



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:37 PM UTC

PDB ID : 6YFC / pdb_00006yfc
Title : Virus-like particle of bacteriophage AVE019
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on : 2020-03-26
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

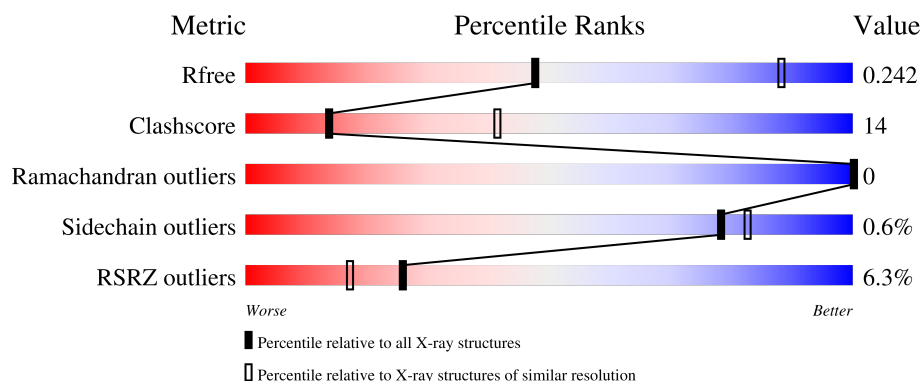
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	124	2% 69% 31%
1	AB	124	6% 60% 33% 6%
1	AC	124	7% 69% 31%
1	AD	124	4% 69% 31%
1	AE	124	14% 56% 37% 6%

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Mol	Chain	Length	Quality of chain
1	AF	124	
1	AG	124	
1	AH	124	
1	AI	124	
1	AJ	124	
1	AK	124	
1	AL	124	
1	AM	124	
1	AN	124	
1	AO	124	
1	AP	124	
1	AQ	124	
1	AR	124	
1	AS	124	
1	AT	124	
1	AU	124	
1	AV	124	
1	AW	124	
1	AX	124	
1	AY	124	
1	AZ	124	
1	BA	124	
1	BB	124	
1	BC	124	
1	BD	124	

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Mol	Chain	Length	Quality of chain
1	BE	124	3% 70% 30%
1	BF	124	3% 63% 31% 6%
1	BG	124	2% 69% 31%
1	BH	124	10% 69% 31%
1	BI	124	8% 61% 31% 6%
1	BJ	124	8% 69% 31%
1	BK	124	8% 64% 36%
1	BL	124	10% 63% 31% 6%
1	BM	124	4% 67% 33%
1	BN	124	7% 65% 35%
1	BO	124	6% 61% 32% 6%
1	BP	124	2% 71% 29%
1	BQ	124	2% 71% 29%
1	BR	124	0% 65% 28% 6%
1	BS	124	3% 70% 30%
1	BT	124	15% 62% 38%
1	BU	124	12% 62% 31% 6%
1	BV	124	10% 70% 30%
1	BW	124	4% 69% 31%
1	BX	124	6% 60% 35% 6%
1	BY	124	4% 67% 33%
1	BZ	124	4% 66% 34%
1	CA	124	8% 60% 33% 6%
1	CB	124	4% 61% 39%
1	CC	124	3% 64% 36%

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

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

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Mol	Chain	Length	Quality of chain
1	EB	124	 3% 65% 32%
1	EC	124	 7% 64% 30% • 6%
1	ED	124	 3% 62% 38%
1	EE	124	 9% 70% 30%
1	EF	124	 4% 64% 30% • 6%
1	EG	124	 10% 66% 34%
1	EH	124	 9% 61% 39%
1	EI	124	 14% 56% 37% • 6%
1	EJ	124	 2% 67% 33%
1	EK	124	 7% 70% 30%
1	EL	124	 8% 59% 35% • 6%
1	EM	124	 8% 72% 28%
1	EN	124	 5% 69% 31%
1	EO	124	 10% 59% 35% • 6%
1	EP	124	 4% 63% 37%
1	EQ	124	 4% 68% 32%
1	ER	124	 10% 60% 34% 6%
1	ES	124	 5% 69% 31%
1	ET	124	 6% 64% 36%
1	EU	124	 6% 64% 30% • 6%
1	EV	124	 14% 65% 35%
1	EW	124	 3% 69% 31%
1	EX	124	 3% 60% 34% 6%
1	EY	124	 6% 64% 36%
1	EZ	124	 3% 71% 29%

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

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Mol	Chain	Length	Quality of chain
1	FZ	124	
1	GA	124	
1	GB	124	
1	GC	124	
1	GD	124	
1	GE	124	
1	GF	124	
1	GG	124	
1	GH	124	
1	GI	124	
1	GJ	124	
1	GK	124	
1	GL	124	
1	GM	124	
1	GN	124	
1	GO	124	
1	GP	124	
1	GQ	124	
1	GR	124	
1	GS	124	
1	GT	124	
1	GU	124	
1	GV	124	
1	GW	124	
1	GX	124	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 169260 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AB	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AC	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AD	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AE	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AF	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AG	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AH	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AI	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AJ	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AK	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AL	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AM	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AN	117	Total	C	N	O	S	0	0	0
			910	569	157	180	4			
1	AO	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			
1	AP	124	Total	C	N	O	S	0	0	0
			955	594	165	192	4			

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

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

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

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

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

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

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

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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

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

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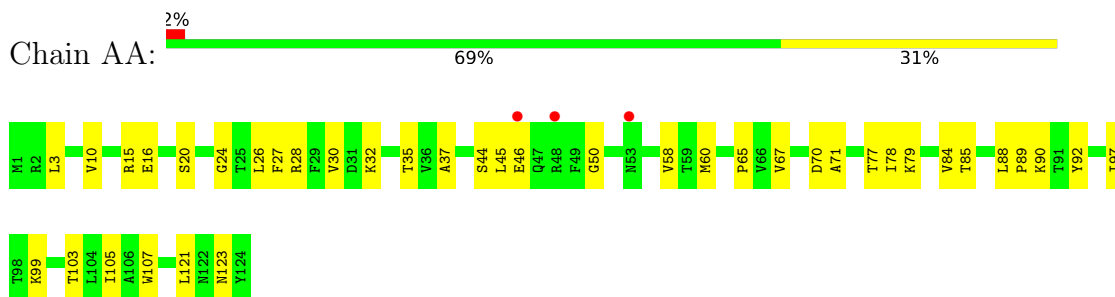
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	FC	1	Total 1	Ca 1	0	0
2	FF	1	Total 1	Ca 1	0	0
2	FI	1	Total 1	Ca 1	0	0
2	FL	1	Total 1	Ca 1	0	0
2	FO	1	Total 1	Ca 1	0	0
2	FR	1	Total 1	Ca 1	0	0
2	FU	1	Total 1	Ca 1	0	0
2	FX	1	Total 1	Ca 1	0	0
2	GA	1	Total 1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

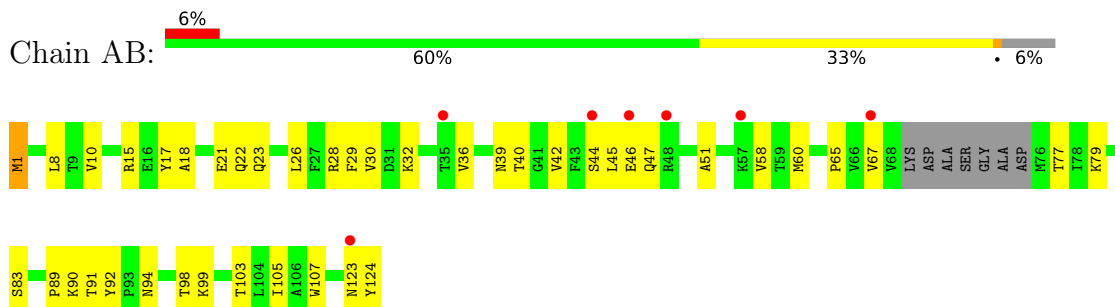
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

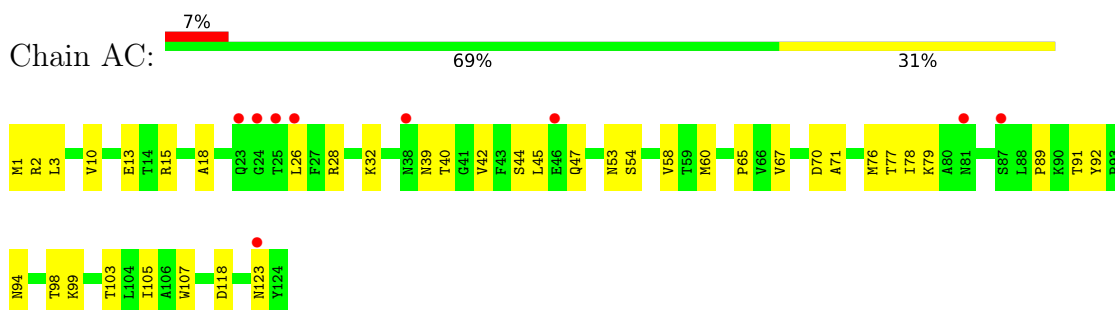
- Molecule 1: coat protein



- Molecule 1: coat protein

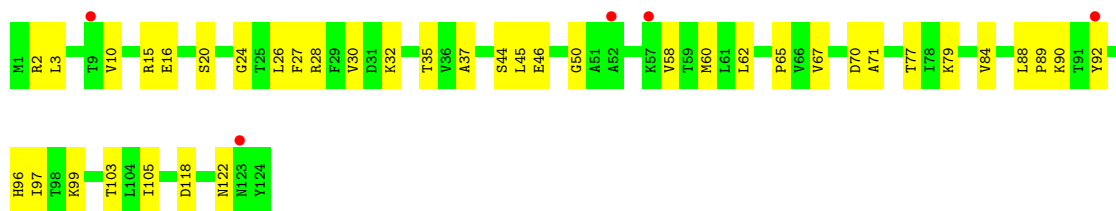


- Molecule 1: coat protein

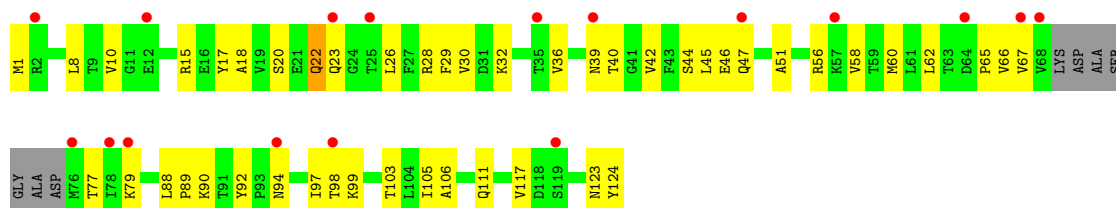


- Molecule 1: coat protein

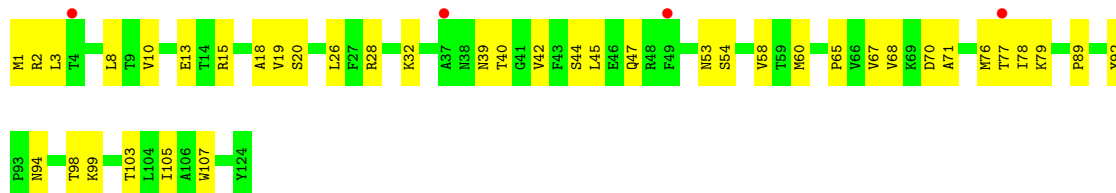




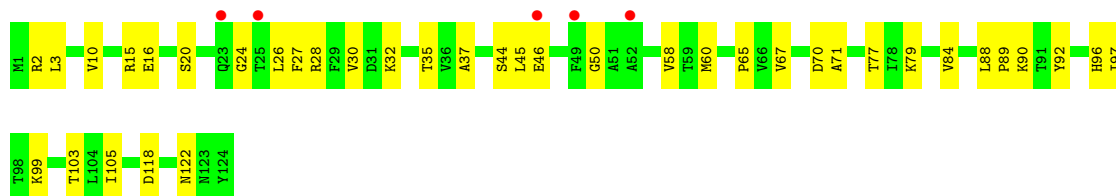
• Molecule 1: coat protein



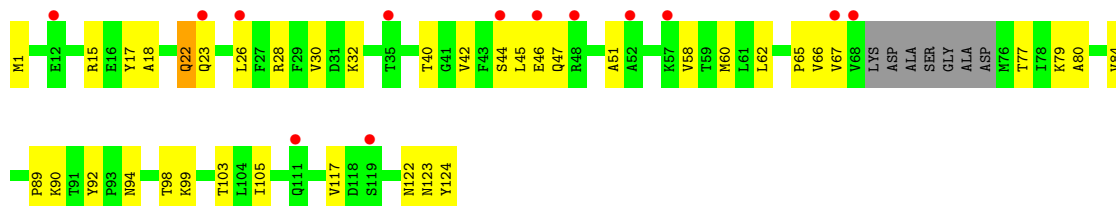
• Molecule 1: coat protein



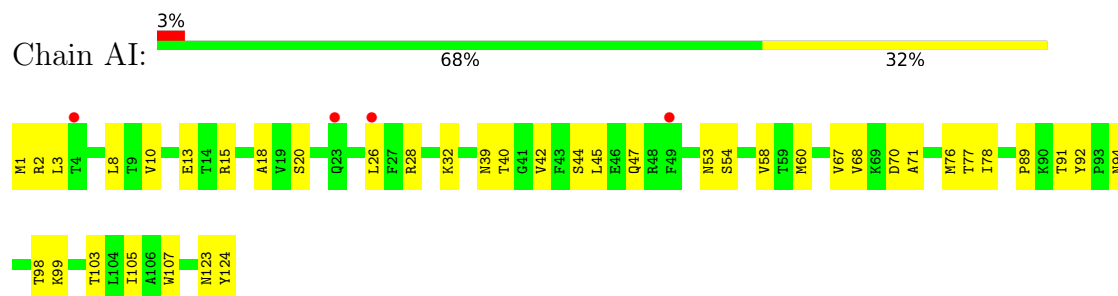
• Molecule 1: coat protein



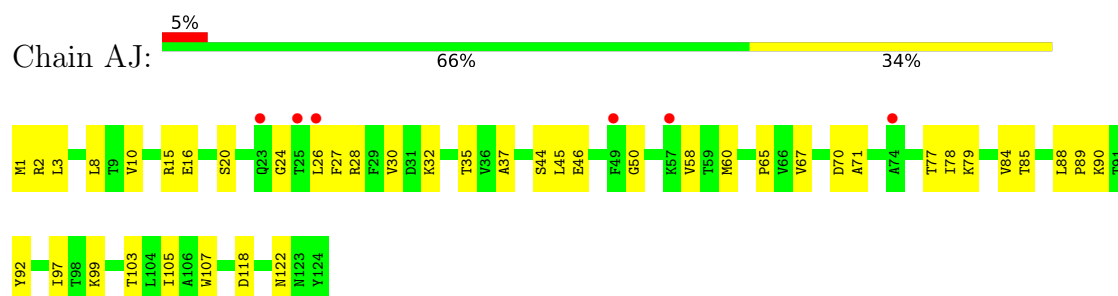
• Molecule 1: coat protein



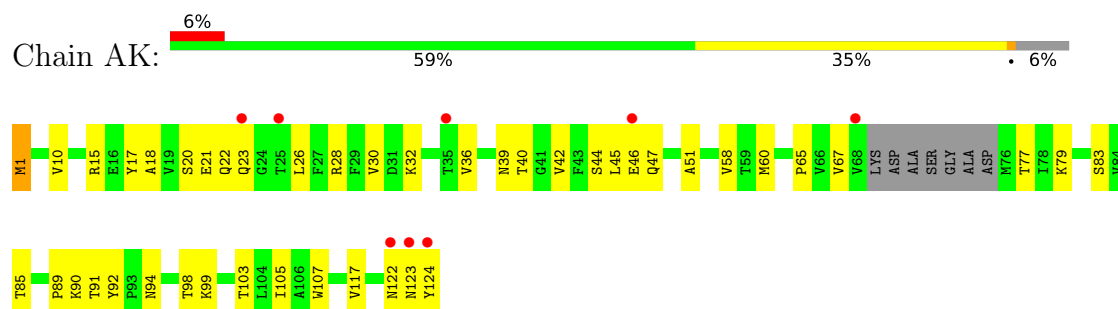
- Molecule 1: coat protein



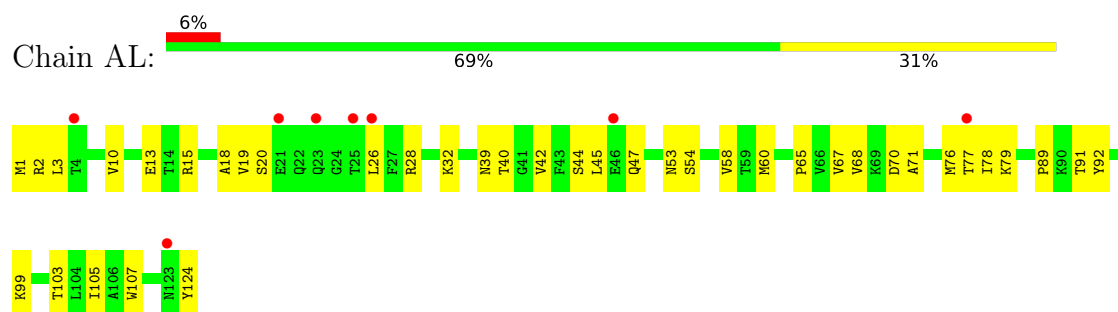
- Molecule 1: coat protein



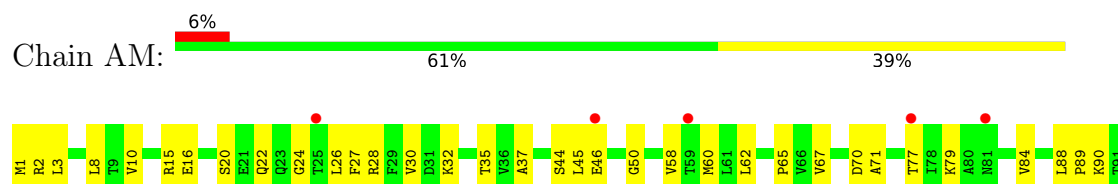
- Molecule 1: coat protein

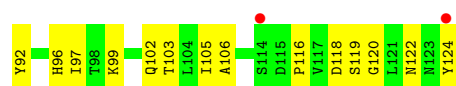


- Molecule 1: coat protein

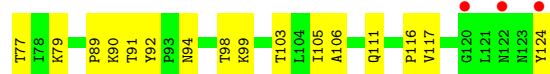


- Molecule 1: coat protein





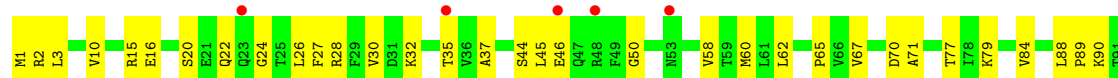
- Molecule 1: coat protein



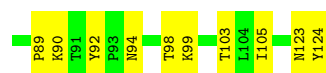
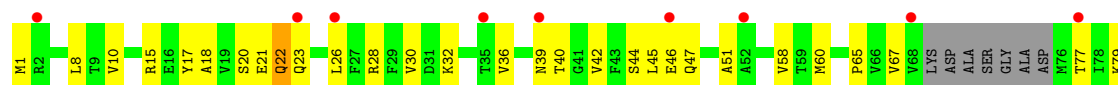
- Molecule 1: coat protein



- Molecule 1: coat protein

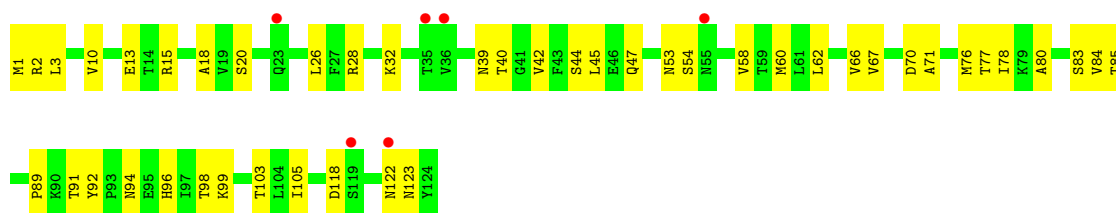


- Molecule 1: coat protein

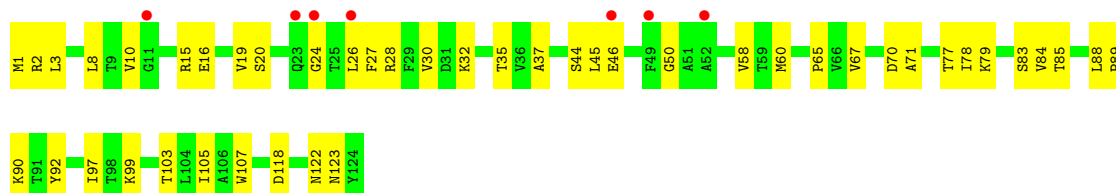


- Molecule 1: coat protein

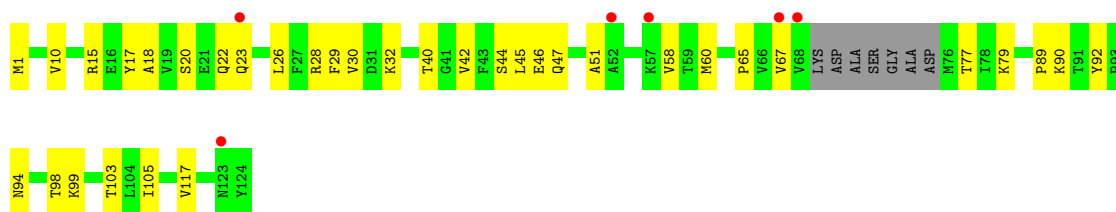




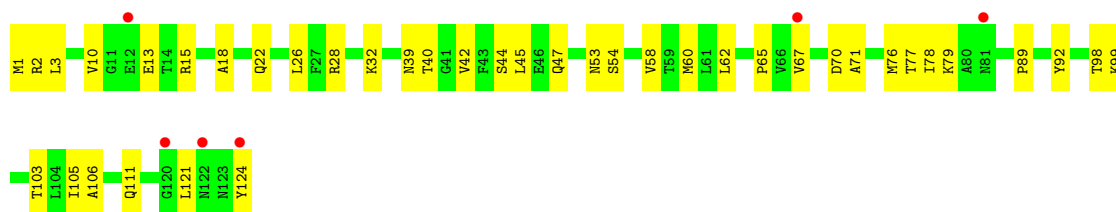
• Molecule 1: coat protein



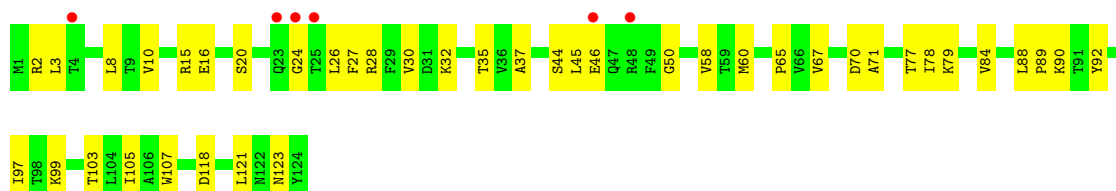
• Molecule 1: coat protein



• Molecule 1: coat protein

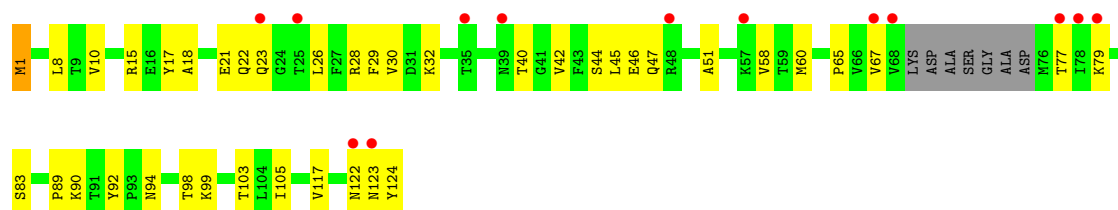


• Molecule 1: coat protein



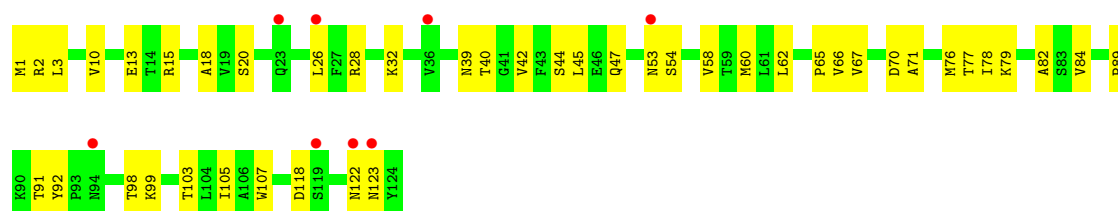
- Molecule 1: coat protein

Chain AW: 



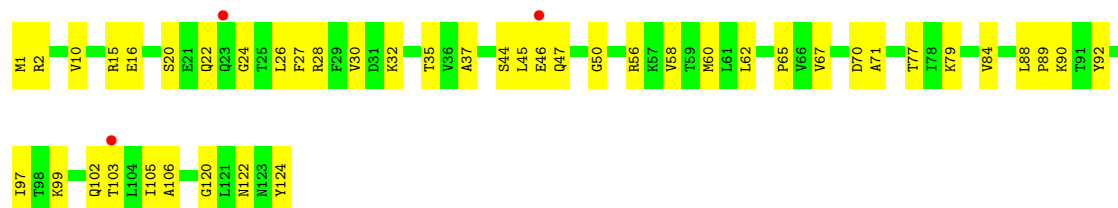
- Molecule 1: coat protein

Chain AX: 



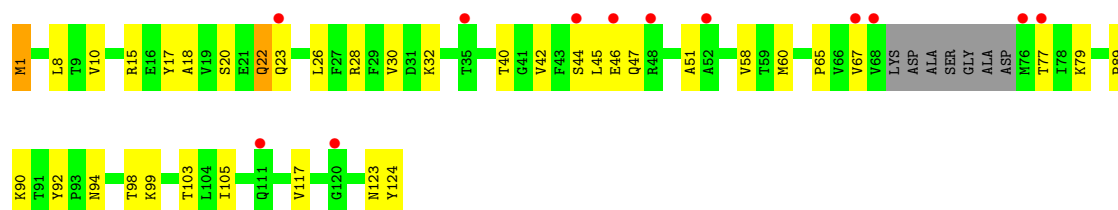
- Molecule 1: coat protein

Chain AY: 



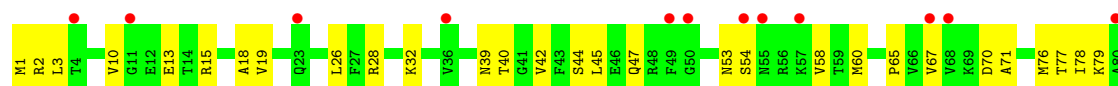
- Molecule 1: coat protein

Chain AZ: 



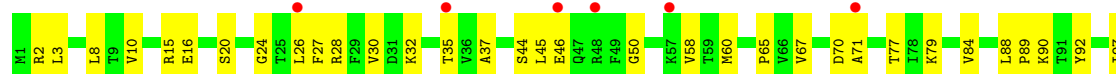
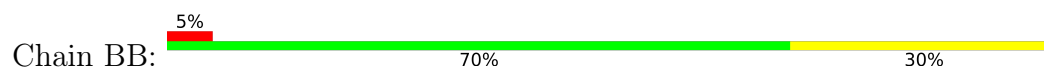
- Molecule 1: coat protein

Chain BA: 

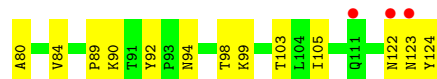
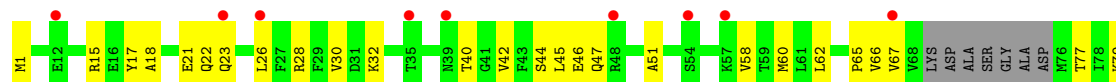




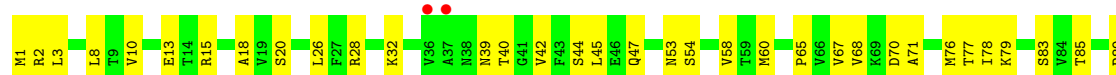
• Molecule 1: coat protein



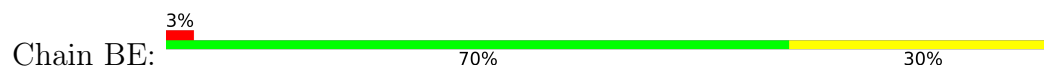
• Molecule 1: coat protein



• Molecule 1: coat protein



• Molecule 1: coat protein

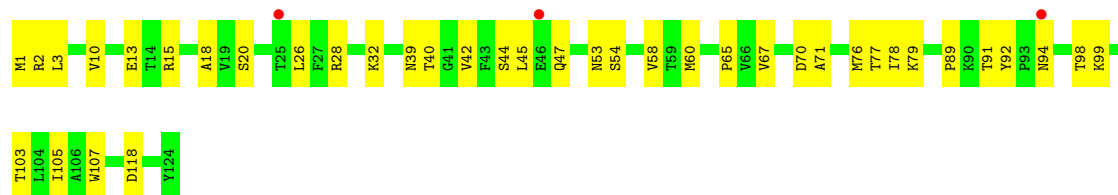


• Molecule 1: coat protein

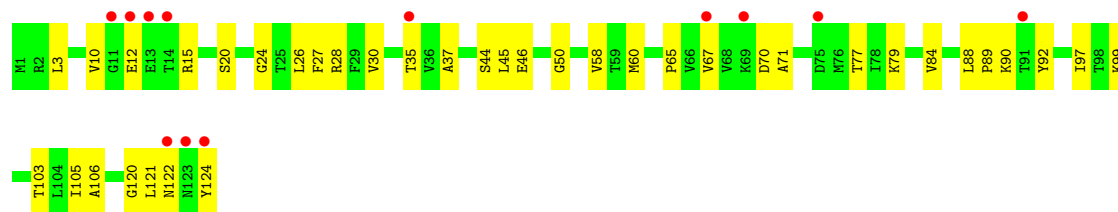




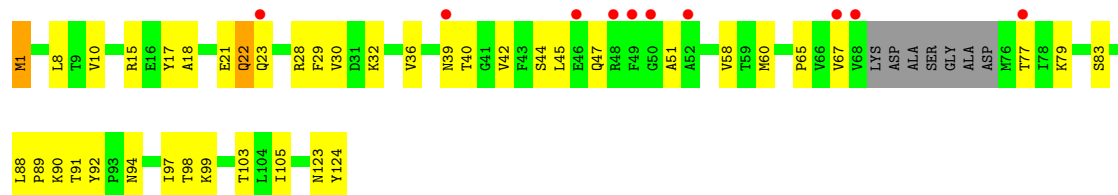
- Molecule 1: coat protein



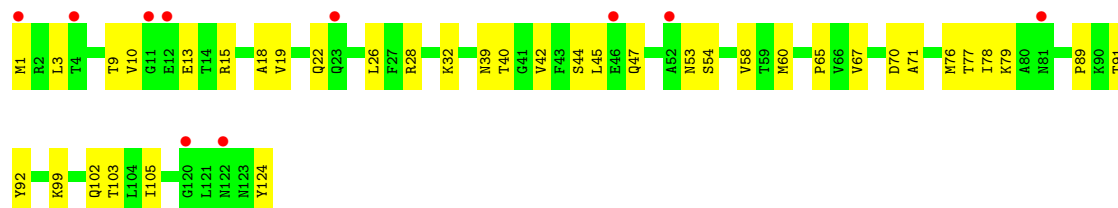
- Molecule 1: coat protein



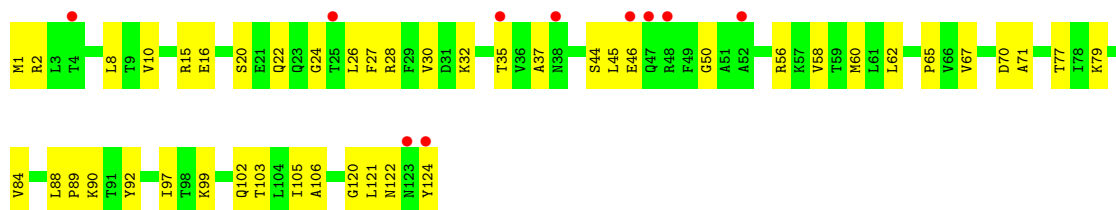
- Molecule 1: coat protein



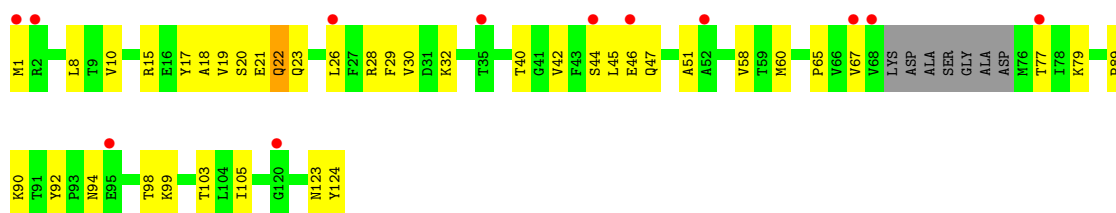
- Molecule 1: coat protein



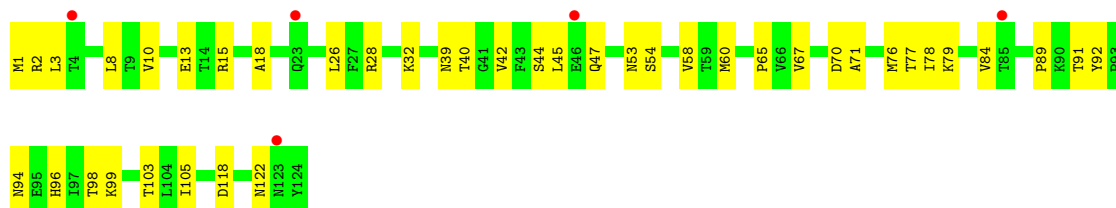
- Molecule 1: coat protein



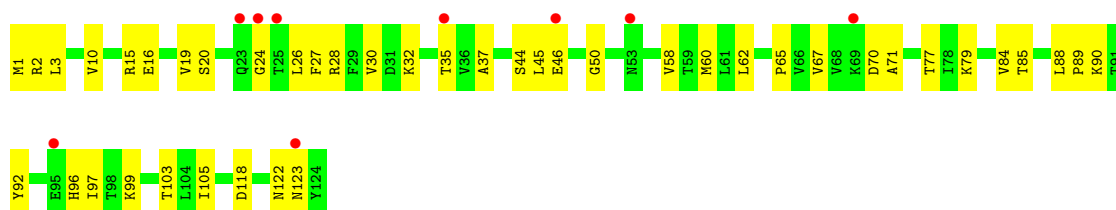
- Molecule 1: coat protein



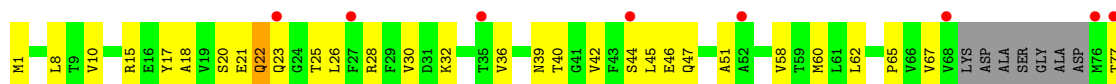
- Molecule 1: coat protein



- Molecule 1: coat protein

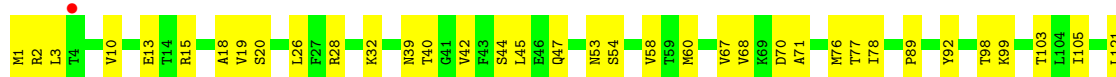
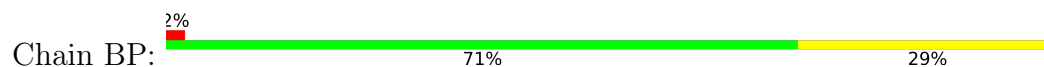


- Molecule 1: coat protein

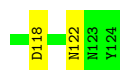
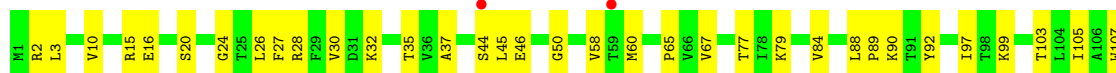
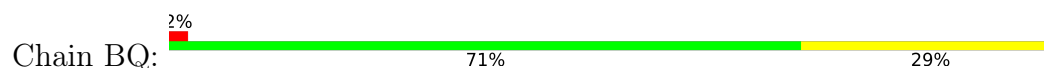




- Molecule 1: coat protein



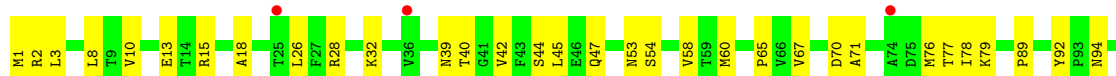
- Molecule 1: coat protein



- Molecule 1: coat protein

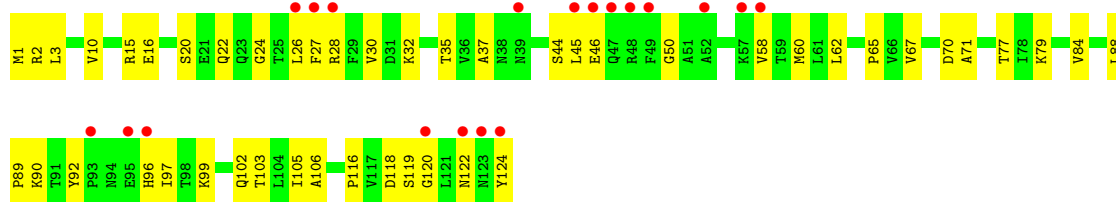


- Molecule 1: coat protein

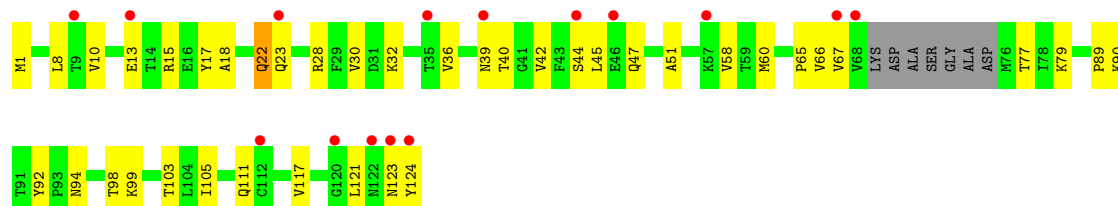


- Molecule 1: coat protein

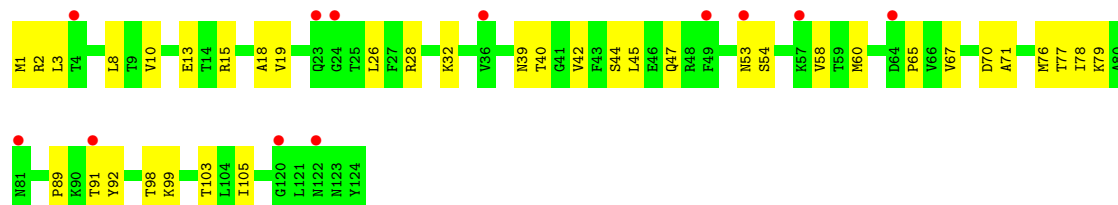




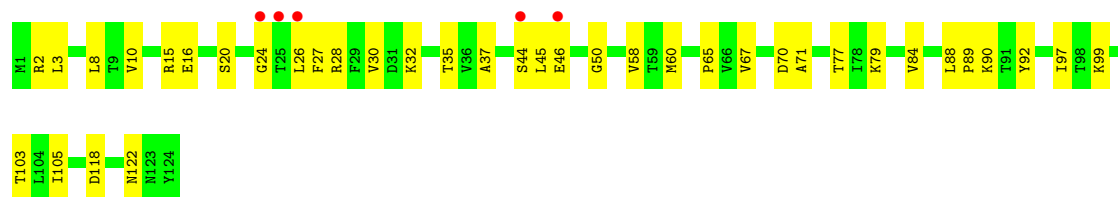
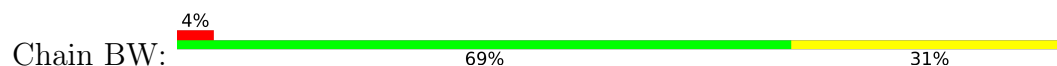
• Molecule 1: coat protein



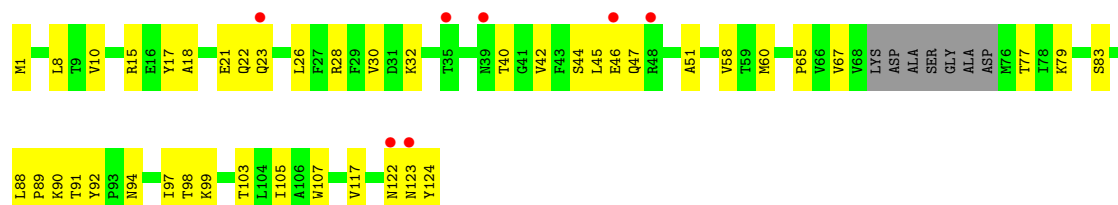
• Molecule 1: coat protein



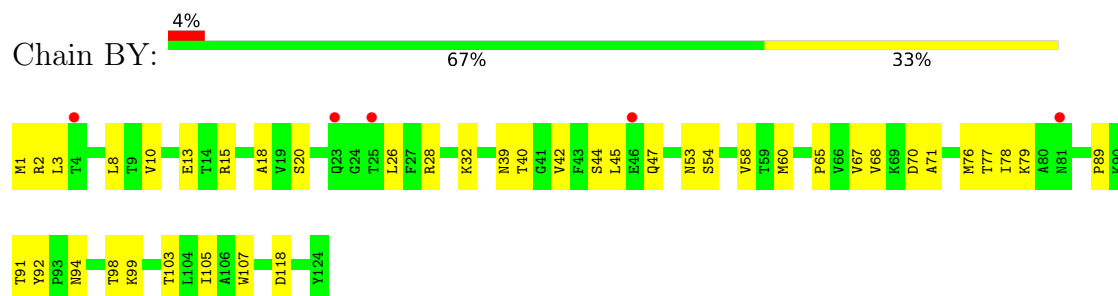
• Molecule 1: coat protein



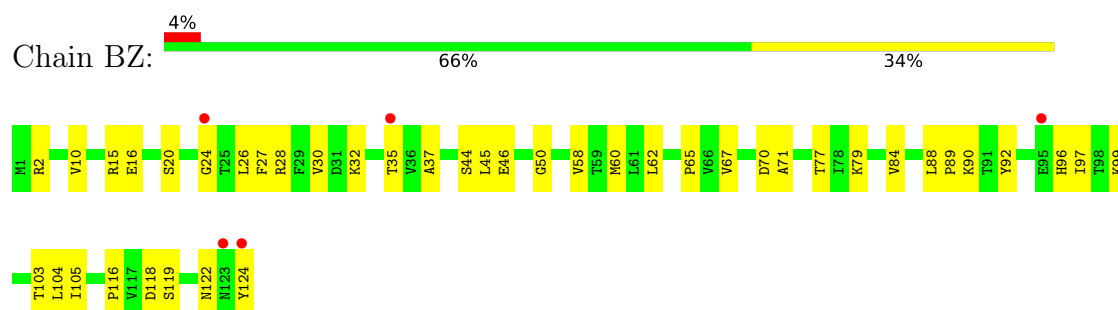
• Molecule 1: coat protein



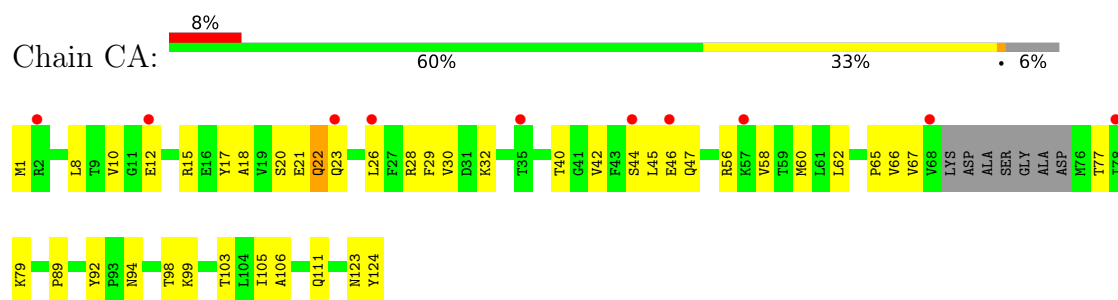
- Molecule 1: coat protein



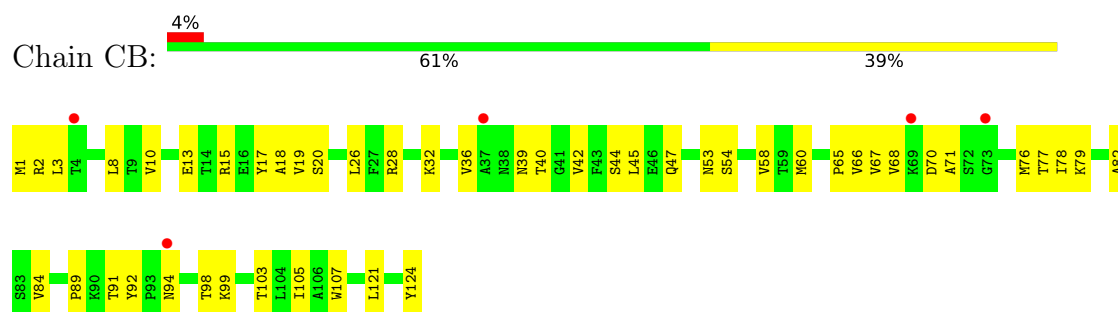
- Molecule 1: coat protein



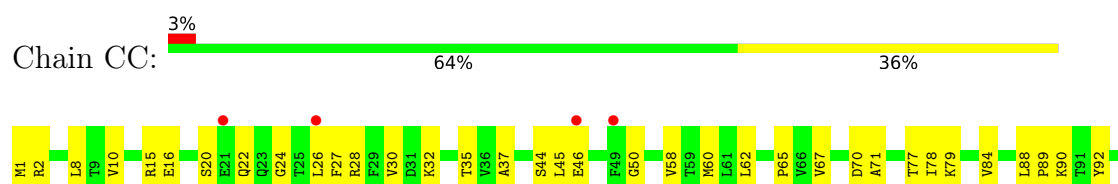
- Molecule 1: coat protein



- Molecule 1: coat protein

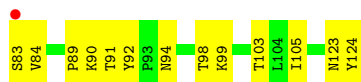


- Molecule 1: coat protein

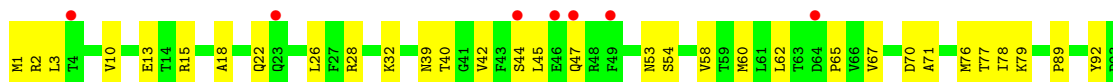




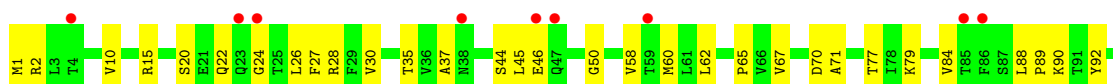
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

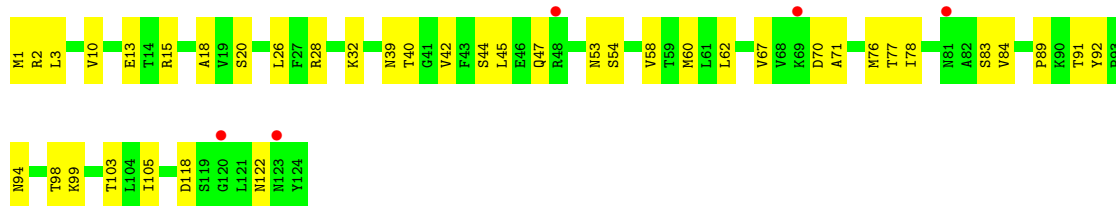


- Molecule 1: coat protein

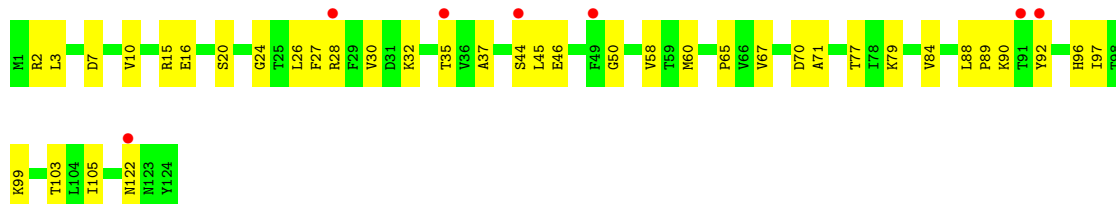


- Molecule 1: coat protein

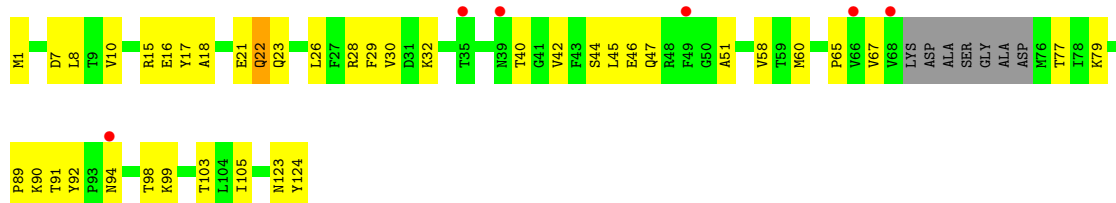




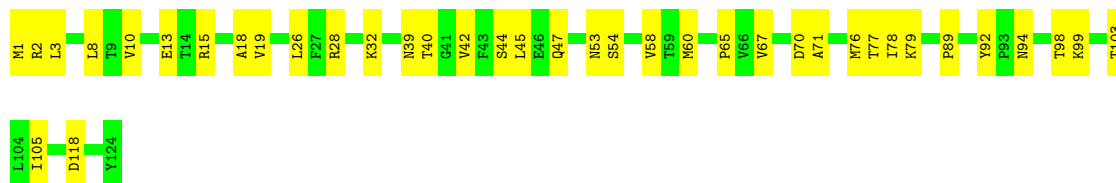
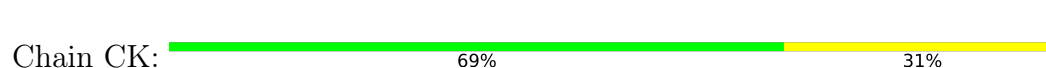
- Molecule 1: coat protein



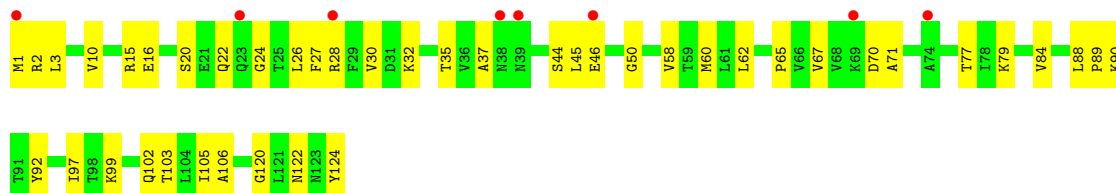
- Molecule 1: coat protein



- Molecule 1: coat protein

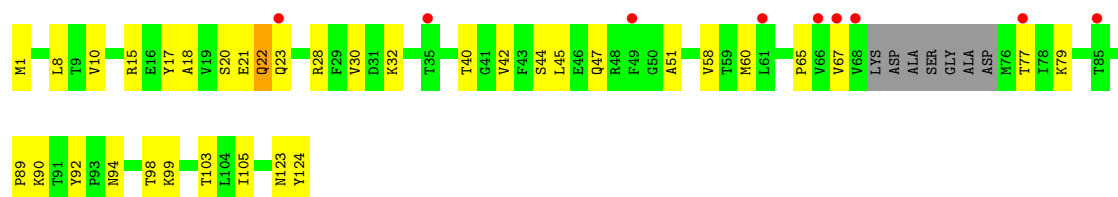


- Molecule 1: coat protein



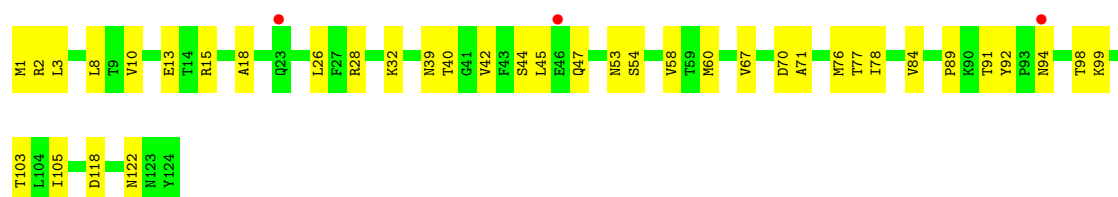
- Molecule 1: coat protein

Chain CM: 



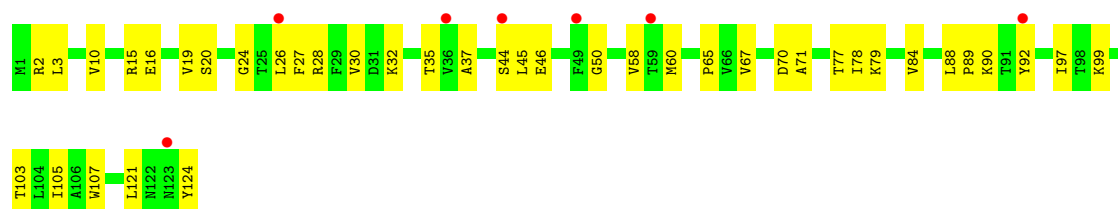
- Molecule 1: coat protein

Chain CN: 



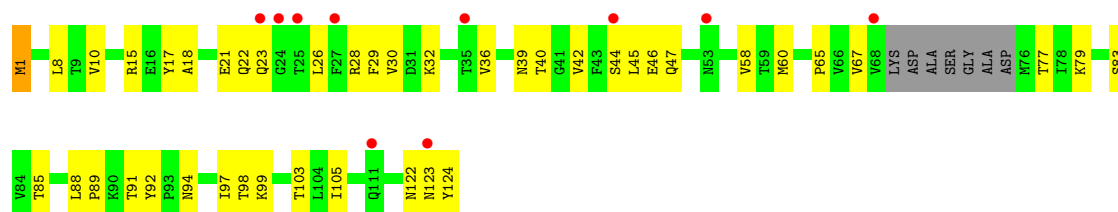
- Molecule 1: coat protein

Chain CO: 



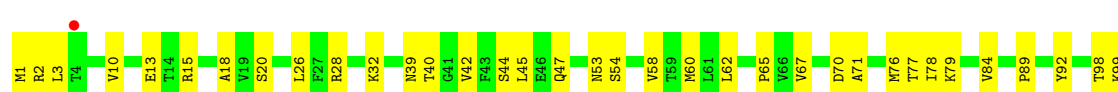
- Molecule 1: coat protein

Chain CP: 



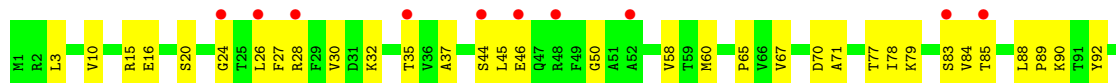
- Molecule 1: coat protein

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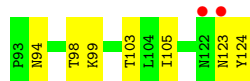
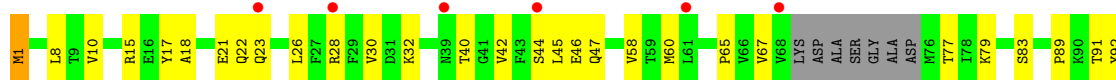




- Molecule 1: coat protein



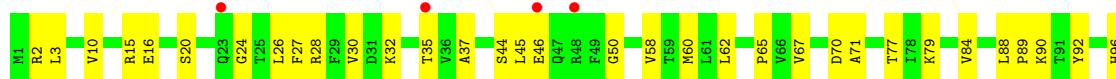
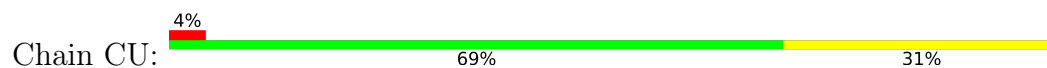
- Molecule 1: coat protein



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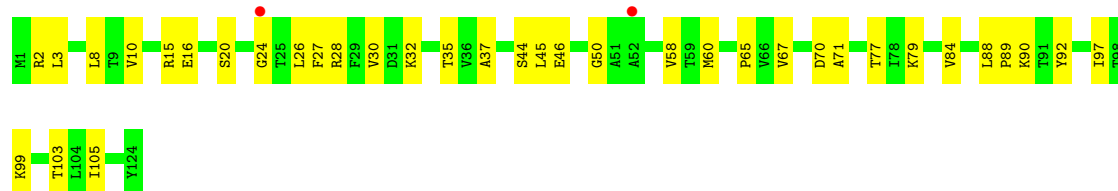
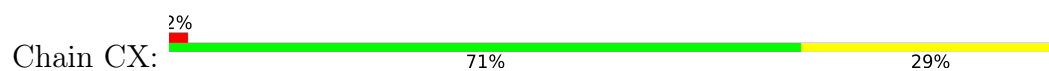




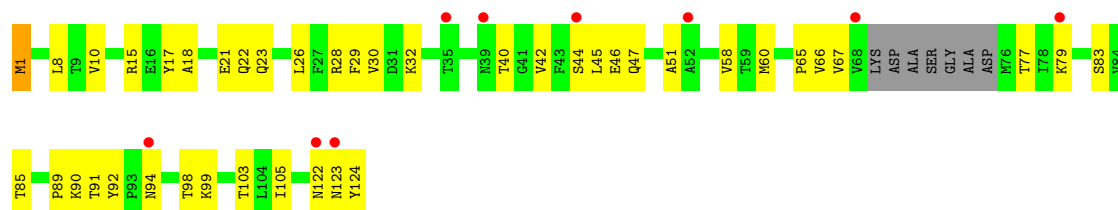
● Molecule 1: coat protein



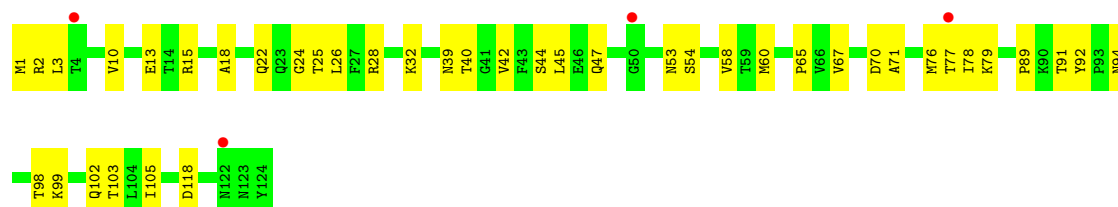
● Molecule 1: coat protein



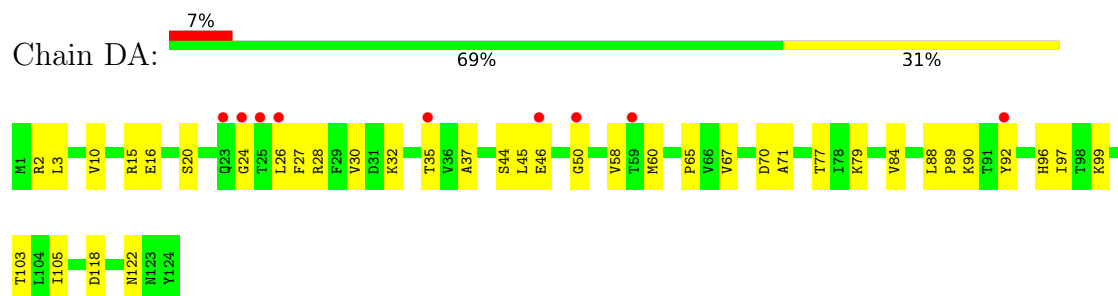
● Molecule 1: coat protein



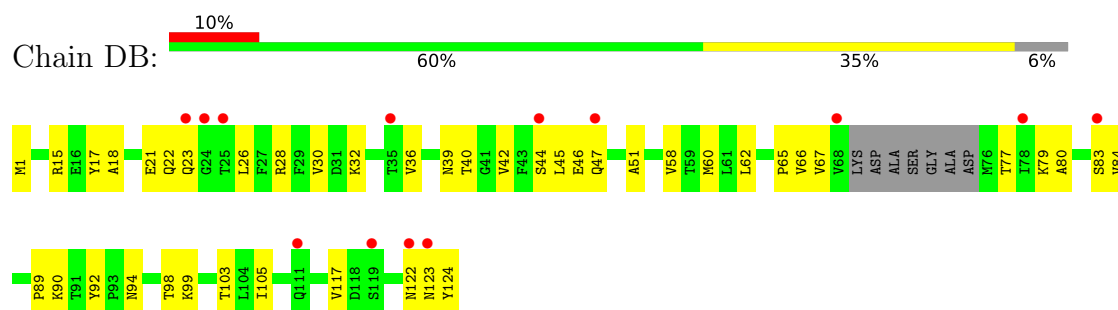
● Molecule 1: coat protein



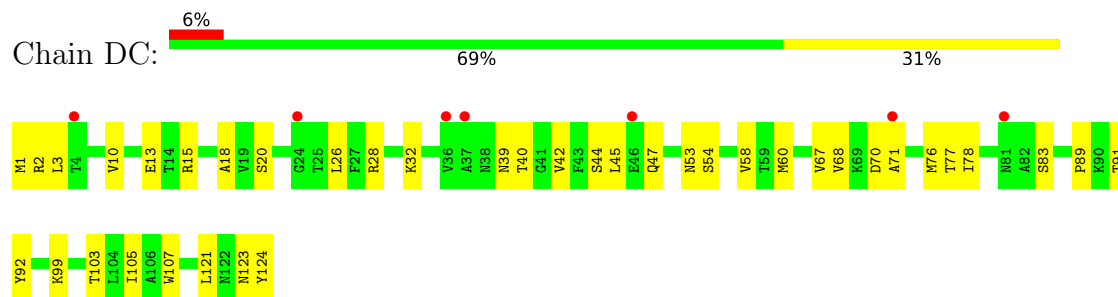
- Molecule 1: coat protein



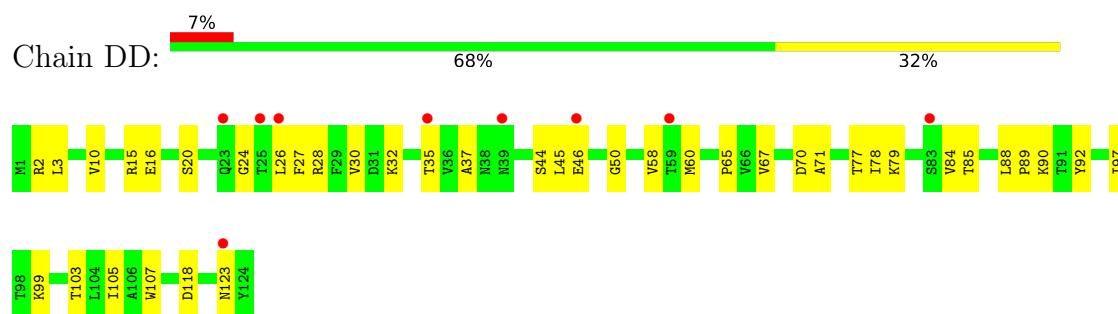
- Molecule 1: coat protein



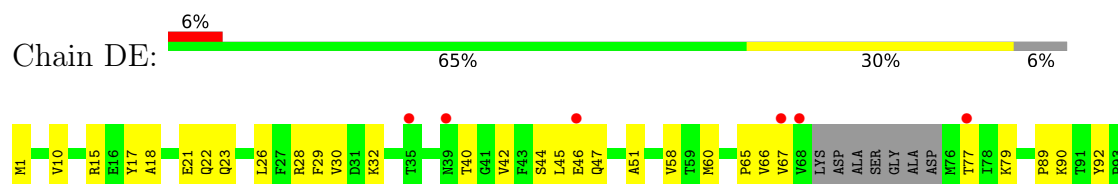
- Molecule 1: coat protein



- Molecule 1: coat protein

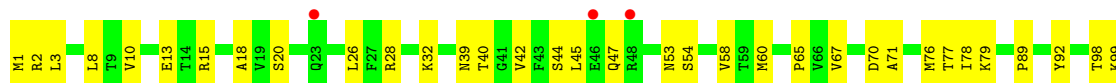


- Molecule 1: coat protein

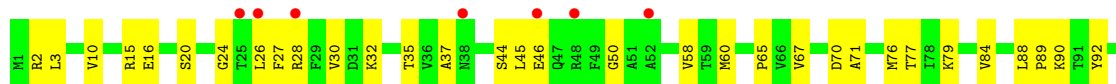
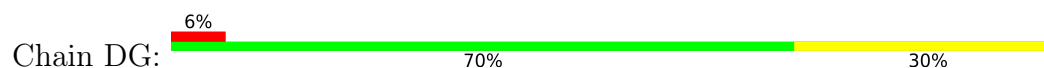




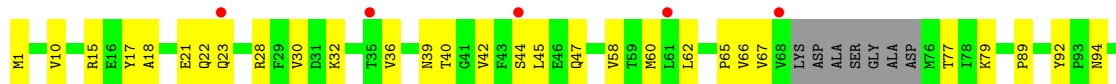
- Molecule 1: coat protein



- Molecule 1: coat protein



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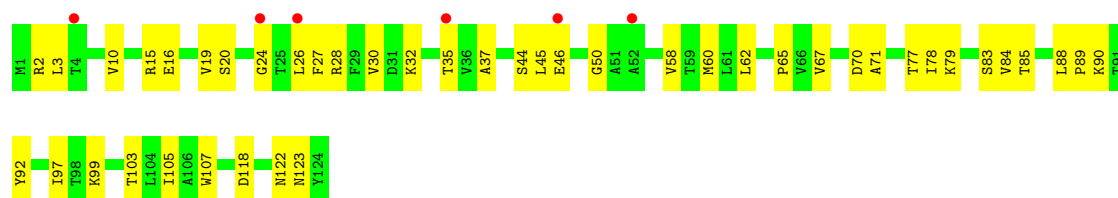


- Molecule 1: coat protein

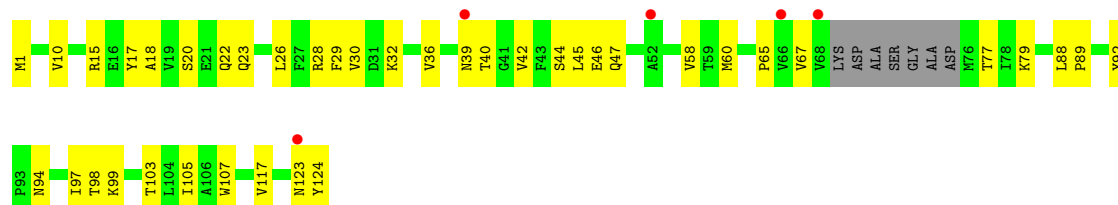


- Molecule 1: coat protein

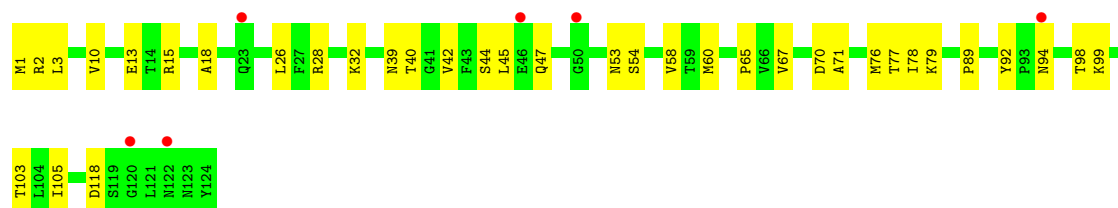
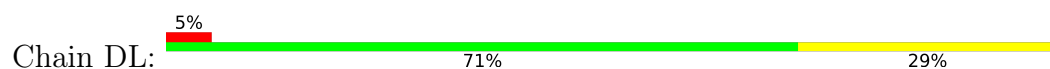




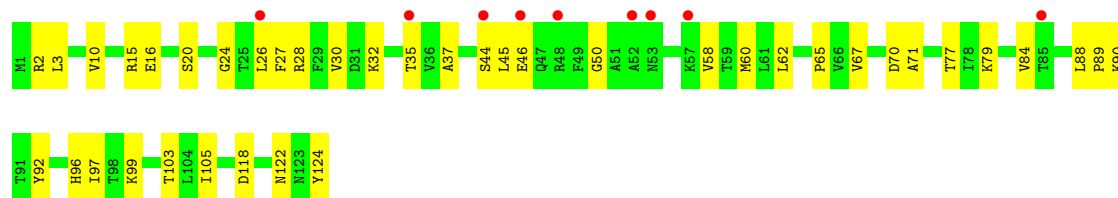
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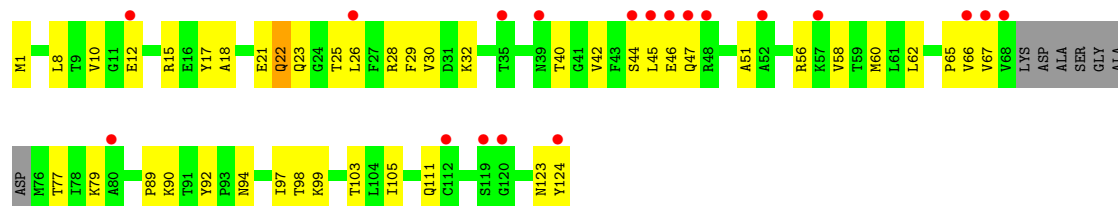
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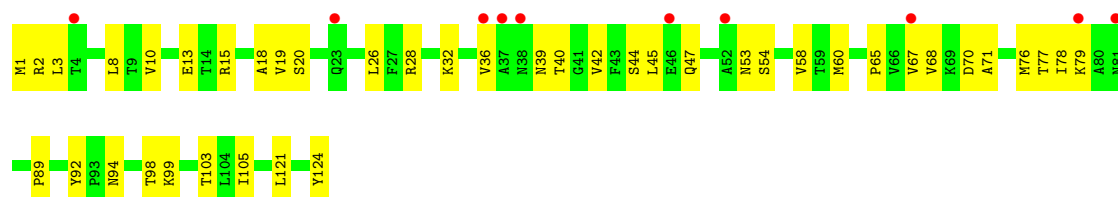
- Molecule 1: coat protein



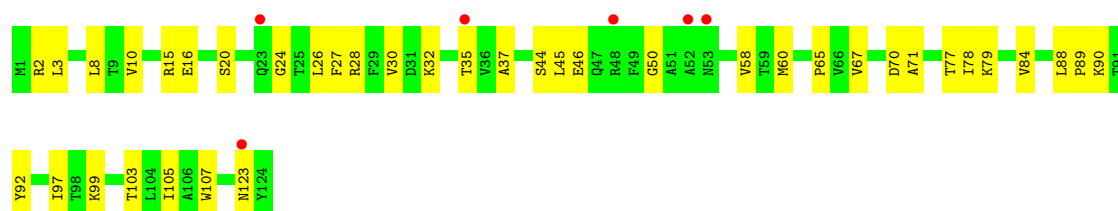
- Molecule 1: coat protein



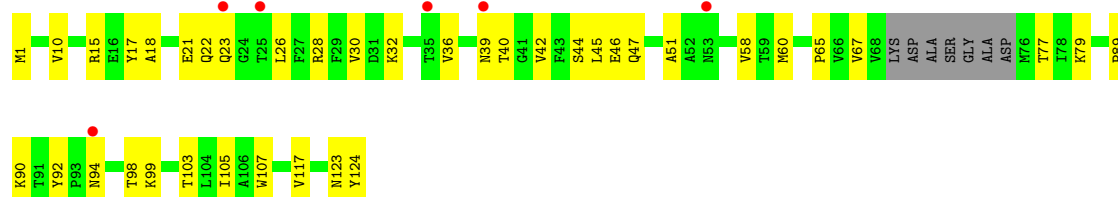
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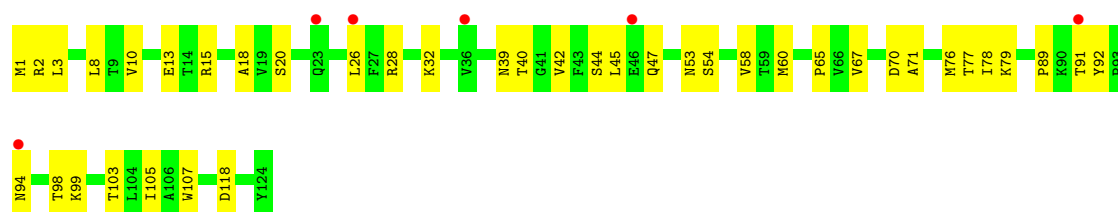
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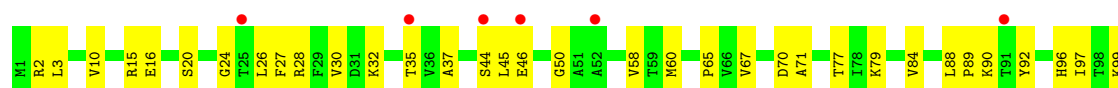
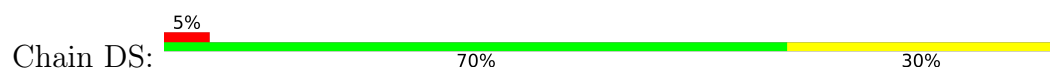
• Molecule 1: coat protein



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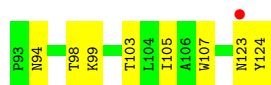




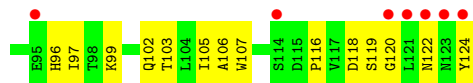
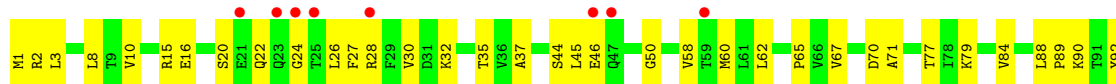
- Molecule 1: coat protein



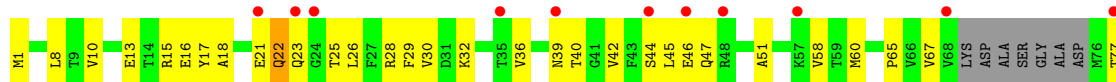
- Molecule 1: coat protein



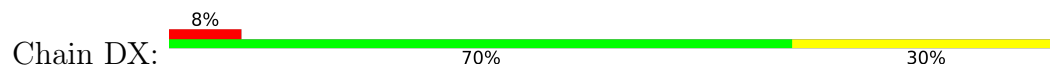
- Molecule 1: coat protein

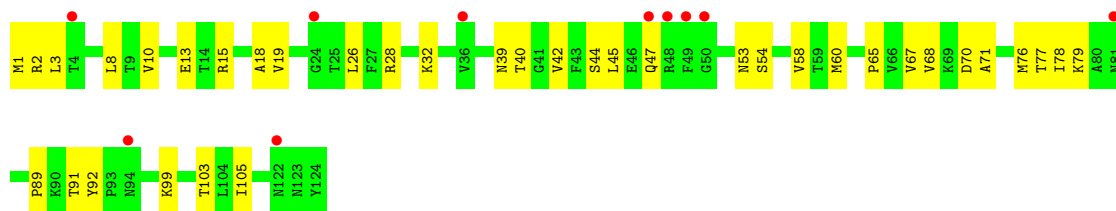


- Molecule 1: coat protein

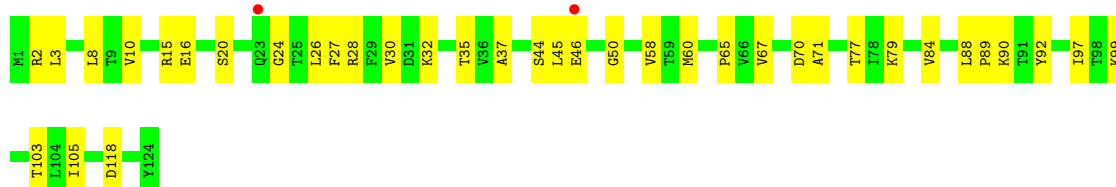
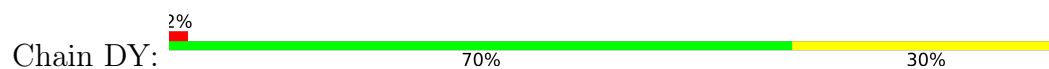


- Molecule 1: coat protein

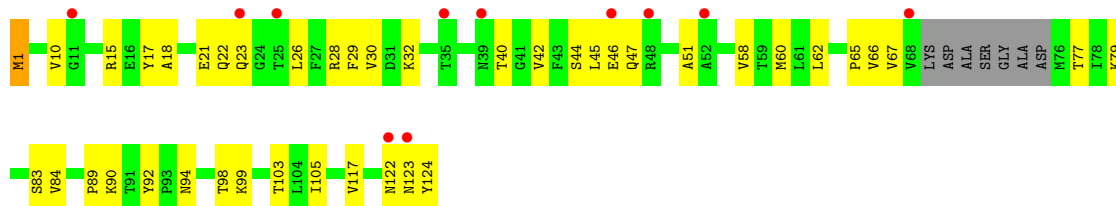




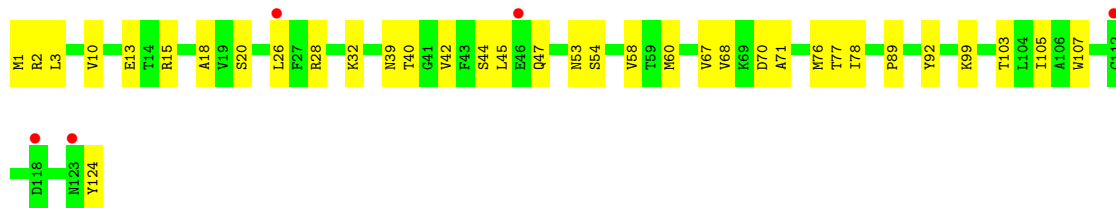
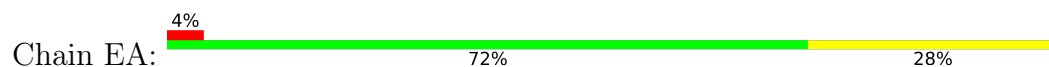
• Molecule 1: coat protein



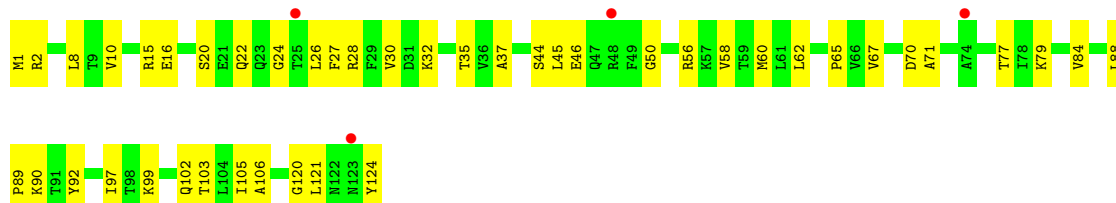
• Molecule 1: coat protein



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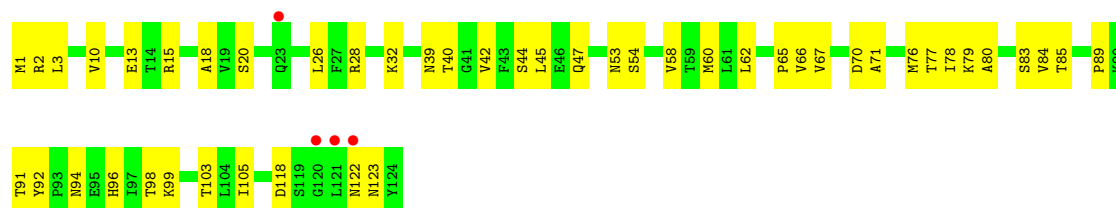
• Molecule 1: coat protein

Chain EC: 



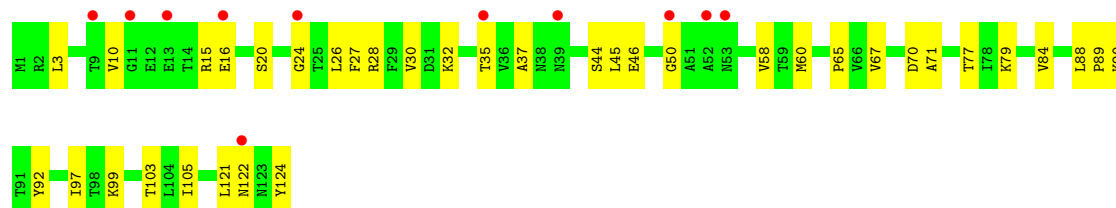
• Molecule 1: coat protein

Chain ED: 



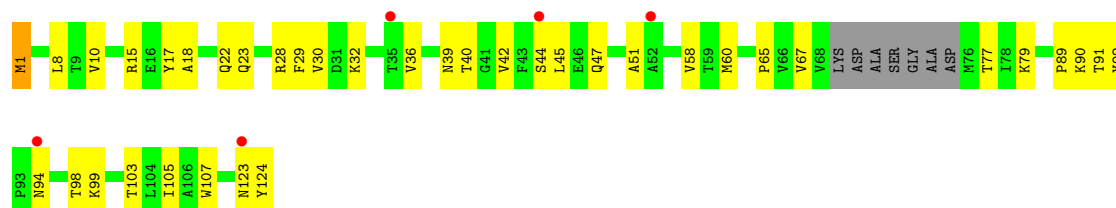
• Molecule 1: coat protein

Chain EE: 



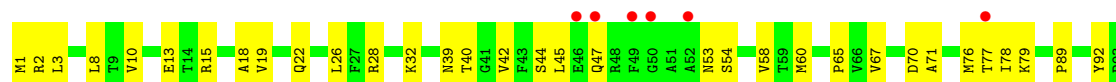
• Molecule 1: coat protein

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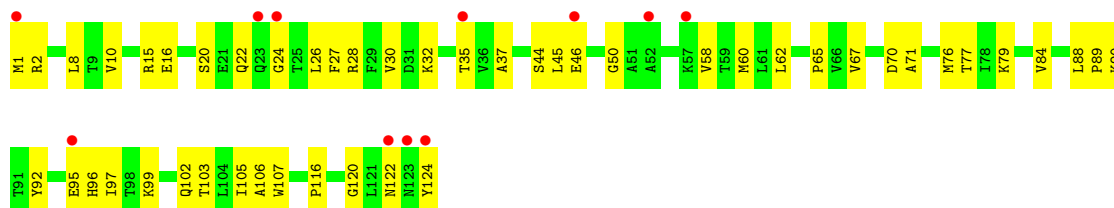
• Molecule 1: coat protein

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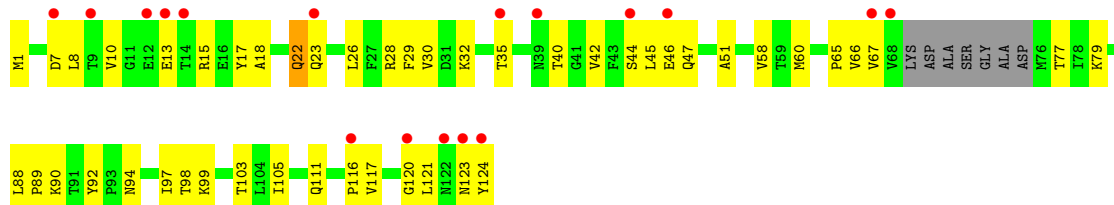




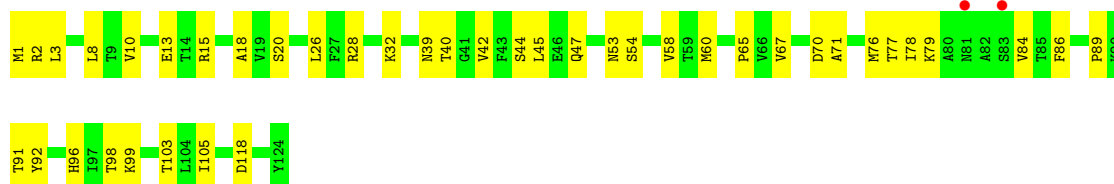
- Molecule 1: coat protein



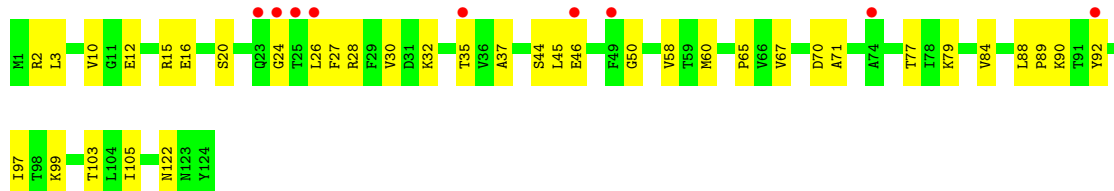
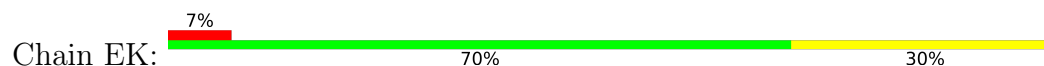
- Molecule 1: coat protein



- Molecule 1: coat protein

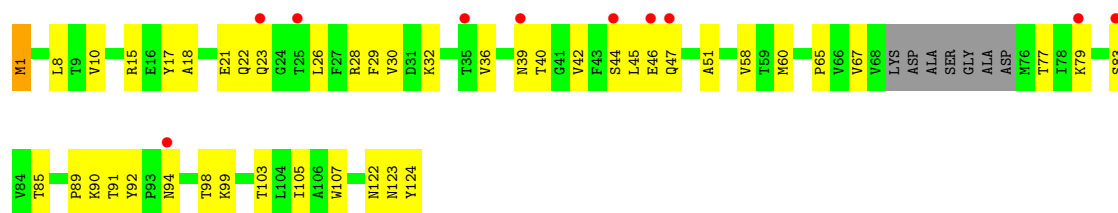


- Molecule 1: coat protein

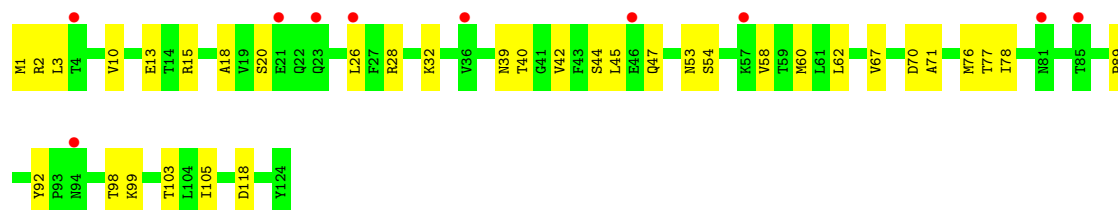
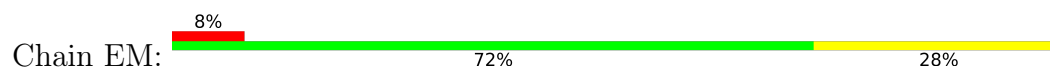


- Molecule 1: coat protein

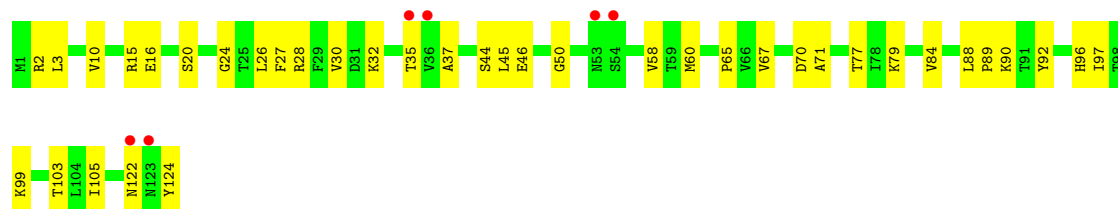




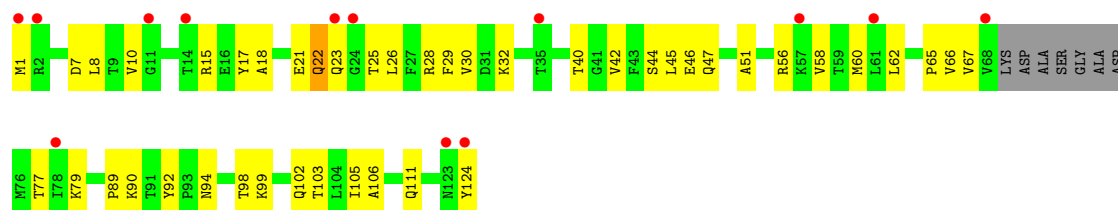
• Molecule 1: coat protein



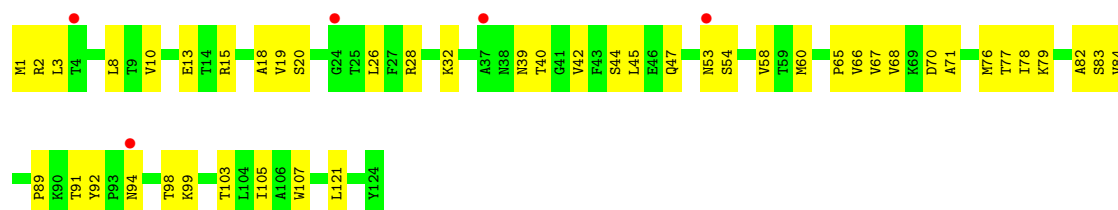
• Molecule 1: coat protein



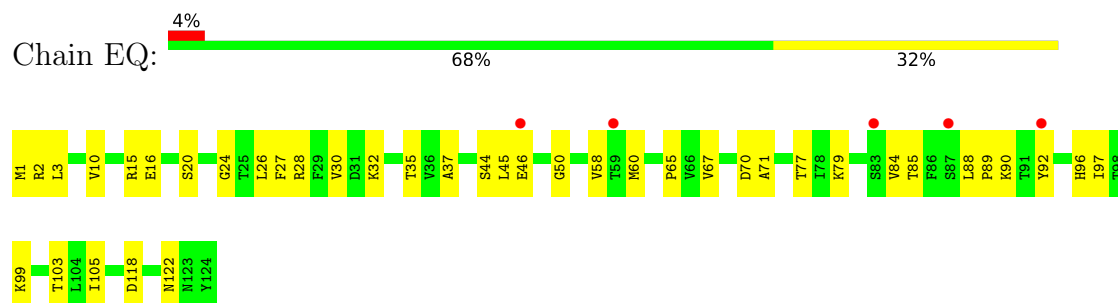
• Molecule 1: coat protein



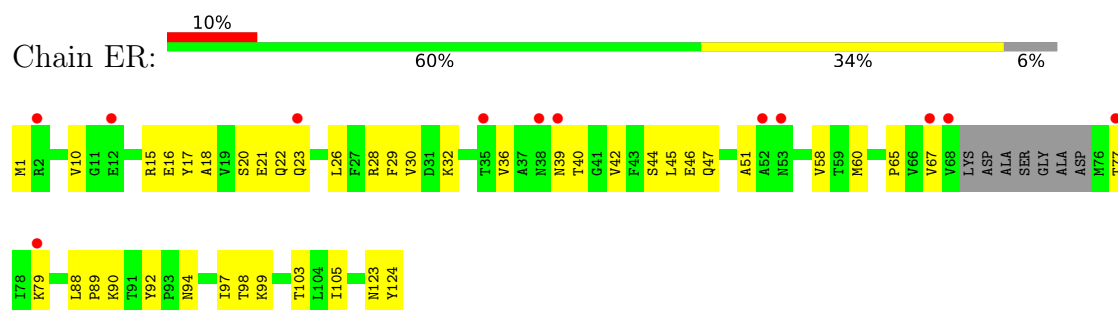
• Molecule 1: coat protein



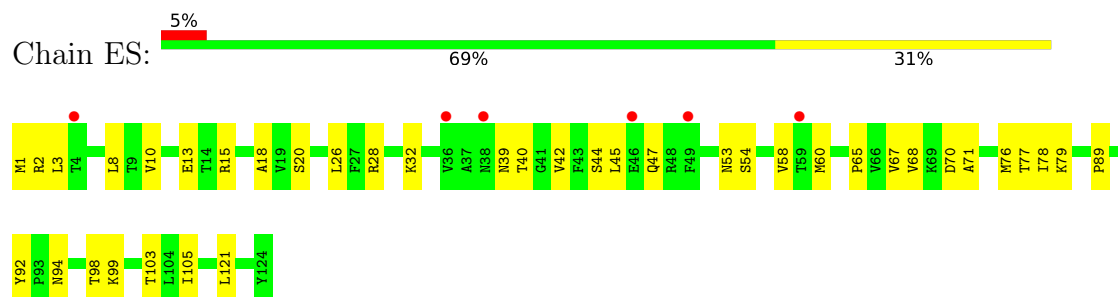
- Molecule 1: coat protein



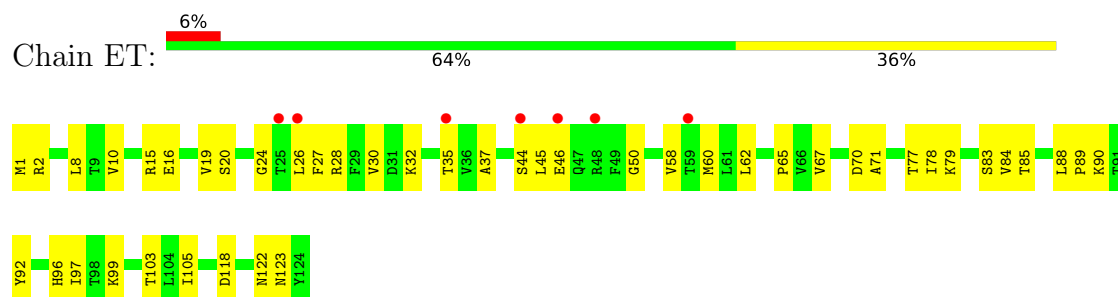
- Molecule 1: coat protein



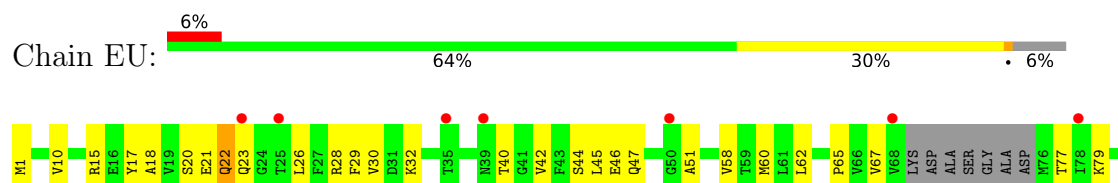
- Molecule 1: coat protein

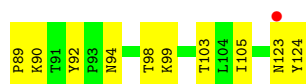


- Molecule 1: coat protein

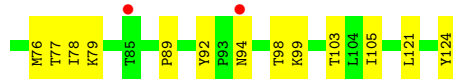
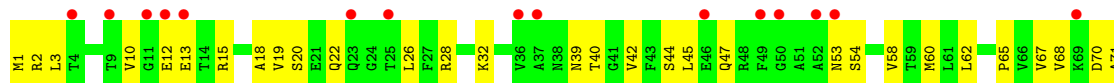


- Molecule 1: coat protein

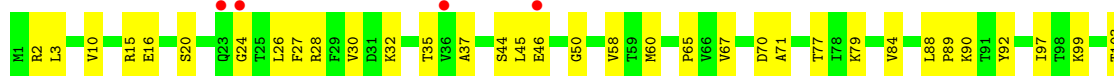
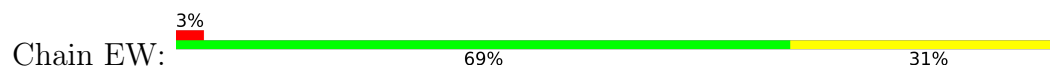




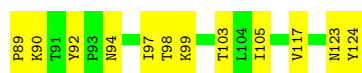
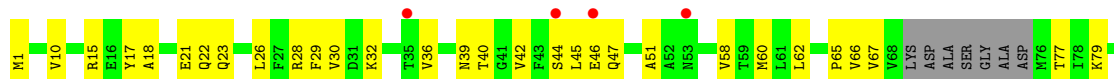
- Molecule 1: coat protein



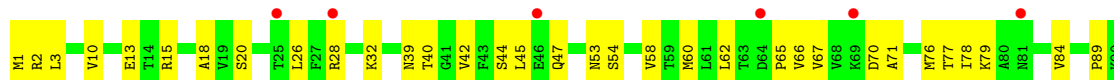
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

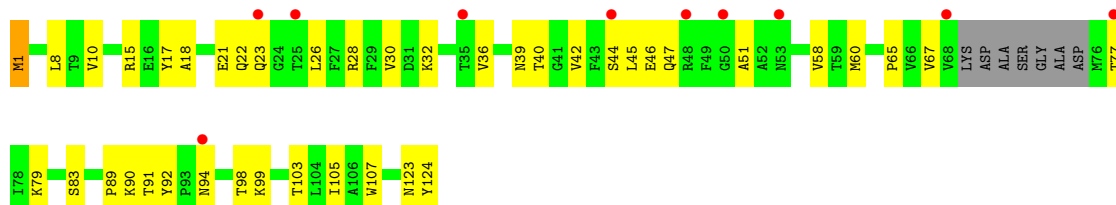


- Molecule 1: coat protein

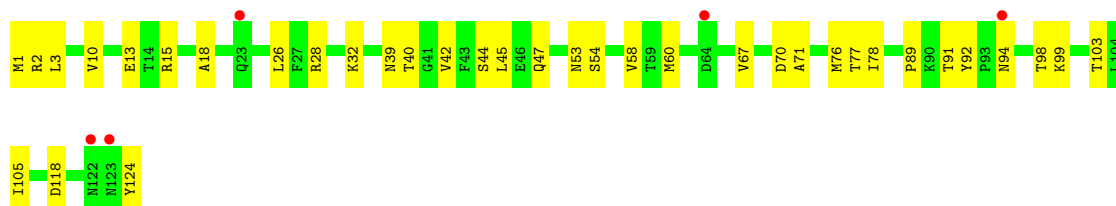
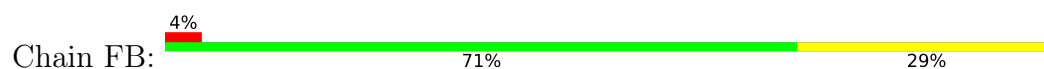




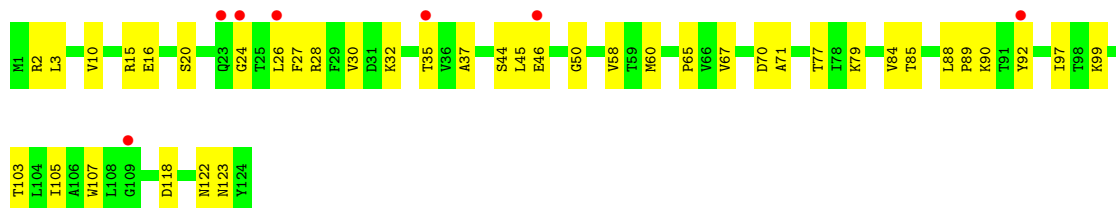
- Molecule 1: coat protein



- Molecule 1: coat protein



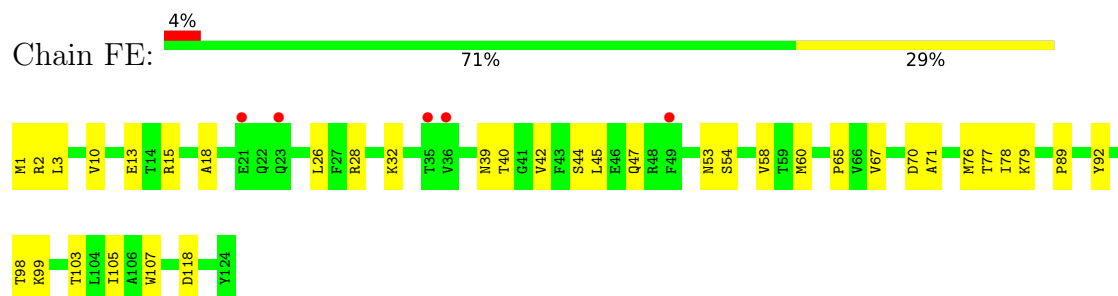
- Molecule 1: coat protein



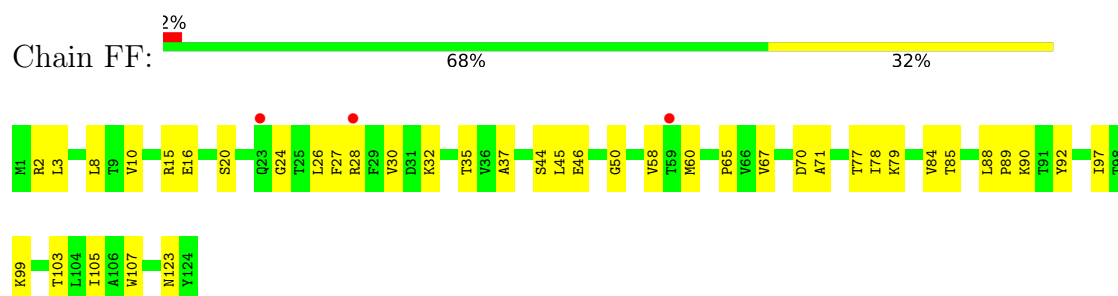
- Molecule 1: coat protein



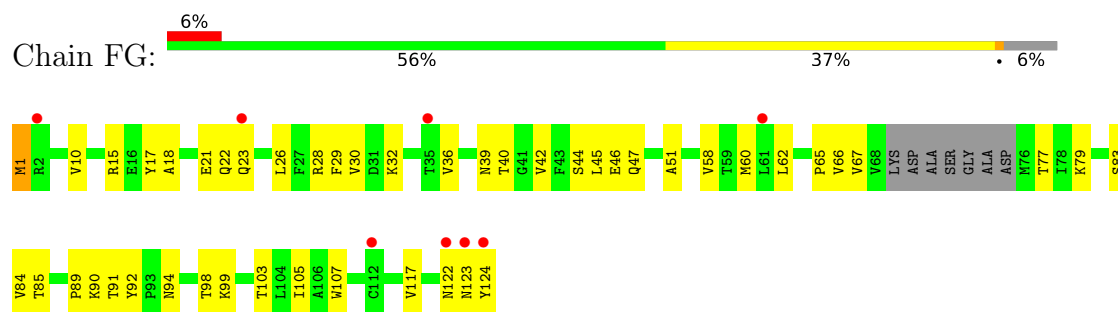
- Molecule 1: coat protein



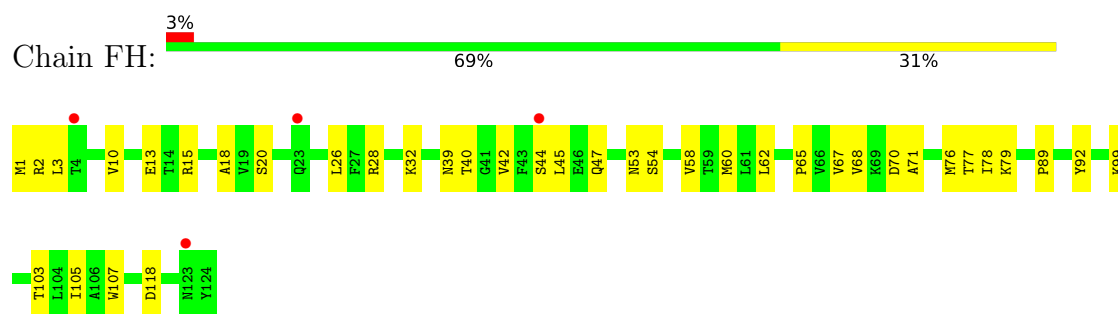
- Molecule 1: coat protein



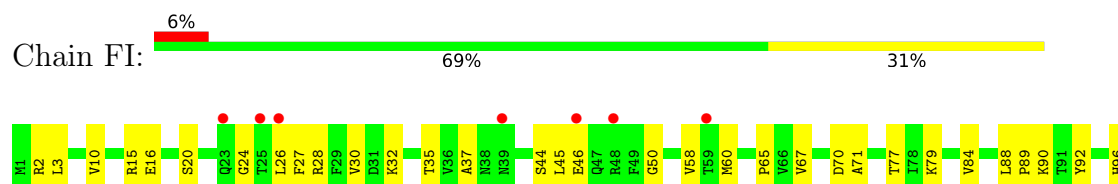
- Molecule 1: coat protein



- Molecule 1: coat protein

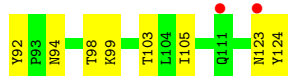
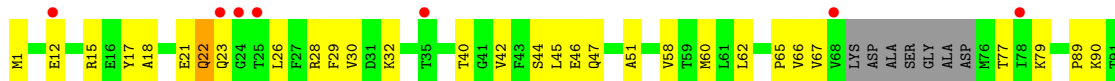


- Molecule 1: coat protein





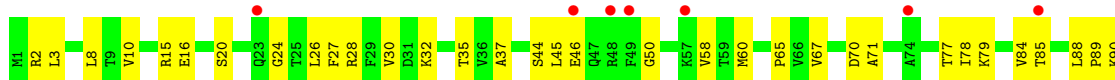
- Molecule 1: coat protein



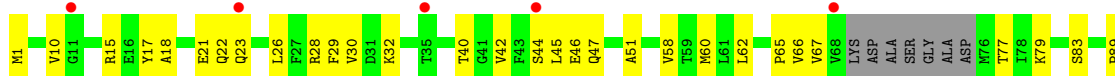
- Molecule 1: coat protein



- Molecule 1: coat protein

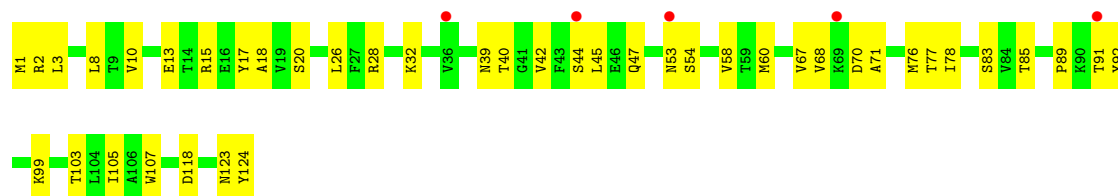


- Molecule 1: coat protein

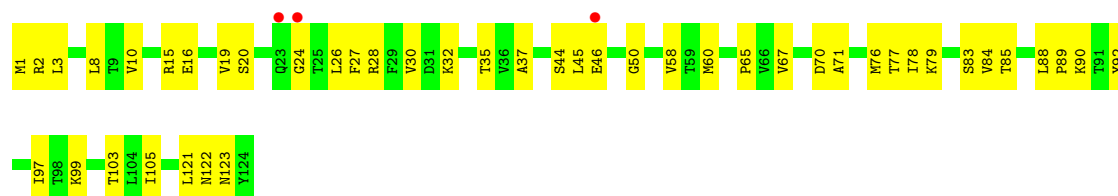


- Molecule 1: coat protein

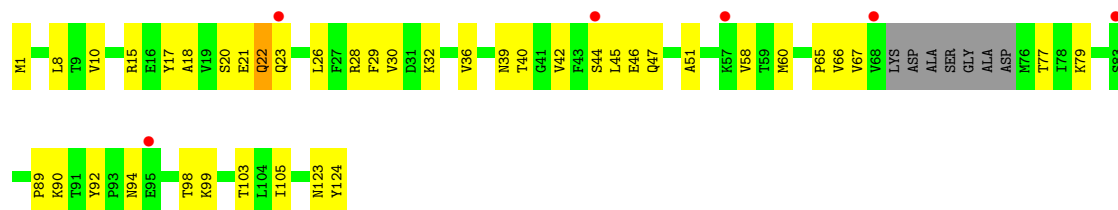




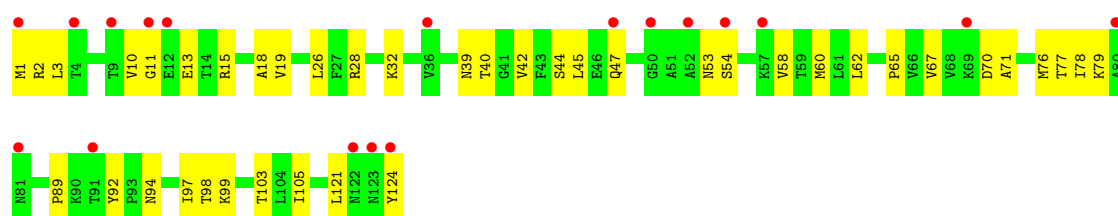
- Molecule 1: coat protein



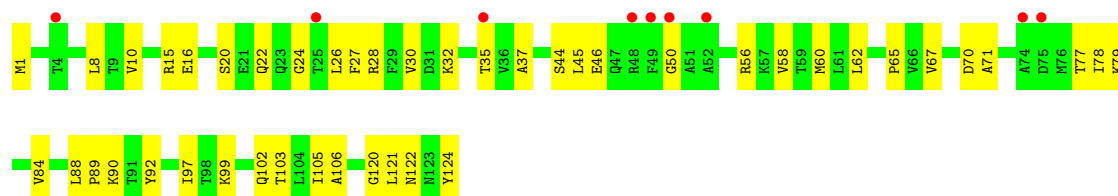
- Molecule 1: coat protein



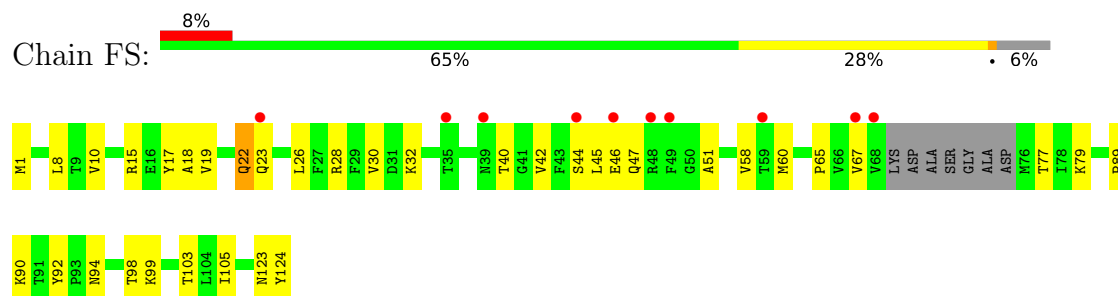
- Molecule 1: coat protein



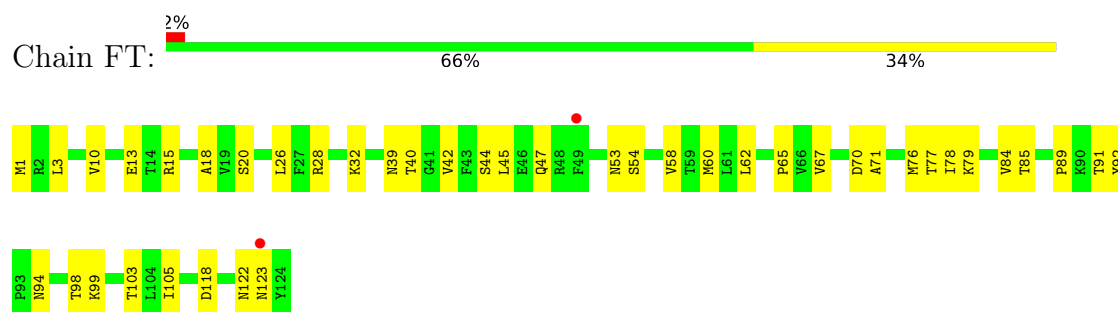
- Molecule 1: coat protein



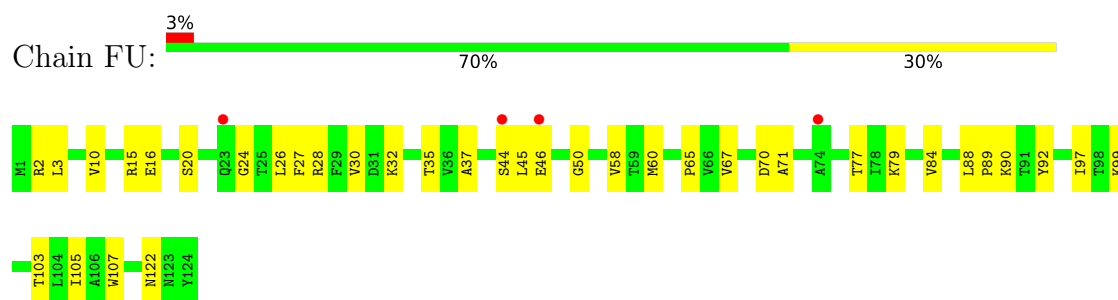
- Molecule 1: coat protein



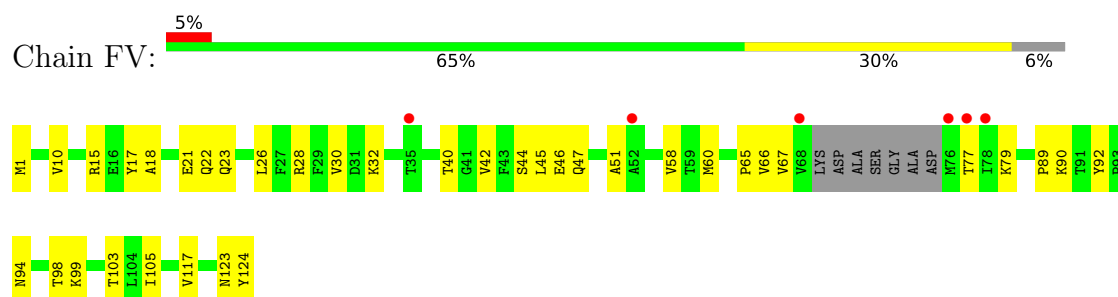
- Molecule 1: coat protein



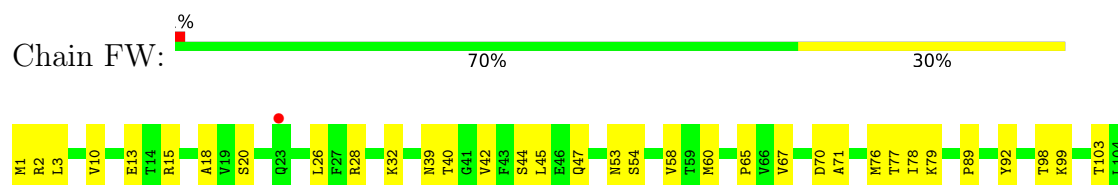
- Molecule 1: coat protein



- Molecule 1: coat protein

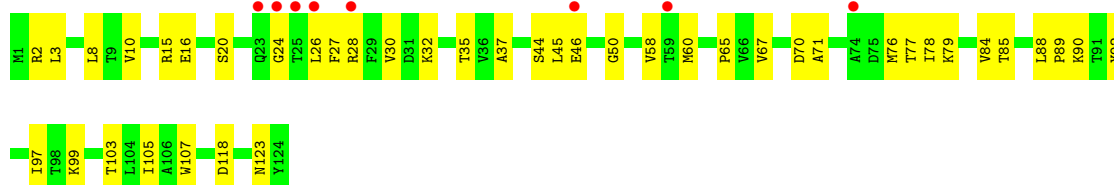


- Molecule 1: coat protein

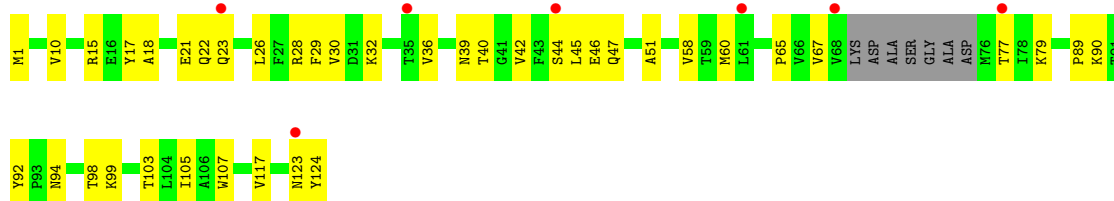




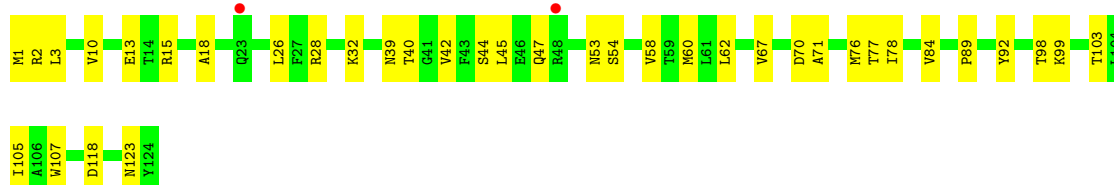
- Molecule 1: coat protein



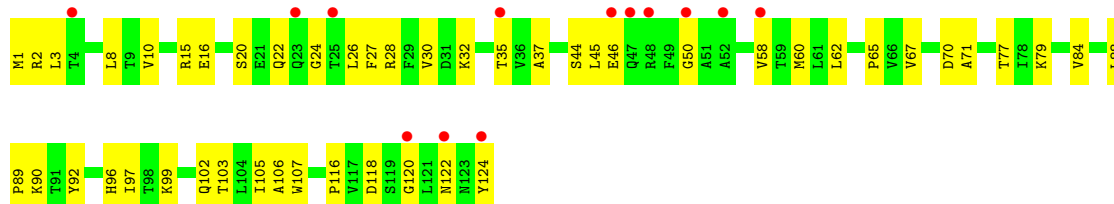
- Molecule 1: coat protein



- Molecule 1: coat protein

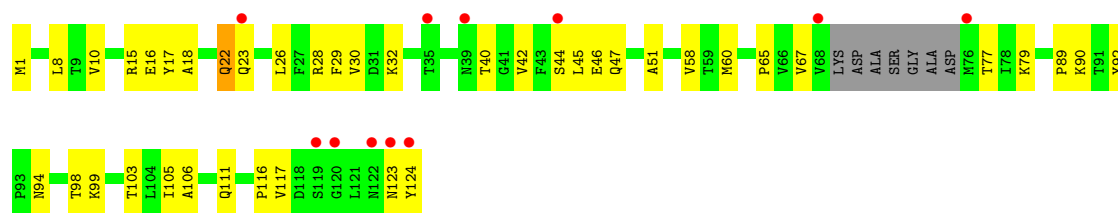


- Molecule 1: coat protein

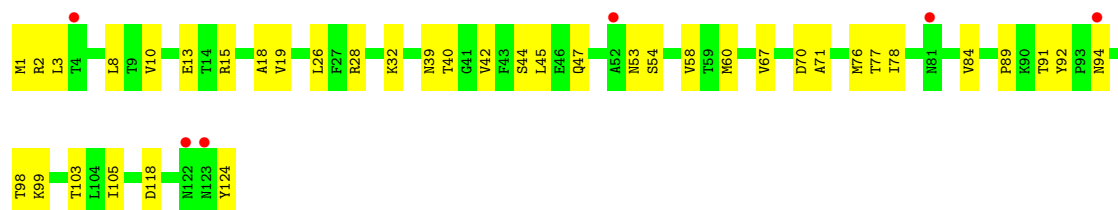


- Molecule 1: coat protein

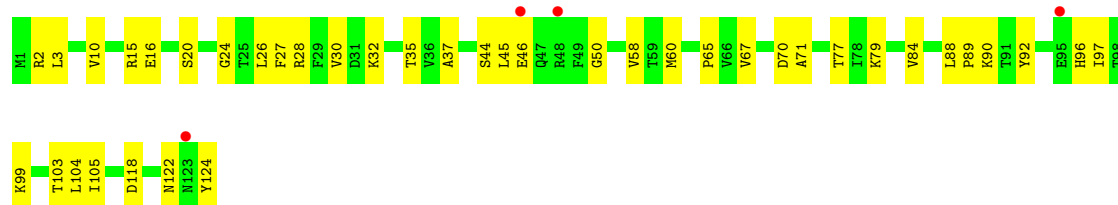




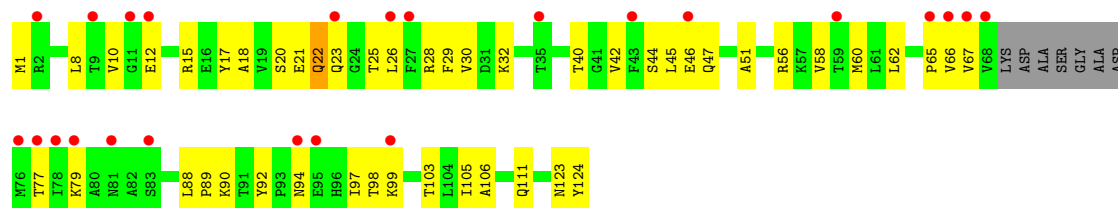
- Molecule 1: coat protein



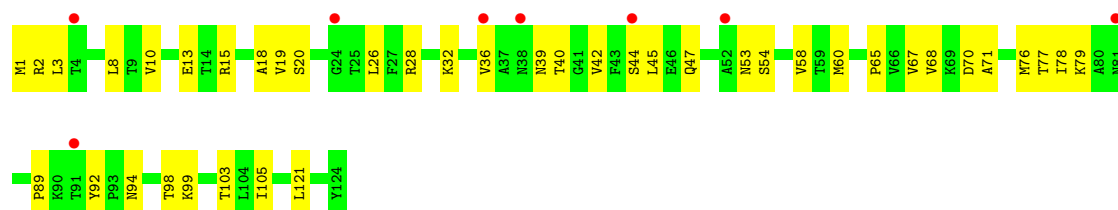
- Molecule 1: coat protein



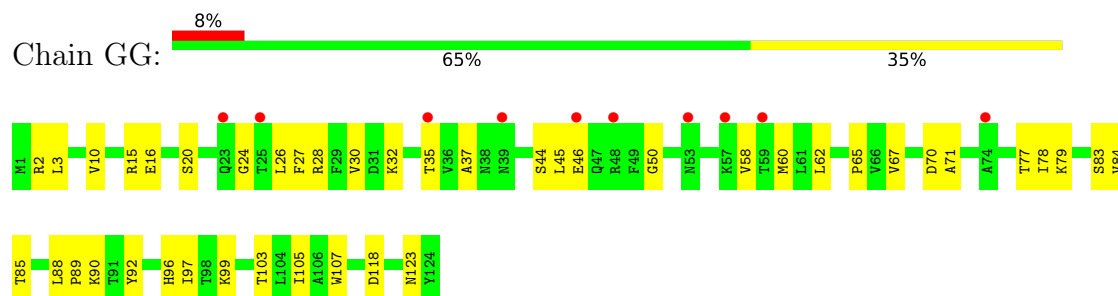
- Molecule 1: coat protein



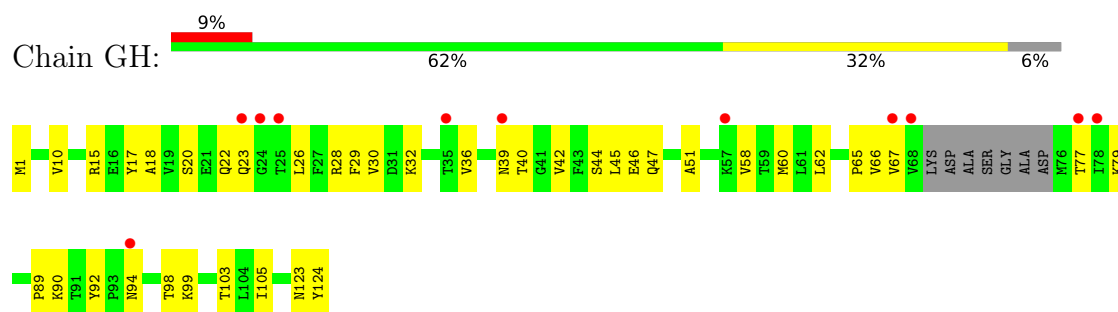
- Molecule 1: coat protein



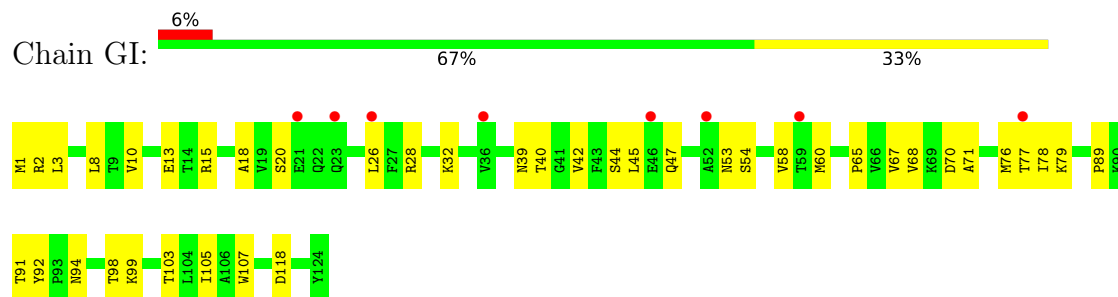
• Molecule 1: coat protein



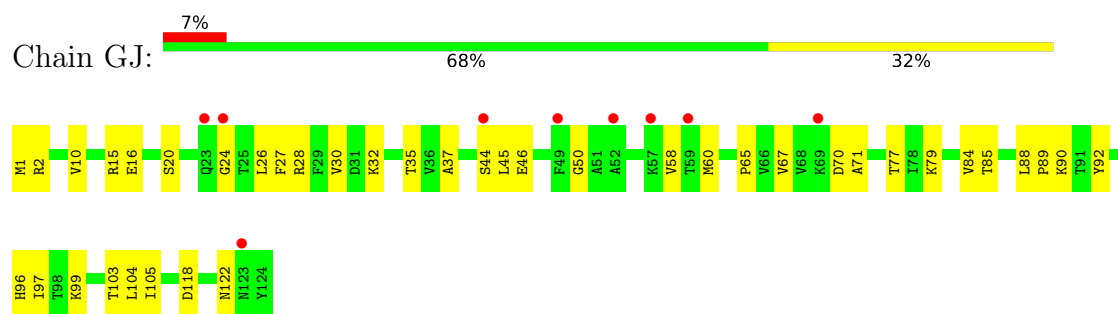
• Molecule 1: coat protein



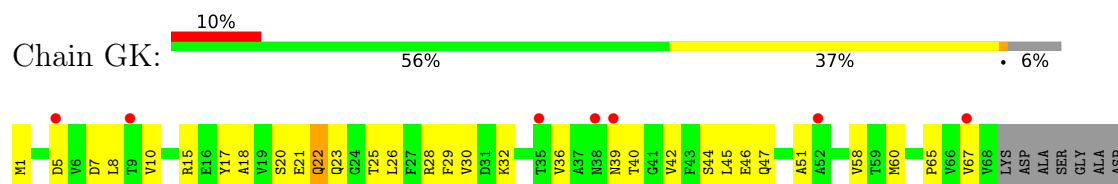
• Molecule 1: coat protein

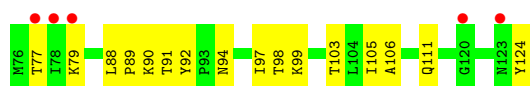


• Molecule 1: coat protein



• Molecule 1: coat protein

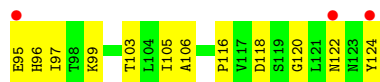
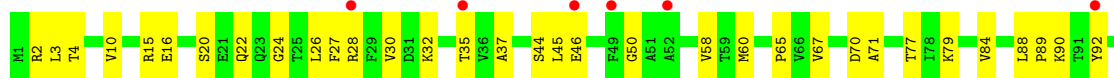




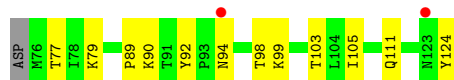
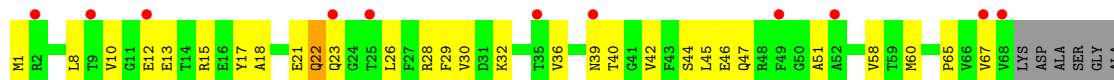
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

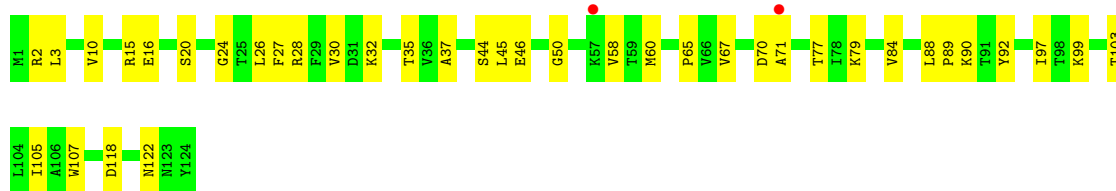


- Molecule 1: coat protein

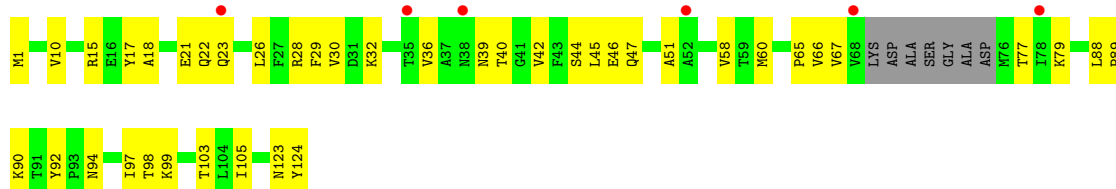


- Molecule 1: coat protein

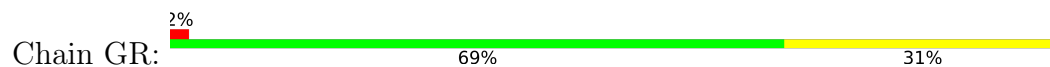




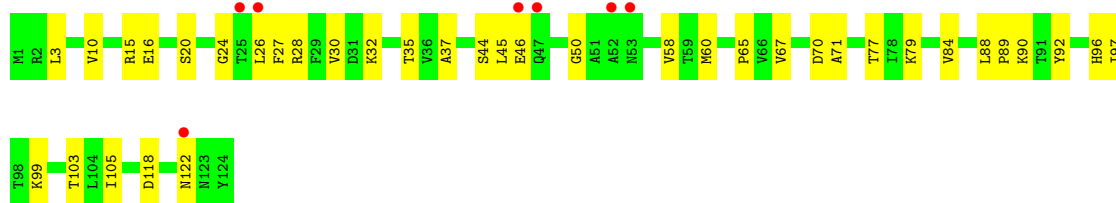
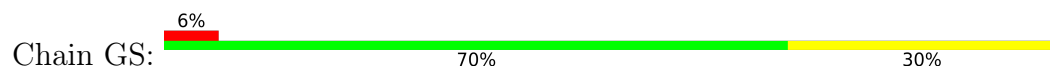
- Molecule 1: coat protein



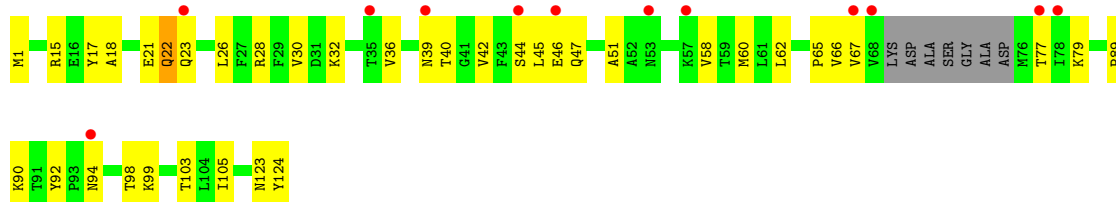
- Molecule 1: coat protein



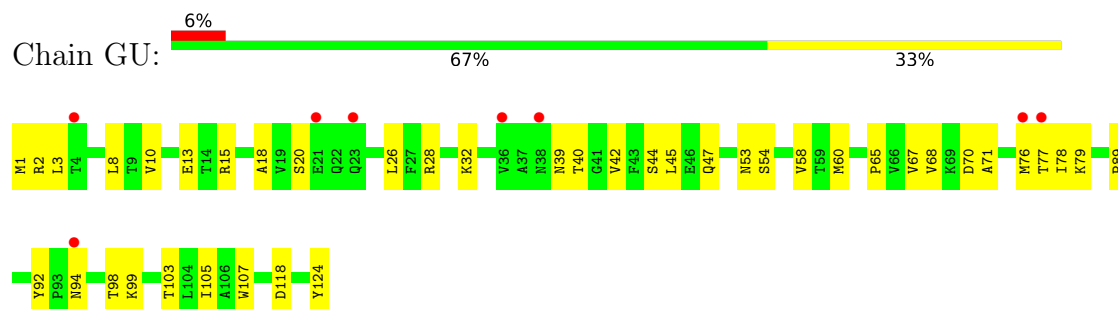
- Molecule 1: coat protein



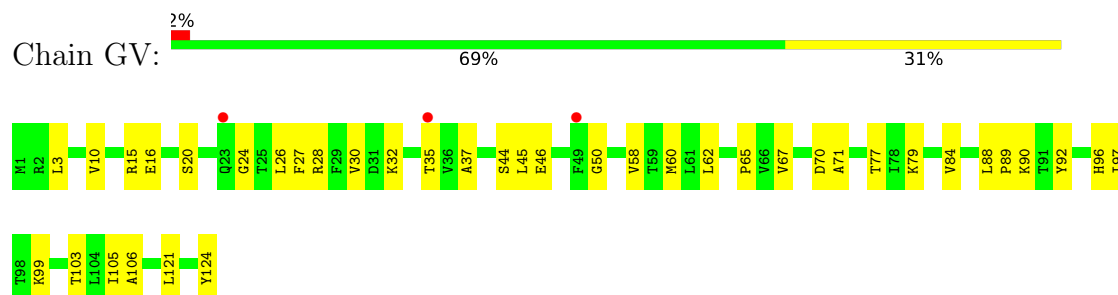
- Molecule 1: coat protein



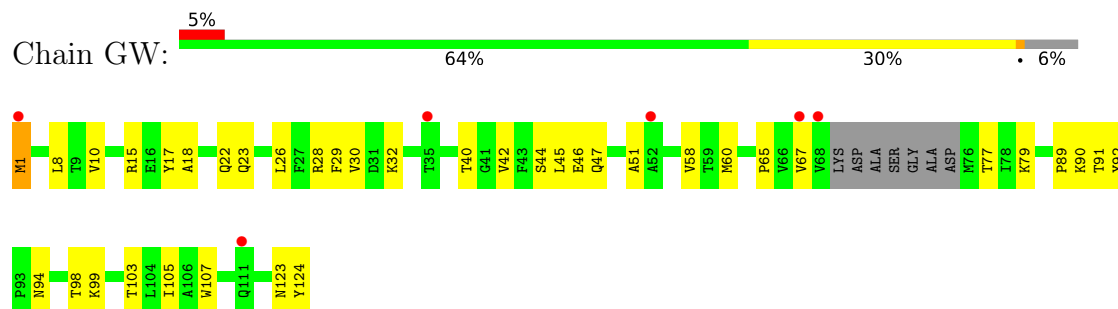
- Molecule 1: coat protein



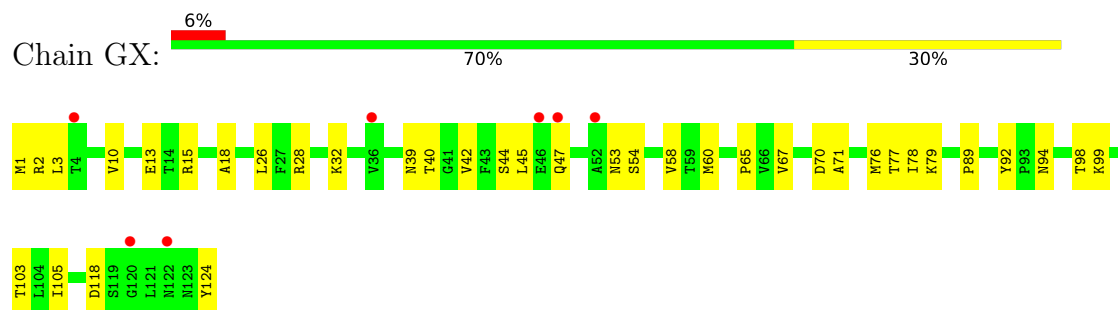
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	269.42Å 277.20Å 277.44Å 103.91° 117.39° 106.96°	Depositor
Resolution (Å)	49.27 – 3.25 49.27 – 3.25	Depositor EDS
% Data completeness (in resolution range)	92.9 (49.27-3.25) 94.1 (49.27-3.25)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.241 , 0.239 0.244 , 0.242	Depositor DCC
R_{free} test set	10025 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å ²)	89.3	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 84.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.026 for k,h,-h-k-l 0.026 for l,-h-k-l,h 0.026 for -h-k-l,l,k	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	169260	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.26	0/969	0.50	0/1314
1	AB	0.28	0/923	0.50	0/1251
1	AC	0.25	0/969	0.47	0/1314
1	AD	0.26	0/969	0.50	0/1314
1	AE	0.28	0/923	0.50	0/1251
1	AF	0.26	0/969	0.47	0/1314
1	AG	0.26	0/969	0.50	0/1314
1	AH	0.28	0/923	0.50	0/1251
1	AI	0.26	0/969	0.47	0/1314
1	AJ	0.26	0/969	0.50	0/1314
1	AK	0.28	0/923	0.50	0/1251
1	AL	0.26	0/969	0.47	0/1314
1	AM	0.26	0/969	0.50	0/1314
1	AN	0.28	0/923	0.50	0/1251
1	AO	0.25	0/969	0.47	0/1314
1	AP	0.26	0/969	0.50	0/1314
1	AQ	0.28	0/923	0.50	0/1251
1	AR	0.26	0/969	0.47	0/1314
1	AS	0.26	0/969	0.50	0/1314
1	AT	0.28	0/923	0.50	0/1251
1	AU	0.25	0/969	0.47	0/1314
1	AV	0.26	0/969	0.50	0/1314
1	AW	0.28	0/923	0.50	0/1251
1	AX	0.25	0/969	0.47	0/1314
1	AY	0.26	0/969	0.50	0/1314
1	AZ	0.28	0/923	0.50	0/1251
1	BA	0.25	0/969	0.47	0/1314
1	BB	0.26	0/969	0.50	0/1314
1	BC	0.28	0/923	0.50	0/1251
1	BD	0.25	0/969	0.47	0/1314
1	BE	0.26	0/969	0.50	0/1314
1	BF	0.28	0/923	0.50	0/1251

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BG	0.25	0/969	0.47	0/1314
1	BH	0.26	0/969	0.50	0/1314
1	BI	0.28	0/923	0.50	0/1251
1	BJ	0.26	0/969	0.47	0/1314
1	BK	0.26	0/969	0.50	0/1314
1	BL	0.28	0/923	0.50	0/1251
1	BM	0.25	0/969	0.47	0/1314
1	BN	0.26	0/969	0.50	0/1314
1	BO	0.28	0/923	0.50	0/1251
1	BP	0.25	0/969	0.47	0/1314
1	BQ	0.26	0/969	0.50	0/1314
1	BR	0.28	0/923	0.50	0/1251
1	BS	0.25	0/969	0.47	0/1314
1	BT	0.26	0/969	0.50	0/1314
1	BU	0.28	0/923	0.50	0/1251
1	BV	0.26	0/969	0.47	0/1314
1	BW	0.26	0/969	0.50	0/1314
1	BX	0.28	0/923	0.50	0/1251
1	BY	0.26	0/969	0.47	0/1314
1	BZ	0.26	0/969	0.50	0/1314
1	CA	0.28	0/923	0.50	0/1251
1	CB	0.25	0/969	0.47	0/1314
1	CC	0.26	0/969	0.50	0/1314
1	CD	0.28	0/923	0.50	0/1251
1	CE	0.26	0/969	0.47	0/1314
1	CF	0.26	0/969	0.50	0/1314
1	CG	0.28	0/923	0.50	0/1251
1	CH	0.26	0/969	0.47	0/1314
1	CI	0.26	0/969	0.50	0/1314
1	CJ	0.28	0/923	0.50	0/1251
1	CK	0.25	0/969	0.47	0/1314
1	CL	0.26	0/969	0.50	0/1314
1	CM	0.28	0/923	0.50	0/1251
1	CN	0.25	0/969	0.47	0/1314
1	CO	0.26	0/969	0.50	0/1314
1	CP	0.28	0/923	0.50	0/1251
1	CQ	0.26	0/969	0.47	0/1314
1	CR	0.26	0/969	0.50	0/1314
1	CS	0.28	0/923	0.50	0/1251
1	CT	0.25	0/969	0.47	0/1314
1	CU	0.26	0/969	0.50	0/1314
1	CV	0.28	0/923	0.50	0/1251
1	CW	0.25	0/969	0.47	0/1314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CX	0.26	0/969	0.50	0/1314
1	CY	0.29	0/923	0.50	0/1251
1	CZ	0.25	0/969	0.47	0/1314
1	DA	0.26	0/969	0.50	0/1314
1	DB	0.28	0/923	0.50	0/1251
1	DC	0.26	0/969	0.47	0/1314
1	DD	0.26	0/969	0.50	0/1314
1	DE	0.28	0/923	0.50	0/1251
1	DF	0.25	0/969	0.47	0/1314
1	DG	0.26	0/969	0.50	0/1314
1	DH	0.28	0/923	0.50	0/1251
1	DI	0.25	0/969	0.47	0/1314
1	DJ	0.26	0/969	0.50	0/1314
1	DK	0.29	0/923	0.50	0/1251
1	DL	0.25	0/969	0.47	0/1314
1	DM	0.26	0/969	0.50	0/1314
1	DN	0.28	0/923	0.50	0/1251
1	DO	0.25	0/969	0.47	0/1314
1	DP	0.26	0/969	0.50	0/1314
1	DQ	0.28	0/923	0.50	0/1251
1	DR	0.26	0/969	0.47	0/1314
1	DS	0.26	0/969	0.50	0/1314
1	DT	0.28	0/923	0.50	0/1251
1	DU	0.25	0/969	0.47	0/1314
1	DV	0.26	0/969	0.50	0/1314
1	DW	0.28	0/923	0.50	0/1251
1	DX	0.25	0/969	0.47	0/1314
1	DY	0.26	0/969	0.50	0/1314
1	DZ	0.28	0/923	0.50	0/1251
1	EA	0.26	0/969	0.47	0/1314
1	EB	0.26	0/969	0.50	0/1314
1	EC	0.28	0/923	0.50	0/1251
1	ED	0.25	0/969	0.47	0/1314
1	EE	0.26	0/969	0.50	0/1314
1	EF	0.28	0/923	0.50	0/1251
1	EG	0.25	0/969	0.47	0/1314
1	EH	0.26	0/969	0.50	0/1314
1	EI	0.28	0/923	0.50	0/1251
1	EJ	0.26	0/969	0.47	0/1314
1	EK	0.26	0/969	0.50	0/1314
1	EL	0.28	0/923	0.50	0/1251
1	EM	0.25	0/969	0.47	0/1314
1	EN	0.26	0/969	0.50	0/1314

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	EO	0.28	0/923	0.50	0/1251
1	EP	0.25	0/969	0.47	0/1314
1	EQ	0.26	0/969	0.50	0/1314
1	ER	0.28	0/923	0.50	0/1251
1	ES	0.26	0/969	0.47	0/1314
1	ET	0.26	0/969	0.50	0/1314
1	EU	0.28	0/923	0.50	0/1251
1	EV	0.26	0/969	0.47	0/1314
1	EW	0.26	0/969	0.50	0/1314
1	EX	0.28	0/923	0.50	0/1251
1	EY	0.25	0/969	0.47	0/1314
1	EZ	0.26	0/969	0.50	0/1314
1	FA	0.28	0/923	0.50	0/1251
1	FB	0.25	0/969	0.47	0/1314
1	FC	0.26	0/969	0.50	0/1314
1	FD	0.28	0/923	0.50	0/1251
1	FE	0.25	0/969	0.47	0/1314
1	FF	0.26	0/969	0.50	0/1314
1	FG	0.28	0/923	0.50	0/1251
1	FH	0.25	0/969	0.47	0/1314
1	FI	0.26	0/969	0.50	0/1314
1	FJ	0.28	0/923	0.50	0/1251
1	FK	0.25	0/969	0.47	0/1314
1	FL	0.26	0/969	0.50	0/1314
1	FM	0.28	0/923	0.50	0/1251
1	FN	0.25	0/969	0.47	0/1314
1	FO	0.26	0/969	0.50	0/1314
1	FP	0.28	0/923	0.50	0/1251
1	FQ	0.25	0/969	0.47	0/1314
1	FR	0.26	0/969	0.50	0/1314
1	FS	0.28	0/923	0.50	0/1251
1	FT	0.25	0/969	0.47	0/1314
1	FU	0.26	0/969	0.50	0/1314
1	FV	0.29	0/923	0.50	0/1251
1	FW	0.25	0/969	0.47	0/1314
1	FX	0.26	0/969	0.50	0/1314
1	FY	0.28	0/923	0.50	0/1251
1	FZ	0.25	0/969	0.47	0/1314
1	GA	0.26	0/969	0.50	0/1314
1	GB	0.28	0/923	0.50	0/1251
1	GC	0.25	0/969	0.47	0/1314
1	GD	0.26	0/969	0.50	0/1314
1	GE	0.28	0/923	0.50	0/1251

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GF	0.25	0/969	0.47	0/1314
1	GG	0.26	0/969	0.50	0/1314
1	GH	0.28	0/923	0.50	0/1251
1	GI	0.26	0/969	0.47	0/1314
1	GJ	0.26	0/969	0.50	0/1314
1	GK	0.28	0/923	0.50	0/1251
1	GL	0.25	0/969	0.47	0/1314
1	GM	0.26	0/969	0.50	0/1314
1	GN	0.28	0/923	0.50	0/1251
1	GO	0.26	0/969	0.47	0/1314
1	GP	0.26	0/969	0.50	0/1314
1	GQ	0.29	0/923	0.50	0/1251
1	GR	0.25	0/969	0.47	0/1314
1	GS	0.26	0/969	0.50	0/1314
1	GT	0.28	0/923	0.50	0/1251
1	GU	0.25	0/969	0.47	0/1314
1	GV	0.26	0/969	0.50	0/1314
1	GW	0.28	0/923	0.50	0/1251
1	GX	0.26	0/969	0.47	0/1314
All	All	0.27	0/171660	0.49	0/232740

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	955	0	947	32	0
1	AB	910	0	907	37	0
1	AC	955	0	947	37	0
1	AD	955	0	947	35	0
1	AE	910	0	907	48	0
1	AF	955	0	947	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AG	955	0	947	33	0
1	AH	910	0	907	37	0
1	AI	955	0	947	38	0
1	AJ	955	0	947	37	0
1	AK	910	0	907	38	0
1	AL	955	0	947	33	0
1	AM	955	0	947	47	0
1	AN	910	0	907	52	2
1	AO	955	0	947	31	0
1	AP	955	0	947	41	0
1	AQ	910	0	907	34	0
1	AR	955	0	947	46	0
1	AS	955	0	947	39	0
1	AT	910	0	907	28	0
1	AU	955	0	947	35	0
1	AV	955	0	947	38	0
1	AW	910	0	907	35	0
1	AX	955	0	947	40	0
1	AY	955	0	947	45	0
1	AZ	910	0	907	32	0
1	BA	955	0	947	34	0
1	BB	955	0	947	30	0
1	BC	910	0	907	35	0
1	BD	955	0	947	42	0
1	BE	955	0	947	31	0
1	BF	910	0	907	33	0
1	BG	955	0	947	31	0
1	BH	955	0	947	38	2
1	BI	910	0	907	34	0
1	BJ	955	0	947	31	1
1	BK	955	0	947	49	0
1	BL	910	0	907	35	0
1	BM	955	0	947	42	0
1	BN	955	0	947	43	0
1	BO	910	0	907	38	0
1	BP	955	0	947	30	0
1	BQ	955	0	947	32	0
1	BR	910	0	907	29	0
1	BS	955	0	947	31	0
1	BT	955	0	947	48	1
1	BU	910	0	907	41	1
1	BV	955	0	947	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BW	955	0	947	32	0
1	BX	910	0	907	38	0
1	BY	955	0	947	33	0
1	BZ	955	0	947	41	0
1	CA	910	0	907	45	1
1	CB	955	0	947	47	0
1	CC	955	0	947	45	0
1	CD	910	0	907	38	0
1	CE	955	0	947	31	0
1	CF	955	0	947	40	0
1	CG	910	0	907	43	1
1	CH	955	0	947	38	0
1	CI	955	0	947	31	1
1	CJ	910	0	907	31	3
1	CK	955	0	947	31	0
1	CL	955	0	947	42	0
1	CM	910	0	907	31	0
1	CN	955	0	947	34	0
1	CO	955	0	947	32	0
1	CP	910	0	907	38	0
1	CQ	955	0	947	36	0
1	CR	955	0	947	37	0
1	CS	910	0	907	32	0
1	CT	955	0	947	37	0
1	CU	955	0	947	34	0
1	CV	910	0	907	37	0
1	CW	955	0	947	34	0
1	CX	955	0	947	31	0
1	CY	910	0	907	37	0
1	CZ	955	0	947	39	0
1	DA	955	0	947	31	0
1	DB	910	0	907	41	0
1	DC	955	0	947	44	0
1	DD	955	0	947	33	0
1	DE	910	0	907	31	0
1	DF	955	0	947	32	0
1	DG	955	0	947	30	0
1	DH	910	0	907	32	0
1	DI	955	0	947	41	0
1	DJ	955	0	947	36	0
1	DK	910	0	907	32	0
1	DL	955	0	947	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DM	955	0	947	35	0
1	DN	910	0	907	46	1
1	DO	955	0	947	42	0
1	DP	955	0	947	32	0
1	DQ	910	0	907	32	0
1	DR	955	0	947	35	0
1	DS	955	0	947	30	0
1	DT	910	0	907	41	0
1	DU	955	0	947	39	0
1	DV	955	0	947	51	1
1	DW	910	0	907	53	1
1	DX	955	0	947	30	0
1	DY	955	0	947	30	0
1	DZ	910	0	907	43	0
1	EA	955	0	947	30	0
1	EB	955	0	947	45	0
1	EC	910	0	907	35	0
1	ED	955	0	947	47	0
1	EE	955	0	947	35	0
1	EF	910	0	907	37	0
1	EG	955	0	947	36	3
1	EH	955	0	947	52	1
1	EI	910	0	907	48	3
1	EJ	955	0	947	37	0
1	EK	955	0	947	29	3
1	EL	910	0	907	40	0
1	EM	955	0	947	33	0
1	EN	955	0	947	33	0
1	EO	910	0	907	48	1
1	EP	955	0	947	45	0
1	EQ	955	0	947	38	0
1	ER	910	0	907	31	1
1	ES	955	0	947	32	0
1	ET	955	0	947	47	0
1	EU	910	0	907	35	0
1	EV	955	0	947	36	1
1	EW	955	0	947	32	0
1	EX	910	0	907	38	0
1	EY	955	0	947	45	0
1	EZ	955	0	947	30	0
1	FA	910	0	907	35	0
1	FB	955	0	947	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	FC	955	0	947	34	0
1	FD	910	0	907	32	0
1	FE	955	0	947	30	0
1	FF	955	0	947	32	0
1	FG	910	0	907	48	0
1	FH	955	0	947	32	0
1	FI	955	0	947	37	0
1	FJ	910	0	907	33	2
1	FK	955	0	947	33	0
1	FL	955	0	947	35	0
1	FM	910	0	907	39	0
1	FN	955	0	947	42	0
1	FO	955	0	947	39	0
1	FP	910	0	907	34	0
1	FQ	955	0	947	34	3
1	FR	955	0	947	49	0
1	FS	910	0	907	34	0
1	FT	955	0	947	38	0
1	FU	955	0	947	31	0
1	FV	910	0	907	31	0
1	FW	955	0	947	30	0
1	FX	955	0	947	37	0
1	FY	910	0	907	32	0
1	FZ	955	0	947	34	0
1	GA	955	0	947	48	1
1	GB	910	0	907	45	2
1	GC	955	0	947	35	0
1	GD	955	0	947	39	0
1	GE	910	0	907	51	1
1	GF	955	0	947	41	0
1	GG	955	0	947	35	0
1	GH	910	0	907	32	0
1	GI	955	0	947	34	0
1	GJ	955	0	947	40	0
1	GK	910	0	907	46	2
1	GL	955	0	947	41	2
1	GM	955	0	947	41	3
1	GN	910	0	907	39	3
1	GO	955	0	947	46	0
1	GP	955	0	947	32	0
1	GQ	910	0	907	32	0
1	GR	955	0	947	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GS	955	0	947	31	0
1	GT	910	0	907	35	0
1	GU	955	0	947	40	0
1	GV	955	0	947	31	0
1	GW	910	0	907	32	0
1	GX	955	0	947	30	0
2	AA	1	0	0	0	0
2	AD	1	0	0	0	0
2	AG	1	0	0	0	0
2	AJ	1	0	0	0	0
2	AM	1	0	0	0	0
2	AP	1	0	0	0	0
2	AS	1	0	0	0	0
2	AV	1	0	0	0	0
2	AY	1	0	0	0	0
2	BB	1	0	0	0	0
2	BE	1	0	0	0	0
2	BH	1	0	0	0	0
2	BK	1	0	0	0	0
2	BN	1	0	0	0	0
2	BQ	1	0	0	0	0
2	BT	1	0	0	0	0
2	BW	1	0	0	0	0
2	BZ	1	0	0	0	0
2	CC	1	0	0	0	0
2	CF	1	0	0	0	0
2	CI	1	0	0	0	0
2	CL	1	0	0	0	0
2	CO	1	0	0	0	0
2	CR	1	0	0	0	0
2	CU	1	0	0	0	0
2	CX	1	0	0	0	0
2	DA	1	0	0	0	0
2	DD	1	0	0	0	0
2	DG	1	0	0	0	0
2	DJ	1	0	0	0	0
2	DM	1	0	0	0	0
2	DP	1	0	0	0	0
2	DS	1	0	0	0	0
2	DV	1	0	0	0	0
2	DY	1	0	0	0	0
2	EB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	EE	1	0	0	0	0
2	EH	1	0	0	0	0
2	EK	1	0	0	0	0
2	EN	1	0	0	0	0
2	EQ	1	0	0	0	0
2	ET	1	0	0	0	0
2	EW	1	0	0	0	0
2	EZ	1	0	0	0	0
2	FC	1	0	0	0	0
2	FF	1	0	0	0	0
2	FI	1	0	0	0	0
2	FL	1	0	0	0	0
2	FO	1	0	0	0	0
2	FR	1	0	0	0	0
2	FU	1	0	0	0	0
2	FX	1	0	0	0	0
2	GA	1	0	0	0	0
2	GD	1	0	0	0	0
2	GG	1	0	0	0	0
2	GJ	1	0	0	0	0
2	GM	1	0	0	0	0
2	GP	1	0	0	0	0
2	GS	1	0	0	0	0
2	GV	1	0	0	0	0
All	All	169260	0	168060	4882	24

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 4882 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BK:15:ARG:HH11	1:DW:103:THR:HG21	1.14	1.12
1:EB:15:ARG:HH11	1:GB:103:THR:HG21	1.17	1.08
1:FP:103:THR:HG21	1:GV:15:ARG:HH11	1.16	1.07
1:CG:103:THR:HG21	1:CL:15:ARG:HH11	1.19	1.05
1:AE:103:THR:HG21	1:GA:15:ARG:HH11	1.23	1.03

The worst 5 of 24 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AN:32:LYS:NZ	1:GB:16:GLU:OE2[1_666]	1.39	0.81
1:BU:32:LYS:NZ	1:DW:16:GLU:OE2[1_554]	1.50	0.70
1:BH:12:GLU:O	1:GK:5:ASP:O[1_655]	1.55	0.65
1:EI:35:THR:CG2	1:GN:12:GLU:OE1[1_545]	1.55	0.65
1:BH:12:GLU:OE1	1:GK:7:ASP:OD1[1_655]	1.57	0.63

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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

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

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GR	122/124 (98%)	122 (100%)	0	0	100	100
1	GS	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	GT	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	GU	122/124 (98%)	122 (100%)	0	0	100	100
1	GV	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
1	GW	113/124 (91%)	110 (97%)	3 (3%)	0	100	100
1	GX	122/124 (98%)	122 (100%)	0	0	100	100
All	All	21420/22320 (96%)	21180 (99%)	240 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	107/107 (100%)	107 (100%)	0	100	100
1	AB	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	AC	107/107 (100%)	107 (100%)	0	100	100
1	AD	107/107 (100%)	107 (100%)	0	100	100
1	AE	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	AF	107/107 (100%)	107 (100%)	0	100	100
1	AG	107/107 (100%)	107 (100%)	0	100	100
1	AH	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	AI	107/107 (100%)	107 (100%)	0	100	100
1	AJ	107/107 (100%)	107 (100%)	0	100	100
1	AK	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	AL	107/107 (100%)	107 (100%)	0	100	100
1	AM	107/107 (100%)	107 (100%)	0	100	100
1	AN	103/107 (96%)	101 (98%)	2 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AO	107/107 (100%)	107 (100%)	0	100	100
1	AP	107/107 (100%)	107 (100%)	0	100	100
1	AQ	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	AR	107/107 (100%)	107 (100%)	0	100	100
1	AS	107/107 (100%)	107 (100%)	0	100	100
1	AT	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	AU	107/107 (100%)	107 (100%)	0	100	100
1	AV	107/107 (100%)	107 (100%)	0	100	100
1	AW	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	AX	107/107 (100%)	107 (100%)	0	100	100
1	AY	107/107 (100%)	107 (100%)	0	100	100
1	AZ	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	BA	107/107 (100%)	107 (100%)	0	100	100
1	BB	107/107 (100%)	107 (100%)	0	100	100
1	BC	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	BD	107/107 (100%)	107 (100%)	0	100	100
1	BE	107/107 (100%)	107 (100%)	0	100	100
1	BF	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	BG	107/107 (100%)	107 (100%)	0	100	100
1	BH	107/107 (100%)	107 (100%)	0	100	100
1	BI	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	BJ	107/107 (100%)	107 (100%)	0	100	100
1	BK	107/107 (100%)	107 (100%)	0	100	100
1	BL	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	BM	107/107 (100%)	107 (100%)	0	100	100
1	BN	107/107 (100%)	107 (100%)	0	100	100
1	BO	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	BP	107/107 (100%)	107 (100%)	0	100	100
1	BQ	107/107 (100%)	107 (100%)	0	100	100
1	BR	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	BS	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BT	107/107 (100%)	107 (100%)	0	100	100
1	BU	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	BV	107/107 (100%)	107 (100%)	0	100	100
1	BW	107/107 (100%)	107 (100%)	0	100	100
1	BX	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	BY	107/107 (100%)	107 (100%)	0	100	100
1	BZ	107/107 (100%)	107 (100%)	0	100	100
1	CA	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	CB	107/107 (100%)	107 (100%)	0	100	100
1	CC	107/107 (100%)	107 (100%)	0	100	100
1	CD	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	CE	107/107 (100%)	107 (100%)	0	100	100
1	CF	107/107 (100%)	107 (100%)	0	100	100
1	CG	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	CH	107/107 (100%)	107 (100%)	0	100	100
1	CI	107/107 (100%)	107 (100%)	0	100	100
1	CJ	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	CK	107/107 (100%)	107 (100%)	0	100	100
1	CL	107/107 (100%)	107 (100%)	0	100	100
1	CM	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	CN	107/107 (100%)	107 (100%)	0	100	100
1	CO	107/107 (100%)	107 (100%)	0	100	100
1	CP	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	CQ	107/107 (100%)	107 (100%)	0	100	100
1	CR	107/107 (100%)	107 (100%)	0	100	100
1	CS	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	CT	107/107 (100%)	107 (100%)	0	100	100
1	CU	107/107 (100%)	107 (100%)	0	100	100
1	CV	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	CW	107/107 (100%)	107 (100%)	0	100	100
1	CX	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CY	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	CZ	107/107 (100%)	107 (100%)	0	100	100
1	DA	107/107 (100%)	107 (100%)	0	100	100
1	DB	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	DC	107/107 (100%)	107 (100%)	0	100	100
1	DD	107/107 (100%)	107 (100%)	0	100	100
1	DE	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	DF	107/107 (100%)	107 (100%)	0	100	100
1	DG	107/107 (100%)	107 (100%)	0	100	100
1	DH	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	DI	107/107 (100%)	107 (100%)	0	100	100
1	DJ	107/107 (100%)	107 (100%)	0	100	100
1	DK	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	DL	107/107 (100%)	107 (100%)	0	100	100
1	DM	107/107 (100%)	107 (100%)	0	100	100
1	DN	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	DO	107/107 (100%)	107 (100%)	0	100	100
1	DP	107/107 (100%)	107 (100%)	0	100	100
1	DQ	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	DR	107/107 (100%)	107 (100%)	0	100	100
1	DS	107/107 (100%)	107 (100%)	0	100	100
1	DT	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	DU	107/107 (100%)	107 (100%)	0	100	100
1	DV	107/107 (100%)	107 (100%)	0	100	100
1	DW	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	DX	107/107 (100%)	107 (100%)	0	100	100
1	DY	107/107 (100%)	107 (100%)	0	100	100
1	DZ	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	EA	107/107 (100%)	107 (100%)	0	100	100
1	EB	107/107 (100%)	107 (100%)	0	100	100
1	EC	103/107 (96%)	101 (98%)	2 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	ED	107/107 (100%)	107 (100%)	0	100	100
1	EE	107/107 (100%)	107 (100%)	0	100	100
1	EF	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	EG	107/107 (100%)	107 (100%)	0	100	100
1	EH	107/107 (100%)	107 (100%)	0	100	100
1	EI	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	EJ	107/107 (100%)	107 (100%)	0	100	100
1	EK	107/107 (100%)	107 (100%)	0	100	100
1	EL	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	EM	107/107 (100%)	107 (100%)	0	100	100
1	EN	107/107 (100%)	107 (100%)	0	100	100
1	EO	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	EP	107/107 (100%)	107 (100%)	0	100	100
1	EQ	107/107 (100%)	107 (100%)	0	100	100
1	ER	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	ES	107/107 (100%)	107 (100%)	0	100	100
1	ET	107/107 (100%)	107 (100%)	0	100	100
1	EU	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	EV	107/107 (100%)	107 (100%)	0	100	100
1	EW	107/107 (100%)	107 (100%)	0	100	100
1	EX	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	EY	107/107 (100%)	107 (100%)	0	100	100
1	EZ	107/107 (100%)	107 (100%)	0	100	100
1	FA	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	FB	107/107 (100%)	107 (100%)	0	100	100
1	FC	107/107 (100%)	107 (100%)	0	100	100
1	FD	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	FE	107/107 (100%)	107 (100%)	0	100	100
1	FF	107/107 (100%)	107 (100%)	0	100	100
1	FG	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	FH	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FI	107/107 (100%)	107 (100%)	0	100	100
1	FJ	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	FK	107/107 (100%)	107 (100%)	0	100	100
1	FL	107/107 (100%)	107 (100%)	0	100	100
1	FM	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	FN	107/107 (100%)	107 (100%)	0	100	100
1	FO	107/107 (100%)	107 (100%)	0	100	100
1	FP	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	FQ	107/107 (100%)	107 (100%)	0	100	100
1	FR	107/107 (100%)	107 (100%)	0	100	100
1	FS	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	FT	107/107 (100%)	107 (100%)	0	100	100
1	FU	107/107 (100%)	107 (100%)	0	100	100
1	FV	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	FW	107/107 (100%)	107 (100%)	0	100	100
1	FX	107/107 (100%)	107 (100%)	0	100	100
1	FY	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	FZ	107/107 (100%)	107 (100%)	0	100	100
1	GA	107/107 (100%)	107 (100%)	0	100	100
1	GB	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	GC	107/107 (100%)	107 (100%)	0	100	100
1	GD	107/107 (100%)	107 (100%)	0	100	100
1	GE	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	GF	107/107 (100%)	107 (100%)	0	100	100
1	GG	107/107 (100%)	107 (100%)	0	100	100
1	GH	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	GI	107/107 (100%)	107 (100%)	0	100	100
1	GJ	107/107 (100%)	107 (100%)	0	100	100
1	GK	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	GL	107/107 (100%)	107 (100%)	0	100	100
1	GM	107/107 (100%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	GN	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	GO	107/107 (100%)	107 (100%)	0	100	100
1	GP	107/107 (100%)	107 (100%)	0	100	100
1	GQ	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	GR	107/107 (100%)	107 (100%)	0	100	100
1	GS	107/107 (100%)	107 (100%)	0	100	100
1	GT	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	GU	107/107 (100%)	107 (100%)	0	100	100
1	GV	107/107 (100%)	107 (100%)	0	100	100
1	GW	103/107 (96%)	101 (98%)	2 (2%)	50	70
1	GX	107/107 (100%)	107 (100%)	0	100	100
All	All	19020/19260 (99%)	18900 (99%)	120 (1%)	78	83

5 of 120 residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 306 such sidechains are listed below:

Mol	Chain	Res	Type
1	FI	110	GLN
1	GK	96	HIS
1	FM	47	GLN
1	FY	96	HIS
1	GQ	81	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	124/124 (100%)	0.49	3 (2%) 59 40	66, 92, 154, 183	0
1	AB	117/124 (94%)	0.43	7 (5%) 27 18	67, 92, 140, 186	0
1	AC	124/124 (100%)	0.54	9 (7%) 21 14	63, 92, 150, 173	0
1	AD	124/124 (100%)	0.45	5 (4%) 42 27	66, 92, 154, 183	0
1	AE	117/124 (94%)	0.99	17 (14%) 6 5	67, 92, 140, 186	0
1	AF	124/124 (100%)	0.47	4 (3%) 50 32	63, 92, 150, 173	0
1	AG	124/124 (100%)	0.46	5 (4%) 42 27	66, 92, 154, 183	0
1	AH	117/124 (94%)	0.74	13 (11%) 10 7	67, 92, 140, 186	0
1	AI	124/124 (100%)	0.42	4 (3%) 50 32	63, 92, 150, 173	0
1	AJ	124/124 (100%)	0.44	6 (4%) 35 23	66, 92, 154, 183	0
1	AK	117/124 (94%)	0.71	8 (6%) 23 15	67, 92, 140, 186	0
1	AL	124/124 (100%)	0.55	8 (6%) 25 16	63, 92, 150, 173	0
1	AM	124/124 (100%)	0.76	7 (5%) 30 20	66, 92, 154, 183	0
1	AN	117/124 (94%)	0.85	13 (11%) 10 7	67, 92, 140, 186	0
1	AO	124/124 (100%)	0.45	6 (4%) 35 23	63, 92, 150, 173	0
1	AP	124/124 (100%)	0.60	8 (6%) 25 16	66, 92, 154, 183	0
1	AQ	117/124 (94%)	0.48	9 (7%) 19 13	67, 92, 140, 186	0
1	AR	124/124 (100%)	0.48	6 (4%) 35 23	63, 92, 150, 173	0
1	AS	124/124 (100%)	0.59	7 (5%) 30 20	66, 92, 154, 183	0
1	AT	117/124 (94%)	0.59	6 (5%) 33 22	67, 92, 140, 186	0
1	AU	124/124 (100%)	0.75	6 (4%) 35 23	63, 92, 150, 173	0
1	AV	124/124 (100%)	0.70	6 (4%) 35 23	66, 92, 154, 183	0
1	AW	117/124 (94%)	0.61	13 (11%) 10 7	67, 92, 140, 186	0
1	AX	124/124 (100%)	0.61	8 (6%) 25 16	63, 92, 150, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AY	124/124 (100%)	0.54	3 (2%) 59 40	66, 92, 154, 183	0
1	AZ	117/124 (94%)	0.63	12 (10%) 12 8	67, 92, 140, 186	0
1	BA	124/124 (100%)	0.76	14 (11%) 10 7	63, 92, 150, 173	0
1	BB	124/124 (100%)	0.38	6 (4%) 35 23	66, 92, 154, 183	0
1	BC	117/124 (94%)	0.62	12 (10%) 12 8	67, 92, 140, 186	0
1	BD	124/124 (100%)	0.48	4 (3%) 50 32	63, 92, 150, 173	0
1	BE	124/124 (100%)	0.56	4 (3%) 50 32	66, 92, 154, 183	0
1	BF	117/124 (94%)	0.47	4 (3%) 48 30	67, 92, 140, 186	0
1	BG	124/124 (100%)	0.48	3 (2%) 59 40	63, 92, 150, 173	0
1	BH	124/124 (100%)	0.67	12 (9%) 13 9	66, 92, 154, 183	0
1	BI	117/124 (94%)	0.53	10 (8%) 16 12	67, 92, 140, 186	0
1	BJ	124/124 (100%)	0.73	10 (8%) 18 12	63, 92, 150, 173	0
1	BK	124/124 (100%)	0.68	10 (8%) 18 12	66, 92, 154, 183	0
1	BL	117/124 (94%)	0.79	12 (10%) 12 8	67, 92, 140, 186	0
1	BM	124/124 (100%)	0.52	5 (4%) 42 27	63, 92, 150, 173	0
1	BN	124/124 (100%)	0.48	9 (7%) 21 14	66, 92, 154, 183	0
1	BO	117/124 (94%)	0.57	8 (6%) 23 15	67, 92, 140, 186	0
1	BP	124/124 (100%)	0.60	3 (2%) 59 40	63, 92, 150, 173	0
1	BQ	124/124 (100%)	0.27	2 (1%) 70 51	66, 92, 154, 183	0
1	BR	117/124 (94%)	0.23	1 (0%) 81 64	67, 92, 140, 186	0
1	BS	124/124 (100%)	0.35	4 (3%) 50 32	63, 92, 150, 173	0
1	BT	124/124 (100%)	1.02	19 (15%) 5 4	66, 92, 154, 183	0
1	BU	117/124 (94%)	0.93	15 (12%) 7 6	67, 92, 140, 186	0
1	BV	124/124 (100%)	0.59	12 (9%) 13 9	63, 92, 150, 173	0
1	BW	124/124 (100%)	0.49	5 (4%) 42 27	66, 92, 154, 183	0
1	BX	117/124 (94%)	0.54	7 (5%) 27 18	67, 92, 140, 186	0
1	BY	124/124 (100%)	0.47	5 (4%) 42 27	63, 92, 150, 173	0
1	BZ	124/124 (100%)	0.51	5 (4%) 42 27	66, 92, 154, 183	0
1	CA	117/124 (94%)	0.78	10 (8%) 16 12	67, 92, 140, 186	0
1	CB	124/124 (100%)	0.47	5 (4%) 42 27	63, 92, 150, 173	0
1	CC	124/124 (100%)	0.46	4 (3%) 50 32	66, 92, 154, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	CD	117/124 (94%)	0.67	11 (9%)	14 10	67, 92, 140, 186	0
1	CE	124/124 (100%)	0.66	10 (8%)	18 12	63, 92, 150, 173	0
1	CF	124/124 (100%)	0.65	10 (8%)	18 12	66, 92, 154, 183	0
1	CG	117/124 (94%)	0.80	14 (11%)	9 7	67, 92, 140, 186	0
1	CH	124/124 (100%)	0.33	5 (4%)	42 27	63, 92, 150, 173	0
1	CI	124/124 (100%)	0.55	7 (5%)	30 20	66, 92, 154, 183	0
1	CJ	117/124 (94%)	0.46	6 (5%)	33 22	67, 92, 140, 186	0
1	CK	124/124 (100%)	0.40	0	100 100	63, 92, 150, 173	0
1	CL	124/124 (100%)	0.51	8 (6%)	25 16	66, 92, 154, 183	0
1	CM	117/124 (94%)	0.66	9 (7%)	19 13	67, 92, 140, 186	0
1	CN	124/124 (100%)	0.39	3 (2%)	59 40	63, 92, 150, 173	0
1	CO	124/124 (100%)	0.45	7 (5%)	30 20	66, 92, 154, 183	0
1	CP	117/124 (94%)	0.64	10 (8%)	16 12	67, 92, 140, 186	0
1	CQ	124/124 (100%)	0.43	2 (1%)	70 51	63, 92, 150, 173	0
1	CR	124/124 (100%)	0.67	12 (9%)	13 9	66, 92, 154, 183	0
1	CS	117/124 (94%)	0.55	8 (6%)	23 15	67, 92, 140, 186	0
1	CT	124/124 (100%)	0.49	5 (4%)	42 27	63, 92, 150, 173	0
1	CU	124/124 (100%)	0.46	5 (4%)	42 27	66, 92, 154, 183	0
1	CV	117/124 (94%)	0.62	7 (5%)	27 18	67, 92, 140, 186	0
1	CW	124/124 (100%)	0.51	5 (4%)	42 27	63, 92, 150, 173	0
1	CX	124/124 (100%)	0.38	2 (1%)	70 51	66, 92, 154, 183	0
1	CY	117/124 (94%)	0.49	9 (7%)	19 13	67, 92, 140, 186	0
1	CZ	124/124 (100%)	0.49	4 (3%)	50 32	63, 92, 150, 173	0
1	DA	124/124 (100%)	0.41	9 (7%)	21 14	66, 92, 154, 183	0
1	DB	117/124 (94%)	0.84	13 (11%)	10 7	67, 92, 140, 186	0
1	DC	124/124 (100%)	0.59	7 (5%)	30 20	63, 92, 150, 173	0
1	DD	124/124 (100%)	0.52	9 (7%)	21 14	66, 92, 154, 183	0
1	DE	117/124 (94%)	0.40	7 (5%)	27 18	67, 92, 140, 186	0
1	DF	124/124 (100%)	0.33	3 (2%)	59 40	63, 92, 150, 173	0
1	DG	124/124 (100%)	0.54	7 (5%)	30 20	66, 92, 154, 183	0
1	DH	117/124 (94%)	0.44	6 (5%)	33 22	67, 92, 140, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	DI	124/124 (100%)	0.42	6 (4%)	35	23	63, 92, 150, 173	0
1	DJ	124/124 (100%)	0.55	6 (4%)	35	23	66, 92, 154, 183	0
1	DK	117/124 (94%)	0.50	5 (4%)	40	25	67, 92, 140, 186	0
1	DL	124/124 (100%)	0.51	6 (4%)	35	23	63, 92, 150, 173	0
1	DM	124/124 (100%)	0.74	9 (7%)	21	14	66, 92, 154, 183	0
1	DN	117/124 (94%)	1.02	19 (16%)	4	3	67, 92, 140, 186	0
1	DO	124/124 (100%)	0.47	10 (8%)	18	12	63, 92, 150, 173	0
1	DP	124/124 (100%)	0.51	6 (4%)	35	23	66, 92, 154, 183	0
1	DQ	117/124 (94%)	0.45	6 (5%)	33	22	67, 92, 140, 186	0
1	DR	124/124 (100%)	0.50	6 (4%)	35	23	63, 92, 150, 173	0
1	DS	124/124 (100%)	0.40	6 (4%)	35	23	66, 92, 154, 183	0
1	DT	117/124 (94%)	0.59	9 (7%)	19	13	67, 92, 140, 186	0
1	DU	124/124 (100%)	0.46	6 (4%)	35	23	63, 92, 150, 173	0
1	DV	124/124 (100%)	0.94	15 (12%)	8	7	66, 92, 154, 183	0
1	DW	117/124 (94%)	1.20	21 (17%)	3	3	67, 92, 140, 186	0
1	DX	124/124 (100%)	0.64	10 (8%)	18	12	63, 92, 150, 173	0
1	DY	124/124 (100%)	0.26	2 (1%)	70	51	66, 92, 154, 183	0
1	DZ	117/124 (94%)	0.65	11 (9%)	14	10	67, 92, 140, 186	0
1	EA	124/124 (100%)	0.50	5 (4%)	42	27	63, 92, 150, 173	0
1	EB	124/124 (100%)	0.53	4 (3%)	50	32	66, 92, 154, 183	0
1	EC	117/124 (94%)	0.39	9 (7%)	19	13	67, 92, 140, 186	0
1	ED	124/124 (100%)	0.42	4 (3%)	50	32	63, 92, 150, 173	0
1	EE	124/124 (100%)	0.58	11 (8%)	15	11	66, 92, 154, 183	0
1	EF	117/124 (94%)	0.54	5 (4%)	40	25	67, 92, 140, 186	0
1	EG	124/124 (100%)	0.82	13 (10%)	11	8	63, 92, 150, 173	0
1	EH	124/124 (100%)	0.77	11 (8%)	15	11	66, 92, 154, 183	0
1	EI	117/124 (94%)	1.01	17 (14%)	6	5	67, 92, 140, 186	0
1	EJ	124/124 (100%)	0.42	2 (1%)	70	51	63, 92, 150, 173	0
1	EK	124/124 (100%)	0.62	9 (7%)	21	14	66, 92, 154, 183	0
1	EL	117/124 (94%)	0.61	10 (8%)	16	12	67, 92, 140, 186	0
1	EM	124/124 (100%)	0.72	10 (8%)	18	12	63, 92, 150, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	EN	124/124 (100%)	0.60	6 (4%)	35	23	66, 92, 154, 183	0
1	EO	117/124 (94%)	0.88	13 (11%)	10	7	67, 92, 140, 186	0
1	EP	124/124 (100%)	0.47	5 (4%)	42	27	63, 92, 150, 173	0
1	EQ	124/124 (100%)	0.62	5 (4%)	42	27	66, 92, 154, 183	0
1	ER	117/124 (94%)	0.78	12 (10%)	12	8	67, 92, 140, 186	0
1	ES	124/124 (100%)	0.58	6 (4%)	35	23	63, 92, 150, 173	0
1	ET	124/124 (100%)	0.64	7 (5%)	30	20	66, 92, 154, 183	0
1	EU	117/124 (94%)	0.58	8 (6%)	23	15	67, 92, 140, 186	0
1	EV	124/124 (100%)	0.75	17 (13%)	6	5	63, 92, 150, 173	0
1	EW	124/124 (100%)	0.50	4 (3%)	50	32	66, 92, 154, 183	0
1	EX	117/124 (94%)	0.57	4 (3%)	48	30	67, 92, 140, 186	0
1	EY	124/124 (100%)	0.55	8 (6%)	25	16	63, 92, 150, 173	0
1	EZ	124/124 (100%)	0.55	4 (3%)	50	32	66, 92, 154, 183	0
1	FA	117/124 (94%)	0.63	10 (8%)	16	12	67, 92, 140, 186	0
1	FB	124/124 (100%)	0.43	5 (4%)	42	27	63, 92, 150, 173	0
1	FC	124/124 (100%)	0.43	7 (5%)	30	20	66, 92, 154, 183	0
1	FD	117/124 (94%)	0.55	12 (10%)	12	8	67, 92, 140, 186	0
1	FE	124/124 (100%)	0.32	5 (4%)	42	27	63, 92, 150, 173	0
1	FF	124/124 (100%)	0.46	3 (2%)	59	40	66, 92, 154, 183	0
1	FG	117/124 (94%)	0.77	8 (6%)	23	15	67, 92, 140, 186	0
1	FH	124/124 (100%)	0.50	4 (3%)	50	32	63, 92, 150, 173	0
1	FI	124/124 (100%)	0.64	7 (5%)	30	20	66, 92, 154, 183	0
1	FJ	117/124 (94%)	0.65	9 (7%)	19	13	67, 92, 140, 186	0
1	FK	124/124 (100%)	0.46	3 (2%)	59	40	63, 92, 150, 173	0
1	FL	124/124 (100%)	0.52	8 (6%)	25	16	66, 92, 154, 183	0
1	FM	117/124 (94%)	0.67	6 (5%)	33	22	67, 92, 140, 186	0
1	FN	124/124 (100%)	0.45	5 (4%)	42	27	63, 92, 150, 173	0
1	FO	124/124 (100%)	0.39	3 (2%)	59	40	66, 92, 154, 183	0
1	FP	117/124 (94%)	0.47	6 (5%)	33	22	67, 92, 140, 186	0
1	FQ	124/124 (100%)	0.93	18 (14%)	6	5	63, 92, 150, 173	0
1	FR	124/124 (100%)	0.62	9 (7%)	21	14	66, 92, 154, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	FS	117/124 (94%)	0.40	10 (8%)	16 12	67, 92, 140, 186	0
1	FT	124/124 (100%)	0.38	2 (1%)	70 51	63, 92, 150, 173	0
1	FU	124/124 (100%)	0.37	4 (3%)	50 32	66, 92, 154, 183	0
1	FV	117/124 (94%)	0.47	6 (5%)	33 22	67, 92, 140, 186	0
1	FW	124/124 (100%)	0.36	1 (0%)	82 67	63, 92, 150, 173	0
1	FX	124/124 (100%)	0.43	8 (6%)	25 16	66, 92, 154, 183	0
1	FY	117/124 (94%)	0.38	7 (5%)	27 18	67, 92, 140, 186	0
1	FZ	124/124 (100%)	0.34	2 (1%)	70 51	63, 92, 150, 173	0
1	GA	124/124 (100%)	0.81	13 (10%)	11 8	66, 92, 154, 183	0
1	GB	117/124 (94%)	0.77	11 (9%)	14 10	67, 92, 140, 186	0
1	GC	124/124 (100%)	0.51	6 (4%)	35 23	63, 92, 150, 173	0
1	GD	124/124 (100%)	0.60	4 (3%)	50 32	66, 92, 154, 183	0
1	GE	117/124 (94%)	1.05	24 (20%)	2 2	67, 92, 140, 186	0
1	GF	124/124 (100%)	0.66	8 (6%)	25 16	63, 92, 150, 173	0
1	GG	124/124 (100%)	0.60	10 (8%)	18 12	66, 92, 154, 183	0
1	GH	117/124 (94%)	0.74	11 (9%)	14 10	67, 92, 140, 186	0
1	GI	124/124 (100%)	0.49	8 (6%)	25 16	63, 92, 150, 173	0
1	GJ	124/124 (100%)	0.59	9 (7%)	21 14	66, 92, 154, 183	0
1	GK	117/124 (94%)	0.68	12 (10%)	12 8	67, 92, 140, 186	0
1	GL	124/124 (100%)	0.79	11 (8%)	15 11	63, 92, 150, 173	0
1	GM	124/124 (100%)	0.61	9 (7%)	21 14	66, 92, 154, 183	0
1	GN	117/124 (94%)	0.84	13 (11%)	10 7	67, 92, 140, 186	0
1	GO	124/124 (100%)	0.38	4 (3%)	50 32	63, 92, 150, 173	0
1	GP	124/124 (100%)	0.23	2 (1%)	70 51	66, 92, 154, 183	0
1	GQ	117/124 (94%)	0.32	6 (5%)	33 22	67, 92, 140, 186	0
1	GR	124/124 (100%)	0.33	3 (2%)	59 40	63, 92, 150, 173	0
1	GS	124/124 (100%)	0.66	7 (5%)	30 20	66, 92, 154, 183	0
1	GT	117/124 (94%)	0.67	12 (10%)	12 8	67, 92, 140, 186	0
1	GU	124/124 (100%)	0.47	8 (6%)	25 16	63, 92, 150, 173	0
1	GV	124/124 (100%)	0.49	3 (2%)	59 40	66, 92, 154, 183	0
1	GW	117/124 (94%)	0.62	6 (5%)	33 22	67, 92, 140, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	GX	124/124 (100%)	0.63	7 (5%) 30 20	63, 92, 150, 173	0
All	All	21900/22320 (98%)	0.57	1382 (6%) 26 17	63, 92, 152, 186	0

The worst 5 of 1382 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DZ	23	GLN	6.0
1	BV	81	ASN	5.7
1	BK	46	GLU	5.2
1	GE	12	GLU	5.1
1	DW	120	GLY	5.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	ET	201	1/1	0.93	0.06	64,64,64,64	0
2	CA	GJ	201	1/1	0.93	0.07	64,64,64,64	0
2	CA	FO	201	1/1	0.94	0.06	64,64,64,64	0
2	CA	GA	201	1/1	0.94	0.06	64,64,64,64	0
2	CA	EH	201	1/1	0.94	0.07	64,64,64,64	0
2	CA	BK	201	1/1	0.95	0.06	64,64,64,64	0
2	CA	AV	201	1/1	0.95	0.07	64,64,64,64	0
2	CA	EN	201	1/1	0.95	0.06	64,64,64,64	0
2	CA	EQ	201	1/1	0.95	0.06	64,64,64,64	0
2	CA	EE	201	1/1	0.96	0.05	64,64,64,64	0
2	CA	GG	201	1/1	0.96	0.05	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	BN	201	1/1	0.96	0.07	64,64,64,64	0
2	CA	AS	201	1/1	0.97	0.05	64,64,64,64	0
2	CA	AP	201	1/1	0.97	0.04	64,64,64,64	0
2	CA	EK	201	1/1	0.97	0.04	64,64,64,64	0
2	CA	BW	201	1/1	0.97	0.05	64,64,64,64	0
2	CA	CL	201	1/1	0.97	0.04	64,64,64,64	0
2	CA	CO	201	1/1	0.97	0.04	64,64,64,64	0
2	CA	DD	201	1/1	0.97	0.06	64,64,64,64	0
2	CA	FX	201	1/1	0.97	0.06	64,64,64,64	0
2	CA	DM	201	1/1	0.97	0.06	64,64,64,64	0
2	CA	GD	201	1/1	0.97	0.08	64,64,64,64	0
2	CA	DS	201	1/1	0.97	0.09	64,64,64,64	0
2	CA	DY	201	1/1	0.97	0.06	64,64,64,64	0
2	CA	GM	201	1/1	0.97	0.09	64,64,64,64	0
2	CA	AY	201	1/1	0.98	0.03	64,64,64,64	0
2	CA	BB	201	1/1	0.98	0.03	64,64,64,64	0
2	CA	CX	201	1/1	0.98	0.04	64,64,64,64	0
2	CA	BE	201	1/1	0.98	0.04	64,64,64,64	0
2	CA	DG	201	1/1	0.98	0.04	64,64,64,64	0
2	CA	EZ	201	1/1	0.98	0.04	64,64,64,64	0
2	CA	FF	201	1/1	0.98	0.10	64,64,64,64	0
2	CA	FI	201	1/1	0.98	0.04	64,64,64,64	0
2	CA	DJ	201	1/1	0.98	0.04	64,64,64,64	0
2	CA	AD	201	1/1	0.98	0.03	64,64,64,64	0
2	CA	DP	201	1/1	0.98	0.04	64,64,64,64	0
2	CA	AJ	201	1/1	0.98	0.05	64,64,64,64	0
2	CA	DV	201	1/1	0.98	0.03	64,64,64,64	0
2	CA	BT	201	1/1	0.98	0.04	64,64,64,64	0
2	CA	AM	201	1/1	0.98	0.04	64,64,64,64	0
2	CA	BZ	201	1/1	0.99	0.05	64,64,64,64	0
2	CA	CC	201	1/1	0.99	0.03	64,64,64,64	0
2	CA	EW	201	1/1	0.99	0.04	64,64,64,64	0
2	CA	CF	201	1/1	0.99	0.07	64,64,64,64	0
2	CA	FC	201	1/1	0.99	0.07	64,64,64,64	0
2	CA	CI	201	1/1	0.99	0.03	64,64,64,64	0
2	CA	AG	201	1/1	0.99	0.07	64,64,64,64	0
2	CA	FL	201	1/1	0.99	0.03	64,64,64,64	0
2	CA	BQ	201	1/1	0.99	0.02	64,64,64,64	0
2	CA	FR	201	1/1	0.99	0.02	64,64,64,64	0
2	CA	CR	201	1/1	0.99	0.07	64,64,64,64	0
2	CA	EB	201	1/1	0.99	0.02	64,64,64,64	0
2	CA	CU	201	1/1	0.99	0.03	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	BH	201	1/1	0.99	0.04	64,64,64,64	0
2	CA	DA	201	1/1	0.99	0.06	64,64,64,64	0
2	CA	AA	201	1/1	0.99	0.03	64,64,64,64	0
2	CA	GP	201	1/1	0.99	0.02	64,64,64,64	0
2	CA	GS	201	1/1	0.99	0.06	64,64,64,64	0
2	CA	GV	201	1/1	0.99	0.03	64,64,64,64	0
2	CA	FU	201	1/1	1.00	0.03	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.