wwPDB X-ray Structure Validation Summary Report (i)

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 (i) 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 (1)) were used in the production of this report:

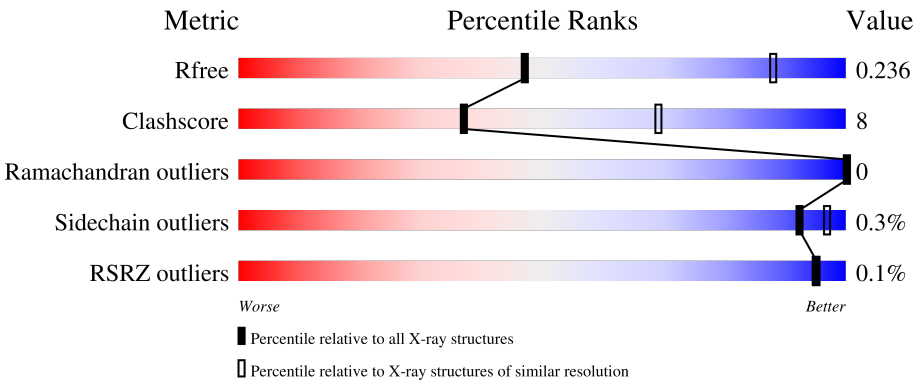
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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 <=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
			Total	C	N	O	S			
1	AB	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AC	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AD	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	AE	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AF	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AG	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	AH	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AI	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AJ	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	AK	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AL	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AM	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	AN	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AO	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
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
			Total	C	N	O	S			
1	AR	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AS	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	AT	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AU	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AV	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	AW	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AX	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	AY	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	AZ	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BA	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BB	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	BC	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BD	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BE	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	BF	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BG	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BH	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	BI	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BJ	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
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
			Total	C	N	O	S			
1	BM	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BN	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	BO	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BP	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BQ	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	BR	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BS	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BT	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	BU	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BV	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BW	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	BX	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BY	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	BZ	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	CA	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CB	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CC	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	CD	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CE	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
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
			Total	C	N	O	S			
1	CH	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CI	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	CJ	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CK	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CL	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	CM	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CN	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CO	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	CP	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CQ	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CR	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	CS	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CT	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CU	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	CV	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CW	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CX	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	CY	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	CZ	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	DA	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	DB	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	DC	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	DD	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	DE	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	DF	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	DG	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	DH	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	DI	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	DJ	141	1104	708	186	206	4	0	0	0
			Total	C	N	O	S			
1	DK	146	1139	728	194	213	4	0	0	0
			Total	C	N	O	S			
1	DL	146	1139	728	194	213	4	0	0	0

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

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

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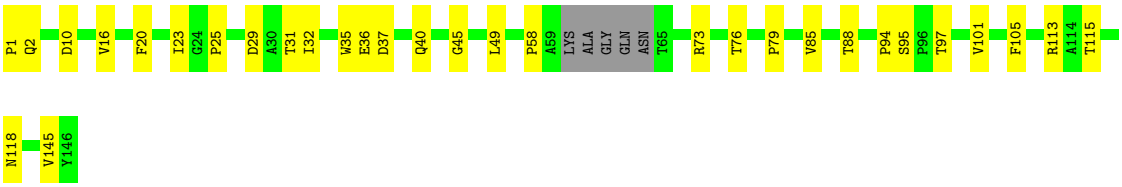
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	BA	2	2	2	0	0
2	BD	2	2	2	0	0
2	BG	2	2	2	0	0
2	BJ	1	1	1	0	0
2	BM	2	2	2	0	0
2	BP	2	2	2	0	0
2	BS	2	2	2	0	0
2	BV	2	2	2	0	0
2	BY	2	2	2	0	0
2	CE	1	1	1	0	0

3 Residue-property plots (i)

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

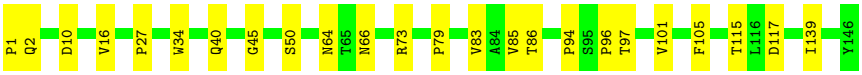
• Molecule 1: coat protein

Chain AA:



• Molecule 1: coat protein

Chain AB:

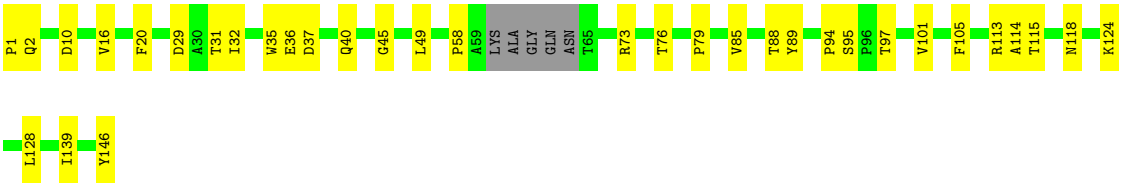


• Molecule 1: coat protein

Chain AC:

• Molecule 1: coat protein

Chain AD:

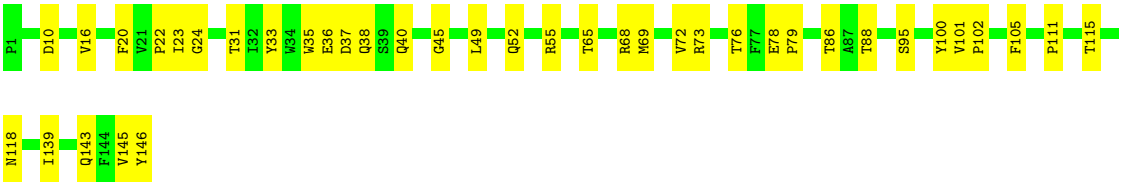


• Molecule 1: coat protein

Chain AE:

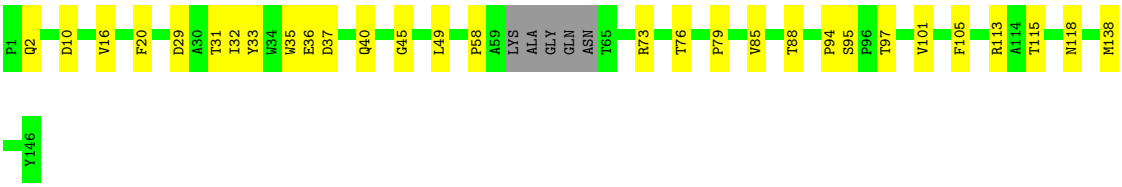
• Molecule 1: coat protein

Chain AF:



• Molecule 1: coat protein

Chain AG:



• Molecule 1: coat protein

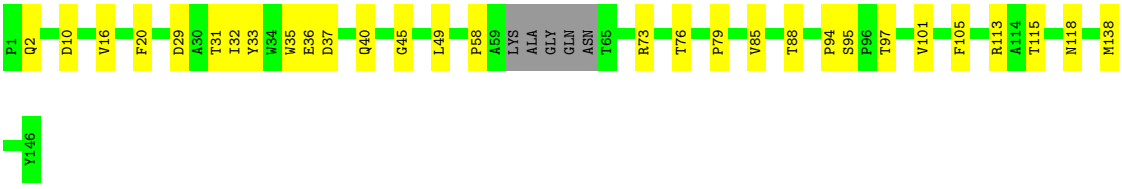
Chain AH:

• Molecule 1: coat protein

Chain AI:

• Molecule 1: coat protein

Chain AJ:



- Molecule 1: coat protein

Chain AK: 84% 16%

P1 Q2 D10 V16 P27 W34 Q40 G45 S50 N66 R73 P79 V83 A84 V85 T86 P94 S95 P96 T97 V101 F105 T115 L116 D117 V145 Y146

- Molecule 1: coat protein

Chain AL: 78% 22%

P1 D10 V16 F20 I23 G24 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 Q52 R55 T65 R68 M69 V72 R73 T76 F77 E78 P79 I80 L81 S95 V101 P102 F105 P111 T115 N118 Y146

- Molecule 1: coat protein

Chain AM: 75% 22% •

P1 Q2 D10 V16 F20 D29 A30 T31 I32 W35 E36 D37 Q40 G45 L49 P58 A59 LYS ALA GLY GLN ASN T65 R73 T76 P79 V85 T86 A87 T88 P94 S95 P96 T97 V101 F105 R113 A114 T115 N118 I139

V145 Y146

- Molecule 1: coat protein

Chain AN: 84% 16%

P1 Q2 D10 V16 P27 W34 Q40 G45 S50 N66 V72 R73 P79 V83 A84 V85 T86 A87 P94 S95 P96 T97 V101 F105 T115 L116 D117 F144 V145 Y146

- Molecule 1: coat protein

Chain AO: 75% 25%

P1 D10 V16 F20 I23 G24 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 Q52 R55 T65 R68 M69 V72 R73 T76 P79 T86 S96 Y100 V101 F105 P111 E112 R113 A114 T115 N118 I139

F144 V145 Y146

- Molecule 1: coat protein

Chain AP: 73% 23% •

P1 Q2 D10 V16 F20 D29 A30 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 P58 A59 LYS ALA GLY GLN ASN T65 R73 T76 P79 V85 T88 P94 S95 P96 T97 V101 F105 V109 R113 A114 T115 N118

K124 L128 F144 V145 Y146

- Molecule 1: coat protein

Chain AQ: 84% 16%

P1 Q2 D10 V16 P27 W34 Q40 G45 S50 N64 T65 N66 V72 R73 P79 V83 A84 V85 P94 S95 P96 T97 V101 F105 T115 L116 D117 F144 V145 Y146

- Molecule 1: coat protein

Chain AR: 80% 20%

P1 D10 V16 F20 I23 G24 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 Q52 R55 T65 R68 M69 V72 R73 T76 P79 S95 V101 F105 P111 T115 N118 Y146

- Molecule 1: coat protein

Chain AS: 71% 26% •

P1 Q2 D10 V16 F20 D29 A30 T31 I32 W35 E36 D37 Q40 G45 L49 P58 A59 LYS ALA GLY GLN ASN T65 R73 T76 P79 V85 T86 A87 T88 Y89 P94 S95 P96 T97 V101 F105 R113 A114 T115 N118 R119

K124 L128 T131 M138 I139 E140 V145 Y146

- Molecule 1: coat protein

Chain AT: 82% 18%

P1 Q2 D10 A11 Q12 V16 P27 W34 Q40 G45 S50 N64 T65 N66 R73 P79 V83 A84 V85 T86 A87 P94 S95 P96 T97 Y100 V101 F105 T115 L116 D117 N118 R119 V145 Y146

- Molecule 1: coat protein

Chain AU: 73% 27%

P1 D10 V16 F20 V21 P22 I23 G24 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 Q52 R55 T65 R68 M69 V72 R73 T76 F77 E78 P79 T86 A87 T88 S95 Y100 V101 P102 K103 A104 F105 P111 E112 R113 A114

T115 N118 F144 V145 Y146

- Molecule 1: coat protein

Chain AV: % 77% 20% •

P1 Q2 D10 V16 F20 D29 A30 T31 I32 W35 E36 D37 Q40 G45 L49 P58 A59 LYS ALA GLY GLN ASN T65 N66 Q67 T76 P79 V85 T88 P94 S95 P96 T97 V101 R113 A114 T115 N118 R119 I139 V145

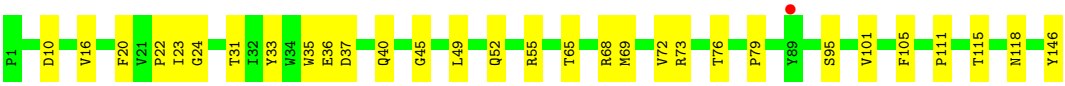
Y146

- Molecule 1: coat protein

Chain AW:

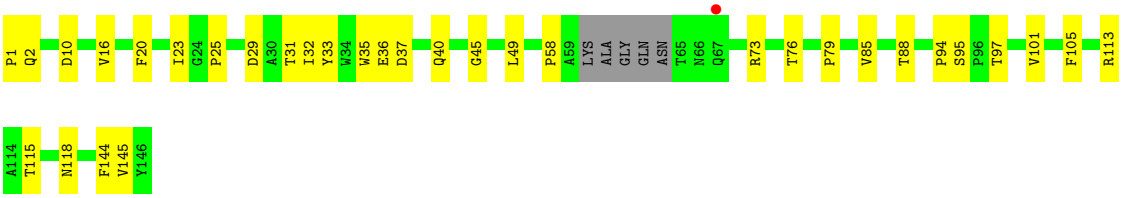
- Molecule 1: coat protein

Chain AX:



- Molecule 1: coat protein

Chain AY:

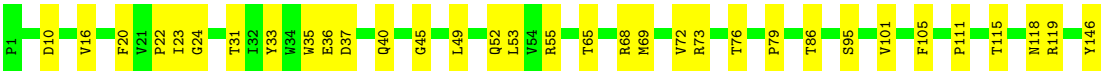


- Molecule 1: coat protein

Chain AZ:

- Molecule 1: coat protein

Chain BA:



- Molecule 1: coat protein

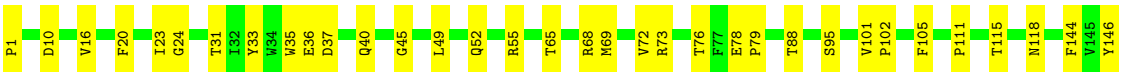
Chain BB:

• Molecule 1: coat protein

Chain BC:

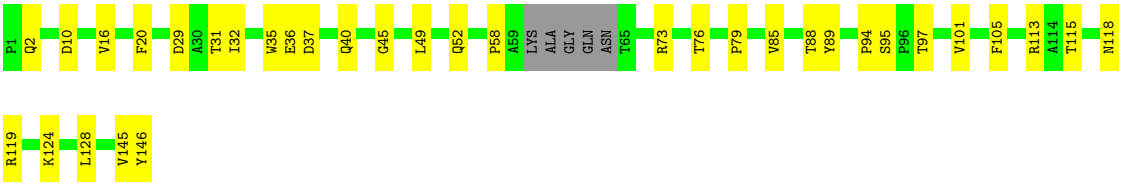
• Molecule 1: coat protein

Chain BD:



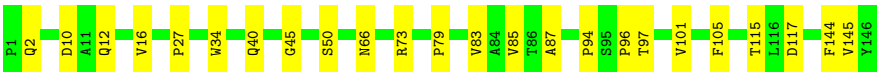
• Molecule 1: coat protein

Chain BE:



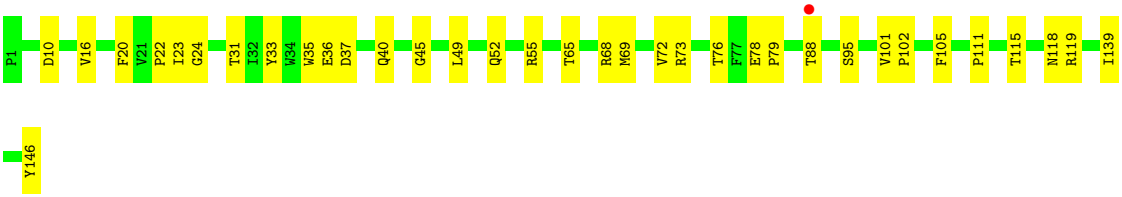
• Molecule 1: coat protein

Chain BF:



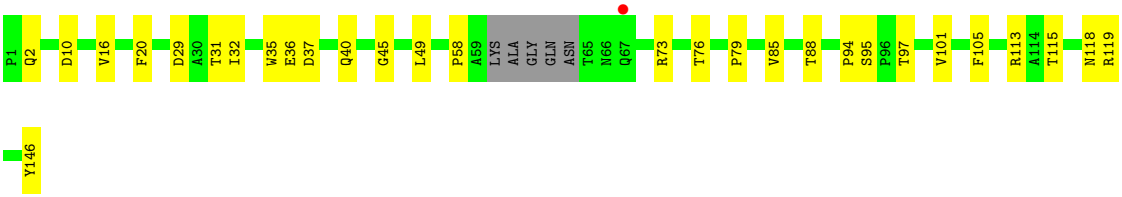
• Molecule 1: coat protein

Chain BG:



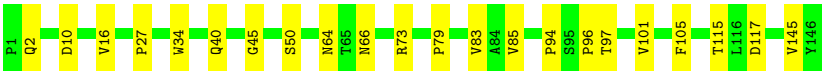
• Molecule 1: coat protein

Chain BH:



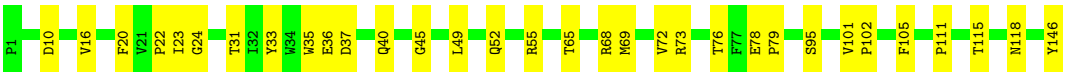
• Molecule 1: coat protein

Chain BI: 85% 15%



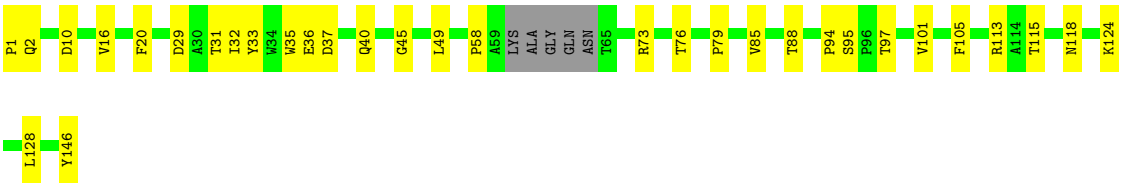
• Molecule 1: coat protein

Chain BJ: 78% 22%



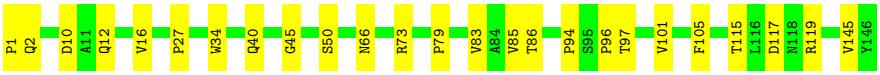
• Molecule 1: coat protein

Chain BK: 75% 22%



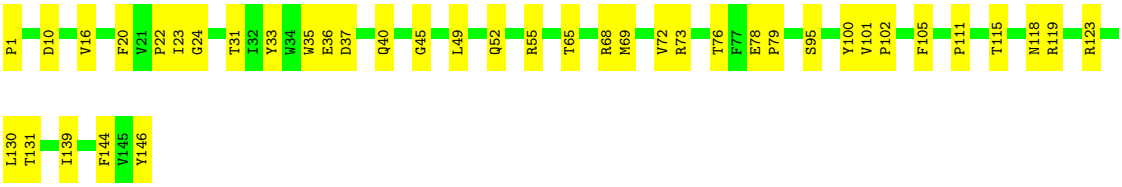
• Molecule 1: coat protein

Chain BL: 83% 17%



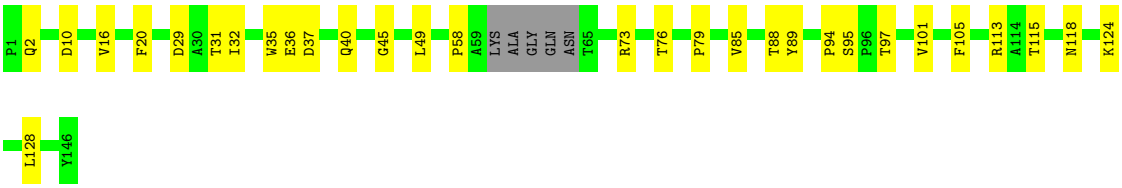
• Molecule 1: coat protein

Chain BM: 73% 27%



• Molecule 1: coat protein

Chain BN:

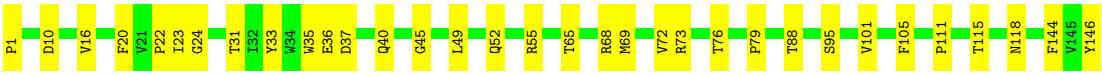


• Molecule 1: coat protein

Chain BO:

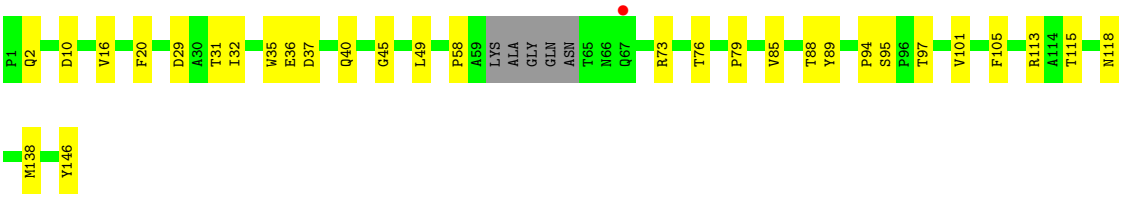
• Molecule 1: coat protein

Chain BP:



• Molecule 1: coat protein

Chain BQ:

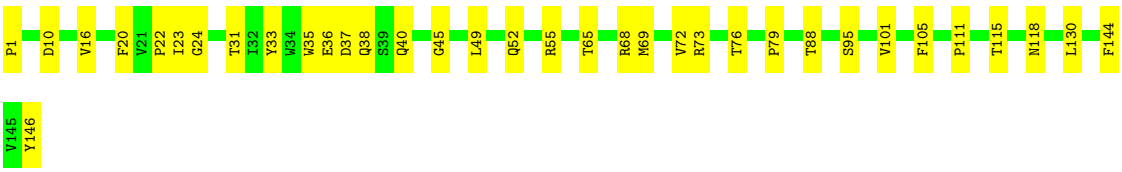


• Molecule 1: coat protein

Chain BR:

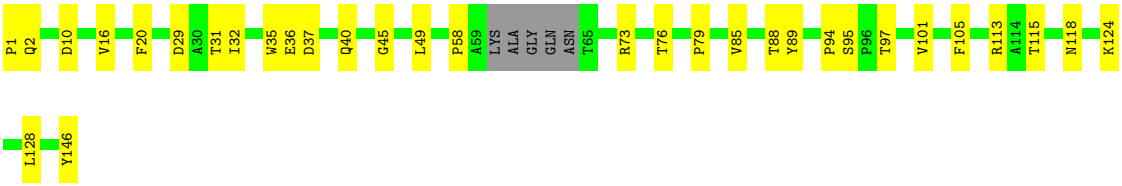
• Molecule 1: coat protein

Chain BS:



• Molecule 1: coat protein

Chain BT: 75% 22% •

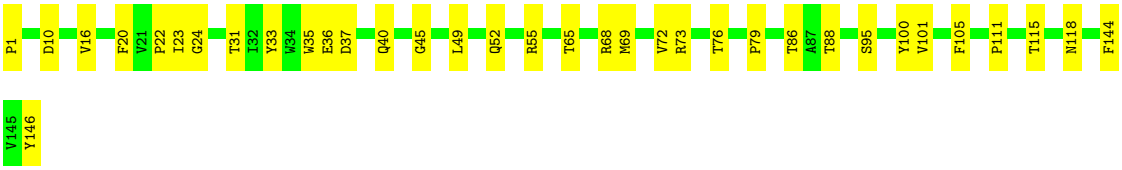


• Molecule 1: coat protein

Chain BU: 84% 16%

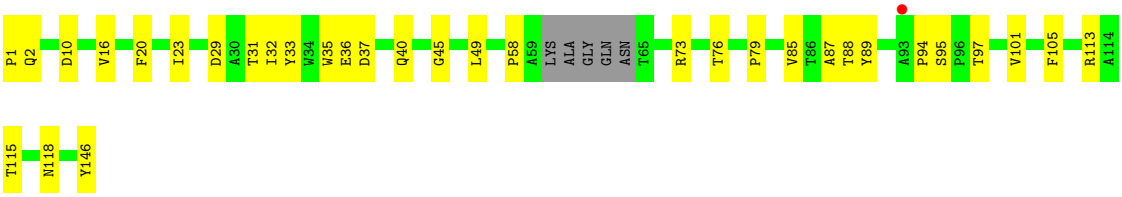
• Molecule 1: coat protein

Chain BV: 76% 24%



• Molecule 1: coat protein

Chain BW: % 74% 23% •

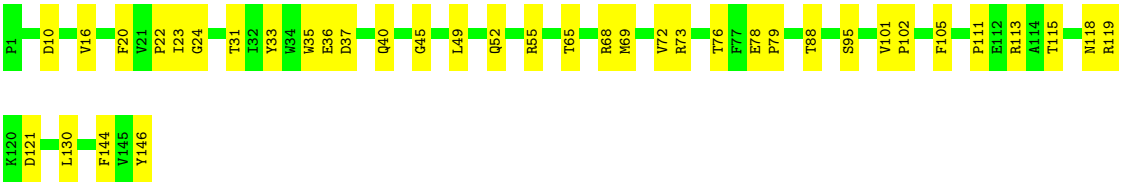


• Molecule 1: coat protein

Chain BX: 84% 16%

• Molecule 1: coat protein

Chain BY: 74% 26%

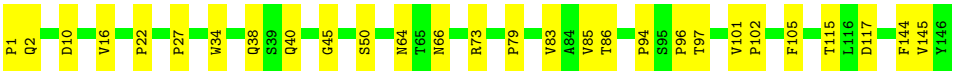


• Molecule 1: coat protein

Chain BZ:

• Molecule 1: coat protein

Chain CA:



• Molecule 1: coat protein

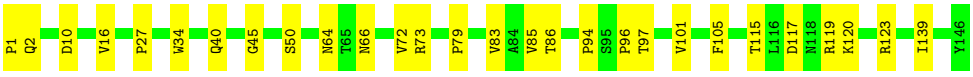
Chain CB:

• Molecule 1: coat protein

Chain CC:

• Molecule 1: coat protein

Chain CD:



• Molecule 1: coat protein

Chain CE: 79% 21%

P1 D10 V16 F20 V21 P22 I23 G24 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 Q52 R55 T65 R68 M69 V72 R73 T76 P79 S95 V101 F105 P111 T115 N118 Y146

• Molecule 1: coat protein

Chain CF: 73% 24% •

P1 Q2 D10 V16 F20 I23 D29 A30 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 P58 A59 LYS ALA GLY GLN ASN T65 R73 T76 P79 V85 T86 A87 T88 Y89 P94 S95 P96 T97 V101 P102 F105 R113 A114

T115 N118 K124 L128 Y146

• Molecule 1: coat protein

Chain CG: 83% 17%

P1 Q2 D10 V16 P27 W34 Q40 G45 S50 N64 T65 N66 R73 P79 V83 A84 V85 T86 P94 S95 P96 T97 V101 F105 T115 L116 D117 N118 R119 V145 Y146

• Molecule 1: coat protein

Chain CH: 77% 23%

P1 D10 V16 F20 V21 P22 I23 G24 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 Q52 R55 T65 R68 M69 V72 R73 T76 P79 T88 S95 V101 F105 P111 E112 R113 A114 T115 N118 R119 Y146

• Molecule 1: coat protein

Chain CI: 79% 18% •

P1 Q2 D10 V16 F20 D29 A30 T31 I32 W35 E36 D37 Q40 G45 L49 P58 A59 LYS ALA GLY GLN ASN T65 T76 P79 V85 T86 A87 T88 P94 S95 P96 T97 V101 R113 A114 T115 N118 Y146

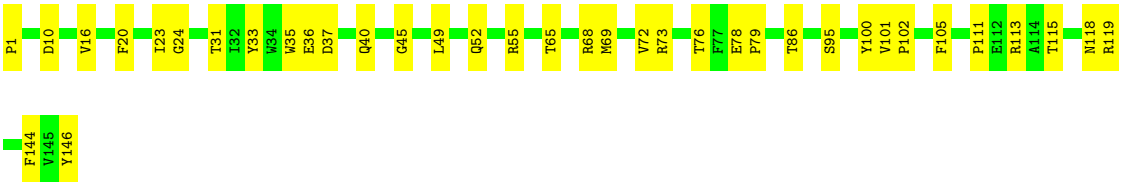
• Molecule 1: coat protein

Chain CJ: 84% 16%

P1 Q2 D10 A11 Q12 V16 P27 W34 Q40 G45 S50 N66 V72 R73 P79 V83 A84 V85 P94 S95 P96 T97 V101 F105 T115 L116 D117 F144 V145 Y146

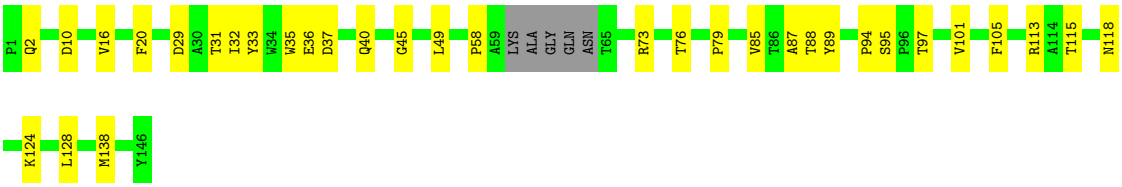
• Molecule 1: coat protein

Chain CK: 75% 25%



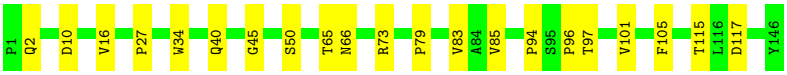
• Molecule 1: coat protein

Chain CL:



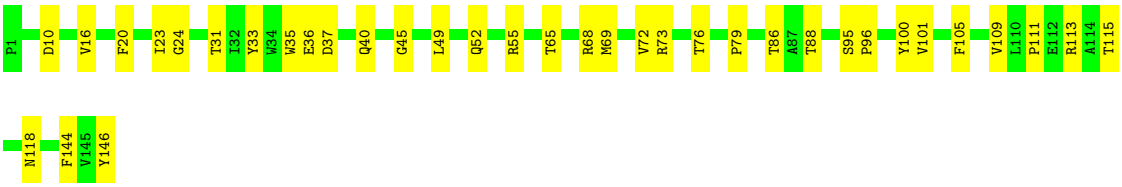
• Molecule 1: coat protein

Chain CM:



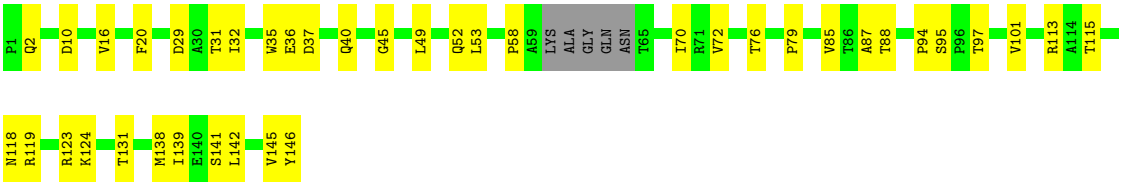
• Molecule 1: coat protein

Chain CN:



• Molecule 1: coat protein

Chain CO:

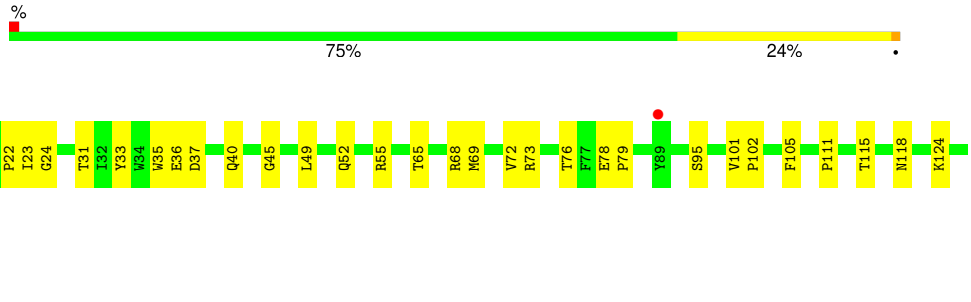


• Molecule 1: coat protein

Chain CP:

• Molecule 1: coat protein

Chain CQ:



• Molecule 1: coat protein

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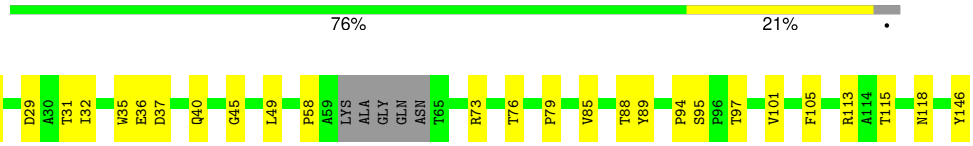
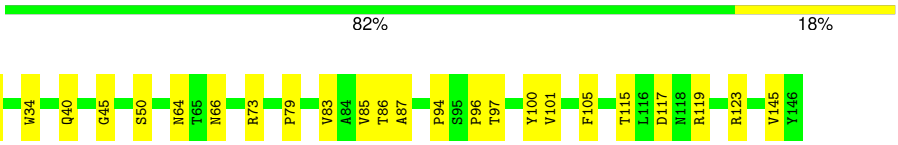


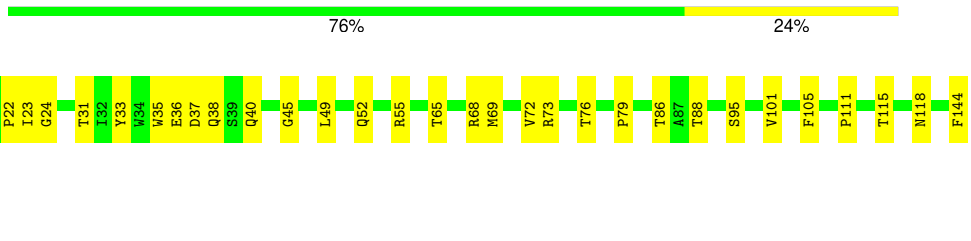
• Molecule 1: coat protein

Chain CS:



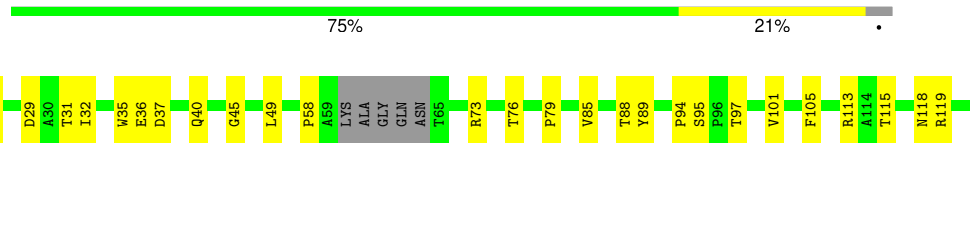
• Molecule 1: coat protein

Chain CT:



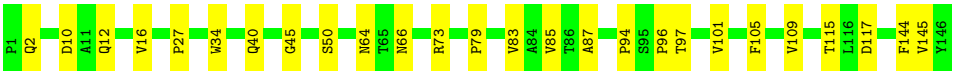
• Molecule 1: coat protein

Chain CU:



• Molecule 1: coat protein

Chain CV:



• Molecule 1: coat protein

Chain CW:

• Molecule 1: coat protein

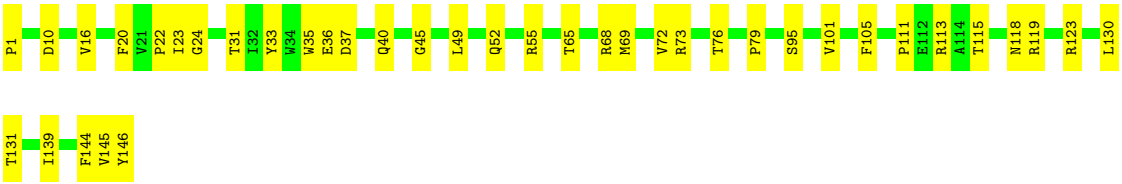
Chain CX:

• Molecule 1: coat protein

Chain CY:

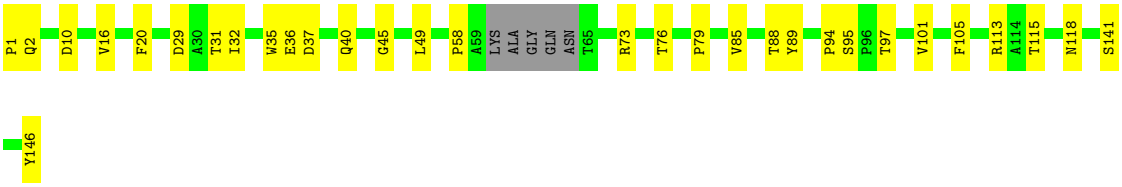
• Molecule 1: coat protein

Chain CZ:



• Molecule 1: coat protein

Chain DA:



• Molecule 1: coat protein

Chain DB: 82% 18%

P1 Q2 D10 A11 Q12 V16 P27 W34 Q40 G45 S50 N64 T65 N66 R73 P79 V83 A84 V85 T86 A87 P94 S95 P96 T97 V101 F105 T115 L116 D117 N118 R119 I139 Y146

- Molecule 1: coat protein

Chain DC: 77% 23%

P1 D10 V16 F20 V21 P22 I23 G24 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 Q52 R55 T65 R68 M69 V72 R73 T76 P79 T88 S95 P96 V101 F105 P111 T115 N118 F144 V145 Y146

- Molecule 1: coat protein

Chain DD: 76% 21% •

P1 Q2 D10 V16 F20 D29 A30 T31 I32 W35 E36 D37 Q40 G45 L49 P58 A59 LYS ALA GLY GLN ASN T65 T76 P79 V85 T88 Y89 P94 S95 P96 T97 V101 R113 A114 T115 N118 I139 V145 Y146

- Molecule 1: coat protein

Chain DE: 82% 18%

P1 Q2 D10 A11 Q12 V16 P27 W34 Q40 G45 S50 N64 T65 N66 R73 P79 V83 A84 V85 T86 A87 P94 S95 P96 T97 V101 F105 T115 L116 D117 F144 V145 Y146

- Molecule 1: coat protein

Chain DF: 77% 23%

P1 D10 V16 F20 I23 G24 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 Q52 R55 T65 R68 M69 V72 R73 T76 P79 T88 S95 V101 F105 P111 T115 N118 L130 F144 V145 Y146

- Molecule 1: coat protein

Chain DG: 72% 25% •

P1 Q2 A9 D10 V16 F20 D29 A30 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 P58 A59 LYS ALA GLY GLN ASN T65 R73 T76 P79 V85 T86 A87 T88 Y89 P94 S95 P96 T97 V101 F105 R113 A114 T115

N118 K124 L128 V145 Y146

- Molecule 1: coat protein

Chain DH: 84% 16%

P1 Q2 D10 A11 Q12 V16 P27 W34 Q40 G45 S50 N64 T65 N66 V72 R73 P79 V83 A84 V85 P94 S95 P96 T97 V101 F105 T115 L116 D117 N118 R119 Y146

• Molecule 1: coat protein

Chain DI: 77% 23%

P1 D10 V16 F20 V21 P22 I23 G24 T31 I32 Y33 W34 W35 E36 D37 Q40 G45 L49 Q52 R55 T65 R68 M69 V72 R73 T76 P79 T88 S95 V101 F105 P111 E112 R113 A114 T115 N118 F144 V145

Y146

• Molecule 1: coat protein

Chain DJ: 72% 25%

P1 Q2 D10 V16 F20 D29 A30 T31 I32 W35 E36 D37 Q40 G45 L49 P58 A59 LYS ALA GLY GLN ASN T65 R73 T76 P79 V85 T88 Y89 P94 S95 P96 T97 V101 F105 R113 A114 T115 N118 K124

L128 T131 I139 E140 S141 Y146

• Molecule 1: coat protein

Chain DK: 75% 25%

P1 Q2 A9 D10 V16 P27 Y33 W34 Q40 G45 S50 M51 Q52 R55 N64 T65 N66 V72 R73 P79 V83 A84 V85 T86 A87 T88 Y89 P94 S95 P96 T97 V101 F105 T115 L116 D117 N118 R119 R123 K124 M125 T131

M138 I139 E140 S141 Y146

• Molecule 1: coat protein

Chain DL: 73% 27%

P1 D10 A11 V16 F20 V21 P22 I23 G24 T31 I32 Y33 W34 W35 E36 D37 Q38 S39 Q40 G45 L49 Q52 R55 T65 R68 M69 V72 R73 T76 P79 T86 A87 T88 S95 Y100 V101 F105 P111 T115 N118

R123 I139 Q143 Y146

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
$< I/\sigma(I) >$ [1]	1.04 (at 3.19Å)	Xtriage
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	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 29.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
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

Xtriage'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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 (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	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(Å^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.