



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2026 – 07:06 PM UTC

PDB ID : 6YFE / pdb_00006yfe
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 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

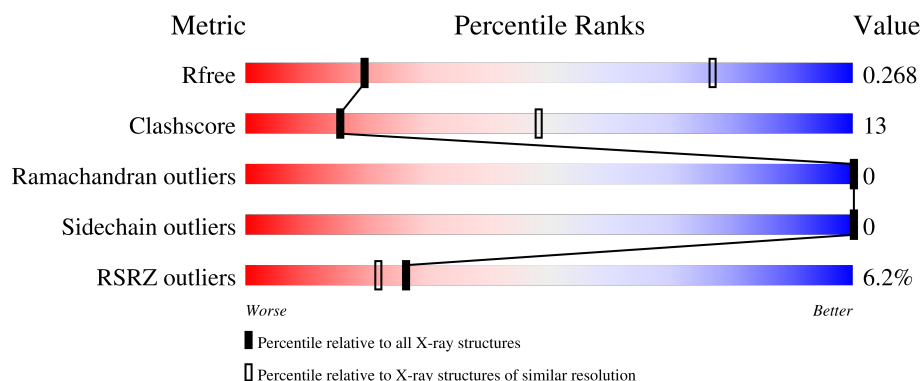
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	3% 74% 26%
1	AB	134	7% 65% 27% 8%
1	AC	134	7% 71% 29%
1	AD	134	9% 81% 19%
1	AE	134	6% 63% 29% 8%

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Mol	Chain	Length	Quality of chain
1	AF	134	
1	AG	134	
1	AH	134	
1	AI	134	
1	AJ	134	
1	AK	134	
1	AL	134	
1	AM	134	
1	AN	134	
1	AO	134	
1	AP	134	
1	AQ	134	
1	AR	134	
1	AS	134	
1	AT	134	
1	AU	134	
1	AV	134	
1	AW	134	
1	AX	134	
1	AY	134	
1	AZ	134	
1	BA	134	
1	BB	134	
1	BC	134	
1	BD	134	

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Mol	Chain	Length	Quality of chain
1	BE	134	4% 74% 26%
1	BF	134	7% 66% 25% 8%
1	BG	134	11% 68% 32%
1	BH	134	8% 72% 28%
1	BI	134	4% 66% 25% 8%
1	BJ	134	4% 70% 30%
1	BK	134	9% 75% 25%
1	BL	134	3% 72% 20% 8%
1	BM	134	3% 78% 22%
1	BN	134	2% 75% 25%
1	BO	134	4% 66% 26% 8%
1	BP	134	6% 68% 32%
1	BQ	134	4% 74% 26%
1	BR	134	6% 66% 26% 8%
1	BS	134	6% 69% 31%
1	BT	134	7% 73% 27%
1	BU	134	6% 66% 25% 8%
1	BV	134	10% 69% 31%
1	BW	134	7% 74% 26%
1	BX	134	4% 63% 29% 8%
1	BY	134	4% 63% 37%
1	BZ	134	4% 80% 20%
1	CA	134	7% 66% 25% 8%
1	CB	134	7% 69% 31%
1	CC	134	% 72% 28%

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Mol	Chain	Length	Quality of chain
1	CD	134	
1	CE	134	
1	CF	134	
1	CG	134	
1	CH	134	
1	CI	134	
1	CJ	134	
1	CK	134	
1	CL	134	
1	CM	134	
1	CN	134	
1	CO	134	
1	CP	134	
1	CQ	134	
1	CR	134	
1	CS	134	
1	CT	134	
1	CU	134	
1	CV	134	
1	CW	134	
1	CX	134	
1	CY	134	
1	CZ	134	
1	DA	134	
1	DB	134	

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Mol	Chain	Length	Quality of chain
1	DC	134	
1	DD	134	
1	DE	134	
1	DF	134	
1	DG	134	
1	DH	134	
1	DI	134	
1	DJ	134	
1	DK	134	
1	DL	134	

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

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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 (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AA	1	Total	Ca	0	0
			1	1		
2	AB	1	Total	Ca	0	0
			1	1		
2	AC	1	Total	Ca	0	0
			1	1		
2	AE	1	Total	Ca	0	0
			1	1		
2	AF	1	Total	Ca	0	0
			1	1		
2	AG	1	Total	Ca	0	0
			1	1		
2	AH	1	Total	Ca	0	0
			1	1		
2	AK	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AM	1	Total 1	Ca 1	0	0
2	AN	1	Total 1	Ca 1	0	0
2	AQ	1	Total 1	Ca 1	0	0
2	AW	1	Total 1	Ca 1	0	0
2	AZ	1	Total 1	Ca 1	0	0
2	BB	1	Total 1	Ca 1	0	0
2	BC	1	Total 1	Ca 1	0	0
2	BF	1	Total 1	Ca 1	0	0
2	BH	1	Total 1	Ca 1	0	0
2	BI	1	Total 1	Ca 1	0	0
2	BK	1	Total 1	Ca 1	0	0
2	BL	1	Total 1	Ca 1	0	0
2	BR	1	Total 1	Ca 1	0	0
2	BT	1	Total 1	Ca 1	0	0
2	BX	1	Total 1	Ca 1	0	0
2	CA	1	Total 1	Ca 1	0	0
2	CC	1	Total 1	Ca 1	0	0
2	CD	1	Total 1	Ca 1	0	0
2	CF	1	Total 1	Ca 1	0	0
2	CJ	1	Total 1	Ca 1	0	0
2	CS	1	Total 1	Ca 1	0	0

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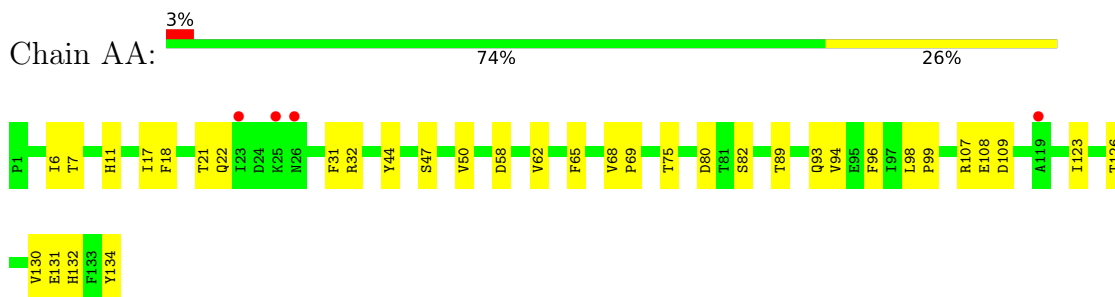
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	CV	1	Total	Ca	0	0
			1	1		

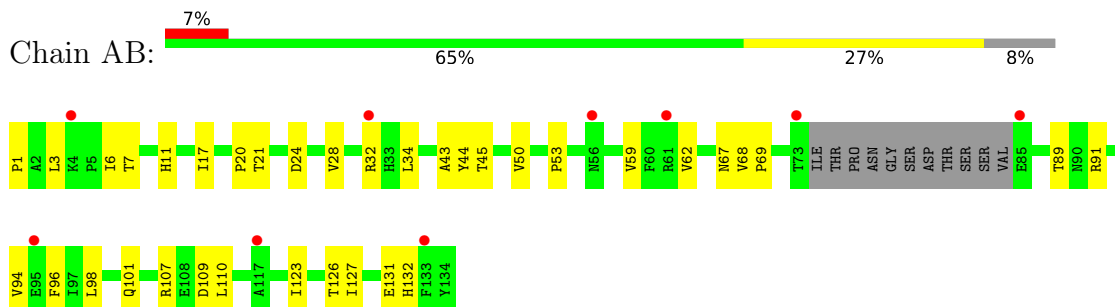
3 Residue-property plots [i](#)

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.

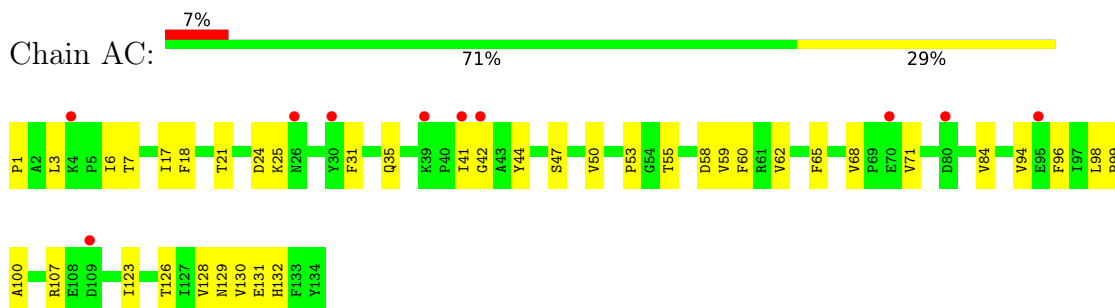
- Molecule 1: coat protein



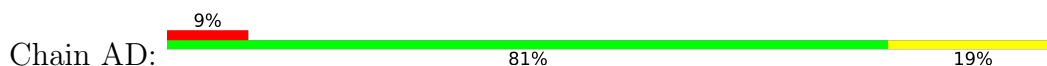
- Molecule 1: coat protein

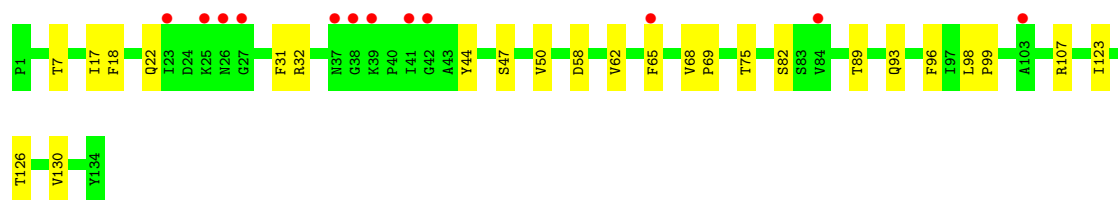


- Molecule 1: coat protein

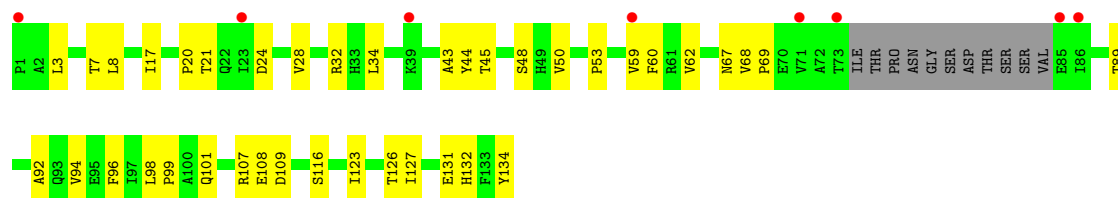


- Molecule 1: coat protein

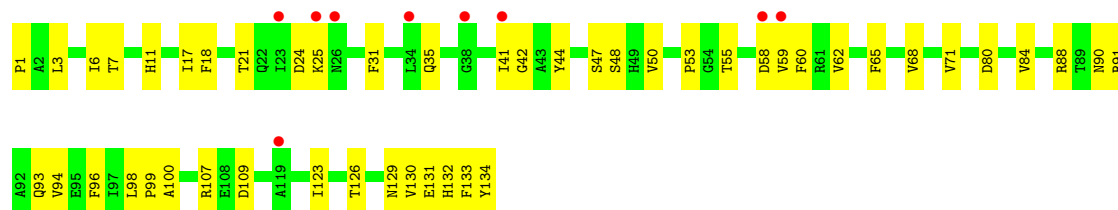




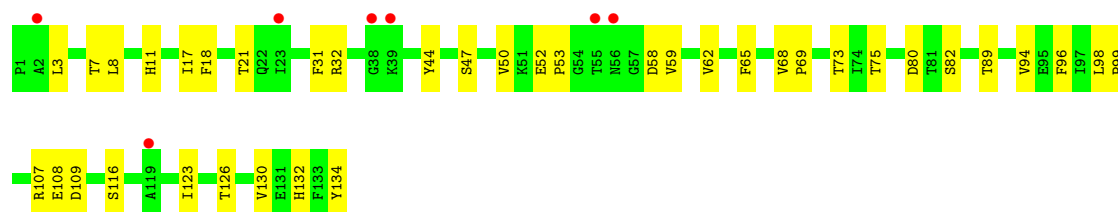
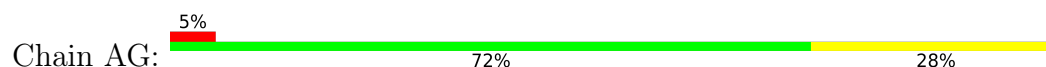
- Molecule 1: coat protein



- Molecule 1: coat protein



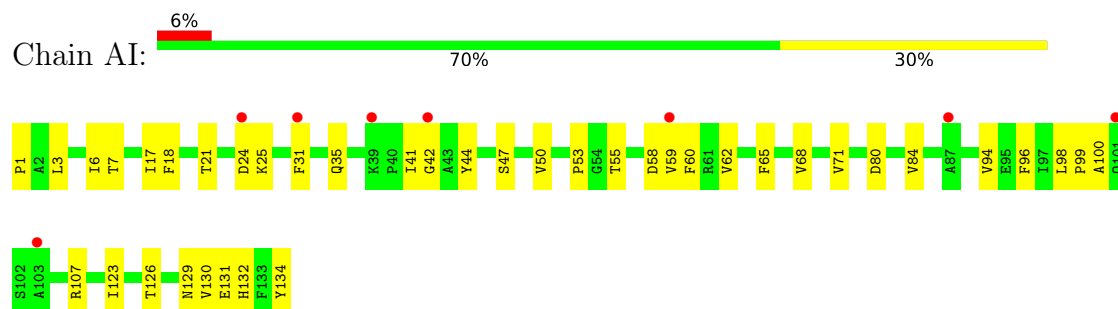
- Molecule 1: coat protein



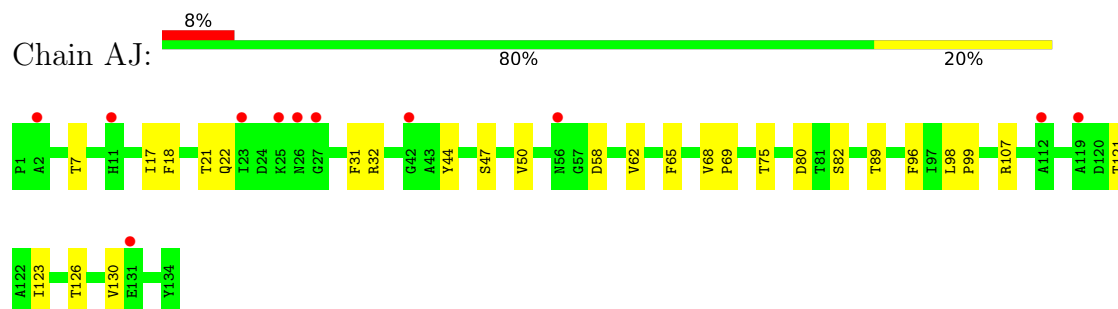
- Molecule 1: coat protein



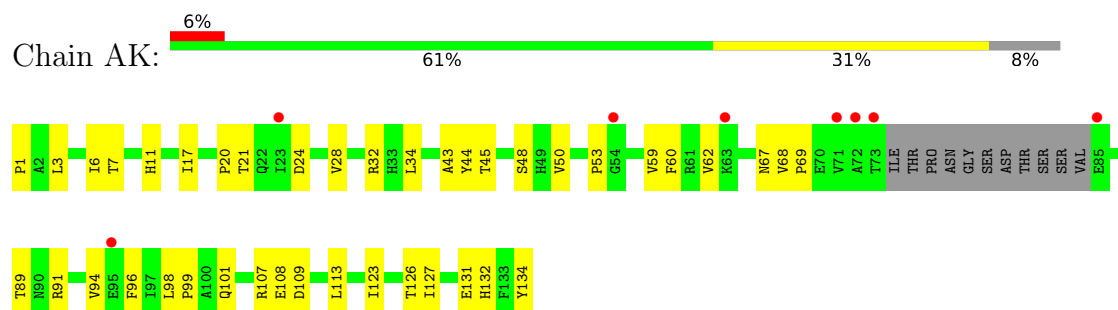
- Molecule 1: coat protein



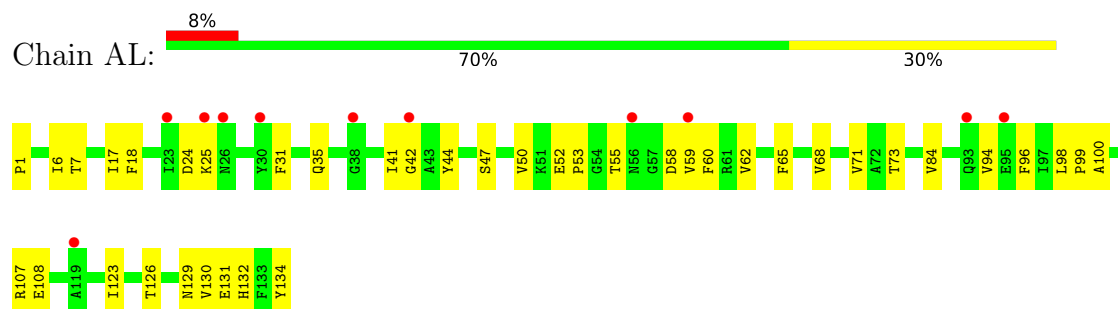
- Molecule 1: coat protein



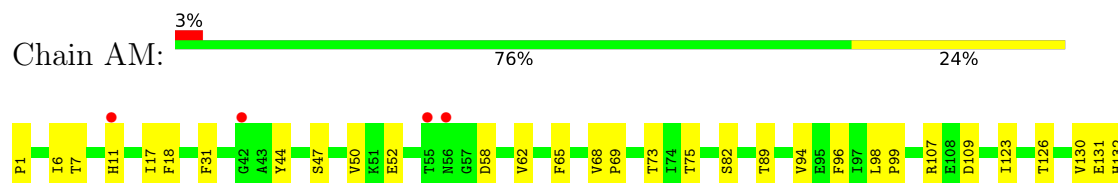
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



F133
Y134

- Molecule 1: coat protein

Chain AN:  4% 66% 25% 8%

P1 A2 L3 I6 T7 I17 P20 T21 T24 V28 R32 R33 L34 A43 Y44 T45 V50 P53 N56 V59 F60 R61 V62 N67 V68 P69 T73 ILE THR PRO ASN GLY ASP THR SER SER SER VAL E85 I86 A87 R88 T89 V94 E95 F96

I97 L98 Q101 R107 E108 D109 I123 T126 I127 E131 F133 Y134

- Molecule 1: coat protein

Chain AO:  4% 75% 25%

P1 A2 L3 T7 I17 F18 Q21 Q22 I23 D24 K25 F31 Q35 I41 Q42 A43 Y44 S47 V50 P53 G54 T55 N56 G57 D58 V59 F60 R61 V62 F65 V68 V71 D80 V84 F96 I97 L98 P99 A100 R107 A119 I123

T126 V130 Y134

- Molecule 1: coat protein

Chain AP:  10% 70% 30%

P1 A2 L3 K4 T7 L8 H11 I17 F18 T21 Q22 I23 D24 K25 N26 Y30 F31 R32 I41 Y44 S47 V50 G54 E52 N56 G57 D58 V62 F65 V68 P69 T73 I74 T75 P76 N77 G78 S79 D80 T81 S82 T89 V94 E95

F96 I97 L98 P99 R107 E108 S116 A119 I123 T126 V130 E131 H132 F133 Y134

- Molecule 1: coat protein

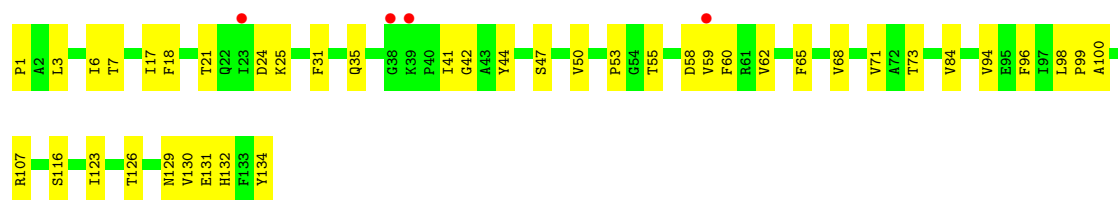
Chain AQ:  6% 64% 28% 8%

P1 A2 L3 I6 T7 H11 I17 P20 T21 Q22 I23 D24 V28 R32 R33 L34 A43 Y44 T45 V50 R51 E52 P53 G54 T55 N56 V59 F60 R61 V62 N67 V68 P69 E70 A72 T73 ILE THR PRO ASN GLY SER SER ASP THR SER SER VAL E85

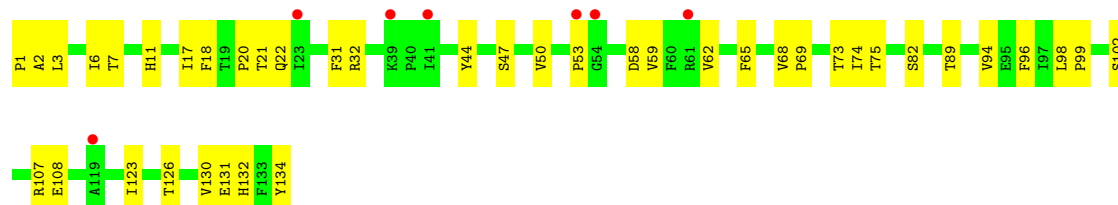
T89 N90 R91 V94 E95 F96 I97 L98 Q101 T105 V106 R107 E108 D109 I123 T126 I127 H132 F133 Y134

- Molecule 1: coat protein

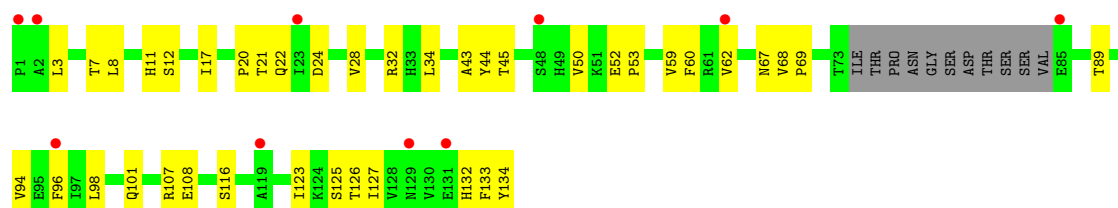
Chain AR:  3% 69% 31%



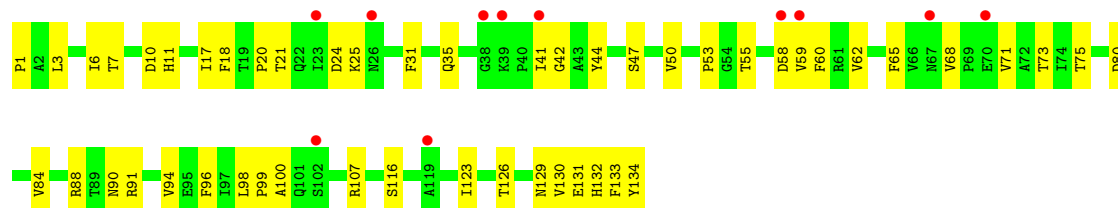
- Molecule 1: coat protein



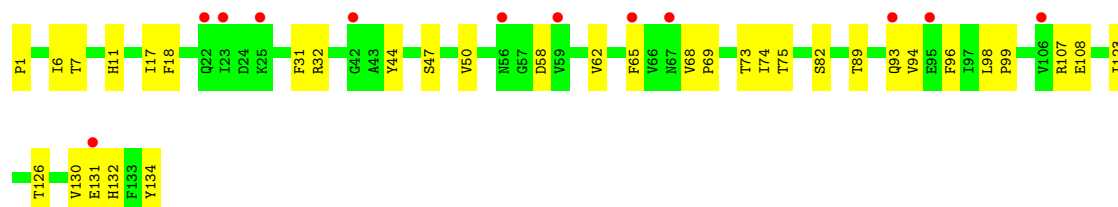
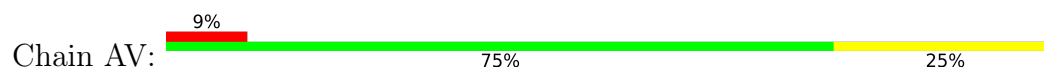
- Molecule 1: coat protein



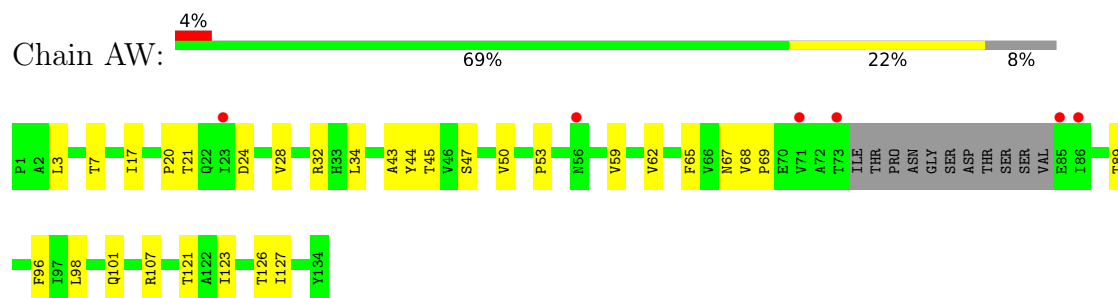
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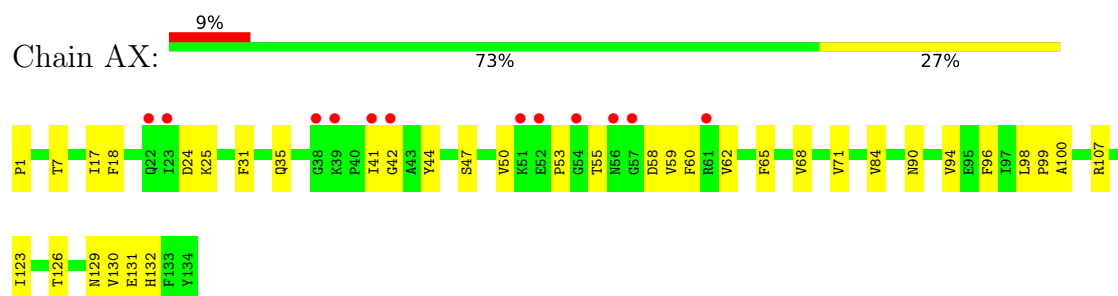
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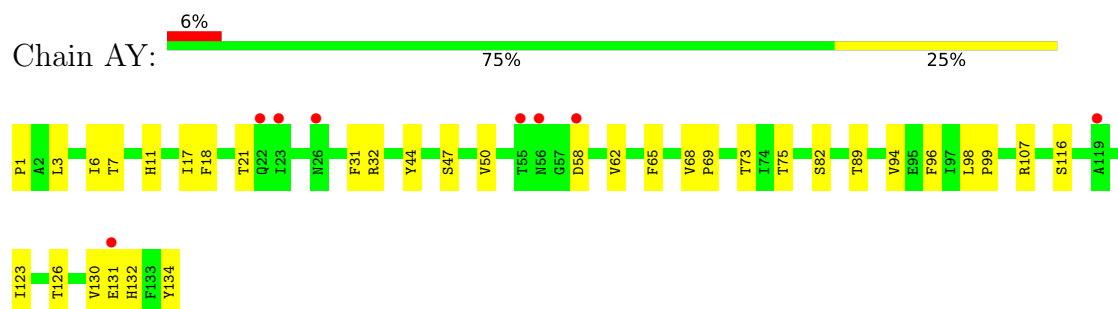
• Molecule 1: coat protein



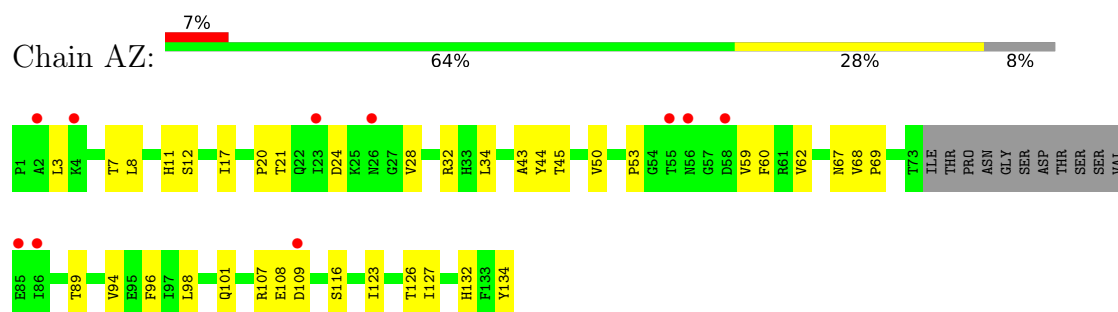
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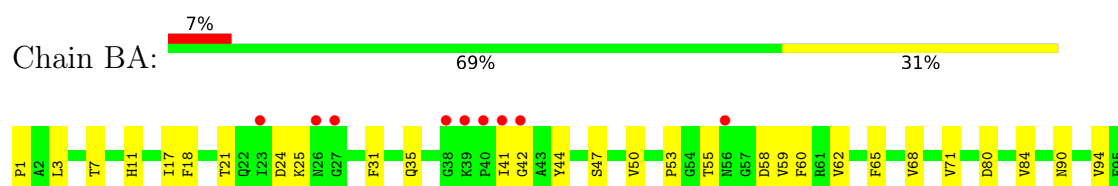
• Molecule 1: coat protein



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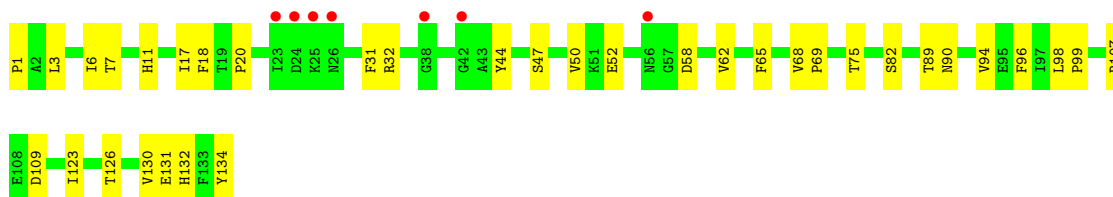
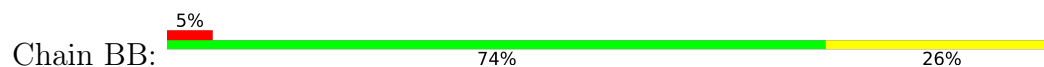


• Molecule 1: coat protein





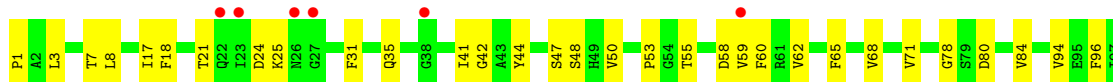
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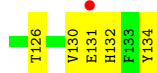
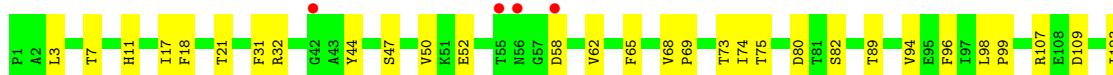
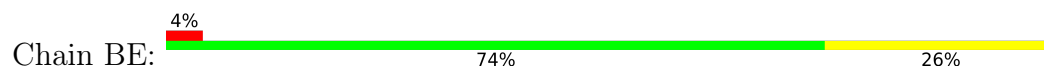
- Molecule 1: coat protein



- Molecule 1: coat protein

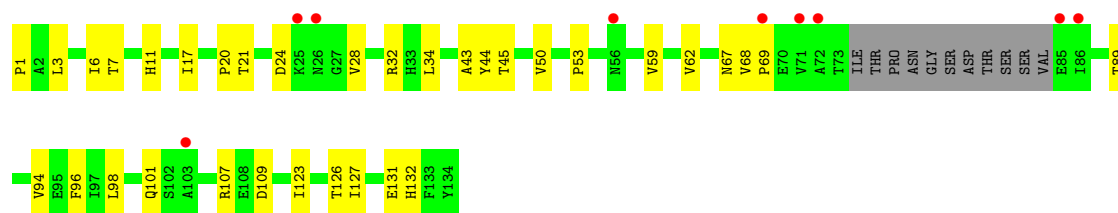


- Molecule 1: coat protein

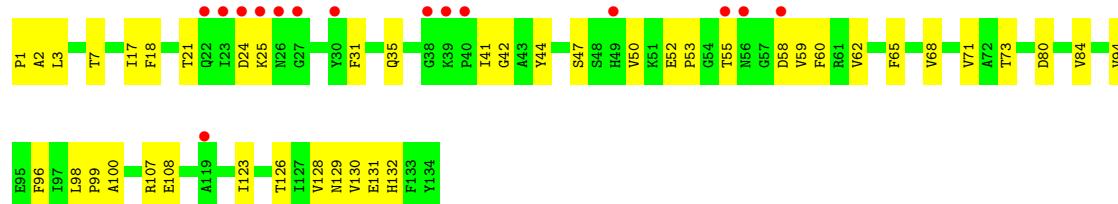


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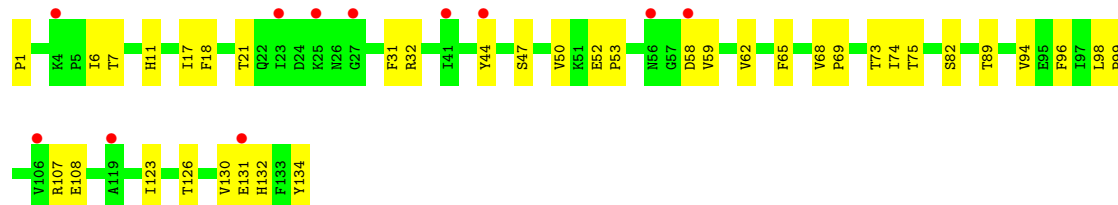
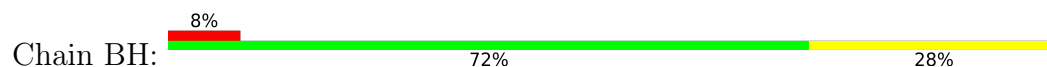




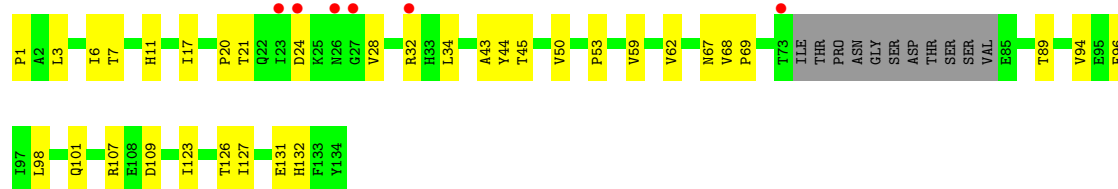
● Molecule 1: coat protein



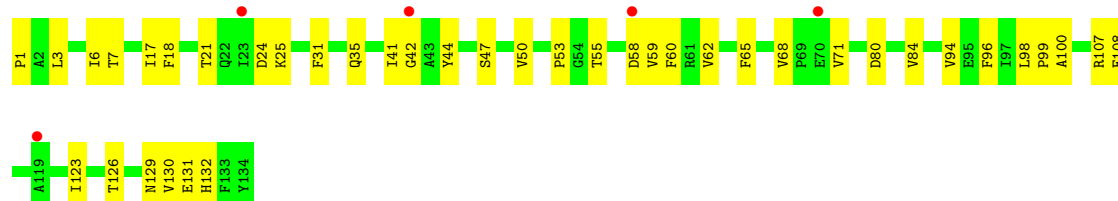
● Molecule 1: coat protein



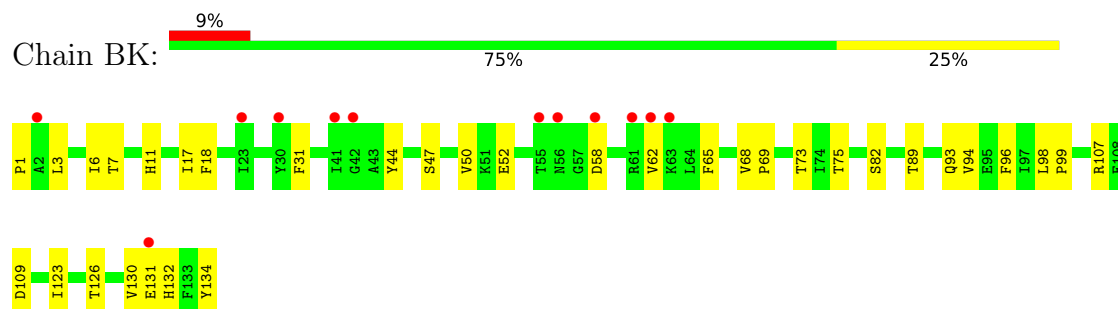
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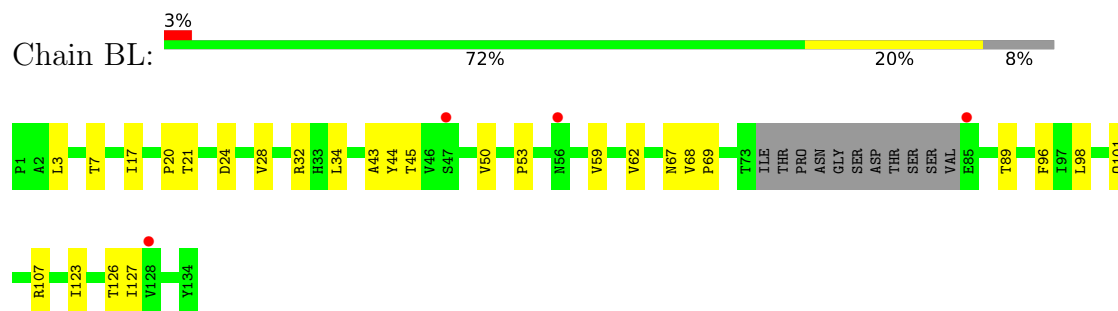
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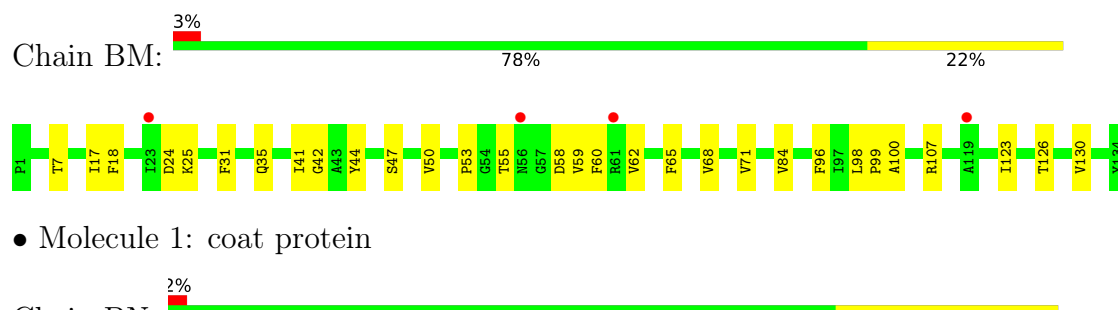
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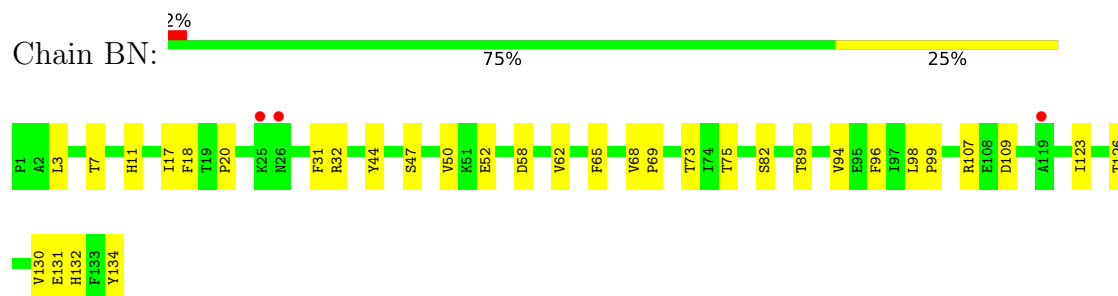
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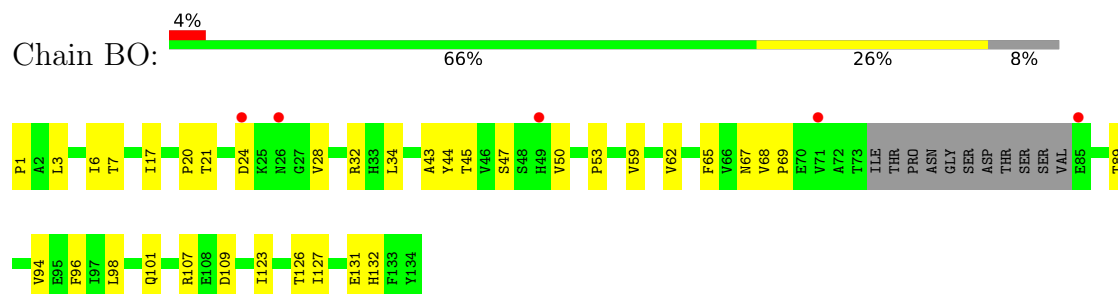
- Molecule 1: coat protein



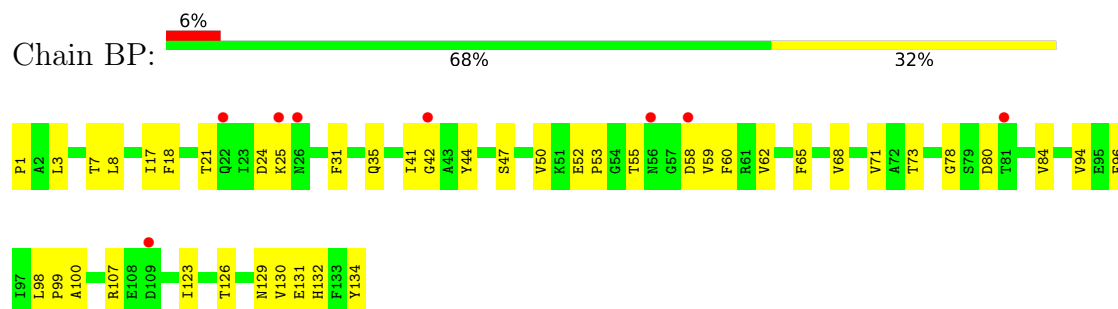
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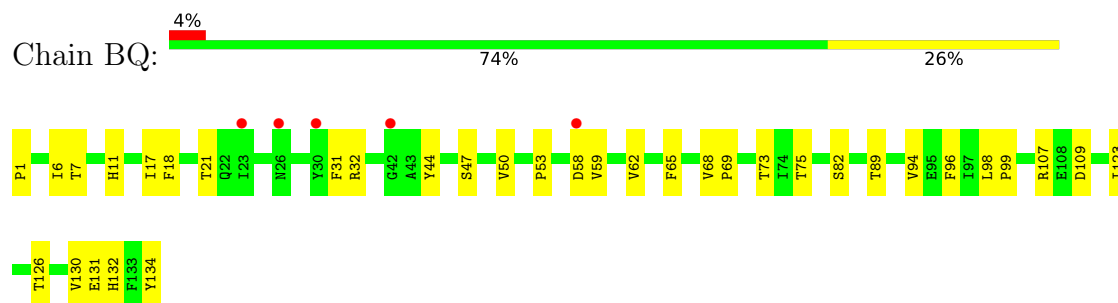
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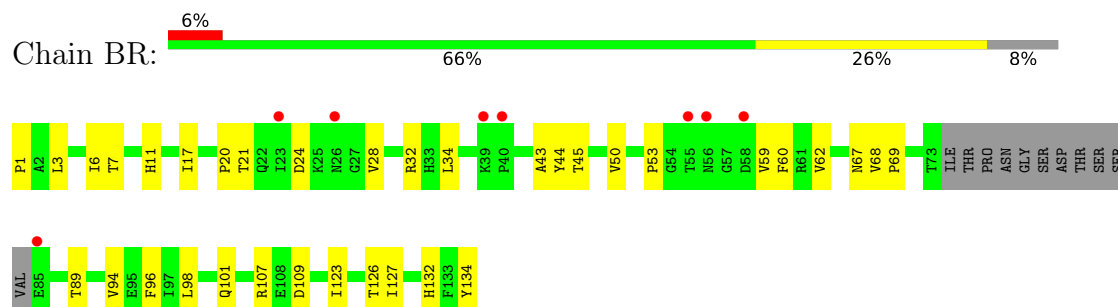
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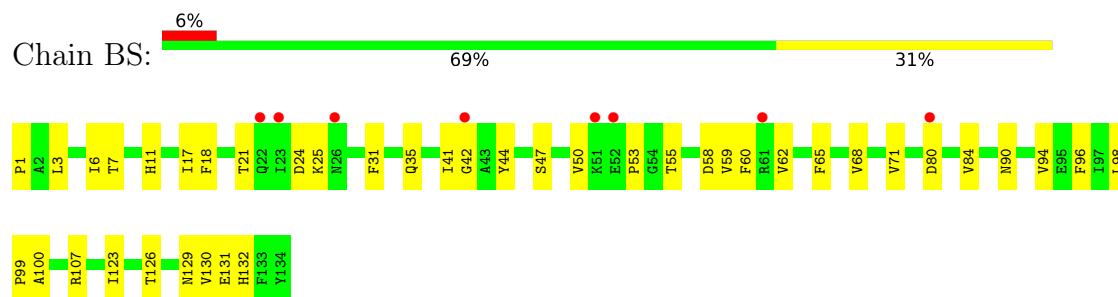
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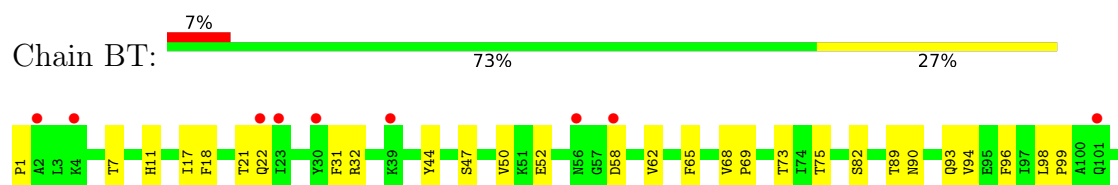
- Molecule 1: coat protein



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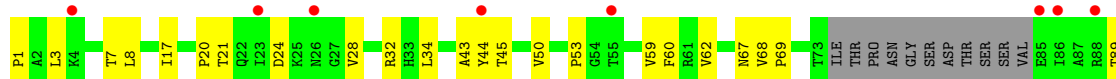


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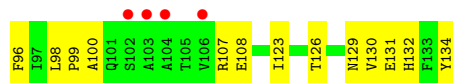




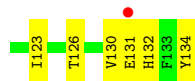
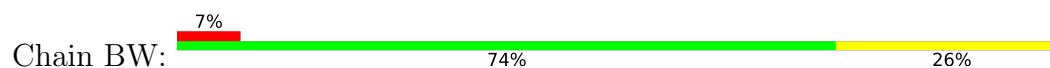
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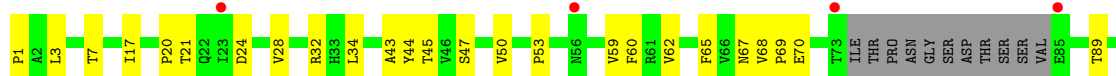
- Molecule 1: coat protein



- Molecule 1: coat protein

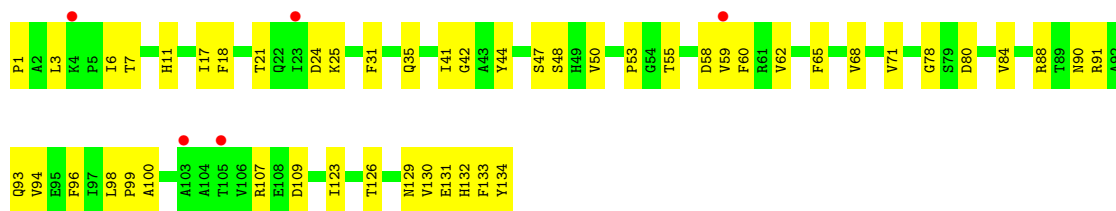


- Molecule 1: coat protein

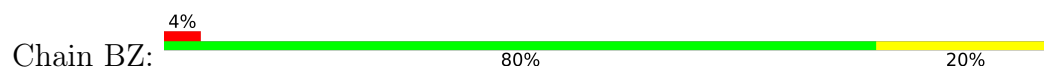


- Molecule 1: coat protein

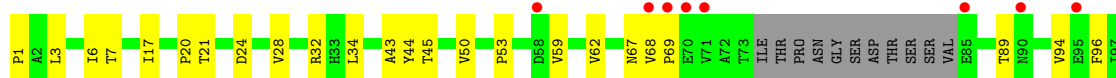




• Molecule 1: coat protein



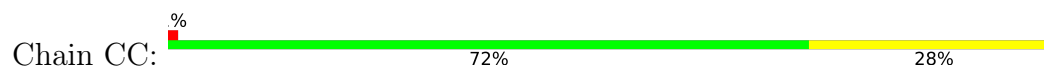
• Molecule 1: coat protein



• Molecule 1: coat protein

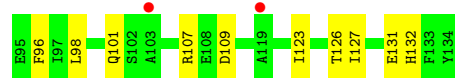
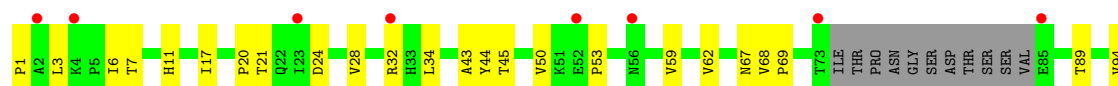


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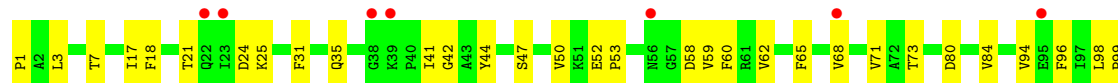
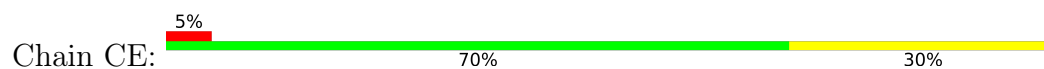


• Molecule 1: coat protein

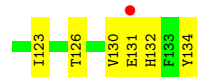
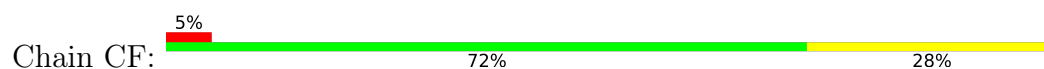




• Molecule 1: coat protein



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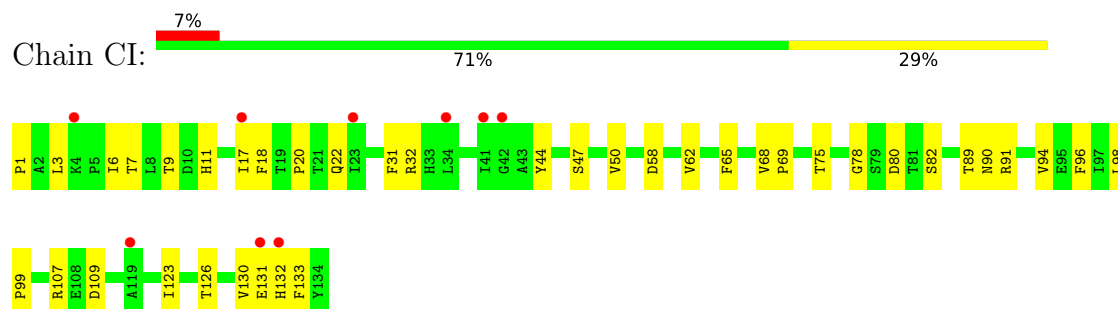
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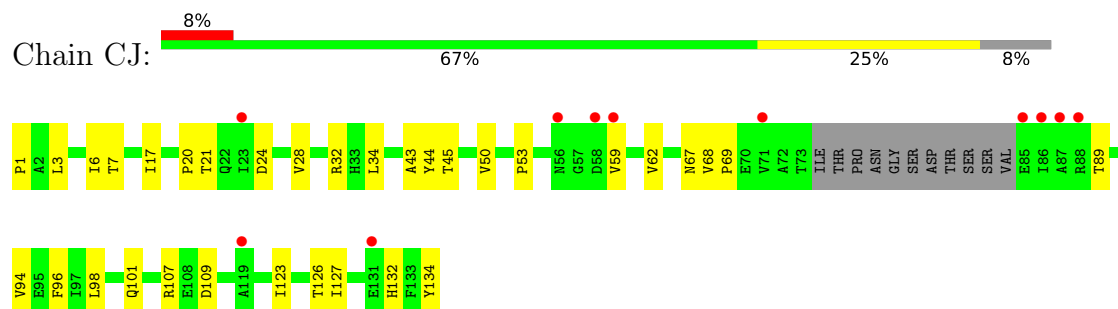
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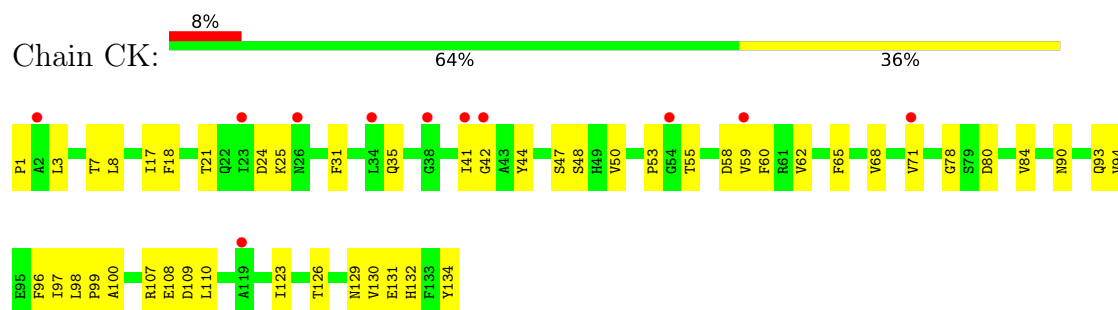
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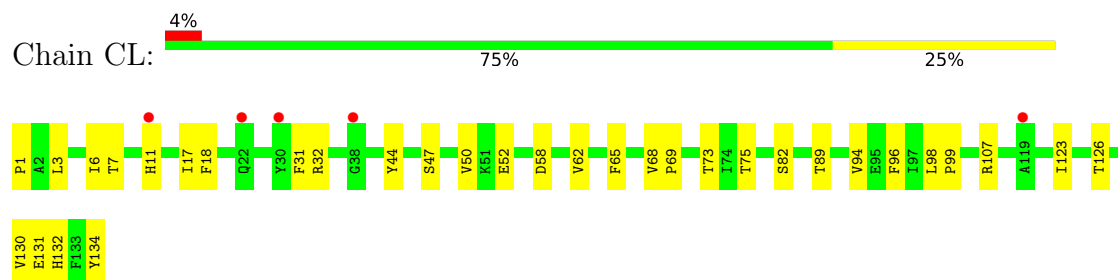
- Molecule 1: coat protein



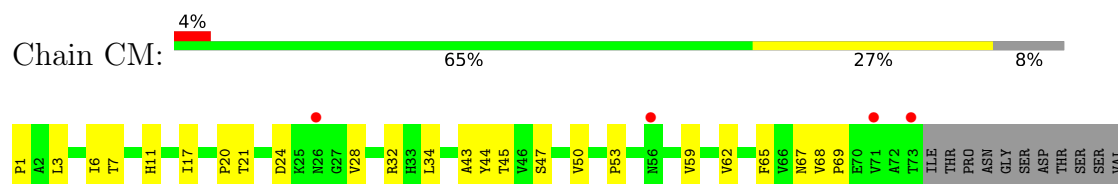
- Molecule 1: coat protein

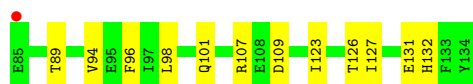


- Molecule 1: coat protein

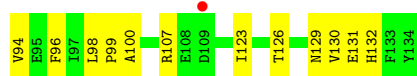
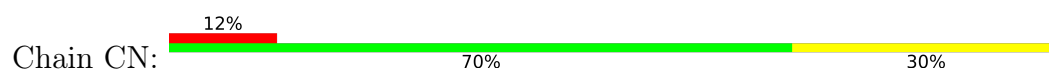


- Molecule 1: coat protein

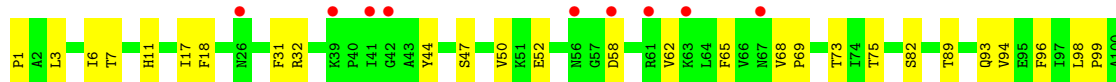
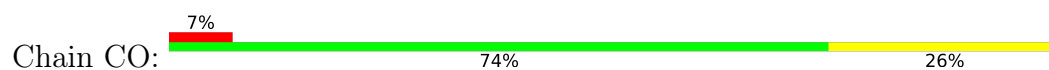




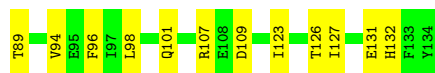
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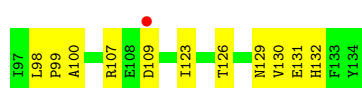
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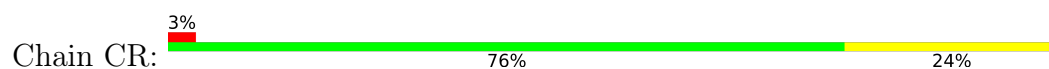
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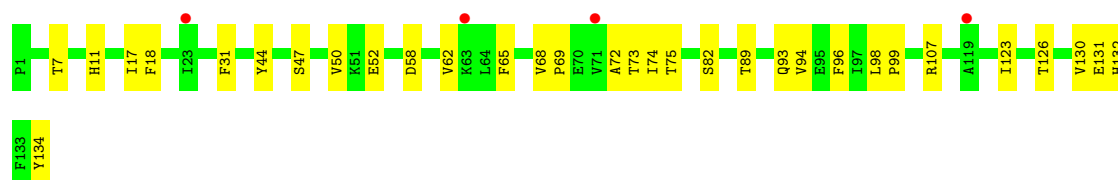


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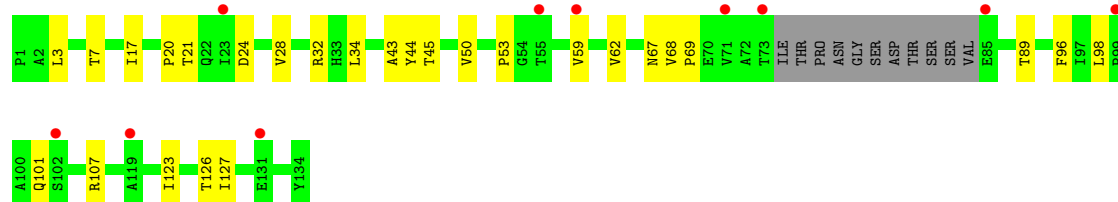
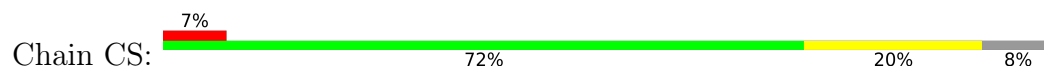


- Molecule 1: coat protein

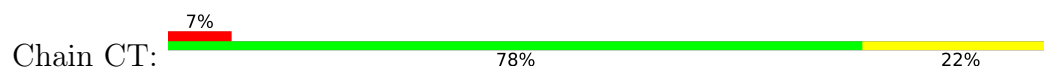




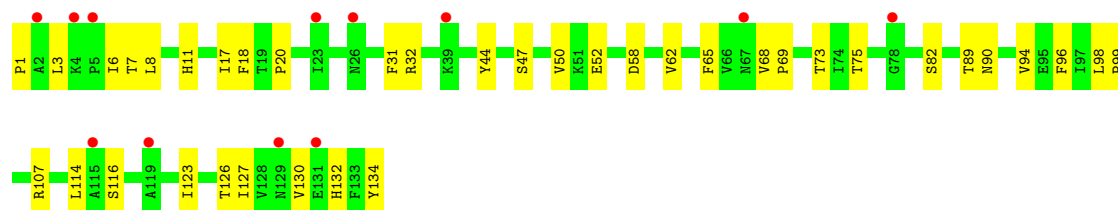
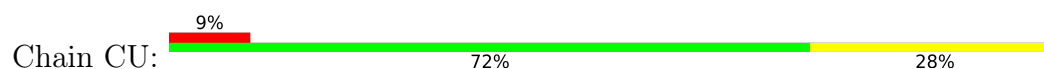
- Molecule 1: coat protein



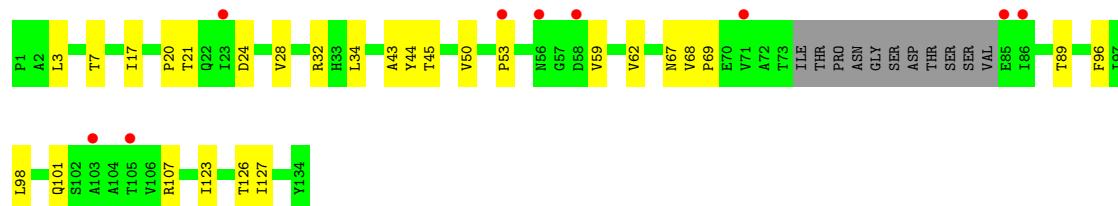
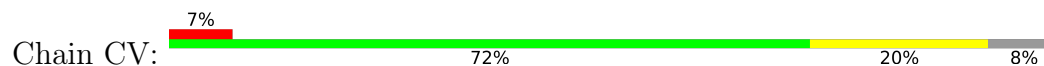
- Molecule 1: coat protein



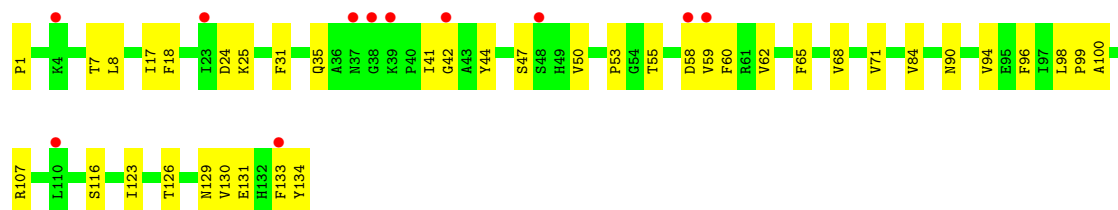
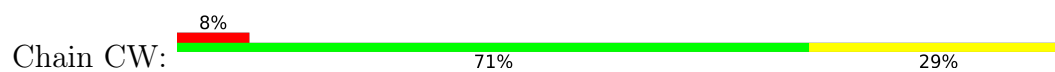
- Molecule 1: coat protein



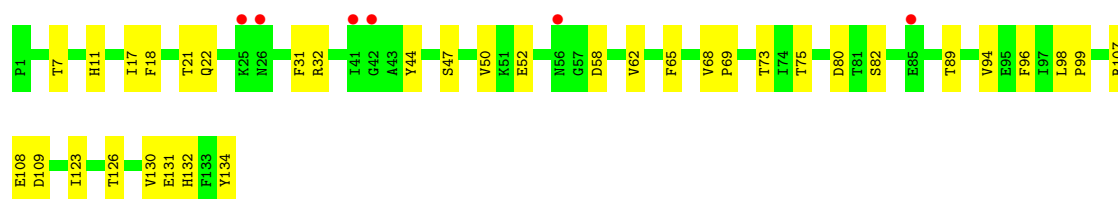
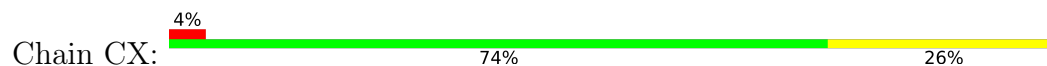
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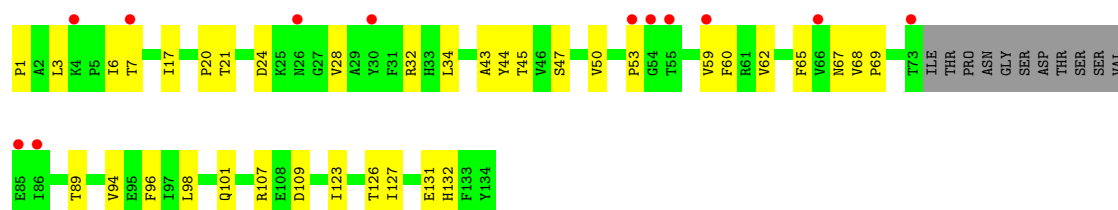
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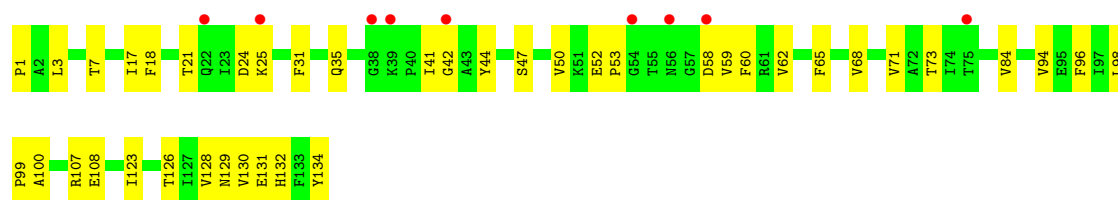
- Molecule 1: coat protein



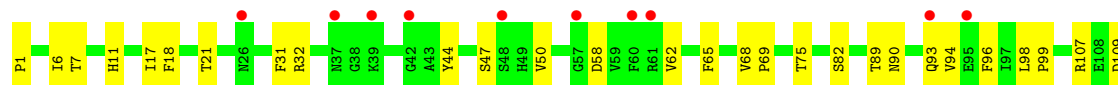
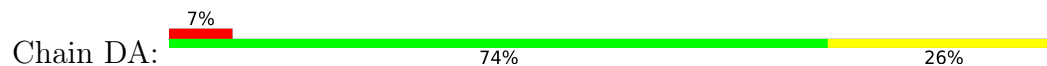
- Molecule 1: coat protein

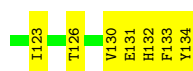


- Molecule 1: coat protein

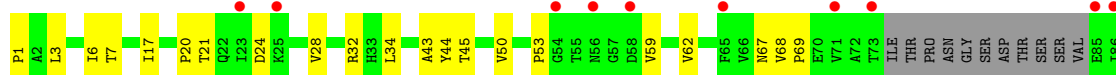


- Molecule 1: coat protein





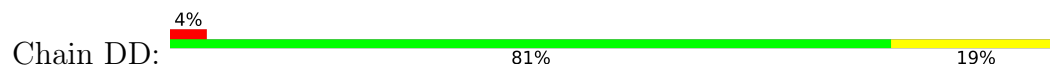
- Molecule 1: coat protein



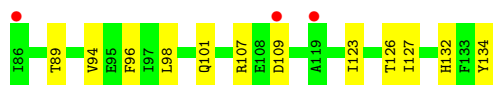
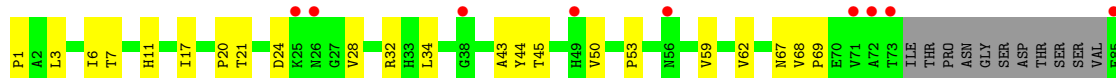
- Molecule 1: coat protein



- Molecule 1: coat protein

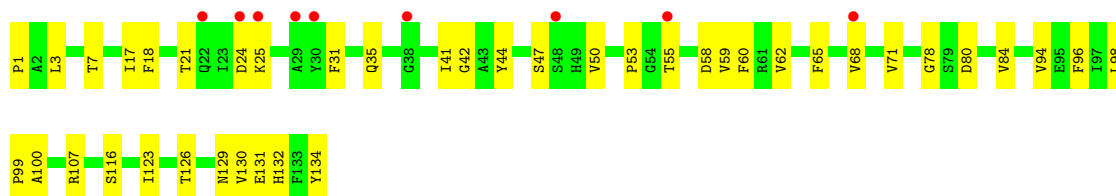


- Molecule 1: coat protein

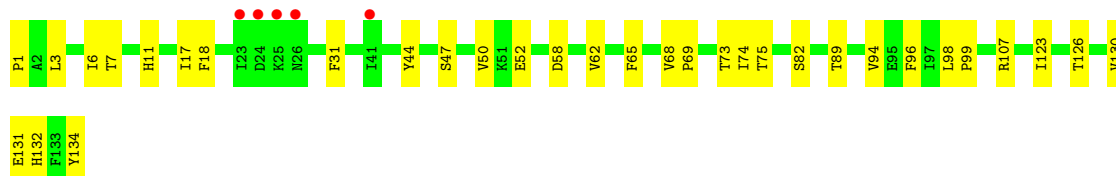
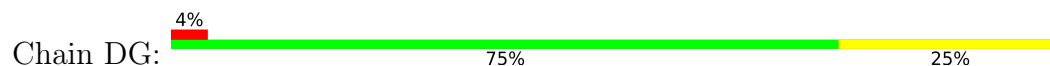


- Molecule 1: coat protein

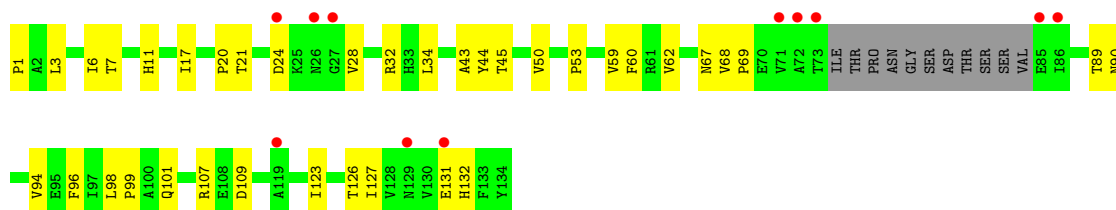




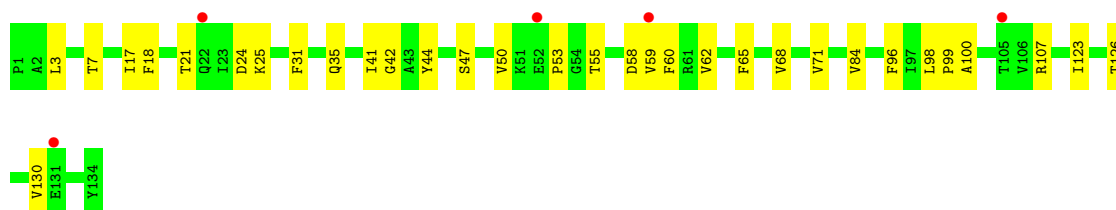
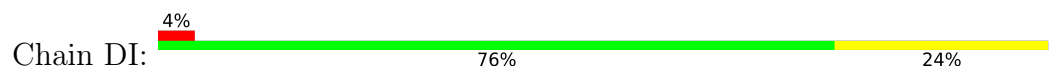
- Molecule 1: coat protein



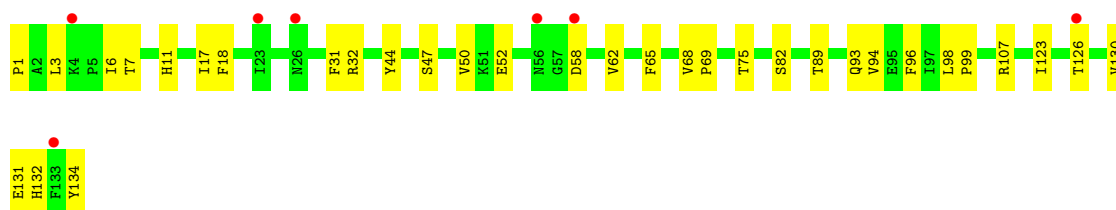
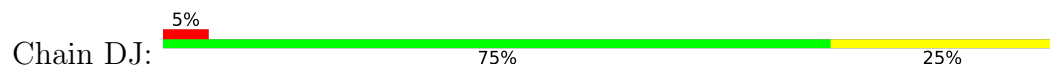
- Molecule 1: coat protein



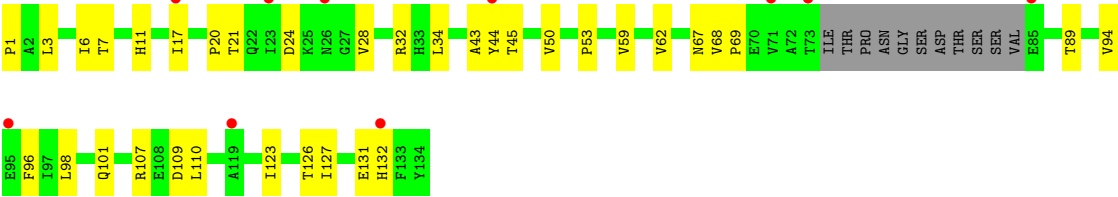
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



● Molecule 1: coat protein



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 41.39 – 3.79	Depositor EDS
% Data completeness (in resolution range)	98.0 (41.39-3.79) 97.9 (41.39-3.79)	Depositor EDS
R_{merge}	0.37	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.261 , 0.267 0.263 , 0.268	Depositor DCC
R_{free} test set	9977 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	102.6	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 81.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	89070	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage'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	0.20	0/1034	0.47	0/1412
1	AB	0.23	0/958	0.50	0/1305
1	AC	0.24	0/1034	0.48	0/1412
1	AD	0.21	0/1034	0.48	0/1412
1	AE	0.23	0/958	0.50	0/1305
1	AF	0.24	0/1034	0.48	0/1412
1	AG	0.21	0/1034	0.47	0/1412
1	AH	0.23	0/958	0.50	0/1305
1	AI	0.24	0/1034	0.48	0/1412
1	AJ	0.21	0/1034	0.48	0/1412
1	AK	0.23	0/958	0.50	0/1305
1	AL	0.24	0/1034	0.47	0/1412
1	AM	0.21	0/1034	0.47	0/1412
1	AN	0.23	0/958	0.50	0/1305
1	AO	0.24	0/1034	0.48	0/1412
1	AP	0.21	0/1034	0.47	0/1412
1	AQ	0.23	0/958	0.50	0/1305
1	AR	0.24	0/1034	0.48	0/1412
1	AS	0.21	0/1034	0.47	0/1412
1	AT	0.23	0/958	0.50	0/1305
1	AU	0.24	0/1034	0.48	0/1412
1	AV	0.21	0/1034	0.47	0/1412
1	AW	0.23	0/958	0.50	0/1305
1	AX	0.24	0/1034	0.48	0/1412
1	AY	0.21	0/1034	0.47	0/1412
1	AZ	0.23	0/958	0.50	0/1305
1	BA	0.24	0/1034	0.48	0/1412
1	BB	0.21	0/1034	0.47	0/1412
1	BC	0.23	0/958	0.50	0/1305
1	BD	0.24	0/1034	0.48	0/1412
1	BE	0.21	0/1034	0.47	0/1412
1	BF	0.23	0/958	0.50	0/1305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BG	0.24	0/1034	0.48	0/1412
1	BH	0.21	0/1034	0.47	0/1412
1	BI	0.23	0/958	0.50	0/1305
1	BJ	0.24	0/1034	0.48	0/1412
1	BK	0.21	0/1034	0.47	0/1412
1	BL	0.23	0/958	0.50	0/1305
1	BM	0.24	0/1034	0.48	0/1412
1	BN	0.21	0/1034	0.47	0/1412
1	BO	0.23	0/958	0.50	0/1305
1	BP	0.24	0/1034	0.48	0/1412
1	BQ	0.21	0/1034	0.47	0/1412
1	BR	0.23	0/958	0.50	0/1305
1	BS	0.24	0/1034	0.48	0/1412
1	BT	0.21	0/1034	0.47	0/1412
1	BU	0.23	0/958	0.50	0/1305
1	BV	0.24	0/1034	0.48	0/1412
1	BW	0.21	0/1034	0.47	0/1412
1	BX	0.23	0/958	0.50	0/1305
1	BY	0.24	0/1034	0.48	0/1412
1	BZ	0.21	0/1034	0.47	0/1412
1	CA	0.23	0/958	0.50	0/1305
1	CB	0.24	0/1034	0.48	0/1412
1	CC	0.21	0/1034	0.48	0/1412
1	CD	0.23	0/958	0.50	0/1305
1	CE	0.24	0/1034	0.48	0/1412
1	CF	0.21	0/1034	0.47	0/1412
1	CG	0.23	0/958	0.50	0/1305
1	CH	0.24	0/1034	0.48	0/1412
1	CI	0.21	0/1034	0.47	0/1412
1	CJ	0.23	0/958	0.50	0/1305
1	CK	0.24	0/1034	0.48	0/1412
1	CL	0.21	0/1034	0.47	0/1412
1	CM	0.23	0/958	0.50	0/1305
1	CN	0.24	0/1034	0.48	0/1412
1	CO	0.21	0/1034	0.47	0/1412
1	CP	0.23	0/958	0.50	0/1305
1	CQ	0.24	0/1034	0.48	0/1412
1	CR	0.21	0/1034	0.47	0/1412
1	CS	0.23	0/958	0.50	0/1305
1	CT	0.24	0/1034	0.48	0/1412
1	CU	0.21	0/1034	0.47	0/1412
1	CV	0.23	0/958	0.50	0/1305
1	CW	0.24	0/1034	0.48	0/1412

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CX	0.21	0/1034	0.47	0/1412
1	CY	0.23	0/958	0.50	0/1305
1	CZ	0.24	0/1034	0.48	0/1412
1	DA	0.21	0/1034	0.47	0/1412
1	DB	0.23	0/958	0.50	0/1305
1	DC	0.24	0/1034	0.47	0/1412
1	DD	0.21	0/1034	0.47	0/1412
1	DE	0.23	0/958	0.50	0/1305
1	DF	0.24	0/1034	0.48	0/1412
1	DG	0.21	0/1034	0.47	0/1412
1	DH	0.23	0/958	0.50	0/1305
1	DI	0.24	0/1034	0.48	0/1412
1	DJ	0.21	0/1034	0.47	0/1412
1	DK	0.23	0/958	0.50	0/1305
1	DL	0.24	0/1034	0.48	0/1412
All	All	0.23	0/90780	0.48	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 ⓘ

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	63	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	47	1
1	AU	1014	0	1020	70	0
1	AV	1014	0	1020	34	0
1	AW	940	0	950	19	1
1	AX	1014	0	1020	35	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	45	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	69	0
1	CL	1014	0	1020	35	0
1	CM	940	0	950	31	0
1	CN	1014	0	1020	38	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	39	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	2402	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 2402 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 ⓘ

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 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	BT	67	ASN
1	DF	67	ASN
1	CB	67	ASN
1	DE	132	HIS
1	DL	11	HIS

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 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 ⓘ

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	134/134 (100%)	0.43	4 (2%) 52 36	64, 102, 139, 208	0
1	AB	123/134 (91%)	0.69	9 (7%) 21 19	67, 109, 164, 214	0
1	AC	134/134 (100%)	0.55	10 (7%) 20 18	66, 105, 140, 217	0
1	AD	134/134 (100%)	0.82	12 (8%) 15 16	64, 102, 139, 208	0
1	AE	123/134 (91%)	0.64	8 (6%) 25 21	67, 109, 164, 214	0
1	AF	134/134 (100%)	0.71	9 (6%) 24 20	66, 105, 140, 217	0
1	AG	134/134 (100%)	0.75	7 (5%) 33 25	64, 102, 139, 208	0
1	AH	123/134 (91%)	0.45	4 (3%) 49 34	67, 109, 164, 214	0
1	AI	134/134 (100%)	0.68	8 (5%) 27 22	66, 105, 140, 217	0
1	AJ	134/134 (100%)	0.62	11 (8%) 17 17	64, 102, 139, 208	0
1	AK	123/134 (91%)	0.63	8 (6%) 25 21	67, 109, 164, 214	0
1	AL	134/134 (100%)	0.61	11 (8%) 17 17	66, 105, 140, 217	0
1	AM	134/134 (100%)	0.34	4 (2%) 52 36	64, 102, 139, 208	0
1	AN	123/134 (91%)	0.41	5 (4%) 41 30	67, 109, 164, 214	0
1	AO	134/134 (100%)	0.43	5 (3%) 45 31	66, 105, 140, 217	0
1	AP	134/134 (100%)	0.74	13 (9%) 13 15	64, 102, 139, 208	0
1	AQ	123/134 (91%)	0.59	8 (6%) 25 21	67, 109, 164, 214	0
1	AR	134/134 (100%)	0.53	4 (2%) 52 36	66, 105, 140, 217	0
1	AS	134/134 (100%)	0.68	7 (5%) 33 25	64, 102, 139, 208	0
1	AT	123/134 (91%)	0.79	10 (8%) 18 17	67, 109, 164, 214	0
1	AU	134/134 (100%)	0.66	11 (8%) 17 17	66, 105, 140, 217	0
1	AV	134/134 (100%)	0.77	12 (8%) 15 16	64, 102, 139, 208	0
1	AW	123/134 (91%)	0.63	6 (4%) 35 26	67, 109, 164, 214	0
1	AX	134/134 (100%)	0.62	12 (8%) 15 16	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%)	0.33	8 (5%) 27 22	64, 102, 139, 208	0
1	AZ	123/134 (91%)	0.65	10 (8%) 18 17	67, 109, 164, 214	0
1	BA	134/134 (100%)	0.54	9 (6%) 24 20	66, 105, 140, 217	0
1	BB	134/134 (100%)	0.46	7 (5%) 33 25	64, 102, 139, 208	0
1	BC	123/134 (91%)	0.55	6 (4%) 35 26	67, 109, 164, 214	0
1	BD	134/134 (100%)	0.63	7 (5%) 33 25	66, 105, 140, 217	0
1	BE	134/134 (100%)	0.51	5 (3%) 45 31	64, 102, 139, 208	0
1	BF	123/134 (91%)	0.73	9 (7%) 21 19	67, 109, 164, 214	0
1	BG	134/134 (100%)	0.72	15 (11%) 10 13	66, 105, 140, 217	0
1	BH	134/134 (100%)	0.52	11 (8%) 17 17	64, 102, 139, 208	0
1	BI	123/134 (91%)	0.44	6 (4%) 35 26	67, 109, 164, 214	0
1	BJ	134/134 (100%)	0.56	5 (3%) 45 31	66, 105, 140, 217	0
1	BK	134/134 (100%)	0.76	12 (8%) 15 16	64, 102, 139, 208	0
1	BL	123/134 (91%)	0.62	4 (3%) 49 34	67, 109, 164, 214	0
1	BM	134/134 (100%)	0.65	4 (2%) 52 36	66, 105, 140, 217	0
1	BN	134/134 (100%)	0.49	3 (2%) 62 44	64, 102, 139, 208	0
1	BO	123/134 (91%)	0.43	5 (4%) 41 30	67, 109, 164, 214	0
1	BP	134/134 (100%)	0.58	8 (5%) 27 22	66, 105, 140, 217	0
1	BQ	134/134 (100%)	0.49	5 (3%) 45 31	64, 102, 139, 208	0
1	BR	123/134 (91%)	0.56	8 (6%) 25 21	67, 109, 164, 214	0
1	BS	134/134 (100%)	0.62	8 (5%) 27 22	66, 105, 140, 217	0
1	BT	134/134 (100%)	0.63	9 (6%) 24 20	64, 102, 139, 208	0
1	BU	123/134 (91%)	0.43	8 (6%) 25 21	67, 109, 164, 214	0
1	BV	134/134 (100%)	0.63	13 (9%) 13 15	66, 105, 140, 217	0
1	BW	134/134 (100%)	0.76	10 (7%) 20 18	64, 102, 139, 208	0
1	BX	123/134 (91%)	0.60	5 (4%) 41 30	67, 109, 164, 214	0
1	BY	134/134 (100%)	0.47	5 (3%) 45 31	66, 105, 140, 217	0
1	BZ	134/134 (100%)	0.52	6 (4%) 38 27	64, 102, 139, 208	0
1	CA	123/134 (91%)	0.62	9 (7%) 21 19	67, 109, 164, 214	0
1	CB	134/134 (100%)	0.68	9 (6%) 24 20	66, 105, 140, 217	0
1	CC	134/134 (100%)	0.38	2 (1%) 72 50	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%)	0.52	10 (8%)	18 17	67, 109, 164, 214	0
1	CE	134/134 (100%)	0.51	7 (5%)	33 25	66, 105, 140, 217	0
1	CF	134/134 (100%)	0.40	7 (5%)	33 25	64, 102, 139, 208	0
1	CG	123/134 (91%)	0.50	6 (4%)	35 26	67, 109, 164, 214	0
1	CH	134/134 (100%)	0.61	8 (5%)	27 22	66, 105, 140, 217	0
1	CI	134/134 (100%)	0.61	9 (6%)	24 20	64, 102, 139, 208	0
1	CJ	123/134 (91%)	0.65	11 (8%)	15 16	67, 109, 164, 214	0
1	CK	134/134 (100%)	0.76	11 (8%)	17 17	66, 105, 140, 217	0
1	CL	134/134 (100%)	0.48	5 (3%)	45 31	64, 102, 139, 208	0
1	CM	123/134 (91%)	0.34	5 (4%)	41 30	67, 109, 164, 214	0
1	CN	134/134 (100%)	0.69	16 (11%)	9 12	66, 105, 140, 217	0
1	CO	134/134 (100%)	0.42	10 (7%)	20 18	64, 102, 139, 208	0
1	CP	123/134 (91%)	0.33	5 (4%)	41 30	67, 109, 164, 214	0
1	CQ	134/134 (100%)	0.50	8 (5%)	27 22	66, 105, 140, 217	0
1	CR	134/134 (100%)	0.57	4 (2%)	52 36	64, 102, 139, 208	0
1	CS	123/134 (91%)	0.73	10 (8%)	18 17	67, 109, 164, 214	0
1	CT	134/134 (100%)	0.79	9 (6%)	24 20	66, 105, 140, 217	0
1	CU	134/134 (100%)	0.72	12 (8%)	15 16	64, 102, 139, 208	0
1	CV	123/134 (91%)	0.63	9 (7%)	21 19	67, 109, 164, 214	0
1	CW	134/134 (100%)	0.69	11 (8%)	17 17	66, 105, 140, 217	0
1	CX	134/134 (100%)	0.43	6 (4%)	38 27	64, 102, 139, 208	0
1	CY	123/134 (91%)	0.58	12 (9%)	13 15	67, 109, 164, 214	0
1	CZ	134/134 (100%)	0.62	9 (6%)	24 20	66, 105, 140, 217	0
1	DA	134/134 (100%)	0.60	10 (7%)	20 18	64, 102, 139, 208	0
1	DB	123/134 (91%)	0.70	11 (8%)	15 16	67, 109, 164, 214	0
1	DC	134/134 (100%)	0.60	5 (3%)	45 31	66, 105, 140, 217	0
1	DD	134/134 (100%)	0.59	6 (4%)	38 27	64, 102, 139, 208	0
1	DE	123/134 (91%)	0.68	12 (9%)	13 15	67, 109, 164, 214	0
1	DF	134/134 (100%)	0.65	9 (6%)	24 20	66, 105, 140, 217	0
1	DG	134/134 (100%)	0.32	5 (3%)	45 31	64, 102, 139, 208	0
1	DH	123/134 (91%)	0.68	11 (8%)	15 16	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%)	0.48	5 (3%) 45 31	66, 105, 140, 217	0
1	DJ	134/134 (100%)	0.44	7 (5%) 33 25	64, 102, 139, 208	0
1	DK	123/134 (91%)	0.61	10 (8%) 18 17	67, 109, 164, 214	0
1	DL	134/134 (100%)	0.60	11 (8%) 17 17	66, 105, 140, 217	0
All	All	11730/12060 (97%)	0.58	731 (6%) 26 22	64, 104, 154, 217	0

The worst 5 of 731 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CZ	56	ASN	8.2
1	AW	56	ASN	6.5
1	BG	56	ASN	6.5
1	BW	26	ASN	6.4
1	CT	23	ILE	6.2

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	AA	201	1/1	0.60	0.14	64,64,64,64	0
2	CA	CV	201	1/1	0.74	0.10	64,64,64,64	0
2	CA	BH	201	1/1	0.83	0.09	64,64,64,64	0
2	CA	BX	201	1/1	0.84	0.09	64,64,64,64	0
2	CA	AZ	201	1/1	0.86	0.09	64,64,64,64	0
2	CA	BB	201	1/1	0.87	0.08	64,64,64,64	0
2	CA	CS	201	1/1	0.88	0.07	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	AE	201	1/1	0.88	0.08	64,64,64,64	0
2	CA	BT	201	1/1	0.90	0.11	64,64,64,64	0
2	CA	BI	201	1/1	0.90	0.10	64,64,64,64	0
2	CA	BL	201	1/1	0.91	0.10	64,64,64,64	0
2	CA	AB	201	1/1	0.91	0.08	64,64,64,64	0
2	CA	AF	201	1/1	0.91	0.07	64,64,64,64	0
2	CA	CD	201	1/1	0.91	0.08	64,64,64,64	0
2	CA	AH	201	1/1	0.91	0.09	64,64,64,64	0
2	CA	AK	201	1/1	0.91	0.08	64,64,64,64	0
2	CA	CF	201	1/1	0.92	0.06	64,64,64,64	0
2	CA	AG	201	1/1	0.92	0.09	64,64,64,64	0
2	CA	BC	201	1/1	0.92	0.06	64,64,64,64	0
2	CA	BR	201	1/1	0.93	0.10	64,64,64,64	0
2	CA	CC	201	1/1	0.93	0.09	64,64,64,64	0
2	CA	AN	201	1/1	0.93	0.12	64,64,64,64	0
2	CA	AW	201	1/1	0.94	0.08	64,64,64,64	0
2	CA	CJ	201	1/1	0.94	0.05	64,64,64,64	0
2	CA	AM	201	1/1	0.96	0.05	64,64,64,64	0
2	CA	CA	201	1/1	0.96	0.13	64,64,64,64	0
2	CA	AC	201	1/1	0.96	0.05	64,64,64,64	0
2	CA	AQ	201	1/1	0.96	0.04	64,64,64,64	0
2	CA	BF	201	1/1	0.97	0.15	64,64,64,64	0
2	CA	BK	201	1/1	0.98	0.09	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.