



Full wwPDB EM Validation Report ⓘ

Apr 2, 2024 – 03:26 PM EDT

PDB ID : 8TOC
EMDB ID : EMD-41443
Title : Acinetobacter phage AP205
Authors : Meng, R.; Xing, Z.; Chang, J.; Zhang, J.
Deposited on : 2023-08-03
Resolution : 3.11 Å (reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>

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:

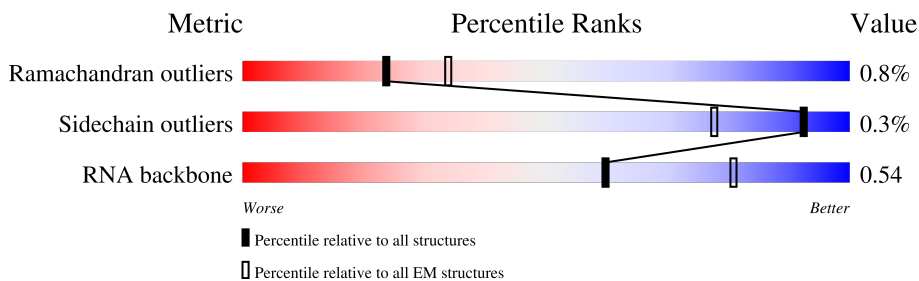
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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.



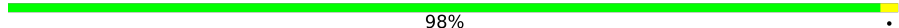
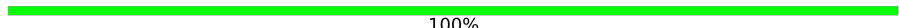
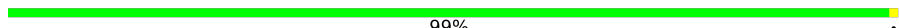
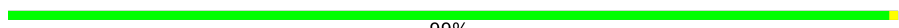
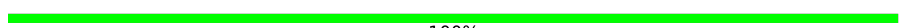








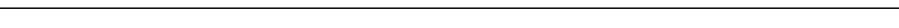

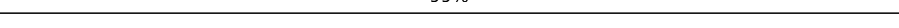
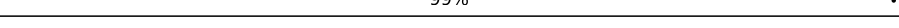
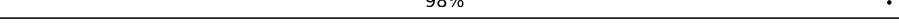
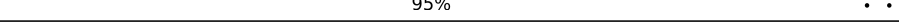
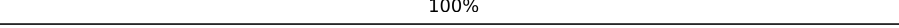
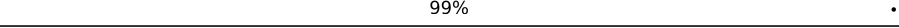
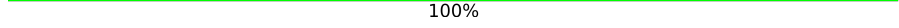
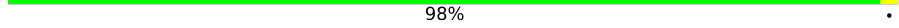
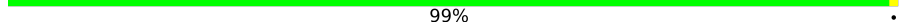
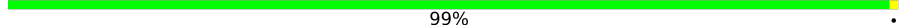
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	4269	
2	a	534	
2	b	534	
3	AB	129	
3	AC	129	
3	AE	129	
3	AF	129	
3	AG	129	

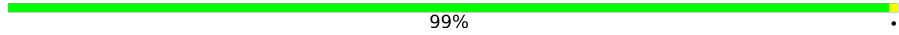
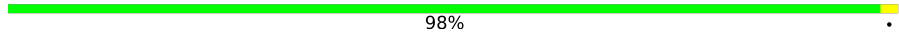
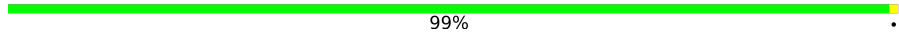
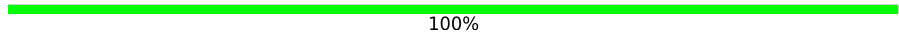
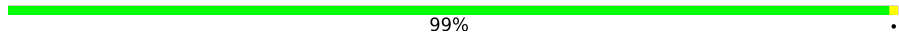
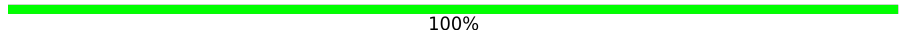
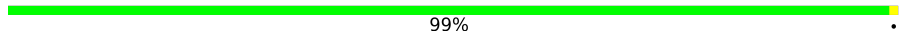
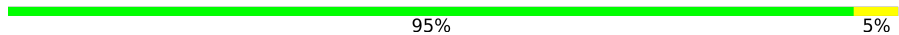
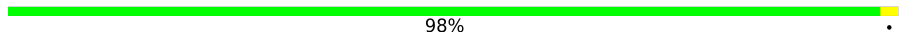
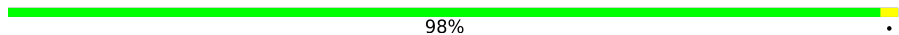
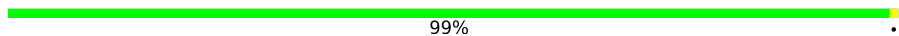
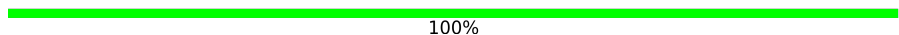
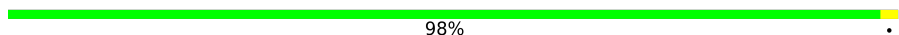


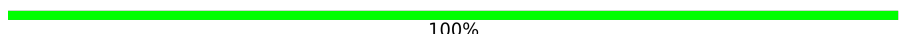
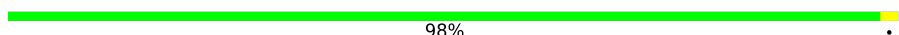
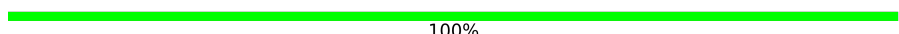
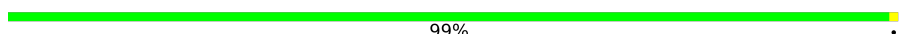
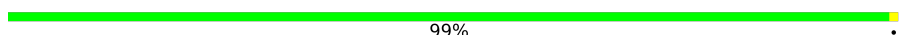
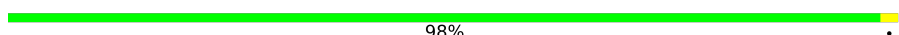
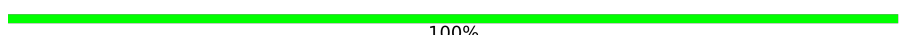
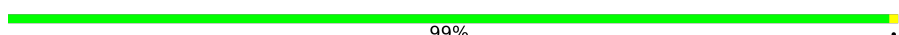
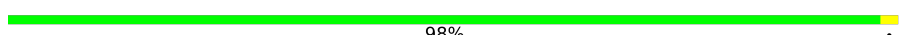
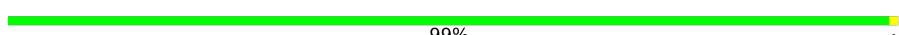
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Mol	Chain	Length	Quality of chain
3	AH	129	 98%
3	AI	129	 100%
3	AJ	129	 99%
3	AK	129	 99%
3	AL	129	 100%
3	AM	129	 99%
3	AN	129	 98%
3	AO	129	 99%
3	AP	129	 99%
3	AQ	129	 98%
3	AS	129	 99%
3	AT	129	 99%
3	AU	129	 100%
3	AV	129	 98%
3	AW	129	 99%
3	AX	129	 99%
3	AY	129	 98%
3	AZ	129	 95%
3	Ac	129	 100%
3	BA	129	 99%
3	BB	129	 100%
3	BC	129	 98%
3	BD	129	 99%
3	BE	129	 99%
3	BF	129	 98%

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Mol	Chain	Length	Quality of chain
3	BG	129	 99%
3	BH	129	 98%
3	BI	129	 99%
3	BJ	129	 100%
3	BK	129	 99%
3	BL	129	 100%
3	BM	129	 99%
3	BN	129	 95% 5%
3	BO	129	 98%
3	BP	129	 98%
3	BQ	129	 99%
3	BS	129	 100%
3	BT	129	 98%
3	BU	129	 98%
3	BV	129	 99%
3	BW	129	 100%
3	BX	129	 98%
3	BY	129	 100%
3	BZ	129	 99%
3	Bc	129	 99%
3	CA	129	 98%
3	CB	129	 100%
3	CC	129	 99%
3	CD	129	 98%
3	CE	129	 99%

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Mol	Chain	Length	Quality of chain
3	CF	129	99%
3	CG	129	99%
3	CH	129	100%
3	CI	129	100%
3	CJ	129	100%
3	CK	129	100%
3	CL	129	99%
3	CM	129	98%
3	CN	129	98%
3	CO	129	100%
3	CP	129	98%
3	CQ	129	98%
3	CS	129	99%
3	CT	129	100%
3	CU	129	100%
3	CV	129	98%
3	CW	129	99%
3	CX	129	98%
3	CY	129	99%
3	CZ	129	99%
3	Cc	129	99%
3	DA	129	99%
3	DB	129	100%
3	DC	129	99%
3	DD	129	98%

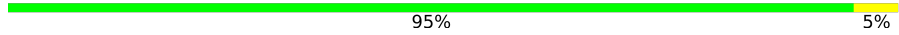
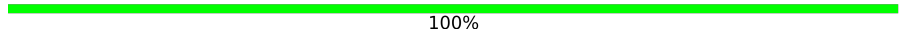
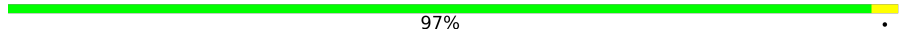
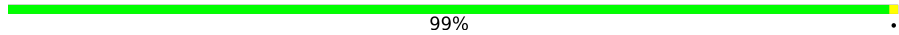
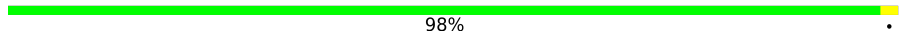
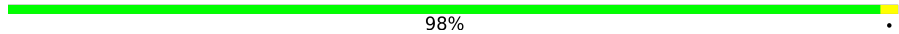
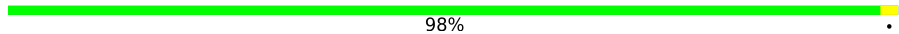
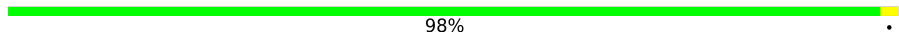
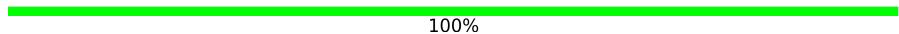
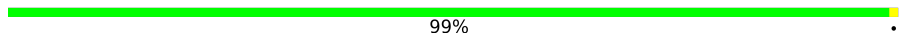
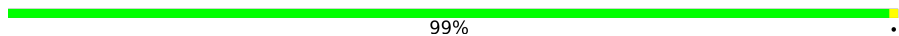
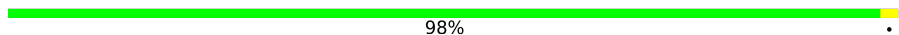
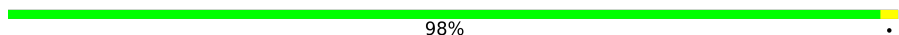
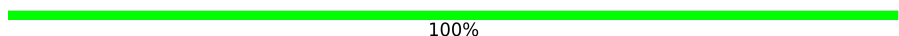

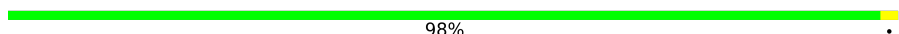
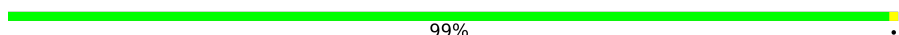
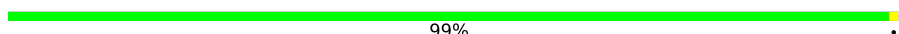
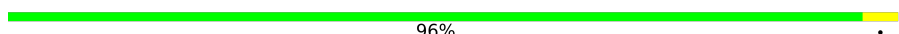
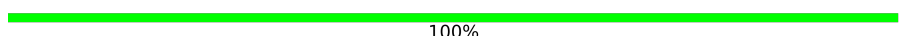
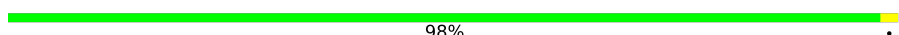
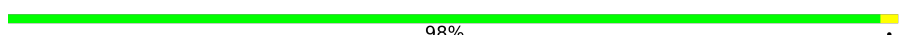
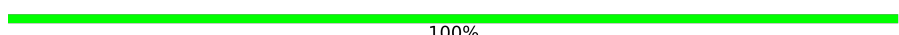
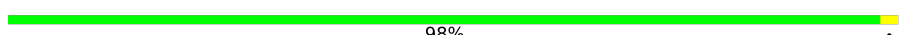
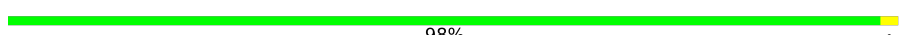
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Mol	Chain	Length	Quality of chain
3	DE	129	100%
3	DF	129	98%
3	DG	129	98%
3	DH	129	100%
3	DI	129	100%
3	DJ	129	100%
3	DK	129	98%
3	DL	129	100%
3	DM	129	99%
3	DN	129	100%
3	DO	129	100%
3	DQ	129	98%
3	DS	129	98%
3	DT	129	98%
3	DU	129	100%
3	DV	129	97%
3	DW	129	99%
3	DX	129	100%
3	DY	129	100%
3	DZ	129	100%
3	Dc	129	100%
3	EA	129	99%
3	EB	129	100%
3	EC	129	100%
3	ED	129	98%

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Mol	Chain	Length	Quality of chain
3	EE	129	 95% 5%
3	EF	129	 100%
3	EG	129	 97%
3	EH	129	 99%
3	EI	129	 98%
3	EJ	129	 98%
3	EK	129	 98%
3	EL	129	 98%
3	EM	129	 100%
3	EN	129	 99%
3	EO	129	 99%
3	EP	129	 98%
3	EQ	129	 98%
3	ES	129	 100%
3	ET	129	 99%
3	EU	129	 98%
3	EV	129	 99%
3	EW	129	 99%
3	EX	129	 96%
3	EY	129	 100%
3	EZ	129	 98%
3	Ec	129	 98%
3	FA	129	 100%
3	FB	129	 98%
3	FC	129	 98%

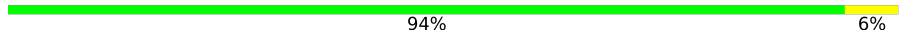
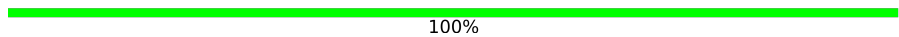
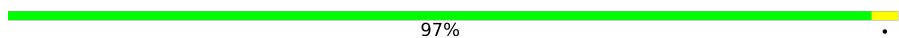
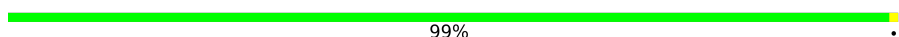

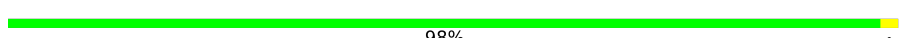
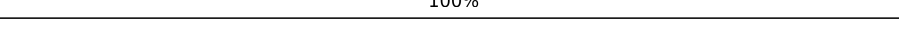



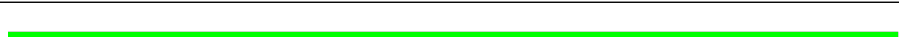


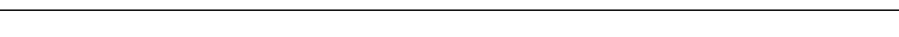
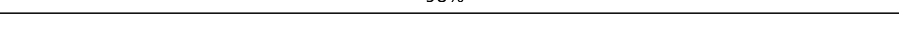
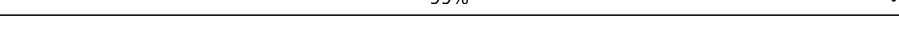
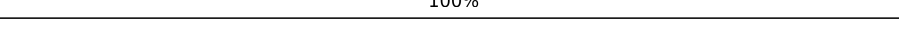
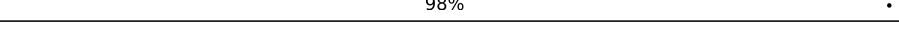
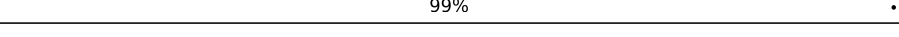
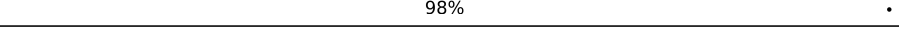
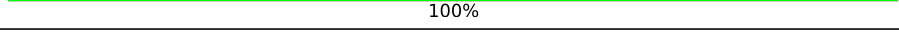
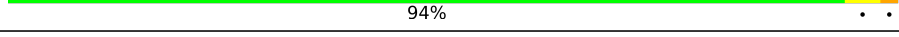
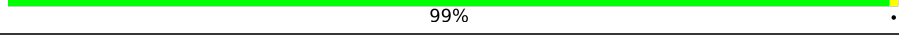
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Mol	Chain	Length	Quality of chain
3	FD	129	100%
3	FE	129	100%
3	FF	129	98%
3	FG	129	100%
3	FH	129	100%
3	FI	129	99%
3	FJ	129	99%
3	FK	129	99%
3	FL	129	98%
3	FM	129	98%
3	FN	129	99%
3	FO	129	99%
3	FP	129	98%
3	FQ	129	100%
3	FS	129	98%
3	FT	129	99%
3	FU	129	100%
3	FV	129	99%
3	FW	129	97%
3	FX	129	98%
3	FY	129	100%
3	FZ	129	98%
3	Fc	129	98%
3	GA	129	99%
3	GB	129	100%

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Mol	Chain	Length	Quality of chain
3	GC	129	 94% 6%
3	GD	129	 100%
3	GE	129	 97%
3	GF	129	 99%
3	GG	129	 99%
3	GH	129	 98%
3	GI	129	 99%
3	GJ	129	 99%
3	GK	129	 99%
3	GL	129	 100%
3	GM	129	 100%
3	GN	129	 98%
3	GO	129	 99%
3	GP	129	 98%
3	GQ	129	 99%
3	GS	129	 100%
3	GT	129	 98%
3	GU	129	 99%
3	GV	129	 98%
3	GW	129	 100%
3	GX	129	 94%
3	GY	129	 99%
3	Gc	129	 100%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 271353 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA chain called RNA (4269-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	R	4269	90441	40490	15694	29988	4269	0	0

- Molecule 2 is a protein called Maturation protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	a	534	4304	2746	765	776	17	0	0
2	b	534	4304	2746	765	776	17	0	0

- Molecule 3 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AB	129	968	602	171	191	4	0	0
3	AC	129	968	602	171	191	4	0	0
3	AE	129	968	602	171	191	4	0	0
3	AF	129	968	602	171	191	4	0	0
3	AG	129	968	602	171	191	4	0	0
3	AH	129	968	602	171	191	4	0	0
3	AI	129	968	602	171	191	4	0	0
3	AJ	129	968	602	171	191	4	0	0
3	AK	129	968	602	171	191	4	0	0
3	AL	129	968	602	171	191	4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O	S		
3	AM	129	968	602	171	191	4	0	0
3	AN	129	968	602	171	191	4	0	0
3	AO	129	968	602	171	191	4	0	0
3	AP	129	968	602	171	191	4	0	0
3	AQ	129	968	602	171	191	4	0	0
3	Ac	129	968	602	171	191	4	0	0
3	AS	129	968	602	171	191	4	0	0
3	AT	129	968	602	171	191	4	0	0
3	AU	129	968	602	171	191	4	0	0
3	AV	129	968	602	171	191	4	0	0
3	AW	129	968	602	171	191	4	0	0
3	AX	129	968	602	171	191	4	0	0
3	AY	129	968	602	171	191	4	0	0
3	AZ	129	968	602	171	191	4	0	0
3	BA	129	968	602	171	191	4	0	0
3	BB	129	968	602	171	191	4	0	0
3	BC	129	968	602	171	191	4	0	0
3	BD	129	968	602	171	191	4	0	0
3	BE	129	968	602	171	191	4	0	0
3	BF	129	968	602	171	191	4	0	0
3	BG	129	968	602	171	191	4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	BH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BI	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BN	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BP	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Bc	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BS	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BT	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BW	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	BZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CA	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CB	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	CC	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CD	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CE	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CF	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CG	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CI	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CN	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CP	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Cc	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CS	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CT	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CW	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	CX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	CZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DA	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DB	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DC	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DD	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DE	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DF	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DG	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DI	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DN	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Dc	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DS	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	DT	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DW	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	DZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EA	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EB	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EC	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	ED	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EE	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EF	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EG	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EI	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EN	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	EO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EP	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Ec	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	ES	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	ET	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EW	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	EZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FA	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FB	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FC	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FD	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FE	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FF	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FG	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FI	129	Total 968	C 602	N 171	O 191	S 4	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace	
3	FJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FN	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FP	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Fc	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FS	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FT	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FW	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FY	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	FZ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GA	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GB	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GC	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GD	129	Total 968	C 602	N 171	O 191	S 4	0	0

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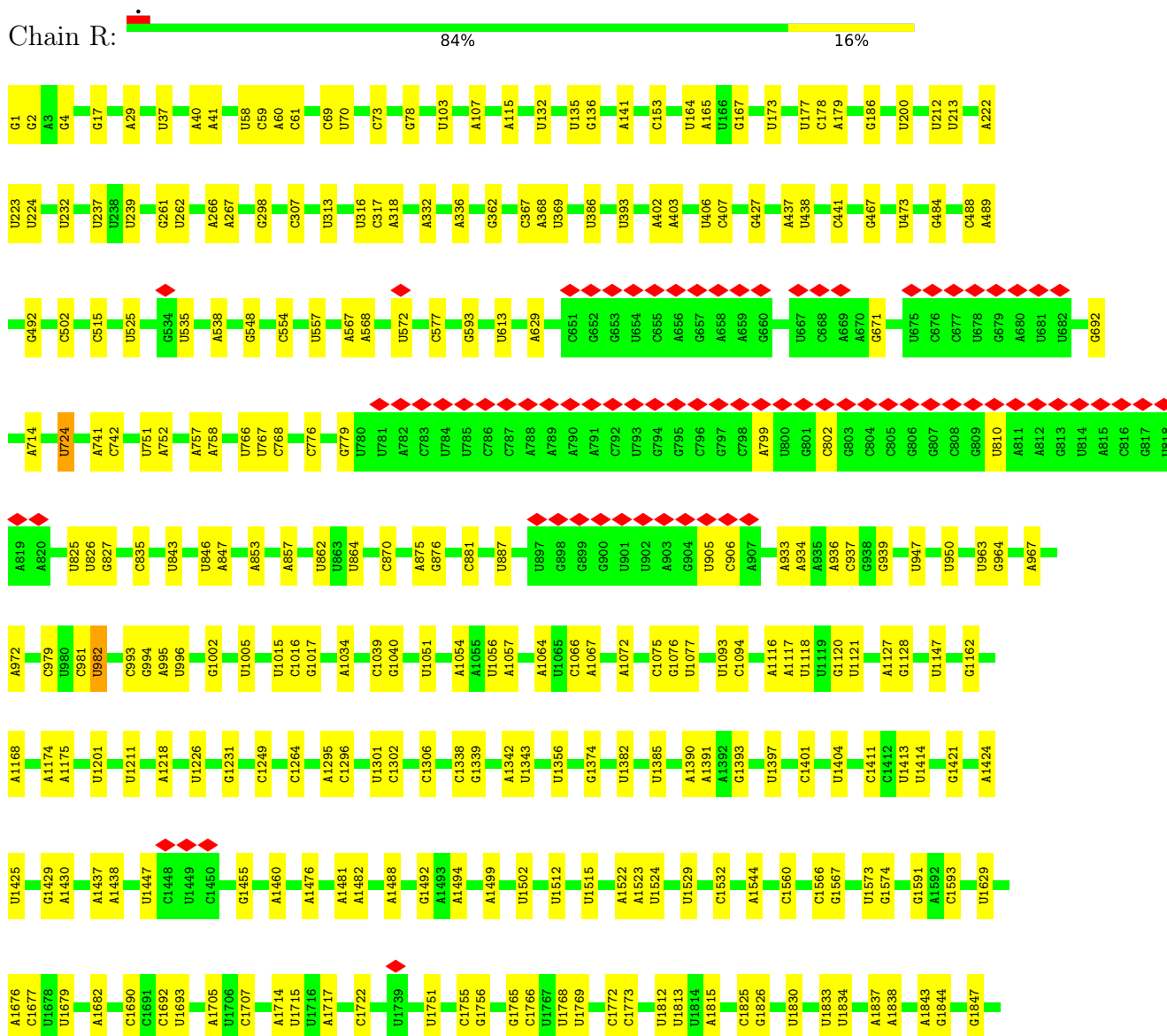
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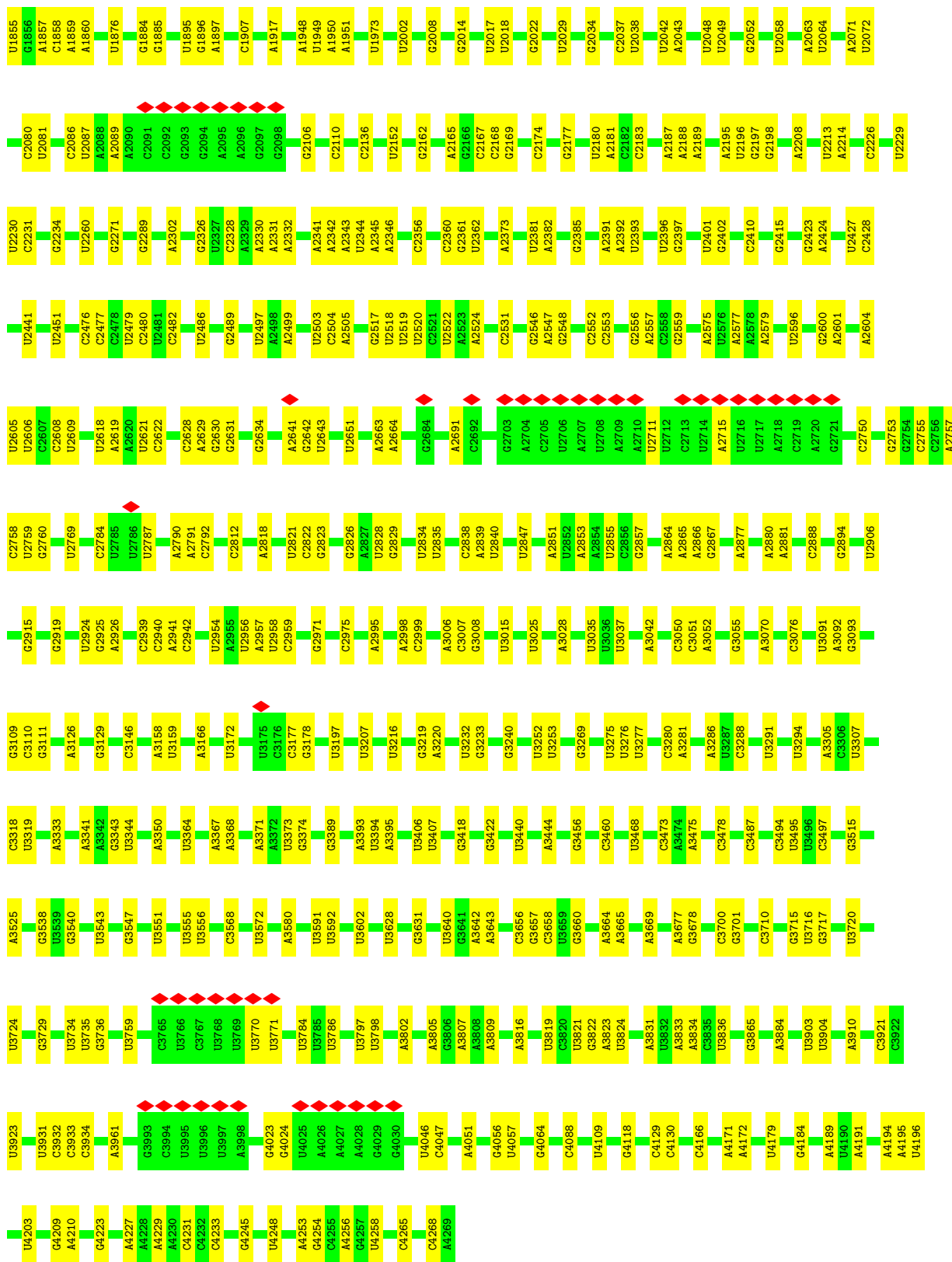
Mol	Chain	Residues	Atoms				AltConf	Trace	
3	GE	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GF	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GG	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GH	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GI	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GJ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GK	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GL	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GM	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GN	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GO	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GP	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GQ	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	Gc	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GS	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GT	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GU	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GV	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GW	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GX	129	Total 968	C 602	N 171	O 191	S 4	0	0
3	GY	129	Total 968	C 602	N 171	O 191	S 4	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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: RNA (4269-MER)





• Molecule 2: Maturation protein

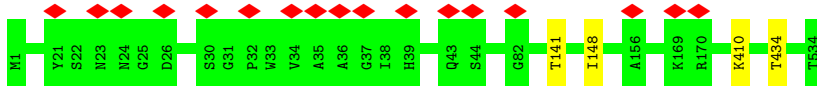
Chain a:

99%



- Molecule 2: Maturation protein

Chain b: 99%



- Molecule 3: Coat protein

Chain AB: 99%



- Molecule 3: Coat protein

Chain AC: 98%



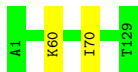
- Molecule 3: Coat protein

Chain AE: 99%



- Molecule 3: Coat protein

Chain AF: 98%



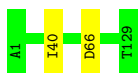
- Molecule 3: Coat protein

Chain AG: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain AH: 98%



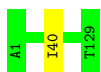
- Molecule 3: Coat protein

Chain AI:  100%

There are no outlier residues recorded for this chain.

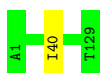
- Molecule 3: Coat protein

Chain AJ:  99%



- Molecule 3: Coat protein

Chain AK:  99%



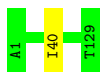
- Molecule 3: Coat protein

Chain AL:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain AM:  99%



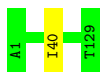
- Molecule 3: Coat protein

Chain AN:  98%



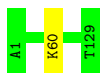
- Molecule 3: Coat protein

Chain AO:  99%



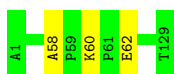
- Molecule 3: Coat protein

Chain AP:  99%



- Molecule 3: Coat protein

Chain AQ:  98%



- Molecule 3: Coat protein

Chain Ac:  100%

There are no outlier residues recorded for this chain.

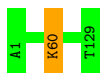
- Molecule 3: Coat protein

Chain AS:  99%



- Molecule 3: Coat protein

Chain AT:  99%



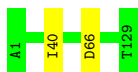
- Molecule 3: Coat protein

Chain AU:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain AV:  98%



- Molecule 3: Coat protein

Chain AW:  99%



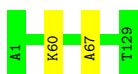
- Molecule 3: Coat protein

Chain AX: 99%



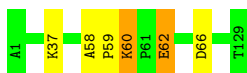
- Molecule 3: Coat protein

Chain AY: 98%



- Molecule 3: Coat protein

Chain AZ: 95%



- Molecule 3: Coat protein

Chain BA: 99%



- Molecule 3: Coat protein

Chain BB: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain BC: 98%



- Molecule 3: Coat protein

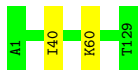
Chain BD: 99%



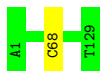
● Molecule 3: Coat protein

Chain BE:  99%

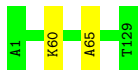
● Molecule 3: Coat protein

Chain BF:  98%

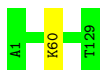
● Molecule 3: Coat protein

Chain BG:  99%

● Molecule 3: Coat protein

Chain BH:  98%

● Molecule 3: Coat protein

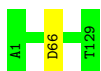
Chain BI:  99%

● Molecule 3: Coat protein

Chain BJ:  100%

There are no outlier residues recorded for this chain.

● Molecule 3: Coat protein

Chain BK:  99%

● Molecule 3: Coat protein

Chain BL:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain BM:  99%



- Molecule 3: Coat protein

Chain BN:  95% 5%



- Molecule 3: Coat protein

Chain BO:  98%



- Molecule 3: Coat protein

Chain BP:  98%



- Molecule 3: Coat protein

Chain BQ:  99%



- Molecule 3: Coat protein

Chain Bc:  99%



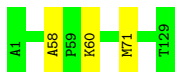
- Molecule 3: Coat protein

Chain BS:  100%

There are no outlier residues recorded for this chain.

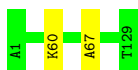
- Molecule 3: Coat protein

Chain BT:  98%



- Molecule 3: Coat protein

Chain BU:  98%



- Molecule 3: Coat protein

Chain BV:  99%



- Molecule 3: Coat protein

Chain BW:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain BX:  98%



- Molecule 3: Coat protein

Chain BY:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain BZ:  99%



- Molecule 3: Coat protein

Chain CA:  98%



- Molecule 3: Coat protein

Chain CB:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain CC:  99%



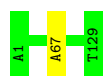
- Molecule 3: Coat protein

Chain CD:  98%



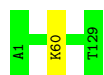
- Molecule 3: Coat protein

Chain CE:  99%



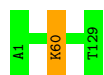
- Molecule 3: Coat protein

Chain CF:  99%



- Molecule 3: Coat protein

Chain CG:  99%



- Molecule 3: Coat protein

Chain CH:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain CI: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain CJ: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain CK: 100%

There are no outlier residues recorded for this chain.

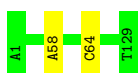
- Molecule 3: Coat protein

Chain CL: 99%



- Molecule 3: Coat protein

Chain CM: 98%



- Molecule 3: Coat protein

Chain CN: 98%



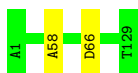
- Molecule 3: Coat protein

Chain CO: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain CP: 98%



- Molecule 3: Coat protein



- Molecule 3: Coat protein



- Molecule 3: Coat protein



- Molecule 3: Coat protein



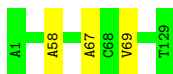
There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein



There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein



- Molecule 3: Coat protein



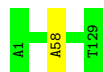
- Molecule 3: Coat protein

Chain CX:  98%



- Molecule 3: Coat protein

Chain CY:  99%



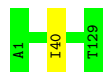
- Molecule 3: Coat protein

Chain CZ:  99%



- Molecule 3: Coat protein

Chain DA:  99%



- Molecule 3: Coat protein

Chain DB:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DC:  99%



- Molecule 3: Coat protein

Chain DD:  98%



- Molecule 3: Coat protein

Chain DE:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DF:  98%



- Molecule 3: Coat protein

Chain DG:  98%



- Molecule 3: Coat protein

Chain DH:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DI:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DJ:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DK:  98%



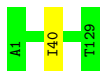
- Molecule 3: Coat protein

Chain DL:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DM:  99%



- Molecule 3: Coat protein

Chain DN: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DO: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DQ: 98%



- Molecule 3: Coat protein

Chain Dc: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DS: 98%



- Molecule 3: Coat protein

Chain DT: 98%



- Molecule 3: Coat protein

Chain DU: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DV: 97%



- Molecule 3: Coat protein

Chain DW: 99%



- Molecule 3: Coat protein

Chain DX: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DY: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain DZ: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain EA: 99%



- Molecule 3: Coat protein

Chain EB: 100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain EC: 100%

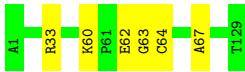
There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain ED: 98%



- Molecule 3: Coat protein

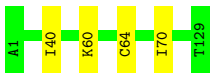


- Molecule 3: Coat protein



There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein



- Molecule 3: Coat protein



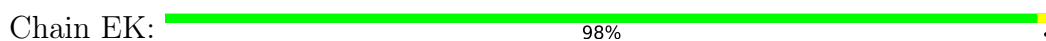
- Molecule 3: Coat protein



- Molecule 3: Coat protein



- Molecule 3: Coat protein



- Molecule 3: Coat protein

Chain EL:  98%



- Molecule 3: Coat protein

Chain EM:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain EN:  99%



- Molecule 3: Coat protein

Chain EO:  99%



- Molecule 3: Coat protein

Chain EP:  98%



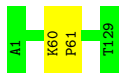
- Molecule 3: Coat protein

Chain EQ:  98%



- Molecule 3: Coat protein

Chain Ec:  98%



- Molecule 3: Coat protein

Chain ES:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain ET:  99%



- Molecule 3: Coat protein

Chain EU:  98%



- Molecule 3: Coat protein

Chain EV:  99%



- Molecule 3: Coat protein

Chain EW:  99%



- Molecule 3: Coat protein

Chain EX:  96%



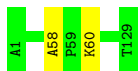
- Molecule 3: Coat protein

Chain EY:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain EZ:  98%



- Molecule 3: Coat protein

Chain FA:  100%

There are no outlier residues recorded for this chain.

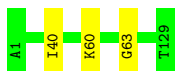
- Molecule 3: Coat protein

Chain FB:  98%



- Molecule 3: Coat protein

Chain FC:  98%



- Molecule 3: Coat protein

Chain FD:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain FE:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain FF:  98%



- Molecule 3: Coat protein

Chain FG:  100%

There are no outlier residues recorded for this chain.

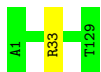
- Molecule 3: Coat protein

Chain FH:  100%

There are no outlier residues recorded for this chain.

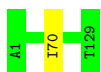
- Molecule 3: Coat protein

Chain FI:  99%



- Molecule 3: Coat protein

Chain FJ:  99%



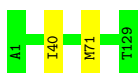
- Molecule 3: Coat protein

Chain FK:  99%



- Molecule 3: Coat protein

Chain FL:  98%



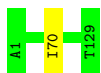
- Molecule 3: Coat protein

Chain FM:  98%



- Molecule 3: Coat protein

Chain FN:  99%



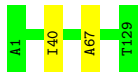
- Molecule 3: Coat protein

Chain FO:  99%



- Molecule 3: Coat protein

Chain FP:  98%



- Molecule 3: Coat protein

Chain FQ:  100%

There are no outlier residues recorded for this chain.

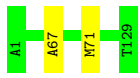
- Molecule 3: Coat protein

Chain Fc:  98%



- Molecule 3: Coat protein

Chain FS:  98%



- Molecule 3: Coat protein

Chain FT:  99%



- Molecule 3: Coat protein

Chain FU:  100%

There are no outlier residues recorded for this chain.

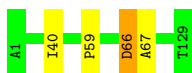
- Molecule 3: Coat protein

Chain FV:  99%



- Molecule 3: Coat protein

Chain FW:  97%



- Molecule 3: Coat protein



- Molecule 3: Coat protein



There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein



- Molecule 3: Coat protein

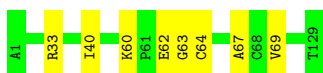


- Molecule 3: Coat protein



There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein



- Molecule 3: Coat protein



There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain GE:  97%



● Molecule 3: Coat protein

Chain GF:  99%



● Molecule 3: Coat protein

Chain GG:  99%



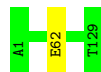
● Molecule 3: Coat protein

Chain GH:  98%



● Molecule 3: Coat protein

Chain GI:  99%



● Molecule 3: Coat protein

Chain GJ:  99%



● Molecule 3: Coat protein

Chain GK:  99%




● Molecule 3: Coat protein

Chain GL:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain GM:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain GN:  98%



- Molecule 3: Coat protein

Chain GO:  99%



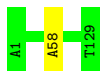
- Molecule 3: Coat protein

Chain GP:  98%



- Molecule 3: Coat protein

Chain GQ:  99%



- Molecule 3: Coat protein

Chain Gc:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Coat protein

Chain GS:  100%

There are no outlier residues recorded for this chain.

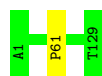
- Molecule 3: Coat protein

Chain GT:  98%



- Molecule 3: Coat protein

Chain GU:  99%



- Molecule 3: Coat protein

Chain GV:  98%



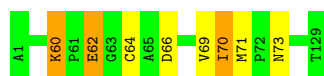
- Molecule 3: Coat protein

Chain GW:  100%

There are no outlier residues recorded for this chain.

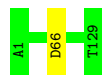
- Molecule 3: Coat protein

Chain GX:  94%



- Molecule 3: Coat protein

Chain GY:  99%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.710	Depositor
Minimum map value	-0.308	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.128	Depositor
Map size (\AA)	487.59998, 487.59998, 487.59998	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	R	0.19	0/101047	0.76	10/157333 (0.0%)
2	a	0.26	0/4409	0.54	0/5964
2	b	0.25	0/4409	0.53	0/5964
3	AB	0.27	0/985	0.52	0/1342
3	AC	0.27	0/985	0.52	0/1342
3	AE	0.30	0/985	0.54	0/1342
3	AF	0.28	0/985	0.51	0/1342
3	AG	0.29	0/985	0.53	0/1342
3	AH	0.28	0/985	0.50	0/1342
3	AI	0.30	0/985	0.52	0/1342
3	AJ	0.29	0/985	0.52	0/1342
3	AK	0.29	0/985	0.53	0/1342
3	AL	0.28	0/985	0.50	0/1342
3	AM	0.29	0/985	0.54	0/1342
3	AN	0.29	0/985	0.51	0/1342
3	AO	0.27	0/985	0.51	0/1342
3	AP	0.30	0/985	0.53	0/1342
3	AQ	0.31	0/985	0.52	0/1342
3	AS	0.30	0/985	0.53	0/1342
3	AT	0.28	0/985	0.53	0/1342
3	AU	0.29	0/985	0.53	0/1342
3	AV	0.29	0/985	0.53	0/1342
3	AW	0.29	0/985	0.54	0/1342
3	AX	0.28	0/985	0.52	0/1342
3	AY	0.29	0/985	0.52	0/1342
3	AZ	0.32	0/985	0.55	0/1342
3	Ac	0.29	0/985	0.53	0/1342
3	BA	0.29	0/985	0.53	0/1342
3	BB	0.29	0/985	0.53	0/1342
3	BC	0.30	0/985	0.56	0/1342
3	BD	0.29	0/985	0.51	0/1342
3	BE	0.29	0/985	0.51	0/1342
3	BF	0.29	0/985	0.52	0/1342
3	BG	0.29	0/985	0.55	1/1342 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	BH	0.29	0/985	0.53	0/1342
3	BI	0.29	0/985	0.53	0/1342
3	BJ	0.29	0/985	0.52	0/1342
3	BK	0.28	0/985	0.53	0/1342
3	BL	0.28	0/985	0.51	0/1342
3	BM	0.28	0/985	0.53	0/1342
3	BN	0.35	0/985	0.55	0/1342
3	BO	0.29	0/985	0.53	0/1342
3	BP	0.29	0/985	0.54	0/1342
3	BQ	0.29	0/985	0.51	0/1342
3	BS	0.30	0/985	0.51	0/1342
3	BT	0.28	0/985	0.53	0/1342
3	BU	0.29	0/985	0.53	0/1342
3	BV	0.32	0/985	0.55	0/1342
3	BW	0.29	0/985	0.53	0/1342
3	BX	0.29	0/985	0.53	0/1342
3	BY	0.29	0/985	0.50	0/1342
3	BZ	0.29	0/985	0.55	0/1342
3	Bc	0.29	0/985	0.53	0/1342
3	CA	0.30	0/985	0.57	0/1342
3	CB	0.29	0/985	0.50	0/1342
3	CC	0.29	0/985	0.53	0/1342
3	CD	0.28	0/985	0.55	0/1342
3	CE	0.30	0/985	0.56	0/1342
3	CF	0.29	0/985	0.52	0/1342
3	CG	0.28	0/985	0.51	0/1342
3	CH	0.29	0/985	0.51	0/1342
3	CI	0.29	0/985	0.53	0/1342
3	CJ	0.30	0/985	0.56	0/1342
3	CK	0.29	0/985	0.53	0/1342
3	CL	0.28	0/985	0.50	0/1342
3	CM	0.27	0/985	0.54	0/1342
3	CN	0.29	0/985	0.56	0/1342
3	CO	0.28	0/985	0.55	0/1342
3	CP	0.28	0/985	0.53	0/1342
3	CQ	0.28	0/985	0.50	0/1342
3	CS	0.28	0/985	0.53	0/1342
3	CT	0.28	0/985	0.51	0/1342
3	CU	0.30	0/985	0.54	0/1342
3	CV	0.28	0/985	0.52	0/1342
3	CW	0.28	0/985	0.50	0/1342
3	CX	0.28	0/985	0.51	0/1342
3	CY	0.28	0/985	0.52	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	CZ	0.28	0/985	0.51	0/1342
3	Cc	0.31	0/985	0.52	0/1342
3	DA	0.29	0/985	0.51	0/1342
3	DB	0.29	0/985	0.54	0/1342
3	DC	0.28	0/985	0.55	0/1342
3	DD	0.29	0/985	0.52	0/1342
3	DE	0.30	0/985	0.53	0/1342
3	DF	0.29	0/985	0.54	0/1342
3	DG	0.29	0/985	0.54	0/1342
3	DH	0.29	0/985	0.51	0/1342
3	DI	0.27	0/985	0.52	0/1342
3	DJ	0.28	0/985	0.52	0/1342
3	DK	0.29	0/985	0.50	0/1342
3	DL	0.29	0/985	0.53	0/1342
3	DM	0.29	0/985	0.52	0/1342
3	DN	0.30	0/985	0.56	0/1342
3	DO	0.27	0/985	0.54	0/1342
3	DQ	0.28	0/985	0.53	0/1342
3	DS	0.29	0/985	0.53	0/1342
3	DT	0.29	0/985	0.53	0/1342
3	DU	0.28	0/985	0.51	0/1342
3	DV	0.29	0/985	0.51	0/1342
3	DW	0.28	0/985	0.52	0/1342
3	DX	0.29	0/985	0.53	0/1342
3	DY	0.31	0/985	0.54	0/1342
3	DZ	0.28	0/985	0.52	0/1342
3	Dc	0.29	0/985	0.50	0/1342
3	EA	0.28	0/985	0.49	0/1342
3	EB	0.29	0/985	0.53	0/1342
3	EC	0.29	0/985	0.51	0/1342
3	ED	0.29	0/985	0.52	0/1342
3	EE	0.31	0/985	0.53	0/1342
3	EF	0.31	0/985	0.54	0/1342
3	EG	0.33	0/985	0.54	0/1342
3	EH	0.30	0/985	0.53	0/1342
3	EI	0.29	0/985	0.53	0/1342
3	EJ	0.30	0/985	0.52	0/1342
3	EK	0.29	0/985	0.55	0/1342
3	EL	0.31	0/985	0.53	0/1342
3	EM	0.28	0/985	0.53	0/1342
3	EN	0.29	0/985	0.53	0/1342
3	EO	0.29	0/985	0.52	0/1342
3	EP	0.29	0/985	0.51	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	EQ	0.29	0/985	0.51	0/1342
3	ES	0.28	0/985	0.52	0/1342
3	ET	0.29	0/985	0.55	1/1342 (0.1%)
3	EU	0.28	0/985	0.54	0/1342
3	EV	0.29	0/985	0.54	0/1342
3	EW	0.29	0/985	0.53	0/1342
3	EX	0.30	0/985	0.55	0/1342
3	EY	0.29	0/985	0.52	0/1342
3	EZ	0.30	0/985	0.52	0/1342
3	Ec	0.31	0/985	0.56	1/1342 (0.1%)
3	FA	0.28	0/985	0.53	0/1342
3	FB	0.28	0/985	0.55	0/1342
3	FC	0.27	0/985	0.49	0/1342
3	FD	0.28	0/985	0.53	0/1342
3	FE	0.29	0/985	0.55	0/1342
3	FF	0.28	0/985	0.53	0/1342
3	FG	0.28	0/985	0.52	0/1342
3	FH	0.29	0/985	0.54	0/1342
3	FI	0.29	0/985	0.54	0/1342
3	FJ	0.29	0/985	0.52	0/1342
3	FK	0.30	0/985	0.52	0/1342
3	FL	0.28	0/985	0.53	0/1342
3	FM	0.28	0/985	0.53	0/1342
3	FN	0.28	0/985	0.52	0/1342
3	FO	0.30	0/985	0.55	0/1342
3	FP	0.29	0/985	0.52	0/1342
3	FQ	0.28	0/985	0.52	0/1342
3	FS	0.28	0/985	0.52	0/1342
3	FT	0.29	0/985	0.52	0/1342
3	FU	0.29	0/985	0.51	0/1342
3	FV	0.28	0/985	0.52	0/1342
3	FW	0.31	0/985	0.56	0/1342
3	FX	0.29	0/985	0.54	0/1342
3	FY	0.28	0/985	0.50	0/1342
3	FZ	0.29	0/985	0.54	0/1342
3	Fc	0.29	0/985	0.56	0/1342
3	GA	0.28	0/985	0.54	0/1342
3	GB	0.29	0/985	0.51	0/1342
3	GC	0.39	0/985	0.57	1/1342 (0.1%)
3	GD	0.28	0/985	0.52	0/1342
3	GE	0.29	0/985	0.54	0/1342
3	GF	0.28	0/985	0.53	0/1342
3	GG	0.28	0/985	0.49	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	GH	0.29	0/985	0.52	0/1342
3	GI	0.29	0/985	0.52	0/1342
3	GJ	0.29	0/985	0.51	0/1342
3	GK	0.29	0/985	0.51	0/1342
3	GL	0.29	0/985	0.51	0/1342
3	GM	0.28	0/985	0.53	0/1342
3	GN	0.29	0/985	0.53	0/1342
3	GO	0.29	0/985	0.52	0/1342
3	GP	0.28	0/985	0.50	0/1342
3	GQ	0.28	0/985	0.52	0/1342
3	GS	0.28	0/985	0.52	0/1342
3	GT	0.29	0/985	0.50	0/1342
3	GU	0.29	0/985	0.51	0/1342
3	GV	0.29	0/985	0.53	0/1342
3	GW	0.29	0/985	0.53	0/1342
3	GX	0.40	0/985	0.58	0/1342
3	GY	0.29	0/985	0.53	0/1342
3	Gc	0.29	0/985	0.52	0/1342
All	All	0.26	0/285195	0.63	14/408137 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BG	68	CYS	CA-CB-SG	7.13	126.83	114.00
1	R	1773	C	N3-C2-O2	-6.86	117.10	121.90
1	R	1094	C	N1-C2-O2	6.72	122.93	118.90
1	R	4223	G	N1-C6-O6	-6.67	115.90	119.90
1	R	4223	G	C5-C6-O6	6.38	132.43	128.60
1	R	1094	C	N3-C2-O2	-6.13	117.61	121.90
3	Ec	60	LYS	C-N-CD	-5.55	108.40	120.60
3	ET	40	ILE	CG1-CB-CG2	-5.50	99.30	111.40
1	R	1773	C	N1-C2-O2	5.37	122.12	118.90
1	R	724	U	N3-C2-O2	-5.23	118.54	122.20
1	R	1772	C	N3-C2-O2	-5.14	118.30	121.90
1	R	982	U	C2-N1-C1'	5.14	123.87	117.70
1	R	3934	C	N3-C2-O2	-5.09	118.34	121.90
3	GC	64	CYS	CA-CB-SG	-5.06	104.89	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

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	
2	a	532/534 (100%)	492 (92%)	38 (7%)	2 (0%)	34	68
2	b	532/534 (100%)	488 (92%)	41 (8%)	3 (1%)	25	59
3	AB	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
3	AC	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	9	36
3	AE	127/129 (98%)	114 (90%)	12 (9%)	1 (1%)	19	53
3	AF	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9	36
3	AG	127/129 (98%)	112 (88%)	15 (12%)	0	100	100
3	AH	127/129 (98%)	120 (94%)	5 (4%)	2 (2%)	9	36
3	AI	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	AJ	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	53
3	AK	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	AL	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	AM	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	AN	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	AO	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	AP	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	AQ	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	6	26
3	AS	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	53
3	AT	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	AU	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	AV	127/129 (98%)	114 (90%)	11 (9%)	2 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AW	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	53
3	AX	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	AY	127/129 (98%)	120 (94%)	5 (4%)	2 (2%)	9	36
3	AZ	127/129 (98%)	115 (91%)	7 (6%)	5 (4%)	3	17
3	Ac	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	BA	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	BB	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
3	BC	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	9	36
3	BD	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	BE	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	53
3	BF	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	BG	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	BH	127/129 (98%)	120 (94%)	5 (4%)	2 (2%)	9	36
3	BI	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	BJ	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	BK	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	BL	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	BM	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	BN	127/129 (98%)	113 (89%)	12 (9%)	2 (2%)	9	36
3	BO	127/129 (98%)	114 (90%)	11 (9%)	2 (2%)	9	36
3	BP	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	BQ	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	BS	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	BT	127/129 (98%)	114 (90%)	11 (9%)	2 (2%)	9	36
3	BU	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	9	36
3	BV	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	53
3	BW	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	BX	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9	36
3	BY	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	BZ	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	Bc	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CA	127/129 (98%)	115 (91%)	10 (8%)	2 (2%)	9	36
3	CB	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
3	CC	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	CD	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	9	36
3	CE	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	CF	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	53
3	CG	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	53
3	CH	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	CI	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	CJ	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	CK	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	CL	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	CM	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	9	36
3	CN	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9	36
3	CO	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	CP	127/129 (98%)	115 (91%)	10 (8%)	2 (2%)	9	36
3	CQ	127/129 (98%)	122 (96%)	3 (2%)	2 (2%)	9	36
3	CS	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	CT	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	CU	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	CV	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	6	26
3	CW	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	53
3	CX	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	53
3	CY	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	53
3	CZ	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	Cc	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	53
3	DA	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	DB	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	DC	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	DD	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9	36
3	DE	127/129 (98%)	121 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	DF	127/129 (98%)	121 (95%)	4 (3%)	2 (2%)	9	36
3	DG	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	19	53
3	DH	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	DI	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	DJ	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	DK	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	9	36
3	DL	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	DM	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	DN	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
3	DO	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
3	DQ	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	53
3	DS	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9	36
3	DT	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	19	53
3	DU	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	DV	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	6	26
3	DW	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	DX	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	DY	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	DZ	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	Dc	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	EA	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	EB	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	EC	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
3	ED	127/129 (98%)	120 (94%)	5 (4%)	2 (2%)	9	36
3	EE	127/129 (98%)	115 (91%)	8 (6%)	4 (3%)	4	22
3	EF	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
3	EG	127/129 (98%)	120 (94%)	3 (2%)	4 (3%)	4	22
3	EH	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	EI	127/129 (98%)	115 (91%)	10 (8%)	2 (2%)	9	36
3	EJ	127/129 (98%)	119 (94%)	5 (4%)	3 (2%)	6	26
3	EK	127/129 (98%)	123 (97%)	2 (2%)	2 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	EL	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	9	36
3	EM	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	EN	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	19	53
3	EO	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	EP	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	9	36
3	EQ	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9	36
3	ES	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	ET	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	53
3	EU	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	19	53
3	EV	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	EW	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	53
3	EX	127/129 (98%)	110 (87%)	13 (10%)	4 (3%)	4	22
3	EY	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
3	EZ	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	9	36
3	Ec	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	19	53
3	FA	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	FB	127/129 (98%)	115 (91%)	9 (7%)	3 (2%)	6	26
3	FC	127/129 (98%)	118 (93%)	6 (5%)	3 (2%)	6	26
3	FD	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
3	FE	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
3	FF	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	FG	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
3	FH	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
3	FI	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	FJ	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	FK	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
3	FL	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	53
3	FM	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9	36
3	FN	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	FO	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	53
3	FP	127/129 (98%)	120 (94%)	5 (4%)	2 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	FQ	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	FS	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	FT	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	FU	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	FV	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	53
3	FW	127/129 (98%)	112 (88%)	11 (9%)	4 (3%)	4	22
3	FX	127/129 (98%)	117 (92%)	8 (6%)	2 (2%)	9	36
3	FY	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
3	FZ	127/129 (98%)	113 (89%)	11 (9%)	3 (2%)	6	26
3	Fc	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9	36
3	GA	127/129 (98%)	116 (91%)	10 (8%)	1 (1%)	19	53
3	GB	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
3	GC	127/129 (98%)	117 (92%)	7 (6%)	3 (2%)	6	26
3	GD	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	GE	127/129 (98%)	119 (94%)	5 (4%)	3 (2%)	6	26
3	GF	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	GG	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	53
3	GH	127/129 (98%)	122 (96%)	3 (2%)	2 (2%)	9	36
3	GI	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	53
3	GJ	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	GK	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	53
3	GL	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
3	GM	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
3	GN	127/129 (98%)	118 (93%)	7 (6%)	2 (2%)	9	36
3	GO	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	GP	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	53
3	GQ	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	53
3	GS	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
3	GT	127/129 (98%)	119 (94%)	6 (5%)	2 (2%)	9	36
3	GU	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	53
3	GV	127/129 (98%)	116 (91%)	9 (7%)	2 (2%)	9	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	GW	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
3	GX	127/129 (98%)	114 (90%)	9 (7%)	4 (3%)	4	22
3	GY	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	53
3	Gc	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
All	All	23670/24030 (98%)	22117 (93%)	1356 (6%)	197 (1%)	24	53

All (197) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	148	ILE
2	b	148	ILE
3	AV	66	ASP
3	AX	70	ILE
3	AY	67	ALA
3	AZ	58	ALA
3	AZ	62	GLU
3	BA	66	ASP
3	BC	66	ASP
3	BK	66	ASP
3	BO	62	GLU
3	Bc	67	ALA
3	BT	58	ALA
3	BU	67	ALA
3	BZ	67	ALA
3	CD	67	ALA
3	CE	67	ALA
3	CM	64	CYS
3	CP	66	ASP
3	CW	67	ALA
3	CY	58	ALA
3	CZ	67	ALA
3	DC	67	ALA
3	DD	67	ALA
3	DT	62	GLU
3	DV	59	PRO
3	ED	66	ASP
3	EK	65	ALA
3	EL	58	ALA
3	EL	59	PRO
3	EN	66	ASP
3	Ec	61	PRO

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Mol	Chain	Res	Type
3	ET	40	ILE
3	EV	67	ALA
3	EX	59	PRO
3	EX	69	VAL
3	FB	67	ALA
3	FF	70	ILE
3	FM	62	GLU
3	FV	67	ALA
3	FW	59	PRO
3	FW	66	ASP
3	FW	67	ALA
3	FZ	58	ALA
3	FZ	61	PRO
3	GA	40	ILE
3	GE	58	ALA
3	GG	70	ILE
3	GN	58	ALA
3	GO	67	ALA
3	GQ	58	ALA
3	GU	61	PRO
3	GV	58	ALA
3	GV	61	PRO
3	AC	67	ALA
3	AF	70	ILE
3	AQ	62	GLU
3	BD	67	ALA
3	BH	65	ALA
3	CA	70	ILE
3	CC	58	ALA
3	CN	66	ASP
3	CN	70	ILE
3	CQ	67	ALA
3	DK	62	GLU
3	DV	58	ALA
3	EJ	66	ASP
3	EP	66	ASP
3	EP	67	ALA
3	EX	70	ILE
3	FB	58	ALA
3	FM	66	ASP
3	FN	70	ILE
3	FO	67	ALA

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Mol	Chain	Res	Type
3	FS	67	ALA
3	FX	66	ASP
3	FZ	67	ALA
3	GC	63	GLY
3	GC	67	ALA
3	GF	70	ILE
3	GX	62	GLU
2	a	141	THR
2	b	141	THR
3	AN	70	ILE
3	AS	58	ALA
3	AZ	66	ASP
3	CA	67	ALA
3	DF	65	ALA
3	EE	64	CYS
3	EE	67	ALA
3	EI	58	ALA
3	GH	70	ILE
3	GX	66	ASP
3	AH	66	ASP
3	AQ	58	ALA
3	BH	60	LYS
3	BT	60	LYS
3	CF	60	LYS
3	CP	58	ALA
3	CV	67	ALA
3	DM	40	ILE
3	DQ	67	ALA
3	EG	60	LYS
3	GK	58	ALA
3	GT	67	ALA
3	GX	60	LYS
3	GX	70	ILE
3	AY	60	LYS
3	AZ	59	PRO
3	AZ	60	LYS
3	BQ	70	ILE
3	CM	58	ALA
3	DD	70	ILE
3	DS	70	ILE
3	EE	60	LYS
3	EJ	70	ILE

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Mol	Chain	Res	Type
3	EO	58	ALA
3	EQ	66	ASP
3	EW	58	ALA
3	EZ	58	ALA
3	FJ	70	ILE
3	FP	67	ALA
3	Fc	40	ILE
3	GE	70	ILE
3	GI	62	GLU
3	GT	58	ALA
2	b	434	THR
3	AE	66	ASP
3	BM	66	ASP
3	BN	64	CYS
3	BU	60	LYS
3	BV	66	ASP
3	BX	70	ILE
3	CS	70	ILE
3	EG	64	CYS
3	EG	70	ILE
3	EH	70	ILE
3	EK	66	ASP
3	EZ	60	LYS
3	FB	70	ILE
3	FC	60	LYS
3	FC	63	GLY
3	GY	66	ASP
3	BP	70	ILE
3	CD	40	ILE
3	CV	58	ALA
3	FC	40	ILE
3	AM	40	ILE
3	AO	40	ILE
3	AW	40	ILE
3	BC	58	ALA
3	EI	70	ILE
3	Fc	61	PRO
3	FW	40	ILE
3	AH	40	ILE
3	AK	40	ILE
3	AQ	60	LYS
3	CG	60	LYS

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Mol	Chain	Res	Type
3	CQ	40	ILE
3	CV	69	VAL
3	CX	40	ILE
3	DG	40	ILE
3	DK	58	ALA
3	DW	40	ILE
3	FT	70	ILE
3	GN	69	VAL
3	GP	40	ILE
3	AF	60	LYS
3	AT	60	LYS
3	AV	40	ILE
3	BE	40	ILE
3	BF	40	ILE
3	BN	38	VAL
3	BO	58	ALA
3	BX	40	ILE
3	Cc	40	ILE
3	DA	40	ILE
3	DV	71	MET
3	ED	40	ILE
3	EX	40	ILE
3	FP	40	ILE
3	GC	40	ILE
3	GE	40	ILE
3	GH	40	ILE
3	AC	40	ILE
3	AJ	40	ILE
3	CL	40	ILE
3	DF	40	ILE
3	DS	40	ILE
3	EE	63	GLY
3	EG	40	ILE
3	EJ	40	ILE
3	EQ	40	ILE
3	EU	58	ALA
3	FL	40	ILE
3	FX	40	ILE
3	GJ	40	ILE

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 PDB entries followed by that with respect to all EM entries.

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	
2	a	466/466 (100%)	461 (99%)	5 (1%)	73	88
2	b	466/466 (100%)	465 (100%)	1 (0%)	93	97
3	AB	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	AC	108/108 (100%)	108 (100%)	0	100	100
3	AE	108/108 (100%)	108 (100%)	0	100	100
3	AF	108/108 (100%)	108 (100%)	0	100	100
3	AG	108/108 (100%)	108 (100%)	0	100	100
3	AH	108/108 (100%)	108 (100%)	0	100	100
3	AI	108/108 (100%)	108 (100%)	0	100	100
3	AJ	108/108 (100%)	108 (100%)	0	100	100
3	AK	108/108 (100%)	108 (100%)	0	100	100
3	AL	108/108 (100%)	108 (100%)	0	100	100
3	AM	108/108 (100%)	108 (100%)	0	100	100
3	AN	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	AO	108/108 (100%)	108 (100%)	0	100	100
3	AP	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	AQ	108/108 (100%)	108 (100%)	0	100	100
3	AS	108/108 (100%)	108 (100%)	0	100	100
3	AT	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	AU	108/108 (100%)	108 (100%)	0	100	100
3	AV	108/108 (100%)	108 (100%)	0	100	100
3	AW	108/108 (100%)	108 (100%)	0	100	100
3	AX	108/108 (100%)	108 (100%)	0	100	100
3	AY	108/108 (100%)	108 (100%)	0	100	100
3	AZ	108/108 (100%)	105 (97%)	3 (3%)	43	72
3	Ac	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	BA	108/108 (100%)	108 (100%)	0	100	100
3	BB	108/108 (100%)	108 (100%)	0	100	100
3	BC	108/108 (100%)	108 (100%)	0	100	100
3	BD	108/108 (100%)	108 (100%)	0	100	100
3	BE	108/108 (100%)	108 (100%)	0	100	100
3	BF	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	BG	108/108 (100%)	108 (100%)	0	100	100
3	BH	108/108 (100%)	108 (100%)	0	100	100
3	BI	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	BJ	108/108 (100%)	108 (100%)	0	100	100
3	BK	108/108 (100%)	108 (100%)	0	100	100
3	BL	108/108 (100%)	108 (100%)	0	100	100
3	BM	108/108 (100%)	108 (100%)	0	100	100
3	BN	108/108 (100%)	104 (96%)	4 (4%)	34	66
3	BO	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	BP	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	BQ	108/108 (100%)	108 (100%)	0	100	100
3	BS	108/108 (100%)	108 (100%)	0	100	100
3	BT	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	BU	108/108 (100%)	108 (100%)	0	100	100
3	BV	108/108 (100%)	108 (100%)	0	100	100
3	BW	108/108 (100%)	108 (100%)	0	100	100
3	BX	108/108 (100%)	108 (100%)	0	100	100
3	BY	108/108 (100%)	108 (100%)	0	100	100
3	BZ	108/108 (100%)	108 (100%)	0	100	100
3	Bc	108/108 (100%)	108 (100%)	0	100	100
3	CA	108/108 (100%)	108 (100%)	0	100	100
3	CB	108/108 (100%)	108 (100%)	0	100	100
3	CC	108/108 (100%)	108 (100%)	0	100	100
3	CD	108/108 (100%)	108 (100%)	0	100	100
3	CE	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	CF	108/108 (100%)	108 (100%)	0	100	100
3	CG	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	CH	108/108 (100%)	108 (100%)	0	100	100
3	CI	108/108 (100%)	108 (100%)	0	100	100
3	CJ	108/108 (100%)	108 (100%)	0	100	100
3	CK	108/108 (100%)	108 (100%)	0	100	100
3	CL	108/108 (100%)	108 (100%)	0	100	100
3	CM	108/108 (100%)	108 (100%)	0	100	100
3	CN	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	CO	108/108 (100%)	108 (100%)	0	100	100
3	CP	108/108 (100%)	108 (100%)	0	100	100
3	CQ	108/108 (100%)	108 (100%)	0	100	100
3	CS	108/108 (100%)	108 (100%)	0	100	100
3	CT	108/108 (100%)	108 (100%)	0	100	100
3	CU	108/108 (100%)	108 (100%)	0	100	100
3	CV	108/108 (100%)	108 (100%)	0	100	100
3	CW	108/108 (100%)	108 (100%)	0	100	100
3	CX	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	CY	108/108 (100%)	108 (100%)	0	100	100
3	CZ	108/108 (100%)	108 (100%)	0	100	100
3	Cc	108/108 (100%)	108 (100%)	0	100	100
3	DA	108/108 (100%)	108 (100%)	0	100	100
3	DB	108/108 (100%)	108 (100%)	0	100	100
3	DC	108/108 (100%)	108 (100%)	0	100	100
3	DD	108/108 (100%)	108 (100%)	0	100	100
3	DE	108/108 (100%)	108 (100%)	0	100	100
3	DF	108/108 (100%)	108 (100%)	0	100	100
3	DG	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	DH	108/108 (100%)	108 (100%)	0	100	100
3	DI	108/108 (100%)	108 (100%)	0	100	100
3	DJ	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	DK	108/108 (100%)	108 (100%)	0	100	100
3	DL	108/108 (100%)	108 (100%)	0	100	100
3	DM	108/108 (100%)	108 (100%)	0	100	100
3	DN	108/108 (100%)	108 (100%)	0	100	100
3	DO	108/108 (100%)	108 (100%)	0	100	100
3	DQ	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	DS	108/108 (100%)	108 (100%)	0	100	100
3	DT	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	DU	108/108 (100%)	108 (100%)	0	100	100
3	DV	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	DW	108/108 (100%)	108 (100%)	0	100	100
3	DX	108/108 (100%)	108 (100%)	0	100	100
3	DY	108/108 (100%)	108 (100%)	0	100	100
3	DZ	108/108 (100%)	108 (100%)	0	100	100
3	Dc	108/108 (100%)	108 (100%)	0	100	100
3	EA	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	EB	108/108 (100%)	108 (100%)	0	100	100
3	EC	108/108 (100%)	108 (100%)	0	100	100
3	ED	108/108 (100%)	108 (100%)	0	100	100
3	EE	108/108 (100%)	106 (98%)	2 (2%)	57	80
3	EF	108/108 (100%)	108 (100%)	0	100	100
3	EG	108/108 (100%)	108 (100%)	0	100	100
3	EH	108/108 (100%)	108 (100%)	0	100	100
3	EI	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	EJ	108/108 (100%)	108 (100%)	0	100	100
3	EK	108/108 (100%)	108 (100%)	0	100	100
3	EL	108/108 (100%)	108 (100%)	0	100	100
3	EM	108/108 (100%)	108 (100%)	0	100	100
3	EN	108/108 (100%)	108 (100%)	0	100	100
3	EO	108/108 (100%)	108 (100%)	0	100	100
3	EP	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	EQ	108/108 (100%)	108 (100%)	0	100	100
3	ES	108/108 (100%)	108 (100%)	0	100	100
3	ET	108/108 (100%)	108 (100%)	0	100	100
3	EU	108/108 (100%)	106 (98%)	2 (2%)	57	80
3	EV	108/108 (100%)	108 (100%)	0	100	100
3	EW	108/108 (100%)	108 (100%)	0	100	100
3	EX	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	EY	108/108 (100%)	108 (100%)	0	100	100
3	EZ	108/108 (100%)	108 (100%)	0	100	100
3	Ec	108/108 (100%)	108 (100%)	0	100	100
3	FA	108/108 (100%)	108 (100%)	0	100	100
3	FB	108/108 (100%)	108 (100%)	0	100	100
3	FC	108/108 (100%)	108 (100%)	0	100	100
3	FD	108/108 (100%)	108 (100%)	0	100	100
3	FE	108/108 (100%)	108 (100%)	0	100	100
3	FF	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	FG	108/108 (100%)	108 (100%)	0	100	100
3	FH	108/108 (100%)	108 (100%)	0	100	100
3	FI	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	FJ	108/108 (100%)	108 (100%)	0	100	100
3	FK	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	FL	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	FM	108/108 (100%)	108 (100%)	0	100	100
3	FN	108/108 (100%)	108 (100%)	0	100	100
3	FO	108/108 (100%)	108 (100%)	0	100	100
3	FP	108/108 (100%)	108 (100%)	0	100	100
3	FQ	108/108 (100%)	108 (100%)	0	100	100
3	FS	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	FT	108/108 (100%)	108 (100%)	0	100	100
3	FU	108/108 (100%)	108 (100%)	0	100	100
3	FV	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	FW	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	FX	108/108 (100%)	108 (100%)	0	100	100
3	FY	108/108 (100%)	108 (100%)	0	100	100
3	FZ	108/108 (100%)	108 (100%)	0	100	100
3	Fc	108/108 (100%)	108 (100%)	0	100	100
3	GA	108/108 (100%)	108 (100%)	0	100	100
3	GB	108/108 (100%)	108 (100%)	0	100	100
3	GC	108/108 (100%)	104 (96%)	4 (4%)	34	66
3	GD	108/108 (100%)	108 (100%)	0	100	100
3	GE	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	GF	108/108 (100%)	108 (100%)	0	100	100
3	GG	108/108 (100%)	108 (100%)	0	100	100
3	GH	108/108 (100%)	108 (100%)	0	100	100
3	GI	108/108 (100%)	108 (100%)	0	100	100
3	GJ	108/108 (100%)	108 (100%)	0	100	100
3	GK	108/108 (100%)	108 (100%)	0	100	100
3	GL	108/108 (100%)	108 (100%)	0	100	100
3	GM	108/108 (100%)	108 (100%)	0	100	100
3	GN	108/108 (100%)	108 (100%)	0	100	100
3	GO	108/108 (100%)	108 (100%)	0	100	100
3	GP	108/108 (100%)	107 (99%)	1 (1%)	78	91
3	GQ	108/108 (100%)	108 (100%)	0	100	100
3	GS	108/108 (100%)	108 (100%)	0	100	100
3	GT	108/108 (100%)	108 (100%)	0	100	100
3	GU	108/108 (100%)	108 (100%)	0	100	100
3	GV	108/108 (100%)	108 (100%)	0	100	100
3	GW	108/108 (100%)	108 (100%)	0	100	100
3	GX	108/108 (100%)	101 (94%)	7 (6%)	17	47
3	GY	108/108 (100%)	108 (100%)	0	100	100
3	Gc	108/108 (100%)	108 (100%)	0	100	100
All	All	20156/20156 (100%)	20101 (100%)	55 (0%)	92	96

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	a	176	ARG
2	a	225	ASN
2	a	258	LYS
2	a	499	ARG
2	a	525	ARG
2	b	410	LYS
3	AB	79	ARG
3	AN	35	ARG
3	AP	60	LYS
3	AT	60	LYS
3	AZ	37	LYS
3	AZ	60	LYS
3	AZ	62	GLU
3	BF	60	LYS
3	BI	60	LYS
3	BN	60	LYS
3	BN	61	PRO
3	BN	62	GLU
3	BN	71	MET
3	BO	35	ARG
3	BP	37	LYS
3	BT	71	MET
3	CG	60	LYS
3	CN	35	ARG
3	CX	33	ARG
3	DG	33	ARG
3	DQ	5	MET
3	DT	33	ARG
3	DV	70	ILE
3	EA	71	MET
3	EE	33	ARG
3	EE	62	GLU
3	EI	33	ARG
3	EU	33	ARG
3	EU	35	ARG
3	EX	35	ARG
3	FF	33	ARG
3	FI	33	ARG
3	FK	33	ARG
3	FL	71	MET
3	FS	71	MET
3	FW	66	ASP

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Mol	Chain	Res	Type
3	GC	33	ARG
3	GC	60	LYS
3	GC	62	GLU
3	GC	69	VAL
3	GE	33	ARG
3	GP	71	MET
3	GX	60	LYS
3	GX	62	GLU
3	GX	64	CYS
3	GX	69	VAL
3	GX	70	ILE
3	GX	71	MET
3	GX	73	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	108	GLN
2	a	272	GLN
2	a	288	GLN
2	a	338	GLN
2	a	356	GLN
2	b	108	GLN
2	b	288	GLN
3	AB	76	GLN
3	AI	75	ASN
3	AK	34	GLN
3	AN	73	ASN
3	AS	111	ASN
3	AW	6	GLN
3	BB	44	ASN
3	BG	34	GLN
3	BT	44	ASN
3	BX	34	GLN
3	BY	34	GLN
3	BZ	111	ASN
3	CA	6	GLN
3	CJ	34	GLN
3	CM	2	ASN
3	CM	34	GLN
3	CZ	2	ASN
3	DH	6	GLN

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Mol	Chain	Res	Type
3	DJ	6	GLN
3	DY	44	ASN
3	DZ	34	GLN
3	EJ	44	ASN
3	EK	111	ASN
3	FB	76	GLN
3	FE	34	GLN
3	FF	44	ASN
3	FK	34	GLN
3	FL	75	ASN
3	FQ	34	GLN
3	GC	73	ASN
3	GH	44	ASN
3	GX	73	ASN
3	GY	111	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	4269/4269 (100%)	689 (16%)	7 (0%)

All (689) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	G
1	R	4	G
1	R	17	G
1	R	29	A
1	R	37	U
1	R	41	A
1	R	58	U
1	R	59	C
1	R	60	A
1	R	61	C
1	R	69	C
1	R	70	U
1	R	73	C
1	R	78	G
1	R	103	U
1	R	107	A
1	R	115	A

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Mol	Chain	Res	Type
1	R	132	U
1	R	135	U
1	R	136	G
1	R	141	A
1	R	153	C
1	R	164	U
1	R	165	A
1	R	167	G
1	R	173	U
1	R	177	U
1	R	178	C
1	R	179	A
1	R	186	G
1	R	200	U
1	R	212	U
1	R	213	U
1	R	222	A
1	R	223	U
1	R	224	U
1	R	232	U
1	R	237	U
1	R	239	U
1	R	261	G
1	R	262	U
1	R	266	A
1	R	267	A
1	R	298	G
1	R	307	C
1	R	313	U
1	R	316	U
1	R	318	A
1	R	332	A
1	R	336	A
1	R	362	G
1	R	367	C
1	R	368	A
1	R	369	U
1	R	386	U
1	R	393	U
1	R	402	A
1	R	403	A
1	R	406	U

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Mol	Chain	Res	Type
1	R	407	C
1	R	427	G
1	R	437	A
1	R	438	U
1	R	441	C
1	R	467	G
1	R	473	U
1	R	484	G
1	R	488	C
1	R	489	A
1	R	492	G
1	R	502	C
1	R	515	C
1	R	525	U
1	R	535	U
1	R	538	A
1	R	548	G
1	R	554	C
1	R	557	U
1	R	567	A
1	R	568	A
1	R	572	U
1	R	577	C
1	R	593	G
1	R	613	U
1	R	629	A
1	R	671	G
1	R	692	G
1	R	714	A
1	R	724	U
1	R	741	A
1	R	742	C
1	R	751	U
1	R	752	A
1	R	757	A
1	R	758	A
1	R	766	U
1	R	767	U
1	R	768	C
1	R	776	C
1	R	779	G
1	R	799	A

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Mol	Chain	Res	Type
1	R	802	C
1	R	810	U
1	R	825	U
1	R	826	U
1	R	827	G
1	R	835	C
1	R	843	U
1	R	846	U
1	R	847	A
1	R	853	A
1	R	857	A
1	R	862	U
1	R	864	U
1	R	870	C
1	R	875	A
1	R	876	G
1	R	881	C
1	R	887	U
1	R	905	U
1	R	906	C
1	R	933	A
1	R	934	A
1	R	936	A
1	R	937	C
1	R	939	G
1	R	947	U
1	R	950	U
1	R	963	U
1	R	964	G
1	R	967	A
1	R	972	A
1	R	979	C
1	R	981	C
1	R	982	U
1	R	993	C
1	R	994	G
1	R	995	A
1	R	996	U
1	R	1002	G
1	R	1005	U
1	R	1015	U
1	R	1016	C

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Mol	Chain	Res	Type
1	R	1017	G
1	R	1034	A
1	R	1039	C
1	R	1040	G
1	R	1051	U
1	R	1054	A
1	R	1056	U
1	R	1057	A
1	R	1064	A
1	R	1066	C
1	R	1067	A
1	R	1072	A
1	R	1075	C
1	R	1076	G
1	R	1077	U
1	R	1093	U
1	R	1116	A
1	R	1117	A
1	R	1118	U
1	R	1120	G
1	R	1121	U
1	R	1127	A
1	R	1128	G
1	R	1147	U
1	R	1162	G
1	R	1168	A
1	R	1174	A
1	R	1175	A
1	R	1201	U
1	R	1211	U
1	R	1218	A
1	R	1226	U
1	R	1231	G
1	R	1249	C
1	R	1264	C
1	R	1295	A
1	R	1296	C
1	R	1301	U
1	R	1302	C
1	R	1306	C
1	R	1338	C
1	R	1339	G

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Mol	Chain	Res	Type
1	R	1342	A
1	R	1343	U
1	R	1356	U
1	R	1374	G
1	R	1382	U
1	R	1385	U
1	R	1390	A
1	R	1391	A
1	R	1393	G
1	R	1397	U
1	R	1401	C
1	R	1404	U
1	R	1411	C
1	R	1413	U
1	R	1414	U
1	R	1421	G
1	R	1424	A
1	R	1425	U
1	R	1429	G
1	R	1430	A
1	R	1437	A
1	R	1438	A
1	R	1447	U
1	R	1455	G
1	R	1460	A
1	R	1476	A
1	R	1481	A
1	R	1482	A
1	R	1488	A
1	R	1492	G
1	R	1494	A
1	R	1499	A
1	R	1502	U
1	R	1512	U
1	R	1515	U
1	R	1522	A
1	R	1523	A
1	R	1524	U
1	R	1529	U
1	R	1532	C
1	R	1544	A
1	R	1560	C

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Mol	Chain	Res	Type
1	R	1566	C
1	R	1567	G
1	R	1573	U
1	R	1574	G
1	R	1591	G
1	R	1593	C
1	R	1629	U
1	R	1676	A
1	R	1677	C
1	R	1679	U
1	R	1682	A
1	R	1690	C
1	R	1692	C
1	R	1693	U
1	R	1705	A
1	R	1707	C
1	R	1714	A
1	R	1715	U
1	R	1717	A
1	R	1722	C
1	R	1751	U
1	R	1755	C
1	R	1756	G
1	R	1765	G
1	R	1766	C
1	R	1768	U
1	R	1769	U
1	R	1812	U
1	R	1813	U
1	R	1815	A
1	R	1825	C
1	R	1826	G
1	R	1830	U
1	R	1833	U
1	R	1834	U
1	R	1837	A
1	R	1838	A
1	R	1843	A
1	R	1844	G
1	R	1847	G
1	R	1855	U
1	R	1857	A

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Mol	Chain	Res	Type
1	R	1858	C
1	R	1859	A
1	R	1860	A
1	R	1876	U
1	R	1884	G
1	R	1885	G
1	R	1895	U
1	R	1896	G
1	R	1897	A
1	R	1907	C
1	R	1917	A
1	R	1948	A
1	R	1949	U
1	R	1950	A
1	R	1951	A
1	R	1973	U
1	R	2002	U
1	R	2008	G
1	R	2014	G
1	R	2017	U
1	R	2018	U
1	R	2022	G
1	R	2029	U
1	R	2034	G
1	R	2037	C
1	R	2038	U
1	R	2042	U
1	R	2043	A
1	R	2048	U
1	R	2049	U
1	R	2052	G
1	R	2058	U
1	R	2063	A
1	R	2064	U
1	R	2071	A
1	R	2072	U
1	R	2080	C
1	R	2081	U
1	R	2086	C
1	R	2087	U
1	R	2089	A
1	R	2106	G

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Mol	Chain	Res	Type
1	R	2110	C
1	R	2136	C
1	R	2152	U
1	R	2162	G
1	R	2165	A
1	R	2167	C
1	R	2168	C
1	R	2169	G
1	R	2174	C
1	R	2177	G
1	R	2180	U
1	R	2181	A
1	R	2183	C
1	R	2187	A
1	R	2188	A
1	R	2189	A
1	R	2195	A
1	R	2196	U
1	R	2197	G
1	R	2198	G
1	R	2208	A
1	R	2213	U
1	R	2214	A
1	R	2226	C
1	R	2229	U
1	R	2230	U
1	R	2231	C
1	R	2234	G
1	R	2260	U
1	R	2271	G
1	R	2289	G
1	R	2302	A
1	R	2326	G
1	R	2328	C
1	R	2330	A
1	R	2331	A
1	R	2332	A
1	R	2341	A
1	R	2342	A
1	R	2343	A
1	R	2344	U
1	R	2345	A

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Mol	Chain	Res	Type
1	R	2346	A
1	R	2356	C
1	R	2360	C
1	R	2361	G
1	R	2362	U
1	R	2373	A
1	R	2381	U
1	R	2382	A
1	R	2385	G
1	R	2391	A
1	R	2392	A
1	R	2393	U
1	R	2396	U
1	R	2397	G
1	R	2401	U
1	R	2402	G
1	R	2410	C
1	R	2415	G
1	R	2423	G
1	R	2424	A
1	R	2427	U
1	R	2428	C
1	R	2441	U
1	R	2451	U
1	R	2476	C
1	R	2477	C
1	R	2479	U
1	R	2480	C
1	R	2482	C
1	R	2486	U
1	R	2489	G
1	R	2497	U
1	R	2499	A
1	R	2503	U
1	R	2504	C
1	R	2505	A
1	R	2517	G
1	R	2518	U
1	R	2519	U
1	R	2520	U
1	R	2522	U
1	R	2524	A

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Mol	Chain	Res	Type
1	R	2531	C
1	R	2546	G
1	R	2547	A
1	R	2548	G
1	R	2552	C
1	R	2553	C
1	R	2556	G
1	R	2557	A
1	R	2559	G
1	R	2575	A
1	R	2577	A
1	R	2579	A
1	R	2596	U
1	R	2600	G
1	R	2601	A
1	R	2604	A
1	R	2605	U
1	R	2606	U
1	R	2608	C
1	R	2609	U
1	R	2618	U
1	R	2619	A
1	R	2621	U
1	R	2622	C
1	R	2628	C
1	R	2629	A
1	R	2630	G
1	R	2631	G
1	R	2634	G
1	R	2641	A
1	R	2642	G
1	R	2643	U
1	R	2651	U
1	R	2663	A
1	R	2664	A
1	R	2691	A
1	R	2711	U
1	R	2715	A
1	R	2750	C
1	R	2753	G
1	R	2755	C
1	R	2757	A

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Mol	Chain	Res	Type
1	R	2758	C
1	R	2759	U
1	R	2760	G
1	R	2769	U
1	R	2784	C
1	R	2787	U
1	R	2790	A
1	R	2791	A
1	R	2792	C
1	R	2812	C
1	R	2818	A
1	R	2821	U
1	R	2822	C
1	R	2823	G
1	R	2826	G
1	R	2828	U
1	R	2829	G
1	R	2834	U
1	R	2835	U
1	R	2838	C
1	R	2839	A
1	R	2840	U
1	R	2847	U
1	R	2851	A
1	R	2853	A
1	R	2855	U
1	R	2857	G
1	R	2864	A
1	R	2865	A
1	R	2866	A
1	R	2867	G
1	R	2877	A
1	R	2880	A
1	R	2881	A
1	R	2888	C
1	R	2894	G
1	R	2906	U
1	R	2915	G
1	R	2919	G
1	R	2924	U
1	R	2925	G
1	R	2926	A

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Mol	Chain	Res	Type
1	R	2939	C
1	R	2940	C
1	R	2941	A
1	R	2942	C
1	R	2954	U
1	R	2956	U
1	R	2957	A
1	R	2958	U
1	R	2959	C
1	R	2971	G
1	R	2975	C
1	R	2995	A
1	R	2998	A
1	R	2999	C
1	R	3006	A
1	R	3007	C
1	R	3008	G
1	R	3015	U
1	R	3025	U
1	R	3028	A
1	R	3035	U
1	R	3037	U
1	R	3042	A
1	R	3050	C
1	R	3051	C
1	R	3052	A
1	R	3055	G
1	R	3070	A
1	R	3076	C
1	R	3091	U
1	R	3092	A
1	R	3093	G
1	R	3109	G
1	R	3110	C
1	R	3111	G
1	R	3126	A
1	R	3129	G
1	R	3146	C
1	R	3158	A
1	R	3159	U
1	R	3166	A
1	R	3172	U

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Mol	Chain	Res	Type
1	R	3177	C
1	R	3178	G
1	R	3197	U
1	R	3207	U
1	R	3216	U
1	R	3219	G
1	R	3220	A
1	R	3232	U
1	R	3233	G
1	R	3240	G
1	R	3252	U
1	R	3253	U
1	R	3269	G
1	R	3275	U
1	R	3276	U
1	R	3277	U
1	R	3280	C
1	R	3281	A
1	R	3286	A
1	R	3288	C
1	R	3291	U
1	R	3294	U
1	R	3305	A
1	R	3307	U
1	R	3318	C
1	R	3319	U
1	R	3333	A
1	R	3341	A
1	R	3343	G
1	R	3344	U
1	R	3350	A
1	R	3364	U
1	R	3367	A
1	R	3368	A
1	R	3371	A
1	R	3373	U
1	R	3374	G
1	R	3389	G
1	R	3393	A
1	R	3394	U
1	R	3395	A
1	R	3406	U

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Mol	Chain	Res	Type
1	R	3407	U
1	R	3418	G
1	R	3422	G
1	R	3440	U
1	R	3444	A
1	R	3456	G
1	R	3460	C
1	R	3468	U
1	R	3473	C
1	R	3475	A
1	R	3478	C
1	R	3487	C
1	R	3494	C
1	R	3495	U
1	R	3497	C
1	R	3515	G
1	R	3525	A
1	R	3538	G
1	R	3540	G
1	R	3543	U
1	R	3547	G
1	R	3551	U
1	R	3555	U
1	R	3556	U
1	R	3568	C
1	R	3572	U
1	R	3580	A
1	R	3591	U
1	R	3592	U
1	R	3602	U
1	R	3628	U
1	R	3631	G
1	R	3640	U
1	R	3642	A
1	R	3643	A
1	R	3656	C
1	R	3657	G
1	R	3658	C
1	R	3660	G
1	R	3664	A
1	R	3665	A
1	R	3669	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	3677	A
1	R	3678	G
1	R	3700	C
1	R	3701	G
1	R	3710	C
1	R	3715	G
1	R	3716	U
1	R	3717	G
1	R	3720	U
1	R	3724	U
1	R	3729	G
1	R	3734	U
1	R	3735	U
1	R	3736	G
1	R	3759	U
1	R	3770	U
1	R	3771	U
1	R	3784	U
1	R	3786	U
1	R	3797	U
1	R	3798	U
1	R	3802	A
1	R	3805	A
1	R	3807	A
1	R	3809	A
1	R	3816	A
1	R	3819	U
1	R	3821	U
1	R	3822	G
1	R	3823	A
1	R	3824	U
1	R	3831	A
1	R	3833	A
1	R	3834	A
1	R	3836	U
1	R	3865	G
1	R	3884	A
1	R	3903	U
1	R	3904	U
1	R	3910	A
1	R	3921	C
1	R	3923	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	3931	U
1	R	3932	C
1	R	3933	C
1	R	3961	A
1	R	4023	G
1	R	4024	G
1	R	4046	U
1	R	4047	C
1	R	4051	A
1	R	4056	G
1	R	4057	U
1	R	4064	G
1	R	4088	C
1	R	4109	U
1	R	4118	G
1	R	4129	C
1	R	4130	C
1	R	4166	C
1	R	4171	A
1	R	4172	A
1	R	4179	U
1	R	4184	G
1	R	4189	A
1	R	4191	A
1	R	4194	A
1	R	4195	A
1	R	4196	U
1	R	4203	U
1	R	4209	G
1	R	4210	A
1	R	4227	A
1	R	4229	A
1	R	4231	C
1	R	4233	C
1	R	4245	G
1	R	4248	U
1	R	4253	A
1	R	4254	G
1	R	4256	A
1	R	4258	U
1	R	4265	C
1	R	4268	C

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	G
1	R	40	A
1	R	60	A
1	R	317	C
1	R	993	C
1	R	2865	A
1	R	3833	A

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

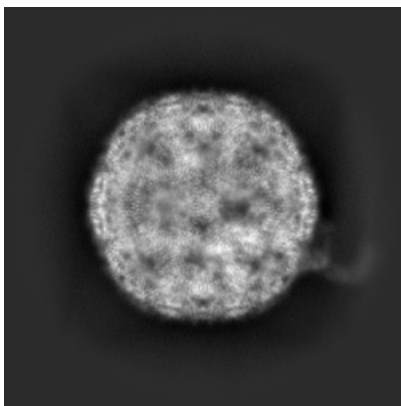
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41443. These allow visual inspection of the internal detail of the map and identification of artifacts.

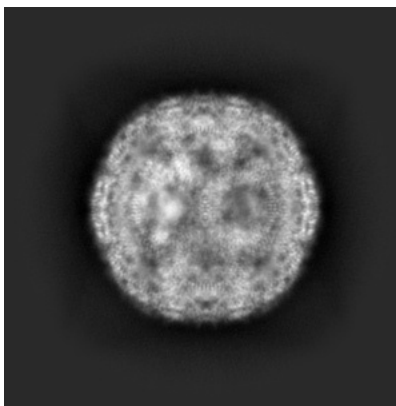
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

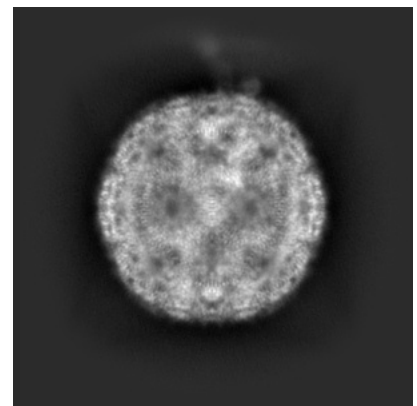
6.1.1 Primary map



X

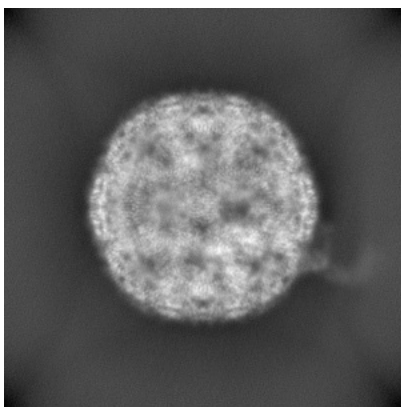


Y

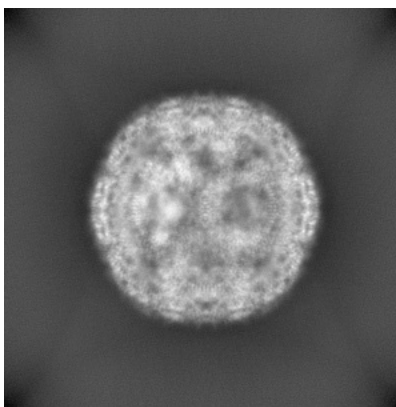


Z

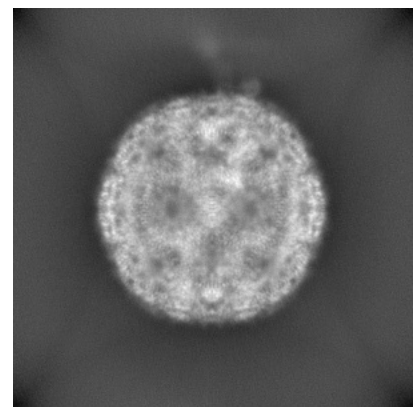
6.1.2 Raw map



X



Y

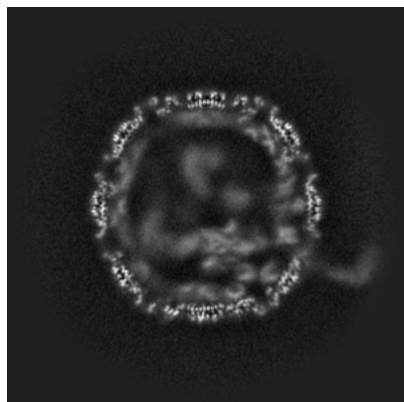


Z

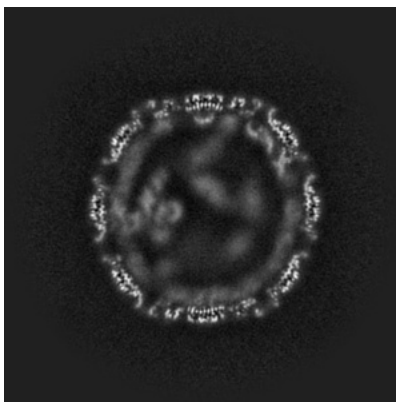
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

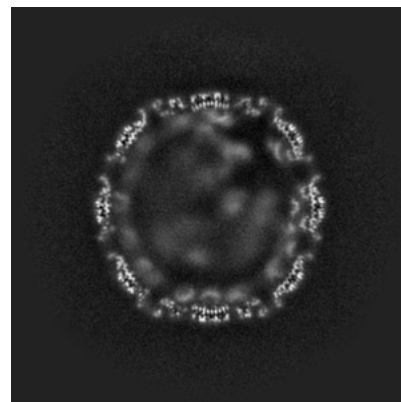
6.2.1 Primary map



X Index: 230

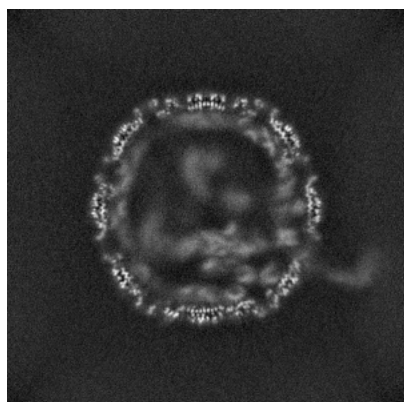


Y Index: 230

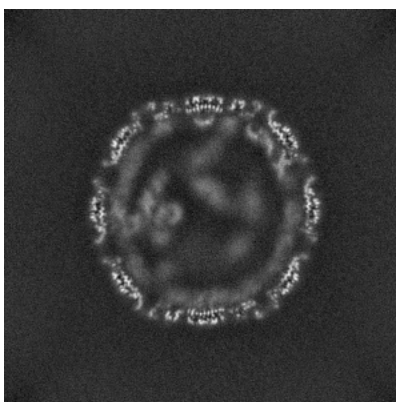


Z Index: 230

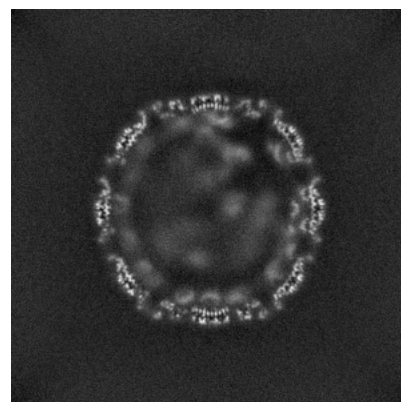
6.2.2 Raw map



X Index: 230



Y Index: 230

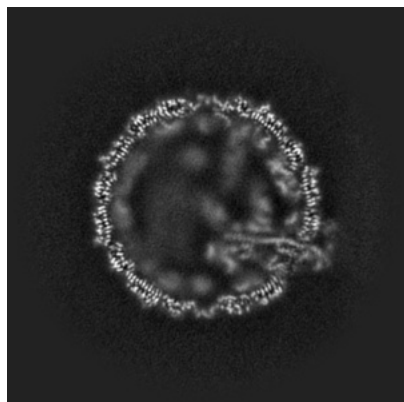


Z Index: 230

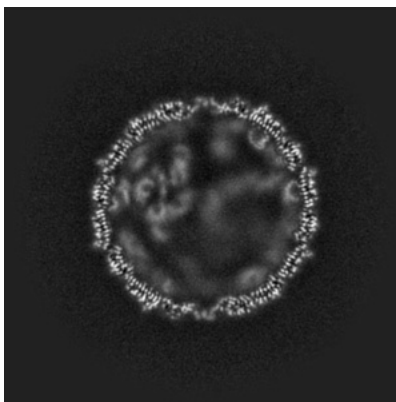
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

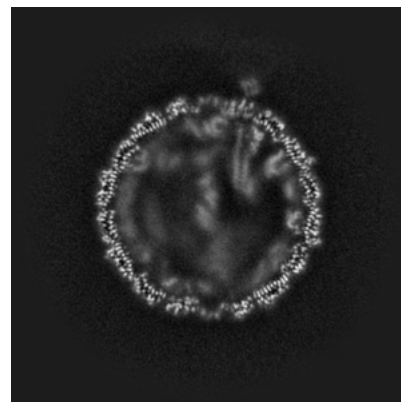
6.3.1 Primary map



X Index: 262

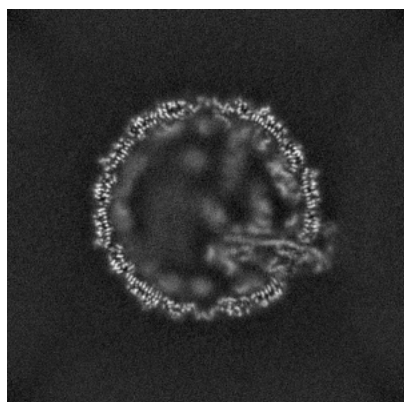


Y Index: 262

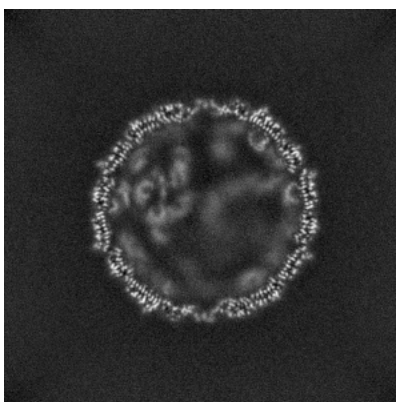


Z Index: 194

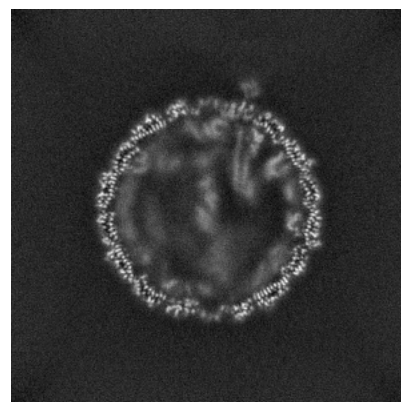
6.3.2 Raw map



X Index: 262



Y Index: 262

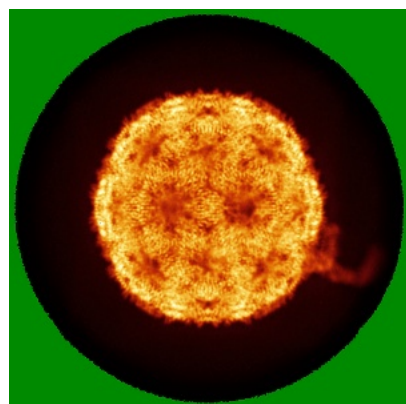


Z Index: 194

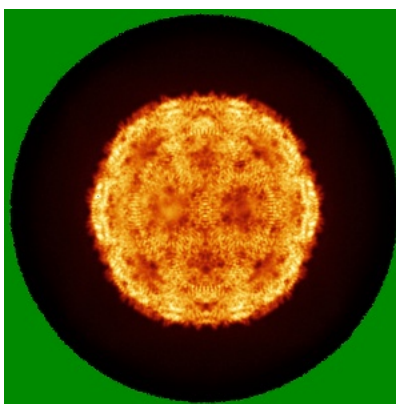
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

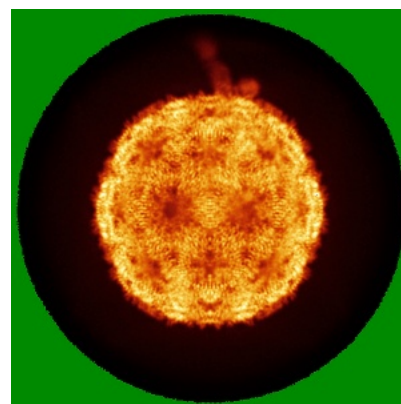
6.4.1 Primary map



X

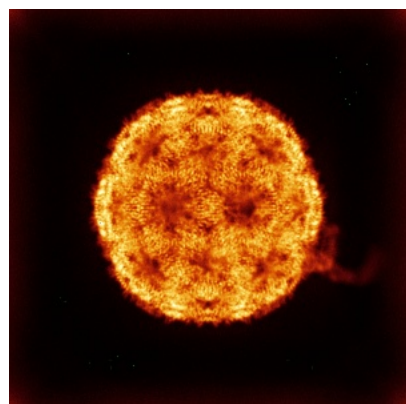


Y

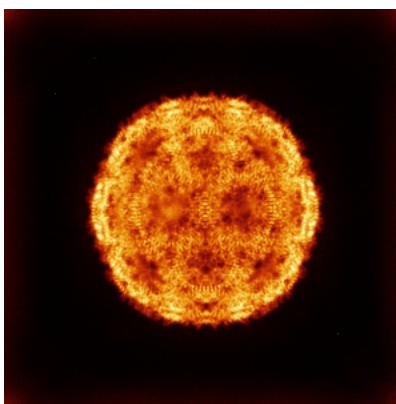


Z

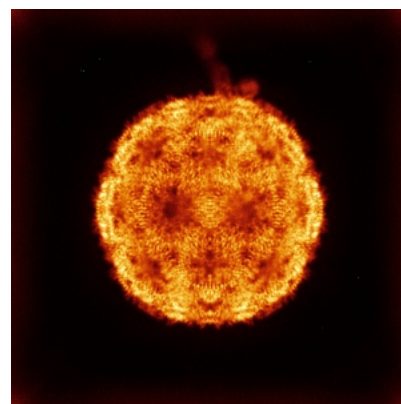
6.4.2 Raw map



X



Y

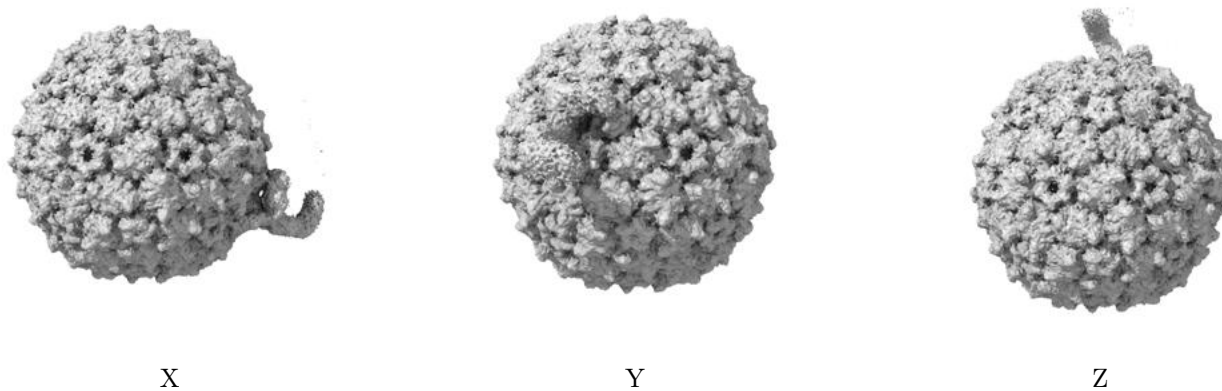


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

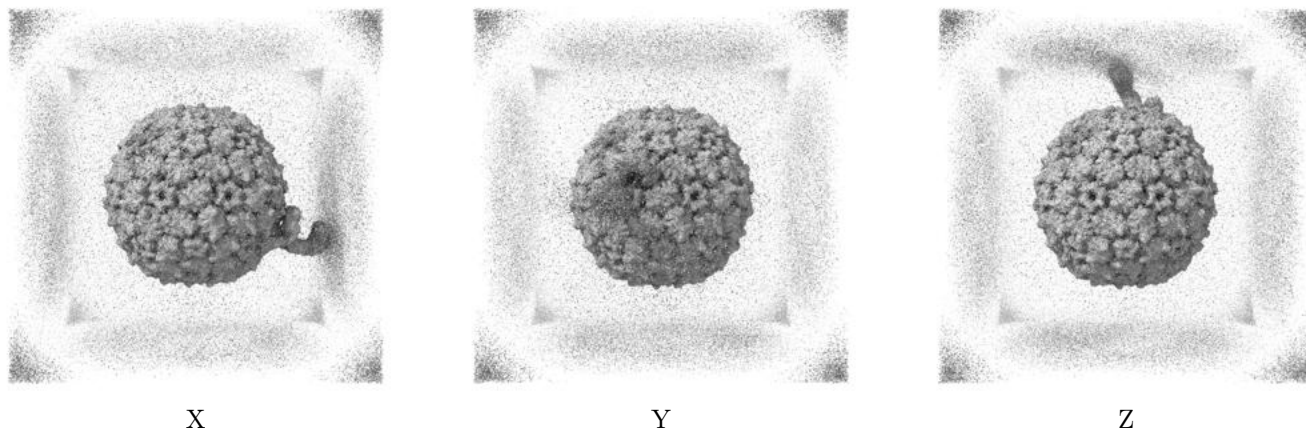
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.128. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

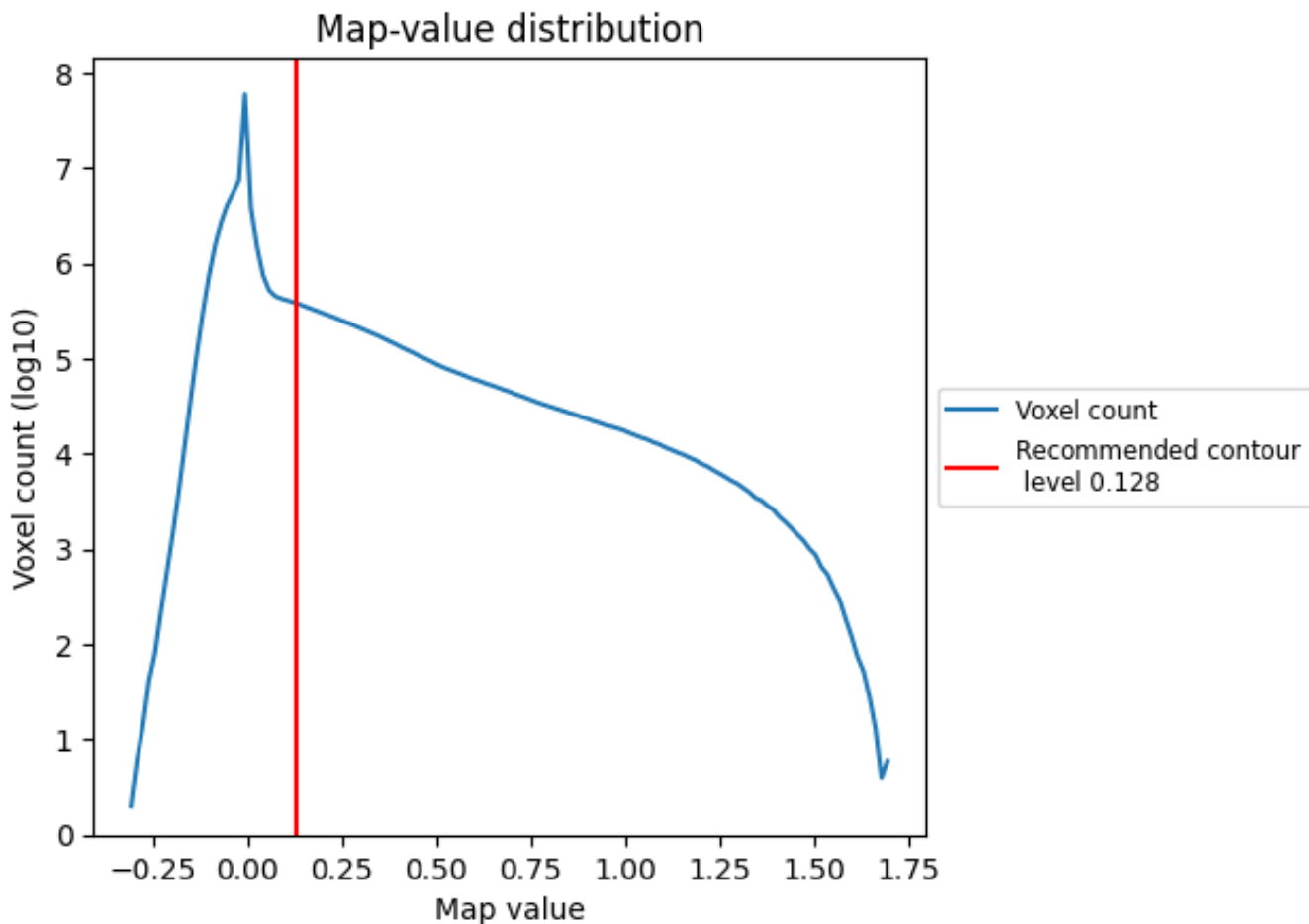
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

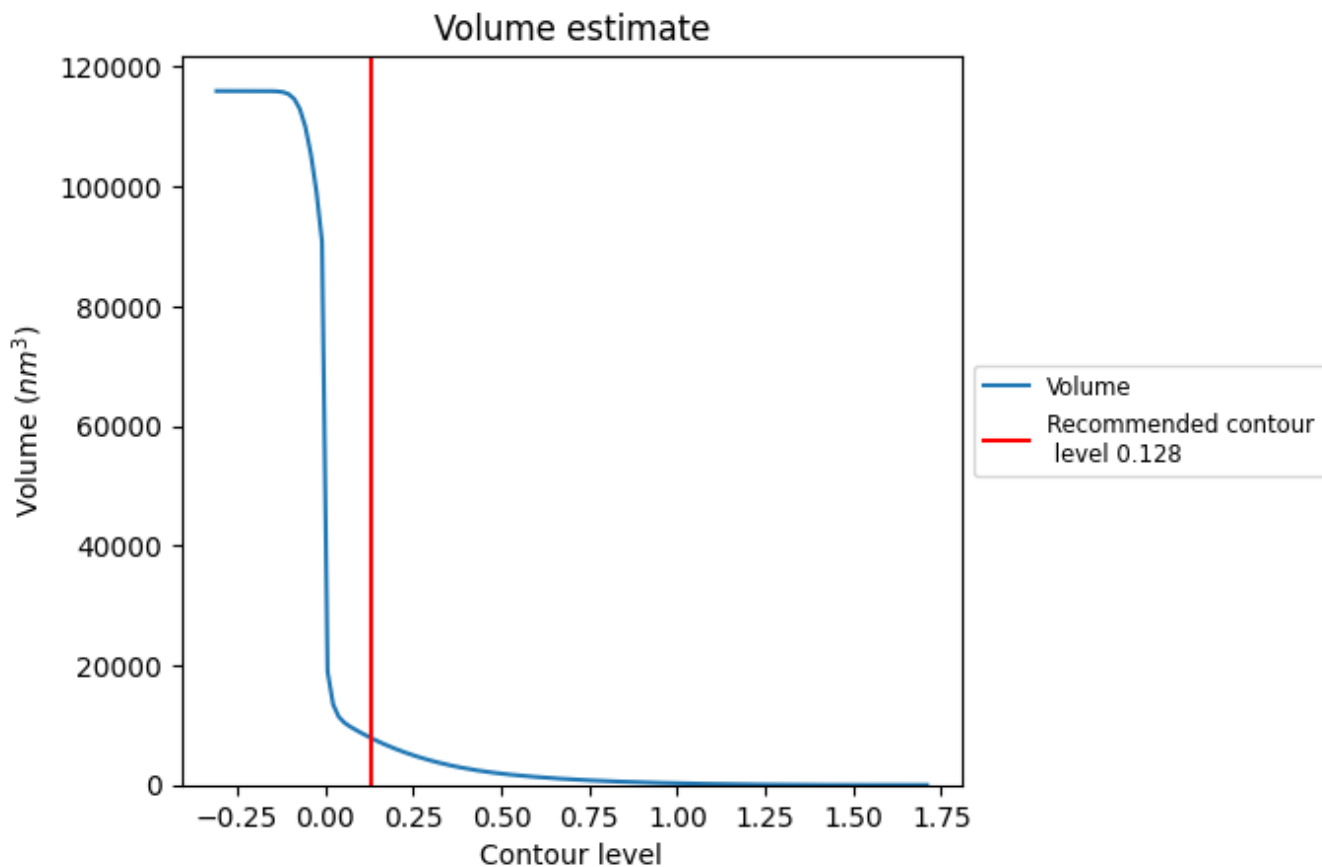
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

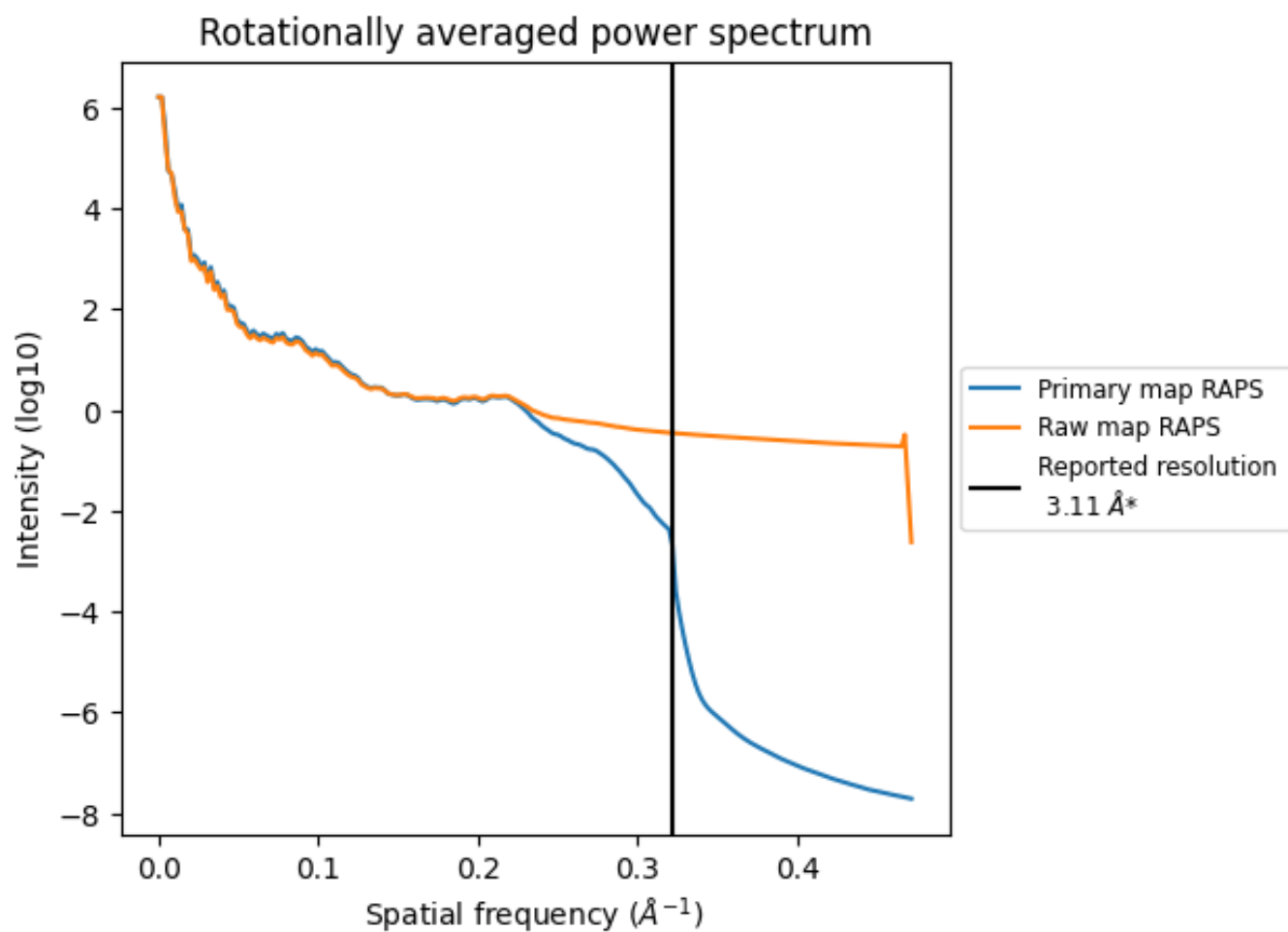
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7917 nm^3 ; this corresponds to an approximate mass of 7152 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

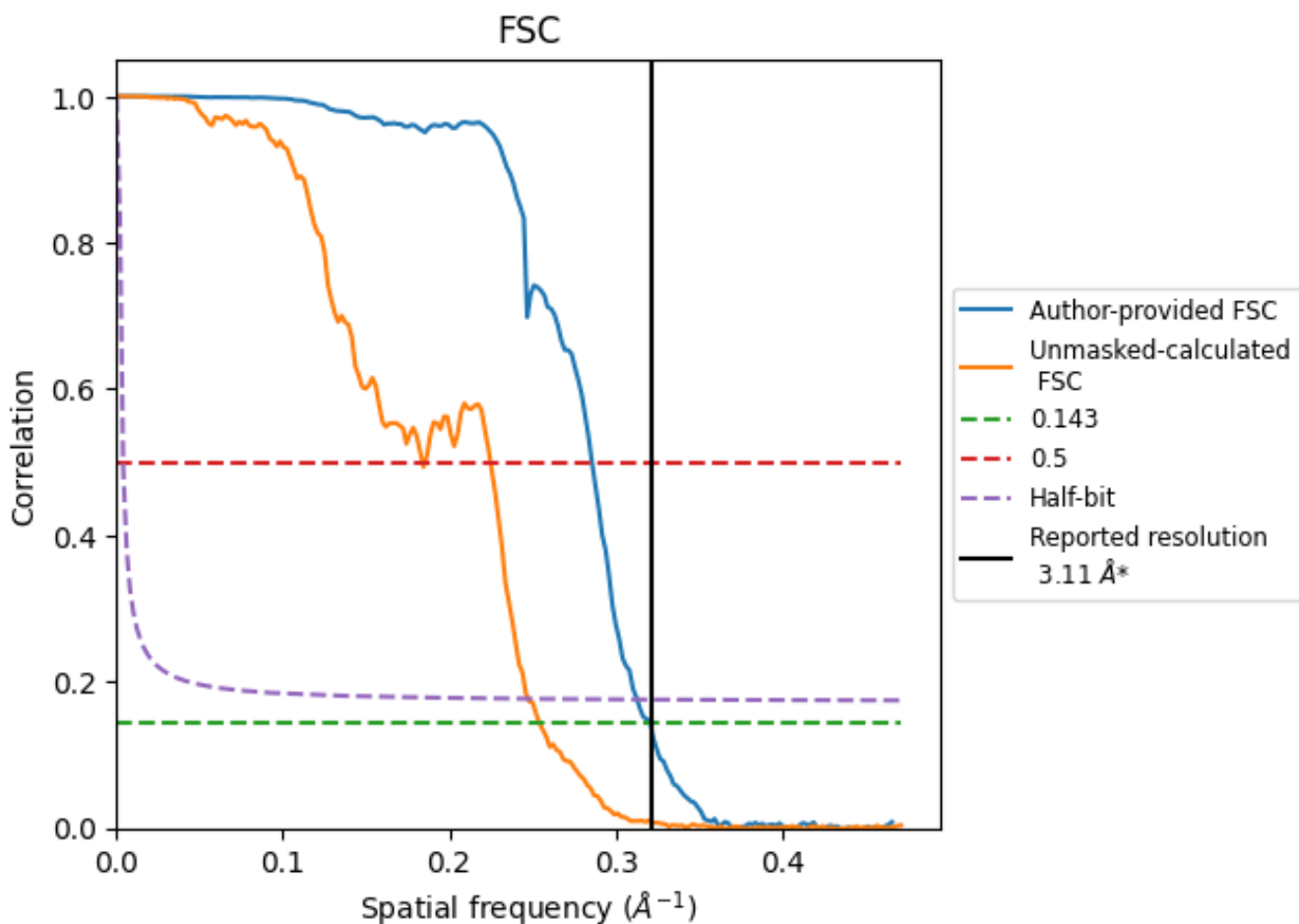


*Reported resolution corresponds to spatial frequency of 0.322 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

8.2 Resolution estimates [i](#)

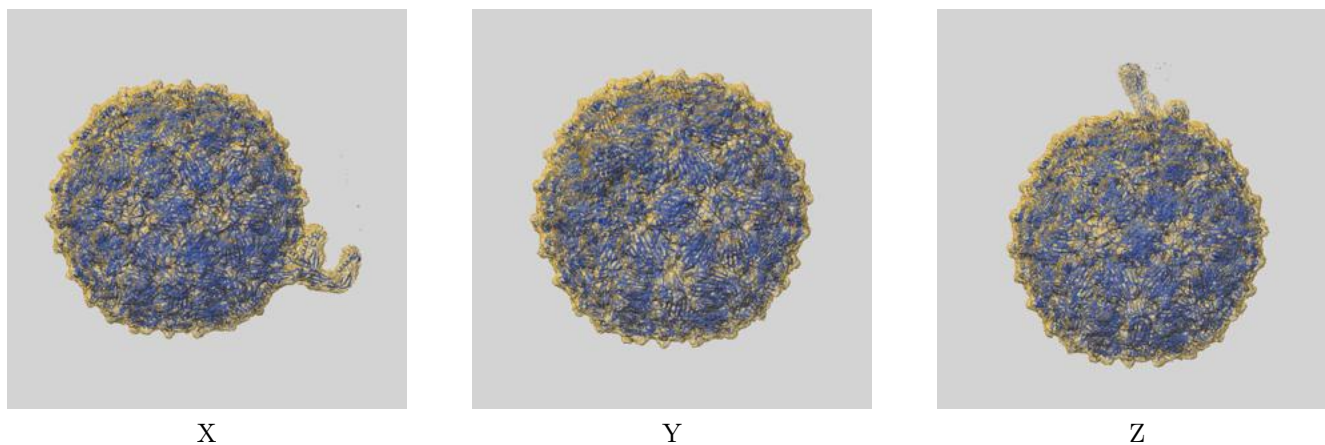
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.12	3.50	3.19
Unmasked-calculated*	3.93	5.44	4.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.11 by more than 10 %

9 Map-model fit [i](#)

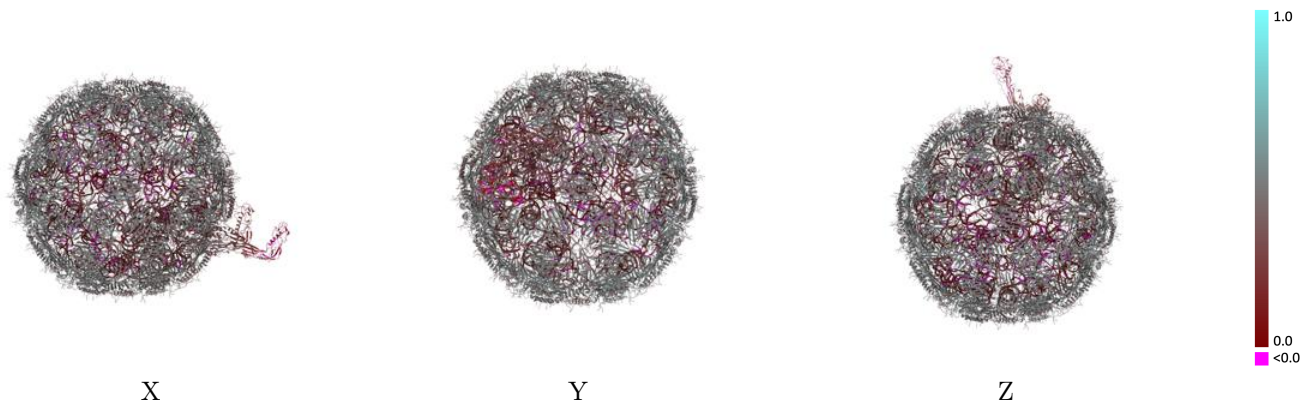
This section contains information regarding the fit between EMDB map EMD-41443 and PDB model 8TOC. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



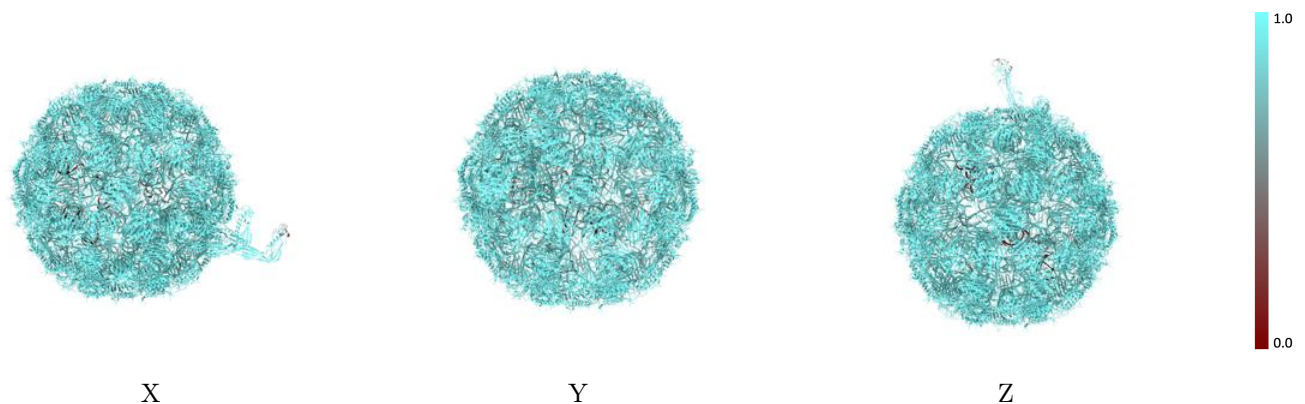
The images above show the 3D surface view of the map at the recommended contour level 0.128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



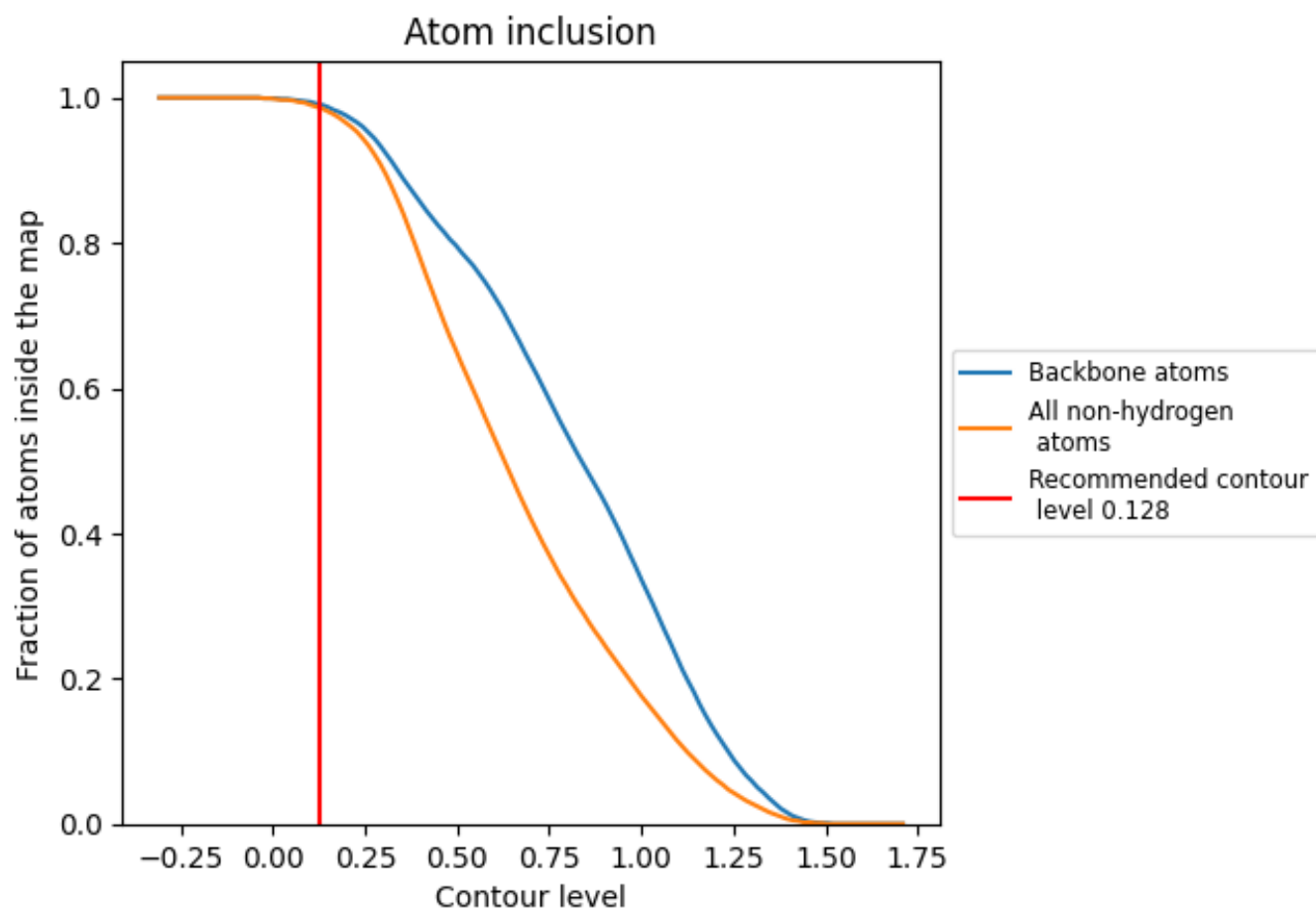
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.128).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (0.128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9860	 0.3540
AB	 1.0000	 0.4070
AC	 1.0000	 0.4160
AE	 1.0000	 0.4640
AF	 0.9990	 0.4650
AG	 1.0000	 0.4690
AH	 1.0000	 0.4680
AI	 1.0000	 0.4600
AJ	 0.9980	 0.4630
AK	 1.0000	 0.4690
AL	 1.0000	 0.4660
AM	 1.0000	 0.4790
AN	 1.0000	 0.4450
AO	 1.0000	 0.4540
AP	 1.0000	 0.4620
AQ	 1.0000	 0.4640
AS	 1.0000	 0.4600
AT	 1.0000	 0.4570
AU	 1.0000	 0.4650
AV	 1.0000	 0.4560
AW	 1.0000	 0.4680
AX	 0.9980	 0.4650
AY	 1.0000	 0.4670
AZ	 1.0000	 0.4650
Ac	 1.0000	 0.4610
BA	 1.0000	 0.4630
BB	 1.0000	 0.4670
BC	 1.0000	 0.4620
BD	 0.9990	 0.4660
BE	 1.0000	 0.4690
BF	 1.0000	 0.4680
BG	 0.9990	 0.4710
BH	 0.9990	 0.4650
BI	 1.0000	 0.4480
BJ	 1.0000	 0.4610























































































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Chain	Atom inclusion	Q-score
BK	 1.0000	 0.4460
BL	 1.0000	 0.4610
BM	 1.0000	 0.4700
BN	 1.0000	 0.4700
BO	 1.0000	 0.4610
BP	 1.0000	 0.4600
BQ	 1.0000	 0.4550
BS	 1.0000	 0.4530
BT	 1.0000	 0.4610
BU	 1.0000	 0.4580
BV	 0.9970	 0.4490
BW	 1.0000	 0.4440
BX	 1.0000	 0.4680
BY	 0.9990	 0.4680
BZ	 1.0000	 0.4670
Bc	 1.0000	 0.4680
CA	 1.0000	 0.4620
CB	 1.0000	 0.4660
CC	 0.9970	 0.4600
CD	 1.0000	 0.4690
CE	 1.0000	 0.4690
CF	 1.0000	 0.4690
CG	 1.0000	 0.4650
CH	 1.0000	 0.4720
CI	 1.0000	 0.4620
CJ	 1.0000	 0.4570
CK	 1.0000	 0.4520
CL	 1.0000	 0.4640
CM	 1.0000	 0.4070
CN	 0.9960	 0.4330
CO	 1.0000	 0.4300
CP	 1.0000	 0.4680
CQ	 0.9990	 0.4660
CS	 1.0000	 0.4740
CT	 1.0000	 0.4700
CU	 1.0000	 0.4740
CV	 1.0000	 0.4650
CW	 1.0000	 0.4630
CX	 0.9990	 0.4650
CY	 1.0000	 0.4700
CZ	 1.0000	 0.4740
Cc	 1.0000	 0.4630





















































































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Chain	Atom inclusion	Q-score
DA	 1.0000	 0.4670
DB	 0.9990	 0.4620
DC	 0.9990	 0.4680
DD	 1.0000	 0.4670
DE	 1.0000	 0.4670
DF	 0.9990	 0.4680
DG	 1.0000	 0.4710
DH	 1.0000	 0.4530
DI	 1.0000	 0.4240
DJ	 1.0000	 0.4480
DK	 0.9990	 0.4760
DL	 1.0000	 0.4660
DM	 0.9990	 0.4720
DN	 0.9990	 0.4270
DO	 0.9990	 0.3930
DQ	 1.0000	 0.4760
DS	 1.0000	 0.4650
DT	 1.0000	 0.4580
DU	 1.0000	 0.4660
DV	 1.0000	 0.4640
DW	 1.0000	 0.4670
DX	 1.0000	 0.4730
DY	 1.0000	 0.4660
DZ	 1.0000	 0.4670
Dc	 0.9990	 0.4670
EA	 1.0000	 0.4680
EB	 1.0000	 0.4600
EC	 1.0000	 0.4540
ED	 1.0000	 0.4560
EE	 1.0000	 0.4620
EF	 1.0000	 0.4570
EG	 0.9990	 0.4640
EH	 1.0000	 0.4620
EI	 0.9990	 0.4590
EJ	 1.0000	 0.4630
EK	 1.0000	 0.4680
EL	 1.0000	 0.4660
EM	 1.0000	 0.4660
EN	 1.0000	 0.4640
EO	 1.0000	 0.4700
EP	 1.0000	 0.4640
EQ	 1.0000	 0.4670











































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Chain	Atom inclusion	Q-score
ES	 1.0000	 0.4650
ET	 0.9990	 0.4640
EU	 1.0000	 0.4410
EV	 0.9990	 0.4380
EW	 1.0000	 0.4500
EX	 1.0000	 0.4690
EY	 0.9980	 0.4630
EZ	 1.0000	 0.4680
Ec	 1.0000	 0.4640
FA	 1.0000	 0.4520
FB	 1.0000	 0.4330
FC	 1.0000	 0.4500
FD	 1.0000	 0.4660
FE	 0.9990	 0.4620
FF	 1.0000	 0.4650
FG	 1.0000	 0.4200
FH	 1.0000	 0.4470
FI	 1.0000	 0.4500
FJ	 1.0000	 0.4710
FK	 1.0000	 0.4630
FL	 1.0000	 0.4660
FM	 1.0000	 0.4660
FN	 0.9990	 0.4660
FO	 1.0000	 0.4620
FP	 1.0000	 0.4730
FQ	 1.0000	 0.4710
FS	 1.0000	 0.4660
FT	 1.0000	 0.4570
FU	 0.9990	 0.4660
FV	 1.0000	 0.4660
FW	 0.9990	 0.4650
FX	 0.9990	 0.4590
FY	 1.0000	 0.4630
FZ	 1.0000	 0.4500
Fc	 1.0000	 0.4710
GA	 1.0000	 0.4320
GB	 0.9990	 0.4630
GC	 1.0000	 0.4690
GD	 1.0000	 0.4700
GE	 1.0000	 0.4710
GF	 1.0000	 0.4640
GG	 1.0000	 0.4720

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Chain	Atom inclusion	Q-score
GH	 1.0000	 0.4570
GI	 1.0000	 0.4630
GJ	 1.0000	 0.4670
GK	 1.0000	 0.4710
GL	 1.0000	 0.4690
GM	 0.9990	 0.4710
GN	 1.0000	 0.4730
GO	 1.0000	 0.4650
GP	 1.0000	 0.4710
GQ	 0.9990	 0.4690
GS	 1.0000	 0.4660
GT	 1.0000	 0.4570
GU	 1.0000	 0.4480
GV	 0.9990	 0.4480
GW	 1.0000	 0.4680
GX	 0.9990	 0.4720
GY	 1.0000	 0.4730
Gc	 1.0000	 0.4660
R	 0.9600	 0.1610
a	 0.9970	 0.2750
b	 0.9600	 0.2190