



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 11:33 AM BST

PDB ID : 6YFA
Title : Virus-like particle of bacteriophage AVE015
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on : 2020-03-26
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

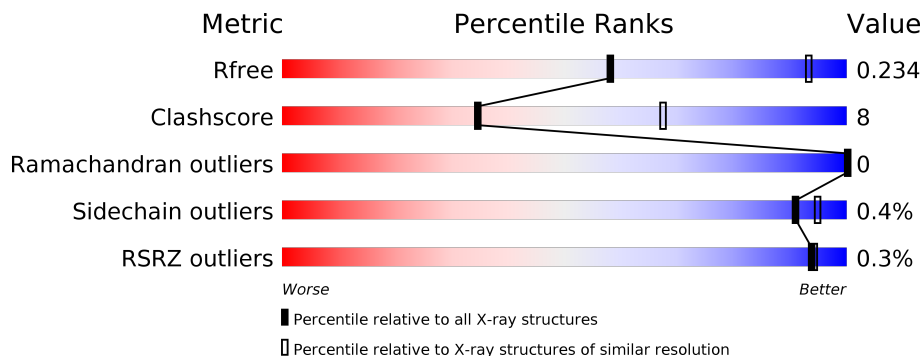
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	AA	167	
1	AB	167	
1	AC	167	
1	AD	167	
1	AE	167	
1	AF	167	


























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Mol	Chain	Length	Quality of chain
1	AG	167	2% 72% 27%
1	AH	167	82% 17%
1	AI	167	75% 25%
1	AJ	167	83% 17%
1	AK	167	83% 16%
1	AL	167	82% 18%
1	AM	167	76% 23%
1	AN	167	84% 15%
1	AO	167	81% 19%
1	AP	167	74% 25%
1	AQ	167	81% 18%
1	AR	167	87% 13%
1	AS	167	75% 25%
1	AT	167	79% 20%
1	AU	167	80% 20%
1	AV	167	75% 24%
1	AW	167	82% 17%
1	AX	167	80% 20%
1	AY	167	75% 25%
1	AZ	167	83% 17%
1	BA	167	80% 20%
1	BB	167	72% 27%
1	BC	167	80% 19%
1	BD	167	87% 13%
1	BE	167	73% 26%





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Mol	Chain	Length	Quality of chain
1	BF	167	 89% 11%
1	BG	167	 83% 17%
1	BH	167	 2% 72% 27%
1	BI	167	 83% 16%
1	BJ	167	 86% 14%
1	BK	167	 1% 83% 17%
1	BL	167	 78% 22%
1	BM	167	 2% 77% 23%
1	BN	167	 71% 28%
1	BO	167	 90% 9%
1	BP	167	 82% 18%
1	BQ	167	 75% 25%
1	BR	167	 81% 19%
1	BS	167	 81% 19%
1	BT	167	 1% 74% 26%
1	BU	167	 79% 20%
1	BV	167	 80% 20%
1	BW	167	 72% 28%
1	BX	167	 4% 80% 20%
1	BY	167	 1% 78% 22%
1	BZ	167	 72% 28%
1	CA	167	 86% 13%
1	CB	167	 86% 14%
1	CC	167	 73% 26%
1	CD	167	 75% 24%

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Mol	Chain	Length	Quality of chain
1	CE	167	 88% 12%
1	CF	167	 75% 25%
1	CG	167	 81% 19%
1	CH	167	 87% 13%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 78980 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AA	167	1316	825	222	267	2	0	0	0
1	AB	167	1316	825	222	267	2	0	0	0
1	AC	167	1316	825	222	267	2	0	0	0
1	AD	167	1316	825	222	267	2	0	0	0
1	AE	167	1316	825	222	267	2	0	0	0
1	AF	167	1316	825	222	267	2	0	0	0
1	AG	167	1316	825	222	267	2	0	0	0
1	AH	167	1316	825	222	267	2	0	0	0
1	AI	167	1316	825	222	267	2	0	0	0
1	AJ	167	1316	825	222	267	2	0	0	0
1	AK	167	1316	825	222	267	2	0	0	0
1	AL	167	1316	825	222	267	2	0	0	0
1	AM	167	1316	825	222	267	2	0	0	0
1	AN	167	1316	825	222	267	2	0	0	0
1	AO	167	1316	825	222	267	2	0	0	0
1	AP	167	1316	825	222	267	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AQ	167	1316	825	222	267	2	0	0	0
1	AR	167	1316	825	222	267	2	0	0	0
1	AS	167	1316	825	222	267	2	0	0	0
1	AT	167	1316	825	222	267	2	0	0	0
1	AU	167	1316	825	222	267	2	0	0	0
1	AV	167	1316	825	222	267	2	0	0	0
1	AW	167	1316	825	222	267	2	0	0	0
1	AX	167	1316	825	222	267	2	0	0	0
1	AY	167	1316	825	222	267	2	0	0	0
1	AZ	167	1316	825	222	267	2	0	0	0
1	BA	167	1316	825	222	267	2	0	0	0
1	BB	167	1316	825	222	267	2	0	0	0
1	BC	167	1316	825	222	267	2	0	0	0
1	BD	167	1316	825	222	267	2	0	0	0
1	BE	167	1316	825	222	267	2	0	0	0
1	BF	167	1316	825	222	267	2	0	0	0
1	BG	167	1316	825	222	267	2	0	0	0
1	BH	167	1316	825	222	267	2	0	0	0
1	BI	167	1316	825	222	267	2	0	0	0
1	BJ	167	1316	825	222	267	2	0	0	0
1	BK	167	1316	825	222	267	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	BL	167	1316	825	222	267	2	0	0	0
1	BM	167	1316	825	222	267	2	0	0	0
1	BN	167	1316	825	222	267	2	0	0	0
1	BO	167	1316	825	222	267	2	0	0	0
1	BP	167	1316	825	222	267	2	0	0	0
1	BQ	167	1316	825	222	267	2	0	0	0
1	BR	167	1316	825	222	267	2	0	0	0
1	BS	167	1316	825	222	267	2	0	0	0
1	BT	167	1316	825	222	267	2	0	0	0
1	BU	167	1316	825	222	267	2	0	0	0
1	BV	167	1316	825	222	267	2	0	0	0
1	BW	167	1316	825	222	267	2	0	0	0
1	BX	167	1316	825	222	267	2	0	0	0
1	BY	167	1316	825	222	267	2	0	0	0
1	BZ	167	1316	825	222	267	2	0	0	0
1	CA	167	1316	825	222	267	2	0	0	0
1	CB	167	1316	825	222	267	2	0	0	0
1	CC	167	1316	825	222	267	2	0	0	0
1	CD	167	1316	825	222	267	2	0	0	0
1	CE	167	1316	825	222	267	2	0	0	0
1	CF	167	1316	825	222	267	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	167	Total	C	N	O	S	0	0	0
			1316	825	222	267	2			
1	CH	167	Total	C	N	O	S	0	0	0
			1316	825	222	267	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AP	1	Total	Ca	0	0
			1	1		
2	AG	1	Total	Ca	0	0
			1	1		
2	AJ	1	Total	Ca	0	0
			1	1		
2	BH	1	Total	Ca	0	0
			1	1		
2	AD	1	Total	Ca	0	0
			1	1		
2	BN	1	Total	Ca	0	0
			1	1		
2	BB	1	Total	Ca	0	0
			1	1		
2	BZ	1	Total	Ca	0	0
			1	1		
2	CC	1	Total	Ca	0	0
			1	1		
2	AV	1	Total	Ca	0	0
			1	1		
2	BE	1	Total	Ca	0	0
			1	1		
2	BT	1	Total	Ca	0	0
			1	1		
2	AA	1	Total	Ca	0	0
			1	1		
2	BQ	1	Total	Ca	0	0
			1	1		
2	BK	1	Total	Ca	0	0
			1	1		
2	BW	1	Total	Ca	0	0
			1	1		
2	AY	1	Total	Ca	0	0
			1	1		

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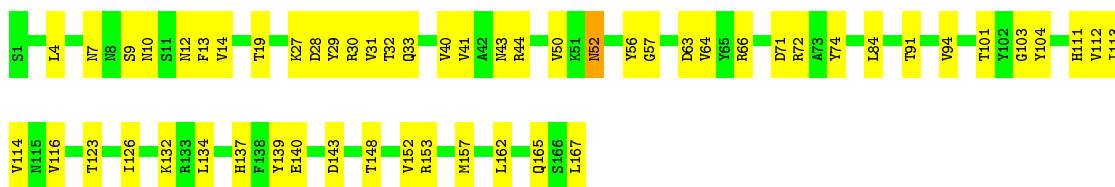
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	CF	1	Total 1	Ca 1	0	0
2	AS	1	Total 1	Ca 1	0	0
2	AM	1	Total 1	Ca 1	0	0

3 Residue-property plots [i](#)


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

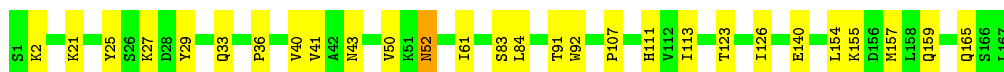
- Molecule 1: coat protein

Chain AA:  67% 32%




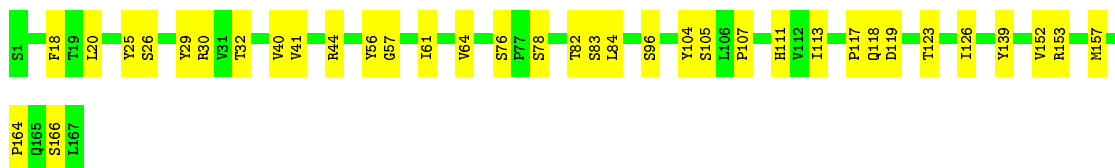
- Molecule 1: coat protein

Chain AB:  83% 16%




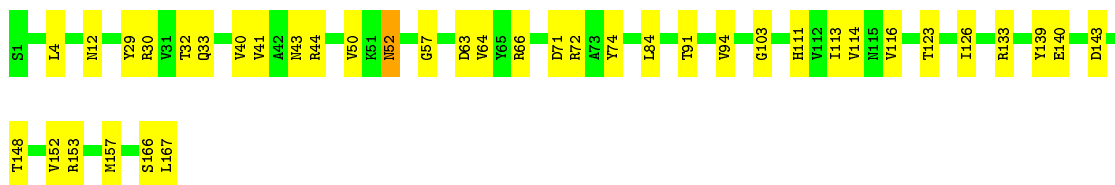
- Molecule 1: coat protein

Chain AC:  78% 22%




- Molecule 1: coat protein

Chain AD:  77% 23%




- Molecule 1: coat protein

Chain AE:  85% 14%




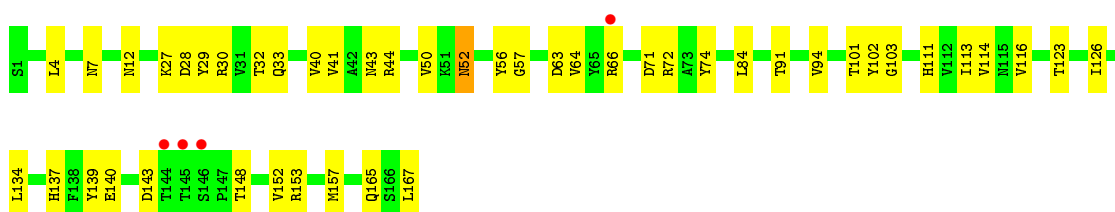
- Molecule 1: coat protein

Chain AF:  83% 17%




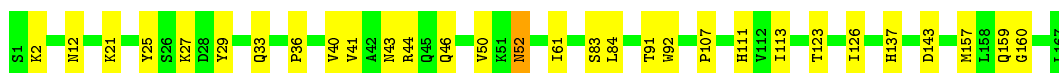
- Molecule 1: coat protein

Chain AG:  2% 72% 27%



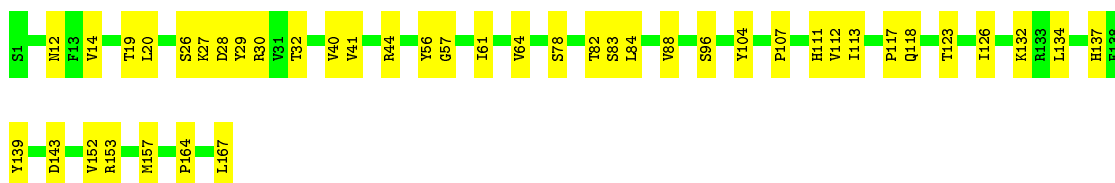
- Molecule 1: coat protein

Chain AH:  82% 17%




- Molecule 1: coat protein

Chain AI:  75% 25%

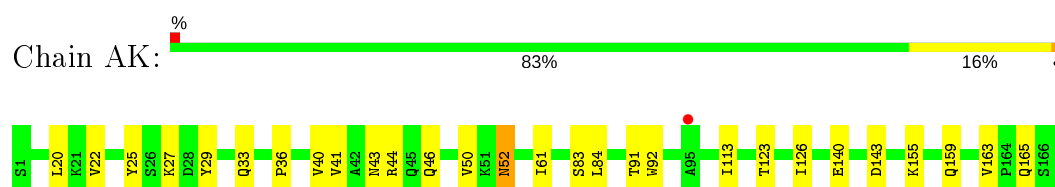


- Molecule 1: coat protein

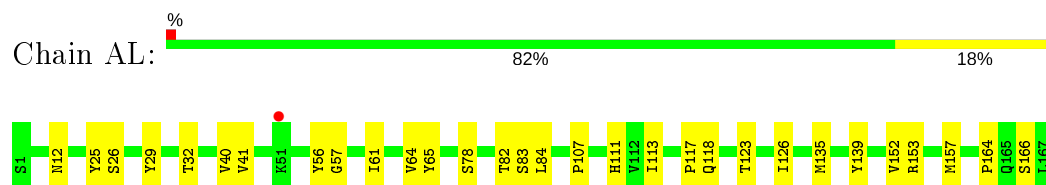
Chain AJ:  83% 17%



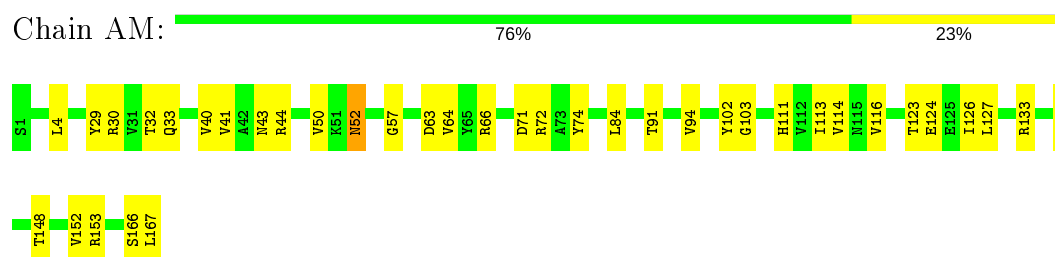
- Molecule 1: coat protein



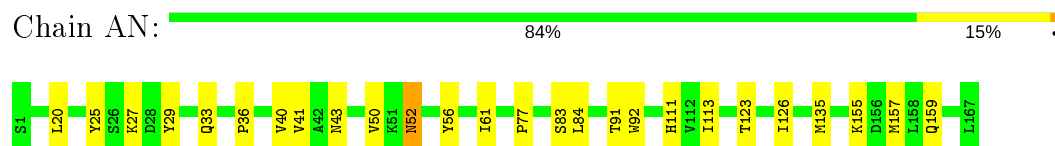
- Molecule 1: coat protein



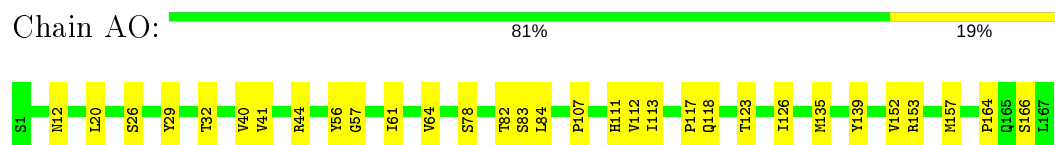
- Molecule 1: coat protein



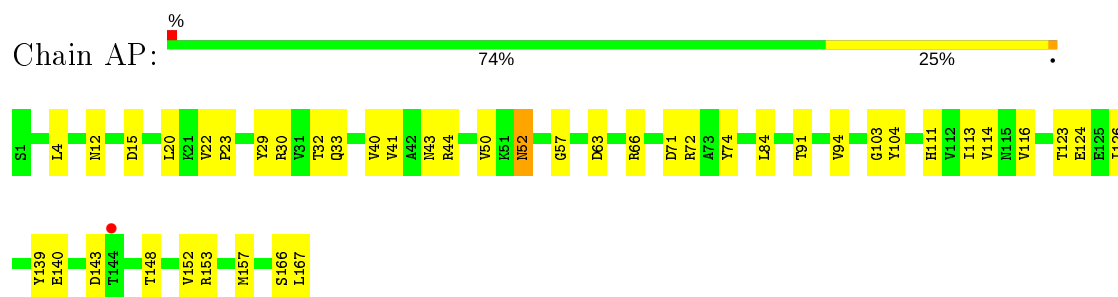
- Molecule 1: coat protein




- Molecule 1: coat protein

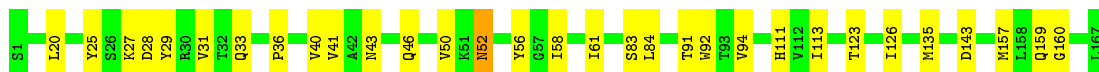


- Molecule 1: coat protein



- Molecule 1: coat protein

Chain AQ:  81% 18%




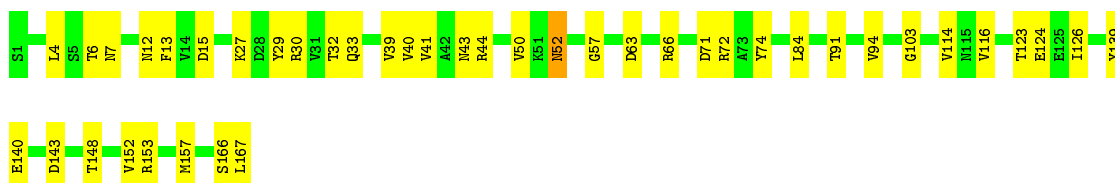
- Molecule 1: coat protein

Chain AR:  87% 13%




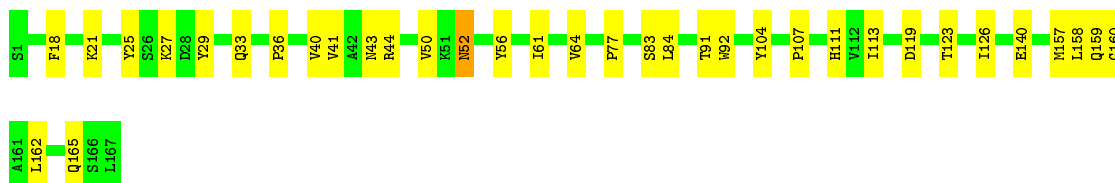
- Molecule 1: coat protein

Chain AS:  75% 25%




- Molecule 1: coat protein

Chain AT:  79% 20%



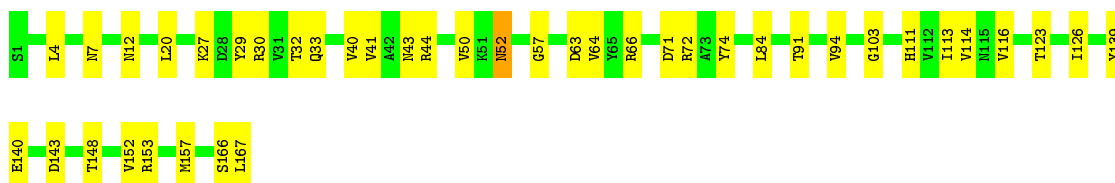
- Molecule 1: coat protein

Chain AU:  80% 20%

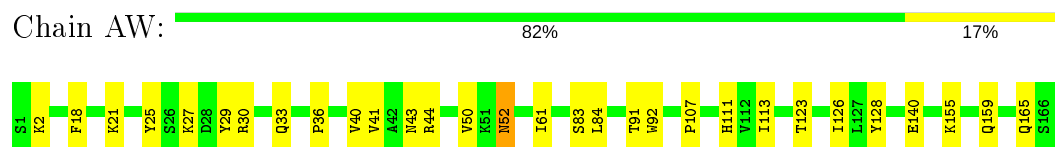


- Molecule 1: coat protein

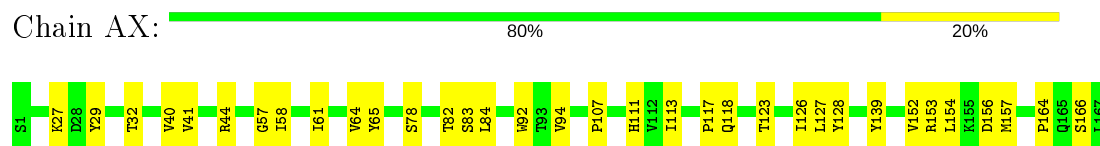
Chain AV:  75% 24%



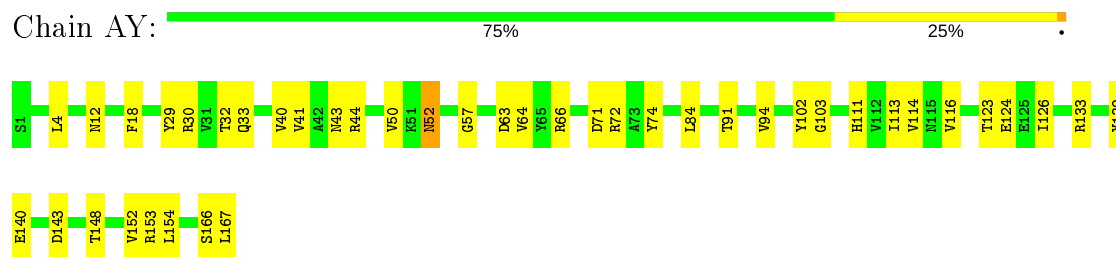
- Molecule 1: coat protein



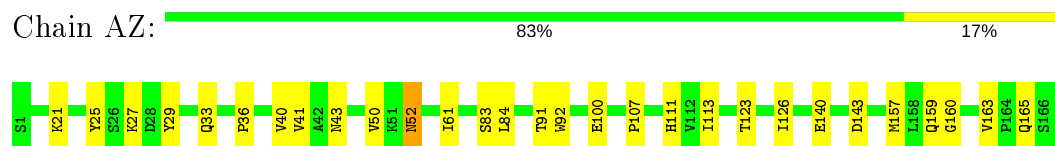
- Molecule 1: coat protein



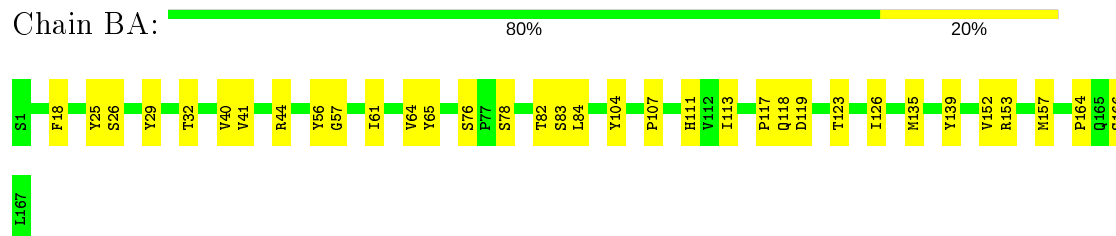
- Molecule 1: coat protein



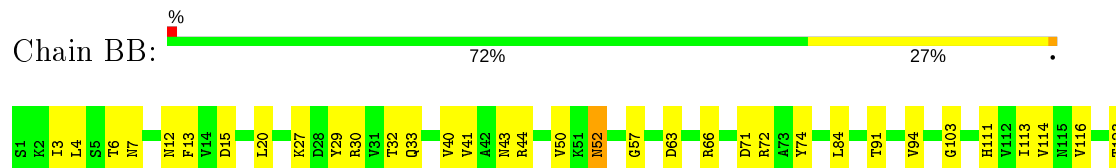
- Molecule 1: coat protein

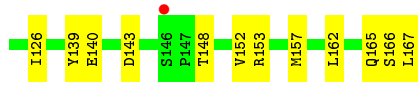


- Molecule 1: coat protein

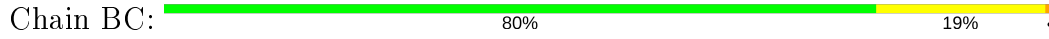


- Molecule 1: coat protein

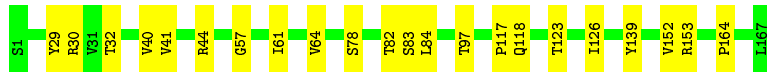
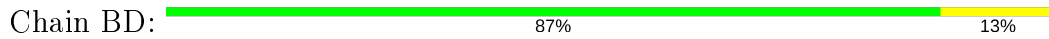




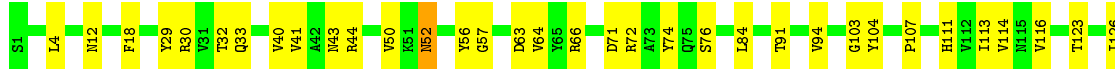
• Molecule 1: coat protein



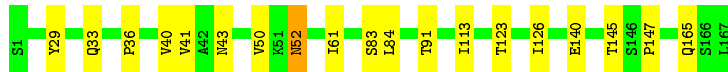
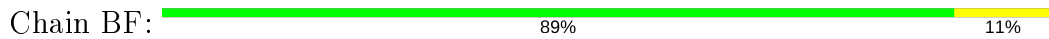
• Molecule 1: coat protein



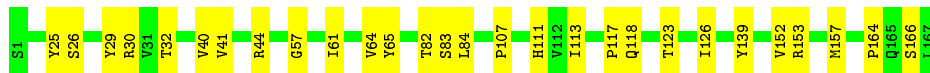
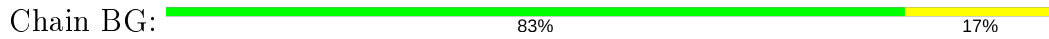
• Molecule 1: coat protein



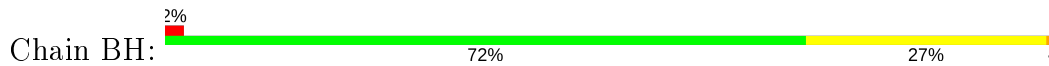
• Molecule 1: coat protein

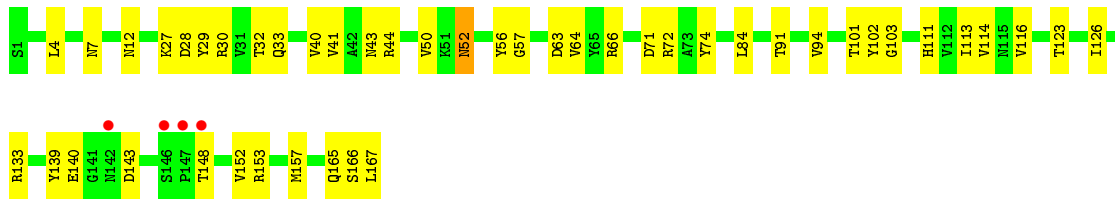


• Molecule 1: coat protein

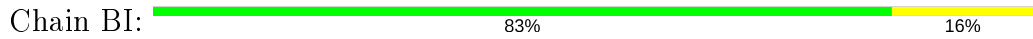


• Molecule 1: coat protein





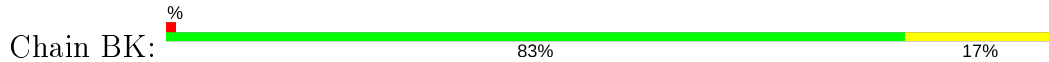
• Molecule 1: coat protein



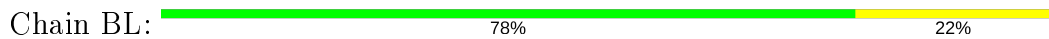
• Molecule 1: coat protein



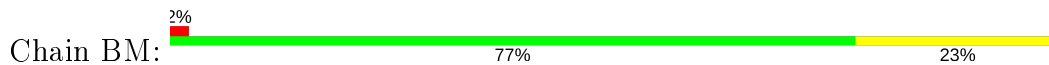
• Molecule 1: coat protein



• Molecule 1: coat protein

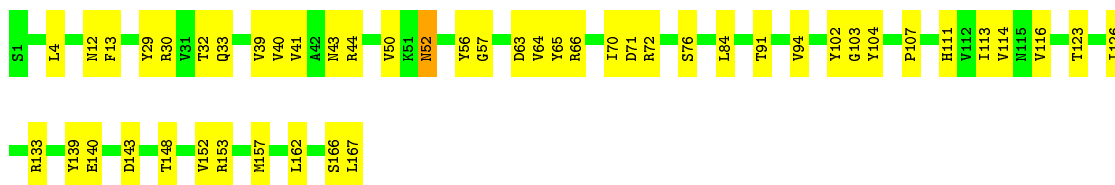


• Molecule 1: coat protein



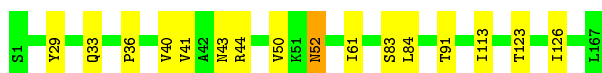
• Molecule 1: coat protein

Chain BN:  71% 28%




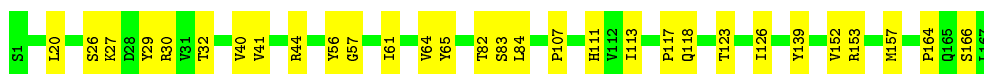
- Molecule 1: coat protein

Chain BO:  90% 9%




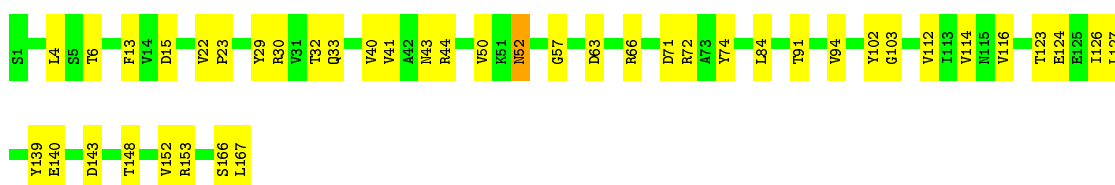
- Molecule 1: coat protein

Chain BP:  82% 18%




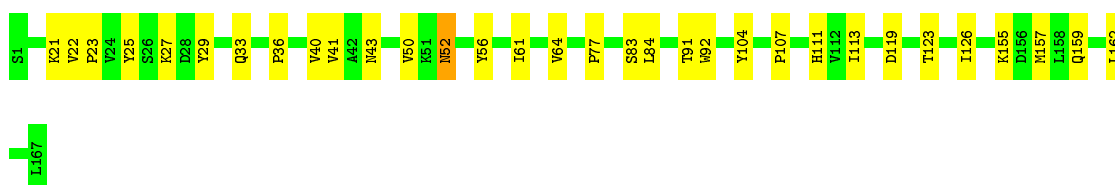
- Molecule 1: coat protein

Chain BQ:  75% 25%




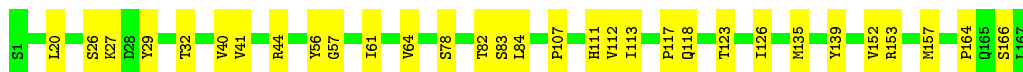
- Molecule 1: coat protein

Chain BR:  81% 19%

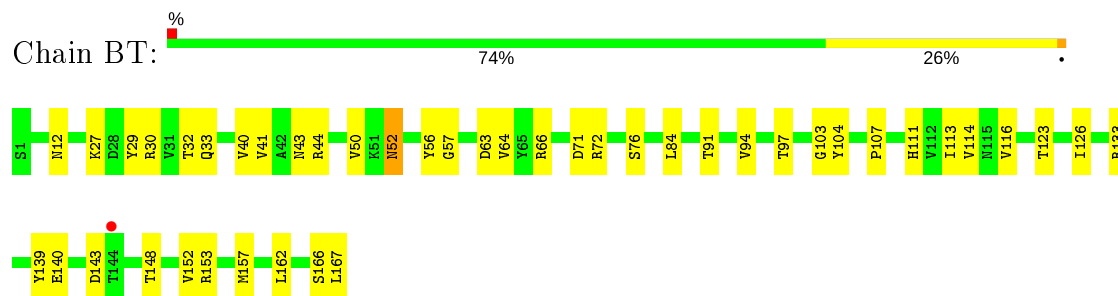


- Molecule 1: coat protein

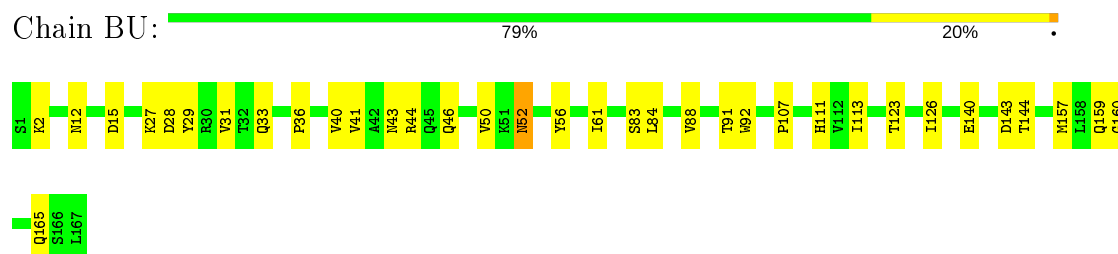
Chain BS:  81% 19%



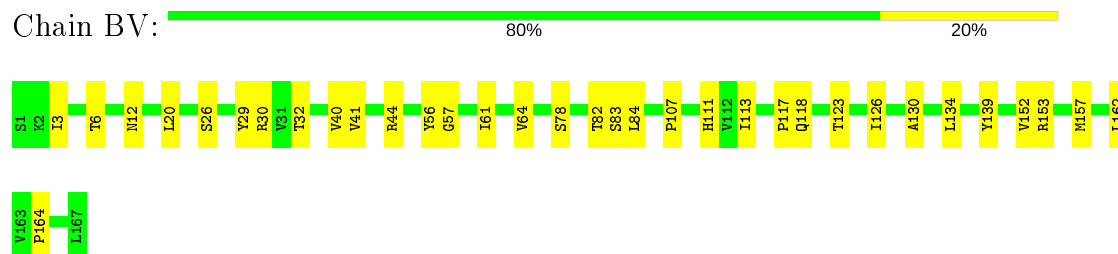
- Molecule 1: coat protein



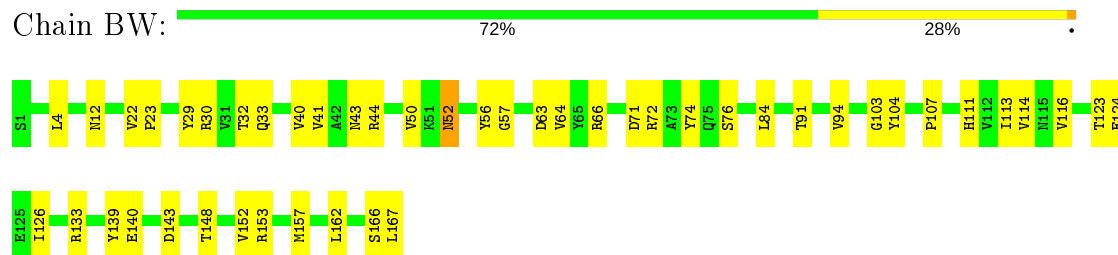
- Molecule 1: coat protein



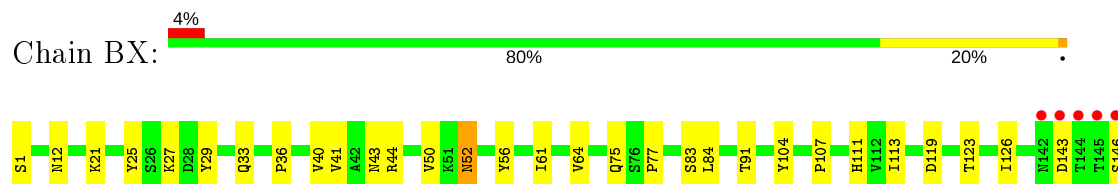
- Molecule 1: coat protein



- Molecule 1: coat protein

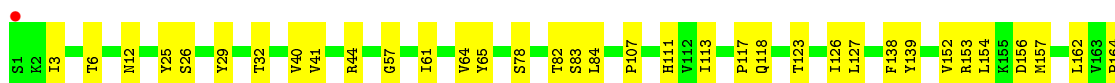
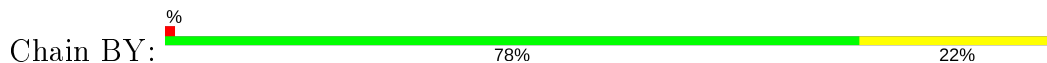


- Molecule 1: coat protein

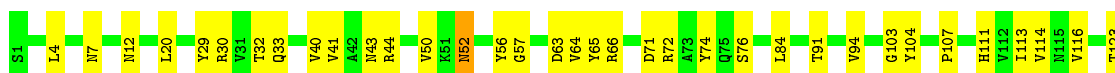




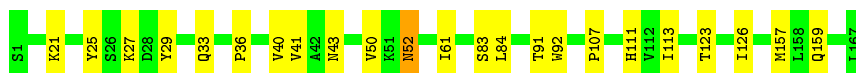
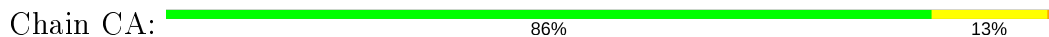
- Molecule 1: coat protein



- Molecule 1: coat protein



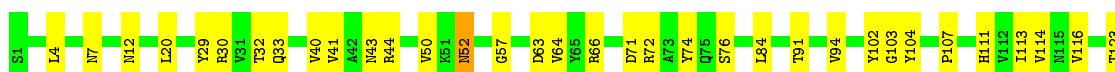
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	559.31Å 559.31Å 559.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.77 – 3.30 61.77 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (61.77-3.30) 99.9 (61.77-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.70	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.231 , 0.233 0.232 , 0.234	Depositor DCC
R_{free} test set	9978 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 24.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	78980	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.36	0/1341	0.58	0/1828
1	AB	0.35	0/1341	0.60	0/1828
1	AC	0.33	0/1341	0.57	0/1828
1	AD	0.36	0/1341	0.58	0/1828
1	AE	0.35	0/1341	0.60	0/1828
1	AF	0.33	0/1341	0.57	0/1828
1	AG	0.36	0/1341	0.58	0/1828
1	AH	0.35	0/1341	0.60	0/1828
1	AI	0.33	0/1341	0.57	0/1828
1	AJ	0.36	0/1341	0.58	0/1828
1	AK	0.35	0/1341	0.60	0/1828
1	AL	0.33	0/1341	0.57	0/1828
1	AM	0.36	0/1341	0.58	0/1828
1	AN	0.35	0/1341	0.60	0/1828
1	AO	0.33	0/1341	0.57	0/1828
1	AP	0.36	0/1341	0.58	0/1828
1	AQ	0.35	0/1341	0.60	0/1828
1	AR	0.33	0/1341	0.57	0/1828
1	AS	0.36	0/1341	0.58	0/1828
1	AT	0.35	0/1341	0.60	0/1828
1	AU	0.33	0/1341	0.57	0/1828
1	AV	0.36	0/1341	0.58	0/1828
1	AW	0.35	0/1341	0.60	0/1828
1	AX	0.33	0/1341	0.57	0/1828
1	AY	0.36	0/1341	0.58	0/1828
1	AZ	0.35	0/1341	0.60	0/1828
1	BA	0.33	0/1341	0.57	0/1828
1	BB	0.36	0/1341	0.58	0/1828
1	BC	0.35	0/1341	0.60	0/1828
1	BD	0.33	0/1341	0.57	0/1828
1	BE	0.36	0/1341	0.58	0/1828
1	BF	0.35	0/1341	0.60	0/1828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BG	0.33	0/1341	0.57	0/1828
1	BH	0.36	0/1341	0.58	0/1828
1	BI	0.35	0/1341	0.60	0/1828
1	BJ	0.33	0/1341	0.57	0/1828
1	BK	0.36	0/1341	0.58	0/1828
1	BL	0.35	0/1341	0.60	0/1828
1	BM	0.33	0/1341	0.57	0/1828
1	BN	0.36	0/1341	0.58	0/1828
1	BO	0.35	0/1341	0.60	0/1828
1	BP	0.33	0/1341	0.57	0/1828
1	BQ	0.36	0/1341	0.58	0/1828
1	BR	0.35	0/1341	0.60	0/1828
1	BS	0.33	0/1341	0.57	0/1828
1	BT	0.36	0/1341	0.58	0/1828
1	BU	0.35	0/1341	0.60	0/1828
1	BV	0.33	0/1341	0.57	0/1828
1	BW	0.36	0/1341	0.58	0/1828
1	BX	0.35	0/1341	0.60	0/1828
1	BY	0.33	0/1341	0.57	0/1828
1	BZ	0.36	0/1341	0.58	0/1828
1	CA	0.35	0/1341	0.60	0/1828
1	CB	0.33	0/1341	0.57	0/1828
1	CC	0.36	0/1341	0.58	0/1828
1	CD	0.35	0/1341	0.60	0/1828
1	CE	0.33	0/1341	0.57	0/1828
1	CF	0.36	0/1341	0.58	0/1828
1	CG	0.35	0/1341	0.60	0/1828
1	CH	0.33	0/1341	0.57	0/1828
All	All	0.35	0/80460	0.58	0/109680

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	1316	0	1295	67	1
1	AB	1316	0	1295	24	0
1	AC	1316	0	1295	41	0
1	AD	1316	0	1295	31	0
1	AE	1316	0	1295	23	0
1	AF	1316	0	1295	24	0
1	AG	1316	0	1295	50	0
1	AH	1316	0	1295	36	0
1	AI	1316	0	1295	56	0
1	AJ	1316	0	1295	17	0
1	AK	1316	0	1295	26	0
1	AL	1316	0	1295	29	0
1	AM	1316	0	1295	34	0
1	AN	1316	0	1295	24	0
1	AO	1316	0	1295	30	0
1	AP	1316	0	1295	35	0
1	AQ	1316	0	1295	32	0
1	AR	1316	0	1295	14	0
1	AS	1316	0	1295	35	0
1	AT	1316	0	1295	36	0
1	AU	1316	0	1295	31	0
1	AV	1316	0	1295	32	0
1	AW	1316	0	1295	29	0
1	AX	1316	0	1295	30	0
1	AY	1316	0	1295	33	0
1	AZ	1316	0	1295	28	0
1	BA	1316	0	1295	38	0
1	BB	1316	0	1295	43	6
1	BC	1316	0	1295	29	0
1	BD	1316	0	1295	14	1
1	BE	1316	0	1295	42	0
1	BF	1316	0	1295	10	0
1	BG	1316	0	1295	26	0
1	BH	1316	0	1295	42	0
1	BI	1316	0	1295	23	0
1	BJ	1316	0	1295	16	2
1	BK	1316	0	1295	18	0
1	BL	1316	0	1295	45	0
1	BM	1316	0	1295	51	0
1	BN	1316	0	1295	47	0
1	BO	1316	0	1295	9	0
1	BP	1316	0	1295	31	0
1	BQ	1316	0	1295	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	1316	0	1295	29	0
1	BS	1316	0	1295	30	0
1	BT	1316	0	1295	44	0
1	BU	1316	0	1295	42	2
1	BV	1316	0	1295	33	0
1	BW	1316	0	1295	39	0
1	BX	1316	0	1295	37	6
1	BY	1316	0	1295	34	0
1	BZ	1316	0	1295	37	0
1	CA	1316	0	1295	21	0
1	CB	1316	0	1295	13	2
1	CC	1316	0	1295	42	0
1	CD	1316	0	1295	56	0
1	CE	1316	0	1295	13	0
1	CF	1316	0	1295	35	0
1	CG	1316	0	1295	28	0
1	CH	1316	0	1295	15	0
2	AA	1	0	0	0	0
2	AD	1	0	0	0	0
2	AG	1	0	0	0	0
2	AJ	1	0	0	0	0
2	AM	1	0	0	0	0
2	AP	1	0	0	0	0
2	AS	1	0	0	0	0
2	AV	1	0	0	0	0
2	AY	1	0	0	0	0
2	BB	1	0	0	0	0
2	BE	1	0	0	0	0
2	BH	1	0	0	0	0
2	BK	1	0	0	0	0
2	BN	1	0	0	0	0
2	BQ	1	0	0	0	0
2	BT	1	0	0	0	0
2	BW	1	0	0	0	0
2	BZ	1	0	0	0	0
2	CC	1	0	0	0	0
2	CF	1	0	0	0	0
All	All	78980	0	77700	1302	10

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 8.

The worst 5 of 1302 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:AA:28:ASP:OD2	1:CD:12:ASN:N	1.98	0.97
1:AA:12:ASN:N	1:CD:28:ASP:OD2	2.01	0.93
1:AI:12:ASN:N	1:BM:28:ASP:OD2	2.05	0.89
1:AA:27:LYS:NZ	1:CD:143:ASP:HB2	1.89	0.88
1:AG:74:TYR:HE2	1:BV:78:SER:HB3	1.40	0.84

The worst 5 of 10 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:BD:97:THR:OG1	1:BU:15:ASP:OD2[18_555]	1.43	0.77
1:BB:13:PHE:O	1:BX:146:SER:OG[18_555]	1.60	0.60
1:BB:13:PHE:O	1:BX:146:SER:CB[18_555]	1.74	0.46
1:BB:13:PHE:C	1:BX:146:SER:OG[18_555]	1.83	0.37
1:BB:13:PHE:N	1:BX:146:SER:OG[18_555]	1.85	0.35

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	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	AB	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	AC	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	AD	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	AE	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	AF	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	AG	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	AH	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	AI	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	AJ	165/167 (99%)	161 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AK	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	AL	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	AM	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	AN	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	AO	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	AP	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	AQ	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	AR	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	AS	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	AT	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	AU	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	AV	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	AW	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	AX	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	AY	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	AZ	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	BA	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	BB	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	BC	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	BD	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	BE	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	BF	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	BG	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	BH	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	BI	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	BJ	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	BK	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	BL	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	BM	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	BN	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	BO	165/167 (99%)	162 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BP	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	BQ	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	BR	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	BS	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	BT	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	BU	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	BV	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	BW	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	BX	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	BY	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	BZ	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	CA	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	CB	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	CC	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	CD	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	CE	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
1	CF	165/167 (99%)	161 (98%)	4 (2%)	0	100	100
1	CG	165/167 (99%)	162 (98%)	3 (2%)	0	100	100
1	CH	165/167 (99%)	163 (99%)	2 (1%)	0	100	100
All	All	9900/10020 (99%)	9720 (98%)	180 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AB	151/151 (100%)	150 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	151/151 (100%)	151 (100%)	0	100	100
1	AD	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AE	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AF	151/151 (100%)	151 (100%)	0	100	100
1	AG	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AH	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AI	151/151 (100%)	151 (100%)	0	100	100
1	AJ	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AK	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AL	151/151 (100%)	151 (100%)	0	100	100
1	AM	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AN	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AO	151/151 (100%)	151 (100%)	0	100	100
1	AP	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AQ	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AR	151/151 (100%)	151 (100%)	0	100	100
1	AS	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AT	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AU	151/151 (100%)	151 (100%)	0	100	100
1	AV	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AW	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AX	151/151 (100%)	151 (100%)	0	100	100
1	AY	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	AZ	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BA	151/151 (100%)	151 (100%)	0	100	100
1	BB	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BC	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BD	151/151 (100%)	151 (100%)	0	100	100
1	BE	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BF	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BG	151/151 (100%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BH	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BI	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BJ	151/151 (100%)	151 (100%)	0	100	100
1	BK	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BL	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BM	151/151 (100%)	151 (100%)	0	100	100
1	BN	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BO	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BP	151/151 (100%)	151 (100%)	0	100	100
1	BQ	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BR	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BS	151/151 (100%)	151 (100%)	0	100	100
1	BT	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BU	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BV	151/151 (100%)	151 (100%)	0	100	100
1	BW	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BX	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	BY	151/151 (100%)	151 (100%)	0	100	100
1	BZ	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	CA	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	CB	151/151 (100%)	151 (100%)	0	100	100
1	CC	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	CD	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	CE	151/151 (100%)	151 (100%)	0	100	100
1	CF	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	CG	151/151 (100%)	150 (99%)	1 (1%)	84	90
1	CH	151/151 (100%)	151 (100%)	0	100	100
All	All	9060/9060 (100%)	9020 (100%)	40 (0%)	91	95

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BB	52	ASN

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Mol	Chain	Res	Type
1	BH	52	ASN
1	CC	52	ASN
1	BE	52	ASN
1	BI	52	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	BD	118	GLN
1	BM	12	ASN
1	CD	12	ASN
1	BE	12	ASN
1	BH	12	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 20 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	167/167 (100%)	-0.04	0 100 100	37, 62, 102, 142	0
1	AB	167/167 (100%)	-0.22	0 100 100	38, 60, 91, 138	0
1	AC	167/167 (100%)	-0.14	0 100 100	41, 67, 106, 126	0
1	AD	167/167 (100%)	-0.30	0 100 100	37, 62, 102, 142	0
1	AE	167/167 (100%)	-0.39	0 100 100	38, 60, 91, 138	0
1	AF	167/167 (100%)	-0.21	0 100 100	41, 67, 106, 126	0
1	AG	167/167 (100%)	0.12	4 (2%) 59 56	37, 62, 102, 142	0
1	AH	167/167 (100%)	-0.07	0 100 100	38, 60, 91, 138	0
1	AI	167/167 (100%)	0.08	0 100 100	41, 67, 106, 126	0
1	AJ	167/167 (100%)	-0.09	0 100 100	37, 62, 102, 142	0
1	AK	167/167 (100%)	-0.30	1 (0%) 89 90	38, 60, 91, 138	0
1	AL	167/167 (100%)	-0.24	1 (0%) 89 90	41, 67, 106, 126	0
1	AM	167/167 (100%)	-0.17	0 100 100	37, 62, 102, 142	0
1	AN	167/167 (100%)	-0.23	0 100 100	38, 60, 91, 138	0
1	AO	167/167 (100%)	-0.23	0 100 100	41, 67, 106, 126	0
1	AP	167/167 (100%)	-0.09	1 (0%) 89 90	37, 62, 102, 142	0
1	AQ	167/167 (100%)	-0.23	0 100 100	38, 60, 91, 138	0
1	AR	167/167 (100%)	-0.10	0 100 100	41, 67, 106, 126	0
1	AS	167/167 (100%)	-0.30	0 100 100	37, 62, 102, 142	0
1	AT	167/167 (100%)	-0.28	0 100 100	38, 60, 91, 138	0
1	AU	167/167 (100%)	-0.20	0 100 100	41, 67, 106, 126	0
1	AV	167/167 (100%)	-0.27	0 100 100	37, 62, 102, 142	0
1	AW	167/167 (100%)	-0.34	0 100 100	38, 60, 91, 138	0
1	AX	167/167 (100%)	-0.23	0 100 100	41, 67, 106, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AY	167/167 (100%)	-0.29	0 100 100	37, 62, 102, 142	0
1	AZ	167/167 (100%)	-0.25	0 100 100	38, 60, 91, 138	0
1	BA	167/167 (100%)	0.02	0 100 100	41, 67, 106, 126	0
1	BB	167/167 (100%)	-0.15	1 (0%) 89 90	37, 62, 102, 142	0
1	BC	167/167 (100%)	-0.18	0 100 100	38, 60, 91, 138	0
1	BD	167/167 (100%)	0.04	0 100 100	41, 67, 106, 126	0
1	BE	167/167 (100%)	-0.23	0 100 100	37, 62, 102, 142	0
1	BF	167/167 (100%)	-0.32	0 100 100	38, 60, 91, 138	0
1	BG	167/167 (100%)	-0.27	0 100 100	41, 67, 106, 126	0
1	BH	167/167 (100%)	-0.05	4 (2%) 59 56	37, 62, 102, 142	0
1	BI	167/167 (100%)	-0.25	0 100 100	38, 60, 91, 138	0
1	BJ	167/167 (100%)	-0.11	0 100 100	41, 67, 106, 126	0
1	BK	167/167 (100%)	-0.26	1 (0%) 89 90	37, 62, 102, 142	0
1	BL	167/167 (100%)	-0.28	0 100 100	38, 60, 91, 138	0
1	BM	167/167 (100%)	-0.03	4 (2%) 59 56	41, 67, 106, 126	0
1	BN	167/167 (100%)	-0.21	0 100 100	37, 62, 102, 142	0
1	BO	167/167 (100%)	-0.19	0 100 100	38, 60, 91, 138	0
1	BP	167/167 (100%)	-0.25	0 100 100	41, 67, 106, 126	0
1	BQ	167/167 (100%)	-0.25	0 100 100	37, 62, 102, 142	0
1	BR	167/167 (100%)	-0.24	0 100 100	38, 60, 91, 138	0
1	BS	167/167 (100%)	-0.18	0 100 100	41, 67, 106, 126	0
1	BT	167/167 (100%)	-0.05	1 (0%) 89 90	37, 62, 102, 142	0
1	BU	167/167 (100%)	-0.11	0 100 100	38, 60, 91, 138	0
1	BV	167/167 (100%)	0.01	0 100 100	41, 67, 106, 126	0
1	BW	167/167 (100%)	-0.29	0 100 100	37, 62, 102, 142	0
1	BX	167/167 (100%)	-0.05	7 (4%) 36 34	38, 60, 91, 138	0
1	BY	167/167 (100%)	-0.12	1 (0%) 89 90	41, 67, 106, 126	0
1	BZ	167/167 (100%)	-0.25	0 100 100	37, 62, 102, 142	0
1	CA	167/167 (100%)	-0.39	0 100 100	38, 60, 91, 138	0
1	CB	167/167 (100%)	-0.16	0 100 100	41, 67, 106, 126	0
1	CC	167/167 (100%)	-0.19	0 100 100	37, 62, 102, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	CD	167/167 (100%)	-0.09	0 100 100	38, 60, 91, 138	0
1	CE	167/167 (100%)	-0.10	0 100 100	41, 67, 106, 126	0
1	CF	167/167 (100%)	-0.18	0 100 100	37, 62, 102, 142	0
1	CG	167/167 (100%)	-0.32	0 100 100	38, 60, 91, 138	0
1	CH	167/167 (100%)	-0.20	0 100 100	41, 67, 106, 126	0
All	All	10020/10020 (100%)	-0.18	26 (0%) 94 94	37, 63, 104, 142	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BX	147	PRO	5.1
1	BX	148	THR	5.0
1	BH	146	SER	4.8
1	BH	147	PRO	4.3
1	BX	143	ASP	3.3

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	CC	201	1/1	0.88	0.15	59,59,59,59	0
2	CA	BK	201	1/1	0.90	0.20	59,59,59,59	0
2	CA	CF	201	1/1	0.90	0.17	59,59,59,59	0
2	CA	AV	201	1/1	0.90	0.17	59,59,59,59	0
2	CA	AA	201	1/1	0.90	0.17	59,59,59,59	0
2	CA	AS	201	1/1	0.91	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	AP	201	1/1	0.91	0.12	59,59,59,59	0
2	CA	BH	201	1/1	0.93	0.18	59,59,59,59	0
2	CA	AG	201	1/1	0.93	0.09	59,59,59,59	0
2	CA	AM	201	1/1	0.94	0.25	59,59,59,59	0
2	CA	BE	201	1/1	0.94	0.13	59,59,59,59	0
2	CA	BZ	201	1/1	0.94	0.22	59,59,59,59	0
2	CA	AJ	201	1/1	0.95	0.12	59,59,59,59	0
2	CA	BT	201	1/1	0.95	0.13	59,59,59,59	0
2	CA	BW	201	1/1	0.95	0.18	59,59,59,59	0
2	CA	AD	201	1/1	0.95	0.12	59,59,59,59	0
2	CA	BB	201	1/1	0.95	0.25	59,59,59,59	0
2	CA	AY	201	1/1	0.96	0.18	59,59,59,59	0
2	CA	BQ	201	1/1	0.96	0.18	59,59,59,59	0
2	CA	BN	201	1/1	0.97	0.18	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.