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AU	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	AV	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AW	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AX	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	AY	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	AZ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BA	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	BB	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BC	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BD	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	BE	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BF	138/140 (99%)	136 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BG	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	BH	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BI	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BJ	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	BK	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BL	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BM	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	BN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BO	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BP	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	BQ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BR	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BS	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	BT	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BU	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BV	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	BW	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BX	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	BY	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	BZ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CA	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CB	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	CC	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CD	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CE	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	CF	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CG	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CH	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	CI	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CJ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CK	138/140 (99%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CL	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CM	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CN	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	CO	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CP	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CQ	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	CR	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CS	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CT	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	CU	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CV	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CW	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	CX	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CY	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	CZ	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	DA	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DB	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DC	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	DD	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DE	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DF	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	DG	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DH	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DI	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	DJ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DK	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DL	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	DM	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DO	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	DP	138/140 (99%)	136 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DQ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DR	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	DS	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DT	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DU	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	DV	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DW	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DX	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	DY	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	DZ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EA	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	EB	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EC	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	ED	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	EE	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EF	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EG	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	EH	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EI	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EJ	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	EK	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EL	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EM	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	EN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EO	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EP	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	EQ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	ER	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	ES	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	ET	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EU	138/140 (99%)	136 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EV	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	EW	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EX	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	EY	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	EZ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FA	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FB	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	FC	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FD	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FE	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	FF	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FG	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FH	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	FI	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FJ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FK	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	FL	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FM	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FN	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	FO	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FP	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FQ	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	FR	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FS	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FT	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	FU	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FV	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FW	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	FX	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FY	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	FZ	138/140 (99%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GA	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GB	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GC	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	GD	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GE	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GF	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	GG	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GH	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GI	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	GJ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GK	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GL	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	GM	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GN	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GO	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	GP	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GQ	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GR	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	GS	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GT	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GU	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
1	GV	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GW	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
1	GX	138/140 (99%)	137 (99%)	1 (1%)	0	100	100
All	All	24840/25200 (99%)	24540 (99%)	300 (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	113/113 (100%)	113 (100%)	0	100	100
1	AB	113/113 (100%)	113 (100%)	0	100	100
1	AC	113/113 (100%)	113 (100%)	0	100	100
1	AD	113/113 (100%)	113 (100%)	0	100	100
1	AE	113/113 (100%)	113 (100%)	0	100	100
1	AF	113/113 (100%)	113 (100%)	0	100	100
1	AG	113/113 (100%)	113 (100%)	0	100	100
1	AH	113/113 (100%)	113 (100%)	0	100	100
1	AI	113/113 (100%)	113 (100%)	0	100	100
1	AJ	113/113 (100%)	113 (100%)	0	100	100
1	AK	113/113 (100%)	113 (100%)	0	100	100
1	AL	113/113 (100%)	113 (100%)	0	100	100
1	AM	113/113 (100%)	113 (100%)	0	100	100
1	AN	113/113 (100%)	113 (100%)	0	100	100
1	AO	113/113 (100%)	113 (100%)	0	100	100
1	AP	113/113 (100%)	113 (100%)	0	100	100
1	AQ	113/113 (100%)	113 (100%)	0	100	100
1	AR	113/113 (100%)	113 (100%)	0	100	100
1	AS	113/113 (100%)	113 (100%)	0	100	100
1	AT	113/113 (100%)	113 (100%)	0	100	100
1	AU	113/113 (100%)	113 (100%)	0	100	100
1	AV	113/113 (100%)	113 (100%)	0	100	100
1	AW	113/113 (100%)	113 (100%)	0	100	100
1	AX	113/113 (100%)	113 (100%)	0	100	100
1	AY	113/113 (100%)	113 (100%)	0	100	100
1	AZ	113/113 (100%)	113 (100%)	0	100	100
1	BA	113/113 (100%)	113 (100%)	0	100	100
1	BB	113/113 (100%)	113 (100%)	0	100	100
1	BC	113/113 (100%)	113 (100%)	0	100	100
1	BD	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BE	113/113 (100%)	113 (100%)	0	100	100
1	BF	113/113 (100%)	113 (100%)	0	100	100
1	BG	113/113 (100%)	113 (100%)	0	100	100
1	BH	113/113 (100%)	113 (100%)	0	100	100
1	BI	113/113 (100%)	113 (100%)	0	100	100
1	BJ	113/113 (100%)	113 (100%)	0	100	100
1	BK	113/113 (100%)	113 (100%)	0	100	100
1	BL	113/113 (100%)	113 (100%)	0	100	100
1	BM	113/113 (100%)	113 (100%)	0	100	100
1	BN	113/113 (100%)	113 (100%)	0	100	100
1	BO	113/113 (100%)	113 (100%)	0	100	100
1	BP	113/113 (100%)	113 (100%)	0	100	100
1	BQ	113/113 (100%)	113 (100%)	0	100	100
1	BR	113/113 (100%)	113 (100%)	0	100	100
1	BS	113/113 (100%)	113 (100%)	0	100	100
1	BT	113/113 (100%)	113 (100%)	0	100	100
1	BU	113/113 (100%)	113 (100%)	0	100	100
1	BV	113/113 (100%)	113 (100%)	0	100	100
1	BW	113/113 (100%)	113 (100%)	0	100	100
1	BX	113/113 (100%)	113 (100%)	0	100	100
1	BY	113/113 (100%)	113 (100%)	0	100	100
1	BZ	113/113 (100%)	113 (100%)	0	100	100
1	CA	113/113 (100%)	113 (100%)	0	100	100
1	CB	113/113 (100%)	113 (100%)	0	100	100
1	CC	113/113 (100%)	113 (100%)	0	100	100
1	CD	113/113 (100%)	113 (100%)	0	100	100
1	CE	113/113 (100%)	113 (100%)	0	100	100
1	CF	113/113 (100%)	113 (100%)	0	100	100
1	CG	113/113 (100%)	113 (100%)	0	100	100
1	CH	113/113 (100%)	113 (100%)	0	100	100
1	CI	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CJ	113/113 (100%)	113 (100%)	0	100	100
1	CK	113/113 (100%)	113 (100%)	0	100	100
1	CL	113/113 (100%)	113 (100%)	0	100	100
1	CM	113/113 (100%)	113 (100%)	0	100	100
1	CN	113/113 (100%)	113 (100%)	0	100	100
1	CO	113/113 (100%)	113 (100%)	0	100	100
1	CP	113/113 (100%)	113 (100%)	0	100	100
1	CQ	113/113 (100%)	113 (100%)	0	100	100
1	CR	113/113 (100%)	113 (100%)	0	100	100
1	CS	113/113 (100%)	113 (100%)	0	100	100
1	CT	113/113 (100%)	113 (100%)	0	100	100
1	CU	113/113 (100%)	113 (100%)	0	100	100
1	CV	113/113 (100%)	113 (100%)	0	100	100
1	CW	113/113 (100%)	113 (100%)	0	100	100
1	CX	113/113 (100%)	113 (100%)	0	100	100
1	CY	113/113 (100%)	113 (100%)	0	100	100
1	CZ	113/113 (100%)	113 (100%)	0	100	100
1	DA	113/113 (100%)	113 (100%)	0	100	100
1	DB	113/113 (100%)	113 (100%)	0	100	100
1	DC	113/113 (100%)	113 (100%)	0	100	100
1	DD	113/113 (100%)	113 (100%)	0	100	100
1	DE	113/113 (100%)	113 (100%)	0	100	100
1	DF	113/113 (100%)	113 (100%)	0	100	100
1	DG	113/113 (100%)	113 (100%)	0	100	100
1	DH	113/113 (100%)	113 (100%)	0	100	100
1	DI	113/113 (100%)	113 (100%)	0	100	100
1	DJ	113/113 (100%)	113 (100%)	0	100	100
1	DK	113/113 (100%)	113 (100%)	0	100	100
1	DL	113/113 (100%)	113 (100%)	0	100	100
1	DM	113/113 (100%)	113 (100%)	0	100	100
1	DN	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DO	113/113 (100%)	113 (100%)	0	100	100
1	DP	113/113 (100%)	113 (100%)	0	100	100
1	DQ	113/113 (100%)	113 (100%)	0	100	100
1	DR	113/113 (100%)	113 (100%)	0	100	100
1	DS	113/113 (100%)	113 (100%)	0	100	100
1	DT	113/113 (100%)	113 (100%)	0	100	100
1	DU	113/113 (100%)	113 (100%)	0	100	100
1	DV	113/113 (100%)	113 (100%)	0	100	100
1	DW	113/113 (100%)	113 (100%)	0	100	100
1	DX	113/113 (100%)	113 (100%)	0	100	100
1	DY	113/113 (100%)	113 (100%)	0	100	100
1	DZ	113/113 (100%)	113 (100%)	0	100	100
1	EA	113/113 (100%)	113 (100%)	0	100	100
1	EB	113/113 (100%)	113 (100%)	0	100	100
1	EC	113/113 (100%)	113 (100%)	0	100	100
1	ED	113/113 (100%)	113 (100%)	0	100	100
1	EE	113/113 (100%)	113 (100%)	0	100	100
1	EF	113/113 (100%)	113 (100%)	0	100	100
1	EG	113/113 (100%)	113 (100%)	0	100	100
1	EH	113/113 (100%)	113 (100%)	0	100	100
1	EI	113/113 (100%)	113 (100%)	0	100	100
1	EJ	113/113 (100%)	113 (100%)	0	100	100
1	EK	113/113 (100%)	113 (100%)	0	100	100
1	EL	113/113 (100%)	113 (100%)	0	100	100
1	EM	113/113 (100%)	113 (100%)	0	100	100
1	EN	113/113 (100%)	113 (100%)	0	100	100
1	EO	113/113 (100%)	113 (100%)	0	100	100
1	EP	113/113 (100%)	113 (100%)	0	100	100
1	EQ	113/113 (100%)	113 (100%)	0	100	100
1	ER	113/113 (100%)	113 (100%)	0	100	100
1	ES	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ET	113/113 (100%)	113 (100%)	0	100	100
1	EU	113/113 (100%)	113 (100%)	0	100	100
1	EV	113/113 (100%)	113 (100%)	0	100	100
1	EW	113/113 (100%)	113 (100%)	0	100	100
1	EX	113/113 (100%)	113 (100%)	0	100	100
1	EY	113/113 (100%)	113 (100%)	0	100	100
1	EZ	113/113 (100%)	113 (100%)	0	100	100
1	FA	113/113 (100%)	113 (100%)	0	100	100
1	FB	113/113 (100%)	113 (100%)	0	100	100
1	FC	113/113 (100%)	113 (100%)	0	100	100
1	FD	113/113 (100%)	113 (100%)	0	100	100
1	FE	113/113 (100%)	113 (100%)	0	100	100
1	FF	113/113 (100%)	113 (100%)	0	100	100
1	FG	113/113 (100%)	113 (100%)	0	100	100
1	FH	113/113 (100%)	113 (100%)	0	100	100
1	FI	113/113 (100%)	113 (100%)	0	100	100
1	FJ	113/113 (100%)	113 (100%)	0	100	100
1	FK	113/113 (100%)	113 (100%)	0	100	100
1	FL	113/113 (100%)	113 (100%)	0	100	100
1	FM	113/113 (100%)	113 (100%)	0	100	100
1	FN	113/113 (100%)	113 (100%)	0	100	100
1	FO	113/113 (100%)	113 (100%)	0	100	100
1	FP	113/113 (100%)	113 (100%)	0	100	100
1	FQ	113/113 (100%)	113 (100%)	0	100	100
1	FR	113/113 (100%)	113 (100%)	0	100	100
1	FS	113/113 (100%)	113 (100%)	0	100	100
1	FT	113/113 (100%)	113 (100%)	0	100	100
1	FU	113/113 (100%)	113 (100%)	0	100	100
1	FV	113/113 (100%)	113 (100%)	0	100	100
1	FW	113/113 (100%)	113 (100%)	0	100	100
1	FX	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FY	113/113 (100%)	113 (100%)	0	100	100
1	FZ	113/113 (100%)	113 (100%)	0	100	100
1	GA	113/113 (100%)	113 (100%)	0	100	100
1	GB	113/113 (100%)	113 (100%)	0	100	100
1	GC	113/113 (100%)	113 (100%)	0	100	100
1	GD	113/113 (100%)	113 (100%)	0	100	100
1	GE	113/113 (100%)	113 (100%)	0	100	100
1	GF	113/113 (100%)	113 (100%)	0	100	100
1	GG	113/113 (100%)	113 (100%)	0	100	100
1	GH	113/113 (100%)	113 (100%)	0	100	100
1	GI	113/113 (100%)	113 (100%)	0	100	100
1	GJ	113/113 (100%)	113 (100%)	0	100	100
1	GK	113/113 (100%)	113 (100%)	0	100	100
1	GL	113/113 (100%)	113 (100%)	0	100	100
1	GM	113/113 (100%)	113 (100%)	0	100	100
1	GN	113/113 (100%)	113 (100%)	0	100	100
1	GO	113/113 (100%)	113 (100%)	0	100	100
1	GP	113/113 (100%)	113 (100%)	0	100	100
1	GQ	113/113 (100%)	113 (100%)	0	100	100
1	GR	113/113 (100%)	113 (100%)	0	100	100
1	GS	113/113 (100%)	113 (100%)	0	100	100
1	GT	113/113 (100%)	113 (100%)	0	100	100
1	GU	113/113 (100%)	113 (100%)	0	100	100
1	GV	113/113 (100%)	113 (100%)	0	100	100
1	GW	113/113 (100%)	113 (100%)	0	100	100
1	GX	113/113 (100%)	113 (100%)	0	100	100
All	All	20340/20340 (100%)	20340 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
1	CX	124	GLN
1	DU	79	ASN
1	GI	79	ASN
1	CZ	79	ASN
1	DJ	124	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	140/140 (100%)	-0.33	0 100 100	17, 32, 64, 77	0
1	AB	140/140 (100%)	-0.33	0 100 100	17, 30, 53, 71	0
1	AC	140/140 (100%)	-0.26	0 100 100	18, 32, 55, 63	0
1	AD	140/140 (100%)	-0.13	0 100 100	17, 32, 64, 77	0
1	AE	140/140 (100%)	-0.22	0 100 100	17, 30, 53, 71	0
1	AF	140/140 (100%)	-0.31	0 100 100	18, 32, 55, 63	0
1	AG	140/140 (100%)	-0.19	1 (0%) 87 81	17, 32, 64, 77	0
1	AH	140/140 (100%)	-0.20	0 100 100	17, 30, 53, 71	0
1	AI	140/140 (100%)	-0.29	0 100 100	18, 32, 55, 63	0
1	AJ	140/140 (100%)	-0.24	0 100 100	17, 32, 64, 77	0
1	AK	140/140 (100%)	-0.39	0 100 100	17, 30, 53, 71	0
1	AL	140/140 (100%)	-0.29	0 100 100	18, 32, 55, 63	0
1	AM	140/140 (100%)	-0.12	1 (0%) 87 81	17, 32, 64, 77	0
1	AN	140/140 (100%)	-0.20	0 100 100	17, 30, 53, 71	0
1	AO	140/140 (100%)	-0.33	0 100 100	18, 32, 55, 63	0
1	AP	140/140 (100%)	0.05	1 (0%) 87 81	17, 32, 64, 77	0
1	AQ	140/140 (100%)	-0.24	0 100 100	17, 30, 53, 71	0
1	AR	140/140 (100%)	-0.12	0 100 100	18, 32, 55, 63	0
1	AS	140/140 (100%)	-0.17	0 100 100	17, 32, 64, 77	0
1	AT	140/140 (100%)	-0.32	0 100 100	17, 30, 53, 71	0
1	AU	140/140 (100%)	-0.37	0 100 100	18, 32, 55, 63	0
1	AV	140/140 (100%)	-0.28	1 (0%) 87 81	17, 32, 64, 77	0
1	AW	140/140 (100%)	-0.44	0 100 100	17, 30, 53, 71	0
1	AX	140/140 (100%)	-0.21	0 100 100	18, 32, 55, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AY	140/140 (100%)	-0.23	1 (0%) 87 81	17, 32, 64, 77	0
1	AZ	140/140 (100%)	-0.24	0 100 100	17, 30, 53, 71	0
1	BA	140/140 (100%)	-0.30	0 100 100	18, 32, 55, 63	0
1	BB	140/140 (100%)	-0.21	1 (0%) 87 81	17, 32, 64, 77	0
1	BC	140/140 (100%)	-0.24	0 100 100	17, 30, 53, 71	0
1	BD	140/140 (100%)	-0.13	0 100 100	18, 32, 55, 63	0
1	BE	140/140 (100%)	-0.06	2 (1%) 75 63	17, 32, 64, 77	0
1	BF	140/140 (100%)	-0.26	0 100 100	17, 30, 53, 71	0
1	BG	140/140 (100%)	-0.40	0 100 100	18, 32, 55, 63	0
1	BH	140/140 (100%)	-0.02	2 (1%) 75 63	17, 32, 64, 77	0
1	BI	140/140 (100%)	-0.23	0 100 100	17, 30, 53, 71	0
1	BJ	140/140 (100%)	-0.25	0 100 100	18, 32, 55, 63	0
1	BK	140/140 (100%)	-0.21	1 (0%) 87 81	17, 32, 64, 77	0
1	BL	140/140 (100%)	-0.17	0 100 100	17, 30, 53, 71	0
1	BM	140/140 (100%)	-0.39	0 100 100	18, 32, 55, 63	0
1	BN	140/140 (100%)	-0.29	0 100 100	17, 32, 64, 77	0
1	BO	140/140 (100%)	-0.26	0 100 100	17, 30, 53, 71	0
1	BP	140/140 (100%)	-0.18	0 100 100	18, 32, 55, 63	0
1	BQ	140/140 (100%)	-0.33	0 100 100	17, 32, 64, 77	0
1	BR	140/140 (100%)	-0.31	0 100 100	17, 30, 53, 71	0
1	BS	140/140 (100%)	-0.29	0 100 100	18, 32, 55, 63	0
1	BT	140/140 (100%)	-0.23	0 100 100	17, 32, 64, 77	0
1	BU	140/140 (100%)	-0.19	0 100 100	17, 30, 53, 71	0
1	BV	140/140 (100%)	-0.35	0 100 100	18, 32, 55, 63	0
1	BW	140/140 (100%)	-0.09	1 (0%) 87 81	17, 32, 64, 77	0
1	BX	140/140 (100%)	-0.24	0 100 100	17, 30, 53, 71	0
1	BY	140/140 (100%)	-0.37	0 100 100	18, 32, 55, 63	0
1	BZ	140/140 (100%)	-0.20	0 100 100	17, 32, 64, 77	0
1	CA	140/140 (100%)	-0.25	0 100 100	17, 30, 53, 71	0
1	CB	140/140 (100%)	-0.13	0 100 100	18, 32, 55, 63	0
1	CC	140/140 (100%)	-0.22	1 (0%) 87 81	17, 32, 64, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	CD	140/140 (100%)	-0.33	0 100 100	17, 30, 53, 71	0
1	CE	140/140 (100%)	-0.33	0 100 100	18, 32, 55, 63	0
1	CF	140/140 (100%)	-0.26	1 (0%) 87 81	17, 32, 64, 77	0
1	CG	140/140 (100%)	-0.25	0 100 100	17, 30, 53, 71	0
1	CH	140/140 (100%)	-0.21	0 100 100	18, 32, 55, 63	0
1	CI	140/140 (100%)	-0.17	0 100 100	17, 32, 64, 77	0
1	CJ	140/140 (100%)	-0.19	0 100 100	17, 30, 53, 71	0
1	CK	140/140 (100%)	-0.33	0 100 100	18, 32, 55, 63	0
1	CL	140/140 (100%)	-0.06	1 (0%) 87 81	17, 32, 64, 77	0
1	CM	140/140 (100%)	-0.26	0 100 100	17, 30, 53, 71	0
1	CN	140/140 (100%)	-0.34	0 100 100	18, 32, 55, 63	0
1	CO	140/140 (100%)	-0.17	0 100 100	17, 32, 64, 77	0
1	CP	140/140 (100%)	-0.26	0 100 100	17, 30, 53, 71	0
1	CQ	140/140 (100%)	-0.18	0 100 100	18, 32, 55, 63	0
1	CR	140/140 (100%)	-0.19	0 100 100	17, 32, 64, 77	0
1	CS	140/140 (100%)	-0.22	0 100 100	17, 30, 53, 71	0
1	CT	140/140 (100%)	-0.36	0 100 100	18, 32, 55, 63	0
1	CU	140/140 (100%)	-0.00	1 (0%) 87 81	17, 32, 64, 77	0
1	CV	140/140 (100%)	-0.29	0 100 100	17, 30, 53, 71	0
1	CW	140/140 (100%)	-0.16	0 100 100	18, 32, 55, 63	0
1	CX	140/140 (100%)	-0.31	0 100 100	17, 32, 64, 77	0
1	CY	140/140 (100%)	-0.29	0 100 100	17, 30, 53, 71	0
1	CZ	140/140 (100%)	-0.30	0 100 100	18, 32, 55, 63	0
1	DA	140/140 (100%)	-0.29	1 (0%) 87 81	17, 32, 64, 77	0
1	DB	140/140 (100%)	-0.42	0 100 100	17, 30, 53, 71	0
1	DC	140/140 (100%)	-0.26	0 100 100	18, 32, 55, 63	0
1	DD	140/140 (100%)	0.03	1 (0%) 87 81	17, 32, 64, 77	0
1	DE	140/140 (100%)	-0.04	0 100 100	17, 30, 53, 71	0
1	DF	140/140 (100%)	-0.17	0 100 100	18, 32, 55, 63	0
1	DG	140/140 (100%)	-0.21	0 100 100	17, 32, 64, 77	0
1	DH	140/140 (100%)	-0.23	0 100 100	17, 30, 53, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	DI	140/140 (100%)	-0.36	0 100 100	18, 32, 55, 63	0
1	DJ	140/140 (100%)	-0.20	1 (0%) 87 81	17, 32, 64, 77	0
1	DK	140/140 (100%)	-0.40	0 100 100	17, 30, 53, 71	0
1	DL	140/140 (100%)	-0.36	0 100 100	18, 32, 55, 63	0
1	DM	140/140 (100%)	-0.22	0 100 100	17, 32, 64, 77	0
1	DN	140/140 (100%)	-0.38	0 100 100	17, 30, 53, 71	0
1	DO	140/140 (100%)	-0.28	0 100 100	18, 32, 55, 63	0
1	DP	140/140 (100%)	-0.22	1 (0%) 87 81	17, 32, 64, 77	0
1	DQ	140/140 (100%)	-0.23	0 100 100	17, 30, 53, 71	0
1	DR	140/140 (100%)	-0.38	0 100 100	18, 32, 55, 63	0
1	DS	140/140 (100%)	-0.23	0 100 100	17, 32, 64, 77	0
1	DT	140/140 (100%)	-0.22	0 100 100	17, 30, 53, 71	0
1	DU	140/140 (100%)	-0.28	0 100 100	18, 32, 55, 63	0
1	DV	140/140 (100%)	-0.22	0 100 100	17, 32, 64, 77	0
1	DW	140/140 (100%)	-0.31	0 100 100	17, 30, 53, 71	0
1	DX	140/140 (100%)	-0.14	0 100 100	18, 32, 55, 63	0
1	DY	140/140 (100%)	-0.18	2 (1%) 75 63	17, 32, 64, 77	0
1	DZ	140/140 (100%)	-0.34	0 100 100	17, 30, 53, 71	0
1	EA	140/140 (100%)	-0.34	0 100 100	18, 32, 55, 63	0
1	EB	140/140 (100%)	-0.18	0 100 100	17, 32, 64, 77	0
1	EC	140/140 (100%)	-0.39	0 100 100	17, 30, 53, 71	0
1	ED	140/140 (100%)	-0.31	1 (0%) 87 81	18, 32, 55, 63	0
1	EE	140/140 (100%)	-0.01	0 100 100	17, 32, 64, 77	0
1	EF	140/140 (100%)	-0.07	0 100 100	17, 30, 53, 71	0
1	EG	140/140 (100%)	-0.25	0 100 100	18, 32, 55, 63	0
1	EH	140/140 (100%)	-0.23	1 (0%) 87 81	17, 32, 64, 77	0
1	EI	140/140 (100%)	-0.24	0 100 100	17, 30, 53, 71	0
1	EJ	140/140 (100%)	-0.18	0 100 100	18, 32, 55, 63	0
1	EK	140/140 (100%)	-0.09	1 (0%) 87 81	17, 32, 64, 77	0
1	EL	140/140 (100%)	-0.23	0 100 100	17, 30, 53, 71	0
1	EM	140/140 (100%)	-0.16	0 100 100	18, 32, 55, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	EN	140/140 (100%)	0.03	2 (1%) 75 63	17, 32, 64, 77	0
1	EO	140/140 (100%)	-0.29	0 100 100	17, 30, 53, 71	0
1	EP	140/140 (100%)	-0.09	0 100 100	18, 32, 55, 63	0
1	EQ	140/140 (100%)	-0.14	0 100 100	17, 32, 64, 77	0
1	ER	140/140 (100%)	-0.19	0 100 100	17, 30, 53, 71	0
1	ES	140/140 (100%)	-0.36	0 100 100	18, 32, 55, 63	0
1	ET	140/140 (100%)	-0.23	0 100 100	17, 32, 64, 77	0
1	EU	140/140 (100%)	-0.20	0 100 100	17, 30, 53, 71	0
1	EV	140/140 (100%)	-0.34	0 100 100	18, 32, 55, 63	0
1	EW	140/140 (100%)	-0.12	0 100 100	17, 32, 64, 77	0
1	EX	140/140 (100%)	-0.24	0 100 100	17, 30, 53, 71	0
1	EY	140/140 (100%)	-0.44	0 100 100	18, 32, 55, 63	0
1	EZ	140/140 (100%)	-0.28	1 (0%) 87 81	17, 32, 64, 77	0
1	FA	140/140 (100%)	-0.18	0 100 100	17, 30, 53, 71	0
1	FB	140/140 (100%)	-0.29	0 100 100	18, 32, 55, 63	0
1	FC	140/140 (100%)	-0.26	0 100 100	17, 32, 64, 77	0
1	FD	140/140 (100%)	-0.31	0 100 100	17, 30, 53, 71	0
1	FE	140/140 (100%)	-0.39	0 100 100	18, 32, 55, 63	0
1	FF	140/140 (100%)	-0.23	0 100 100	17, 32, 64, 77	0
1	FG	140/140 (100%)	-0.35	0 100 100	17, 30, 53, 71	0
1	FH	140/140 (100%)	-0.27	0 100 100	18, 32, 55, 63	0
1	FI	140/140 (100%)	-0.29	0 100 100	17, 32, 64, 77	0
1	FJ	140/140 (100%)	-0.22	0 100 100	17, 30, 53, 71	0
1	FK	140/140 (100%)	-0.34	0 100 100	18, 32, 55, 63	0
1	FL	140/140 (100%)	-0.19	1 (0%) 87 81	17, 32, 64, 77	0
1	FM	140/140 (100%)	-0.21	0 100 100	17, 30, 53, 71	0
1	FN	140/140 (100%)	-0.11	0 100 100	18, 32, 55, 63	0
1	FO	140/140 (100%)	-0.23	1 (0%) 87 81	17, 32, 64, 77	0
1	FP	140/140 (100%)	-0.22	0 100 100	17, 30, 53, 71	0
1	FQ	140/140 (100%)	-0.26	0 100 100	18, 32, 55, 63	0
1	FR	140/140 (100%)	-0.21	1 (0%) 87 81	17, 32, 64, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	FS	140/140 (100%)	-0.30	0 100 100	17, 30, 53, 71	0
1	FT	140/140 (100%)	-0.17	0 100 100	18, 32, 55, 63	0
1	FU	140/140 (100%)	-0.18	1 (0%) 87 81	17, 32, 64, 77	0
1	FV	140/140 (100%)	-0.19	0 100 100	17, 30, 53, 71	0
1	FW	140/140 (100%)	-0.27	0 100 100	18, 32, 55, 63	0
1	FX	140/140 (100%)	-0.26	1 (0%) 87 81	17, 32, 64, 77	0
1	FY	140/140 (100%)	-0.23	0 100 100	17, 30, 53, 71	0
1	FZ	140/140 (100%)	-0.24	0 100 100	18, 32, 55, 63	0
1	GA	140/140 (100%)	-0.10	1 (0%) 87 81	17, 32, 64, 77	0
1	GB	140/140 (100%)	-0.28	0 100 100	17, 30, 53, 71	0
1	GC	140/140 (100%)	-0.21	0 100 100	18, 32, 55, 63	0
1	GD	140/140 (100%)	-0.01	2 (1%) 75 63	17, 32, 64, 77	0
1	GE	140/140 (100%)	-0.35	0 100 100	17, 30, 53, 71	0
1	GF	140/140 (100%)	-0.27	0 100 100	18, 32, 55, 63	0
1	GG	140/140 (100%)	-0.24	0 100 100	17, 32, 64, 77	0
1	GH	140/140 (100%)	-0.27	0 100 100	17, 30, 53, 71	0
1	GI	140/140 (100%)	-0.13	0 100 100	18, 32, 55, 63	0
1	GJ	140/140 (100%)	-0.32	1 (0%) 87 81	17, 32, 64, 77	0
1	GK	140/140 (100%)	-0.36	0 100 100	17, 30, 53, 71	0
1	GL	140/140 (100%)	-0.36	0 100 100	18, 32, 55, 63	0
1	GM	140/140 (100%)	-0.13	1 (0%) 87 81	17, 32, 64, 77	0
1	GN	140/140 (100%)	-0.27	0 100 100	17, 30, 53, 71	0
1	GO	140/140 (100%)	-0.19	0 100 100	18, 32, 55, 63	0
1	GP	140/140 (100%)	-0.22	0 100 100	17, 32, 64, 77	0
1	GQ	140/140 (100%)	-0.36	0 100 100	17, 30, 53, 71	0
1	GR	140/140 (100%)	-0.31	0 100 100	18, 32, 55, 63	0
1	GS	140/140 (100%)	-0.16	0 100 100	17, 32, 64, 77	0
1	GT	140/140 (100%)	-0.30	0 100 100	17, 30, 53, 71	0
1	GU	140/140 (100%)	-0.39	0 100 100	18, 32, 55, 63	0
1	GV	140/140 (100%)	-0.09	1 (0%) 87 81	17, 32, 64, 77	0
1	GW	140/140 (100%)	-0.43	0 100 100	17, 30, 53, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	GX	140/140 (100%)	-0.08	0 100 100	18, 32, 55, 63	0
All	All	25200/25200 (100%)	-0.24	39 (0%) 95 94	17, 32, 59, 77	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	FR	60	THR	3.2
1	AG	60	THR	3.1
1	BE	59	ILE	3.1
1	DP	60	THR	3.1
1	AV	60	THR	3.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.