



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 10:32 PM EDT

PDB ID : 6YFK
Title : Virus-like particle of bacteriophage ESE007
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on : 2020-03-26
Resolution : 3.70 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

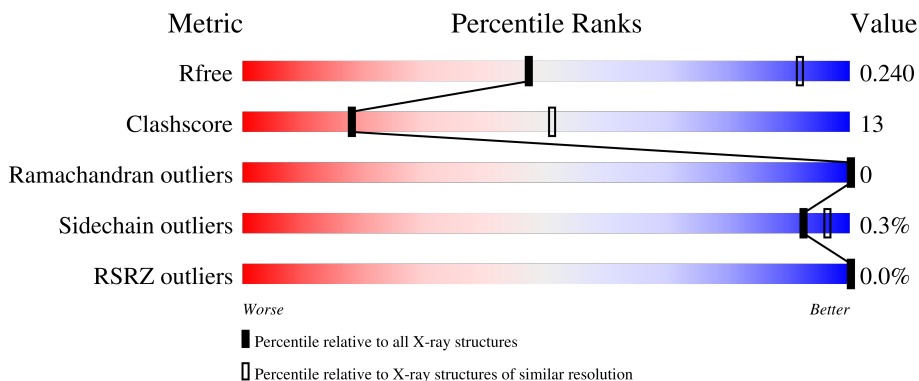
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	137	71% (green), 29% (yellow)
1	AB	137	60% (green), 40% (yellow)
1	AC	137	77% (green), 22% (yellow), 1% (orange)
1	AD	137	64% (green), 36% (yellow)
1	AE	137	64% (green), 36% (yellow)

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Mol	Chain	Length	Quality of chain	
1	AF	137	71%	28%
1	AG	137	74%	26%
1	AH	137	63%	37%
1	AI	137	73%	26%
1	AJ	137	69%	31%
1	AK	137	62%	38%
1	AL	137	74%	26%
1	AM	137	70%	30%
1	AN	137	64%	36%
1	AO	137	75%	24%
1	AP	137	70%	30%
1	AQ	137	58%	42%
1	AR	137	70%	29%
1	AS	137	69%	31%
1	AT	137	63%	37%
1	AU	137	74%	25%
1	AV	137	68%	32%
1	AW	137	68%	32%
1	AX	137	74%	26%
1	AY	137	69%	31%
1	AZ	137	68%	32%
1	BA	137	74%	26%
1	BB	137	72%	28%
1	BC	137	59%	41%
1	BD	137	74%	25%


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Mol	Chain	Length	Quality of chain
1	BE	137	72% 28%
1	BF	137	61% 39%
1	BG	137	77% 23%
1	BH	137	64% 36%
1	BI	137	61% 39%
1	BJ	137	71% 28%
1	BK	137	66% 34%
1	BL	137	69% 31%
1	BM	137	74% 26%
1	BN	137	74% 26%
1	BO	137	59% 41%
1	BP	137	73% 26%
1	BQ	137	72% 28%
1	BR	137	64% 36%
1	BS	137	74% 25%
1	BT	137	69% 31%
1	BU	137	68% 32%
1	BV	137	74% 26%
1	BW	137	68% 32%
1	BX	137	64% 36%
1	BY	137	74% 25%
1	BZ	137	69% 31%
1	CA	137	61% 39%
1	CB	137	73% 26%
1	CC	137	72% 28%

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Mol	Chain	Length	Quality of chain
1	CD	137	 63% 37%
1	CE	137	 74% 26%
1	CF	137	 70% 30%
1	CG	137	 64% 36%
1	CH	137	 74% 25%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 62180 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	137	1036	656	178	200	2	0	0	0
1	AB	137	1036	656	178	200	2	0	0	0
1	AC	137	1036	656	178	200	2	0	0	0
1	AD	137	1036	656	178	200	2	0	0	0
1	AE	137	1036	656	178	200	2	0	0	0
1	AF	137	1036	656	178	200	2	0	0	0
1	AG	137	1036	656	178	200	2	0	0	0
1	AH	137	1036	656	178	200	2	0	0	0
1	AI	137	1036	656	178	200	2	0	0	0
1	AJ	137	1036	656	178	200	2	0	0	0
1	AK	137	1036	656	178	200	2	0	0	0
1	AL	137	1036	656	178	200	2	0	0	0
1	AM	137	1036	656	178	200	2	0	0	0
1	AN	137	1036	656	178	200	2	0	0	0
1	AO	137	1036	656	178	200	2	0	0	0
1	AP	137	1036	656	178	200	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AQ	137	1036	656	178	200	2	0	0	0
1	AR	137	1036	656	178	200	2	0	0	0
1	AS	137	1036	656	178	200	2	0	0	0
1	AT	137	1036	656	178	200	2	0	0	0
1	AU	137	1036	656	178	200	2	0	0	0
1	AV	137	1036	656	178	200	2	0	0	0
1	AW	137	1036	656	178	200	2	0	0	0
1	AX	137	1036	656	178	200	2	0	0	0
1	AY	137	1036	656	178	200	2	0	0	0
1	AZ	137	1036	656	178	200	2	0	0	0
1	BA	137	1036	656	178	200	2	0	0	0
1	BB	137	1036	656	178	200	2	0	0	0
1	BC	137	1036	656	178	200	2	0	0	0
1	BD	137	1036	656	178	200	2	0	0	0
1	BE	137	1036	656	178	200	2	0	0	0
1	BF	137	1036	656	178	200	2	0	0	0
1	BG	137	1036	656	178	200	2	0	0	0
1	BH	137	1036	656	178	200	2	0	0	0
1	BI	137	1036	656	178	200	2	0	0	0
1	BJ	137	1036	656	178	200	2	0	0	0
1	BK	137	1036	656	178	200	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	BL	137	1036	656	178	200	2	0	0	0
1	BM	137	1036	656	178	200	2	0	0	0
1	BN	137	1036	656	178	200	2	0	0	0
1	BO	137	1036	656	178	200	2	0	0	0
1	BP	137	1036	656	178	200	2	0	0	0
1	BQ	137	1036	656	178	200	2	0	0	0
1	BR	137	1036	656	178	200	2	0	0	0
1	BS	137	1036	656	178	200	2	0	0	0
1	BT	137	1036	656	178	200	2	0	0	0
1	BU	137	1036	656	178	200	2	0	0	0
1	BV	137	1036	656	178	200	2	0	0	0
1	BW	137	1036	656	178	200	2	0	0	0
1	BX	137	1036	656	178	200	2	0	0	0
1	BY	137	1036	656	178	200	2	0	0	0
1	BZ	137	1036	656	178	200	2	0	0	0
1	CA	137	1036	656	178	200	2	0	0	0
1	CB	137	1036	656	178	200	2	0	0	0
1	CC	137	1036	656	178	200	2	0	0	0
1	CD	137	1036	656	178	200	2	0	0	0
1	CE	137	1036	656	178	200	2	0	0	0
1	CF	137	1036	656	178	200	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CG	137	Total	C	N	O	S	0	0	0
			1036	656	178	200	2			
1	CH	137	Total	C	N	O	S	0	0	0
			1036	656	178	200	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AF	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	AL	1	Total	Ca	0	0
			1	1		
2	AO	1	Total	Ca	0	0
			1	1		
2	AP	1	Total	Ca	0	0
			1	1		
2	AU	1	Total	Ca	0	0
			1	1		
2	AX	1	Total	Ca	0	0
			1	1		
2	BA	1	Total	Ca	0	0
			1	1		
2	BB	1	Total	Ca	0	0
			1	1		
2	BD	1	Total	Ca	0	0
			1	1		
2	BJ	1	Total	Ca	0	0
			1	1		
2	BM	1	Total	Ca	0	0
			1	1		
2	BN	1	Total	Ca	0	0
			1	1		
2	BP	1	Total	Ca	0	0
			1	1		
2	BV	1	Total	Ca	0	0
			1	1		
2	BY	1	Total	Ca	0	0
			1	1		

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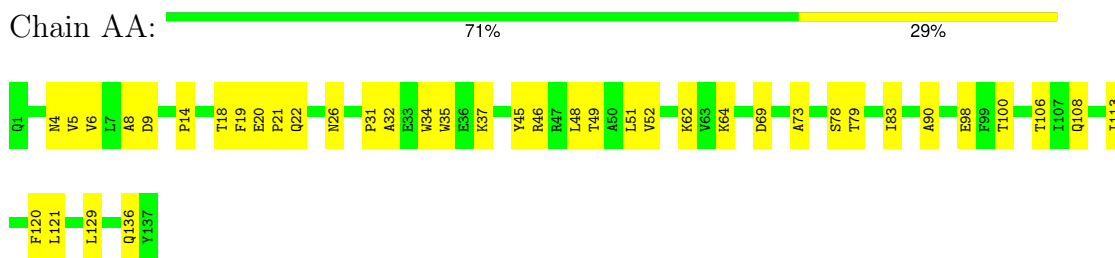
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BZ	1	Total 1	Ca 1	0	0
2	CC	1	Total 1	Ca 1	0	0
2	CH	1	Total 1	Ca 1	0	0

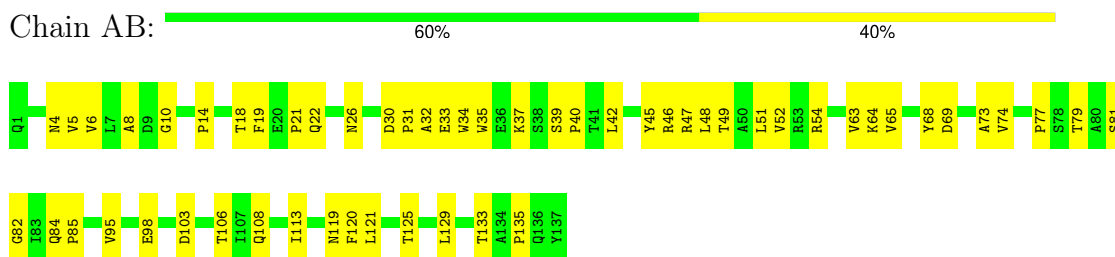
3 Residue-property plots [i](#)

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.

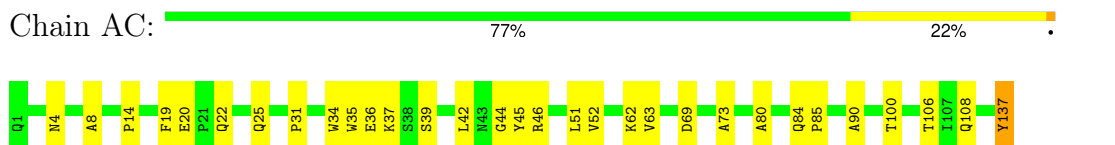
- Molecule 1: coat protein



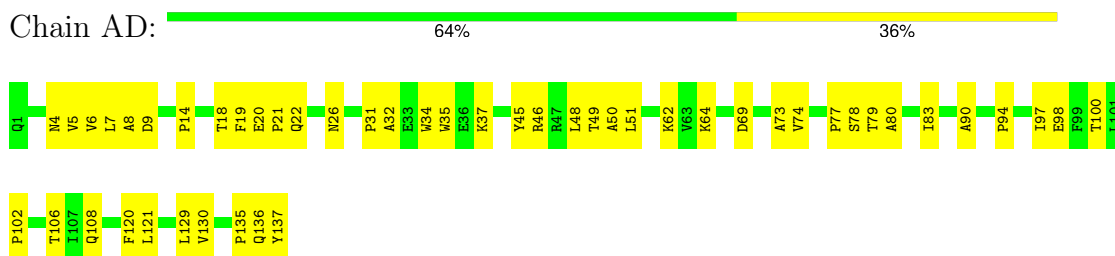
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



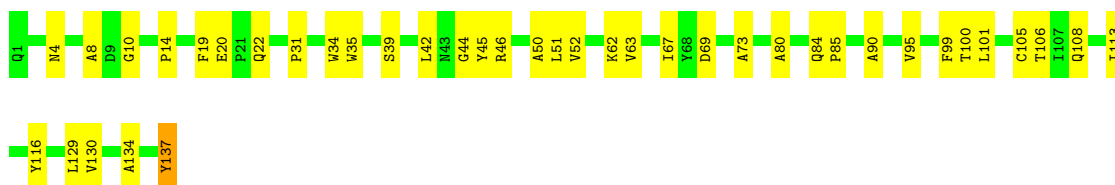
- Molecule 1: coat protein

Chain AE:  64% 36%




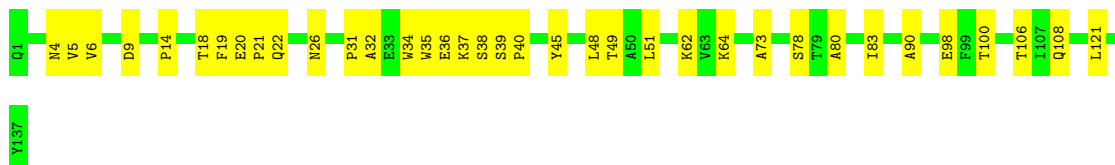
- Molecule 1: coat protein

Chain AF:  71% 28%



- Molecule 1: coat protein

Chain AG:  74% 26%



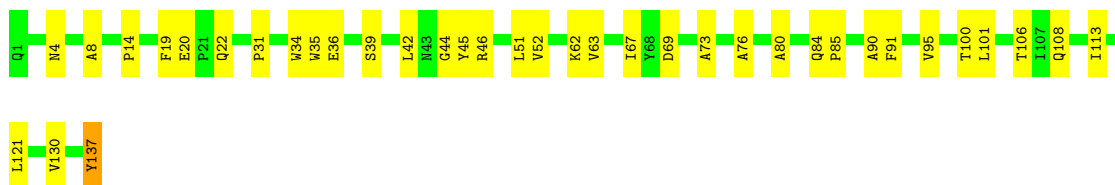
- Molecule 1: coat protein

Chain AH:  63% 37%

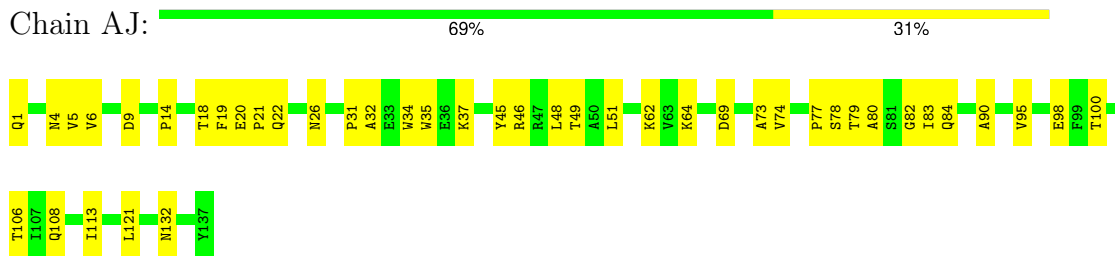


- Molecule 1: coat protein

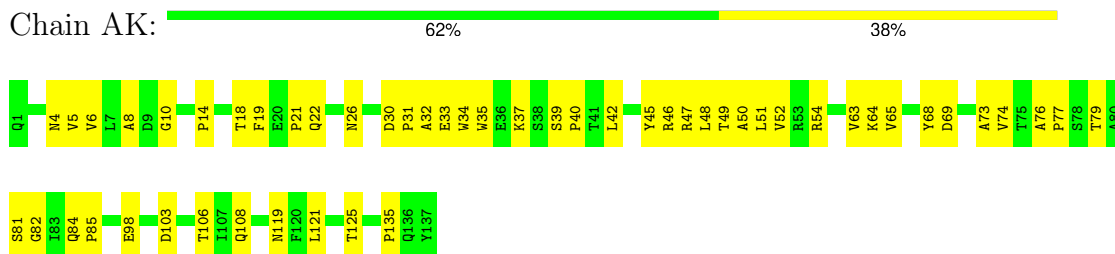
Chain AI:  73% 26%



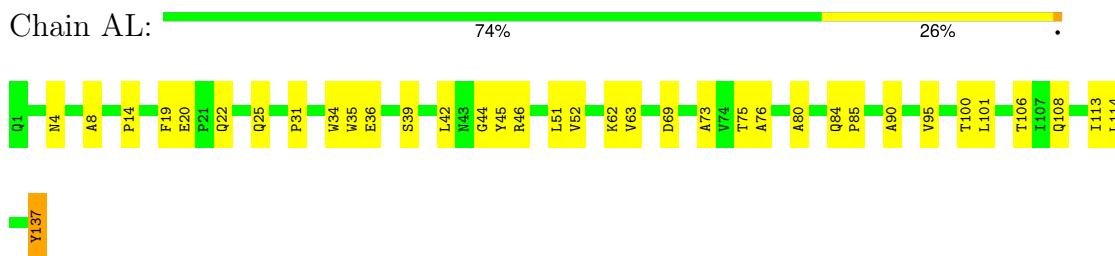
- Molecule 1: coat protein



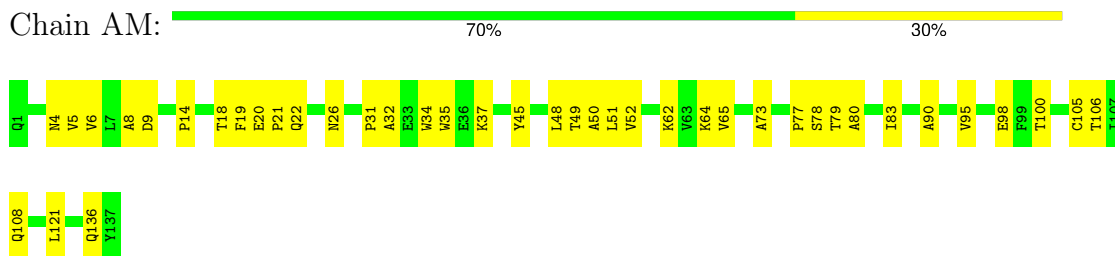
- Molecule 1: coat protein



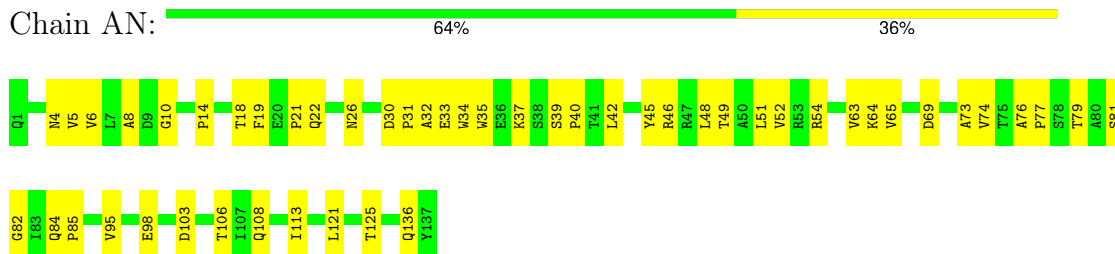
- Molecule 1: coat protein




- Molecule 1: coat protein



- Molecule 1: coat protein



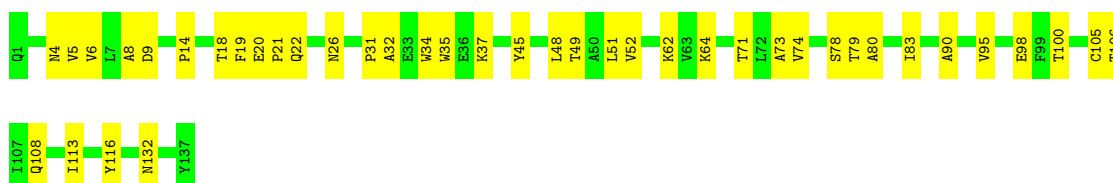
- Molecule 1: coat protein

Chain AO:  75% 24%



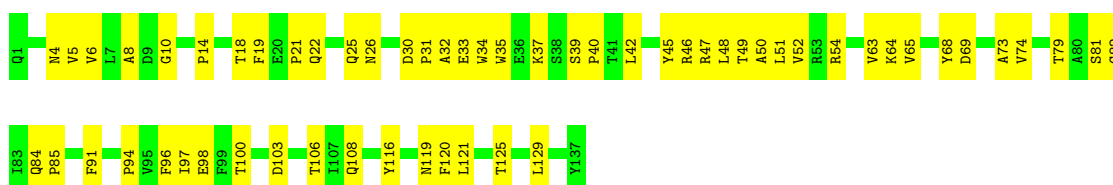
- Molecule 1: coat protein

Chain AP:  70% 30%



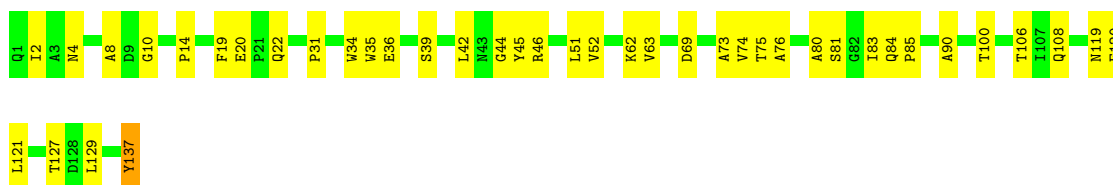
- Molecule 1: coat protein

Chain AQ:  58% 42%



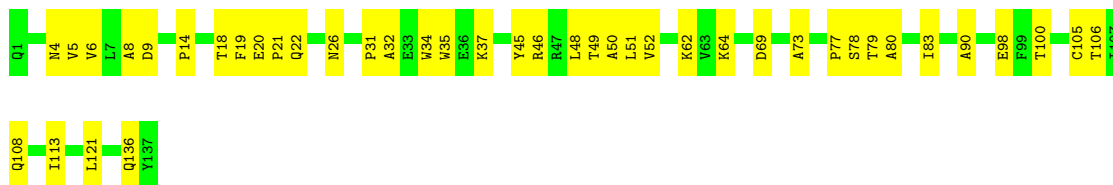
- Molecule 1: coat protein

Chain AR:  70% 29%



- Molecule 1: coat protein

Chain AS:  69% 31%

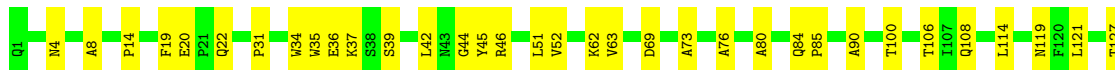


- Molecule 1: coat protein

Chain AT:  63% 37%



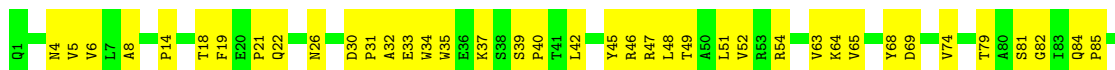
• Molecule 1: coat protein



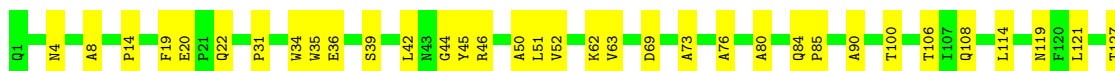
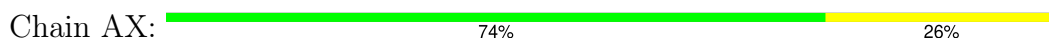
• Molecule 1: coat protein



• Molecule 1: coat protein

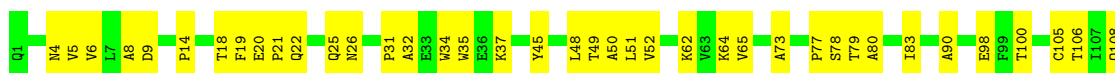


• Molecule 1: coat protein

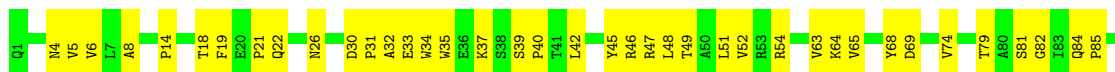


• Molecule 1: coat protein

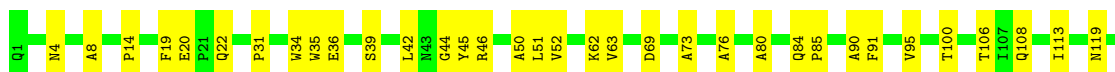




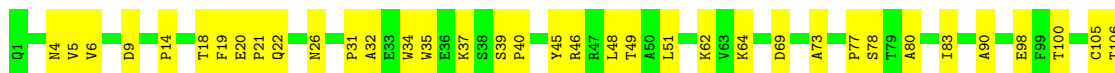
- Molecule 1: coat protein



- Molecule 1: coat protein



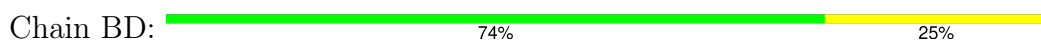
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

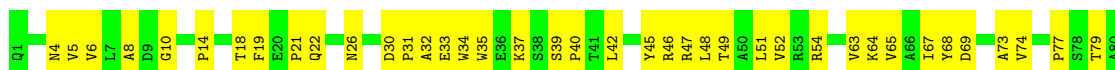




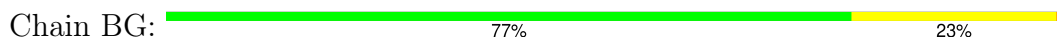
• Molecule 1: coat protein



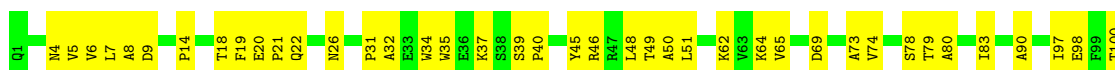
• Molecule 1: coat protein



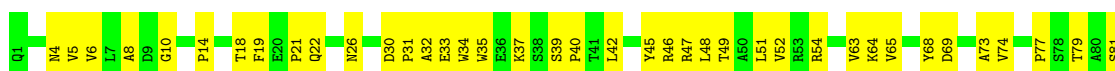
• Molecule 1: coat protein



• Molecule 1: coat protein



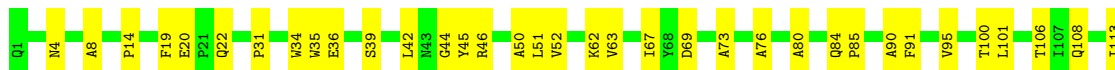
• Molecule 1: coat protein





- Molecule 1: coat protein

Chain BJ: 71% 28%



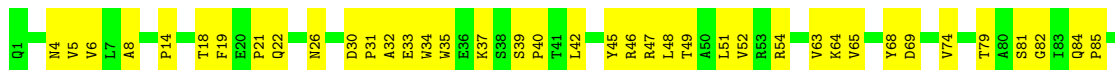
- Molecule 1: coat protein

Chain BK: 66% 34%



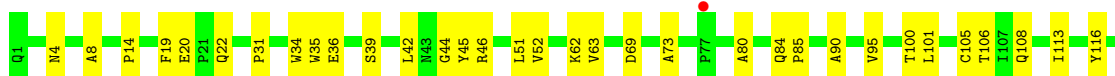
- Molecule 1: coat protein

Chain BL: 69% 31%



- Molecule 1: coat protein

Chain BM: 74% 26%

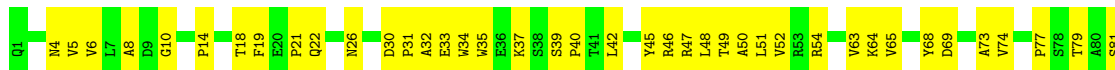


- Molecule 1: coat protein

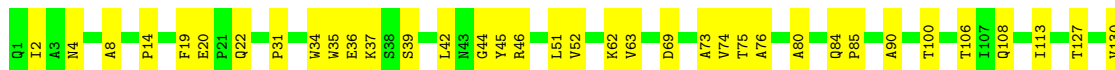
Chain BN: 74% 26%



- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein





Y137

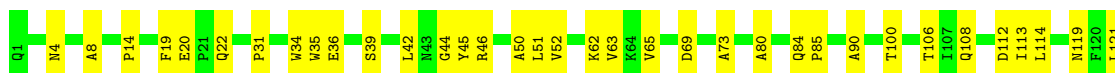
- Molecule 1: coat protein

T106
I107
Q108
I113
N132
Q136
Y137

- Molecule 1: coat protein

E98
D103
T106
I107
Q108
L121
Y137

- Molecule 1: coat protein



Y137

- Molecule 1: coat protein

Q108
I113
A117
L121
T125
Q136
Y137

- Molecule 1: coat protein

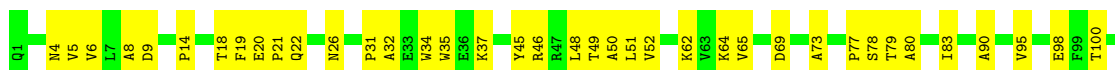




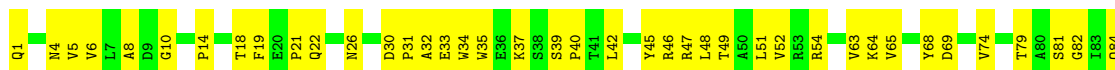
- Molecule 1: coat protein



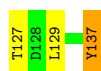
- Molecule 1: coat protein



- Molecule 1: coat protein

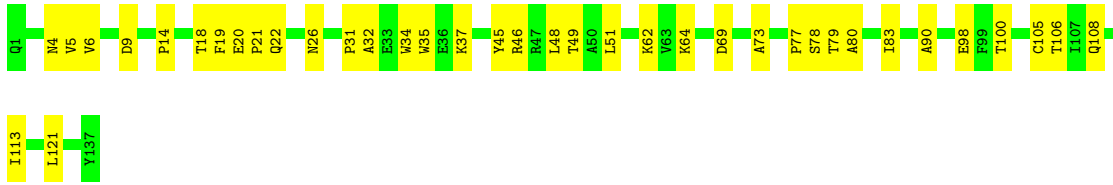


- Molecule 1: coat protein



- Molecule 1: coat protein





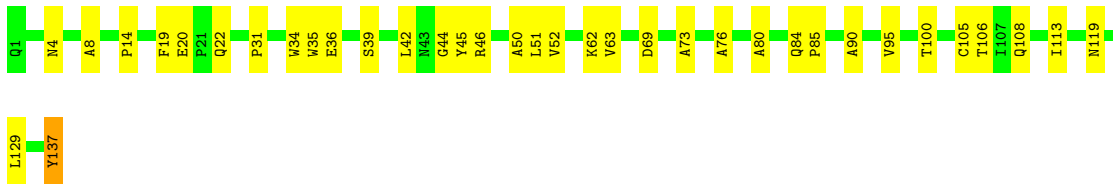
- Molecule 1: coat protein

Chain CD: 63% 37%



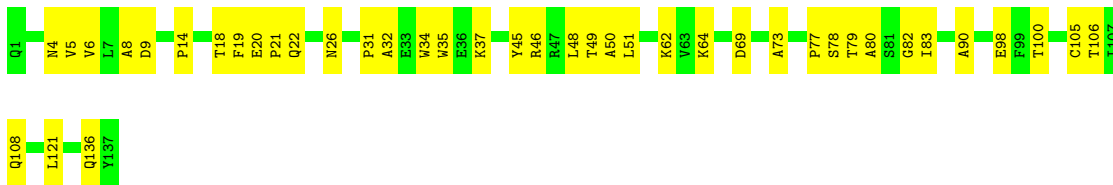
- Molecule 1: coat protein

Chain CE: 74% 26%



- Molecule 1: coat protein

Chain CF: 70% 30%



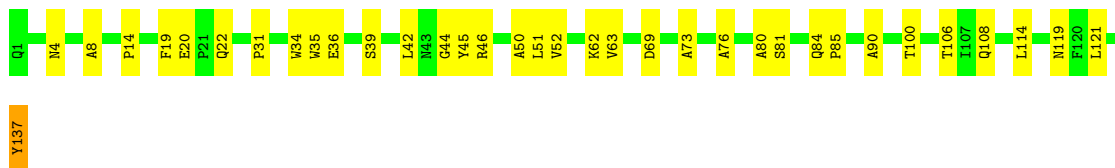
- Molecule 1: coat protein

Chain CG: 64% 36%



- Molecule 1: coat protein

Chain CH: 74% 25%



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	278.20Å 278.20Å 661.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.00 – 3.70 38.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	64.8 (38.00-3.70) 64.9 (38.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.14 3260	Depositor
R, R_{free}	0.235 , 0.237 0.238 , 0.240	Depositor DCC
R_{free} test set	5033 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.026 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.024 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.027 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l 0.024 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3* k-1/3*l 0.029 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k- 1/3*l,4/3*h-4/3*k-1/3*l 0.024 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3 *k-1/3*l 0.043 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	62180	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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	0.32	0/1059	0.53	0/1451
1	AB	0.34	0/1059	0.54	0/1451
1	AC	0.34	0/1059	0.55	0/1451
1	AD	0.33	0/1059	0.53	0/1451
1	AE	0.34	0/1059	0.54	0/1451
1	AF	0.34	0/1059	0.56	0/1451
1	AG	0.33	0/1059	0.53	0/1451
1	AH	0.34	0/1059	0.54	0/1451
1	AI	0.34	0/1059	0.56	0/1451
1	AJ	0.33	0/1059	0.54	0/1451
1	AK	0.34	0/1059	0.54	0/1451
1	AL	0.34	0/1059	0.56	0/1451
1	AM	0.33	0/1059	0.53	0/1451
1	AN	0.34	0/1059	0.54	0/1451
1	AO	0.34	0/1059	0.55	0/1451
1	AP	0.33	0/1059	0.54	0/1451
1	AQ	0.34	0/1059	0.54	0/1451
1	AR	0.34	0/1059	0.55	0/1451
1	AS	0.33	0/1059	0.54	0/1451
1	AT	0.34	0/1059	0.54	0/1451
1	AU	0.34	0/1059	0.55	0/1451
1	AV	0.32	0/1059	0.54	0/1451
1	AW	0.34	0/1059	0.54	0/1451
1	AX	0.34	0/1059	0.56	0/1451
1	AY	0.33	0/1059	0.53	0/1451
1	AZ	0.34	0/1059	0.54	0/1451
1	BA	0.34	0/1059	0.55	0/1451
1	BB	0.33	0/1059	0.53	0/1451
1	BC	0.34	0/1059	0.54	0/1451
1	BD	0.34	0/1059	0.56	0/1451
1	BE	0.33	0/1059	0.53	0/1451
1	BF	0.34	0/1059	0.54	0/1451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BG	0.34	0/1059	0.55	0/1451
1	BH	0.33	0/1059	0.54	0/1451
1	BI	0.34	0/1059	0.54	0/1451
1	BJ	0.34	0/1059	0.56	0/1451
1	BK	0.33	0/1059	0.53	0/1451
1	BL	0.34	0/1059	0.54	0/1451
1	BM	0.34	0/1059	0.55	0/1451
1	BN	0.33	0/1059	0.53	0/1451
1	BO	0.34	0/1059	0.54	0/1451
1	BP	0.34	0/1059	0.56	0/1451
1	BQ	0.33	0/1059	0.54	0/1451
1	BR	0.34	0/1059	0.54	0/1451
1	BS	0.34	0/1059	0.56	0/1451
1	BT	0.33	0/1059	0.53	0/1451
1	BU	0.34	0/1059	0.54	0/1451
1	BV	0.34	0/1059	0.56	0/1451
1	BW	0.33	0/1059	0.54	0/1451
1	BX	0.34	0/1059	0.54	0/1451
1	BY	0.34	0/1059	0.55	0/1451
1	BZ	0.33	0/1059	0.53	0/1451
1	CA	0.34	0/1059	0.54	0/1451
1	CB	0.34	0/1059	0.55	0/1451
1	CC	0.32	0/1059	0.53	0/1451
1	CD	0.34	0/1059	0.54	0/1451
1	CE	0.34	0/1059	0.55	0/1451
1	CF	0.32	0/1059	0.54	0/1451
1	CG	0.34	0/1059	0.54	0/1451
1	CH	0.34	0/1059	0.55	0/1451
All	All	0.34	0/63540	0.54	0/87060

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	1036	0	1040	31	0
1	AB	1036	0	1040	44	0
1	AC	1036	0	1040	20	0
1	AD	1036	0	1040	53	0
1	AE	1036	0	1040	41	0
1	AF	1036	0	1040	33	0
1	AG	1036	0	1040	22	0
1	AH	1036	0	1040	39	0
1	AI	1036	0	1040	32	0
1	AJ	1036	0	1040	33	0
1	AK	1036	0	1040	46	0
1	AL	1036	0	1040	29	0
1	AM	1036	0	1040	32	0
1	AN	1036	0	1040	41	0
1	AO	1036	0	1040	28	0
1	AP	1036	0	1040	32	0
1	AQ	1036	0	1040	58	0
1	AR	1036	0	1040	40	0
1	AS	1036	0	1040	32	0
1	AT	1036	0	1040	42	0
1	AU	1036	0	1040	29	0
1	AV	1036	0	1040	34	0
1	AW	1036	0	1040	31	0
1	AX	1036	0	1040	30	0
1	AY	1036	0	1040	39	0
1	AZ	1036	0	1040	33	0
1	BA	1036	0	1040	30	0
1	BB	1036	0	1040	25	0
1	BC	1036	0	1040	45	0
1	BD	1036	0	1040	30	0
1	BE	1036	0	1040	31	0
1	BF	1036	0	1040	45	0
1	BG	1036	0	1040	23	0
1	BH	1036	0	1040	46	0
1	BI	1036	0	1040	42	0
1	BJ	1036	0	1040	39	0
1	BK	1036	0	1040	41	0
1	BL	1036	0	1040	33	0
1	BM	1036	0	1040	29	0
1	BN	1036	0	1040	23	0
1	BO	1036	0	1040	43	0
1	BP	1036	0	1040	28	0
1	BQ	1036	0	1040	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BR	1036	0	1040	39	0
1	BS	1036	0	1040	31	0
1	BT	1036	0	1040	34	0
1	BU	1036	0	1040	32	0
1	BV	1036	0	1040	29	0
1	BW	1036	0	1040	35	0
1	BX	1036	0	1040	40	0
1	BY	1036	0	1040	30	0
1	BZ	1036	0	1040	34	0
1	CA	1036	0	1040	56	0
1	CB	1036	0	1040	34	0
1	CC	1036	0	1040	26	0
1	CD	1036	0	1040	40	0
1	CE	1036	0	1040	32	0
1	CF	1036	0	1040	33	0
1	CG	1036	0	1040	40	0
1	CH	1036	0	1040	29	0
2	AF	1	0	0	0	0
2	AG	1	0	0	0	0
2	AJ	1	0	0	0	0
2	AL	1	0	0	0	0
2	AO	1	0	0	0	0
2	AP	1	0	0	0	0
2	AU	1	0	0	0	0
2	AX	1	0	0	0	0
2	BA	1	0	0	0	0
2	BB	1	0	0	0	0
2	BD	1	0	0	0	0
2	BJ	1	0	0	0	0
2	BM	1	0	0	0	0
2	BN	1	0	0	0	0
2	BP	1	0	0	0	0
2	BV	1	0	0	0	0
2	BY	1	0	0	0	0
2	BZ	1	0	0	0	0
2	CC	1	0	0	0	0
2	CH	1	0	0	0	0
All	All	62180	0	62400	1676	0

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

The worst 5 of 1676 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:AD:79:THR:HB	1:AR:80:ALA:HA	1.19	1.16
1:BY:80:ALA:HA	1:CF:79:THR:HB	1.33	1.11
1:BE:79:THR:HB	1:CH:80:ALA:HA	1.31	1.10
1:BH:79:THR:HB	1:CB:80:ALA:HA	1.15	1.09
1:AY:79:THR:HB	1:BD:80:ALA:HA	1.37	1.07

There are no symmetry-related clashes.

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	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AB	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AC	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AD	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AE	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AF	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AG	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AH	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AI	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AJ	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AK	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AL	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AM	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AN	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AO	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AP	135/137 (98%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AQ	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AR	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AS	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AT	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AU	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AV	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AW	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AX	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	AY	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	AZ	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BA	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BB	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BC	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BD	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BE	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BF	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BG	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BH	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BI	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BJ	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BK	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BL	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BM	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BN	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BO	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BP	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BQ	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BR	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BS	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BT	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BU	135/137 (98%)	132 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BV	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BW	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BX	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	BY	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	BZ	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CA	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CB	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	CC	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CD	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CE	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	CF	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CG	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
1	CH	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
All	All	8100/8220 (98%)	7940 (98%)	160 (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	111/111 (100%)	111 (100%)	0	100	100
1	AB	111/111 (100%)	111 (100%)	0	100	100
1	AC	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AD	111/111 (100%)	111 (100%)	0	100	100
1	AE	111/111 (100%)	111 (100%)	0	100	100
1	AF	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AG	111/111 (100%)	111 (100%)	0	100	100
1	AH	111/111 (100%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AI	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AJ	111/111 (100%)	111 (100%)	0	100	100
1	AK	111/111 (100%)	111 (100%)	0	100	100
1	AL	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AM	111/111 (100%)	111 (100%)	0	100	100
1	AN	111/111 (100%)	111 (100%)	0	100	100
1	AO	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AP	111/111 (100%)	111 (100%)	0	100	100
1	AQ	111/111 (100%)	111 (100%)	0	100	100
1	AR	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AS	111/111 (100%)	111 (100%)	0	100	100
1	AT	111/111 (100%)	111 (100%)	0	100	100
1	AU	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AV	111/111 (100%)	111 (100%)	0	100	100
1	AW	111/111 (100%)	111 (100%)	0	100	100
1	AX	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	AY	111/111 (100%)	111 (100%)	0	100	100
1	AZ	111/111 (100%)	111 (100%)	0	100	100
1	BA	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BB	111/111 (100%)	111 (100%)	0	100	100
1	BC	111/111 (100%)	111 (100%)	0	100	100
1	BD	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BE	111/111 (100%)	111 (100%)	0	100	100
1	BF	111/111 (100%)	111 (100%)	0	100	100
1	BG	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BH	111/111 (100%)	111 (100%)	0	100	100
1	BI	111/111 (100%)	111 (100%)	0	100	100
1	BJ	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BK	111/111 (100%)	111 (100%)	0	100	100
1	BL	111/111 (100%)	111 (100%)	0	100	100
1	BM	111/111 (100%)	110 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BN	111/111 (100%)	111 (100%)	0	100	100
1	BO	111/111 (100%)	111 (100%)	0	100	100
1	BP	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BQ	111/111 (100%)	111 (100%)	0	100	100
1	BR	111/111 (100%)	111 (100%)	0	100	100
1	BS	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BT	111/111 (100%)	111 (100%)	0	100	100
1	BU	111/111 (100%)	111 (100%)	0	100	100
1	BV	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BW	111/111 (100%)	111 (100%)	0	100	100
1	BX	111/111 (100%)	111 (100%)	0	100	100
1	BY	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	BZ	111/111 (100%)	111 (100%)	0	100	100
1	CA	111/111 (100%)	111 (100%)	0	100	100
1	CB	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	CC	111/111 (100%)	111 (100%)	0	100	100
1	CD	111/111 (100%)	111 (100%)	0	100	100
1	CE	111/111 (100%)	110 (99%)	1 (1%)	78	88
1	CF	111/111 (100%)	111 (100%)	0	100	100
1	CG	111/111 (100%)	111 (100%)	0	100	100
1	CH	111/111 (100%)	110 (99%)	1 (1%)	78	88
All	All	6660/6660 (100%)	6640 (100%)	20 (0%)	92	96

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BS	137	TYR
1	CB	137	TYR
1	CH	137	TYR
1	CE	137	TYR
1	AU	137	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	BJ	119	ASN
1	BR	136	GLN
1	BK	1	GLN
1	BO	55	ASN
1	BW	1	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](#)

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 [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	137/137 (100%)	-0.60	0	100	100	58, 84, 108, 123	0
1	AB	137/137 (100%)	-0.58	0	100	100	57, 83, 104, 118	0
1	AC	137/137 (100%)	-0.39	0	100	100	56, 85, 114, 137	0
1	AD	137/137 (100%)	-0.56	0	100	100	58, 84, 108, 123	0
1	AE	137/137 (100%)	-0.55	0	100	100	57, 83, 104, 118	0
1	AF	137/137 (100%)	-0.47	0	100	100	56, 85, 114, 137	0
1	AG	137/137 (100%)	-0.58	0	100	100	58, 84, 108, 123	0
1	AH	137/137 (100%)	-0.59	0	100	100	57, 83, 104, 118	0
1	AI	137/137 (100%)	-0.55	0	100	100	56, 85, 114, 137	0
1	AJ	137/137 (100%)	-0.60	0	100	100	58, 84, 108, 123	0
1	AK	137/137 (100%)	-0.58	0	100	100	57, 83, 104, 118	0
1	AL	137/137 (100%)	-0.60	0	100	100	56, 85, 114, 137	0
1	AM	137/137 (100%)	-0.63	0	100	100	58, 84, 108, 123	0
1	AN	137/137 (100%)	-0.62	0	100	100	57, 83, 104, 118	0
1	AO	137/137 (100%)	-0.53	0	100	100	56, 85, 114, 137	0
1	AP	137/137 (100%)	-0.69	0	100	100	58, 84, 108, 123	0
1	AQ	137/137 (100%)	-0.62	0	100	100	57, 83, 104, 118	0
1	AR	137/137 (100%)	-0.44	0	100	100	56, 85, 114, 137	0
1	AS	137/137 (100%)	-0.63	0	100	100	58, 84, 108, 123	0
1	AT	137/137 (100%)	-0.62	0	100	100	57, 83, 104, 118	0
1	AU	137/137 (100%)	-0.61	0	100	100	56, 85, 114, 137	0
1	AV	137/137 (100%)	-0.62	0	100	100	58, 84, 108, 123	0
1	AW	137/137 (100%)	-0.53	0	100	100	57, 83, 104, 118	0
1	AX	137/137 (100%)	-0.57	0	100	100	56, 85, 114, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AY	137/137 (100%)	-0.64	0 100 100	58, 84, 108, 123	0
1	AZ	137/137 (100%)	-0.56	0 100 100	57, 83, 104, 118	0
1	BA	137/137 (100%)	-0.45	0 100 100	56, 85, 114, 137	0
1	BB	137/137 (100%)	-0.63	0 100 100	58, 84, 108, 123	0
1	BC	137/137 (100%)	-0.59	0 100 100	57, 83, 104, 118	0
1	BD	137/137 (100%)	-0.54	0 100 100	56, 85, 114, 137	0
1	BE	137/137 (100%)	-0.61	0 100 100	58, 84, 108, 123	0
1	BF	137/137 (100%)	-0.63	0 100 100	57, 83, 104, 118	0
1	BG	137/137 (100%)	-0.64	0 100 100	56, 85, 114, 137	0
1	BH	137/137 (100%)	-0.61	0 100 100	58, 84, 108, 123	0
1	BI	137/137 (100%)	-0.66	0 100 100	57, 83, 104, 118	0
1	BJ	137/137 (100%)	-0.49	0 100 100	56, 85, 114, 137	0
1	BK	137/137 (100%)	-0.57	1 (0%) 87 81	58, 84, 108, 123	0
1	BL	137/137 (100%)	-0.68	0 100 100	57, 83, 104, 118	0
1	BM	137/137 (100%)	-0.57	1 (0%) 87 81	56, 85, 114, 137	0
1	BN	137/137 (100%)	-0.54	0 100 100	58, 84, 108, 123	0
1	BO	137/137 (100%)	-0.60	0 100 100	57, 83, 104, 118	0
1	BP	137/137 (100%)	-0.55	0 100 100	56, 85, 114, 137	0
1	BQ	137/137 (100%)	-0.59	0 100 100	58, 84, 108, 123	0
1	BR	137/137 (100%)	-0.69	0 100 100	57, 83, 104, 118	0
1	BS	137/137 (100%)	-0.57	0 100 100	56, 85, 114, 137	0
1	BT	137/137 (100%)	-0.58	0 100 100	58, 84, 108, 123	0
1	BU	137/137 (100%)	-0.63	0 100 100	57, 83, 104, 118	0
1	BV	137/137 (100%)	-0.56	0 100 100	56, 85, 114, 137	0
1	BW	137/137 (100%)	-0.70	0 100 100	58, 84, 108, 123	0
1	BX	137/137 (100%)	-0.62	0 100 100	57, 83, 104, 118	0
1	BY	137/137 (100%)	-0.53	0 100 100	56, 85, 114, 137	0
1	BZ	137/137 (100%)	-0.57	0 100 100	58, 84, 108, 123	0
1	CA	137/137 (100%)	-0.67	0 100 100	57, 83, 104, 118	0
1	CB	137/137 (100%)	-0.55	0 100 100	56, 85, 114, 137	0
1	CC	137/137 (100%)	-0.56	0 100 100	58, 84, 108, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	CD	137/137 (100%)	-0.64	0 100 100	57, 83, 104, 118	0
1	CE	137/137 (100%)	-0.59	0 100 100	56, 85, 114, 137	0
1	CF	137/137 (100%)	-0.53	0 100 100	58, 84, 108, 123	0
1	CG	137/137 (100%)	-0.60	0 100 100	57, 83, 104, 118	0
1	CH	137/137 (100%)	-0.57	0 100 100	56, 85, 114, 137	0
All	All	8220/8220 (100%)	-0.58	2 (0%) 100 100	56, 84, 108, 137	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BK	12	ALA	2.5
1	BM	77	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	BP	201	1/1	0.82	0.21	51,51,51,51	0
2	CA	AG	201	1/1	0.87	0.14	51,51,51,51	0
2	CA	BV	201	1/1	0.90	0.14	51,51,51,51	0
2	CA	BB	201	1/1	0.92	0.12	51,51,51,51	0
2	CA	AP	201	1/1	0.93	0.26	51,51,51,51	0
2	CA	BY	201	1/1	0.94	0.26	51,51,51,51	0
2	CA	AL	201	1/1	0.95	0.24	51,51,51,51	0
2	CA	BZ	201	1/1	0.95	0.17	51,51,51,51	0
2	CA	BD	201	1/1	0.96	0.29	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	BN	201	1/1	0.96	0.20	51,51,51,51	0
2	CA	CC	201	1/1	0.96	0.25	51,51,51,51	0
2	CA	AU	201	1/1	0.97	0.20	51,51,51,51	0
2	CA	BJ	201	1/1	0.97	0.18	51,51,51,51	0
2	CA	AJ	201	1/1	0.98	0.24	51,51,51,51	0
2	CA	AO	201	1/1	0.98	0.17	51,51,51,51	0
2	CA	AX	201	1/1	0.98	0.24	51,51,51,51	0
2	CA	BM	201	1/1	0.98	0.15	51,51,51,51	0
2	CA	BA	201	1/1	0.98	0.18	51,51,51,51	0
2	CA	CH	201	1/1	0.98	0.19	51,51,51,51	0
2	CA	AF	201	1/1	0.99	0.26	51,51,51,51	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.