



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 11:01 PM EDT

PDB ID : 6YFN
Title : Virus-like particle of bacteriophage ESE058
Authors : Rumnieks, J.; Kalnins, G.; Sisovs, M.; Lieknina, I.; Tars, K.
Deposited on : 2020-03-26
Resolution : 3.19 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

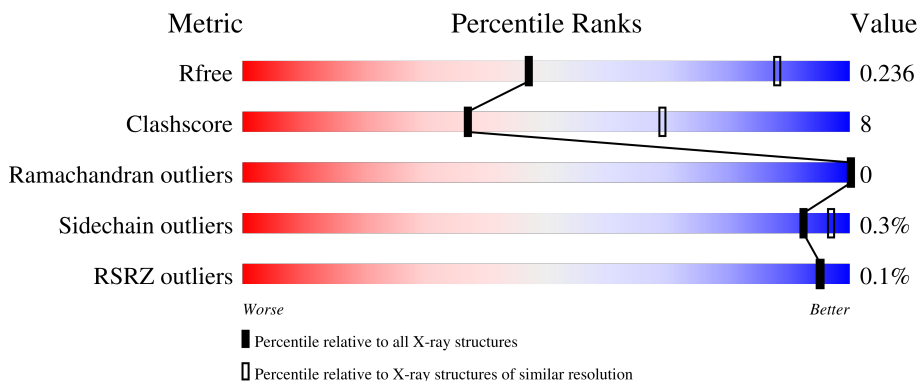
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	 75% 21%
1	AB	146	 84% 16%
1	AC	146	 77% 23%
1	AD	146	 73% 23%
1	AE	146	 75% 25%


























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Mol	Chain	Length	Quality of chain
1	AF	146	73% 27%
1	AG	146	77% 20% .
1	AH	146	84% 16%
1	AI	146	79% 21%
1	AJ	146	77% 20% .
1	AK	146	84% 16%
1	AL	146	78% 22%
1	AM	146	75% 22% .
1	AN	146	84% 16%
1	AO	146	75% 25%
1	AP	146	73% 23% .
1	AQ	146	84% 16%
1	AR	146	80% 20%
1	AS	146	71% 26% .
1	AT	146	82% 18%
1	AU	146	73% 27%
1	AV	146	% 77% 20% .
1	AW	146	85% 15%
1	AX	146	% 79% 21%
1	AY	146	% 74% 23% .
1	AZ	146	82% 18%
1	BA	146	77% 23%
1	BB	146	75% 22% .
1	BC	146	86% 14%
1	BD	146	77% 23%

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Mol	Chain	Length	Quality of chain
1	BE	146	 73% 23%
1	BF	146	 84% 16%
1	BG	146	 % 76% 24%
1	BH	146	 % 77% 20%
1	BI	146	 85% 15%
1	BJ	146	 78% 22%
1	BK	146	 75% 22%
1	BL	146	 83% 17%
1	BM	146	 73% 27%
1	BN	146	 76% 21%
1	BO	146	 84% 16%
1	BP	146	 77% 23%
1	BQ	146	 % 76% 21%
1	BR	146	 84% 16%
1	BS	146	 76% 24%
1	BT	146	 75% 22%
1	BU	146	 84% 16%
1	BV	146	 76% 24%
1	BW	146	 % 74% 23%
1	BX	146	 84% 16%
1	BY	146	 74% 26%
1	BZ	146	 68% 29%
1	CA	146	 81% 19%
1	CB	146	 76% 23%
1	CC	146	 76% 21%











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Mol	Chain	Length	Quality of chain
1	CD	146	81% 19%
1	CE	146	79% 21%
1	CF	146	73% 24% .
1	CG	146	83% 17%
1	CH	146	77% 23%
1	CI	146	79% 18% .
1	CJ	146	84% 16%
1	CK	146	75% 25%
1	CL	146	74% 23% .
1	CM	146	86% 14%
1	CN	146	75% 25%
1	CO	146	69% 27% .
1	CP	146	81% 19%
1	CQ	146	75% 24% .
1	CR	146	76% 21% .
1	CS	146	82% 18%
1	CT	146	76% 24%
1	CU	146	75% 21% .
1	CV	146	82% 18%
1	CW	146	77% 23%
1	CX	146	77% 20% .
1	CY	146	85% 15%
1	CZ	146	73% 27%
1	DA	146	75% 21% .
1	DB	146	82% 18%

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Mol	Chain	Length	Quality of chain	
1	DC	146		77% 23%
1	DD	146		76% 21% .
1	DE	146		82% 18%
1	DF	146		77% 23%
1	DG	146		72% 25% .
1	DH	146		84% 16%
1	DI	146		77% 23%
1	DJ	146		72% 25% .
1	DK	146		75% 25%
1	DL	146		73% 27%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 101490 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	141	1104	708	186	206	4	0	0	0
1	AB	146	1139	728	194	213	4	0	0	0
1	AC	146	1139	728	194	213	4	0	0	0
1	AD	141	1104	708	186	206	4	0	0	0
1	AE	146	1139	728	194	213	4	0	0	0
1	AF	146	1139	728	194	213	4	0	0	0
1	AG	141	1104	708	186	206	4	0	0	0
1	AH	146	1139	728	194	213	4	0	0	0
1	AI	146	1139	728	194	213	4	0	0	0
1	AJ	141	1104	708	186	206	4	0	0	0
1	AK	146	1139	728	194	213	4	0	0	0
1	AL	146	1139	728	194	213	4	0	0	0
1	AM	141	1104	708	186	206	4	0	0	0
1	AN	146	1139	728	194	213	4	0	0	0
1	AO	146	1139	728	194	213	4	0	0	0
1	AP	141	1104	708	186	206	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AQ	146	1139	728	194	213	4	0	0	0
1	AR	146	1139	728	194	213	4	0	0	0
1	AS	141	1104	708	186	206	4	0	0	0
1	AT	146	1139	728	194	213	4	0	0	0
1	AU	146	1139	728	194	213	4	0	0	0
1	AV	141	1104	708	186	206	4	0	0	0
1	AW	146	1139	728	194	213	4	0	0	0
1	AX	146	1139	728	194	213	4	0	0	0
1	AY	141	1104	708	186	206	4	0	0	0
1	AZ	146	1139	728	194	213	4	0	0	0
1	BA	146	1139	728	194	213	4	0	0	0
1	BB	141	1104	708	186	206	4	0	0	0
1	BC	146	1139	728	194	213	4	0	0	0
1	BD	146	1139	728	194	213	4	0	0	0
1	BE	141	1104	708	186	206	4	0	0	0
1	BF	146	1139	728	194	213	4	0	0	0
1	BG	146	1139	728	194	213	4	0	0	0
1	BH	141	1104	708	186	206	4	0	0	0
1	BI	146	1139	728	194	213	4	0	0	0
1	BJ	146	1139	728	194	213	4	0	0	0
1	BK	141	1104	708	186	206	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	BL	146	1139	728	194	213	4	0	0	0
1	BM	146	1139	728	194	213	4	0	0	0
1	BN	141	1104	708	186	206	4	0	0	0
1	BO	146	1139	728	194	213	4	0	0	0
1	BP	146	1139	728	194	213	4	0	0	0
1	BQ	141	1104	708	186	206	4	0	0	0
1	BR	146	1139	728	194	213	4	0	0	0
1	BS	146	1139	728	194	213	4	0	0	0
1	BT	141	1104	708	186	206	4	0	0	0
1	BU	146	1139	728	194	213	4	0	0	0
1	BV	146	1139	728	194	213	4	0	0	0
1	BW	141	1104	708	186	206	4	0	0	0
1	BX	146	1139	728	194	213	4	0	0	0
1	BY	146	1139	728	194	213	4	0	0	0
1	BZ	141	1104	708	186	206	4	0	0	0
1	CA	146	1139	728	194	213	4	0	0	0
1	CB	146	1139	728	194	213	4	0	0	0
1	CC	141	1104	708	186	206	4	0	0	0
1	CD	146	1139	728	194	213	4	0	0	0
1	CE	146	1139	728	194	213	4	0	0	0
1	CF	141	1104	708	186	206	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	CG	146	1139	728	194	213	4	0	0	0
1	CH	146	1139	728	194	213	4	0	0	0
1	CI	141	1104	708	186	206	4	0	0	0
1	CJ	146	1139	728	194	213	4	0	0	0
1	CK	146	1139	728	194	213	4	0	0	0
1	CL	141	1104	708	186	206	4	0	0	0
1	CM	146	1139	728	194	213	4	0	0	0
1	CN	146	1139	728	194	213	4	0	0	0
1	CO	141	1104	708	186	206	4	0	0	0
1	CP	146	1139	728	194	213	4	0	0	0
1	CQ	146	1139	728	194	213	4	0	0	0
1	CR	141	1104	708	186	206	4	0	0	0
1	CS	146	1139	728	194	213	4	0	0	0
1	CT	146	1139	728	194	213	4	0	0	0
1	CU	141	1104	708	186	206	4	0	0	0
1	CV	146	1139	728	194	213	4	0	0	0
1	CW	146	1139	728	194	213	4	0	0	0
1	CX	141	1104	708	186	206	4	0	0	0
1	CY	146	1139	728	194	213	4	0	0	0
1	CZ	146	1139	728	194	213	4	0	0	0
1	DA	141	1104	708	186	206	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DB	146	Total	C	N	O	S	0	0	0
			1139	728	194	213	4			
1	DC	146	Total	C	N	O	S	0	0	0
			1139	728	194	213	4			
1	DD	141	Total	C	N	O	S	0	0	0
			1104	708	186	206	4			
1	DE	146	Total	C	N	O	S	0	0	0
			1139	728	194	213	4			
1	DF	146	Total	C	N	O	S	0	0	0
			1139	728	194	213	4			
1	DG	141	Total	C	N	O	S	0	0	0
			1104	708	186	206	4			
1	DH	146	Total	C	N	O	S	0	0	0
			1139	728	194	213	4			
1	DI	146	Total	C	N	O	S	0	0	0
			1139	728	194	213	4			
1	DJ	141	Total	C	N	O	S	0	0	0
			1104	708	186	206	4			
1	DK	146	Total	C	N	O	S	0	0	0
			1139	728	194	213	4			
1	DL	146	Total	C	N	O	S	0	0	0
			1139	728	194	213	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	AC	2	Total	Ca	0	0
			2	2		
2	AF	2	Total	Ca	0	0
			2	2		
2	AI	1	Total	Ca	0	0
			1	1		
2	AL	1	Total	Ca	0	0
			1	1		
2	AO	2	Total	Ca	0	0
			2	2		
2	AR	1	Total	Ca	0	0
			1	1		
2	AU	2	Total	Ca	0	0
			2	2		
2	AX	1	Total	Ca	0	0
			1	1		

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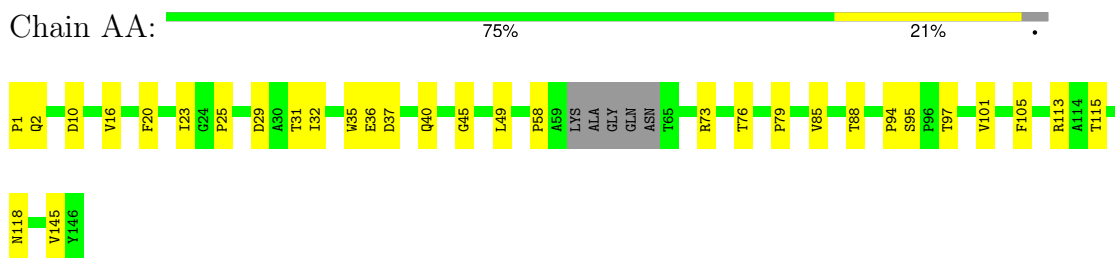
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BA	2	Total 2	Ca 2	0	0
2	BD	2	Total 2	Ca 2	0	0
2	BG	2	Total 2	Ca 2	0	0
2	BJ	1	Total 1	Ca 1	0	0
2	BM	2	Total 2	Ca 2	0	0
2	BP	2	Total 2	Ca 2	0	0
2	BS	2	Total 2	Ca 2	0	0
2	BV	2	Total 2	Ca 2	0	0
2	BY	2	Total 2	Ca 2	0	0
2	CE	1	Total 1	Ca 1	0	0

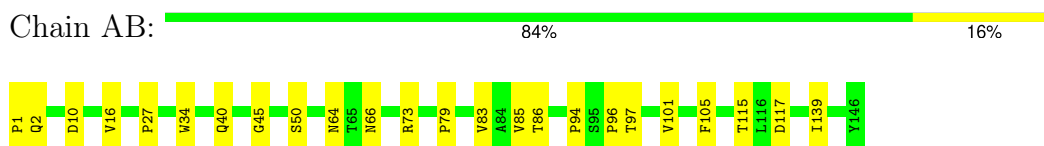
3 Residue-property plots [i](#)

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.

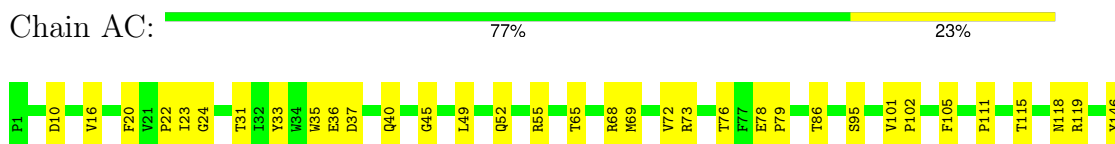
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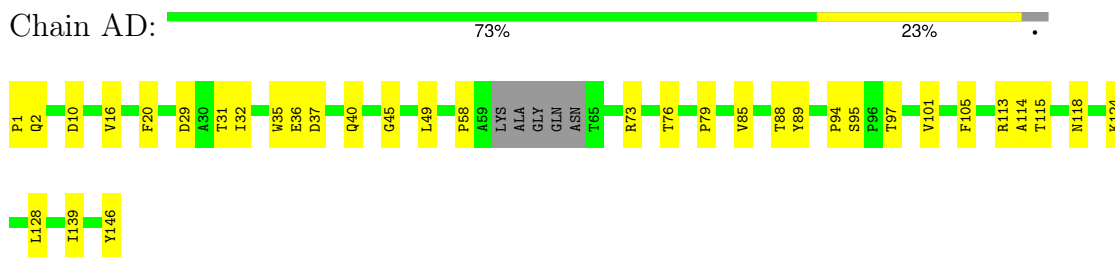
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein

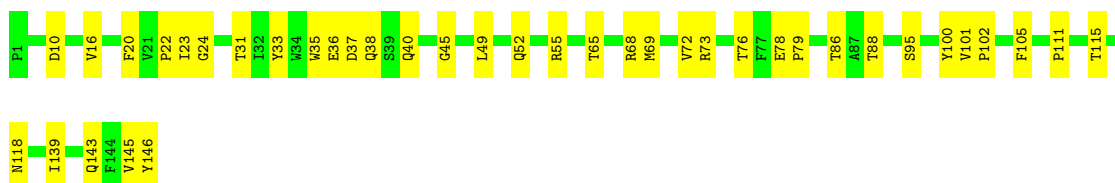


- Molecule 1: coat protein

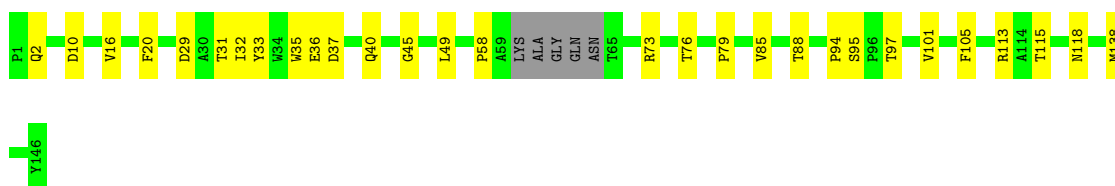
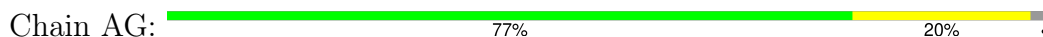




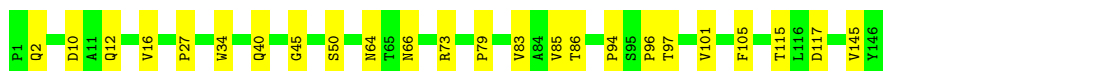
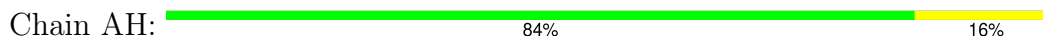
- Molecule 1: coat protein



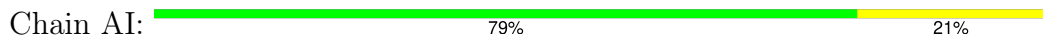
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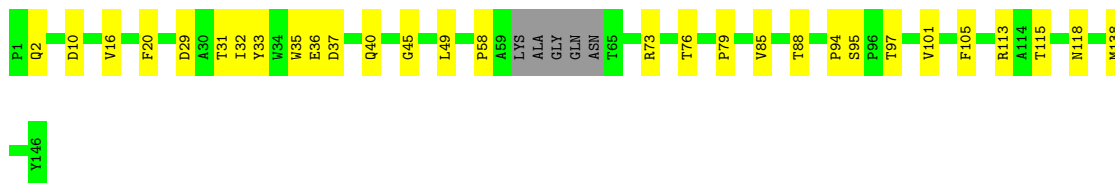
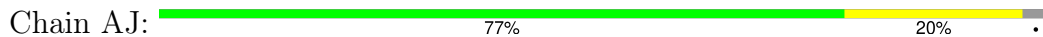
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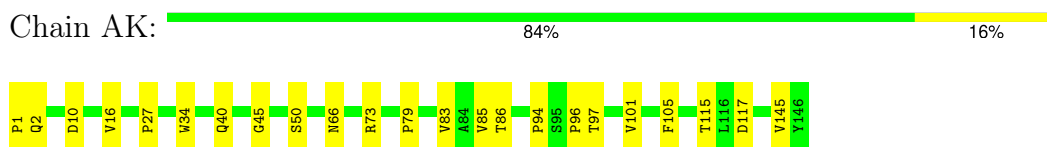
- Molecule 1: coat protein



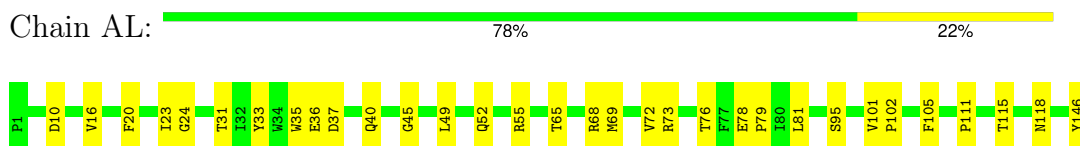
- Molecule 1: coat protein



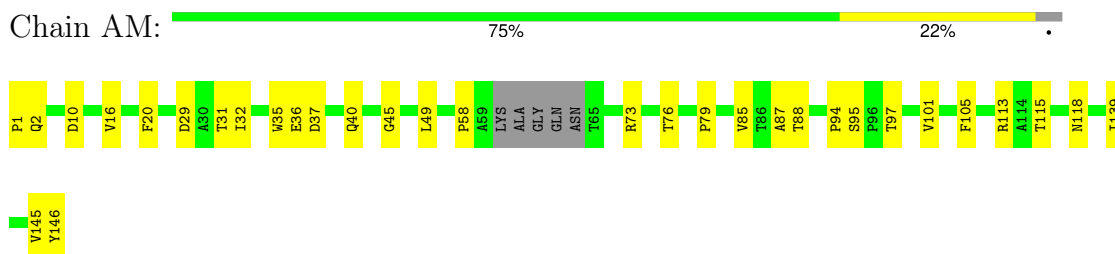
- Molecule 1: coat protein



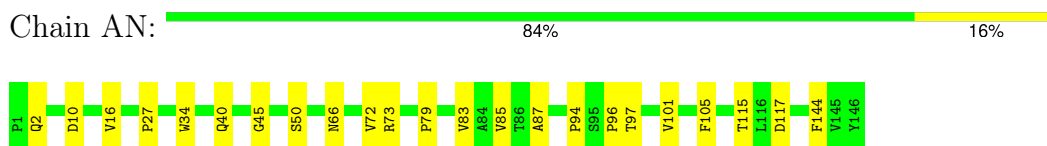
- Molecule 1: coat protein



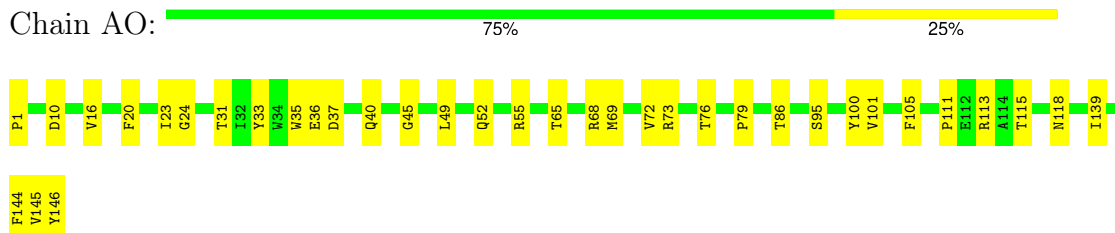
- Molecule 1: coat protein



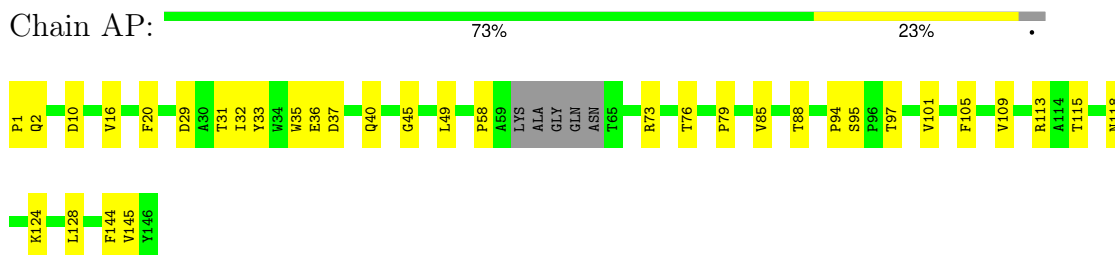
- Molecule 1: coat protein



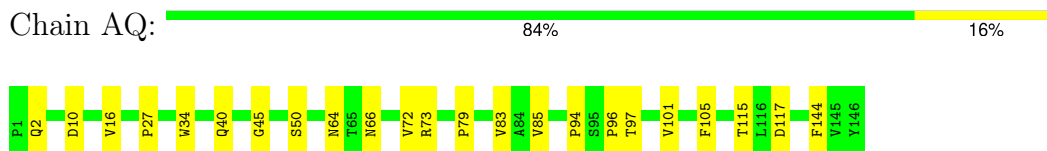
- Molecule 1: coat protein



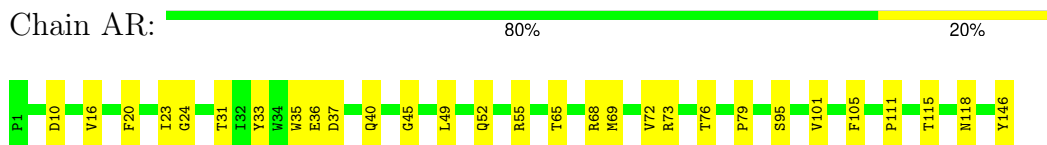
- Molecule 1: coat protein



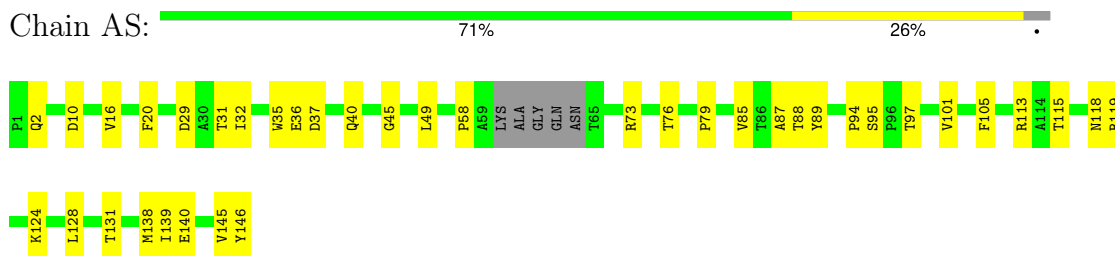
- Molecule 1: coat protein



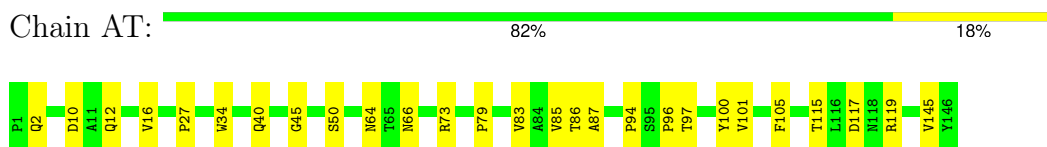
- Molecule 1: coat protein



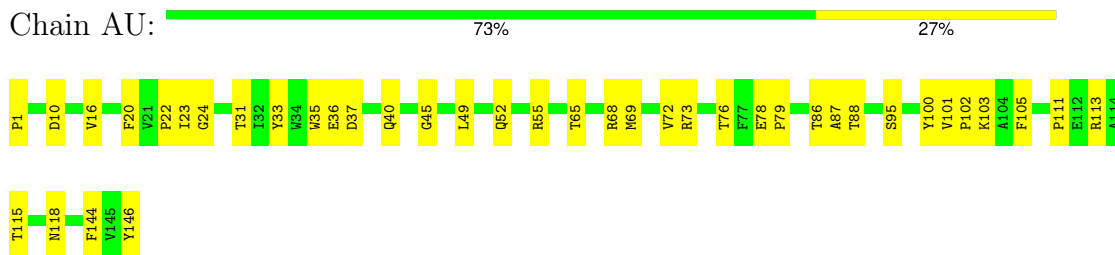
- Molecule 1: coat protein



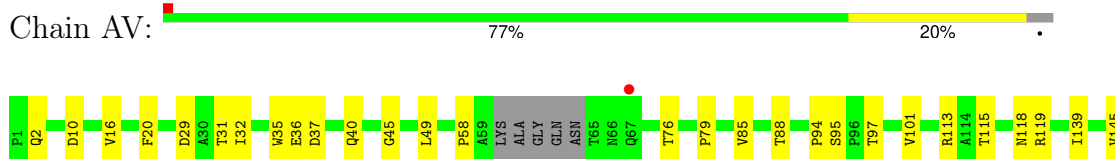
- Molecule 1: coat protein



- Molecule 1: coat protein




- Molecule 1: coat protein




Y146


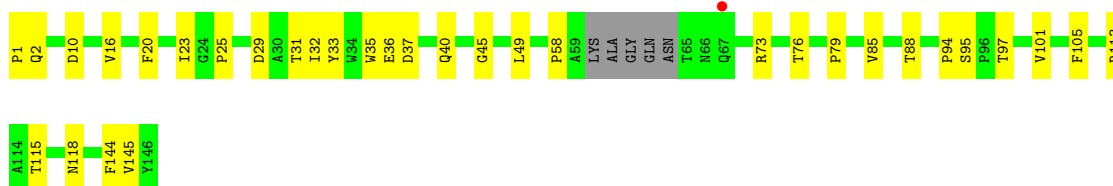
- Molecule 1: coat protein

Chain AW:  85% 15%


- Molecule 1: coat protein

Chain AX:  79% 21%


- Molecule 1: coat protein

Chain AY:  74% 23%


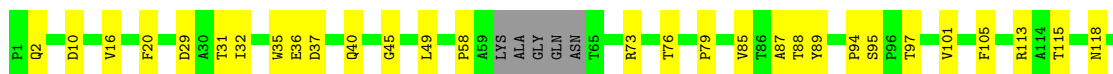
- Molecule 1: coat protein

Chain AZ:  82% 18%

- Molecule 1: coat protein

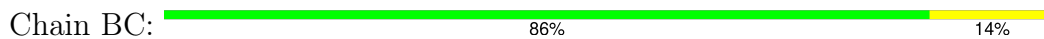
Chain BA:  77% 23%

- Molecule 1: coat protein

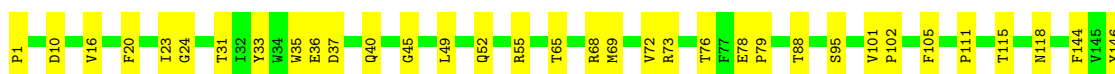
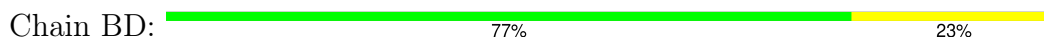
Chain BB:  75% 22%



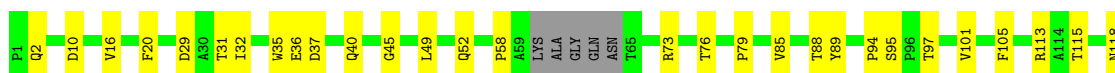
• Molecule 1: coat protein



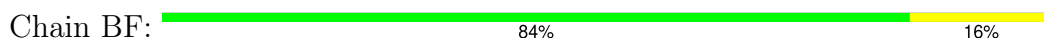
• Molecule 1: coat protein



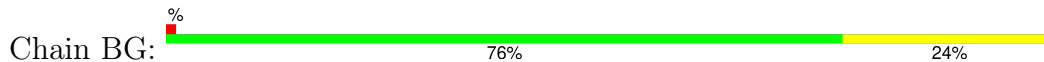
• Molecule 1: coat protein



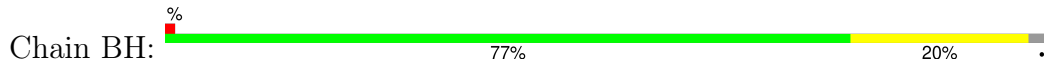
• Molecule 1: coat protein

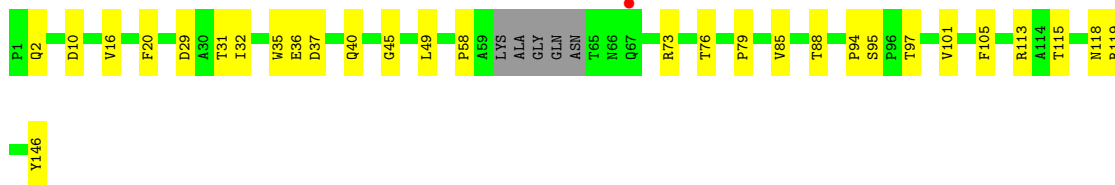


• Molecule 1: coat protein

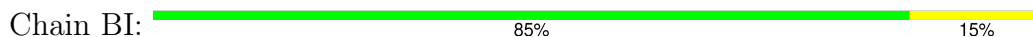


• Molecule 1: coat protein

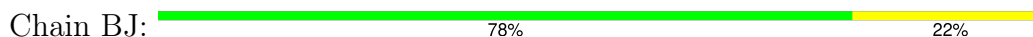




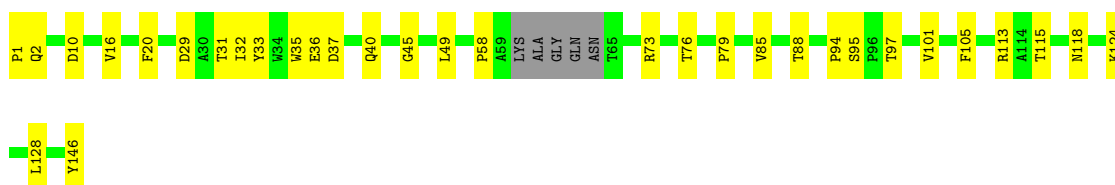
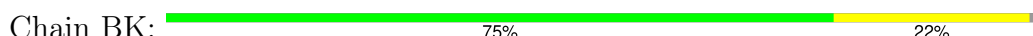
• Molecule 1: coat protein



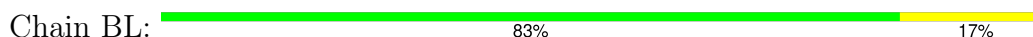
• Molecule 1: coat protein



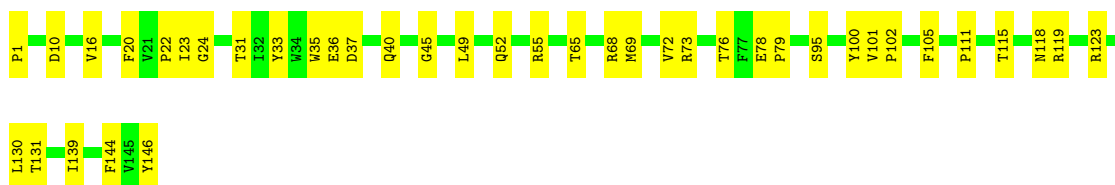
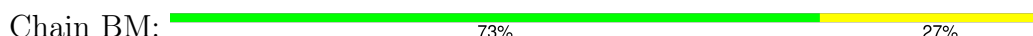
• Molecule 1: coat protein




• Molecule 1: coat protein

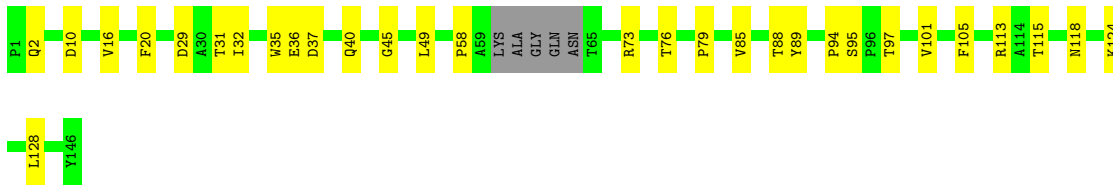


• Molecule 1: coat protein




• Molecule 1: coat protein

Chain BN:  76% 21%




- Molecule 1: coat protein

Chain BO:  84% 16%




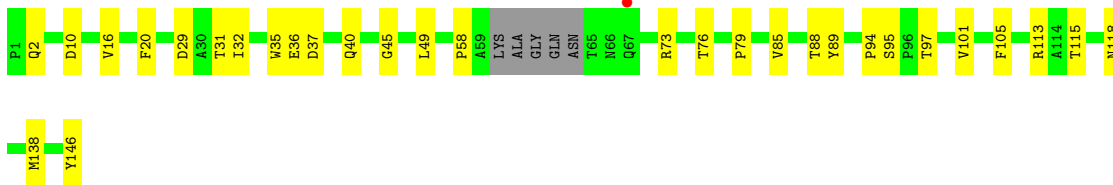
- Molecule 1: coat protein

Chain BP:  77% 23%




- Molecule 1: coat protein

Chain BQ:  76% 21%




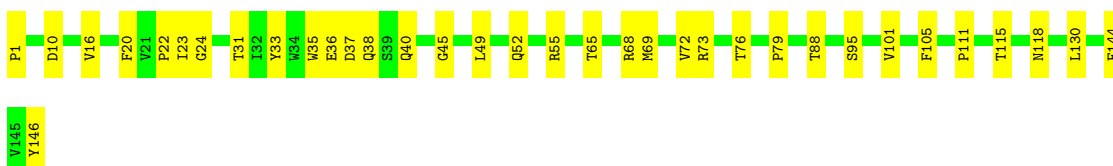
- Molecule 1: coat protein

Chain BR:  84% 16%

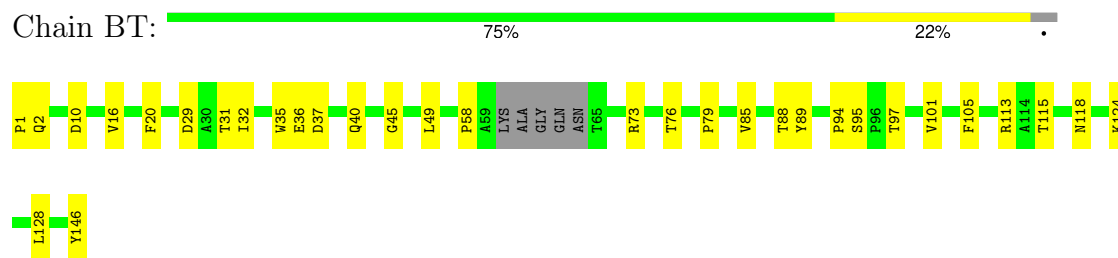


- Molecule 1: coat protein

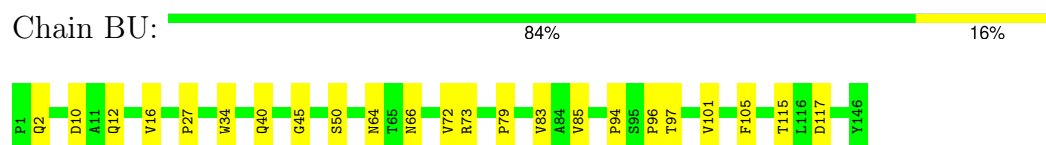
Chain BS:  76% 24%



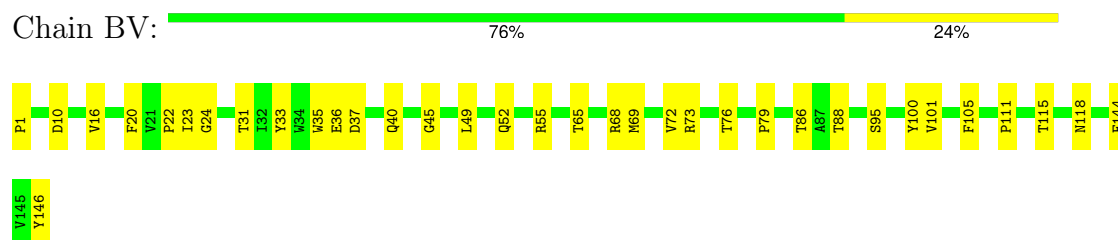
- Molecule 1: coat protein



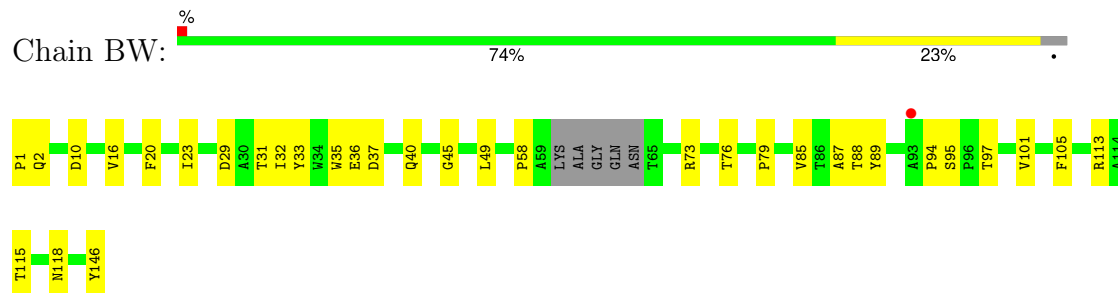
- Molecule 1: coat protein



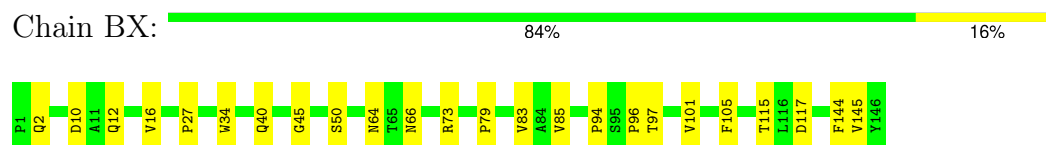
- Molecule 1: coat protein



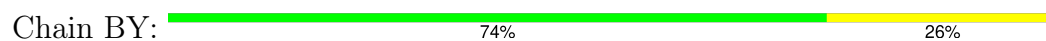
- Molecule 1: coat protein



- Molecule 1: coat protein

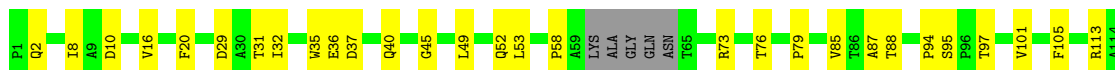


- Molecule 1: coat protein

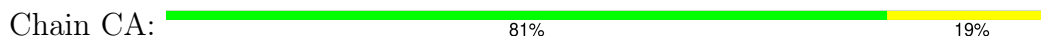




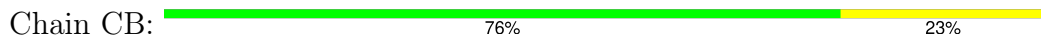
- Molecule 1: coat protein



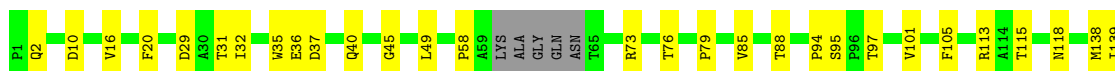
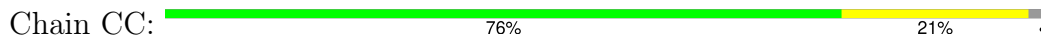
- Molecule 1: coat protein



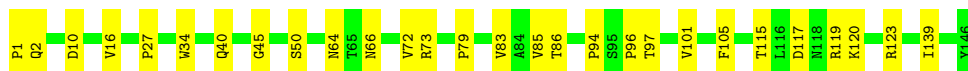
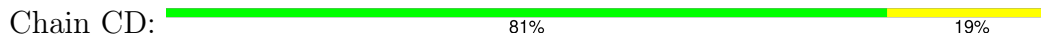
- Molecule 1: coat protein



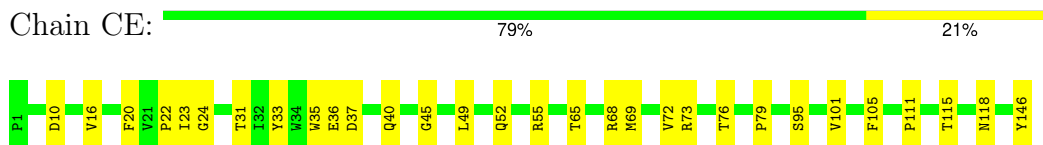
- Molecule 1: coat protein



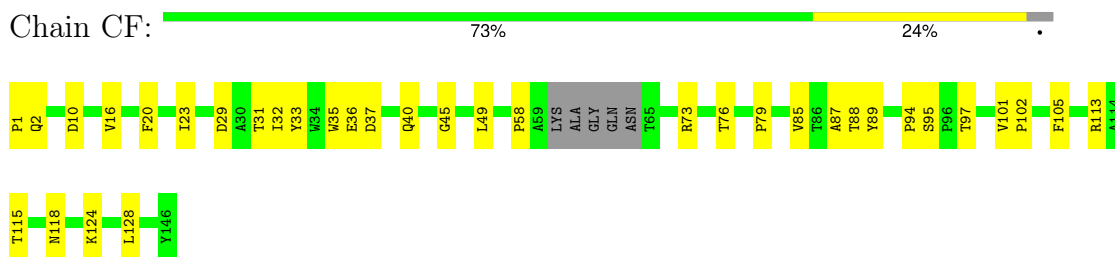
- Molecule 1: coat protein



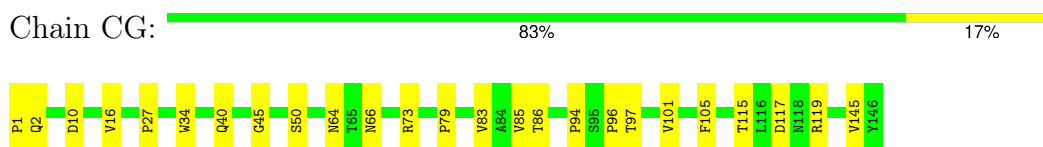
- Molecule 1: coat protein



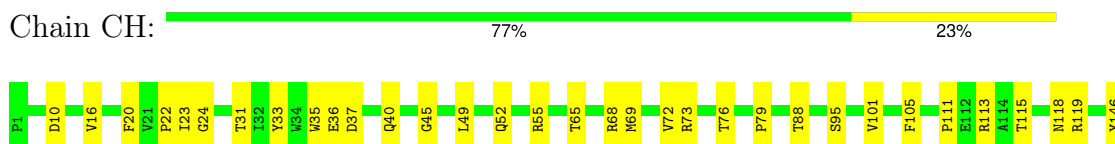
- Molecule 1: coat protein



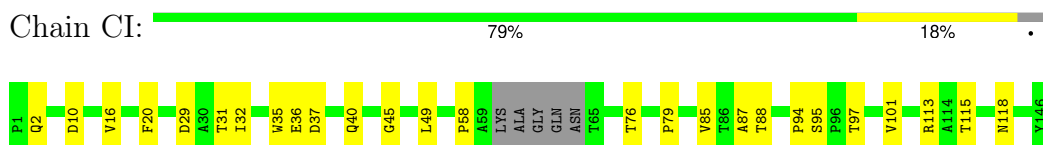
- Molecule 1: coat protein



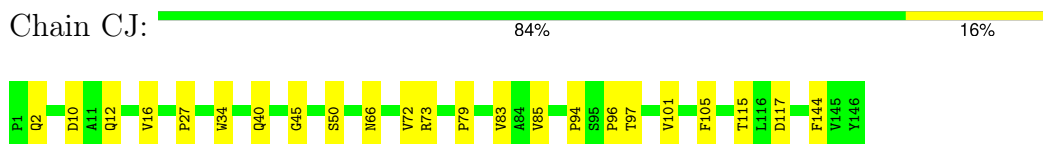
- Molecule 1: coat protein



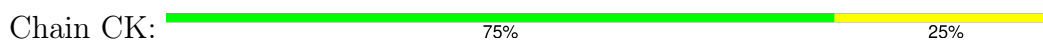
- Molecule 1: coat protein



- Molecule 1: coat protein

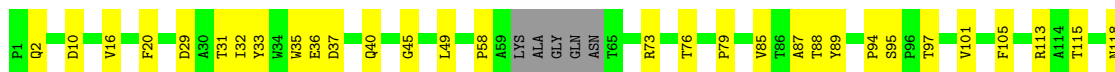


- Molecule 1: coat protein





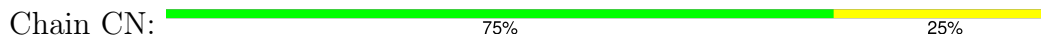
- Molecule 1: coat protein



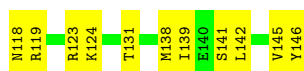
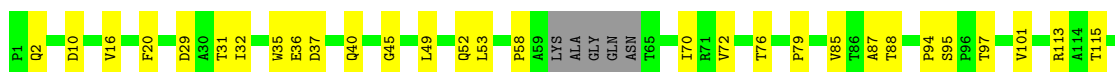
- Molecule 1: coat protein



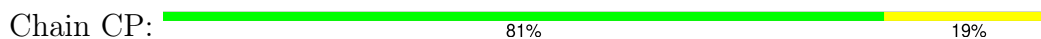
- Molecule 1: coat protein



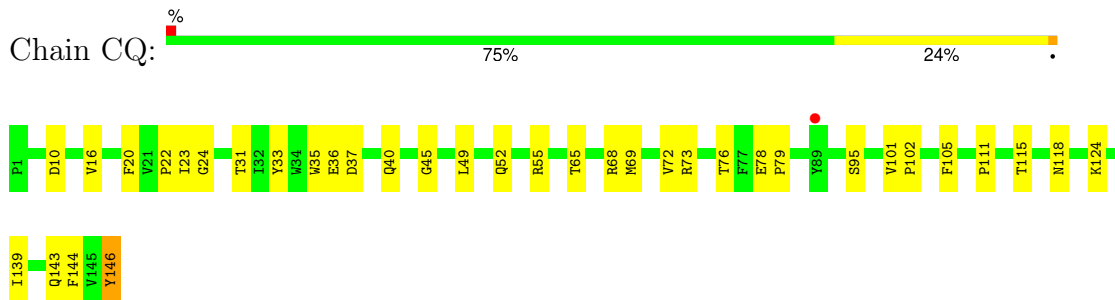
- Molecule 1: coat protein



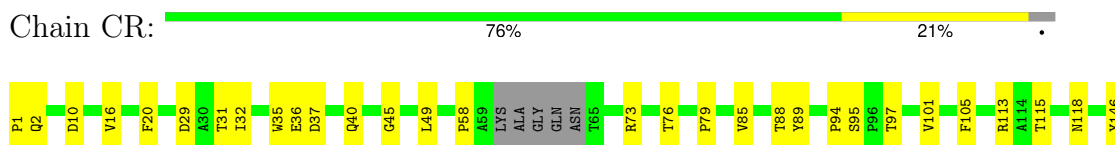
- Molecule 1: coat protein



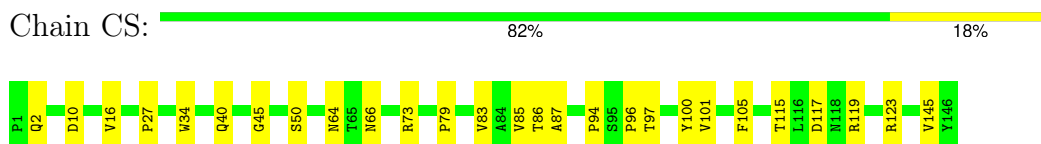
- Molecule 1: coat protein



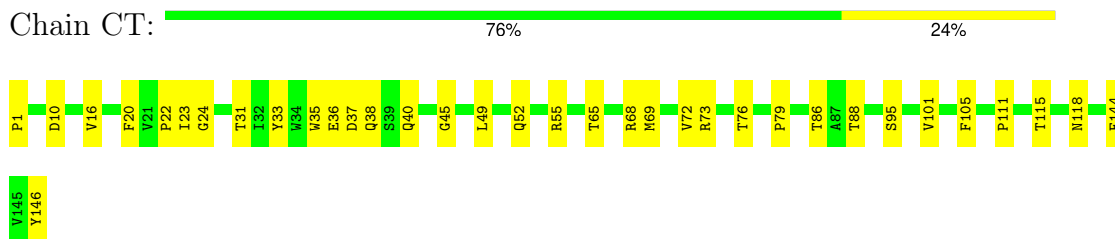
- Molecule 1: coat protein



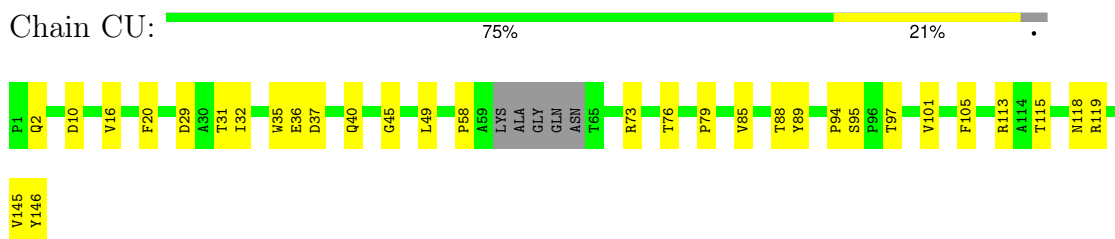
- Molecule 1: coat protein



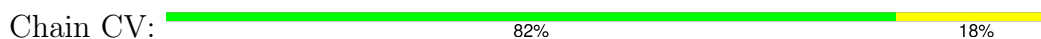
- Molecule 1: coat protein



- Molecule 1: coat protein

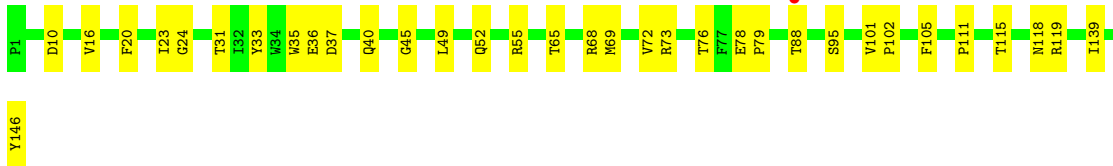
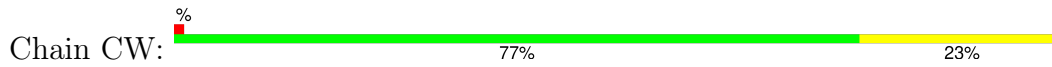


- Molecule 1: coat protein

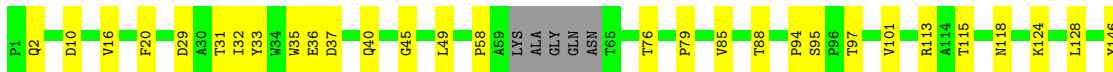
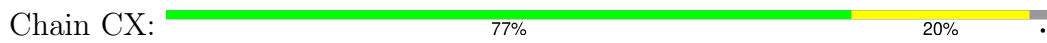




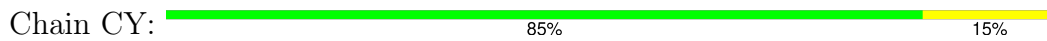
- Molecule 1: coat protein



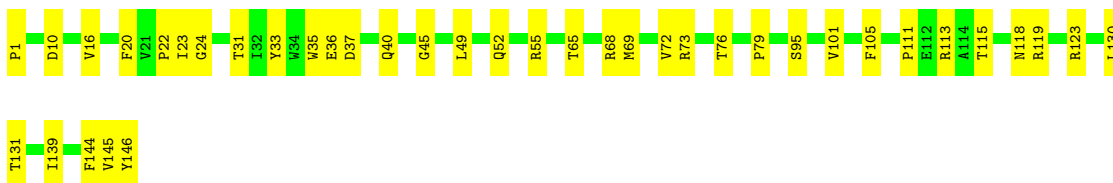
- Molecule 1: coat protein



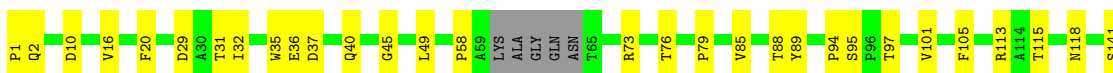
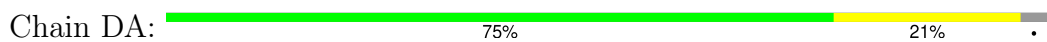
- Molecule 1: coat protein




- Molecule 1: coat protein



- Molecule 1: coat protein




- Molecule 1: coat protein

Chain DB:  82% 18%




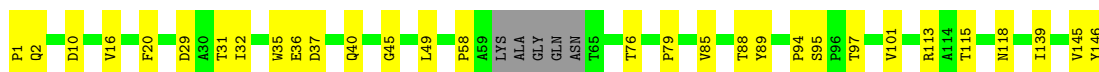
- Molecule 1: coat protein

Chain DC:  77% 23%




- Molecule 1: coat protein

Chain DD:  76% 21%




- Molecule 1: coat protein

Chain DE:  82% 18%



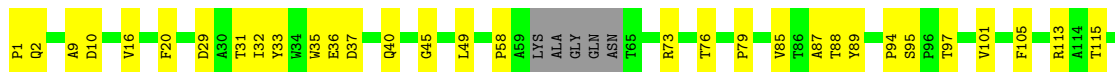
- Molecule 1: coat protein

Chain DF:  77% 23%




- Molecule 1: coat protein

Chain DG:  72% 25%




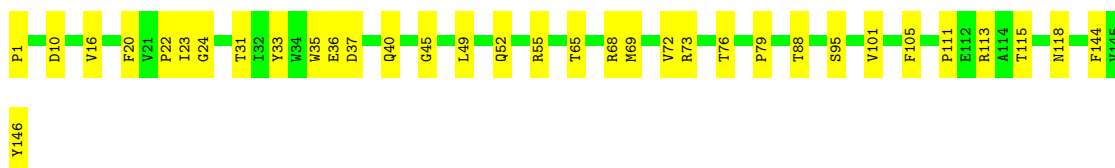
- Molecule 1: coat protein

Chain DH:  84% 16%



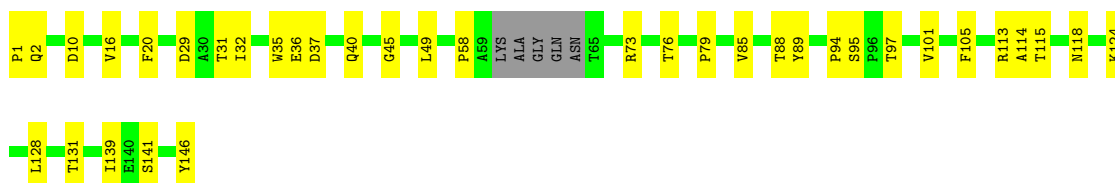
- Molecule 1: coat protein

Chain DI:  77% 23%




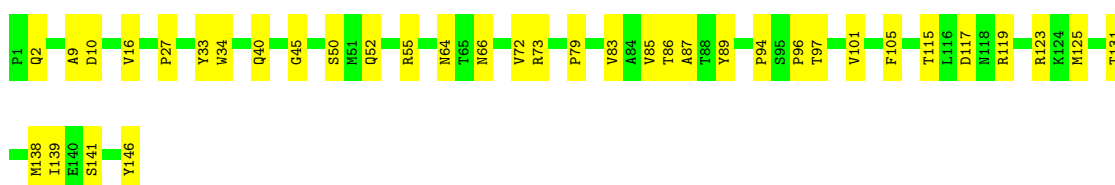
- Molecule 1: coat protein

Chain DJ:  72% 25% .




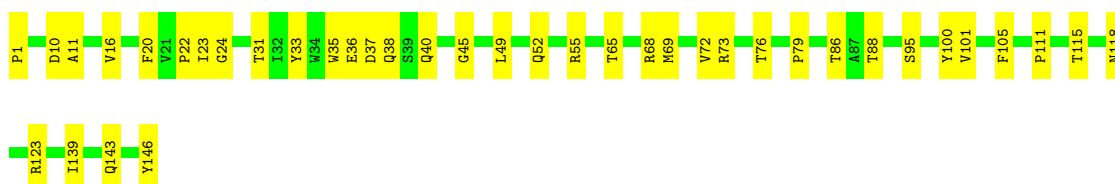
- Molecule 1: coat protein

Chain DK:  75% 25%



- Molecule 1: coat protein

Chain DL:  73% 27%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	500.89Å 500.89Å 287.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.26 – 3.19 49.26 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.26-3.19) 99.8 (49.26-3.19)	Depositor EDS
R_{merge}	0.80	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.231 , 0.234 0.233 , 0.236	Depositor DCC
R_{free} test set	9997 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtrriage
Anisotropy	0.122	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	101490	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.25% 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	0.31	0/1133	0.49	0/1550
1	AB	0.35	0/1169	0.53	0/1599
1	AC	0.31	0/1169	0.50	0/1599
1	AD	0.32	0/1133	0.49	0/1550
1	AE	0.35	0/1169	0.53	0/1599
1	AF	0.31	0/1169	0.50	0/1599
1	AG	0.32	0/1133	0.49	0/1550
1	AH	0.35	0/1169	0.53	0/1599
1	AI	0.31	0/1169	0.50	0/1599
1	AJ	0.31	0/1133	0.49	0/1550
1	AK	0.35	0/1169	0.53	0/1599
1	AL	0.31	0/1169	0.50	0/1599
1	AM	0.32	0/1133	0.49	0/1550
1	AN	0.35	0/1169	0.53	0/1599
1	AO	0.31	0/1169	0.50	0/1599
1	AP	0.32	0/1133	0.49	0/1550
1	AQ	0.35	0/1169	0.52	0/1599
1	AR	0.31	0/1169	0.50	0/1599
1	AS	0.32	0/1133	0.49	0/1550
1	AT	0.35	0/1169	0.53	0/1599
1	AU	0.31	0/1169	0.50	0/1599
1	AV	0.32	0/1133	0.49	0/1550
1	AW	0.35	0/1169	0.53	0/1599
1	AX	0.31	0/1169	0.50	0/1599
1	AY	0.31	0/1133	0.49	0/1550
1	AZ	0.35	0/1169	0.53	0/1599
1	BA	0.31	0/1169	0.50	0/1599
1	BB	0.32	0/1133	0.49	0/1550
1	BC	0.35	0/1169	0.53	0/1599
1	BD	0.31	0/1169	0.50	0/1599
1	BE	0.31	0/1133	0.49	0/1550
1	BF	0.35	0/1169	0.53	0/1599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BG	0.31	0/1169	0.50	0/1599
1	BH	0.32	0/1133	0.49	0/1550
1	BI	0.35	0/1169	0.53	0/1599
1	BJ	0.31	0/1169	0.50	0/1599
1	BK	0.31	0/1133	0.49	0/1550
1	BL	0.35	0/1169	0.53	0/1599
1	BM	0.31	0/1169	0.50	0/1599
1	BN	0.31	0/1133	0.49	0/1550
1	BO	0.35	0/1169	0.53	0/1599
1	BP	0.31	0/1169	0.49	0/1599
1	BQ	0.31	0/1133	0.49	0/1550
1	BR	0.35	0/1169	0.53	0/1599
1	BS	0.31	0/1169	0.49	0/1599
1	BT	0.32	0/1133	0.49	0/1550
1	BU	0.35	0/1169	0.53	0/1599
1	BV	0.31	0/1169	0.50	0/1599
1	BW	0.32	0/1133	0.49	0/1550
1	BX	0.35	0/1169	0.52	0/1599
1	BY	0.31	0/1169	0.50	0/1599
1	BZ	0.32	0/1133	0.49	0/1550
1	CA	0.35	0/1169	0.53	0/1599
1	CB	0.31	0/1169	0.50	0/1599
1	CC	0.31	0/1133	0.49	0/1550
1	CD	0.35	0/1169	0.53	0/1599
1	CE	0.31	0/1169	0.50	0/1599
1	CF	0.31	0/1133	0.49	0/1550
1	CG	0.35	0/1169	0.53	0/1599
1	CH	0.31	0/1169	0.50	0/1599
1	CI	0.31	0/1133	0.49	0/1550
1	CJ	0.34	0/1169	0.53	0/1599
1	CK	0.31	0/1169	0.50	0/1599
1	CL	0.31	0/1133	0.49	0/1550
1	CM	0.35	0/1169	0.52	0/1599
1	CN	0.31	0/1169	0.50	0/1599
1	CO	0.31	0/1133	0.49	0/1550
1	CP	0.35	0/1169	0.53	0/1599
1	CQ	0.31	0/1169	0.50	0/1599
1	CR	0.31	0/1133	0.49	0/1550
1	CS	0.35	0/1169	0.53	0/1599
1	CT	0.31	0/1169	0.50	0/1599
1	CU	0.31	0/1133	0.49	0/1550
1	CV	0.34	0/1169	0.53	0/1599
1	CW	0.31	0/1169	0.50	0/1599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	CX	0.31	0/1133	0.49	0/1550
1	CY	0.35	0/1169	0.53	0/1599
1	CZ	0.31	0/1169	0.50	0/1599
1	DA	0.32	0/1133	0.49	0/1550
1	DB	0.34	0/1169	0.53	0/1599
1	DC	0.31	0/1169	0.50	0/1599
1	DD	0.31	0/1133	0.49	0/1550
1	DE	0.35	0/1169	0.53	0/1599
1	DF	0.31	0/1169	0.50	0/1599
1	DG	0.31	0/1133	0.49	0/1550
1	DH	0.35	0/1169	0.53	0/1599
1	DI	0.31	0/1169	0.50	0/1599
1	DJ	0.31	0/1133	0.49	0/1550
1	DK	0.35	0/1169	0.53	0/1599
1	DL	0.31	0/1169	0.50	0/1599
All	All	0.33	0/104130	0.50	0/142440

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	1104	0	1101	22	0
1	AB	1139	0	1137	20	0
1	AC	1139	0	1137	24	0
1	AD	1104	0	1101	24	0
1	AE	1139	0	1137	34	0
1	AF	1139	0	1137	32	0
1	AG	1104	0	1101	21	0
1	AH	1139	0	1137	18	0
1	AI	1139	0	1137	18	0
1	AJ	1104	0	1101	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AK	1139	0	1137	18	0
1	AL	1139	0	1137	19	0
1	AM	1104	0	1101	25	0
1	AN	1139	0	1137	17	0
1	AO	1139	0	1137	24	0
1	AP	1104	0	1101	24	0
1	AQ	1139	0	1137	19	0
1	AR	1139	0	1137	17	0
1	AS	1104	0	1101	28	0
1	AT	1139	0	1137	22	0
1	AU	1139	0	1137	31	0
1	AV	1104	0	1101	20	0
1	AW	1139	0	1137	16	0
1	AX	1139	0	1137	18	0
1	AY	1104	0	1101	24	0
1	AZ	1139	0	1137	22	0
1	BA	1139	0	1137	22	0
1	BB	1104	0	1101	22	0
1	BC	1139	0	1137	15	0
1	BD	1139	0	1137	23	0
1	BE	1104	0	1101	24	0
1	BF	1139	0	1137	18	0
1	BG	1139	0	1137	23	0
1	BH	1104	0	1101	19	0
1	BI	1139	0	1137	16	0
1	BJ	1139	0	1137	20	0
1	BK	1104	0	1101	21	0
1	BL	1139	0	1137	19	0
1	BM	1139	0	1137	31	0
1	BN	1104	0	1101	19	0
1	BO	1139	0	1137	18	0
1	BP	1139	0	1137	23	0
1	BQ	1104	0	1101	20	0
1	BR	1139	0	1137	17	0
1	BS	1139	0	1137	24	0
1	BT	1104	0	1101	23	0
1	BU	1139	0	1137	17	0
1	BV	1139	0	1137	24	0
1	BW	1104	0	1101	24	0
1	BX	1139	0	1137	18	0
1	BY	1139	0	1137	26	0
1	BZ	1104	0	1101	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	1139	0	1137	25	0
1	CB	1139	0	1137	24	0
1	CC	1104	0	1101	21	0
1	CD	1139	0	1137	22	0
1	CE	1139	0	1137	19	0
1	CF	1104	0	1101	26	0
1	CG	1139	0	1137	20	0
1	CH	1139	0	1137	24	0
1	CI	1104	0	1101	17	0
1	CJ	1139	0	1137	18	0
1	CK	1139	0	1137	27	0
1	CL	1104	0	1101	27	0
1	CM	1139	0	1137	15	0
1	CN	1139	0	1137	26	0
1	CO	1104	0	1101	36	0
1	CP	1139	0	1137	24	0
1	CQ	1139	0	1137	24	0
1	CR	1104	0	1101	21	0
1	CS	1139	0	1137	25	0
1	CT	1139	0	1137	26	0
1	CU	1104	0	1101	22	0
1	CV	1139	0	1137	20	0
1	CW	1139	0	1137	22	0
1	CX	1104	0	1101	20	0
1	CY	1139	0	1137	16	0
1	CZ	1139	0	1137	31	0
1	DA	1104	0	1101	22	0
1	DB	1139	0	1137	21	0
1	DC	1139	0	1137	22	0
1	DD	1104	0	1101	22	0
1	DE	1139	0	1137	23	0
1	DF	1139	0	1137	21	0
1	DG	1104	0	1101	28	0
1	DH	1139	0	1137	19	0
1	DI	1139	0	1137	23	0
1	DJ	1104	0	1101	26	0
1	DK	1139	0	1137	35	0
1	DL	1139	0	1137	32	0
2	AC	2	0	0	0	0
2	AF	2	0	0	0	0
2	AI	1	0	0	0	0
2	AL	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AO	2	0	0	0	0
2	AR	1	0	0	0	0
2	AU	2	0	0	0	0
2	AX	1	0	0	0	0
2	BA	2	0	0	0	0
2	BD	2	0	0	0	0
2	BG	2	0	0	0	0
2	BJ	1	0	0	0	0
2	BM	2	0	0	0	0
2	BP	2	0	0	0	0
2	BS	2	0	0	0	0
2	BV	2	0	0	0	0
2	BY	2	0	0	0	0
2	CE	1	0	0	0	0
All	All	101490	0	101250	1590	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 8.

The worst 5 of 1590 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:BZ:146:TYR:CE2	1:DL:22:PRO:HG2	2.07	0.89
1:AF:22:PRO:HG2	1:CO:146:TYR:CE2	2.13	0.83
1:CS:86:THR:HG21	1:DK:87:ALA:HB3	1.64	0.80
1:AU:86:THR:HB	1:CL:87:ALA:CB	2.21	0.70
1:BW:89:TYR:HA	1:DL:88:THR:OG1	1.93	0.69

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	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	AB	144/146 (99%)	144 (100%)	0	0	100	100
1	AC	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	AD	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	AE	144/146 (99%)	144 (100%)	0	0	100	100
1	AF	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	AG	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	AH	144/146 (99%)	144 (100%)	0	0	100	100
1	AI	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	AJ	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	AK	144/146 (99%)	144 (100%)	0	0	100	100
1	AL	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	AM	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	AN	144/146 (99%)	144 (100%)	0	0	100	100
1	AO	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	AP	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	AQ	144/146 (99%)	144 (100%)	0	0	100	100
1	AR	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	AS	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	AT	144/146 (99%)	144 (100%)	0	0	100	100
1	AU	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	AV	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	AW	144/146 (99%)	144 (100%)	0	0	100	100
1	AX	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	AY	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	AZ	144/146 (99%)	144 (100%)	0	0	100	100
1	BA	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	BB	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	BC	144/146 (99%)	144 (100%)	0	0	100	100
1	BD	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	BE	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	BF	144/146 (99%)	144 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BG	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	BH	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	BI	144/146 (99%)	144 (100%)	0	0	100	100
1	BJ	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	BK	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	BL	144/146 (99%)	144 (100%)	0	0	100	100
1	BM	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	BN	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	BO	144/146 (99%)	144 (100%)	0	0	100	100
1	BP	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	BQ	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	BR	144/146 (99%)	144 (100%)	0	0	100	100
1	BS	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	BT	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	BU	144/146 (99%)	144 (100%)	0	0	100	100
1	BV	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	BW	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	BX	144/146 (99%)	144 (100%)	0	0	100	100
1	BY	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	BZ	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	CA	144/146 (99%)	144 (100%)	0	0	100	100
1	CB	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	CC	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	CD	144/146 (99%)	144 (100%)	0	0	100	100
1	CE	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	CF	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	CG	144/146 (99%)	144 (100%)	0	0	100	100
1	CH	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	CI	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	CJ	144/146 (99%)	144 (100%)	0	0	100	100
1	CK	144/146 (99%)	143 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CL	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	CM	144/146 (99%)	144 (100%)	0	0	100	100
1	CN	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	CO	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	CP	144/146 (99%)	144 (100%)	0	0	100	100
1	CQ	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	CR	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	CS	144/146 (99%)	144 (100%)	0	0	100	100
1	CT	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	CU	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	CV	144/146 (99%)	144 (100%)	0	0	100	100
1	CW	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	CX	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	CY	144/146 (99%)	144 (100%)	0	0	100	100
1	CZ	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	DA	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	DB	144/146 (99%)	144 (100%)	0	0	100	100
1	DC	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	DD	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	DE	144/146 (99%)	144 (100%)	0	0	100	100
1	DF	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	DG	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	DH	144/146 (99%)	144 (100%)	0	0	100	100
1	DI	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
1	DJ	137/146 (94%)	136 (99%)	1 (1%)	0	100	100
1	DK	144/146 (99%)	144 (100%)	0	0	100	100
1	DL	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
All	All	12750/13140 (97%)	12690 (100%)	60 (0%)	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	119/122 (98%)	119 (100%)	0	100	100
1	AB	122/122 (100%)	122 (100%)	0	100	100
1	AC	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	AD	119/122 (98%)	119 (100%)	0	100	100
1	AE	122/122 (100%)	122 (100%)	0	100	100
1	AF	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	AG	119/122 (98%)	119 (100%)	0	100	100
1	AH	122/122 (100%)	122 (100%)	0	100	100
1	AI	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	AJ	119/122 (98%)	119 (100%)	0	100	100
1	AK	122/122 (100%)	122 (100%)	0	100	100
1	AL	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	AM	119/122 (98%)	119 (100%)	0	100	100
1	AN	122/122 (100%)	122 (100%)	0	100	100
1	AO	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	AP	119/122 (98%)	119 (100%)	0	100	100
1	AQ	122/122 (100%)	122 (100%)	0	100	100
1	AR	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	AS	119/122 (98%)	119 (100%)	0	100	100
1	AT	122/122 (100%)	122 (100%)	0	100	100
1	AU	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	AV	119/122 (98%)	119 (100%)	0	100	100
1	AW	122/122 (100%)	122 (100%)	0	100	100
1	AX	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	AY	119/122 (98%)	119 (100%)	0	100	100
1	AZ	122/122 (100%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	BB	119/122 (98%)	119 (100%)	0	100	100
1	BC	122/122 (100%)	122 (100%)	0	100	100
1	BD	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	BE	119/122 (98%)	119 (100%)	0	100	100
1	BF	122/122 (100%)	122 (100%)	0	100	100
1	BG	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	BH	119/122 (98%)	119 (100%)	0	100	100
1	BI	122/122 (100%)	122 (100%)	0	100	100
1	BJ	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	BK	119/122 (98%)	119 (100%)	0	100	100
1	BL	122/122 (100%)	122 (100%)	0	100	100
1	BM	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	BN	119/122 (98%)	119 (100%)	0	100	100
1	BO	122/122 (100%)	122 (100%)	0	100	100
1	BP	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	BQ	119/122 (98%)	119 (100%)	0	100	100
1	BR	122/122 (100%)	122 (100%)	0	100	100
1	BS	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	BT	119/122 (98%)	119 (100%)	0	100	100
1	BU	122/122 (100%)	122 (100%)	0	100	100
1	BV	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	BW	119/122 (98%)	119 (100%)	0	100	100
1	BX	122/122 (100%)	122 (100%)	0	100	100
1	BY	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	BZ	119/122 (98%)	119 (100%)	0	100	100
1	CA	122/122 (100%)	122 (100%)	0	100	100
1	CB	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	CC	119/122 (98%)	119 (100%)	0	100	100
1	CD	122/122 (100%)	122 (100%)	0	100	100
1	CE	122/122 (100%)	121 (99%)	1 (1%)	81	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CF	119/122 (98%)	119 (100%)	0	100	100
1	CG	122/122 (100%)	122 (100%)	0	100	100
1	CH	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	CI	119/122 (98%)	119 (100%)	0	100	100
1	CJ	122/122 (100%)	122 (100%)	0	100	100
1	CK	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	CL	119/122 (98%)	119 (100%)	0	100	100
1	CM	122/122 (100%)	122 (100%)	0	100	100
1	CN	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	CO	119/122 (98%)	119 (100%)	0	100	100
1	CP	122/122 (100%)	122 (100%)	0	100	100
1	CQ	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	CR	119/122 (98%)	119 (100%)	0	100	100
1	CS	122/122 (100%)	122 (100%)	0	100	100
1	CT	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	CU	119/122 (98%)	119 (100%)	0	100	100
1	CV	122/122 (100%)	122 (100%)	0	100	100
1	CW	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	CX	119/122 (98%)	119 (100%)	0	100	100
1	CY	122/122 (100%)	122 (100%)	0	100	100
1	CZ	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	DA	119/122 (98%)	119 (100%)	0	100	100
1	DB	122/122 (100%)	122 (100%)	0	100	100
1	DC	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	DD	119/122 (98%)	119 (100%)	0	100	100
1	DE	122/122 (100%)	122 (100%)	0	100	100
1	DF	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	DG	119/122 (98%)	119 (100%)	0	100	100
1	DH	122/122 (100%)	122 (100%)	0	100	100
1	DI	122/122 (100%)	121 (99%)	1 (1%)	81	92
1	DJ	119/122 (98%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DK	122/122 (100%)	122 (100%)	0	100	100
1	DL	122/122 (100%)	121 (99%)	1 (1%)	81	92
All	All	10890/10980 (99%)	10860 (100%)	30 (0%)	92	97

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BS	146	TYR
1	DF	146	TYR
1	CB	146	TYR
1	DL	146	TYR
1	CW	146	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	AG	40	GLN
1	AP	40	GLN
1	BQ	40	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 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	141/146 (96%)	-0.46	0 100 100	36, 58, 86, 115	0
1	AB	146/146 (100%)	-0.45	0 100 100	40, 58, 79, 102	0
1	AC	146/146 (100%)	-0.35	0 100 100	42, 58, 80, 105	0
1	AD	141/146 (96%)	-0.42	0 100 100	36, 58, 86, 115	0
1	AE	146/146 (100%)	-0.14	0 100 100	40, 58, 79, 102	0
1	AF	146/146 (100%)	-0.25	0 100 100	42, 58, 80, 105	0
1	AG	141/146 (96%)	-0.36	0 100 100	36, 58, 86, 115	0
1	AH	146/146 (100%)	-0.47	0 100 100	40, 58, 79, 102	0
1	AI	146/146 (100%)	-0.42	0 100 100	42, 58, 80, 105	0
1	AJ	141/146 (96%)	-0.47	0 100 100	36, 58, 86, 115	0
1	AK	146/146 (100%)	-0.43	0 100 100	40, 58, 79, 102	0
1	AL	146/146 (100%)	-0.37	0 100 100	42, 58, 80, 105	0
1	AM	141/146 (96%)	-0.41	0 100 100	36, 58, 86, 115	0
1	AN	146/146 (100%)	-0.45	0 100 100	40, 58, 79, 102	0
1	AO	146/146 (100%)	-0.40	0 100 100	42, 58, 80, 105	0
1	AP	141/146 (96%)	-0.45	0 100 100	36, 58, 86, 115	0
1	AQ	146/146 (100%)	-0.47	0 100 100	40, 58, 79, 102	0
1	AR	146/146 (100%)	-0.41	0 100 100	42, 58, 80, 105	0
1	AS	141/146 (96%)	-0.46	0 100 100	36, 58, 86, 115	0
1	AT	146/146 (100%)	-0.33	0 100 100	40, 58, 79, 102	0
1	AU	146/146 (100%)	-0.52	0 100 100	42, 58, 80, 105	0
1	AV	141/146 (96%)	-0.41	1 (0%) 87 81	36, 58, 86, 115	0
1	AW	146/146 (100%)	-0.45	0 100 100	40, 58, 79, 102	0
1	AX	146/146 (100%)	-0.36	1 (0%) 87 81	42, 58, 80, 105	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AY	141/146 (96%)	-0.49	1 (0%) 87 81	36, 58, 86, 115	0
1	AZ	146/146 (100%)	-0.42	0 100 100	40, 58, 79, 102	0
1	BA	146/146 (100%)	-0.33	0 100 100	42, 58, 80, 105	0
1	BB	141/146 (96%)	-0.39	0 100 100	36, 58, 86, 115	0
1	BC	146/146 (100%)	-0.48	0 100 100	40, 58, 79, 102	0
1	BD	146/146 (100%)	-0.45	0 100 100	42, 58, 80, 105	0
1	BE	141/146 (96%)	-0.43	0 100 100	36, 58, 86, 115	0
1	BF	146/146 (100%)	-0.44	0 100 100	40, 58, 79, 102	0
1	BG	146/146 (100%)	-0.32	1 (0%) 87 81	42, 58, 80, 105	0
1	BH	141/146 (96%)	-0.45	1 (0%) 87 81	36, 58, 86, 115	0
1	BI	146/146 (100%)	-0.40	0 100 100	40, 58, 79, 102	0
1	BJ	146/146 (100%)	-0.37	0 100 100	42, 58, 80, 105	0
1	BK	141/146 (96%)	-0.48	0 100 100	36, 58, 86, 115	0
1	BL	146/146 (100%)	-0.52	0 100 100	40, 58, 79, 102	0
1	BM	146/146 (100%)	-0.43	0 100 100	42, 58, 80, 105	0
1	BN	141/146 (96%)	-0.41	0 100 100	36, 58, 86, 115	0
1	BO	146/146 (100%)	-0.48	0 100 100	40, 58, 79, 102	0
1	BP	146/146 (100%)	-0.45	0 100 100	42, 58, 80, 105	0
1	BQ	141/146 (96%)	-0.34	1 (0%) 87 81	36, 58, 86, 115	0
1	BR	146/146 (100%)	-0.40	0 100 100	40, 58, 79, 102	0
1	BS	146/146 (100%)	-0.44	0 100 100	42, 58, 80, 105	0
1	BT	141/146 (96%)	-0.52	0 100 100	36, 58, 86, 115	0
1	BU	146/146 (100%)	-0.42	0 100 100	40, 58, 79, 102	0
1	BV	146/146 (100%)	-0.42	0 100 100	42, 58, 80, 105	0
1	BW	141/146 (96%)	-0.31	1 (0%) 87 81	36, 58, 86, 115	0
1	BX	146/146 (100%)	-0.46	0 100 100	40, 58, 79, 102	0
1	BY	146/146 (100%)	-0.46	0 100 100	42, 58, 80, 105	0
1	BZ	141/146 (96%)	-0.10	0 100 100	36, 58, 86, 115	0
1	CA	146/146 (100%)	-0.37	0 100 100	40, 58, 79, 102	0
1	CB	146/146 (100%)	-0.28	0 100 100	42, 58, 80, 105	0
1	CC	141/146 (96%)	-0.37	0 100 100	36, 58, 86, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	CD	146/146 (100%)	-0.49	0 100 100	40, 58, 79, 102	0
1	CE	146/146 (100%)	-0.48	0 100 100	42, 58, 80, 105	0
1	CF	141/146 (96%)	-0.33	0 100 100	36, 58, 86, 115	0
1	CG	146/146 (100%)	-0.51	0 100 100	40, 58, 79, 102	0
1	CH	146/146 (100%)	-0.37	0 100 100	42, 58, 80, 105	0
1	CI	141/146 (96%)	-0.37	0 100 100	36, 58, 86, 115	0
1	CJ	146/146 (100%)	-0.44	0 100 100	40, 58, 79, 102	0
1	CK	146/146 (100%)	-0.41	0 100 100	42, 58, 80, 105	0
1	CL	141/146 (96%)	-0.37	0 100 100	36, 58, 86, 115	0
1	CM	146/146 (100%)	-0.48	0 100 100	40, 58, 79, 102	0
1	CN	146/146 (100%)	-0.32	0 100 100	42, 58, 80, 105	0
1	CO	141/146 (96%)	-0.21	0 100 100	36, 58, 86, 115	0
1	CP	146/146 (100%)	-0.43	0 100 100	40, 58, 79, 102	0
1	CQ	146/146 (100%)	-0.30	1 (0%) 87 81	42, 58, 80, 105	0
1	CR	141/146 (96%)	-0.40	0 100 100	36, 58, 86, 115	0
1	CS	146/146 (100%)	-0.34	0 100 100	40, 58, 79, 102	0
1	CT	146/146 (100%)	-0.51	0 100 100	42, 58, 80, 105	0
1	CU	141/146 (96%)	-0.42	0 100 100	36, 58, 86, 115	0
1	CV	146/146 (100%)	-0.39	0 100 100	40, 58, 79, 102	0
1	CW	146/146 (100%)	-0.43	1 (0%) 87 81	42, 58, 80, 105	0
1	CX	141/146 (96%)	-0.34	0 100 100	36, 58, 86, 115	0
1	CY	146/146 (100%)	-0.45	0 100 100	40, 58, 79, 102	0
1	CZ	146/146 (100%)	-0.40	0 100 100	42, 58, 80, 105	0
1	DA	141/146 (96%)	-0.44	0 100 100	36, 58, 86, 115	0
1	DB	146/146 (100%)	-0.49	0 100 100	40, 58, 79, 102	0
1	DC	146/146 (100%)	-0.44	0 100 100	42, 58, 80, 105	0
1	DD	141/146 (96%)	-0.51	0 100 100	36, 58, 86, 115	0
1	DE	146/146 (100%)	-0.33	0 100 100	40, 58, 79, 102	0
1	DF	146/146 (100%)	-0.31	0 100 100	42, 58, 80, 105	0
1	DG	141/146 (96%)	-0.42	0 100 100	36, 58, 86, 115	0
1	DH	146/146 (100%)	-0.47	0 100 100	40, 58, 79, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	DI	146/146 (100%)	-0.39	0 100 100	42, 58, 80, 105	0
1	DJ	141/146 (96%)	-0.34	0 100 100	36, 58, 86, 115	0
1	DK	146/146 (100%)	-0.27	0 100 100	40, 58, 79, 102	0
1	DL	146/146 (100%)	-0.37	0 100 100	42, 58, 80, 105	0
All	All	12990/13140 (98%)	-0.40	9 (0%) 95 95	36, 58, 84, 115	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BG	88	THR	3.6
1	AX	89	TYR	3.0
1	AV	67	GLN	2.9
1	CQ	89	TYR	2.8
1	CW	88	THR	2.6

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	AC	202	1/1	0.72	0.22	78,78,78,78	0
2	CA	BA	202	1/1	0.81	0.19	78,78,78,78	0
2	CA	AR	201	1/1	0.85	0.19	78,78,78,78	0
2	CA	BY	201	1/1	0.85	0.22	78,78,78,78	0
2	CA	BD	202	1/1	0.86	0.10	78,78,78,78	0
2	CA	BV	202	1/1	0.87	0.18	78,78,78,78	0
2	CA	AI	201	1/1	0.91	0.15	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CA	BP	201	1/1	0.91	0.12	78,78,78,78	0
2	CA	AX	201	1/1	0.92	0.18	78,78,78,78	0
2	CA	AO	202	1/1	0.92	0.10	78,78,78,78	0
2	CA	BP	202	1/1	0.93	0.12	78,78,78,78	0
2	CA	BS	201	1/1	0.93	0.14	78,78,78,78	0
2	CA	BJ	201	1/1	0.93	0.10	78,78,78,78	0
2	CA	BA	201	1/1	0.93	0.14	78,78,78,78	0
2	CA	BM	202	1/1	0.95	0.13	78,78,78,78	0
2	CA	AO	201	1/1	0.95	0.05	78,78,78,78	0
2	CA	AU	201	1/1	0.95	0.10	78,78,78,78	0
2	CA	AU	202	1/1	0.95	0.13	78,78,78,78	0
2	CA	BS	202	1/1	0.95	0.13	78,78,78,78	0
2	CA	BV	201	1/1	0.95	0.17	78,78,78,78	0
2	CA	BG	201	1/1	0.95	0.20	78,78,78,78	0
2	CA	AF	202	1/1	0.95	0.19	78,78,78,78	0
2	CA	BY	202	1/1	0.95	0.13	78,78,78,78	0
2	CA	AC	201	1/1	0.96	0.23	78,78,78,78	0
2	CA	AF	201	1/1	0.96	0.20	78,78,78,78	0
2	CA	CE	201	1/1	0.96	0.14	78,78,78,78	0
2	CA	BD	201	1/1	0.97	0.10	78,78,78,78	0
2	CA	AL	201	1/1	0.97	0.14	78,78,78,78	0
2	CA	BG	202	1/1	0.99	0.17	78,78,78,78	0
2	CA	BM	201	1/1	0.99	0.10	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.