



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 10:12 PM EDT

PDB ID : 6YFH
Title : Virus-like particle of bacteriophage EMS014
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on : 2020-03-26
Resolution : 3.89 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

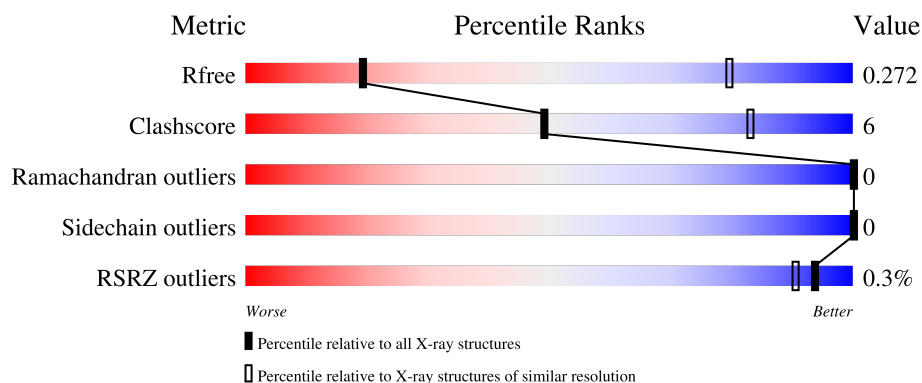
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	156	 82% 18%
1	AB	156	 85% 15%
1	AC	156	 83% 17%
1	AD	156	 83% 17%
1	AE	156	 85% 15%



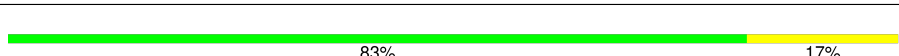
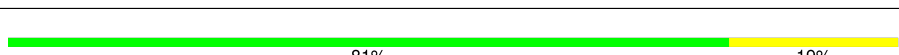
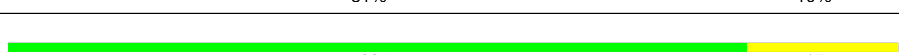

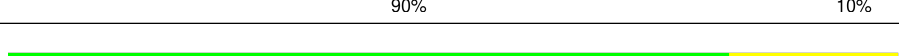
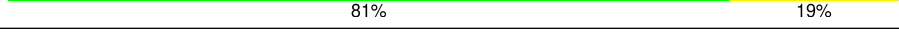




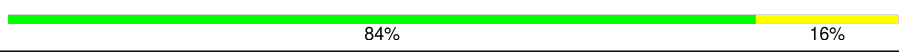



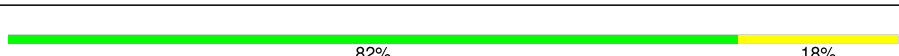
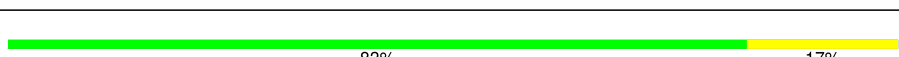






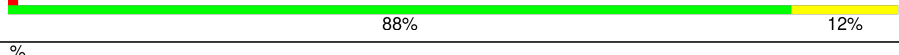
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Mol	Chain	Length	Quality of chain
1	AF	156	 83%17%
1	AG	156	 85%15%
1	AH	156	 83%17%
1	AI	156	 91%9%
1	AJ	156	 81%19%
1	AK	156	 2%84%16%
1	AL	156	 83%17%
1	AM	156	 83%17%
1	AN	156	 85%15%
1	AO	156	 86%14%
1	AP	156	 0%85%15%
1	AQ	156	 0%85%15%
1	AR	156	 0%87%13%
1	AS	156	 80%20%
1	AT	156	 0%86%14%
1	AU	156	 0%83%17%
1	AV	156	 0%82%18%
1	AW	156	 86%14%
1	AX	156	 84%16%
1	AY	156	 82%18%
1	AZ	156	 84%16%
1	BA	156	 83%17%
1	BB	156	 83%17%
1	BC	156	 0%82%18%
1	BD	156	 87%13%


























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Mol	Chain	Length	Quality of chain	
1	BE	156		
1	BF	156		
1	BG	156		
1	BH	156		
1	BI	156		
1	BJ	156		
1	BK	156		
1	BL	156		
1	BM	156		
1	BN	156		
1	BO	156		
1	BP	156		
1	BQ	156		
1	BR	156		
1	BS	156		
1	BT	156		
1	BU	156		
1	BV	156		
1	BW	156		
1	BX	156		
1	BY	156		
1	BZ	156		
1	CA	156		
1	CB	156		
1	CC	156		











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Mol	Chain	Length	Quality of chain
1	CD	156	 80% 20%
1	CE	156	 90% 10%
1	CF	156	 83% 17%
1	CG	156	 85% 15%
1	CH	156	 90% 10%
1	CI	156	 85% 15%
1	CJ	156	 85% 15%
1	CK	156	 86% 14%
1	CL	156	 81% 19%
1	CM	156	 86% 14%
1	CN	156	 84% 16%
1	CO	156	 81% 19%
1	CP	156	 83% 17%
1	CQ	156	 90% 10%
1	CR	156	 82% 18%
1	CS	156	 85% 15%
1	CT	156	 81% 19%
1	CU	156	 85% 15%
1	CV	156	 85% 15%
1	CW	156	 83% 17%
1	CX	156	 83% 17%
1	CY	156	 88% 12%
1	CZ	156	 88% 12%
1	DA	156	 83% 17%
1	DB	156	 86% 14%

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Mol	Chain	Length	Quality of chain
1	DC	156	 90% 10%
1	DD	156	 82% 18%
1	DE	156	 85% 15%
1	DF	156	 83% 17%
1	DG	156	 82% 18%
1	DH	156	 85% 15%
1	DI	156	 89% 11%
1	DJ	156	 82% 18%
1	DK	156	 84% 16%
1	DL	156	 83% 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 104400 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	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AB	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AC	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AD	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AE	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AF	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AG	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AH	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AI	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AJ	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AK	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AL	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AM	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AN	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AO	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AP	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AR	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AS	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AT	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AU	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AV	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AW	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AX	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AY	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	AZ	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BA	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BB	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BC	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BD	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BE	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BF	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BG	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BH	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BI	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BJ	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BK	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BM	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BN	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BO	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BP	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BQ	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BR	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BS	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BT	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BU	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BV	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BW	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BX	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BY	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	BZ	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CA	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CB	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CC	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CD	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CE	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CF	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CH	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CI	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CJ	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CK	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CL	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CM	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CN	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CO	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CP	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CQ	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CR	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CS	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CT	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CU	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CV	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CW	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CX	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CY	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	CZ	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			
1	DA	156	Total	C	N	O	S	0	0	0
			1160	732	198	223	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DB	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0
1	DC	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0
1	DD	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0
1	DE	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0
1	DF	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0
1	DG	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0
1	DH	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0
1	DI	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0
1	DJ	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0
1	DK	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0
1	DL	156	Total 1160	C 732	N 198	O 223	S 7	0	0	0

3 Residue-property plots [i](#)


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

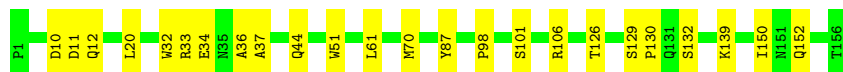
- Molecule 1: coat protein

Chain AA:  82% 18%




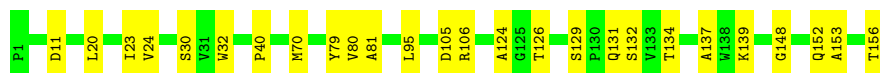
- Molecule 1: coat protein

Chain AB:  85% 15%




- Molecule 1: coat protein

Chain AC:  83% 17%




- Molecule 1: coat protein

Chain AD:  83% 17%




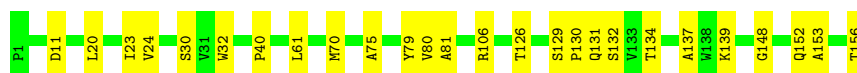
- Molecule 1: coat protein

Chain AE:  85% 15%



- Molecule 1: coat protein

Chain AF:  83% 17%



- Molecule 1: coat protein

Chain AG: 85% 15%



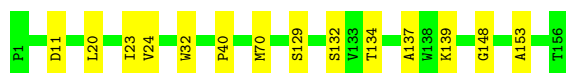
- Molecule 1: coat protein

Chain AH: 83% 17%



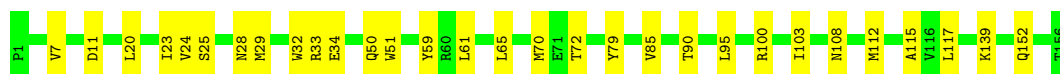
- Molecule 1: coat protein

Chain AI: 91% 9%



- Molecule 1: coat protein

Chain AJ: 81% 19%



- Molecule 1: coat protein

Chain AK: 84% 16% 2%



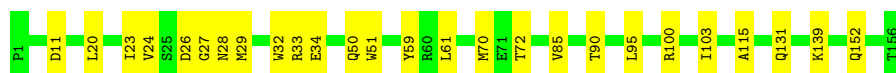
- Molecule 1: coat protein

Chain AL: 83% 17%



- Molecule 1: coat protein

Chain AM: 83% 17%



- Molecule 1: coat protein

Chain AN: 85% 15%



- Molecule 1: coat protein

Chain AO: 86% 14%



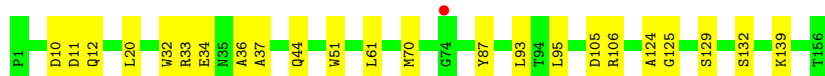
- Molecule 1: coat protein

Chain AP: 85% 15%



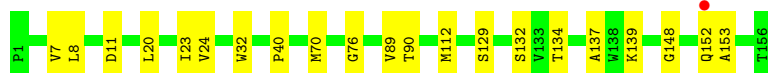
- Molecule 1: coat protein

Chain AQ: 85% 15%



- Molecule 1: coat protein

Chain AR: 87% 13%



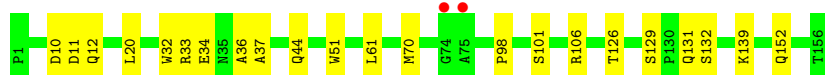
- Molecule 1: coat protein

Chain AS: 80% 20%

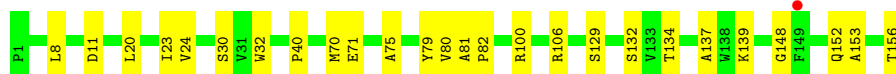
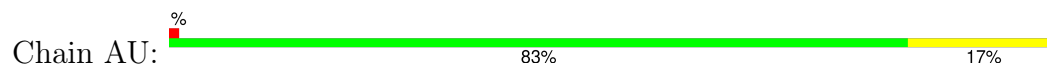


- Molecule 1: coat protein

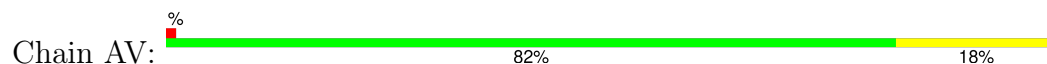
Chain AT: 86% 14%



- Molecule 1: coat protein



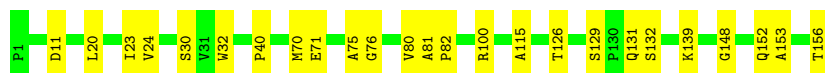
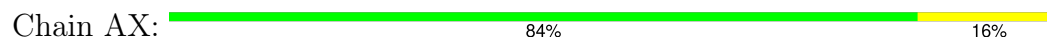
- Molecule 1: coat protein



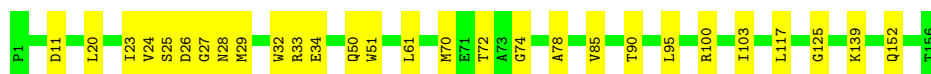
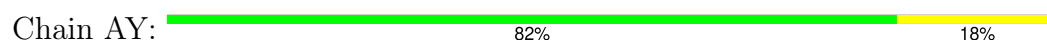
- Molecule 1: coat protein



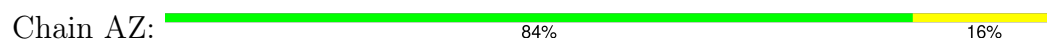
- Molecule 1: coat protein



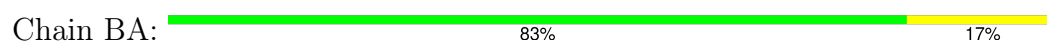
- Molecule 1: coat protein

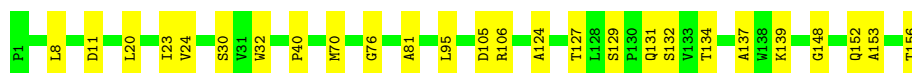


- Molecule 1: coat protein

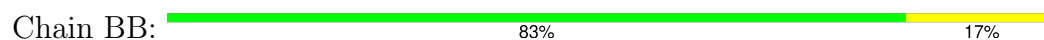


- Molecule 1: coat protein

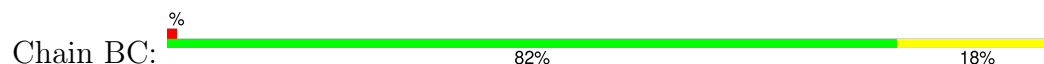




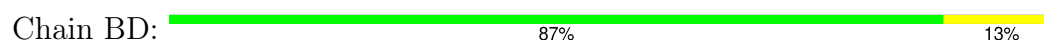
- Molecule 1: coat protein



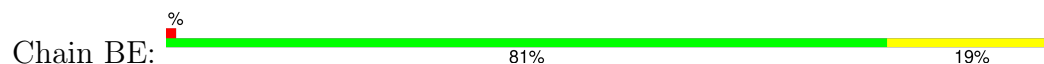
- Molecule 1: coat protein



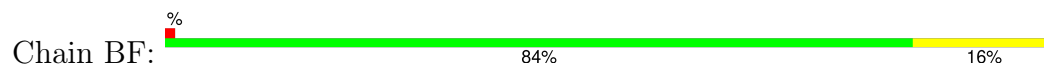
- Molecule 1: coat protein



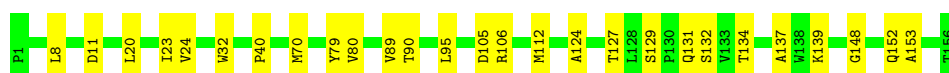
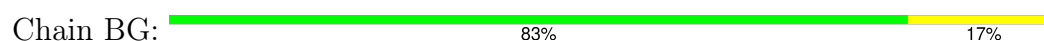
- Molecule 1: coat protein



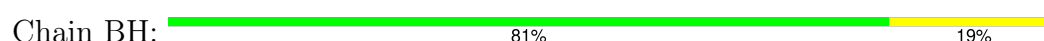
- Molecule 1: coat protein



- Molecule 1: coat protein



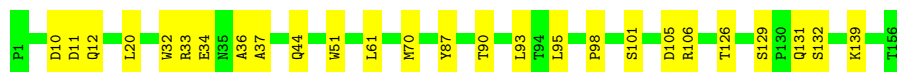
- Molecule 1: coat protein





- Molecule 1: coat protein

Chain BI: 83% 17%



- Molecule 1: coat protein

Chain BJ: 90% 10%



- Molecule 1: coat protein

Chain BK: 81% 19%



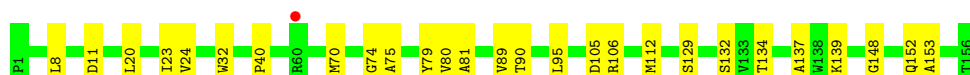
- Molecule 1: coat protein

Chain BL: 83% 17%



- Molecule 1: coat protein

Chain BM: 83% 17%



- Molecule 1: coat protein

Chain BN: 80% 20%



- Molecule 1: coat protein

Chain BO: 84% 16%



- Molecule 1: coat protein

Chain BP: 84% 16%



- Molecule 1: coat protein

Chain BQ: 87% 13%



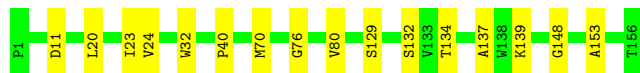
- Molecule 1: coat protein

Chain BR: 86% 14%



- Molecule 1: coat protein

Chain BS: 90% 10%



- Molecule 1: coat protein

Chain BT: 82% 18%



- Molecule 1: coat protein

Chain BU: 83% 17%

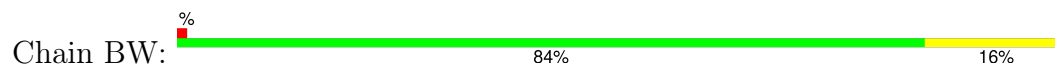


- Molecule 1: coat protein

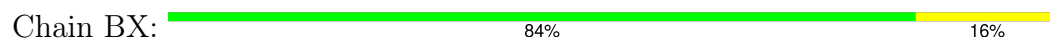
Chain BV: 85% 15%



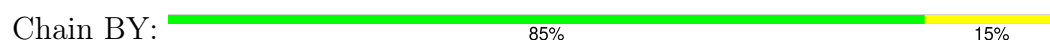
- Molecule 1: coat protein



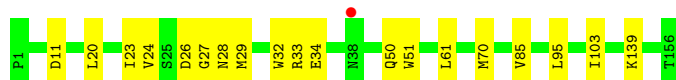
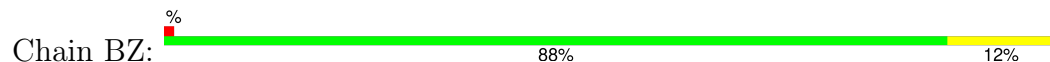
- Molecule 1: coat protein



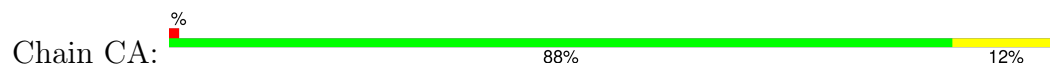
- Molecule 1: coat protein



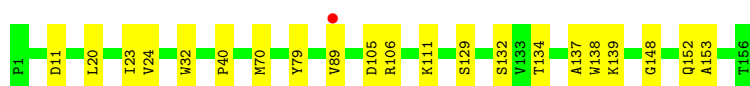
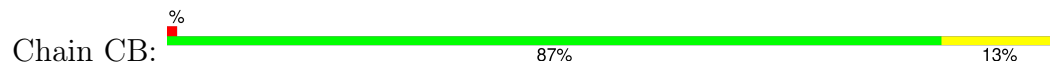
- Molecule 1: coat protein



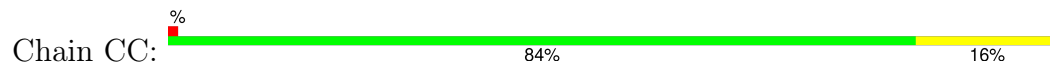
- Molecule 1: coat protein



- Molecule 1: coat protein

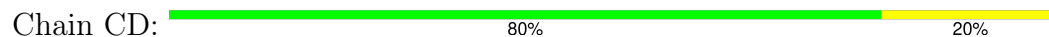


- Molecule 1: coat protein





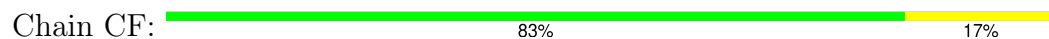
- Molecule 1: coat protein



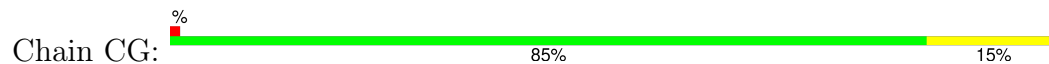
- Molecule 1: coat protein



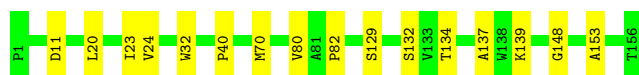
- Molecule 1: coat protein



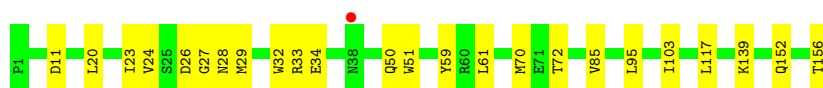
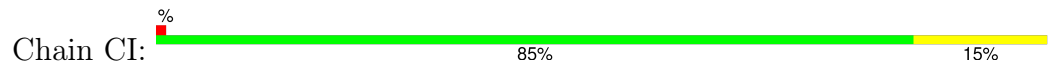
- Molecule 1: coat protein



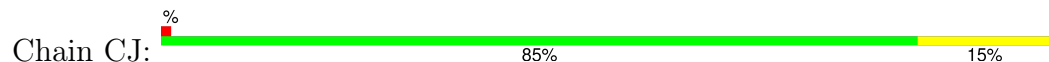
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

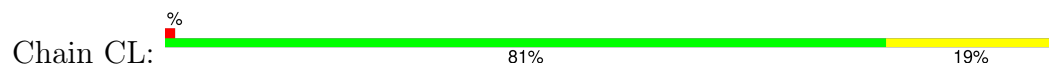




- Molecule 1: coat protein



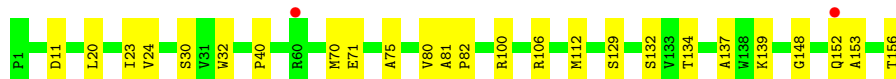
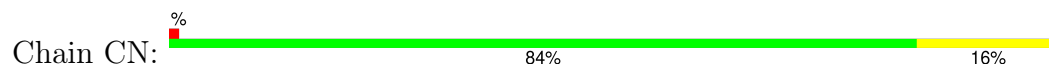
- Molecule 1: coat protein



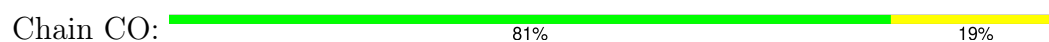
- Molecule 1: coat protein



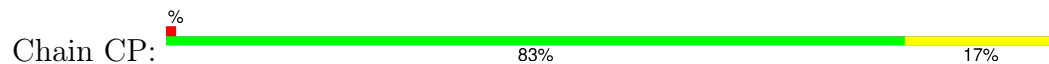
- Molecule 1: coat protein



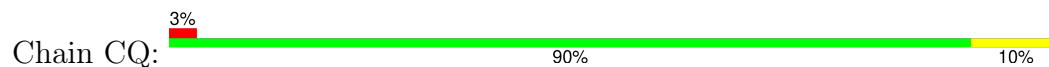
- Molecule 1: coat protein



- Molecule 1: coat protein

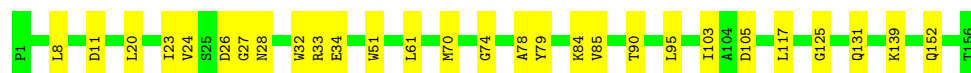
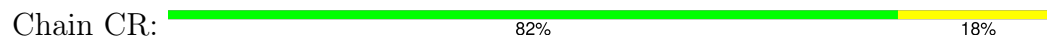


- Molecule 1: coat protein

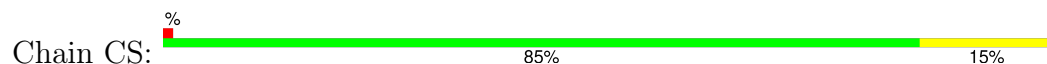




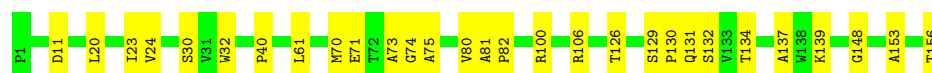
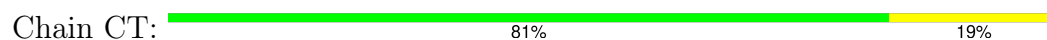
- Molecule 1: coat protein



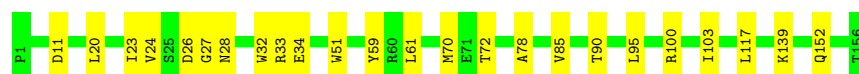
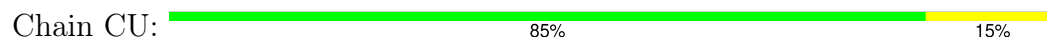
- Molecule 1: coat protein



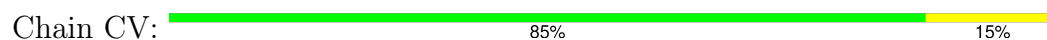
- Molecule 1: coat protein



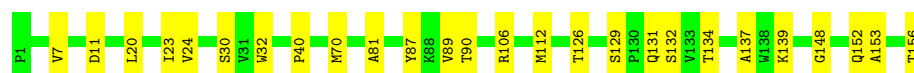
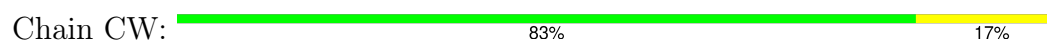
- Molecule 1: coat protein



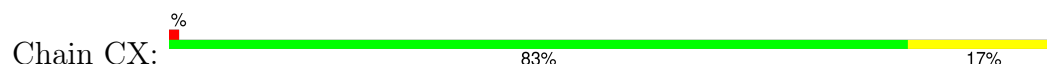
- Molecule 1: coat protein

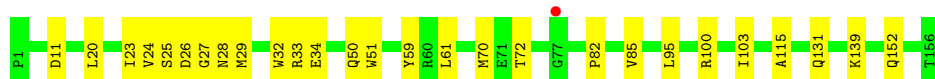


- Molecule 1: coat protein



- Molecule 1: coat protein





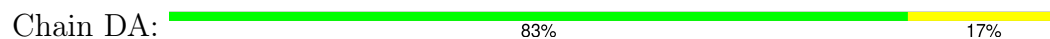
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



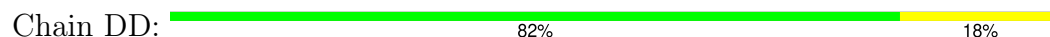
- Molecule 1: coat protein



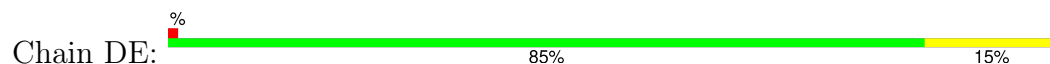
- Molecule 1: coat protein



- Molecule 1: coat protein

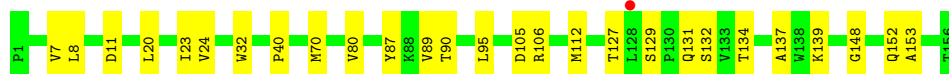
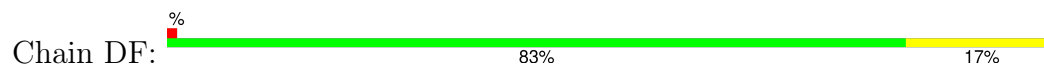


- Molecule 1: coat protein

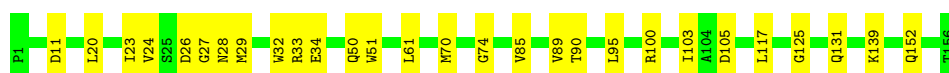
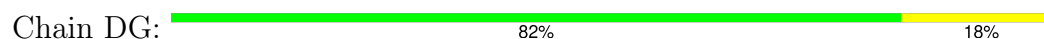




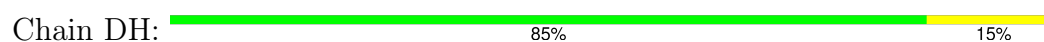
- Molecule 1: coat protein



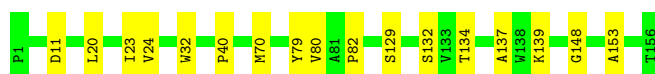
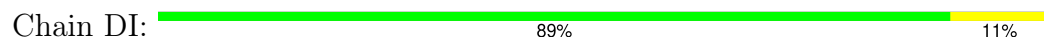
- Molecule 1: coat protein



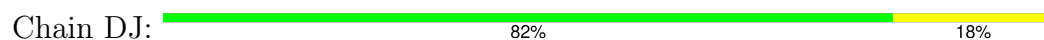
- Molecule 1: coat protein



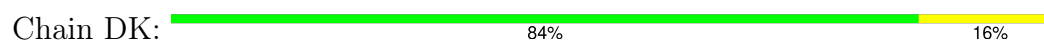
- Molecule 1: coat protein



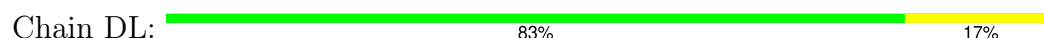
- Molecule 1: coat protein

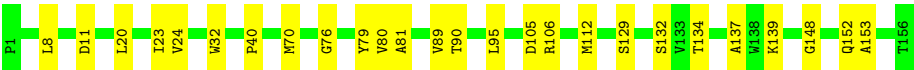


- Molecule 1: coat protein



- Molecule 1: coat protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	287.11Å 492.50Å 553.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 3.89 49.41 – 3.89	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.36-3.89) 99.2 (49.41-3.89)	Depositor EDS
R_{merge}	0.86	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.267 , 0.270 0.269 , 0.272	Depositor DCC
R_{free} test set	10019 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å ²)	127.7	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 106.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.100 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.136 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	104400	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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

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	0.30	0/1183	0.51	0/1612
1	AB	0.29	0/1183	0.48	0/1612
1	AC	0.29	0/1183	0.50	0/1612
1	AD	0.30	0/1183	0.51	0/1612
1	AE	0.29	0/1183	0.48	0/1612
1	AF	0.29	0/1183	0.50	0/1612
1	AG	0.30	0/1183	0.51	0/1612
1	AH	0.29	0/1183	0.48	0/1612
1	AI	0.29	0/1183	0.50	0/1612
1	AJ	0.30	0/1183	0.51	0/1612
1	AK	0.29	0/1183	0.48	0/1612
1	AL	0.29	0/1183	0.50	0/1612
1	AM	0.30	0/1183	0.51	0/1612
1	AN	0.29	0/1183	0.48	0/1612
1	AO	0.29	0/1183	0.50	0/1612
1	AP	0.31	0/1183	0.51	0/1612
1	AQ	0.29	0/1183	0.48	0/1612
1	AR	0.29	0/1183	0.50	0/1612
1	AS	0.30	0/1183	0.51	0/1612
1	AT	0.29	0/1183	0.48	0/1612
1	AU	0.29	0/1183	0.50	0/1612
1	AV	0.30	0/1183	0.51	0/1612
1	AW	0.29	0/1183	0.48	0/1612
1	AX	0.29	0/1183	0.50	0/1612
1	AY	0.30	0/1183	0.51	0/1612
1	AZ	0.29	0/1183	0.48	0/1612
1	BA	0.29	0/1183	0.50	0/1612
1	BB	0.30	0/1183	0.51	0/1612
1	BC	0.29	0/1183	0.48	0/1612
1	BD	0.29	0/1183	0.50	0/1612
1	BE	0.30	0/1183	0.51	0/1612
1	BF	0.29	0/1183	0.48	0/1612
1	BG	0.29	0/1183	0.50	0/1612
1	BH	0.30	0/1183	0.51	0/1612

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BI	0.29	0/1183	0.48	0/1612
1	BJ	0.29	0/1183	0.50	0/1612
1	BK	0.30	0/1183	0.51	0/1612
1	BL	0.29	0/1183	0.48	0/1612
1	BM	0.29	0/1183	0.50	0/1612
1	BN	0.30	0/1183	0.51	0/1612
1	BO	0.29	0/1183	0.48	0/1612
1	BP	0.29	0/1183	0.50	0/1612
1	BQ	0.30	0/1183	0.51	0/1612
1	BR	0.29	0/1183	0.48	0/1612
1	BS	0.29	0/1183	0.50	0/1612
1	BT	0.30	0/1183	0.51	0/1612
1	BU	0.29	0/1183	0.48	0/1612
1	BV	0.29	0/1183	0.50	0/1612
1	BW	0.30	0/1183	0.51	0/1612
1	BX	0.29	0/1183	0.48	0/1612
1	BY	0.29	0/1183	0.50	0/1612
1	BZ	0.30	0/1183	0.51	0/1612
1	CA	0.29	0/1183	0.48	0/1612
1	CB	0.29	0/1183	0.50	0/1612
1	CC	0.30	0/1183	0.51	0/1612
1	CD	0.29	0/1183	0.48	0/1612
1	CE	0.29	0/1183	0.50	0/1612
1	CF	0.30	0/1183	0.51	0/1612
1	CG	0.30	0/1183	0.48	0/1612
1	CH	0.29	0/1183	0.50	0/1612
1	CI	0.31	0/1183	0.51	0/1612
1	CJ	0.29	0/1183	0.48	0/1612
1	CK	0.29	0/1183	0.50	0/1612
1	CL	0.30	0/1183	0.51	0/1612
1	CM	0.29	0/1183	0.48	0/1612
1	CN	0.29	0/1183	0.50	0/1612
1	CO	0.30	0/1183	0.51	0/1612
1	CP	0.29	0/1183	0.48	0/1612
1	CQ	0.29	0/1183	0.50	0/1612
1	CR	0.30	0/1183	0.51	0/1612
1	CS	0.29	0/1183	0.48	0/1612
1	CT	0.29	0/1183	0.50	0/1612
1	CU	0.30	0/1183	0.51	0/1612
1	CV	0.30	0/1183	0.48	0/1612
1	CW	0.29	0/1183	0.50	0/1612
1	CX	0.30	0/1183	0.51	0/1612
1	CY	0.29	0/1183	0.48	0/1612

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CZ	0.29	0/1183	0.50	0/1612
1	DA	0.30	0/1183	0.51	0/1612
1	DB	0.29	0/1183	0.48	0/1612
1	DC	0.29	0/1183	0.50	0/1612
1	DD	0.30	0/1183	0.51	0/1612
1	DE	0.29	0/1183	0.48	0/1612
1	DF	0.29	0/1183	0.50	0/1612
1	DG	0.31	0/1183	0.51	0/1612
1	DH	0.30	0/1183	0.48	0/1612
1	DI	0.29	0/1183	0.50	0/1612
1	DJ	0.30	0/1183	0.51	0/1612
1	DK	0.30	0/1183	0.48	0/1612
1	DL	0.29	0/1183	0.50	0/1612
All	All	0.30	0/106470	0.50	0/145080

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	1160	0	1172	20	0
1	AB	1160	0	1172	19	0
1	AC	1160	0	1172	23	0
1	AD	1160	0	1172	22	0
1	AE	1160	0	1172	19	0
1	AF	1160	0	1172	25	0
1	AG	1160	0	1172	18	0
1	AH	1160	0	1172	22	1
1	AI	1160	0	1172	8	0
1	AJ	1160	0	1172	25	0
1	AK	1160	0	1172	20	0
1	AL	1160	0	1172	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AM	1160	0	1172	20	0
1	AN	1160	0	1172	18	0
1	AO	1160	0	1172	24	0
1	AP	1160	0	1172	18	0
1	AQ	1160	0	1172	19	0
1	AR	1160	0	1172	16	0
1	AS	1160	0	1172	26	0
1	AT	1160	0	1172	16	0
1	AU	1160	0	1172	23	0
1	AV	1160	0	1172	25	0
1	AW	1160	0	1172	16	0
1	AX	1160	0	1172	23	0
1	AY	1160	0	1172	20	0
1	AZ	1160	0	1172	23	0
1	BA	1160	0	1172	23	0
1	BB	1160	0	1172	21	0
1	BC	1160	0	1172	26	0
1	BD	1160	0	1172	18	0
1	BE	1160	0	1172	28	0
1	BF	1160	0	1172	18	0
1	BG	1160	0	1172	26	0
1	BH	1160	0	1172	22	0
1	BI	1160	0	1172	23	0
1	BJ	1160	0	1172	9	0
1	BK	1160	0	1172	23	0
1	BL	1160	0	1172	19	0
1	BM	1160	0	1172	23	0
1	BN	1160	0	1172	22	0
1	BO	1160	0	1172	20	0
1	BP	1160	0	1172	21	0
1	BQ	1160	0	1172	10	1
1	BR	1160	0	1172	16	0
1	BS	1160	0	1172	11	0
1	BT	1160	0	1172	21	0
1	BU	1160	0	1172	20	0
1	BV	1160	0	1172	24	0
1	BW	1160	0	1172	19	0
1	BX	1160	0	1172	19	0
1	BY	1160	0	1172	24	0
1	BZ	1160	0	1172	10	0
1	CA	1160	0	1172	12	0
1	CB	1160	0	1172	21	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CC	1160	0	1172	18	0
1	CD	1160	0	1172	26	1
1	CE	1160	0	1172	9	0
1	CF	1160	0	1172	18	1
1	CG	1160	0	1172	18	0
1	CH	1160	0	1172	10	1
1	CI	1160	0	1172	20	0
1	CJ	1160	0	1172	18	0
1	CK	1160	0	1172	18	0
1	CL	1160	0	1172	23	0
1	CM	1160	0	1172	16	0
1	CN	1160	0	1172	20	0
1	CO	1160	0	1172	22	1
1	CP	1160	0	1172	20	0
1	CQ	1160	0	1172	10	0
1	CR	1160	0	1172	23	0
1	CS	1160	0	1172	19	0
1	CT	1160	0	1172	27	0
1	CU	1160	0	1172	16	0
1	CV	1160	0	1172	18	0
1	CW	1160	0	1172	22	0
1	CX	1160	0	1172	23	0
1	CY	1160	0	1172	11	0
1	CZ	1160	0	1172	14	0
1	DA	1160	0	1172	21	0
1	DB	1160	0	1172	17	0
1	DC	1160	0	1172	10	0
1	DD	1160	0	1172	22	0
1	DE	1160	0	1172	18	0
1	DF	1160	0	1172	24	0
1	DG	1160	0	1172	23	0
1	DH	1160	0	1172	19	0
1	DI	1160	0	1172	11	1
1	DJ	1160	0	1172	22	0
1	DK	1160	0	1172	19	0
1	DL	1160	0	1172	20	0
All	All	104400	0	105480	1247	4

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 6.

The worst 5 of 1247 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:AV:79:TYR:OH	1:CT:82:PRO:O	1.89	0.90
1:AV:78:ALA:HA	1:CT:75:ALA:O	1.80	0.82
1:AM:23:ILE:HG22	1:AM:24:VAL:HG23	1.67	0.77
1:AG:23:ILE:HG22	1:AG:24:VAL:HG23	1.67	0.77
1:AS:23:ILE:HG22	1:AS:24:VAL:HG23	1.67	0.77

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:13:THR:OG1	1:CD:13:THR:OG1[7_555]	1.60	0.60
1:BQ:82:PRO:O	1:CB:79:TYR:OH[3_555]	2.03	0.17
1:CF:79:TYR:OH	1:CH:82:PRO:O[3_555]	2.05	0.15
1:CO:79:TYR:OH	1:DI:82:PRO:O[3_555]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	AB	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AC	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AD	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	AE	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AF	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AG	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	AH	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AI	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AJ	154/156 (99%)	152 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AK	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AL	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AM	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	AN	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AO	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AP	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	AQ	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AR	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AS	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	AT	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AU	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AV	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	AW	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AX	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	AY	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	AZ	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BA	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BB	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	BC	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BD	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BE	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	BF	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BG	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BH	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	BI	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BJ	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BK	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	BL	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BM	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BN	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	BO	154/156 (99%)	153 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BP	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BQ	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	BR	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BS	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BT	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	BU	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BV	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BW	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	BX	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BY	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	BZ	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	CA	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CB	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CC	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	CD	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CE	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CF	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	CG	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CH	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CI	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	CJ	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CK	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CL	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	CM	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CN	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CO	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	CP	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CQ	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CR	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	CS	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CT	154/156 (99%)	153 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CU	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	CV	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CW	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CX	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	CY	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	CZ	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	DA	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	DB	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	DC	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	DD	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	DE	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	DF	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	DG	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	DH	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	DI	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	DJ	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
1	DK	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
1	DL	154/156 (99%)	153 (99%)	1 (1%)	0	100	100
All	All	13860/14040 (99%)	13740 (99%)	120 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	123/123 (100%)	123 (100%)	0	100	100
1	AB	123/123 (100%)	123 (100%)	0	100	100
1	AC	123/123 (100%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AD	123/123 (100%)	123 (100%)	0	100	100
1	AE	123/123 (100%)	123 (100%)	0	100	100
1	AF	123/123 (100%)	123 (100%)	0	100	100
1	AG	123/123 (100%)	123 (100%)	0	100	100
1	AH	123/123 (100%)	123 (100%)	0	100	100
1	AI	123/123 (100%)	123 (100%)	0	100	100
1	AJ	123/123 (100%)	123 (100%)	0	100	100
1	AK	123/123 (100%)	123 (100%)	0	100	100
1	AL	123/123 (100%)	123 (100%)	0	100	100
1	AM	123/123 (100%)	123 (100%)	0	100	100
1	AN	123/123 (100%)	123 (100%)	0	100	100
1	AO	123/123 (100%)	123 (100%)	0	100	100
1	AP	123/123 (100%)	123 (100%)	0	100	100
1	AQ	123/123 (100%)	123 (100%)	0	100	100
1	AR	123/123 (100%)	123 (100%)	0	100	100
1	AS	123/123 (100%)	123 (100%)	0	100	100
1	AT	123/123 (100%)	123 (100%)	0	100	100
1	AU	123/123 (100%)	123 (100%)	0	100	100
1	AV	123/123 (100%)	123 (100%)	0	100	100
1	AW	123/123 (100%)	123 (100%)	0	100	100
1	AX	123/123 (100%)	123 (100%)	0	100	100
1	AY	123/123 (100%)	123 (100%)	0	100	100
1	AZ	123/123 (100%)	123 (100%)	0	100	100
1	BA	123/123 (100%)	123 (100%)	0	100	100
1	BB	123/123 (100%)	123 (100%)	0	100	100
1	BC	123/123 (100%)	123 (100%)	0	100	100
1	BD	123/123 (100%)	123 (100%)	0	100	100
1	BE	123/123 (100%)	123 (100%)	0	100	100
1	BF	123/123 (100%)	123 (100%)	0	100	100
1	BG	123/123 (100%)	123 (100%)	0	100	100
1	BH	123/123 (100%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BI	123/123 (100%)	123 (100%)	0	100	100
1	BJ	123/123 (100%)	123 (100%)	0	100	100
1	BK	123/123 (100%)	123 (100%)	0	100	100
1	BL	123/123 (100%)	123 (100%)	0	100	100
1	BM	123/123 (100%)	123 (100%)	0	100	100
1	BN	123/123 (100%)	123 (100%)	0	100	100
1	BO	123/123 (100%)	123 (100%)	0	100	100
1	BP	123/123 (100%)	123 (100%)	0	100	100
1	BQ	123/123 (100%)	123 (100%)	0	100	100
1	BR	123/123 (100%)	123 (100%)	0	100	100
1	BS	123/123 (100%)	123 (100%)	0	100	100
1	BT	123/123 (100%)	123 (100%)	0	100	100
1	BU	123/123 (100%)	123 (100%)	0	100	100
1	BV	123/123 (100%)	123 (100%)	0	100	100
1	BW	123/123 (100%)	123 (100%)	0	100	100
1	BX	123/123 (100%)	123 (100%)	0	100	100
1	BY	123/123 (100%)	123 (100%)	0	100	100
1	BZ	123/123 (100%)	123 (100%)	0	100	100
1	CA	123/123 (100%)	123 (100%)	0	100	100
1	CB	123/123 (100%)	123 (100%)	0	100	100
1	CC	123/123 (100%)	123 (100%)	0	100	100
1	CD	123/123 (100%)	123 (100%)	0	100	100
1	CE	123/123 (100%)	123 (100%)	0	100	100
1	CF	123/123 (100%)	123 (100%)	0	100	100
1	CG	123/123 (100%)	123 (100%)	0	100	100
1	CH	123/123 (100%)	123 (100%)	0	100	100
1	CI	123/123 (100%)	123 (100%)	0	100	100
1	CJ	123/123 (100%)	123 (100%)	0	100	100
1	CK	123/123 (100%)	123 (100%)	0	100	100
1	CL	123/123 (100%)	123 (100%)	0	100	100
1	CM	123/123 (100%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CN	123/123 (100%)	123 (100%)	0	100	100
1	CO	123/123 (100%)	123 (100%)	0	100	100
1	CP	123/123 (100%)	123 (100%)	0	100	100
1	CQ	123/123 (100%)	123 (100%)	0	100	100
1	CR	123/123 (100%)	123 (100%)	0	100	100
1	CS	123/123 (100%)	123 (100%)	0	100	100
1	CT	123/123 (100%)	123 (100%)	0	100	100
1	CU	123/123 (100%)	123 (100%)	0	100	100
1	CV	123/123 (100%)	123 (100%)	0	100	100
1	CW	123/123 (100%)	123 (100%)	0	100	100
1	CX	123/123 (100%)	123 (100%)	0	100	100
1	CY	123/123 (100%)	123 (100%)	0	100	100
1	CZ	123/123 (100%)	123 (100%)	0	100	100
1	DA	123/123 (100%)	123 (100%)	0	100	100
1	DB	123/123 (100%)	123 (100%)	0	100	100
1	DC	123/123 (100%)	123 (100%)	0	100	100
1	DD	123/123 (100%)	123 (100%)	0	100	100
1	DE	123/123 (100%)	123 (100%)	0	100	100
1	DF	123/123 (100%)	123 (100%)	0	100	100
1	DG	123/123 (100%)	123 (100%)	0	100	100
1	DH	123/123 (100%)	123 (100%)	0	100	100
1	DI	123/123 (100%)	123 (100%)	0	100	100
1	DJ	123/123 (100%)	123 (100%)	0	100	100
1	DK	123/123 (100%)	123 (100%)	0	100	100
1	DL	123/123 (100%)	123 (100%)	0	100	100
All	All	11070/11070 (100%)	11070 (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 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	CC	131	GLN

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Mol	Chain	Res	Type
1	CQ	50	GLN
1	CE	50	GLN
1	CK	152	GLN
1	CT	152	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	156/156 (100%)	-0.33	0 100 100	68, 108, 158, 204	0
1	AB	156/156 (100%)	-0.18	0 100 100	63, 106, 148, 193	0
1	AC	156/156 (100%)	-0.20	0 100 100	73, 116, 157, 176	0
1	AD	156/156 (100%)	-0.26	0 100 100	68, 108, 158, 204	0
1	AE	156/156 (100%)	-0.28	0 100 100	63, 106, 148, 193	0
1	AF	156/156 (100%)	-0.09	0 100 100	73, 116, 157, 176	0
1	AG	156/156 (100%)	-0.26	0 100 100	68, 108, 158, 204	0
1	AH	156/156 (100%)	-0.20	0 100 100	63, 106, 148, 193	0
1	AI	156/156 (100%)	-0.12	0 100 100	73, 116, 157, 176	0
1	AJ	156/156 (100%)	-0.14	0 100 100	68, 108, 158, 204	0
1	AK	156/156 (100%)	-0.24	3 (1%) 66 57	63, 106, 148, 193	0
1	AL	156/156 (100%)	-0.38	0 100 100	73, 116, 157, 176	0
1	AM	156/156 (100%)	-0.30	0 100 100	68, 108, 158, 204	0
1	AN	156/156 (100%)	-0.19	0 100 100	63, 106, 148, 193	0
1	AO	156/156 (100%)	-0.13	0 100 100	73, 116, 157, 176	0
1	AP	156/156 (100%)	-0.30	1 (0%) 89 84	68, 108, 158, 204	0
1	AQ	156/156 (100%)	-0.31	1 (0%) 89 84	63, 106, 148, 193	0
1	AR	156/156 (100%)	-0.14	1 (0%) 89 84	73, 116, 157, 176	0
1	AS	156/156 (100%)	-0.30	0 100 100	68, 108, 158, 204	0
1	AT	156/156 (100%)	-0.28	2 (1%) 77 68	63, 106, 148, 193	0
1	AU	156/156 (100%)	-0.19	1 (0%) 89 84	73, 116, 157, 176	0
1	AV	156/156 (100%)	-0.27	1 (0%) 89 84	68, 108, 158, 204	0
1	AW	156/156 (100%)	-0.27	0 100 100	63, 106, 148, 193	0
1	AX	156/156 (100%)	-0.18	0 100 100	73, 116, 157, 176	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AY	156/156 (100%)	-0.37	0 100 100	68, 108, 158, 204	0
1	AZ	156/156 (100%)	-0.31	0 100 100	63, 106, 148, 193	0
1	BA	156/156 (100%)	-0.29	0 100 100	73, 116, 157, 176	0
1	BB	156/156 (100%)	-0.16	0 100 100	68, 108, 158, 204	0
1	BC	156/156 (100%)	-0.10	2 (1%) 77 68	63, 106, 148, 193	0
1	BD	156/156 (100%)	0.08	0 100 100	73, 116, 157, 176	0
1	BE	156/156 (100%)	-0.17	1 (0%) 89 84	68, 108, 158, 204	0
1	BF	156/156 (100%)	-0.24	2 (1%) 77 68	63, 106, 148, 193	0
1	BG	156/156 (100%)	-0.13	0 100 100	73, 116, 157, 176	0
1	BH	156/156 (100%)	-0.38	0 100 100	68, 108, 158, 204	0
1	BI	156/156 (100%)	-0.29	0 100 100	63, 106, 148, 193	0
1	BJ	156/156 (100%)	-0.27	0 100 100	73, 116, 157, 176	0
1	BK	156/156 (100%)	-0.29	0 100 100	68, 108, 158, 204	0
1	BL	156/156 (100%)	-0.36	0 100 100	63, 106, 148, 193	0
1	BM	156/156 (100%)	-0.31	1 (0%) 89 84	73, 116, 157, 176	0
1	BN	156/156 (100%)	-0.29	0 100 100	68, 108, 158, 204	0
1	BO	156/156 (100%)	-0.24	0 100 100	63, 106, 148, 193	0
1	BP	156/156 (100%)	-0.28	0 100 100	73, 116, 157, 176	0
1	BQ	156/156 (100%)	-0.29	0 100 100	68, 108, 158, 204	0
1	BR	156/156 (100%)	-0.32	0 100 100	63, 106, 148, 193	0
1	BS	156/156 (100%)	-0.33	0 100 100	73, 116, 157, 176	0
1	BT	156/156 (100%)	-0.29	0 100 100	68, 108, 158, 204	0
1	BU	156/156 (100%)	-0.37	0 100 100	63, 106, 148, 193	0
1	BV	156/156 (100%)	-0.13	0 100 100	73, 116, 157, 176	0
1	BW	156/156 (100%)	-0.26	1 (0%) 89 84	68, 108, 158, 204	0
1	BX	156/156 (100%)	-0.28	0 100 100	63, 106, 148, 193	0
1	BY	156/156 (100%)	-0.36	0 100 100	73, 116, 157, 176	0
1	BZ	156/156 (100%)	-0.28	1 (0%) 89 84	68, 108, 158, 204	0
1	CA	156/156 (100%)	-0.31	2 (1%) 77 68	63, 106, 148, 193	0
1	CB	156/156 (100%)	-0.02	1 (0%) 89 84	73, 116, 157, 176	0
1	CC	156/156 (100%)	-0.23	1 (0%) 89 84	68, 108, 158, 204	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	CD	156/156 (100%)	-0.27	0 100 100	63, 106, 148, 193	0
1	CE	156/156 (100%)	-0.17	0 100 100	73, 116, 157, 176	0
1	CF	156/156 (100%)	-0.26	0 100 100	68, 108, 158, 204	0
1	CG	156/156 (100%)	-0.20	1 (0%) 89 84	63, 106, 148, 193	0
1	CH	156/156 (100%)	-0.26	0 100 100	73, 116, 157, 176	0
1	CI	156/156 (100%)	-0.16	1 (0%) 89 84	68, 108, 158, 204	0
1	CJ	156/156 (100%)	-0.21	1 (0%) 89 84	63, 106, 148, 193	0
1	CK	156/156 (100%)	-0.14	0 100 100	73, 116, 157, 176	0
1	CL	156/156 (100%)	-0.31	1 (0%) 89 84	68, 108, 158, 204	0
1	CM	156/156 (100%)	-0.28	0 100 100	63, 106, 148, 193	0
1	CN	156/156 (100%)	-0.17	2 (1%) 77 68	73, 116, 157, 176	0
1	CO	156/156 (100%)	-0.28	0 100 100	68, 108, 158, 204	0
1	CP	156/156 (100%)	-0.20	1 (0%) 89 84	63, 106, 148, 193	0
1	CQ	156/156 (100%)	-0.07	4 (2%) 56 45	73, 116, 157, 176	0
1	CR	156/156 (100%)	-0.31	0 100 100	68, 108, 158, 204	0
1	CS	156/156 (100%)	-0.19	2 (1%) 77 68	63, 106, 148, 193	0
1	CT	156/156 (100%)	-0.20	0 100 100	73, 116, 157, 176	0
1	CU	156/156 (100%)	-0.27	0 100 100	68, 108, 158, 204	0
1	CV	156/156 (100%)	-0.25	0 100 100	63, 106, 148, 193	0
1	CW	156/156 (100%)	-0.32	0 100 100	73, 116, 157, 176	0
1	CX	156/156 (100%)	-0.21	1 (0%) 89 84	68, 108, 158, 204	0
1	CY	156/156 (100%)	-0.20	0 100 100	63, 106, 148, 193	0
1	CZ	156/156 (100%)	-0.20	0 100 100	73, 116, 157, 176	0
1	DA	156/156 (100%)	-0.27	0 100 100	68, 108, 158, 204	0
1	DB	156/156 (100%)	-0.22	0 100 100	63, 106, 148, 193	0
1	DC	156/156 (100%)	-0.34	0 100 100	73, 116, 157, 176	0
1	DD	156/156 (100%)	-0.26	0 100 100	68, 108, 158, 204	0
1	DE	156/156 (100%)	-0.14	2 (1%) 77 68	63, 106, 148, 193	0
1	DF	156/156 (100%)	-0.11	1 (0%) 89 84	73, 116, 157, 176	0
1	DG	156/156 (100%)	-0.38	0 100 100	68, 108, 158, 204	0
1	DH	156/156 (100%)	-0.21	0 100 100	63, 106, 148, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	DI	156/156 (100%)	-0.21	0	100	100	73, 116, 157, 176	0
1	DJ	156/156 (100%)	-0.24	0	100	100	68, 108, 158, 204	0
1	DK	156/156 (100%)	-0.27	0	100	100	63, 106, 148, 193	0
1	DL	156/156 (100%)	-0.21	0	100	100	73, 116, 157, 176	0
All	All	14040/14040 (100%)	-0.24	39 (0%)	94	90	63, 110, 157, 204	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AK	74	GLY	3.8
1	CI	38	ASN	3.6
1	BF	75	ALA	3.5
1	CQ	88	LYS	3.3
1	CN	152	GLN	3.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.