



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 12, 2020 – 08:58 AM GMT

PDB ID : 6YFE
Title : Virus-like particle of Beihai levi-like virus 19
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on : 2020-03-26
Resolution : 3.79 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.15.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.15.1

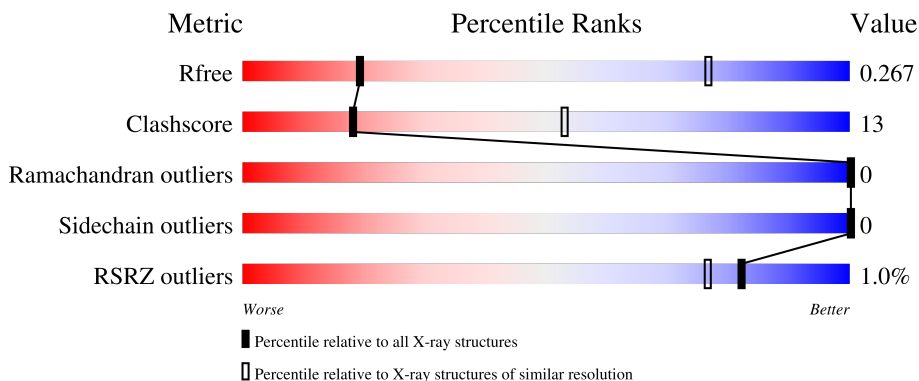
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	134	 74% 26%
1	AB	134	 65% 27% 8%
1	AC	134	 71% 29%
1	AD	134	 81% 19%
1	AE	134	 63% 29% 8%

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Mol	Chain	Length	Quality of chain
1	AF	134	% 64% 36%
1	AG	134	% 72% 28%
1	AH	134	% 64% 28% 8%
1	AI	134	% 70% 30%
1	AJ	134	% 80% 20%
1	AK	134	% 61% 31% 8%
1	AL	134	% 70% 30%
1	AM	134	% 76% 24%
1	AN	134	4% 66% 25% 8%
1	AO	134	% 75% 25%
1	AP	134	% 70% 30%
1	AQ	134	% 64% 28% 8%
1	AR	134	% 69% 31%
1	AS	134	% 69% 31%
1	AT	134	2% 62% 30% 8%
1	AU	134	% 63% 37%
1	AV	134	% 75% 25%
1	AW	134	% 69% 22% 8%
1	AX	134	% 74% 26%
1	AY	134	2% 75% 25%
1	AZ	134	2% 64% 28% 8%
1	BA	134	% 69% 31%
1	BB	134	% 74% 26%
1	BC	134	% 65% 27% 8%
1	BD	134	% 68% 32%

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Mol	Chain	Length	Quality of chain	
1	BE	134	74%	26%
1	BF	134	66%	25% 8%
1	BG	134	68%	32%
1	BH	134	72%	28%
1	BI	134	66%	25% 8%
1	BJ	134	70%	30%
1	BK	134	75%	25%
1	BL	134	72%	20% 8%
1	BM	134	78%	22%
1	BN	134	75%	25%
1	BO	134	66%	26% 8%
1	BP	134	68%	32%
1	BQ	134	74%	26%
1	BR	134	66%	26% 8%
1	BS	134	69%	31%
1	BT	134	73%	27%
1	BU	134	66%	25% 8%
1	BV	134	69%	31%
1	BW	134	74%	26%
1	BX	134	63%	29% 8%
1	BY	134	63%	37%
1	BZ	134	80%	20%
1	CA	134	66%	25% 8%
1	CB	134	69%	31%
1	CC	134	72%	28%











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Mol	Chain	Length	Quality of chain
1	CD	134	2% 66% 25% 8%
1	CE	134	% 70% 30%
1	CF	134	72% 28%
1	CG	134	% 66% 26% 8%
1	CH	134	66% 34%
1	CI	134	% 71% 29%
1	CJ	134	4% 67% 25% 8%
1	CK	134	% 65% 35%
1	CL	134	75% 25%
1	CM	134	% 65% 27% 8%
1	CN	134	% 70% 30%
1	CO	134	74% 26%
1	CP	134	2% 65% 27% 8%
1	CQ	134	69% 31%
1	CR	134	% 76% 24%
1	CS	134	% 72% 20% 8%
1	CT	134	2% 78% 22%
1	CU	134	72% 28%
1	CV	134	2% 72% 20% 8%
1	CW	134	71% 29%
1	CX	134	74% 26%
1	CY	134	% 65% 27% 8%
1	CZ	134	% 69% 31%
1	DA	134	% 74% 26%
1	DB	134	% 67% 25% 8%

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Mol	Chain	Length	Quality of chain
1	DC	134	 70% 30%
1	DD	134	 81% 19%
1	DE	134	 66% 25% 8%
1	DF	134	 69% 31%
1	DG	134	 75% 25%
1	DH	134	 64% 28% 8%
1	DI	134	 76% 24%
1	DJ	134	 75% 25%
1	DK	134	 66% 26% 8%
1	DL	134	 70% 30%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 89070 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called coat protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	AA	134	1014	642	174	198	0	0	0
1	AB	123	940	599	162	179	0	0	0
1	AC	134	1014	642	174	198	0	0	0
1	AD	134	1014	642	174	198	0	0	0
1	AE	123	940	599	162	179	0	0	0
1	AF	134	1014	642	174	198	0	0	0
1	AG	134	1014	642	174	198	0	0	0
1	AH	123	940	599	162	179	0	0	0
1	AI	134	1014	642	174	198	0	0	0
1	AJ	134	1014	642	174	198	0	0	0
1	AK	123	940	599	162	179	0	0	0
1	AL	134	1014	642	174	198	0	0	0
1	AM	134	1014	642	174	198	0	0	0
1	AN	123	940	599	162	179	0	0	0
1	AO	134	1014	642	174	198	0	0	0
1	AP	134	1014	642	174	198	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	AQ	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	AR	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	AS	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	AT	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	AU	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	AV	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	AW	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	AX	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	AY	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	AZ	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	BA	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BB	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BC	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	BD	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BE	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BF	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	BG	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BH	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BI	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	BJ	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BK	134	Total	C	N	O	0	0	0
			1014	642	174	198			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	BL	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	BM	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BN	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BO	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	BP	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BQ	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BR	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	BS	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BT	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BU	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	BV	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BW	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BX	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	BY	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	BZ	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CA	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	CB	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CC	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CD	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	CE	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CF	134	Total	C	N	O	0	0	0
			1014	642	174	198			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	CG	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	CH	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CI	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CJ	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	CK	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CL	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CM	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	CN	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CO	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CP	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	CQ	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CR	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CS	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	CT	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CU	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CV	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	CW	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CX	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	CY	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	CZ	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	DA	134	Total	C	N	O	0	0	0
			1014	642	174	198			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	DB	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	DC	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	DD	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	DE	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	DF	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	DG	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	DH	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	DI	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	DJ	134	Total	C	N	O	0	0	0
			1014	642	174	198			
1	DK	123	Total	C	N	O	0	0	0
			940	599	162	179			
1	DL	134	Total	C	N	O	0	0	0
			1014	642	174	198			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AK	1	Total	Ca	0	0
			1	1		
2	AB	1	Total	Ca	0	0
			1	1		
2	BL	1	Total	Ca	0	0
			1	1		
2	CV	1	Total	Ca	0	0
			1	1		
2	AW	1	Total	Ca	0	0
			1	1		
2	AN	1	Total	Ca	0	0
			1	1		
2	BI	1	Total	Ca	0	0
			1	1		
2	CA	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BB	1	Total Ca 1 1	0	0
2	BT	1	Total Ca 1 1	0	0
2	AE	1	Total Ca 1 1	0	0
2	BF	1	Total Ca 1 1	0	0
2	BX	1	Total Ca 1 1	0	0
2	AA	1	Total Ca 1 1	0	0
2	BC	1	Total Ca 1 1	0	0
2	AM	1	Total Ca 1 1	0	0
2	CC	1	Total Ca 1 1	0	0
2	CJ	1	Total Ca 1 1	0	0
2	BR	1	Total Ca 1 1	0	0
2	AZ	1	Total Ca 1 1	0	0
2	BK	1	Total Ca 1 1	0	0
2	CF	1	Total Ca 1 1	0	0
2	AG	1	Total Ca 1 1	0	0
2	AQ	1	Total Ca 1 1	0	0
2	AH	1	Total Ca 1 1	0	0
2	AC	1	Total Ca 1 1	0	0
2	CD	1	Total Ca 1 1	0	0
2	CS	1	Total Ca 1 1	0	0
2	AF	1	Total Ca 1 1	0	0

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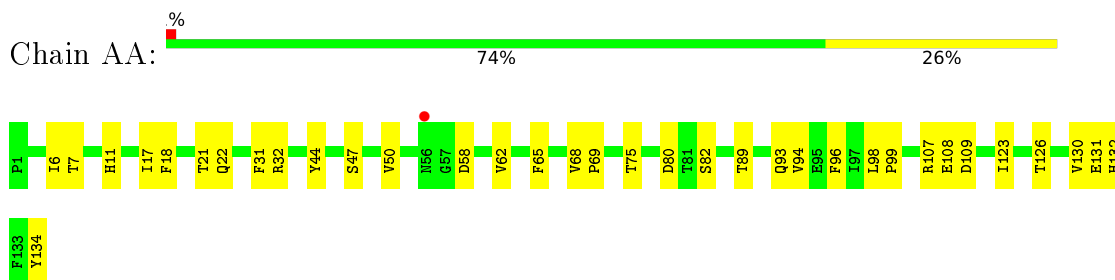
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BH	1	Total	Ca	0	0
			1	1		

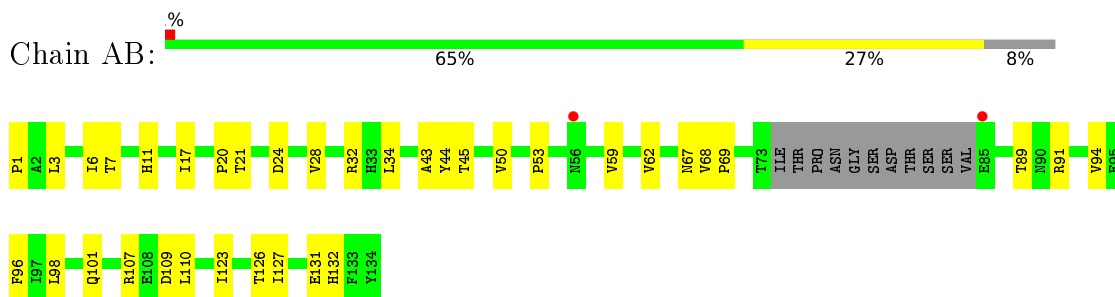
3 Residue-property plots [i](#)

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.

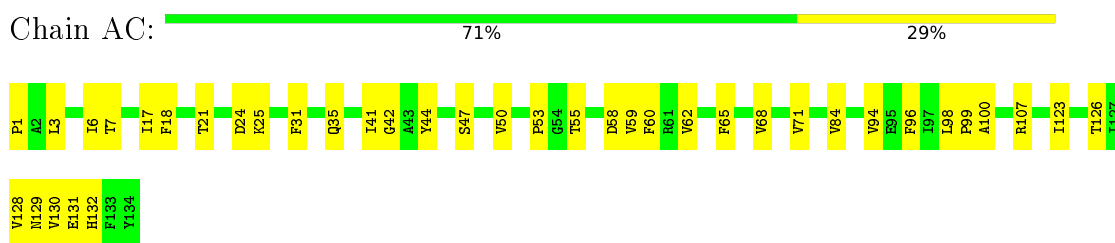
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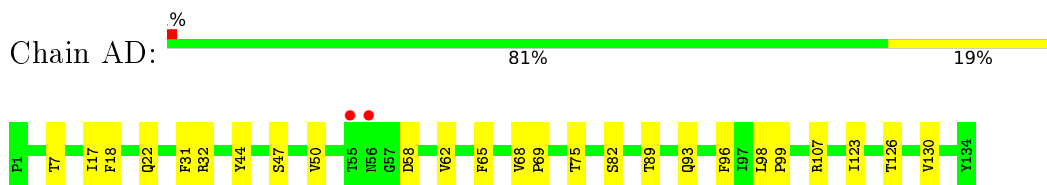
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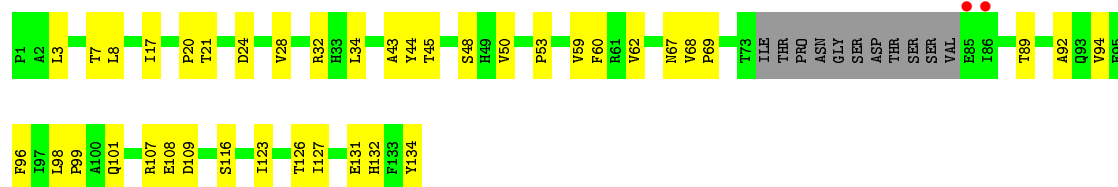
- Molecule 1: coat protein



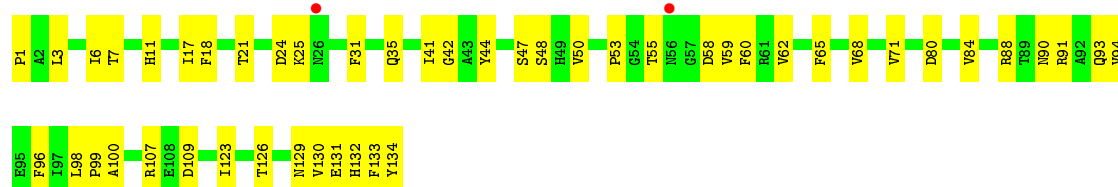
- Molecule 1: coat protein



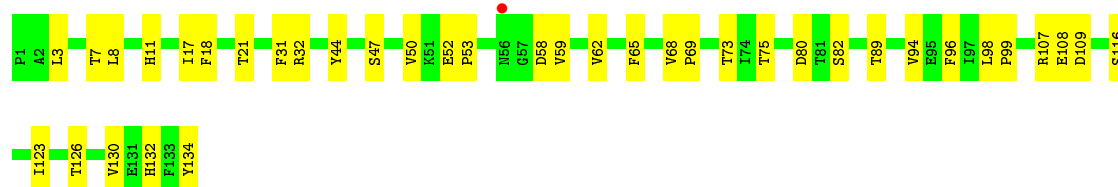
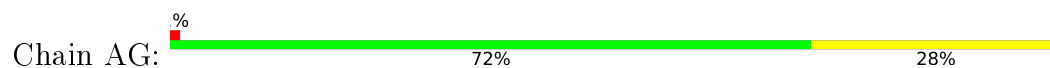
- Molecule 1: coat protein



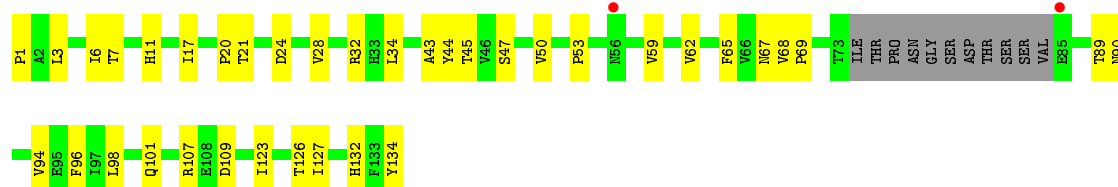
- Molecule 1: coat protein



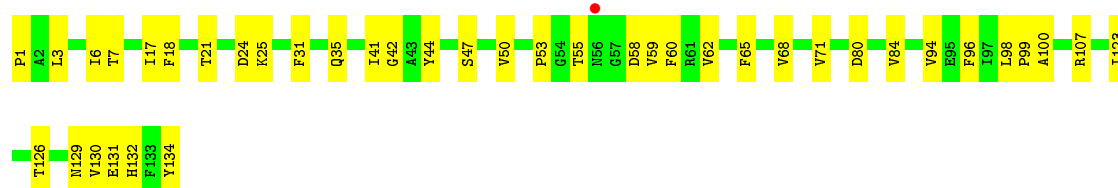
- Molecule 1: coat protein



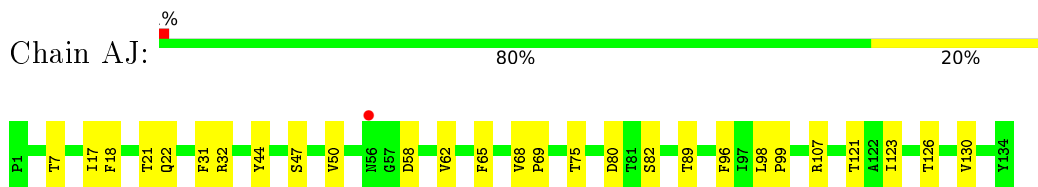
- Molecule 1: coat protein



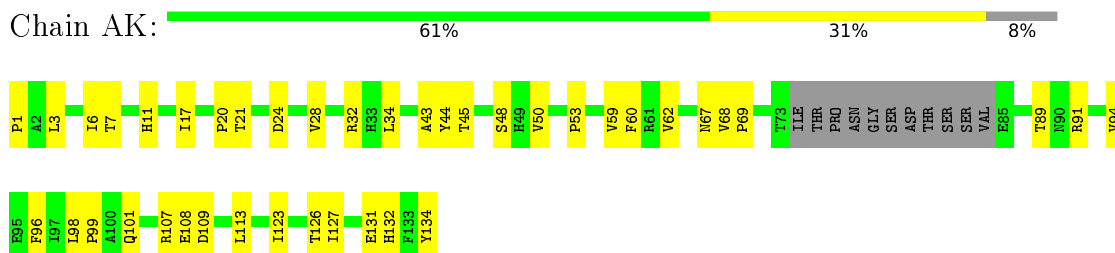
- Molecule 1: coat protein



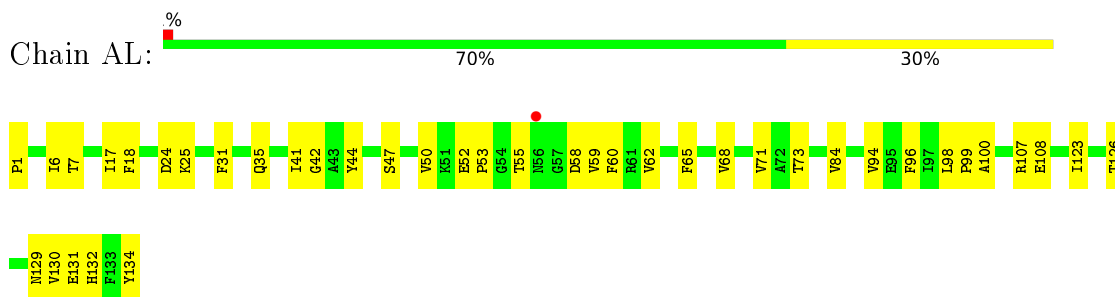
• Molecule 1: coat protein



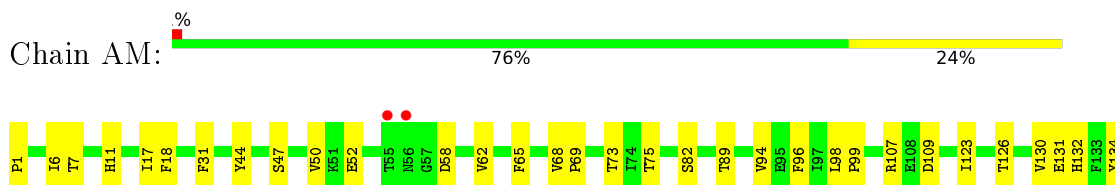
• Molecule 1: coat protein



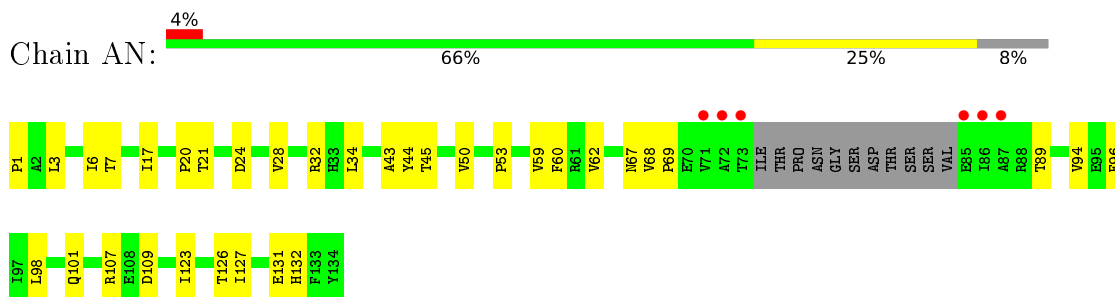
• Molecule 1: coat protein



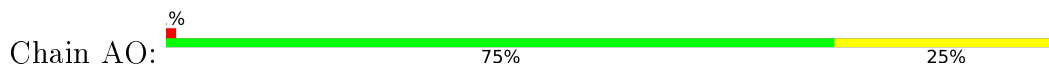
• Molecule 1: coat protein

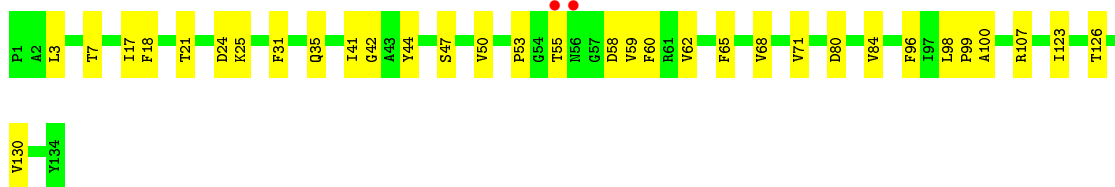


• Molecule 1: coat protein

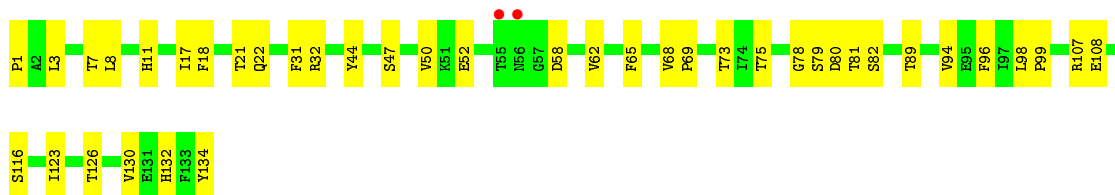


• Molecule 1: coat protein

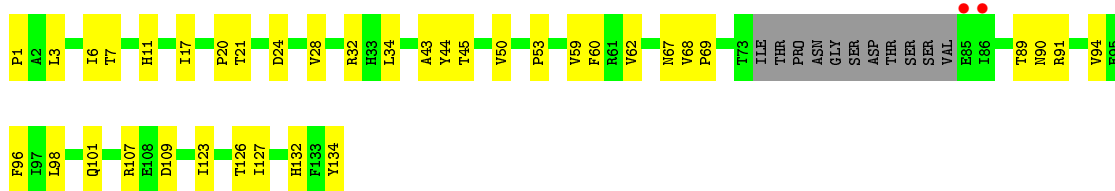




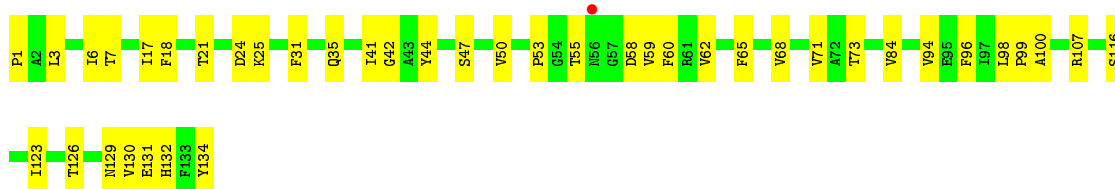
- Molecule 1: coat protein



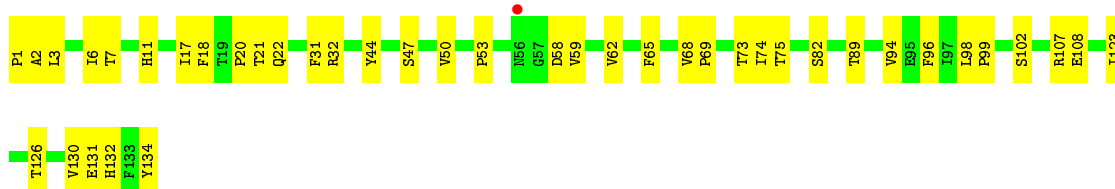
- Molecule 1: coat protein



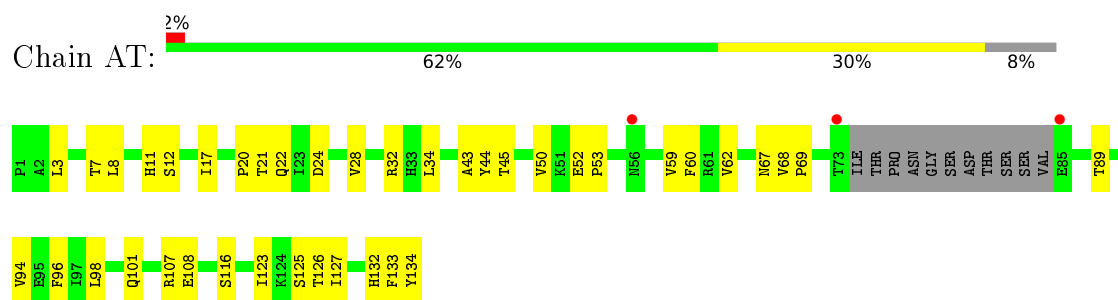
- Molecule 1: coat protein



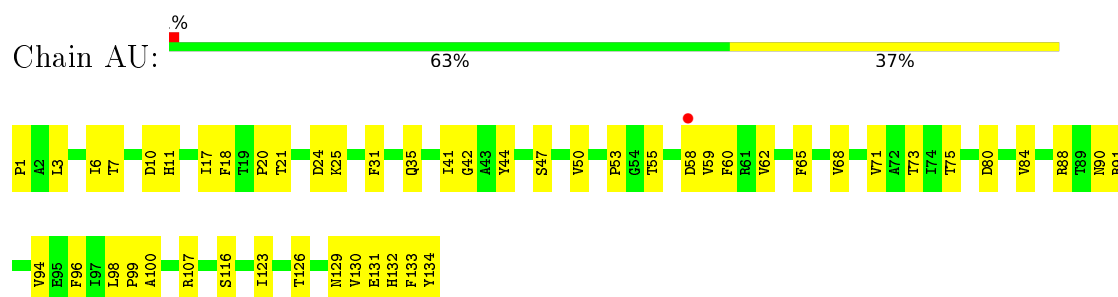
- Molecule 1: coat protein



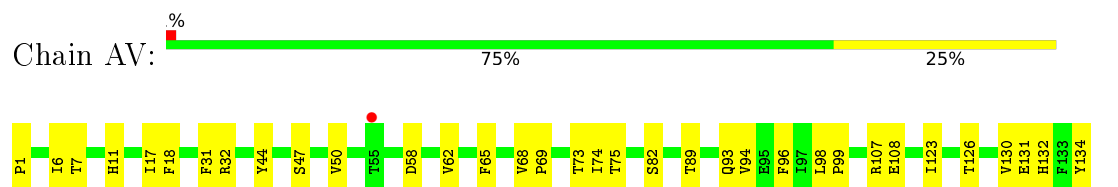
- Molecule 1: coat protein



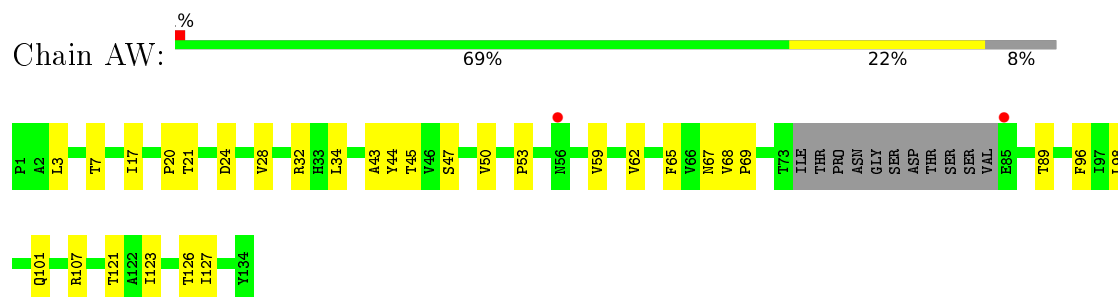
- Molecule 1: coat protein



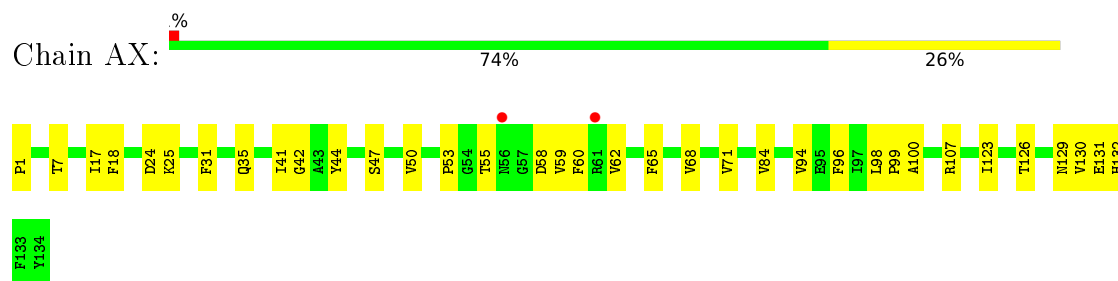
- Molecule 1: coat protein



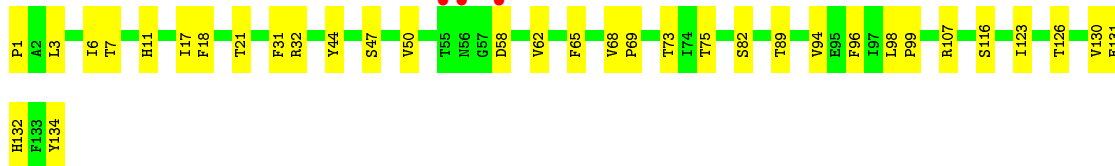
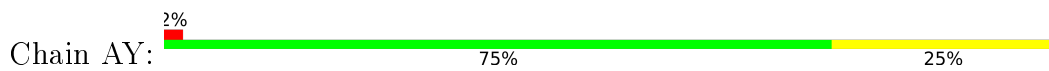
- Molecule 1: coat protein



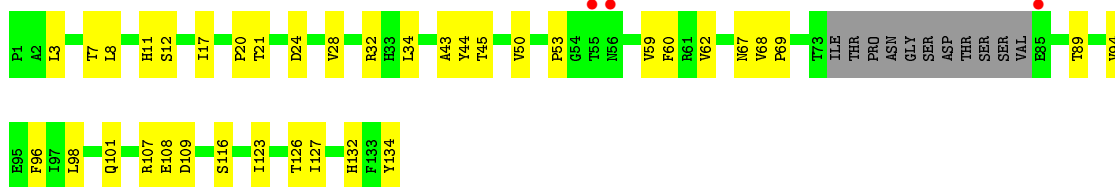
- Molecule 1: coat protein



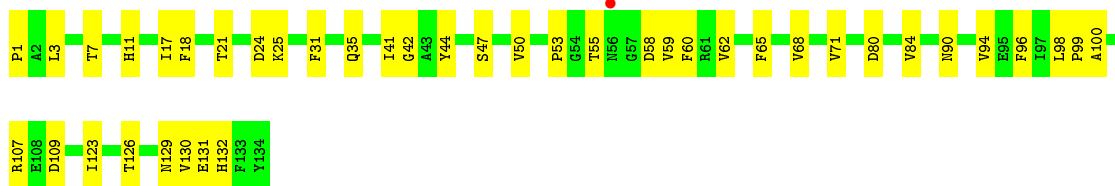
- Molecule 1: coat protein



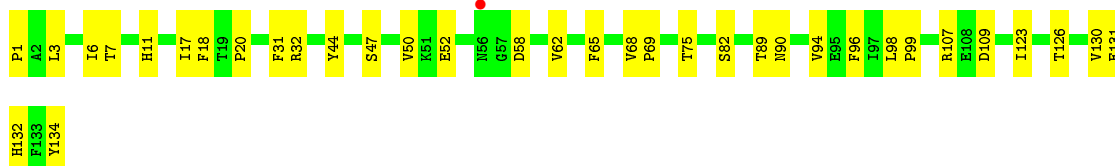
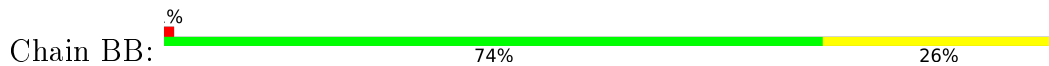
• Molecule 1: coat protein



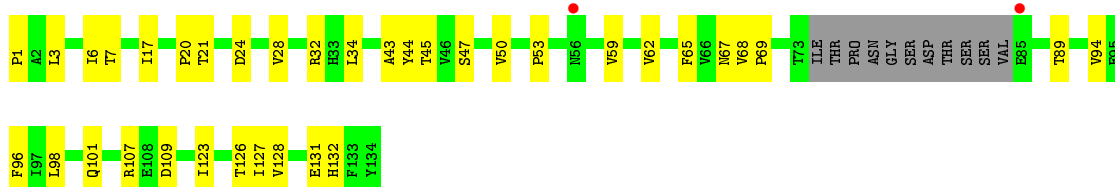
• Molecule 1: coat protein



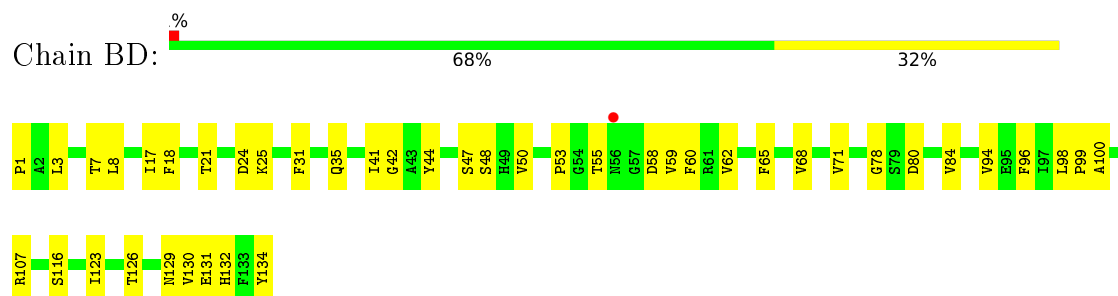
• Molecule 1: coat protein



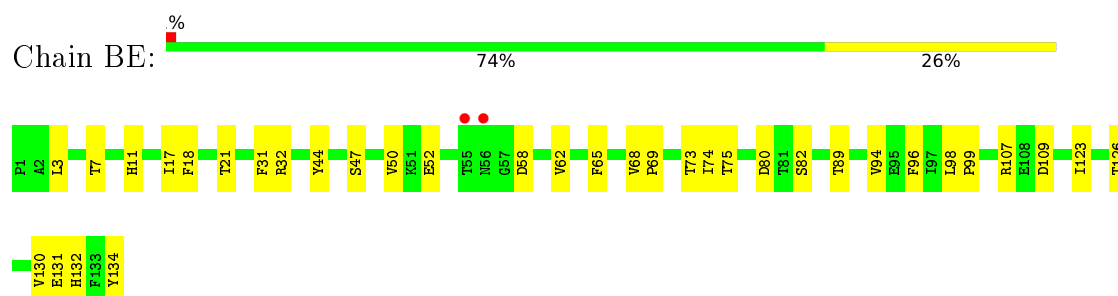
• Molecule 1: coat protein



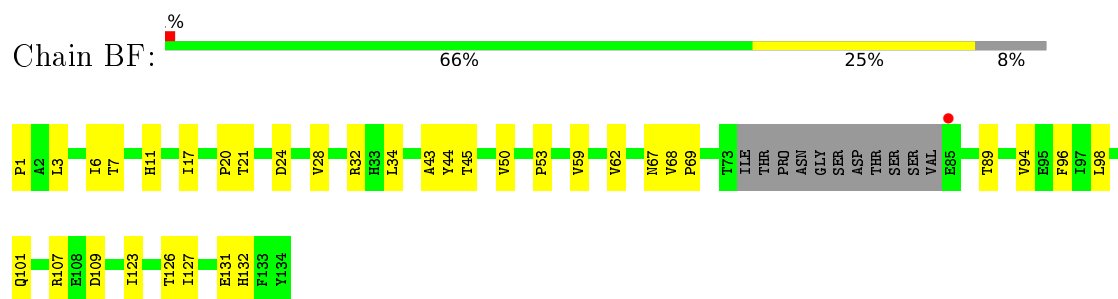
- Molecule 1: coat protein



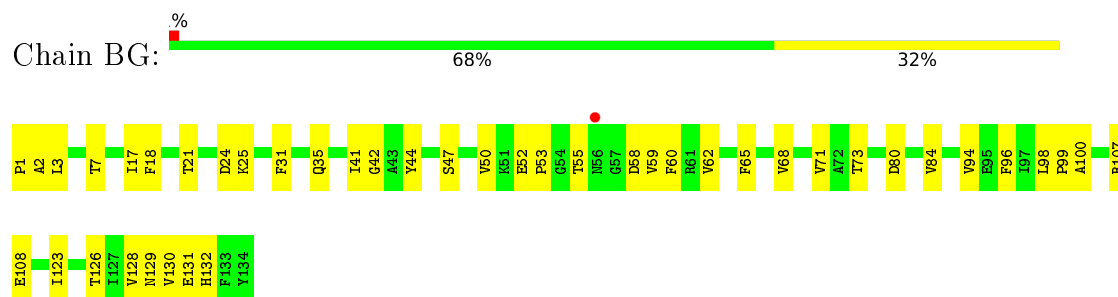
- Molecule 1: coat protein



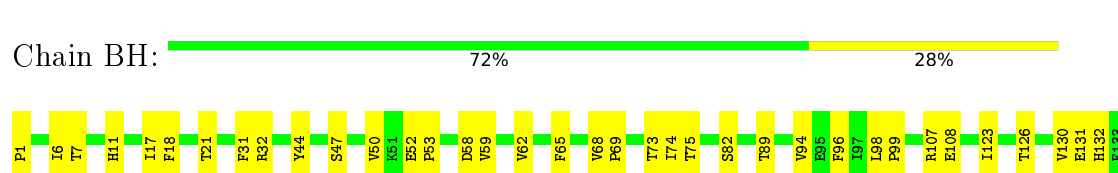
- Molecule 1: coat protein



- Molecule 1: coat protein

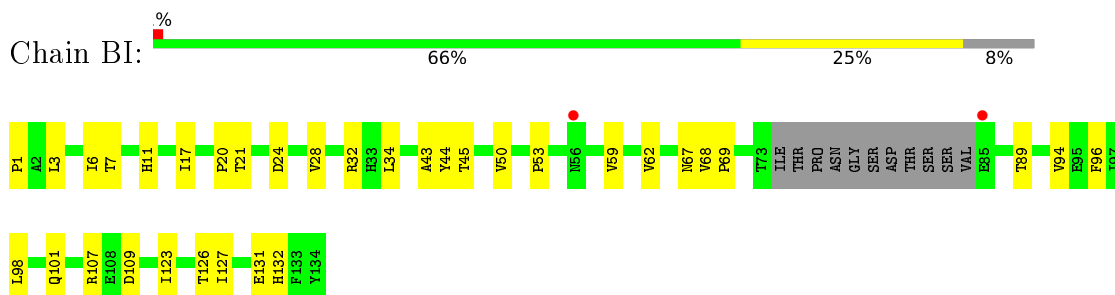


- Molecule 1: coat protein

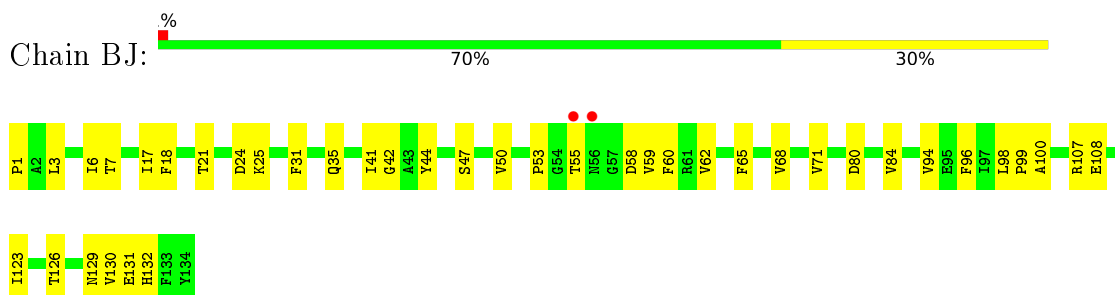


Y134

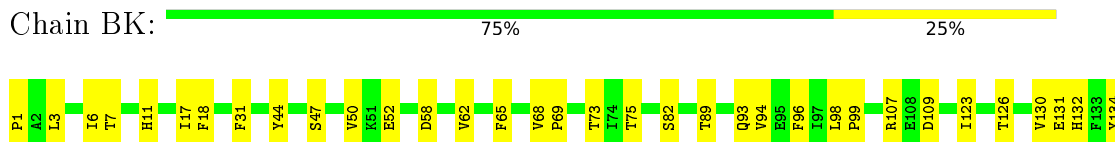
- Molecule 1: coat protein



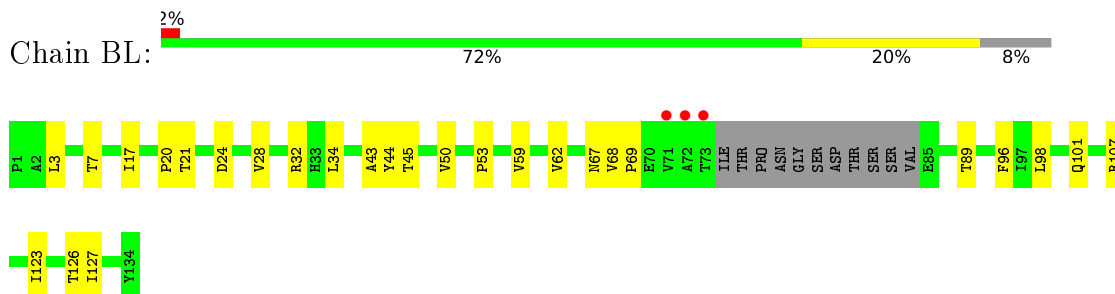
- Molecule 1: coat protein



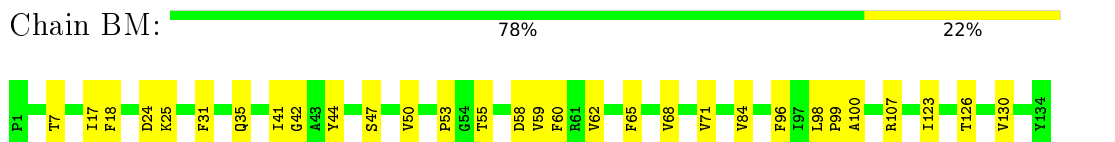
- Molecule 1: coat protein



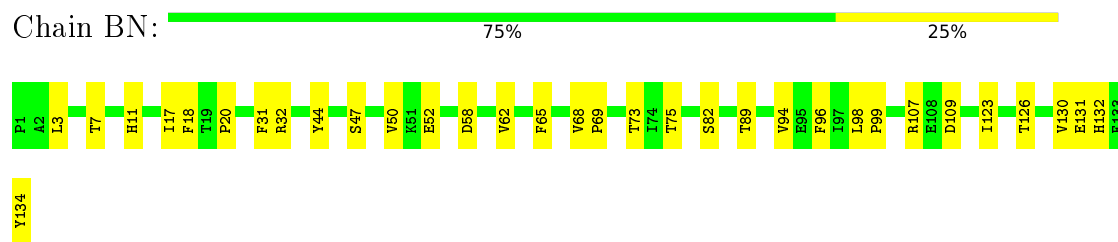
- Molecule 1: coat protein



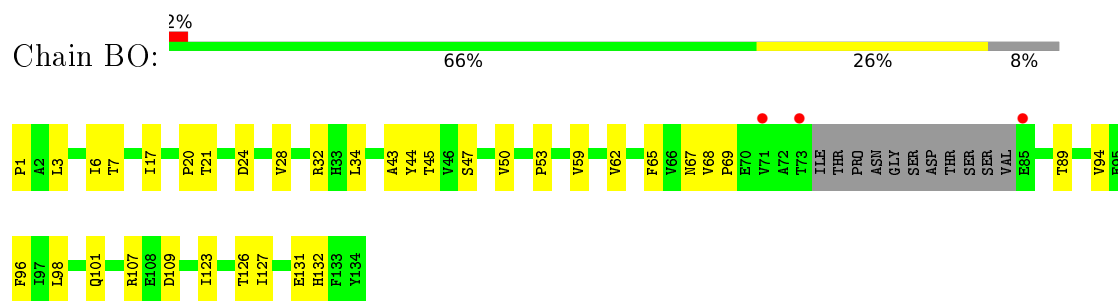
- Molecule 1: coat protein



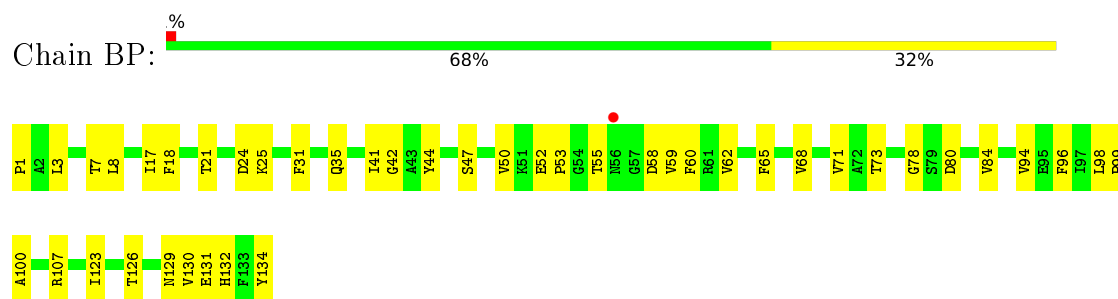
- Molecule 1: coat protein



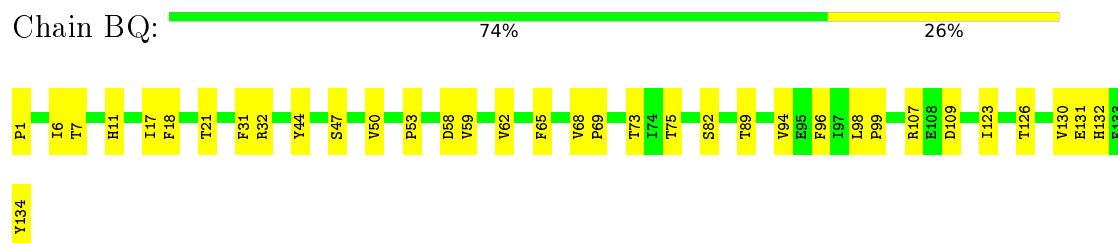
- Molecule 1: coat protein



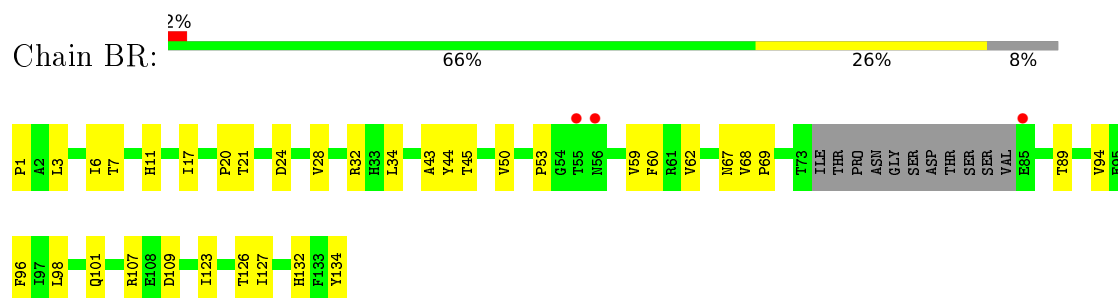
- Molecule 1: coat protein



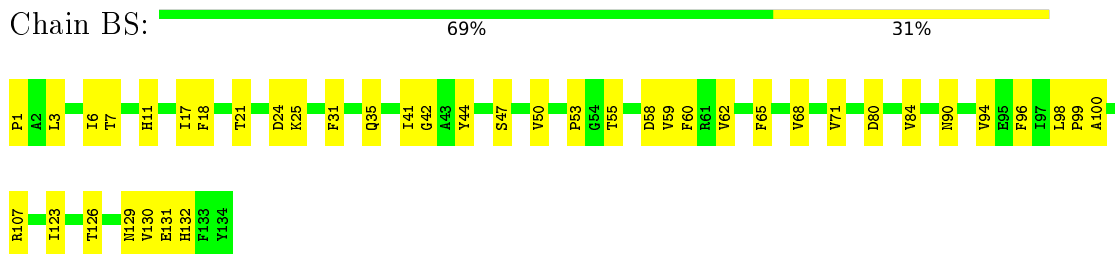
- Molecule 1: coat protein



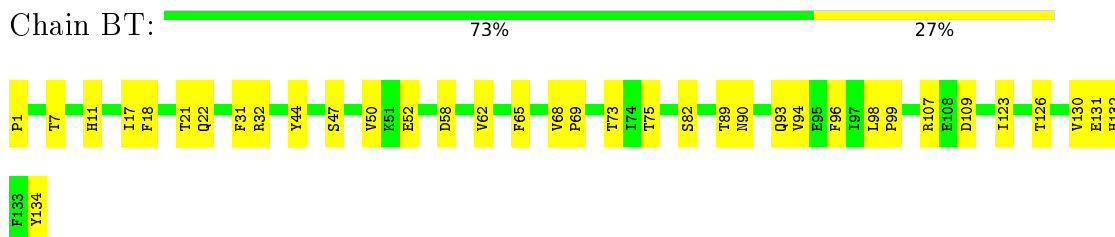
- Molecule 1: coat protein



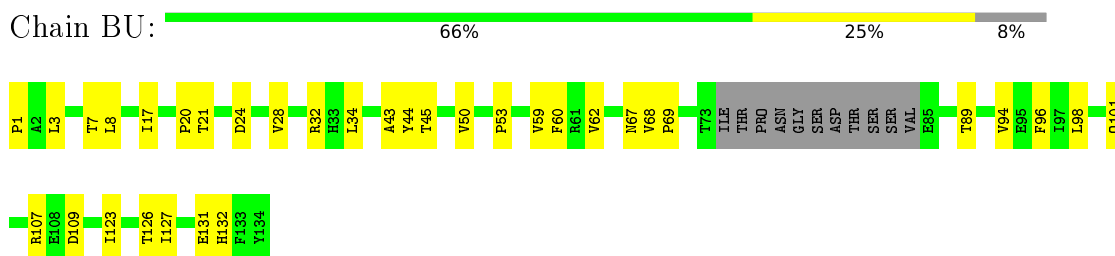
- Molecule 1: coat protein



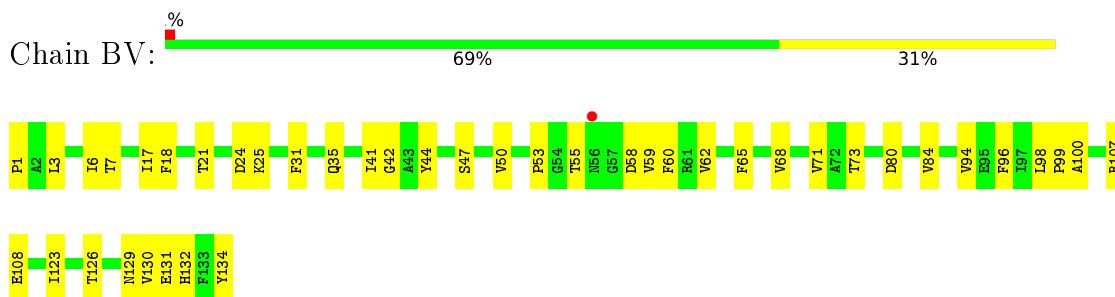
- Molecule 1: coat protein



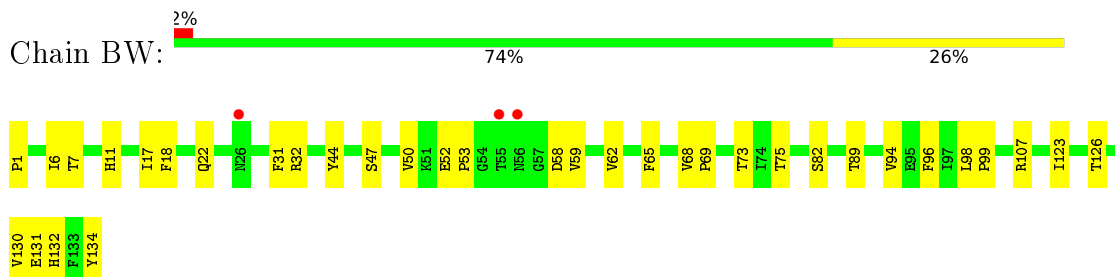
- Molecule 1: coat protein



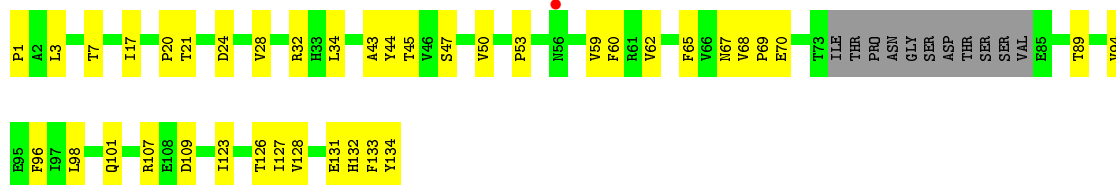
- Molecule 1: coat protein



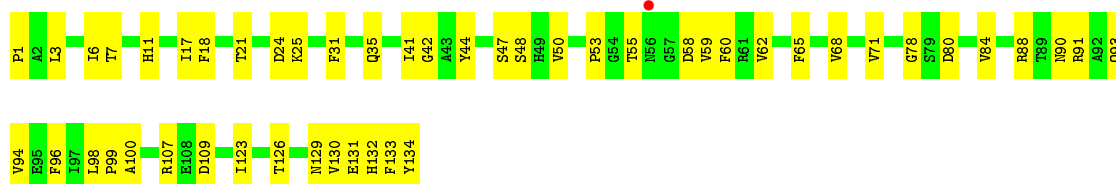
- Molecule 1: coat protein



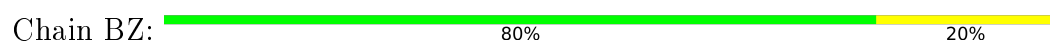
- Molecule 1: coat protein



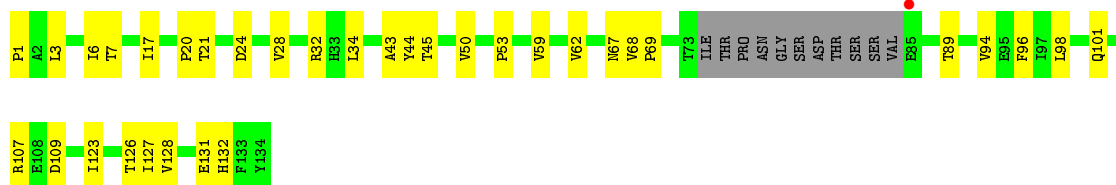
- Molecule 1: coat protein



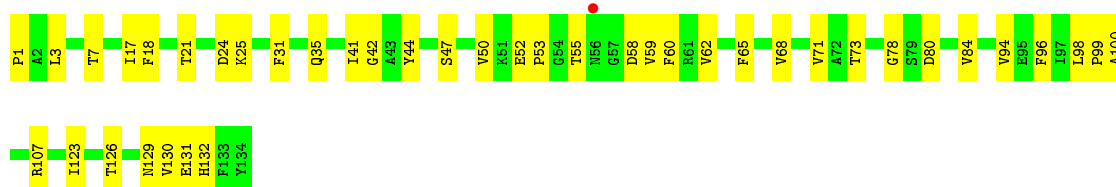
- Molecule 1: coat protein



- Molecule 1: coat protein

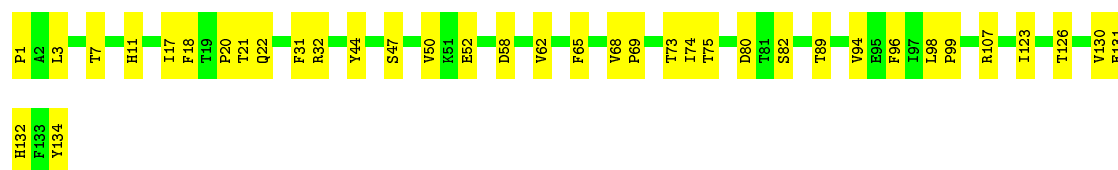


- Molecule 1: coat protein



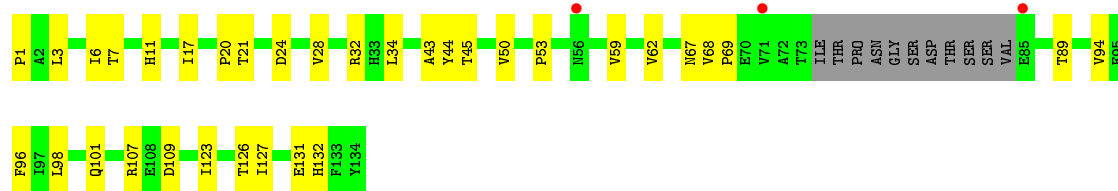
- Molecule 1: coat protein

Chain CC:  72% 28%




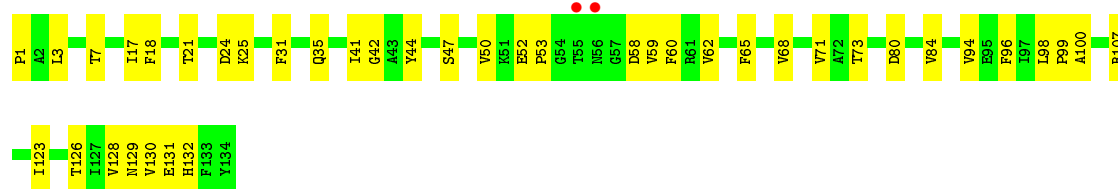
• Molecule 1: coat protein

Chain CD:  2% 66% 25% 8%



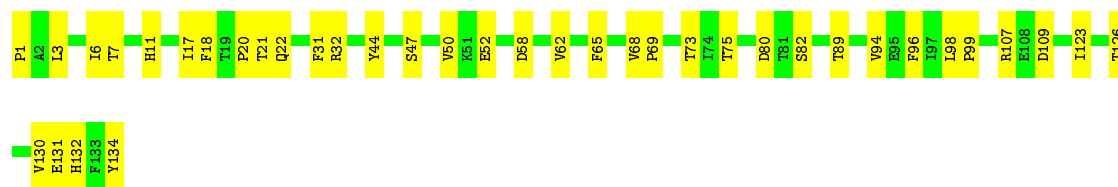
• Molecule 1: coat protein

Chain CE:  70% 30%



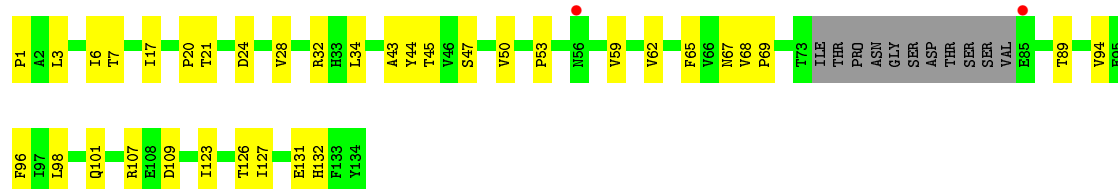
• Molecule 1: coat protein

Chain CF:  72% 28%



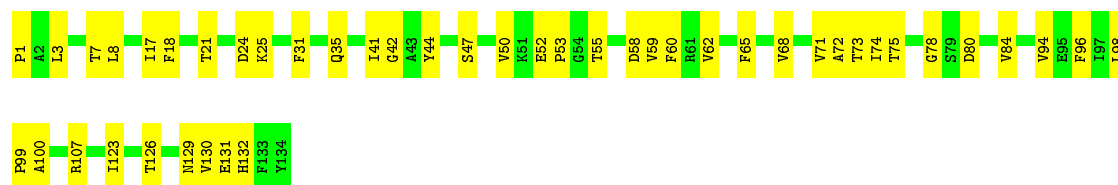
• Molecule 1: coat protein

Chain CG:  66% 26% 8%




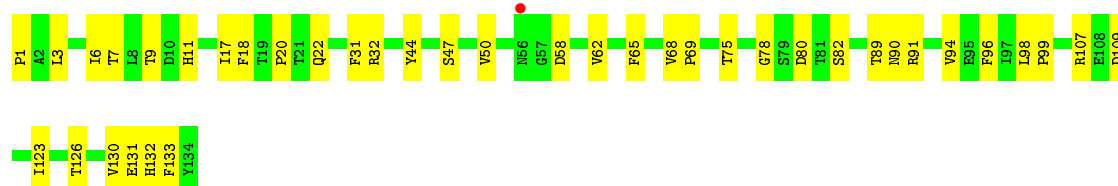
- Molecule 1: coat protein

Chain CH:  66% 34%



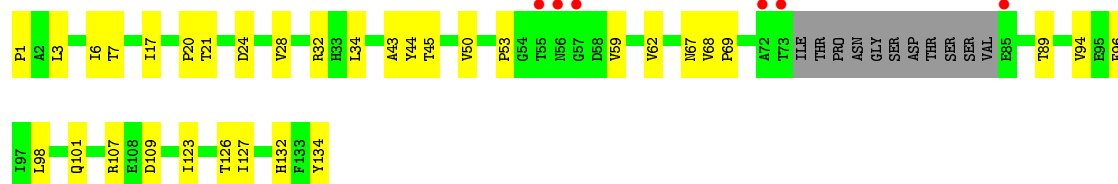
- Molecule 1: coat protein

Chain CI:  71% 29%



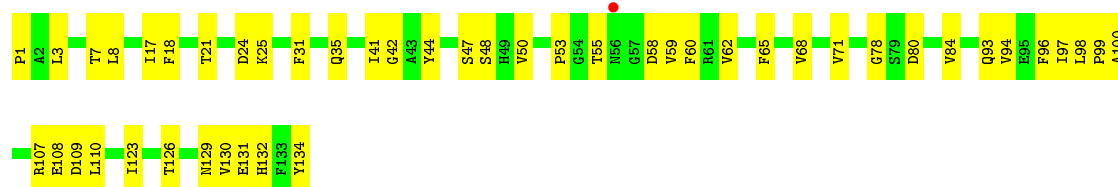
- Molecule 1: coat protein

Chain CJ:  4% 67% 25% 8%




- Molecule 1: coat protein

Chain CK:  65% 35%

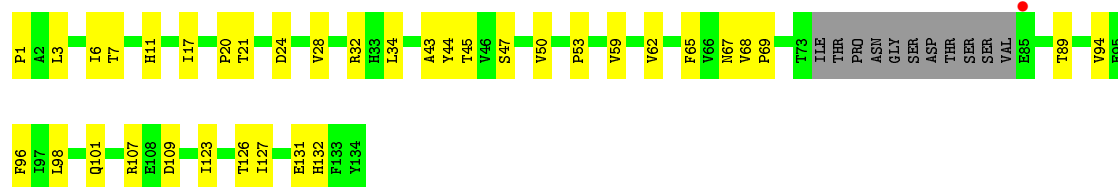


- Molecule 1: coat protein

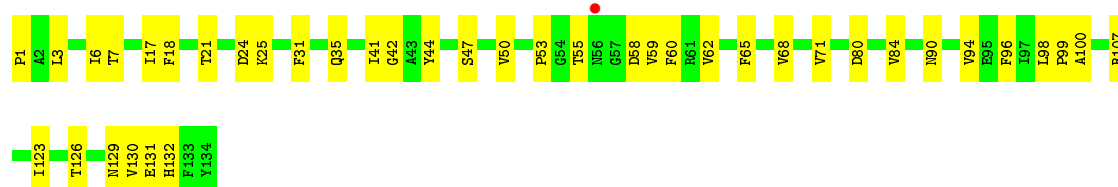
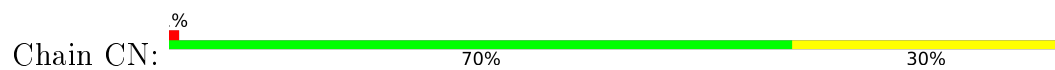
Chain CL:  75% 25%



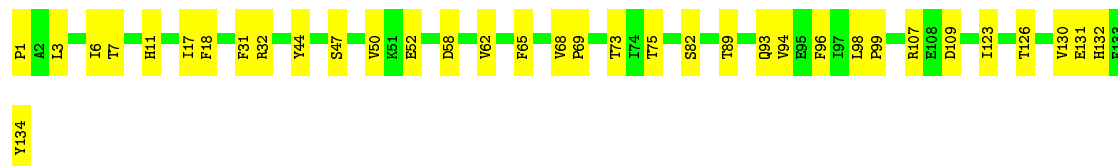
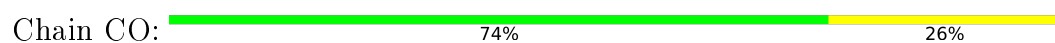
- Molecule 1: coat protein



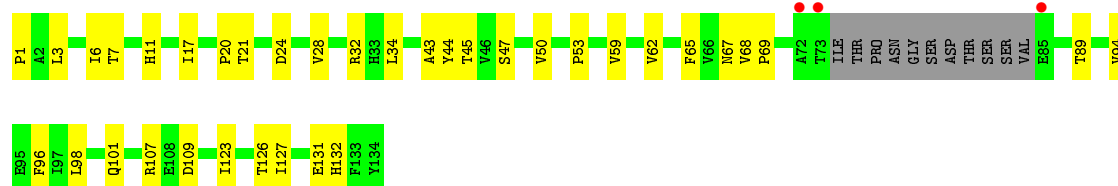
- Molecule 1: coat protein



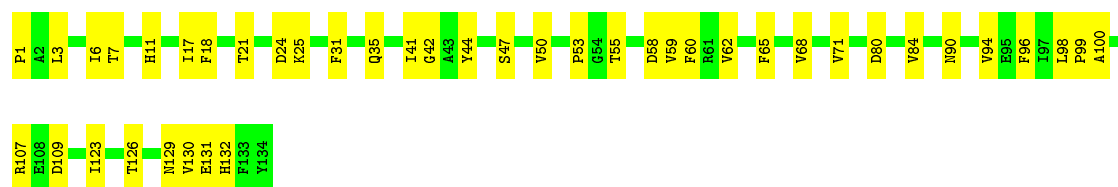
- Molecule 1: coat protein



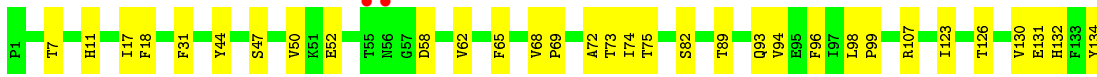
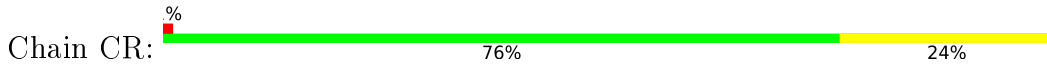
- Molecule 1: coat protein



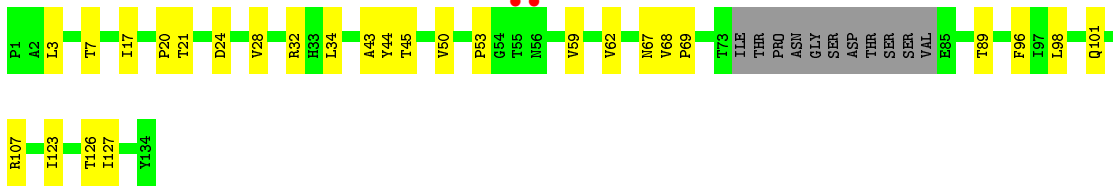
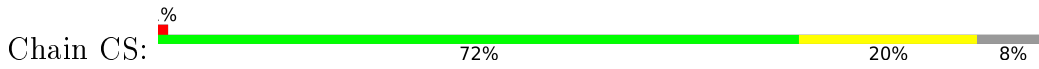
- Molecule 1: coat protein



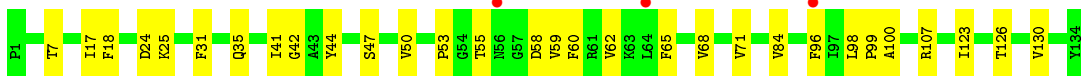
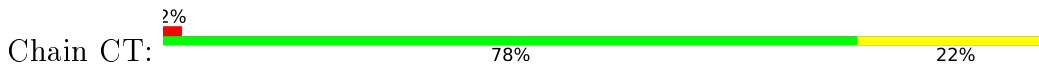
• Molecule 1: coat protein



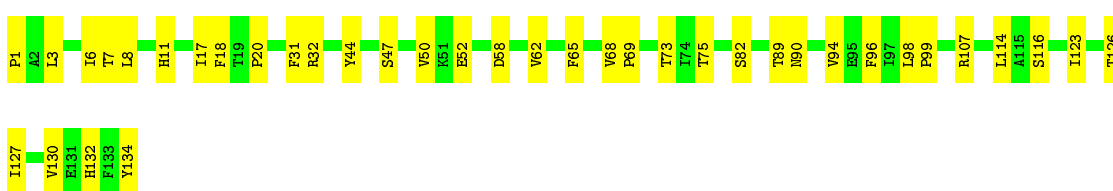
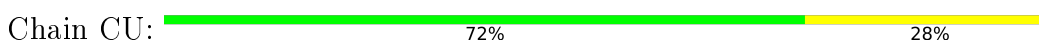
• Molecule 1: coat protein



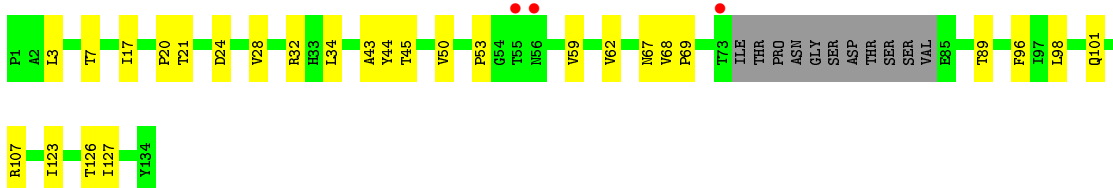
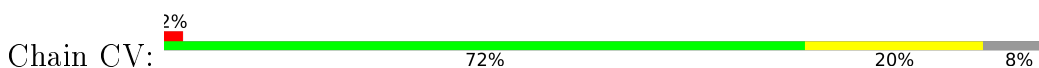
• Molecule 1: coat protein



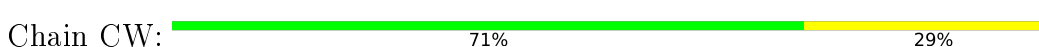
• Molecule 1: coat protein

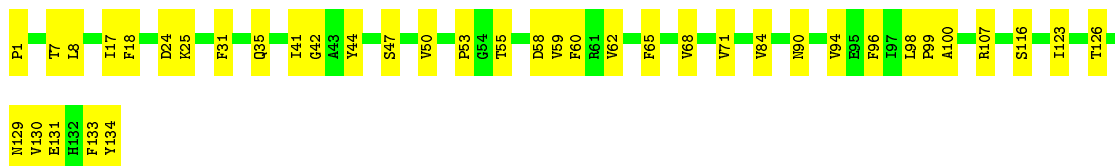


• Molecule 1: coat protein

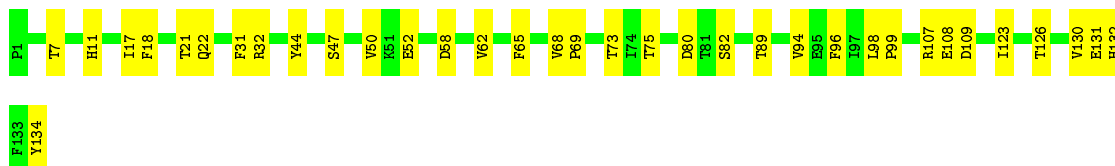
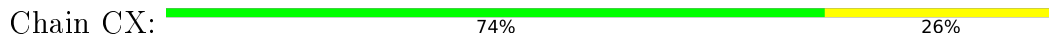


• Molecule 1: coat protein

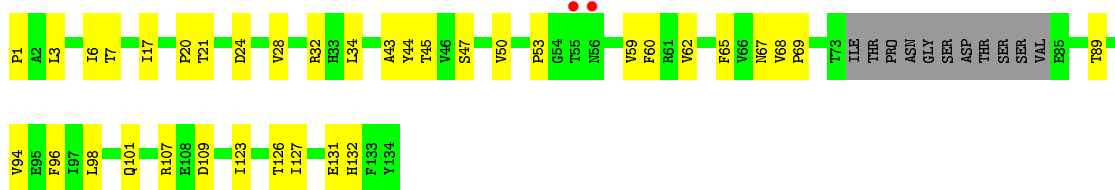




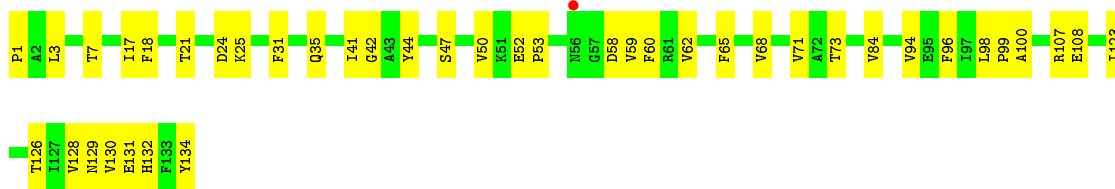
• Molecule 1: coat protein



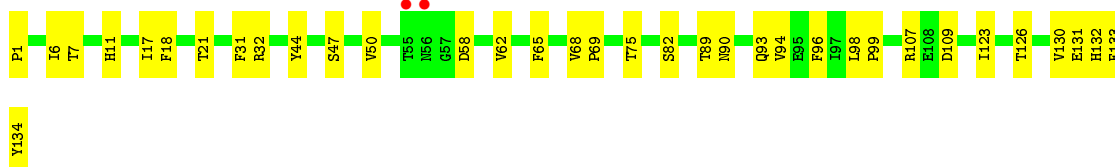
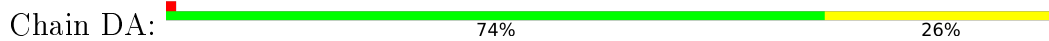
• Molecule 1: coat protein



• Molecule 1: coat protein

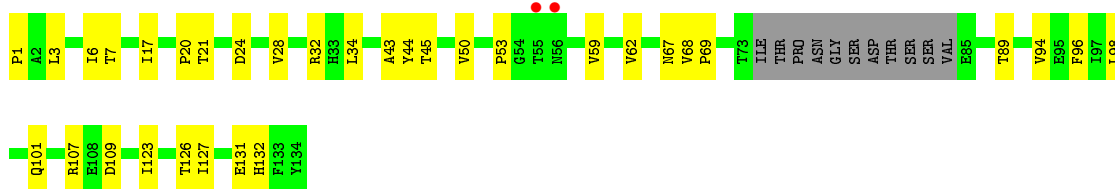


• Molecule 1: coat protein

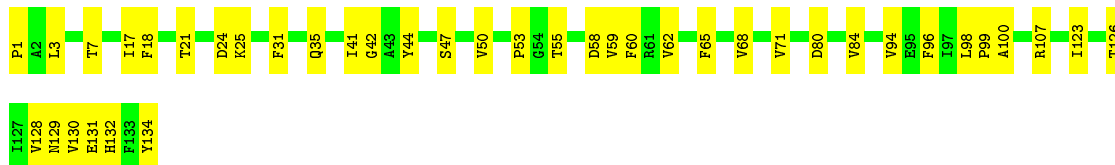


• Molecule 1: coat protein

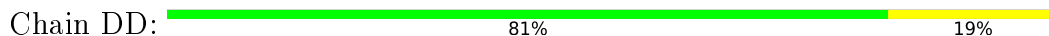




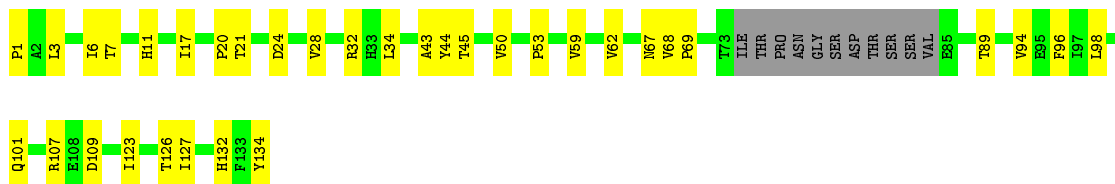
• Molecule 1: coat protein



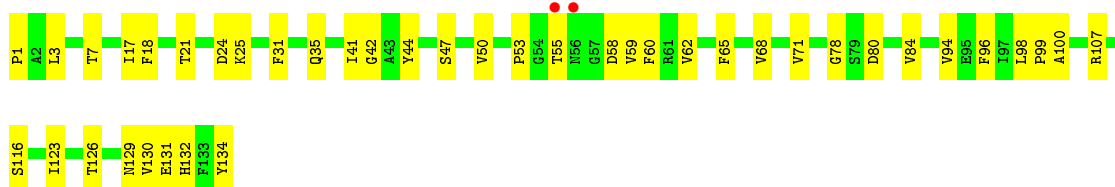
• Molecule 1: coat protein



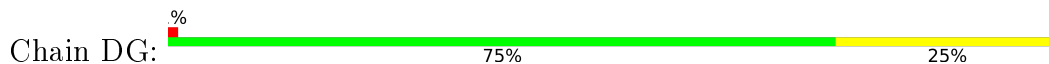
• Molecule 1: coat protein



• Molecule 1: coat protein



• Molecule 1: coat protein

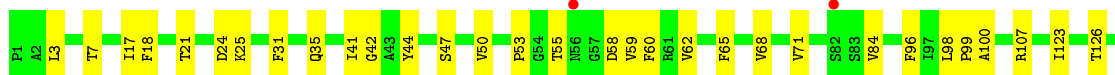
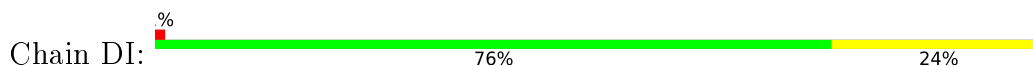




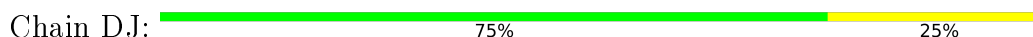
• Molecule 1: coat protein



• Molecule 1: coat protein



• Molecule 1: coat protein



• Molecule 1: coat protein



• Molecule 1: coat protein



I123	I124	I125	I126	I127	I128
M129	V130	E131	H132	F133	Y134

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	298.11Å 325.05Å 346.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.39 – 3.79 49.43 – 3.79	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.39-3.79) 98.0 (49.43-3.79)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.77Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.261 , 0.267 0.262 , 0.267	Depositor DCC
R_{free} test set	9977 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	102.6	Xtrriage
Anisotropy	0.195	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	89070	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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	0.29	0/1034	0.51	0/1412
1	AB	0.33	0/958	0.52	0/1305
1	AC	0.31	0/1034	0.52	0/1412
1	AD	0.29	0/1034	0.51	0/1412
1	AE	0.33	0/958	0.52	0/1305
1	AF	0.31	0/1034	0.52	0/1412
1	AG	0.29	0/1034	0.51	0/1412
1	AH	0.33	0/958	0.52	0/1305
1	AI	0.31	0/1034	0.52	0/1412
1	AJ	0.29	0/1034	0.51	0/1412
1	AK	0.33	0/958	0.52	0/1305
1	AL	0.31	0/1034	0.52	0/1412
1	AM	0.29	0/1034	0.51	0/1412
1	AN	0.33	0/958	0.52	0/1305
1	AO	0.31	0/1034	0.52	0/1412
1	AP	0.29	0/1034	0.51	0/1412
1	AQ	0.33	0/958	0.52	0/1305
1	AR	0.31	0/1034	0.52	0/1412
1	AS	0.29	0/1034	0.51	0/1412
1	AT	0.33	0/958	0.52	0/1305
1	AU	0.31	0/1034	0.52	0/1412
1	AV	0.29	0/1034	0.51	0/1412
1	AW	0.33	0/958	0.52	0/1305
1	AX	0.31	0/1034	0.52	0/1412
1	AY	0.29	0/1034	0.51	0/1412
1	AZ	0.33	0/958	0.52	0/1305
1	BA	0.31	0/1034	0.52	0/1412
1	BB	0.29	0/1034	0.51	0/1412
1	BC	0.33	0/958	0.52	0/1305
1	BD	0.31	0/1034	0.52	0/1412
1	BE	0.29	0/1034	0.51	0/1412
1	BF	0.33	0/958	0.52	0/1305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BG	0.31	0/1034	0.52	0/1412
1	BH	0.29	0/1034	0.51	0/1412
1	BI	0.33	0/958	0.52	0/1305
1	BJ	0.31	0/1034	0.52	0/1412
1	BK	0.29	0/1034	0.51	0/1412
1	BL	0.33	0/958	0.52	0/1305
1	BM	0.31	0/1034	0.52	0/1412
1	BN	0.29	0/1034	0.51	0/1412
1	BO	0.33	0/958	0.52	0/1305
1	BP	0.31	0/1034	0.52	0/1412
1	BQ	0.29	0/1034	0.51	0/1412
1	BR	0.33	0/958	0.52	0/1305
1	BS	0.31	0/1034	0.52	0/1412
1	BT	0.29	0/1034	0.51	0/1412
1	BU	0.33	0/958	0.52	0/1305
1	BV	0.31	0/1034	0.52	0/1412
1	BW	0.29	0/1034	0.51	0/1412
1	BX	0.33	0/958	0.52	0/1305
1	BY	0.31	0/1034	0.52	0/1412
1	BZ	0.29	0/1034	0.51	0/1412
1	CA	0.33	0/958	0.52	0/1305
1	CB	0.31	0/1034	0.52	0/1412
1	CC	0.29	0/1034	0.51	0/1412
1	CD	0.33	0/958	0.52	0/1305
1	CE	0.31	0/1034	0.52	0/1412
1	CF	0.29	0/1034	0.51	0/1412
1	CG	0.33	0/958	0.52	0/1305
1	CH	0.31	0/1034	0.52	0/1412
1	CI	0.29	0/1034	0.51	0/1412
1	CJ	0.33	0/958	0.52	0/1305
1	CK	0.31	0/1034	0.52	0/1412
1	CL	0.29	0/1034	0.51	0/1412
1	CM	0.33	0/958	0.52	0/1305
1	CN	0.31	0/1034	0.52	0/1412
1	CO	0.29	0/1034	0.51	0/1412
1	CP	0.33	0/958	0.52	0/1305
1	CQ	0.31	0/1034	0.52	0/1412
1	CR	0.29	0/1034	0.51	0/1412
1	CS	0.33	0/958	0.52	0/1305
1	CT	0.31	0/1034	0.52	0/1412
1	CU	0.29	0/1034	0.51	0/1412
1	CV	0.33	0/958	0.52	0/1305
1	CW	0.31	0/1034	0.52	0/1412

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CX	0.29	0/1034	0.51	0/1412
1	CY	0.33	0/958	0.52	0/1305
1	CZ	0.31	0/1034	0.52	0/1412
1	DA	0.29	0/1034	0.51	0/1412
1	DB	0.33	0/958	0.52	0/1305
1	DC	0.31	0/1034	0.52	0/1412
1	DD	0.29	0/1034	0.51	0/1412
1	DE	0.33	0/958	0.52	0/1305
1	DF	0.31	0/1034	0.52	0/1412
1	DG	0.29	0/1034	0.51	0/1412
1	DH	0.33	0/958	0.52	0/1305
1	DI	0.31	0/1034	0.52	0/1412
1	DJ	0.29	0/1034	0.51	0/1412
1	DK	0.33	0/958	0.52	0/1305
1	DL	0.31	0/1034	0.52	0/1412
All	All	0.31	0/90780	0.52	0/123870

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	1014	0	1020	44	0
1	AB	940	0	950	38	0
1	AC	1014	0	1020	41	0
1	AD	1014	0	1020	17	0
1	AE	940	0	950	47	0
1	AF	1014	0	1020	65	0
1	AG	1014	0	1020	38	0
1	AH	940	0	950	36	0
1	AI	1014	0	1020	39	0
1	AJ	1014	0	1020	19	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AK	940	0	950	46	0
1	AL	1014	0	1020	39	0
1	AM	1014	0	1020	28	0
1	AN	940	0	950	33	0
1	AO	1014	0	1020	24	0
1	AP	1014	0	1020	62	0
1	AQ	940	0	950	42	0
1	AR	1014	0	1020	40	0
1	AS	1014	0	1020	43	0
1	AT	940	0	950	46	1
1	AU	1014	0	1020	67	0
1	AV	1014	0	1020	34	0
1	AW	940	0	950	19	1
1	AX	1014	0	1020	34	0
1	AY	1014	0	1020	33	0
1	AZ	940	0	950	33	1
1	BA	1014	0	1020	42	0
1	BB	1014	0	1020	38	0
1	BC	940	0	950	32	0
1	BD	1014	0	1020	44	0
1	BE	1014	0	1020	32	0
1	BF	940	0	950	34	0
1	BG	1014	0	1020	42	0
1	BH	1014	0	1020	36	0
1	BI	940	0	950	32	0
1	BJ	1014	0	1020	38	0
1	BK	1014	0	1020	34	0
1	BL	940	0	950	17	0
1	BM	1014	0	1020	21	0
1	BN	1014	0	1020	34	0
1	BO	940	0	950	33	0
1	BP	1014	0	1020	39	0
1	BQ	1014	0	1020	35	0
1	BR	940	0	950	33	0
1	BS	1014	0	1020	38	0
1	BT	1014	0	1020	39	0
1	BU	940	0	950	29	0
1	BV	1014	0	1020	45	0
1	BW	1014	0	1020	34	0
1	BX	940	0	950	38	0
1	BY	1014	0	1020	67	0
1	BZ	1014	0	1020	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	940	0	950	31	0
1	CB	1014	0	1020	40	0
1	CC	1014	0	1020	35	0
1	CD	940	0	950	28	0
1	CE	1014	0	1020	41	0
1	CF	1014	0	1020	37	0
1	CG	940	0	950	29	0
1	CH	1014	0	1020	53	0
1	CI	1014	0	1020	50	0
1	CJ	940	0	950	29	0
1	CK	1014	0	1020	66	0
1	CL	1014	0	1020	35	0
1	CM	940	0	950	31	0
1	CN	1014	0	1020	37	0
1	CO	1014	0	1020	33	0
1	CP	940	0	950	32	0
1	CQ	1014	0	1020	41	0
1	CR	1014	0	1020	30	0
1	CS	940	0	950	21	0
1	CT	1014	0	1020	21	0
1	CU	1014	0	1020	50	0
1	CV	940	0	950	18	0
1	CW	1014	0	1020	38	0
1	CX	1014	0	1020	37	0
1	CY	940	0	950	36	0
1	CZ	1014	0	1020	39	0
1	DA	1014	0	1020	40	0
1	DB	940	0	950	31	0
1	DC	1014	0	1020	38	0
1	DD	1014	0	1020	19	0
1	DE	940	0	950	27	0
1	DF	1014	0	1020	39	0
1	DG	1014	0	1020	32	0
1	DH	940	0	950	36	0
1	DI	1014	0	1020	23	0
1	DJ	1014	0	1020	35	0
1	DK	940	0	950	34	0
1	DL	1014	0	1020	41	0
2	AA	1	0	0	0	0
2	AB	1	0	0	0	0
2	AC	1	0	0	0	0
2	AE	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AF	1	0	0	0	0
2	AG	1	0	0	0	0
2	AH	1	0	0	0	0
2	AK	1	0	0	0	0
2	AM	1	0	0	0	0
2	AN	1	0	0	0	0
2	AQ	1	0	0	0	0
2	AW	1	0	0	0	0
2	AZ	1	0	0	0	0
2	BB	1	0	0	0	0
2	BC	1	0	0	0	0
2	BF	1	0	0	0	0
2	BH	1	0	0	0	0
2	BI	1	0	0	0	0
2	BK	1	0	0	0	0
2	BL	1	0	0	0	0
2	BR	1	0	0	0	0
2	BT	1	0	0	0	0
2	BX	1	0	0	0	0
2	CA	1	0	0	0	0
2	CC	1	0	0	0	0
2	CD	1	0	0	0	0
2	CF	1	0	0	0	0
2	CJ	1	0	0	0	0
2	CS	1	0	0	0	0
2	CV	1	0	0	0	0
All	All	89070	0	89700	2396	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 2396 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:AR:1:PRO:HD3	1:CH:131:GLU:HB3	1.39	1.03
1:AU:129:ASN:O	1:CI:32:ARG:NH1	1.91	1.02
1:AP:134:TYR:CD1	1:AU:3:LEU:HD23	1.96	1.01
1:AC:1:PRO:HD3	1:BV:131:GLU:HB3	1.46	0.97
1:AF:1:PRO:HD3	1:BY:131:GLU:HB3	1.47	0.97

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AW:121:THR:OG1	1:AZ:12:SER:O[4_565]	1.95	0.25
1:AJ:121:THR:OG1	1:AT:12:SER:O[4_566]	2.10	0.10

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	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AB	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	AC	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AD	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AE	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	AF	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AG	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AH	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	AI	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AJ	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AK	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	AL	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AM	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AN	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	AO	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AP	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AQ	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	AR	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AS	132/134 (98%)	130 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AT	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	AU	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AV	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AW	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	AX	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AY	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	AZ	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	BA	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BB	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BC	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	BD	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BE	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BF	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	BG	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BH	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BI	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	BJ	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BK	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BL	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	BM	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BN	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BO	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	BP	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BQ	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BR	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	BS	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BT	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BU	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	BV	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BW	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BX	119/134 (89%)	117 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BY	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	BZ	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CA	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	CB	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CC	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CD	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	CE	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CF	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CG	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	CH	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CI	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CJ	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	CK	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CL	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CM	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	CN	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CO	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CP	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	CQ	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CR	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CS	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	CT	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CU	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CV	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	CW	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CX	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	CY	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	CZ	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	DA	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	DB	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	DC	132/134 (98%)	130 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DD	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	DE	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	DF	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	DG	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	DH	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	DI	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	DJ	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
1	DK	119/134 (89%)	117 (98%)	2 (2%)	0	100	100
1	DL	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
All	All	11490/12060 (95%)	11310 (98%)	180 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	112/112 (100%)	112 (100%)	0	100	100
1	AB	102/112 (91%)	102 (100%)	0	100	100
1	AC	112/112 (100%)	112 (100%)	0	100	100
1	AD	112/112 (100%)	112 (100%)	0	100	100
1	AE	102/112 (91%)	102 (100%)	0	100	100
1	AF	112/112 (100%)	112 (100%)	0	100	100
1	AG	112/112 (100%)	112 (100%)	0	100	100
1	AH	102/112 (91%)	102 (100%)	0	100	100
1	AI	112/112 (100%)	112 (100%)	0	100	100
1	AJ	112/112 (100%)	112 (100%)	0	100	100
1	AK	102/112 (91%)	102 (100%)	0	100	100
1	AL	112/112 (100%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AM	112/112 (100%)	112 (100%)	0	100	100
1	AN	102/112 (91%)	102 (100%)	0	100	100
1	AO	112/112 (100%)	112 (100%)	0	100	100
1	AP	112/112 (100%)	112 (100%)	0	100	100
1	AQ	102/112 (91%)	102 (100%)	0	100	100
1	AR	112/112 (100%)	112 (100%)	0	100	100
1	AS	112/112 (100%)	112 (100%)	0	100	100
1	AT	102/112 (91%)	102 (100%)	0	100	100
1	AU	112/112 (100%)	112 (100%)	0	100	100
1	AV	112/112 (100%)	112 (100%)	0	100	100
1	AW	102/112 (91%)	102 (100%)	0	100	100
1	AX	112/112 (100%)	112 (100%)	0	100	100
1	AY	112/112 (100%)	112 (100%)	0	100	100
1	AZ	102/112 (91%)	102 (100%)	0	100	100
1	BA	112/112 (100%)	112 (100%)	0	100	100
1	BB	112/112 (100%)	112 (100%)	0	100	100
1	BC	102/112 (91%)	102 (100%)	0	100	100
1	BD	112/112 (100%)	112 (100%)	0	100	100
1	BE	112/112 (100%)	112 (100%)	0	100	100
1	BF	102/112 (91%)	102 (100%)	0	100	100
1	BG	112/112 (100%)	112 (100%)	0	100	100
1	BH	112/112 (100%)	112 (100%)	0	100	100
1	BI	102/112 (91%)	102 (100%)	0	100	100
1	BJ	112/112 (100%)	112 (100%)	0	100	100
1	BK	112/112 (100%)	112 (100%)	0	100	100
1	BL	102/112 (91%)	102 (100%)	0	100	100
1	BM	112/112 (100%)	112 (100%)	0	100	100
1	BN	112/112 (100%)	112 (100%)	0	100	100
1	BO	102/112 (91%)	102 (100%)	0	100	100
1	BP	112/112 (100%)	112 (100%)	0	100	100
1	BQ	112/112 (100%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BR	102/112 (91%)	102 (100%)	0	100	100
1	BS	112/112 (100%)	112 (100%)	0	100	100
1	BT	112/112 (100%)	112 (100%)	0	100	100
1	BU	102/112 (91%)	102 (100%)	0	100	100
1	BV	112/112 (100%)	112 (100%)	0	100	100
1	BW	112/112 (100%)	112 (100%)	0	100	100
1	BX	102/112 (91%)	102 (100%)	0	100	100
1	BY	112/112 (100%)	112 (100%)	0	100	100
1	BZ	112/112 (100%)	112 (100%)	0	100	100
1	CA	102/112 (91%)	102 (100%)	0	100	100
1	CB	112/112 (100%)	112 (100%)	0	100	100
1	CC	112/112 (100%)	112 (100%)	0	100	100
1	CD	102/112 (91%)	102 (100%)	0	100	100
1	CE	112/112 (100%)	112 (100%)	0	100	100
1	CF	112/112 (100%)	112 (100%)	0	100	100
1	CG	102/112 (91%)	102 (100%)	0	100	100
1	CH	112/112 (100%)	112 (100%)	0	100	100
1	CI	112/112 (100%)	112 (100%)	0	100	100
1	CJ	102/112 (91%)	102 (100%)	0	100	100
1	CK	112/112 (100%)	112 (100%)	0	100	100
1	CL	112/112 (100%)	112 (100%)	0	100	100
1	CM	102/112 (91%)	102 (100%)	0	100	100
1	CN	112/112 (100%)	112 (100%)	0	100	100
1	CO	112/112 (100%)	112 (100%)	0	100	100
1	CP	102/112 (91%)	102 (100%)	0	100	100
1	CQ	112/112 (100%)	112 (100%)	0	100	100
1	CR	112/112 (100%)	112 (100%)	0	100	100
1	CS	102/112 (91%)	102 (100%)	0	100	100
1	CT	112/112 (100%)	112 (100%)	0	100	100
1	CU	112/112 (100%)	112 (100%)	0	100	100
1	CV	102/112 (91%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CW	112/112 (100%)	112 (100%)	0	100	100
1	CX	112/112 (100%)	112 (100%)	0	100	100
1	CY	102/112 (91%)	102 (100%)	0	100	100
1	CZ	112/112 (100%)	112 (100%)	0	100	100
1	DA	112/112 (100%)	112 (100%)	0	100	100
1	DB	102/112 (91%)	102 (100%)	0	100	100
1	DC	112/112 (100%)	112 (100%)	0	100	100
1	DD	112/112 (100%)	112 (100%)	0	100	100
1	DE	102/112 (91%)	102 (100%)	0	100	100
1	DF	112/112 (100%)	112 (100%)	0	100	100
1	DG	112/112 (100%)	112 (100%)	0	100	100
1	DH	102/112 (91%)	102 (100%)	0	100	100
1	DI	112/112 (100%)	112 (100%)	0	100	100
1	DJ	112/112 (100%)	112 (100%)	0	100	100
1	DK	102/112 (91%)	102 (100%)	0	100	100
1	DL	112/112 (100%)	112 (100%)	0	100	100
All	All	9780/10080 (97%)	9780 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	BO	132	HIS
1	DG	90	ASN
1	CR	90	ASN
1	AS	90	ASN
1	CJ	132	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 30 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 i

6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	AA	134/134 (100%)	-0.32	1 (0%) 87 83	64, 102, 139, 208	0
1	AB	123/134 (91%)	-0.27	2 (1%) 72 64	67, 109, 164, 214	0
1	AC	134/134 (100%)	-0.36	0 100 100	66, 105, 140, 217	0
1	AD	134/134 (100%)	-0.23	2 (1%) 73 66	64, 102, 139, 208	0
1	AE	123/134 (91%)	-0.30	2 (1%) 72 64	67, 109, 164, 214	0
1	AF	134/134 (100%)	-0.21	2 (1%) 73 66	66, 105, 140, 217	0
1	AG	134/134 (100%)	-0.21	1 (0%) 87 83	64, 102, 139, 208	0
1	AH	123/134 (91%)	-0.33	2 (1%) 72 64	67, 109, 164, 214	0
1	AI	134/134 (100%)	-0.23	1 (0%) 87 83	66, 105, 140, 217	0
1	AJ	134/134 (100%)	-0.23	1 (0%) 87 83	64, 102, 139, 208	0
1	AK	123/134 (91%)	-0.31	0 100 100	67, 109, 164, 214	0
1	AL	134/134 (100%)	-0.26	1 (0%) 87 83	66, 105, 140, 217	0
1	AM	134/134 (100%)	-0.42	2 (1%) 73 66	64, 102, 139, 208	0
1	AN	123/134 (91%)	-0.15	6 (4%) 29 25	67, 109, 164, 214	0
1	AO	134/134 (100%)	-0.22	2 (1%) 73 66	66, 105, 140, 217	0
1	AP	134/134 (100%)	-0.17	2 (1%) 73 66	64, 102, 139, 208	0
1	AQ	123/134 (91%)	-0.24	2 (1%) 72 64	67, 109, 164, 214	0
1	AR	134/134 (100%)	-0.08	1 (0%) 87 83	66, 105, 140, 217	0
1	AS	134/134 (100%)	-0.21	1 (0%) 87 83	64, 102, 139, 208	0
1	AT	123/134 (91%)	-0.25	3 (2%) 59 50	67, 109, 164, 214	0
1	AU	134/134 (100%)	-0.07	1 (0%) 87 83	66, 105, 140, 217	0
1	AV	134/134 (100%)	-0.25	1 (0%) 87 83	64, 102, 139, 208	0
1	AW	123/134 (91%)	-0.28	2 (1%) 72 64	67, 109, 164, 214	0
1	AX	134/134 (100%)	-0.18	2 (1%) 73 66	66, 105, 140, 217	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AY	134/134 (100%)	-0.17	3 (2%) 62 54	64, 102, 139, 208	0
1	AZ	123/134 (91%)	-0.24	3 (2%) 59 50	67, 109, 164, 214	0
1	BA	134/134 (100%)	-0.33	1 (0%) 87 83	66, 105, 140, 217	0
1	BB	134/134 (100%)	-0.19	1 (0%) 87 83	64, 102, 139, 208	0
1	BC	123/134 (91%)	-0.22	2 (1%) 72 64	67, 109, 164, 214	0
1	BD	134/134 (100%)	-0.14	1 (0%) 87 83	66, 105, 140, 217	0
1	BE	134/134 (100%)	-0.36	2 (1%) 73 66	64, 102, 139, 208	0
1	BF	123/134 (91%)	-0.33	1 (0%) 86 81	67, 109, 164, 214	0
1	BG	134/134 (100%)	-0.32	1 (0%) 87 83	66, 105, 140, 217	0
1	BH	134/134 (100%)	-0.50	0 100 100	64, 102, 139, 208	0
1	BI	123/134 (91%)	-0.23	2 (1%) 72 64	67, 109, 164, 214	0
1	BJ	134/134 (100%)	-0.32	2 (1%) 73 66	66, 105, 140, 217	0
1	BK	134/134 (100%)	-0.38	0 100 100	64, 102, 139, 208	0
1	BL	123/134 (91%)	-0.19	3 (2%) 59 50	67, 109, 164, 214	0
1	BM	134/134 (100%)	-0.24	0 100 100	66, 105, 140, 217	0
1	BN	134/134 (100%)	-0.31	0 100 100	64, 102, 139, 208	0
1	BO	123/134 (91%)	-0.22	3 (2%) 59 50	67, 109, 164, 214	0
1	BP	134/134 (100%)	-0.18	1 (0%) 87 83	66, 105, 140, 217	0
1	BQ	134/134 (100%)	-0.54	0 100 100	64, 102, 139, 208	0
1	BR	123/134 (91%)	-0.27	3 (2%) 59 50	67, 109, 164, 214	0
1	BS	134/134 (100%)	-0.41	0 100 100	66, 105, 140, 217	0
1	BT	134/134 (100%)	-0.50	0 100 100	64, 102, 139, 208	0
1	BU	123/134 (91%)	-0.34	0 100 100	67, 109, 164, 214	0
1	BV	134/134 (100%)	-0.36	1 (0%) 87 83	66, 105, 140, 217	0
1	BW	134/134 (100%)	-0.13	3 (2%) 62 54	64, 102, 139, 208	0
1	BX	123/134 (91%)	-0.19	1 (0%) 86 81	67, 109, 164, 214	0
1	BY	134/134 (100%)	-0.24	1 (0%) 87 83	66, 105, 140, 217	0
1	BZ	134/134 (100%)	-0.36	0 100 100	64, 102, 139, 208	0
1	CA	123/134 (91%)	-0.23	1 (0%) 86 81	67, 109, 164, 214	0
1	CB	134/134 (100%)	-0.17	1 (0%) 87 83	66, 105, 140, 217	0
1	CC	134/134 (100%)	-0.40	0 100 100	64, 102, 139, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	CD	123/134 (91%)	-0.11	3 (2%) 59 50	67, 109, 164, 214	0
1	CE	134/134 (100%)	-0.18	2 (1%) 73 66	66, 105, 140, 217	0
1	CF	134/134 (100%)	-0.20	0 100 100	64, 102, 139, 208	0
1	CG	123/134 (91%)	-0.51	2 (1%) 72 64	67, 109, 164, 214	0
1	CH	134/134 (100%)	-0.43	0 100 100	66, 105, 140, 217	0
1	CI	134/134 (100%)	-0.15	1 (0%) 87 83	64, 102, 139, 208	0
1	CJ	123/134 (91%)	-0.03	6 (4%) 29 25	67, 109, 164, 214	0
1	CK	134/134 (100%)	-0.21	1 (0%) 87 83	66, 105, 140, 217	0
1	CL	134/134 (100%)	-0.32	0 100 100	64, 102, 139, 208	0
1	CM	123/134 (91%)	-0.49	1 (0%) 86 81	67, 109, 164, 214	0
1	CN	134/134 (100%)	-0.29	1 (0%) 87 83	66, 105, 140, 217	0
1	CO	134/134 (100%)	-0.47	0 100 100	64, 102, 139, 208	0
1	CP	123/134 (91%)	-0.26	3 (2%) 59 50	67, 109, 164, 214	0
1	CQ	134/134 (100%)	-0.24	0 100 100	66, 105, 140, 217	0
1	CR	134/134 (100%)	-0.28	2 (1%) 73 66	64, 102, 139, 208	0
1	CS	123/134 (91%)	-0.28	2 (1%) 72 64	67, 109, 164, 214	0
1	CT	134/134 (100%)	-0.10	3 (2%) 62 54	66, 105, 140, 217	0
1	CU	134/134 (100%)	-0.23	0 100 100	64, 102, 139, 208	0
1	CV	123/134 (91%)	-0.22	3 (2%) 59 50	67, 109, 164, 214	0
1	CW	134/134 (100%)	-0.23	0 100 100	66, 105, 140, 217	0
1	CX	134/134 (100%)	-0.40	0 100 100	64, 102, 139, 208	0
1	CY	123/134 (91%)	-0.24	2 (1%) 72 64	67, 109, 164, 214	0
1	CZ	134/134 (100%)	-0.27	1 (0%) 87 83	66, 105, 140, 217	0
1	DA	134/134 (100%)	-0.35	2 (1%) 73 66	64, 102, 139, 208	0
1	DB	123/134 (91%)	-0.38	2 (1%) 72 64	67, 109, 164, 214	0
1	DC	134/134 (100%)	-0.38	0 100 100	66, 105, 140, 217	0
1	DD	134/134 (100%)	-0.28	0 100 100	64, 102, 139, 208	0
1	DE	123/134 (91%)	-0.26	0 100 100	67, 109, 164, 214	0
1	DF	134/134 (100%)	-0.23	2 (1%) 73 66	66, 105, 140, 217	0
1	DG	134/134 (100%)	-0.38	1 (0%) 87 83	64, 102, 139, 208	0
1	DH	123/134 (91%)	-0.12	4 (3%) 46 38	67, 109, 164, 214	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	DI	134/134 (100%)	-0.13	2 (1%) 73 66	66, 105, 140, 217	0
1	DJ	134/134 (100%)	-0.47	0 100 100	64, 102, 139, 208	0
1	DK	123/134 (91%)	-0.33	0 100 100	67, 109, 164, 214	0
1	DL	134/134 (100%)	-0.44	0 100 100	66, 105, 140, 217	0
All	All	11730/12060 (97%)	-0.28	123 (1%) 82 76	64, 104, 154, 217	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DH	85	GLU	8.4
1	CJ	85	GLU	5.6
1	AN	85	GLU	5.5
1	CE	56	ASN	5.1
1	DH	72	ALA	5.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	AA	201	1/1	0.52	0.22	64,64,64,64	0
2	CA	AZ	201	1/1	0.79	0.17	64,64,64,64	0
2	CA	AN	201	1/1	0.79	0.26	64,64,64,64	0
2	CA	AE	201	1/1	0.81	0.15	64,64,64,64	0
2	CA	CV	201	1/1	0.83	0.19	64,64,64,64	0
2	CA	CJ	201	1/1	0.86	0.13	64,64,64,64	0
2	CA	AF	201	1/1	0.87	0.24	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	AW	201	1/1	0.89	0.25	64,64,64,64	0
2	CA	BB	201	1/1	0.90	0.16	64,64,64,64	0
2	CA	BL	201	1/1	0.91	0.26	64,64,64,64	0
2	CA	AH	201	1/1	0.91	0.34	64,64,64,64	0
2	CA	BR	201	1/1	0.92	0.20	64,64,64,64	0
2	CA	CS	201	1/1	0.93	0.20	64,64,64,64	0
2	CA	AM	201	1/1	0.93	0.12	64,64,64,64	0
2	CA	AG	201	1/1	0.93	0.20	64,64,64,64	0
2	CA	BH	201	1/1	0.94	0.16	64,64,64,64	0
2	CA	BX	201	1/1	0.94	0.22	64,64,64,64	0
2	CA	BF	201	1/1	0.94	0.23	64,64,64,64	0
2	CA	AK	201	1/1	0.94	0.17	64,64,64,64	0
2	CA	AC	201	1/1	0.94	0.34	64,64,64,64	0
2	CA	AQ	201	1/1	0.94	0.35	64,64,64,64	0
2	CA	CA	201	1/1	0.95	0.30	64,64,64,64	0
2	CA	BK	201	1/1	0.95	0.21	64,64,64,64	0
2	CA	CC	201	1/1	0.95	0.09	64,64,64,64	0
2	CA	AB	201	1/1	0.96	0.09	64,64,64,64	0
2	CA	BT	201	1/1	0.97	0.30	64,64,64,64	0
2	CA	BC	201	1/1	0.97	0.27	64,64,64,64	0
2	CA	BI	201	1/1	0.97	0.30	64,64,64,64	0
2	CA	CF	201	1/1	0.98	0.14	64,64,64,64	0
2	CA	CD	201	1/1	0.98	0.24	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.