



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 11:51 PM EDT

PDB ID : 6YFU
Title : Virus-like particle of Wenzhou levi-like virus 4
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on : 2020-03-26
Resolution : 4.02 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
Xtrriage (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

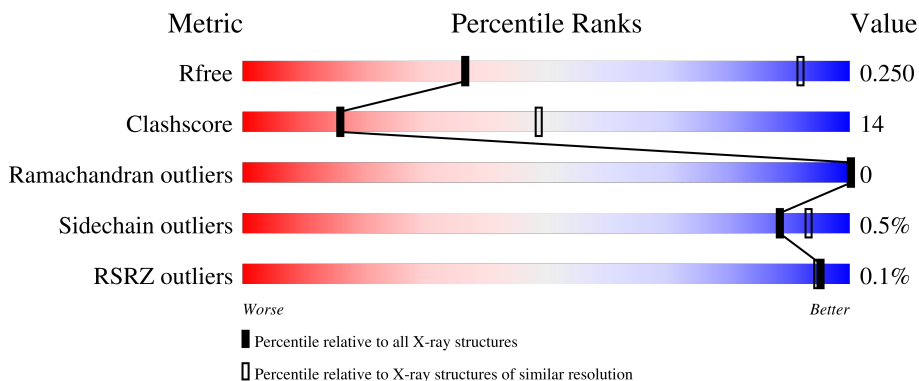
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.02 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.











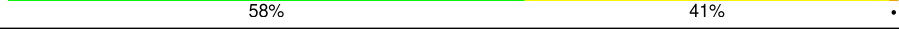

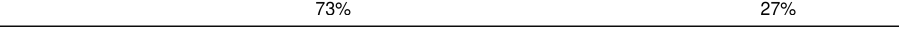
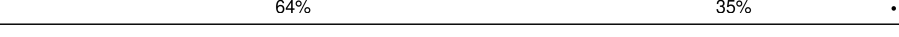

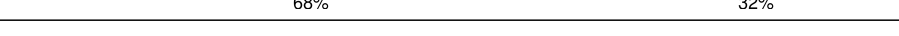


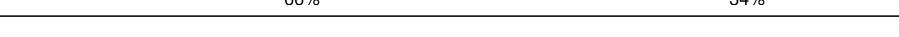

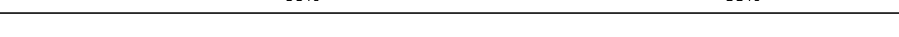






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1098 (4.34-3.70)
Clashscore	141614	1159 (4.34-3.70)
Ramachandran outliers	138981	1118 (4.34-3.70)
Sidechain outliers	138945	1108 (4.34-3.70)
RSRZ outliers	127900	1034 (4.38-3.66)

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	146	64% (green), 36% (yellow)
1	AB	146	60% (green), 40% (yellow), 0% (orange), 0% (red)
1	AC	146	64% (green), 36% (yellow), 0% (orange), 0% (red)
1	AD	146	71% (green), 29% (yellow), 0% (orange), 0% (red)
1	AE	146	66% (green), 33% (yellow), 0% (orange), 0% (red)

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Mol	Chain	Length	Quality of chain
1	AF	146	 64% 35%
1	AG	146	 71% 29%
1	AH	146	 62% 37%
1	AI	146	 71% 28%
1	AJ	146	 72% 28%
1	AK	146	 66% 33%
1	AL	146	 71% 29%
1	AM	146	 70% 30%
1	AN	146	 % 58% 41%
1	AO	146	 67% 32%
1	AP	146	 73% 27%
1	AQ	146	 64% 35%
1	AR	146	 68% 32%
1	AS	146	 68% 32%
1	AT	146	 74% 25%
1	AU	146	 68% 32%
1	AV	146	 66% 34%
1	AW	146	 65% 34%
1	AX	146	 66% 33%
1	AY	146	 62% 38%
1	AZ	146	 64% 35%
1	BA	146	 68% 31%
1	BB	146	 66% 34%
1	BC	146	 62% 37%
1	BD	146	 77% 23%


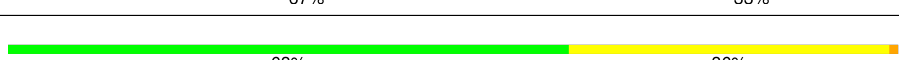
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Mol	Chain	Length	Quality of chain	
1	BE	146	64%	36%
1	BF	146	66%	34%
1	BG	146	79%	20%
1	BH	146	64%	36%
1	BI	146	65%	34%
1	BJ	146	70%	29%
1	BK	146	65%	35%
1	BL	146	64%	35%
1	BM	146	69%	30%
1	BN	146	73%	27%
1	BO	146	63%	36%
1	BP	146	71%	29%
1	BQ	146	64%	36%
1	BR	146	68%	31%
1	BS	146	71%	29%
1	BT	146	65%	35%
1	BU	146	68%	32%
1	BV	146	65%	34%
1	BW	146	64%	36%
1	BX	146	65%	34%
1	BY	146	62%	38%
1	BZ	146	66%	34%
1	CA	146	74%	25%
1	CB	146	68%	32%
1	CC	146	64%	36%

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Mol	Chain	Length	Quality of chain
1	CD	146	 <p>% 65% 34% .</p>
1	CE	146	 <p>% 68% 31% .</p>
1	CF	146	 <p>% 67% 33% .</p>
1	CG	146	 <p>% 63% 36% .</p>
1	CH	146	 <p>% 71% 29% .</p>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 66540 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	146	1109	706	187	213	3	0	0	0
1	AB	146	1109	706	187	213	3	0	0	0
1	AC	146	1109	706	187	213	3	0	0	0
1	AD	146	1109	706	187	213	3	0	0	0
1	AE	146	1109	706	187	213	3	0	0	0
1	AF	146	1109	706	187	213	3	0	0	0
1	AG	146	1109	706	187	213	3	0	0	0
1	AH	146	1109	706	187	213	3	0	0	0
1	AI	146	1109	706	187	213	3	0	0	0
1	AJ	146	1109	706	187	213	3	0	0	0
1	AK	146	1109	706	187	213	3	0	0	0
1	AL	146	1109	706	187	213	3	0	0	0
1	AM	146	1109	706	187	213	3	0	0	0
1	AN	146	1109	706	187	213	3	0	0	0
1	AO	146	1109	706	187	213	3	0	0	0
1	AP	146	1109	706	187	213	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AQ	146	1109	706	187	213	3	0	0	0
1	AR	146	1109	706	187	213	3	0	0	0
1	AS	146	1109	706	187	213	3	0	0	0
1	AT	146	1109	706	187	213	3	0	0	0
1	AU	146	1109	706	187	213	3	0	0	0
1	AV	146	1109	706	187	213	3	0	0	0
1	AW	146	1109	706	187	213	3	0	0	0
1	AX	146	1109	706	187	213	3	0	0	0
1	AY	146	1109	706	187	213	3	0	0	0
1	AZ	146	1109	706	187	213	3	0	0	0
1	BA	146	1109	706	187	213	3	0	0	0
1	BB	146	1109	706	187	213	3	0	0	0
1	BC	146	1109	706	187	213	3	0	0	0
1	BD	146	1109	706	187	213	3	0	0	0
1	BE	146	1109	706	187	213	3	0	0	0
1	BF	146	1109	706	187	213	3	0	0	0
1	BG	146	1109	706	187	213	3	0	0	0
1	BH	146	1109	706	187	213	3	0	0	0
1	BI	146	1109	706	187	213	3	0	0	0
1	BJ	146	1109	706	187	213	3	0	0	0
1	BK	146	1109	706	187	213	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BL	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BM	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BN	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BO	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BP	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BQ	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BR	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BS	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BT	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BU	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BV	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BW	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BX	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BY	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	BZ	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	CA	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	CB	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	CC	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	CD	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	CE	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			
1	CF	146	Total	C	N	O	S	0	0	0
			1109	706	187	213	3			

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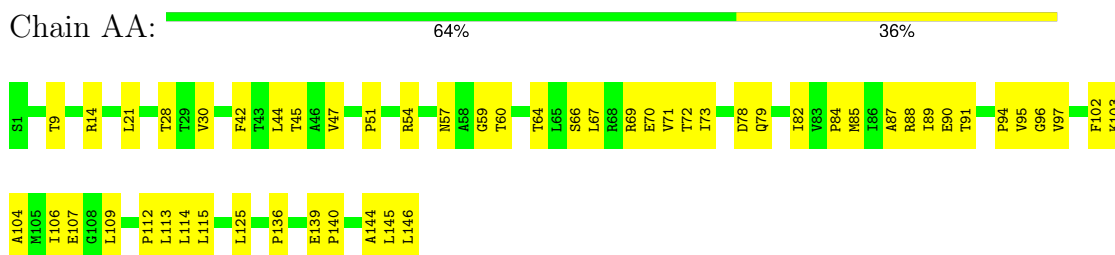
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	CG	146	Total 1109	C 706	N 187	O 213	S 3	0	0	0
1	CH	146	Total 1109	C 706	N 187	O 213	S 3	0	0	0

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.

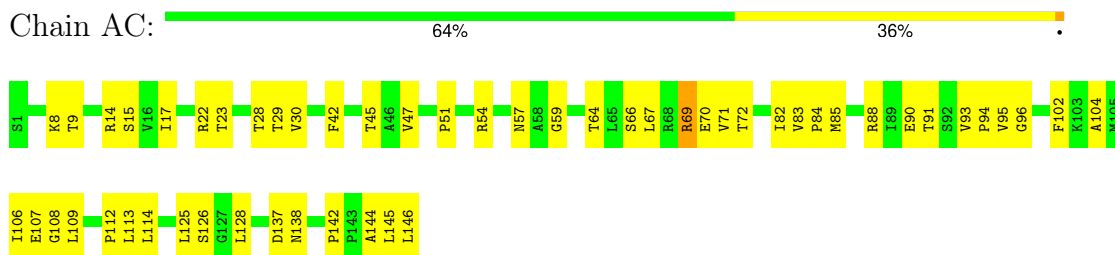
- Molecule 1: coat protein



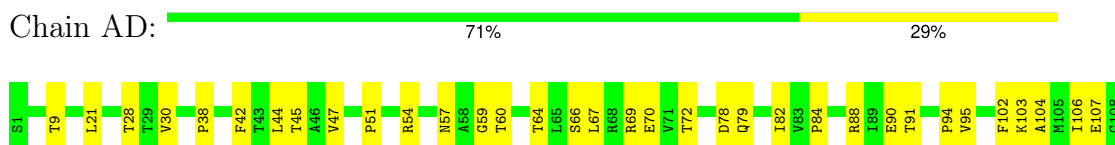
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein





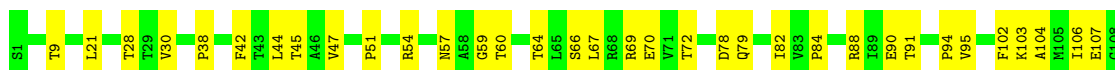
- Molecule 1: coat protein



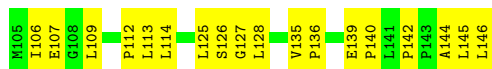
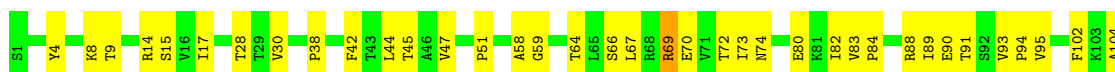
- Molecule 1: coat protein



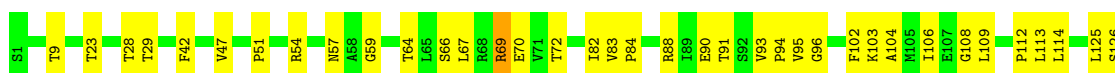
- Molecule 1: coat protein



- Molecule 1: coat protein

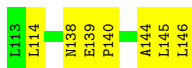


- Molecule 1: coat protein

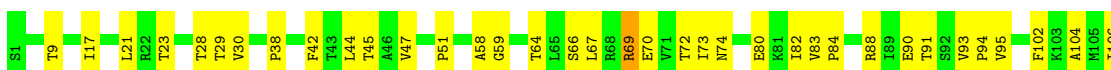




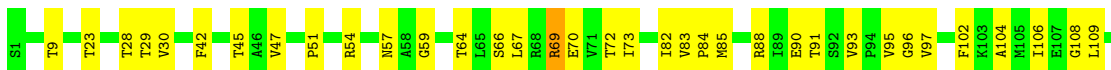
- Molecule 1: coat protein



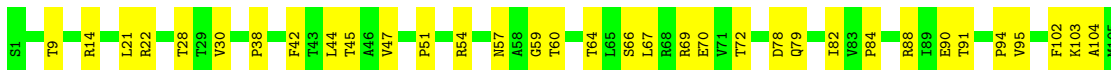
- Molecule 1: coat protein



- Molecule 1: coat protein

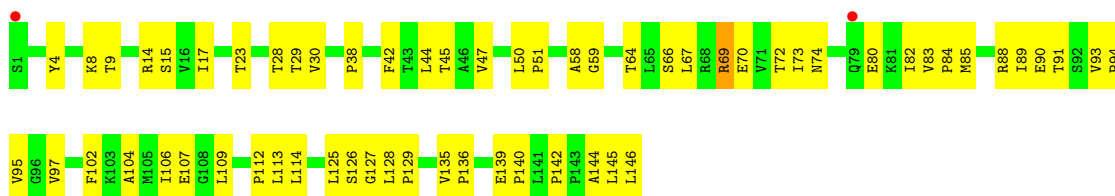


- Molecule 1: coat protein



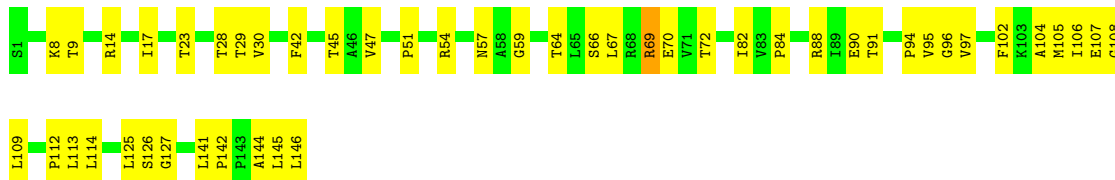
- Molecule 1: coat protein





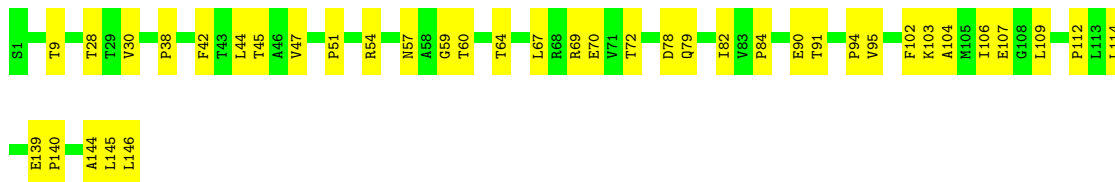
- Molecule 1: coat protein

Chain AO: 67% 32%



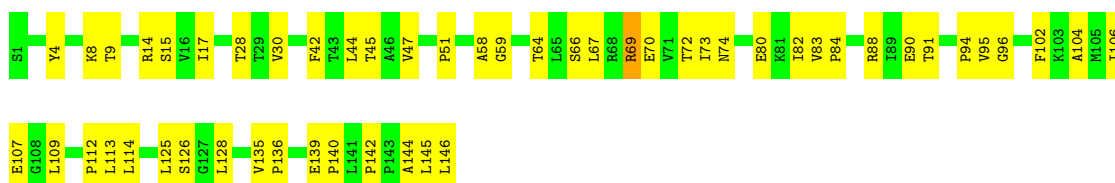
- Molecule 1: coat protein

Chain AP: 73% 27%



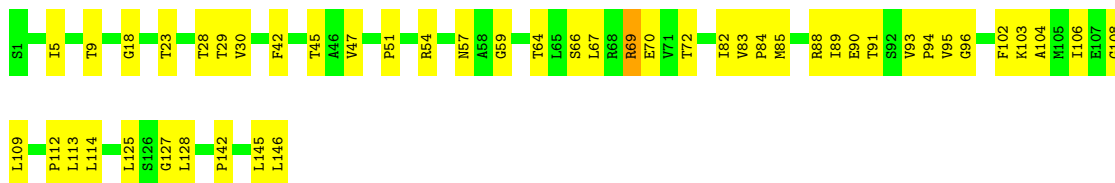
- Molecule 1: coat protein

Chain AQ: 64% 35%



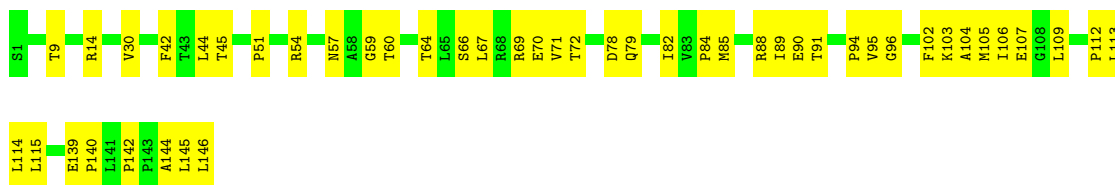
- Molecule 1: coat protein

Chain AR: 68% 32%



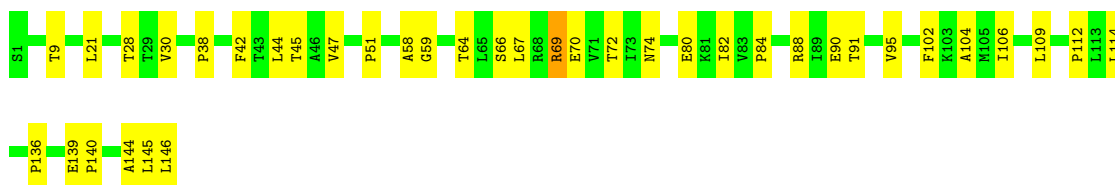
- Molecule 1: coat protein

Chain AS:  68% 32%



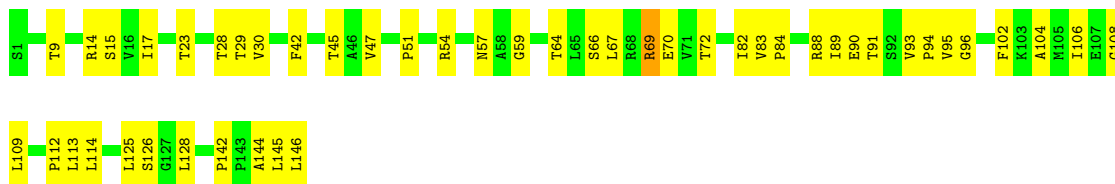
- Molecule 1: coat protein

Chain AT:  74% 25%



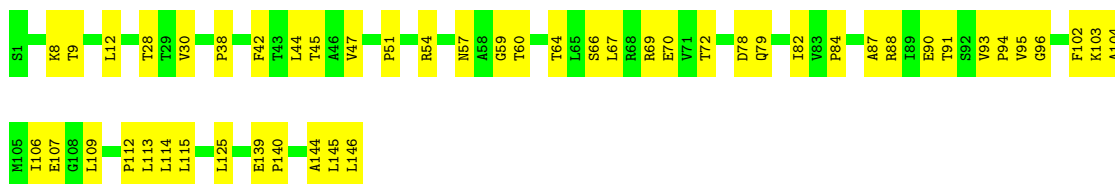
- Molecule 1: coat protein

Chain AU:  68% 32%



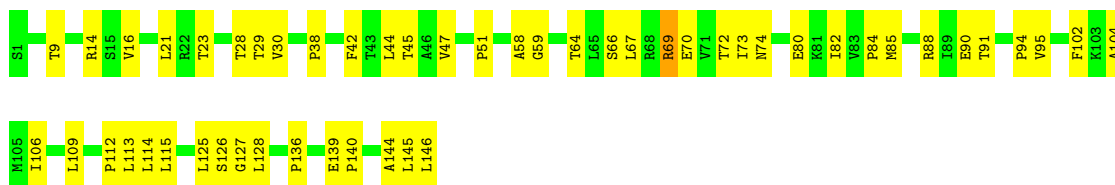
- Molecule 1: coat protein

Chain AV:  66% 34%



- Molecule 1: coat protein

Chain AW:  65% 34%



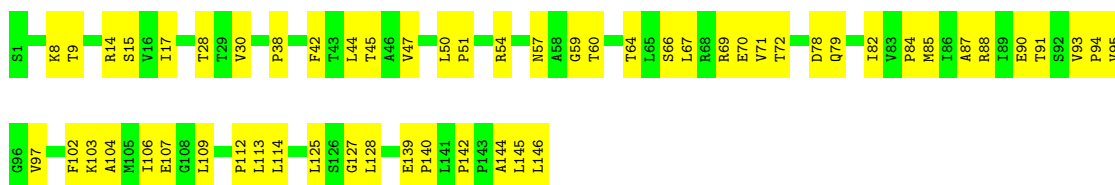
- Molecule 1: coat protein

Chain AX:  66% 33%



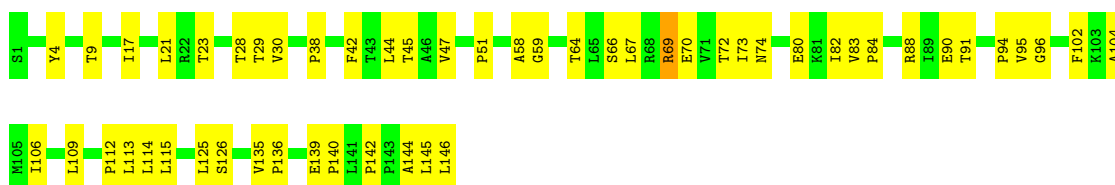
- Molecule 1: coat protein

Chain AY:  62% 38%



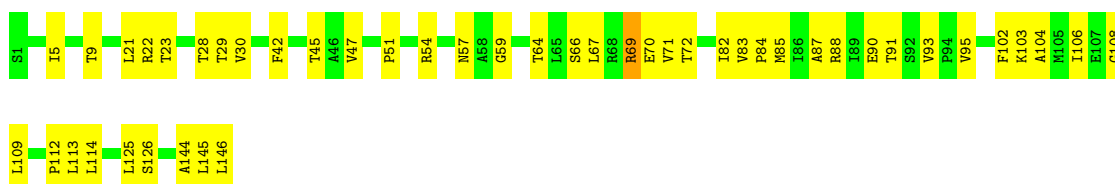
- Molecule 1: coat protein

Chain AZ:  64% 35%



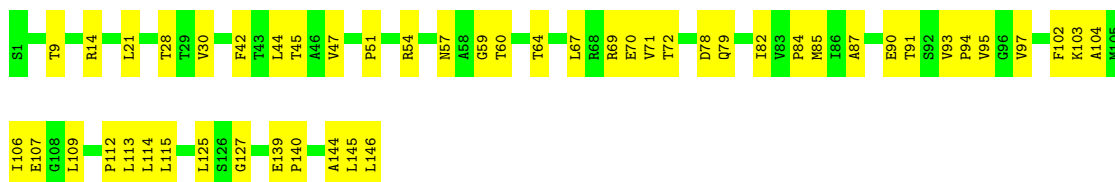
- Molecule 1: coat protein

Chain BA:  68% 31%



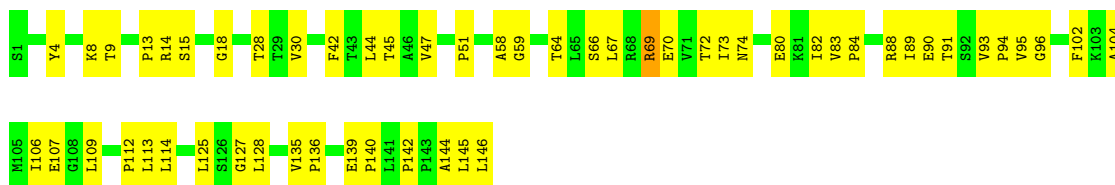
- Molecule 1: coat protein

Chain BB:  66% 34%




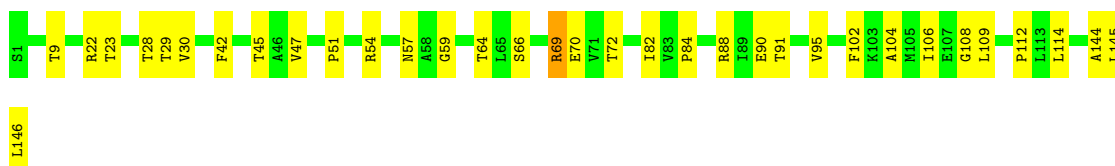
- Molecule 1: coat protein

Chain BC:  62% 37%



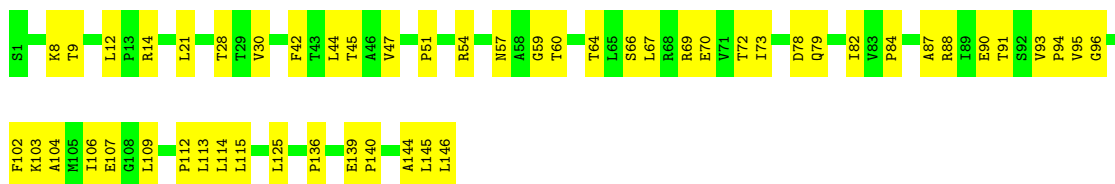
- Molecule 1: coat protein

Chain BD:  77% 23%



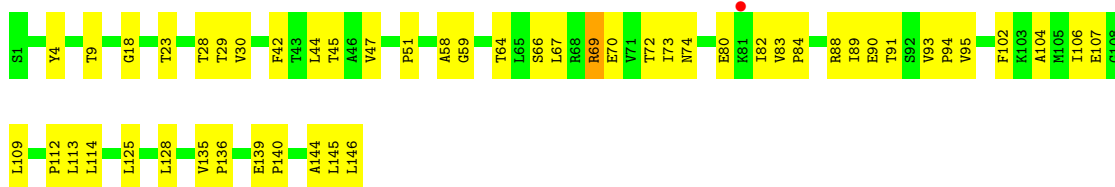
- Molecule 1: coat protein

Chain BE:  64% 36%




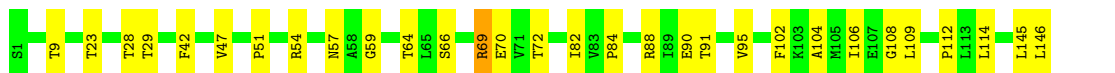
- Molecule 1: coat protein

Chain BF:  66% 34%



- Molecule 1: coat protein

Chain BG:  79% 20%



- Molecule 1: coat protein

Chain BH:  64% 36%



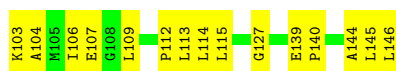
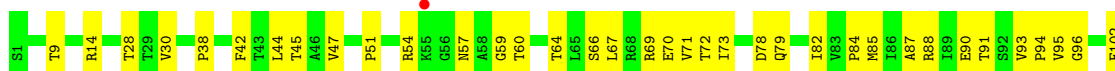
• Molecule 1: coat protein



• Molecule 1: coat protein



• Molecule 1: coat protein

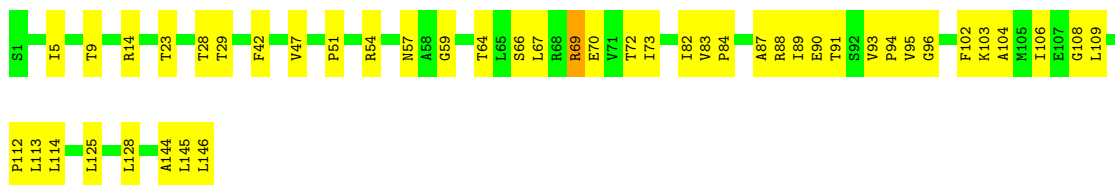


• Molecule 1: coat protein



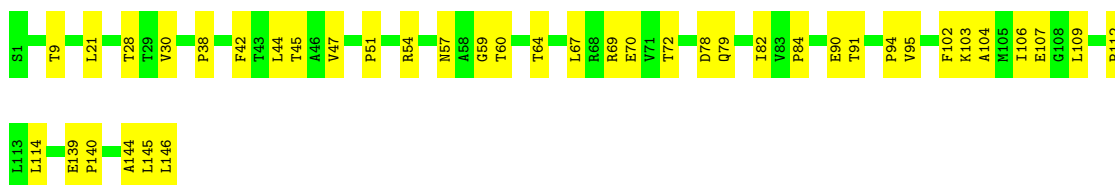
• Molecule 1: coat protein

Chain BM:  69% 30%



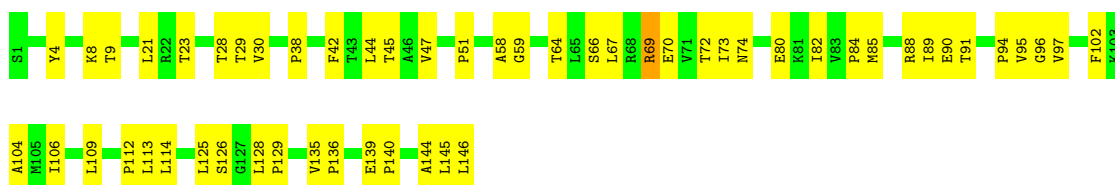
- Molecule 1: coat protein

Chain BN:  73% 27%



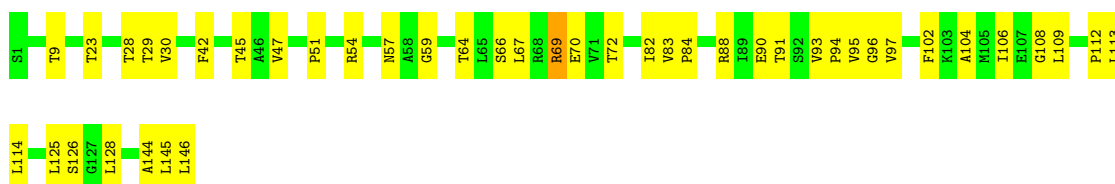
- Molecule 1: coat protein

Chain BO:  63% 36%



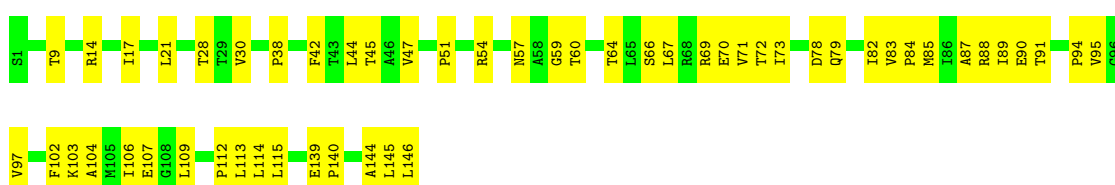
- Molecule 1: coat protein

Chain BP:  71% 29%

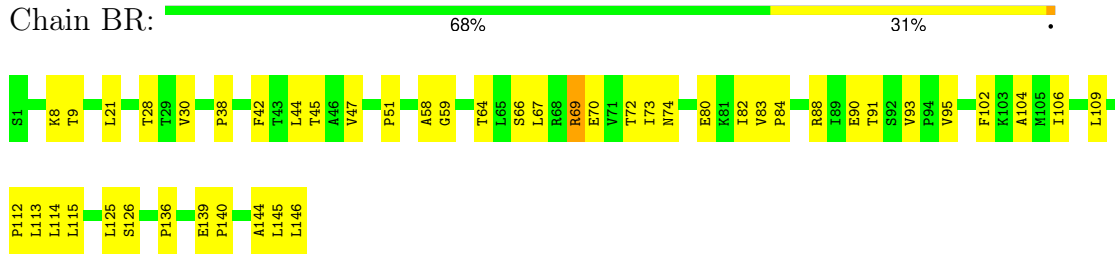


- Molecule 1: coat protein

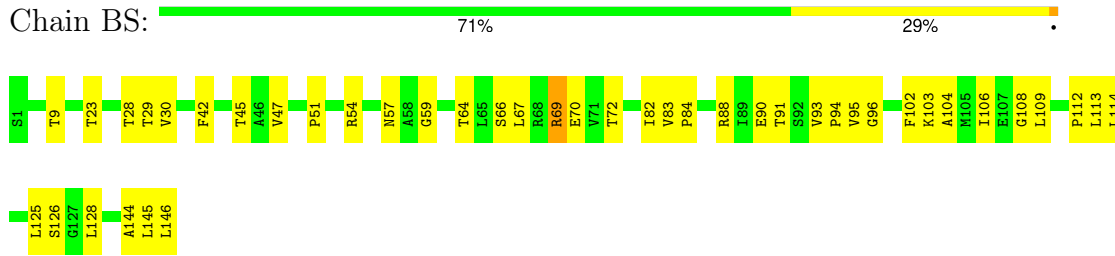
Chain BQ:  64% 36%



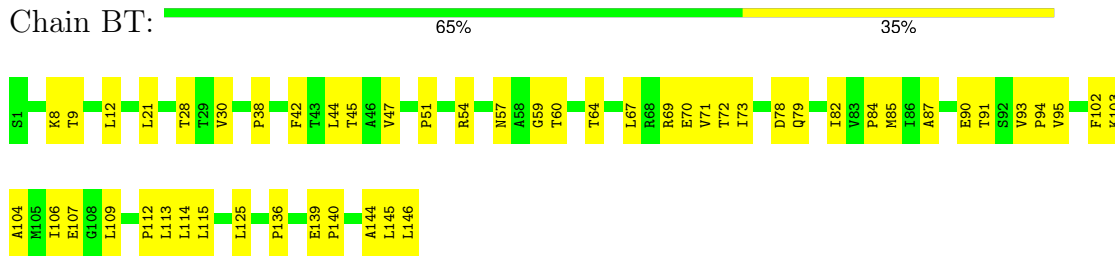
- Molecule 1: coat protein



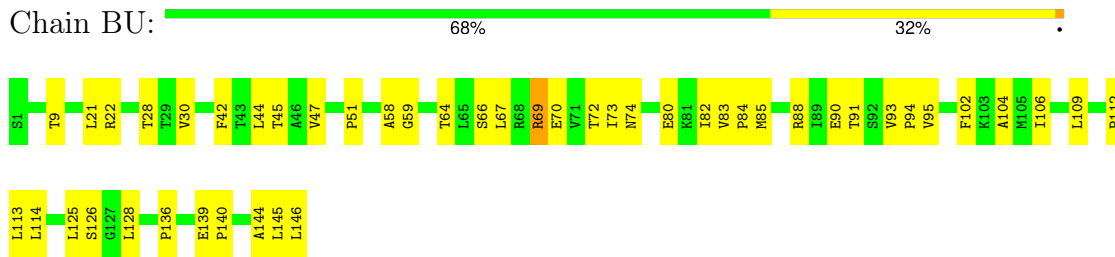
- Molecule 1: coat protein



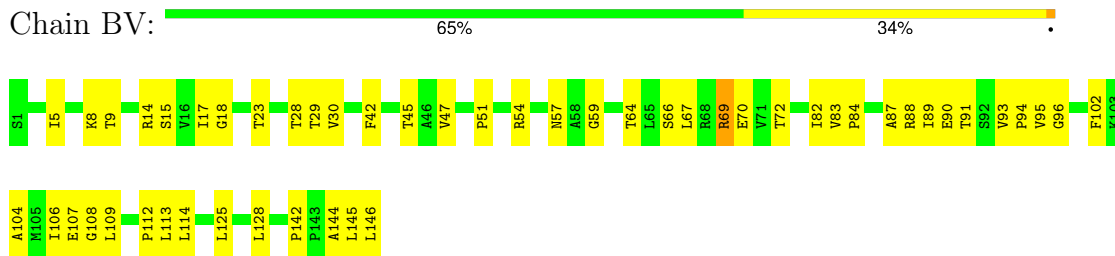
- Molecule 1: coat protein



- Molecule 1: coat protein

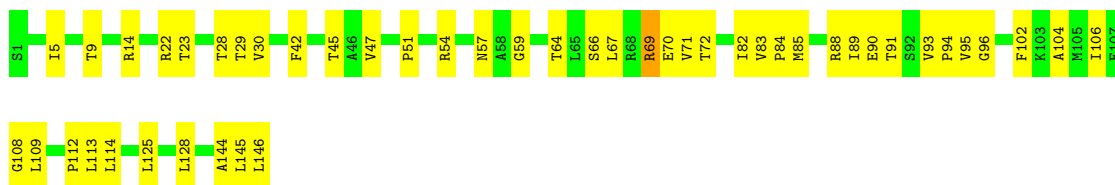


- Molecule 1: coat protein



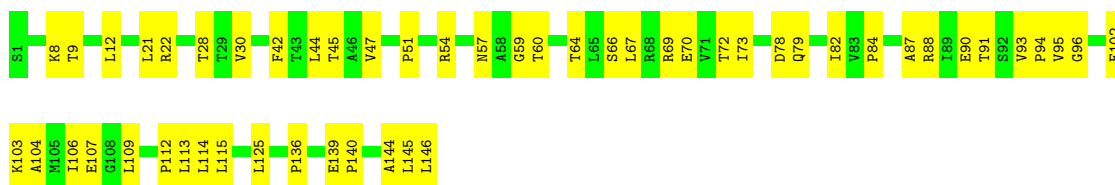
- Molecule 1: coat protein

Chain CB:  68% 32%



• Molecule 1: coat protein

Chain CC:  64% 36%



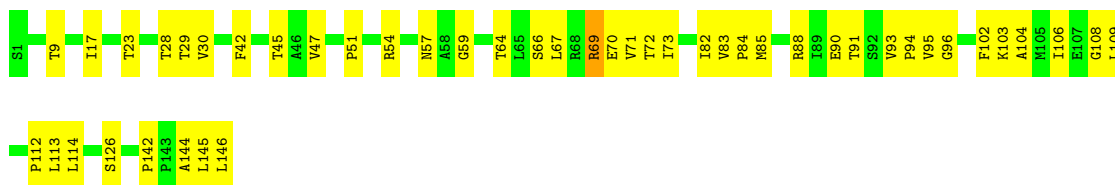
• Molecule 1: coat protein

Chain CD:  65% 34%



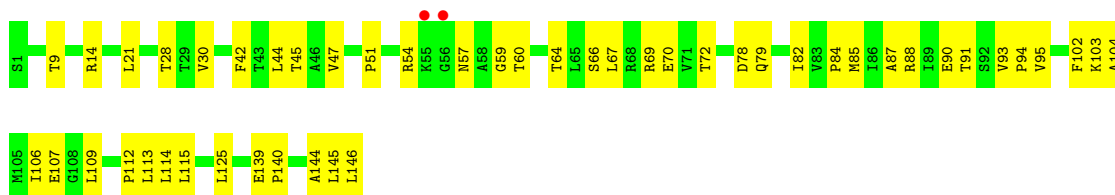
• Molecule 1: coat protein

Chain CE:  68% 31%



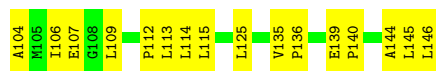
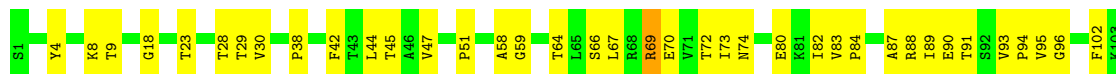
• Molecule 1: coat protein

Chain CF:  67% 33%



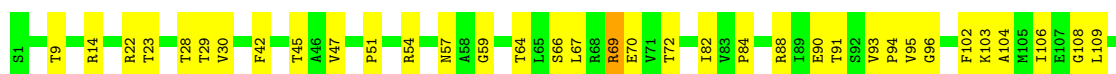
- Molecule 1: coat protein

Chain CG:  63% 36%



- Molecule 1: coat protein

Chain CH:  71% 29%



4 Data and refinement statistics i

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	551.80Å 551.80Å 551.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 4.02 49.96 – 4.02	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.96-4.02) 99.6 (49.96-4.02)	Depositor EDS
R_{merge}	0.88	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 4.00Å)	Xtrriage
Refinement program	PHENIX 1.14 3260	Depositor
R, R_{free}	0.242 , 0.250 0.242 , 0.250	Depositor DCC
R_{free} test set	4983 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å ²)	172.3	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 90.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.075 for -l,-k,-h	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	66540	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.10% 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	0.31	0/1131	0.58	0/1547
1	AB	0.32	0/1131	0.58	0/1547
1	AC	0.31	0/1131	0.57	0/1547
1	AD	0.31	0/1131	0.58	0/1547
1	AE	0.32	0/1131	0.58	0/1547
1	AF	0.31	0/1131	0.57	0/1547
1	AG	0.31	0/1131	0.58	0/1547
1	AH	0.32	0/1131	0.58	0/1547
1	AI	0.31	0/1131	0.57	0/1547
1	AJ	0.31	0/1131	0.58	0/1547
1	AK	0.32	0/1131	0.58	0/1547
1	AL	0.31	0/1131	0.57	0/1547
1	AM	0.31	0/1131	0.58	0/1547
1	AN	0.32	0/1131	0.58	0/1547
1	AO	0.31	0/1131	0.57	0/1547
1	AP	0.31	0/1131	0.58	0/1547
1	AQ	0.32	0/1131	0.58	0/1547
1	AR	0.31	0/1131	0.57	0/1547
1	AS	0.31	0/1131	0.58	0/1547
1	AT	0.32	0/1131	0.58	0/1547
1	AU	0.31	0/1131	0.57	0/1547
1	AV	0.31	0/1131	0.58	0/1547
1	AW	0.32	0/1131	0.58	0/1547
1	AX	0.31	0/1131	0.57	0/1547
1	AY	0.31	0/1131	0.58	0/1547
1	AZ	0.32	0/1131	0.58	0/1547
1	BA	0.31	0/1131	0.57	0/1547
1	BB	0.31	0/1131	0.58	0/1547
1	BC	0.32	0/1131	0.58	0/1547
1	BD	0.31	0/1131	0.57	0/1547
1	BE	0.31	0/1131	0.58	0/1547
1	BF	0.32	0/1131	0.58	0/1547
1	BG	0.31	0/1131	0.57	0/1547
1	BH	0.31	0/1131	0.58	0/1547

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BI	0.32	0/1131	0.58	0/1547
1	BJ	0.31	0/1131	0.57	0/1547
1	BK	0.31	0/1131	0.58	0/1547
1	BL	0.32	0/1131	0.58	0/1547
1	BM	0.31	0/1131	0.57	0/1547
1	BN	0.31	0/1131	0.58	0/1547
1	BO	0.32	0/1131	0.58	0/1547
1	BP	0.31	0/1131	0.57	0/1547
1	BQ	0.31	0/1131	0.58	0/1547
1	BR	0.32	0/1131	0.58	0/1547
1	BS	0.31	0/1131	0.57	0/1547
1	BT	0.31	0/1131	0.58	0/1547
1	BU	0.32	0/1131	0.58	0/1547
1	BV	0.31	0/1131	0.57	0/1547
1	BW	0.31	0/1131	0.58	0/1547
1	BX	0.32	0/1131	0.58	0/1547
1	BY	0.31	0/1131	0.57	0/1547
1	BZ	0.31	0/1131	0.58	0/1547
1	CA	0.32	0/1131	0.58	0/1547
1	CB	0.31	0/1131	0.57	0/1547
1	CC	0.31	0/1131	0.58	0/1547
1	CD	0.32	0/1131	0.58	0/1547
1	CE	0.31	0/1131	0.57	0/1547
1	CF	0.31	0/1131	0.58	0/1547
1	CG	0.32	0/1131	0.58	0/1547
1	CH	0.31	0/1131	0.57	0/1547
All	All	0.31	0/67860	0.58	0/92820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	1109	0	1159	45	0
1	AB	1109	0	1159	53	0
1	AC	1109	0	1159	46	2
1	AD	1109	0	1159	29	0
1	AE	1109	0	1159	43	0
1	AF	1109	0	1159	53	0
1	AG	1109	0	1159	28	0
1	AH	1109	0	1159	51	0
1	AI	1109	0	1159	35	0
1	AJ	1109	0	1159	28	2
1	AK	1109	0	1159	40	0
1	AL	1109	0	1159	38	0
1	AM	1109	0	1159	31	1
1	AN	1109	0	1159	57	0
1	AO	1109	0	1159	44	0
1	AP	1109	0	1159	27	0
1	AQ	1109	0	1159	44	0
1	AR	1109	0	1159	47	0
1	AS	1109	0	1159	41	0
1	AT	1109	0	1159	25	0
1	AU	1109	0	1159	40	0
1	AV	1109	0	1159	40	0
1	AW	1109	0	1159	41	0
1	AX	1109	0	1159	42	0
1	AY	1109	0	1159	48	0
1	AZ	1109	0	1159	43	0
1	BA	1109	0	1159	39	0
1	BB	1109	0	1159	42	0
1	BC	1109	0	1159	49	0
1	BD	1109	0	1159	24	0
1	BE	1109	0	1159	41	0
1	BF	1109	0	1159	41	0
1	BG	1109	0	1159	21	0
1	BH	1109	0	1159	41	0
1	BI	1109	0	1159	43	0
1	BJ	1109	0	1159	37	0
1	BK	1109	0	1159	46	0
1	BL	1109	0	1159	47	0
1	BM	1109	0	1159	42	0
1	BN	1109	0	1159	28	0
1	BO	1109	0	1159	45	0
1	BP	1109	0	1159	39	0
1	BQ	1109	0	1159	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	1109	0	1159	37	0
1	BS	1109	0	1159	36	0
1	BT	1109	0	1159	42	0
1	BU	1109	0	1159	41	0
1	BV	1109	0	1159	46	0
1	BW	1109	0	1159	49	0
1	BX	1109	0	1159	44	0
1	BY	1109	0	1159	51	0
1	BZ	1109	0	1159	43	1
1	CA	1109	0	1159	27	0
1	CB	1109	0	1159	40	0
1	CC	1109	0	1159	44	0
1	CD	1109	0	1159	48	0
1	CE	1109	0	1159	39	0
1	CF	1109	0	1159	38	0
1	CG	1109	0	1159	48	0
1	CH	1109	0	1159	34	0
All	All	66540	0	69540	1973	3

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

The worst 5 of 1973 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:AF:128:LEU:HD23	1:AM:21:LEU:HD13	1.51	0.91
1:AE:21:LEU:HD13	1:AN:128:LEU:HD23	1.59	0.82
1:BA:93:VAL:HG11	1:BI:125:LEU:HG	1.64	0.79
1:AR:128:LEU:HD23	1:CC:21:LEU:HD13	1.64	0.78
1:AO:126:SER:HA	1:BK:38:PRO:HG3	1.66	0.77

All (3) 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:AM:14:ARG:NH2	1:BZ:138:ASN:O[20_555]	2.06	0.14
1:AC:137:ASP:C	1:AJ:138:ASN:OD1[11_566]	2.13	0.07
1:AC:138:ASN:N	1:AJ:138:ASN:OD1[11_566]	2.18	0.02

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	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AB	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AC	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AD	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AE	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AF	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AG	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AH	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AI	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AJ	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AK	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AL	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AM	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AN	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AO	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AP	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AQ	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AR	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AS	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AT	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AU	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AV	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AW	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AX	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	AY	144/146 (99%)	142 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AZ	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BA	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BB	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BC	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BD	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BE	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BF	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BG	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BH	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BI	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BJ	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BK	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BL	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BM	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BN	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BO	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BP	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BQ	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BR	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BS	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BT	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BU	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BV	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BW	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BX	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BY	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	BZ	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	CA	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	CB	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	CC	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	CD	144/146 (99%)	142 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CE	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	CF	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	CG	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	CH	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
All	All	8640/8760 (99%)	8520 (99%)	120 (1%)	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	130/130 (100%)	130 (100%)	0	100	100
1	AB	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AC	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AD	130/130 (100%)	130 (100%)	0	100	100
1	AE	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AF	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AG	130/130 (100%)	130 (100%)	0	100	100
1	AH	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AI	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AJ	130/130 (100%)	130 (100%)	0	100	100
1	AK	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AL	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AM	130/130 (100%)	130 (100%)	0	100	100
1	AN	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AO	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AP	130/130 (100%)	130 (100%)	0	100	100
1	AQ	130/130 (100%)	129 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AR	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AS	130/130 (100%)	130 (100%)	0	100	100
1	AT	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AU	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AV	130/130 (100%)	130 (100%)	0	100	100
1	AW	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AX	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	AY	130/130 (100%)	130 (100%)	0	100	100
1	AZ	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BA	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BB	130/130 (100%)	130 (100%)	0	100	100
1	BC	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BD	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BE	130/130 (100%)	130 (100%)	0	100	100
1	BF	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BG	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BH	130/130 (100%)	130 (100%)	0	100	100
1	BI	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BJ	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BK	130/130 (100%)	130 (100%)	0	100	100
1	BL	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BM	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BN	130/130 (100%)	130 (100%)	0	100	100
1	BO	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BP	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BQ	130/130 (100%)	130 (100%)	0	100	100
1	BR	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BS	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BT	130/130 (100%)	130 (100%)	0	100	100
1	BU	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BV	130/130 (100%)	129 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BW	130/130 (100%)	130 (100%)	0	100	100
1	BX	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BY	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	BZ	130/130 (100%)	130 (100%)	0	100	100
1	CA	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	CB	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	CC	130/130 (100%)	130 (100%)	0	100	100
1	CD	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	CE	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	CF	130/130 (100%)	130 (100%)	0	100	100
1	CG	130/130 (100%)	129 (99%)	1 (1%)	81	89
1	CH	130/130 (100%)	129 (99%)	1 (1%)	81	89
All	All	7800/7800 (100%)	7760 (100%)	40 (0%)	88	93

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

Mol	Chain	Res	Type
1	BR	69	ARG
1	CB	69	ARG
1	BS	69	ARG
1	BX	69	ARG
1	CE	69	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 [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	146/146 (100%)	-0.52	0 100 100	119, 157, 210, 242	0
1	AB	146/146 (100%)	-0.53	0 100 100	119, 156, 213, 251	0
1	AC	146/146 (100%)	-0.40	0 100 100	119, 157, 210, 241	0
1	AD	146/146 (100%)	-0.38	0 100 100	119, 157, 210, 242	0
1	AE	146/146 (100%)	-0.44	0 100 100	119, 156, 213, 251	0
1	AF	146/146 (100%)	-0.51	0 100 100	119, 157, 210, 241	0
1	AG	146/146 (100%)	-0.41	0 100 100	119, 157, 210, 242	0
1	AH	146/146 (100%)	-0.48	0 100 100	119, 156, 213, 251	0
1	AI	146/146 (100%)	-0.44	0 100 100	119, 157, 210, 241	0
1	AJ	146/146 (100%)	-0.31	0 100 100	119, 157, 210, 242	0
1	AK	146/146 (100%)	-0.47	0 100 100	119, 156, 213, 251	0
1	AL	146/146 (100%)	-0.50	0 100 100	119, 157, 210, 241	0
1	AM	146/146 (100%)	-0.47	0 100 100	119, 157, 210, 242	0
1	AN	146/146 (100%)	-0.39	2 (1%) 75 65	119, 156, 213, 251	0
1	AO	146/146 (100%)	-0.50	0 100 100	119, 157, 210, 241	0
1	AP	146/146 (100%)	-0.45	0 100 100	119, 157, 210, 242	0
1	AQ	146/146 (100%)	-0.46	0 100 100	119, 156, 213, 251	0
1	AR	146/146 (100%)	-0.47	0 100 100	119, 157, 210, 241	0
1	AS	146/146 (100%)	-0.42	0 100 100	119, 157, 210, 242	0
1	AT	146/146 (100%)	-0.51	0 100 100	119, 156, 213, 251	0
1	AU	146/146 (100%)	-0.50	0 100 100	119, 157, 210, 241	0
1	AV	146/146 (100%)	-0.44	0 100 100	119, 157, 210, 242	0
1	AW	146/146 (100%)	-0.51	0 100 100	119, 156, 213, 251	0
1	AX	146/146 (100%)	-0.52	0 100 100	119, 157, 210, 241	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AY	146/146 (100%)	-0.37	0 100 100	119, 157, 210, 242	0
1	AZ	146/146 (100%)	-0.47	0 100 100	119, 156, 213, 251	0
1	BA	146/146 (100%)	-0.46	0 100 100	119, 157, 210, 241	0
1	BB	146/146 (100%)	-0.35	0 100 100	119, 157, 210, 242	0
1	BC	146/146 (100%)	-0.36	0 100 100	119, 156, 213, 251	0
1	BD	146/146 (100%)	-0.46	0 100 100	119, 157, 210, 241	0
1	BE	146/146 (100%)	-0.39	0 100 100	119, 157, 210, 242	0
1	BF	146/146 (100%)	-0.35	1 (0%) 87 82	119, 156, 213, 251	0
1	BG	146/146 (100%)	-0.51	0 100 100	119, 157, 210, 241	0
1	BH	146/146 (100%)	-0.43	0 100 100	119, 157, 210, 242	0
1	BI	146/146 (100%)	-0.40	1 (0%) 87 82	119, 156, 213, 251	0
1	BJ	146/146 (100%)	-0.47	0 100 100	119, 157, 210, 241	0
1	BK	146/146 (100%)	-0.43	1 (0%) 87 82	119, 157, 210, 242	0
1	BL	146/146 (100%)	-0.39	0 100 100	119, 156, 213, 251	0
1	BM	146/146 (100%)	-0.46	0 100 100	119, 157, 210, 241	0
1	BN	146/146 (100%)	-0.51	0 100 100	119, 157, 210, 242	0
1	BO	146/146 (100%)	-0.56	0 100 100	119, 156, 213, 251	0
1	BP	146/146 (100%)	-0.38	0 100 100	119, 157, 210, 241	0
1	BQ	146/146 (100%)	-0.45	0 100 100	119, 157, 210, 242	0
1	BR	146/146 (100%)	-0.44	0 100 100	119, 156, 213, 251	0
1	BS	146/146 (100%)	-0.43	0 100 100	119, 157, 210, 241	0
1	BT	146/146 (100%)	-0.42	0 100 100	119, 157, 210, 242	0
1	BU	146/146 (100%)	-0.51	0 100 100	119, 156, 213, 251	0
1	BV	146/146 (100%)	-0.55	0 100 100	119, 157, 210, 241	0
1	BW	146/146 (100%)	-0.35	1 (0%) 87 82	119, 157, 210, 242	0
1	BX	146/146 (100%)	-0.40	0 100 100	119, 156, 213, 251	0
1	BY	146/146 (100%)	-0.48	0 100 100	119, 157, 210, 241	0
1	BZ	146/146 (100%)	-0.38	0 100 100	119, 157, 210, 242	0
1	CA	146/146 (100%)	-0.43	0 100 100	119, 156, 213, 251	0
1	CB	146/146 (100%)	-0.38	0 100 100	119, 157, 210, 241	0
1	CC	146/146 (100%)	-0.25	0 100 100	119, 157, 210, 242	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	CD	146/146 (100%)	-0.37	1 (0%) 87 82	119, 156, 213, 251	0
1	CE	146/146 (100%)	-0.38	0 100 100	119, 157, 210, 241	0
1	CF	146/146 (100%)	-0.37	2 (1%) 75 65	119, 157, 210, 242	0
1	CG	146/146 (100%)	-0.46	0 100 100	119, 156, 213, 251	0
1	CH	146/146 (100%)	-0.52	0 100 100	119, 157, 210, 241	0
All	All	8760/8760 (100%)	-0.44	9 (0%) 95 94	119, 157, 214, 251	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CF	55	LYS	3.9
1	CF	56	GLY	2.9
1	BW	55	LYS	2.4
1	AN	79	GLN	2.4
1	CD	14	ARG	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.