wwPDB EM Validation Summary Report (i)

Apr 2, 2024 – 02:34 PM EDT

PDB ID	:	8TWC
EMDB ID	:	EMD-41666
Title	:	Acinetobacter phage AP205 T=3 VLP
Authors	:	Meng, R.; Xing, Z.; Zhang, J.
Deposited on	:	2023-08-20
Resolution	:	3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

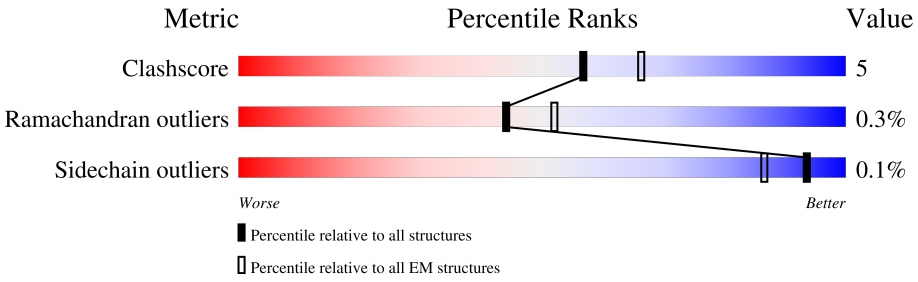
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	AB	129	88% 12%
1	AC	129	88% 12%
1	AD	129	89% 11%
1	AE	129	85% 15%
1	AF	129	80% 20%
1	AG	129	78% 22%
1	AH	129	84% 15%
1	AI	129	87% 13%

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Mol	Chain	Length	Quality of chain
1	AJ	129	91% 9%
1	AK	129	85% 15%
1	AL	129	91% 9%
1	AM	129	86% 14%
1	AN	129	89% 11%
1	AO	129	92% 8%
1	AP	129	91% 9%
1	AQ	129	81% 19%
1	AR	129	83% 17%
1	AS	129	83% 17%
1	AT	129	81% 19%
1	AU	129	92% 8%
1	AV	129	83% 17%
1	AW	129	87% 13%
1	AX	129	89% 11%
1	AY	129	90% 10%
1	AZ	129	83% 17%
1	BA	129	84% 16%
1	BB	129	84% 16%
1	BC	129	84% 16%
1	BD	129	88% 12%
1	BE	129	86% 14%
1	BF	129	85% 14%
1	BG	129	90% 10%
1	BH	129	84% 16%

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Mol	Chain	Length	Quality of chain
1	BI	129	84% 16%
1	BJ	129	86% 14%
1	BK	129	83% 17%
1	BL	129	84% 16%
1	BM	129	89% 11%
1	BN	129	84% 16%
1	BO	129	84% 16%
1	BP	129	92% 8%
1	BQ	129	84% 16%
1	BR	129	88% 12%
1	BS	129	90% 10%
1	BT	129	87% 13%
1	BU	129	86% 12%
1	BV	129	88% 12%
1	BW	129	85% 15%
1	BX	129	82% 17%
1	BY	129	82% 18%
1	BZ	129	93% 7%
1	CA	129	89% 11%
1	CB	129	87% 13%
1	CC	129	91% 9%
1	CD	129	90% 10%
1	CE	129	83% 17%
1	CF	129	91% 9%
1	CG	129	83% 16%

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Mol	Chain	Length	Quality of chain
1	CH	129	85% 15%
1	CI	129	89% 11%
1	CJ	129	86% 14%
1	CK	129	89% 11%
1	CL	129	84% 16%
1	CM	129	88% 12%
1	CN	129	88% 12%
1	CO	129	83% 17%
1	CP	129	83% 17%
1	CQ	129	83% 17%
1	CR	129	78% 22%
1	CS	129	88% 12%
1	CT	129	84% 16%
1	CU	129	82% 18%
1	CV	129	85% 15%
1	CW	129	91% 9%
1	CX	129	92% 8%
1	CY	129	88% 12%
1	CZ	129	86% 14%
1	DA	129	91% 9%
1	DB	129	88% 12%
1	DC	129	88% 12%
1	DD	129	89% 11%
1	DE	129	83% 17%
1	DF	129	87% 13%

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Mol	Chain	Length	Quality of chain
1	DG	129	88% 12%
1	DH	129	87% 13%
1	DI	129	91% 9%
1	DJ	129	89% 11%
1	DK	129	82% 18%
1	DL	129	87% 13%
1	DM	129	85% 15%
1	DN	129	84% 16%
1	DO	129	86% 14%
1	DP	129	81% 19%
1	DQ	129	86% 13%
1	DR	129	88% 12%
1	DS	129	85% 15%
1	DT	129	81% 19%
1	DU	129	91% 9%
1	DV	129	87% 13%
1	DW	129	90% 10%
1	DX	129	91% 9%
1	DY	129	88% 12%
1	DZ	129	82% 18%
1	EA	129	88% 12%
1	EB	129	91% 9%
1	EC	129	87% 13%
1	ED	129	88% 12%
1	EE	129	83% 17%

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Mol	Chain	Length	Quality of chain
1	EF	129	83% 17%
1	EG	129	85% 15%
1	EH	129	90% 10%
1	EI	129	88% 12%
1	EJ	129	88% 12%
1	EK	129	89% 11%
1	EL	129	83% 16%
1	EM	129	88% 12%
1	EN	129	89% 11%
1	EO	129	89% 11%
1	EP	129	89% 11%
1	EQ	129	90% 10%
1	ER	129	84% 16%
1	ES	129	79% 21%
1	ET	129	85% 15%
1	EU	129	84% 15%
1	EV	129	89% 11%
1	EW	129	89% 11%
1	EX	129	90% 9%
1	EY	129	88% 12%
1	EZ	129	87% 13%
1	FA	129	84% 15%
1	FB	129	86% 14%
1	FC	129	91% 9%
1	FD	129	84% 16%

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Mol	Chain	Length	Quality of chain
1	FE	129	91% 9%
1	FF	129	85% 15%
1	FG	129	79% 21%
1	FH	129	89% 11%
1	FI	129	83% 17%
1	FJ	129	81% 19%
1	FK	129	88% 12%
1	FL	129	85% 15%
1	FM	129	89% 11%
1	FN	129	87% 13%
1	FO	129	82% 18%
1	FP	129	89% 11%
1	FQ	129	87% 13%
1	FR	129	89% 11%
1	FS	129	87% 13%
1	FT	129	81% 19%
1	FU	129	84% 16%
1	FV	129	84% 16%
1	FW	129	86% 14%
1	FX	129	90% 10%
1	FY	129	81% 19%
1	FZ	129	87% 13%
1	GA	129	84% 16%
1	GB	129	86% 14%
1	GC	129	89% 11%

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Mol	Chain	Length	Quality of chain
1	GD	129	83% 17%
1	GE	129	84% 15%
1	GF	129	89% 11%
1	GG	129	89% 11%
1	GH	129	88% 12%
1	GI	129	89% 11%
1	GJ	129	90% 10%
1	GK	129	85% 15%
1	GL	129	85% 15%
1	GM	129	88% 12%
1	GN	129	83% 16%
1	GO	129	92% 8%
1	GP	129	91% 9%
1	GQ	129	84% 16%
1	GR	129	88% 12%
1	GS	129	91% 9%
1	GT	129	87% 13%
1	GU	129	88% 12%
1	GV	129	90% 10%
1	GW	129	81% 19%
1	GX	129	88% 12%
1	GY	129	78% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 174240 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 protein called Coat protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AB	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AC	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AD	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AE	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AF	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AG	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AH	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AI	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AJ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AK	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AL	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AM	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AN	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AO	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AP	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AQ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AR	129	Total	C	N	O	S	0	0
			968	602	171	191	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AS	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AT	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AU	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AV	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AW	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AX	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AY	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	AZ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BA	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BB	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BC	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BD	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BE	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BF	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BG	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BH	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BI	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BJ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BK	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BL	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BM	129	Total	C	N	O	S	0	0
			968	602	171	191	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BN	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BO	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BP	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BQ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BR	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BS	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BT	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BU	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BV	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BW	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BX	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BY	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	BZ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CA	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CB	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CC	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CD	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CE	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CF	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CG	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CH	129	Total	C	N	O	S	0	0
			968	602	171	191	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CI	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CJ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CK	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CL	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CM	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CN	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CO	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CP	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CQ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CR	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CS	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CT	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CU	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CV	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CW	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CX	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CY	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	CZ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DA	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DB	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DC	129	Total	C	N	O	S	0	0
			968	602	171	191	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DD	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DE	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DF	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DG	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DH	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DI	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DJ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DK	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DL	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DM	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DN	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DO	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DP	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DQ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DR	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DS	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DT	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DU	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DV	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DW	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DX	129	Total	C	N	O	S	0	0
			968	602	171	191	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	DY	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	DZ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EA	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EB	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EC	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	ED	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EE	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EF	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EG	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EH	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EI	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EJ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EK	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EL	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EM	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EN	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EO	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EP	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EQ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	ER	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	ES	129	Total	C	N	O	S	0	0
			968	602	171	191	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	ET	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EU	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EV	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EW	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EX	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EY	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	EZ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FA	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FB	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FC	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FD	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FE	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FF	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FG	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FH	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FI	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FJ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FK	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FL	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FM	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FN	129	Total	C	N	O	S	0	0
			968	602	171	191	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	FO	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FP	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FQ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FR	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FS	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FT	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FU	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FV	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FW	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FX	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FY	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	FZ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GA	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GB	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GC	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GD	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GE	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GF	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GG	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GH	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GI	129	Total	C	N	O	S	0	0
			968	602	171	191	4		

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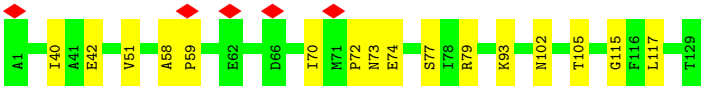
Mol	Chain	Residues	Atoms					AltConf	Trace
1	GJ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GK	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GL	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GM	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GN	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GO	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GP	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GQ	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GR	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GS	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GT	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GU	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GV	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GW	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GX	129	Total	C	N	O	S	0	0
			968	602	171	191	4		
1	GY	129	Total	C	N	O	S	0	0
			968	602	171	191	4		

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.

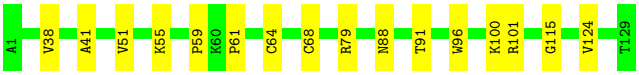
• Molecule 1: Coat protein

Chain AB:



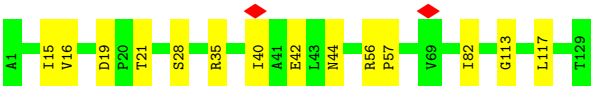
• Molecule 1: Coat protein

Chain AC:



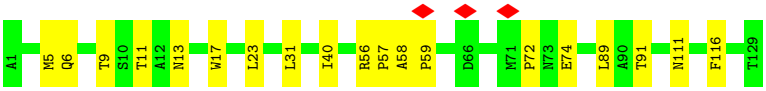
• Molecule 1: Coat protein

Chain AD:



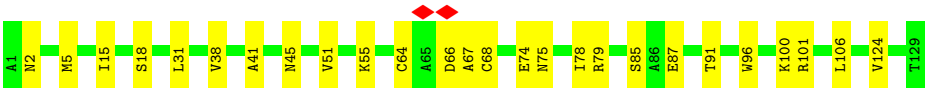
• Molecule 1: Coat protein

Chain AE:



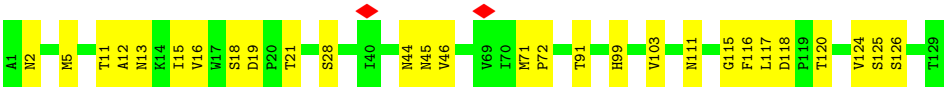
• Molecule 1: Coat protein

Chain AF:



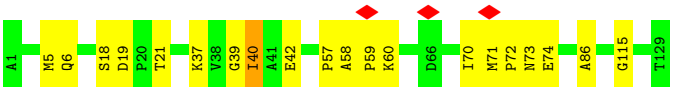
• Molecule 1: Coat protein

Chain AG:



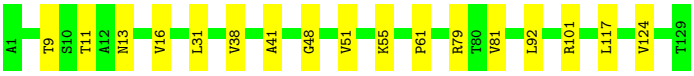
• Molecule 1: Coat protein

Chain AH:



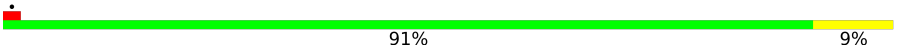
• Molecule 1: Coat protein

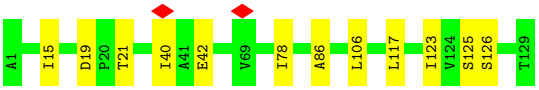
Chain AI:



• Molecule 1: Coat protein

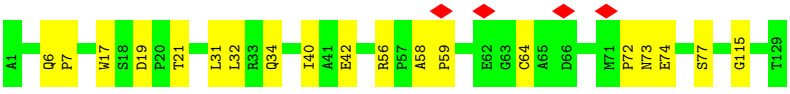
Chain AJ:





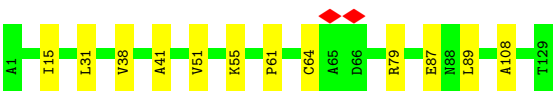
• Molecule 1: Coat protein

Chain AK:



• Molecule 1: Coat protein

Chain AL:

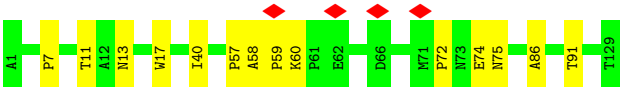


• Molecule 1: Coat protein

Chain AM:

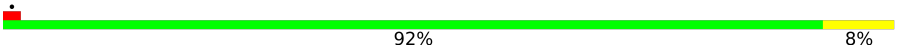
• Molecule 1: Coat protein

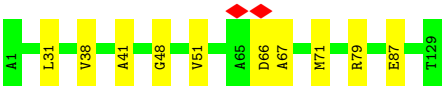
Chain AN:



• Molecule 1: Coat protein

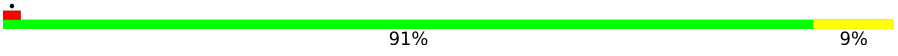
Chain AO:

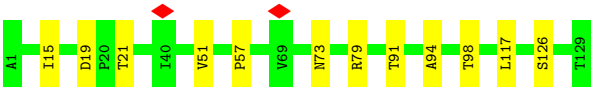




• Molecule 1: Coat protein

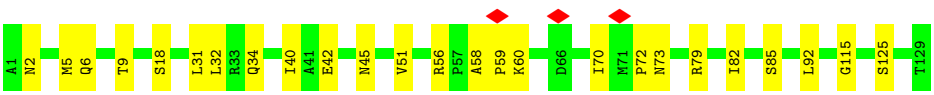
Chain AP:





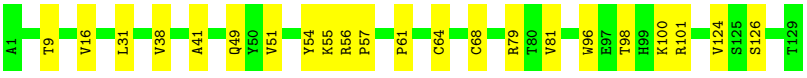
• Molecule 1: Coat protein

Chain AQ:



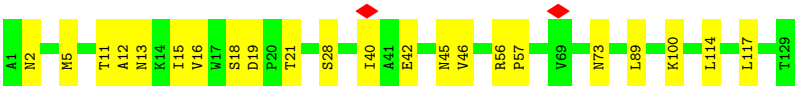
• Molecule 1: Coat protein

Chain AR:



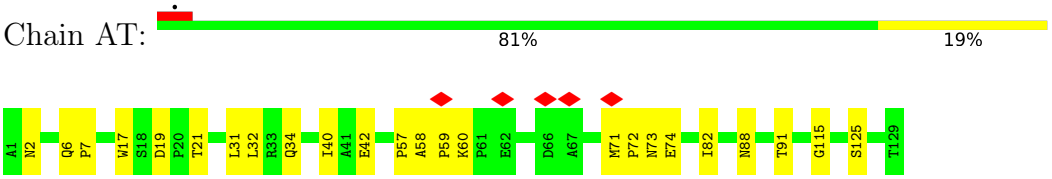
• Molecule 1: Coat protein

Chain AS:



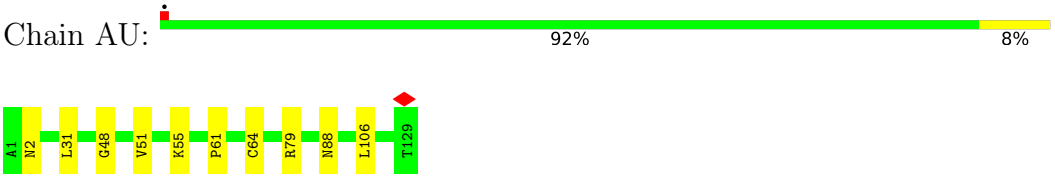
• Molecule 1: Coat protein

Chain AT:



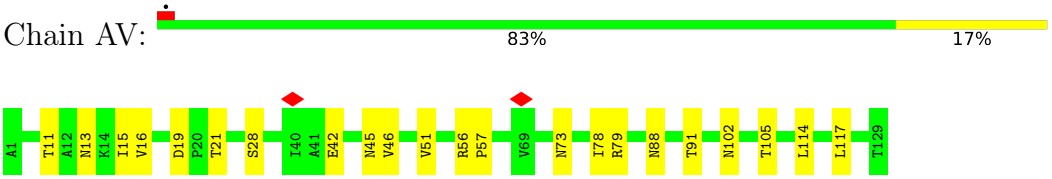
• Molecule 1: Coat protein

Chain AU:



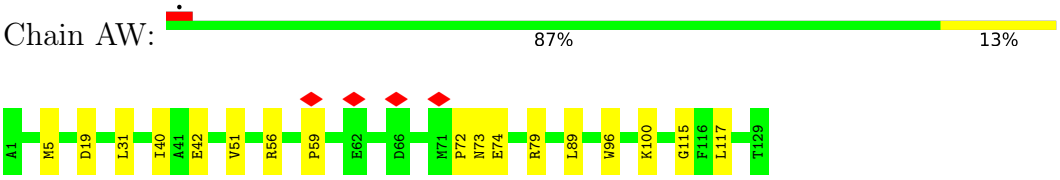
• Molecule 1: Coat protein

Chain AV:



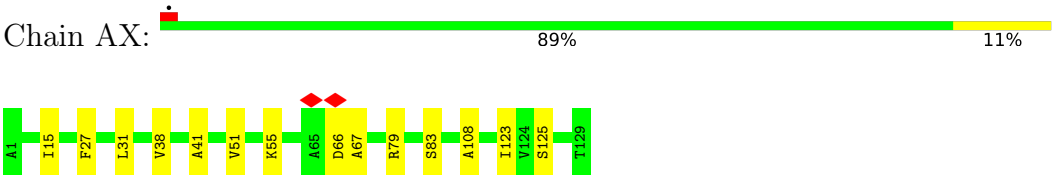
• Molecule 1: Coat protein

Chain AW:



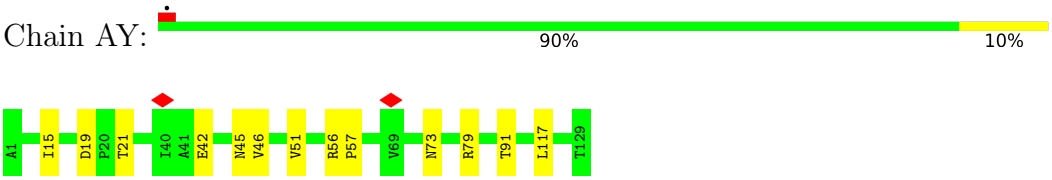
• Molecule 1: Coat protein

Chain AX:



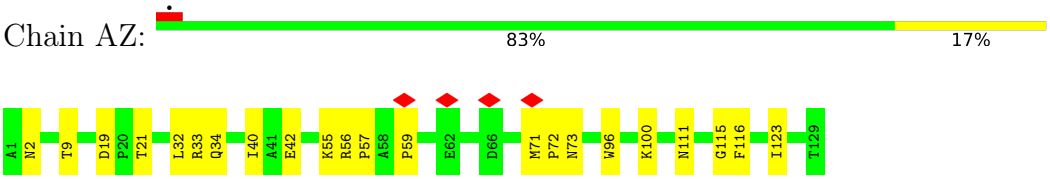
• Molecule 1: Coat protein

Chain AY:



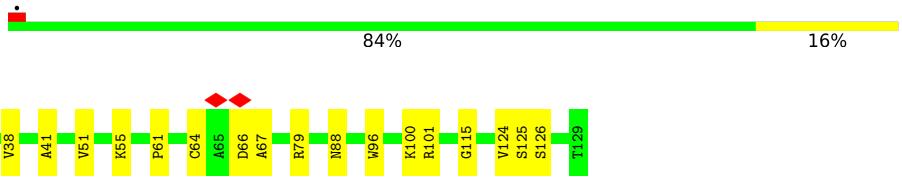
• Molecule 1: Coat protein

Chain AZ:



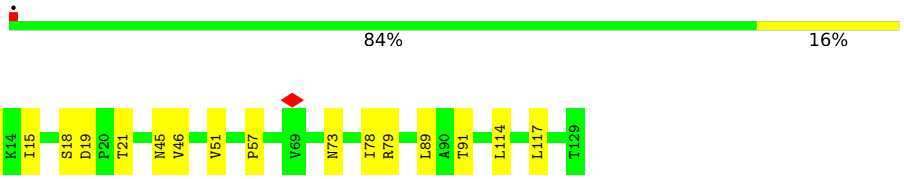
• Molecule 1: Coat protein

Chain BA:



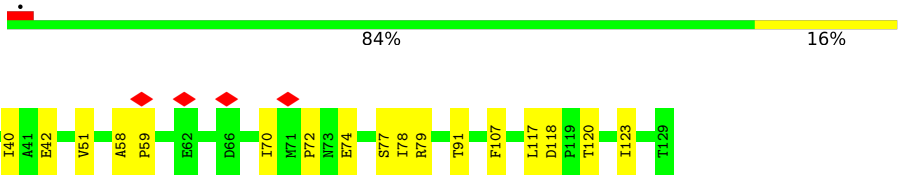
• Molecule 1: Coat protein

Chain BB:



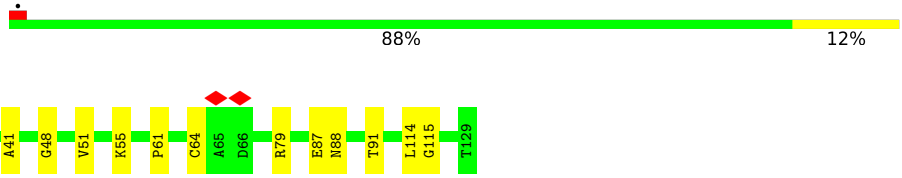
• Molecule 1: Coat protein

Chain BC:



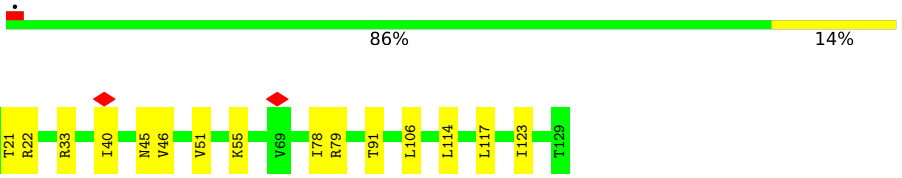
• Molecule 1: Coat protein

Chain BD:



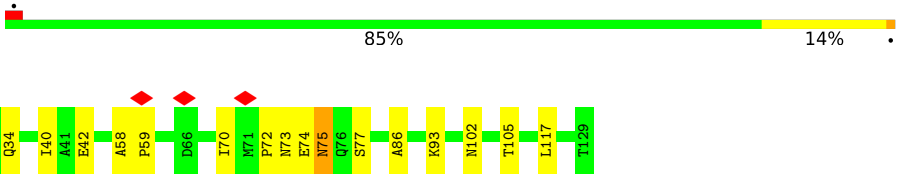
• Molecule 1: Coat protein

Chain BE:



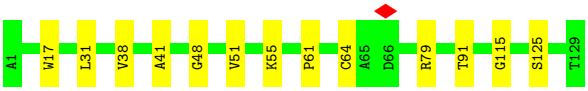
• Molecule 1: Coat protein

Chain BF:



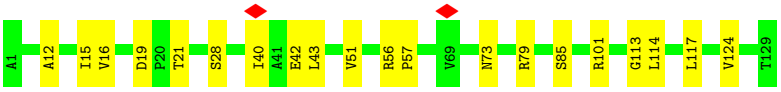
• Molecule 1: Coat protein

Chain BG:



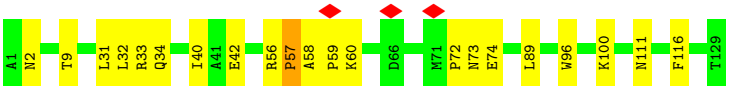
• Molecule 1: Coat protein

Chain BH:



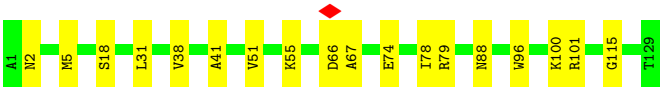
• Molecule 1: Coat protein

Chain BI:



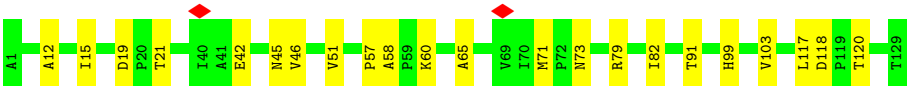
• Molecule 1: Coat protein

Chain BJ:



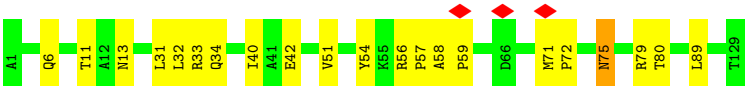
• Molecule 1: Coat protein

Chain BK:



• Molecule 1: Coat protein

Chain BL:

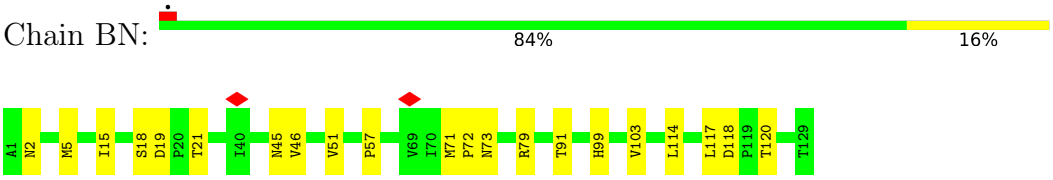


• Molecule 1: Coat protein

Chain BM:

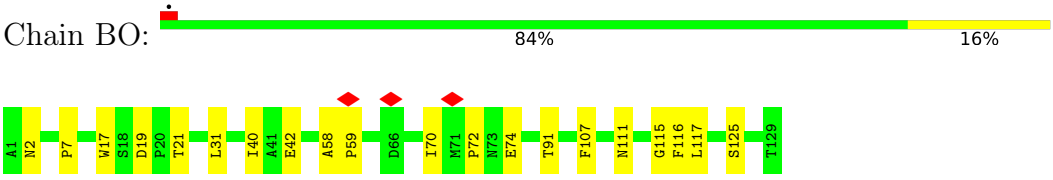
• Molecule 1: Coat protein

Chain BN:



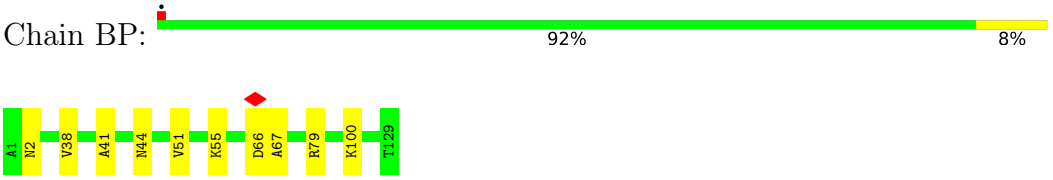
• Molecule 1: Coat protein

Chain BO:



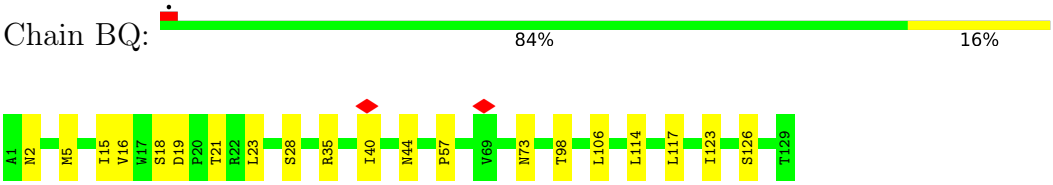
• Molecule 1: Coat protein

Chain BP:



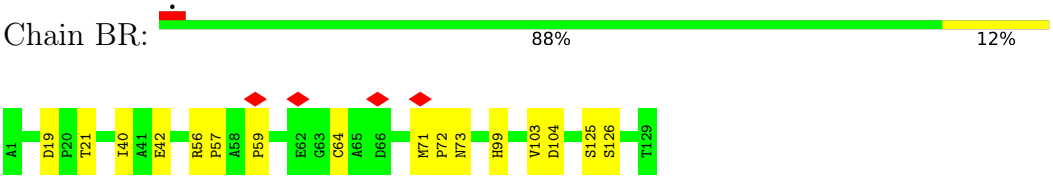
• Molecule 1: Coat protein

Chain BQ:



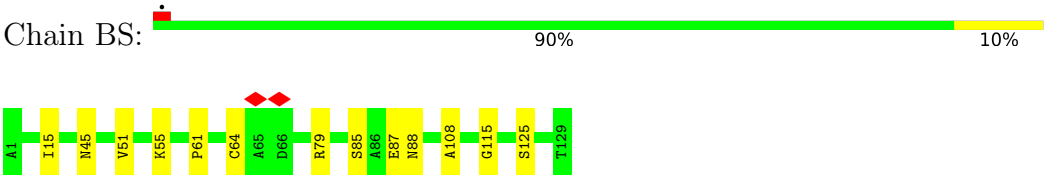
• Molecule 1: Coat protein

Chain BR:



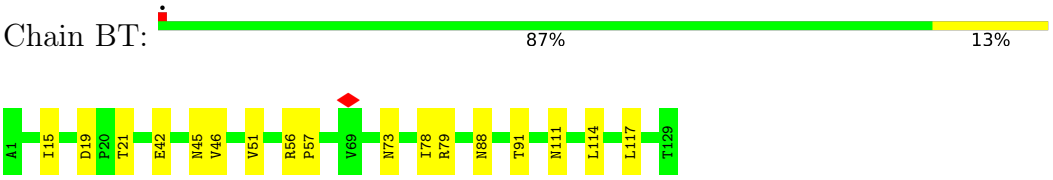
• Molecule 1: Coat protein

Chain BS:



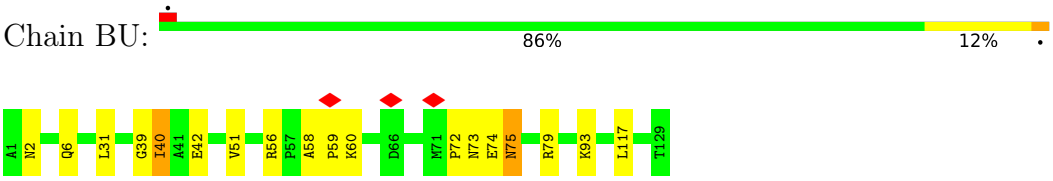
• Molecule 1: Coat protein

Chain BT:



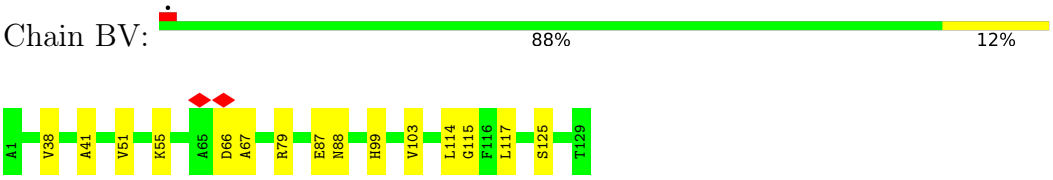
• Molecule 1: Coat protein

Chain BU:



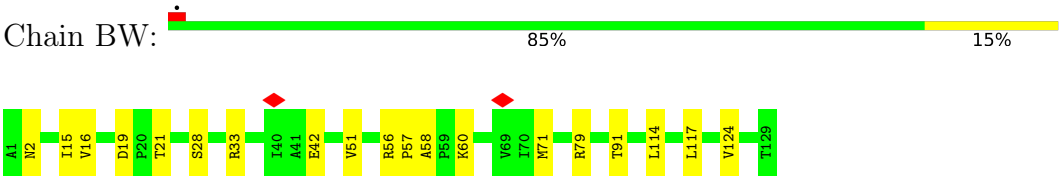
• Molecule 1: Coat protein

Chain BV:



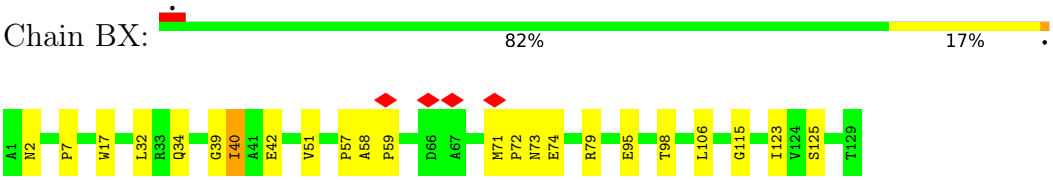
• Molecule 1: Coat protein

Chain BW:



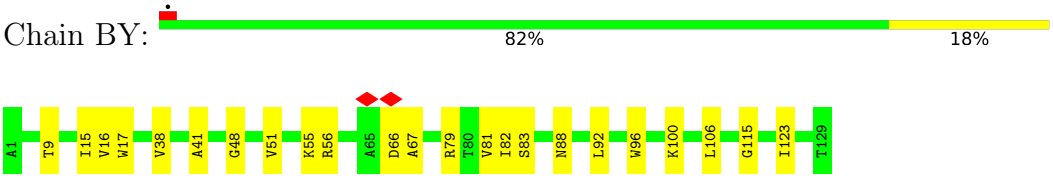
• Molecule 1: Coat protein

Chain BX:



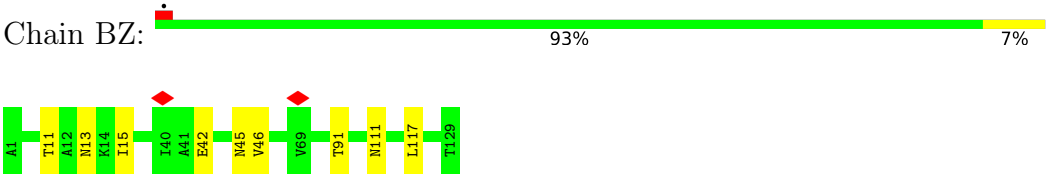
• Molecule 1: Coat protein

Chain BY:



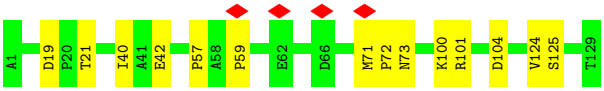
• Molecule 1: Coat protein

Chain BZ:



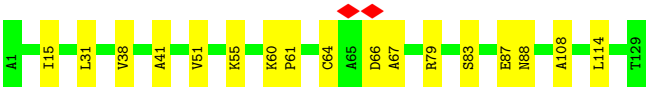
• Molecule 1: Coat protein

Chain CA:



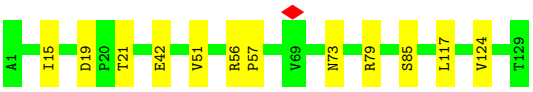
• Molecule 1: Coat protein

Chain CB:



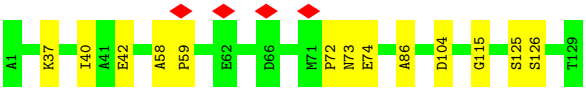
• Molecule 1: Coat protein

Chain CC:



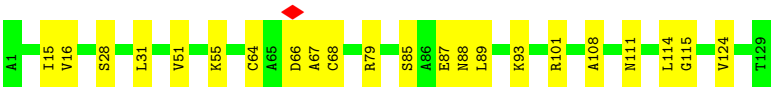
• Molecule 1: Coat protein

Chain CD:



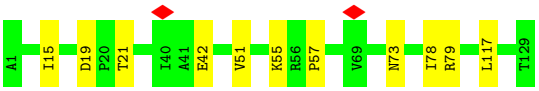
• Molecule 1: Coat protein

Chain CE:



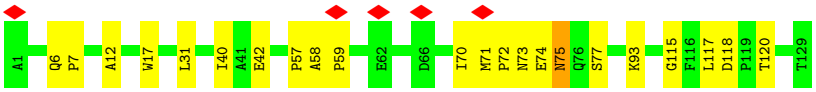
• Molecule 1: Coat protein

Chain CF:



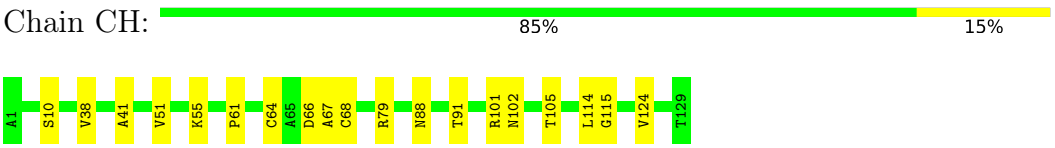
• Molecule 1: Coat protein

Chain CG:



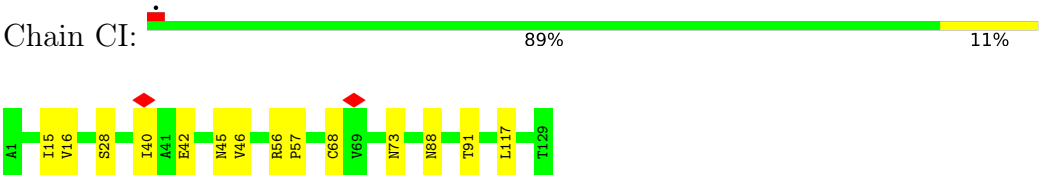
• Molecule 1: Coat protein

Chain CH:



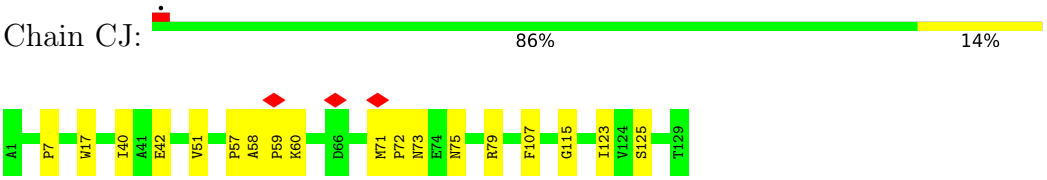
• Molecule 1: Coat protein

Chain CI:



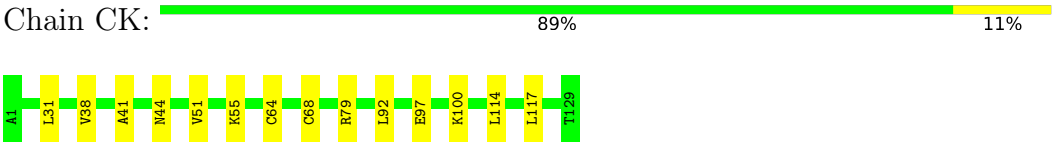
• Molecule 1: Coat protein

Chain CJ:



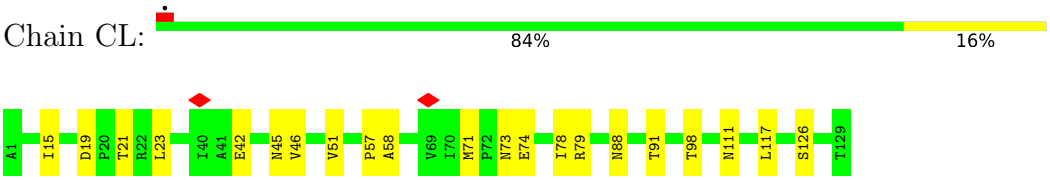
• Molecule 1: Coat protein

Chain CK:



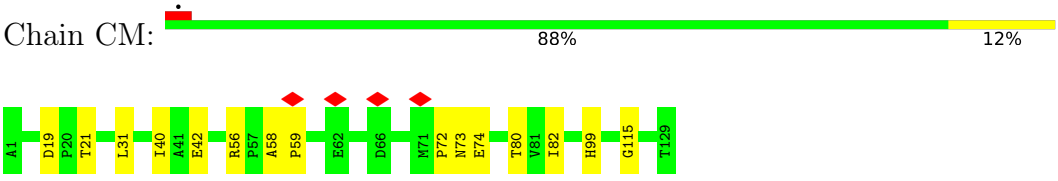
• Molecule 1: Coat protein

Chain CL:



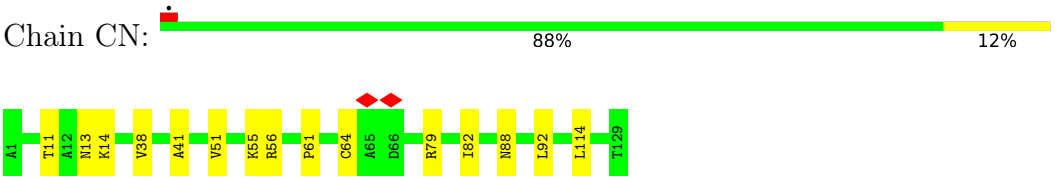
• Molecule 1: Coat protein

Chain CM:



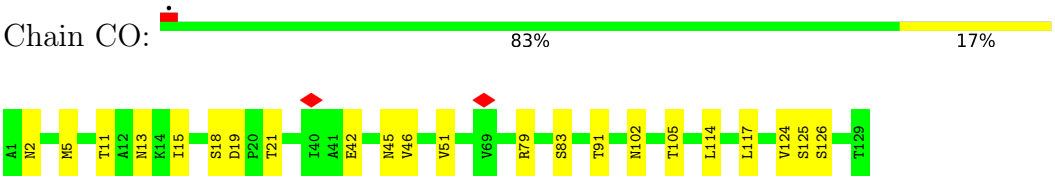
• Molecule 1: Coat protein

Chain CN:



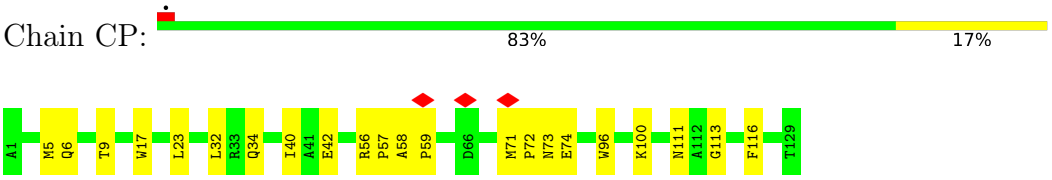
• Molecule 1: Coat protein

Chain CO:



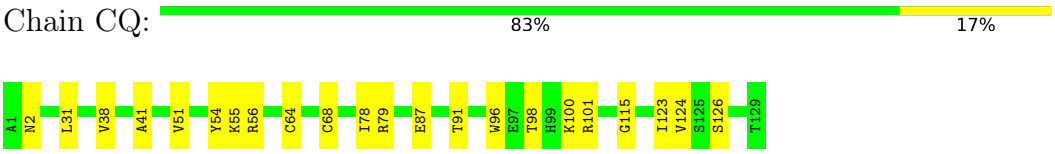
• Molecule 1: Coat protein

Chain CP:



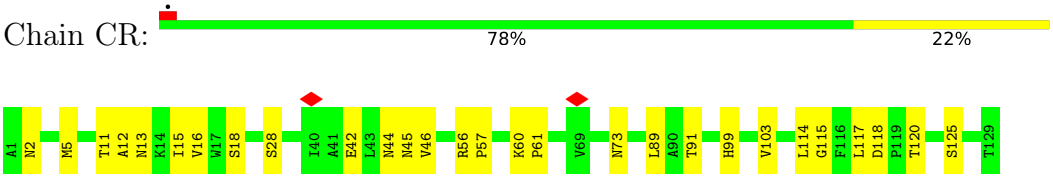
• Molecule 1: Coat protein

Chain CQ:



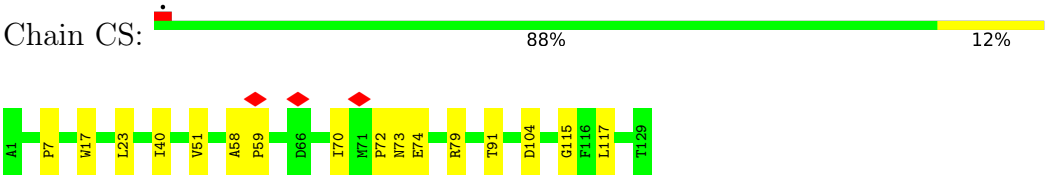
• Molecule 1: Coat protein

Chain CR:



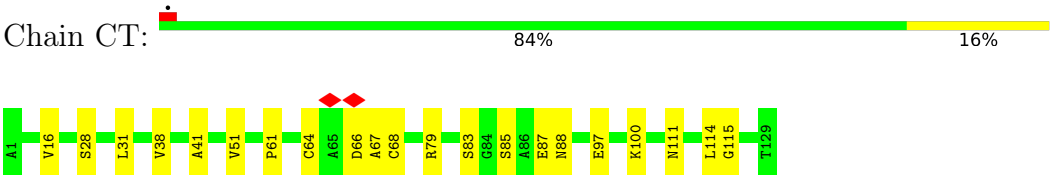
• Molecule 1: Coat protein

Chain CS:



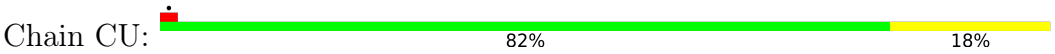
• Molecule 1: Coat protein

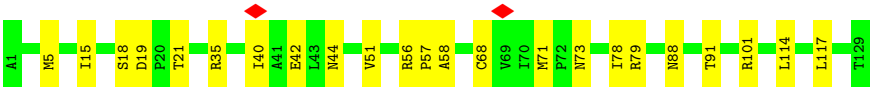
Chain CT:



• Molecule 1: Coat protein

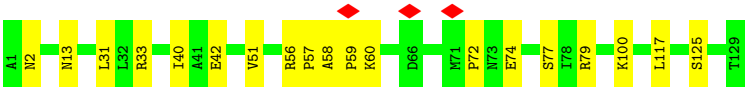
Chain CU:





• Molecule 1: Coat protein

Chain CV:

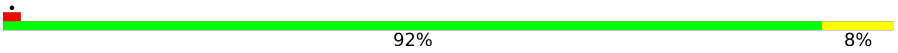


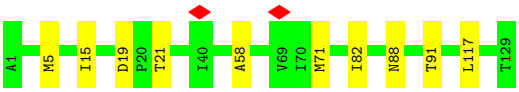
• Molecule 1: Coat protein

Chain CW:

• Molecule 1: Coat protein

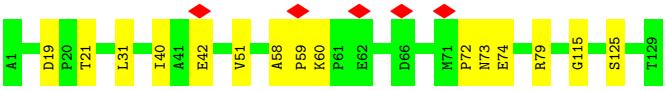
Chain CX:





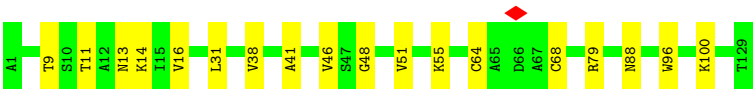
• Molecule 1: Coat protein

Chain CY:



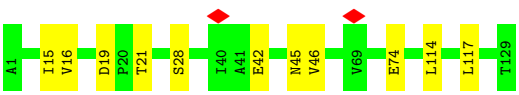
• Molecule 1: Coat protein

Chain CZ:



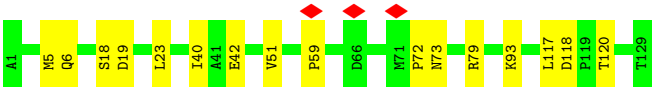
• Molecule 1: Coat protein

Chain DA:



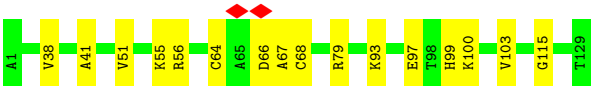
• Molecule 1: Coat protein

Chain DB:



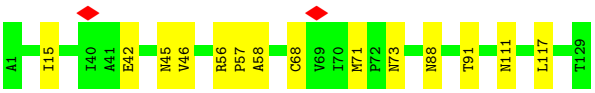
• Molecule 1: Coat protein

Chain DC:



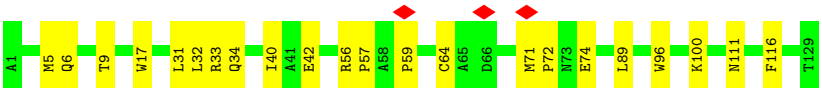
• Molecule 1: Coat protein

Chain DD:



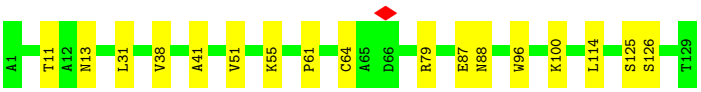
• Molecule 1: Coat protein

Chain DE:



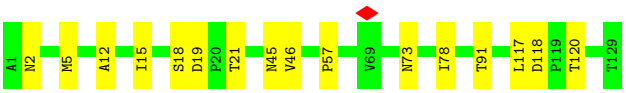
• Molecule 1: Coat protein

Chain DF:



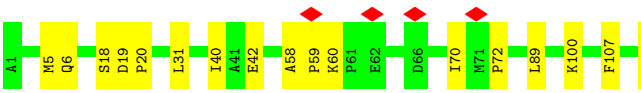
• Molecule 1: Coat protein

Chain DG:



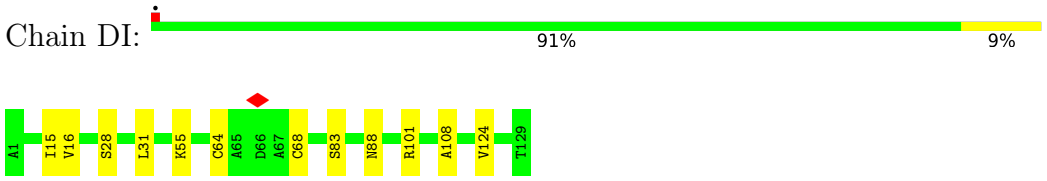
• Molecule 1: Coat protein

Chain DH:



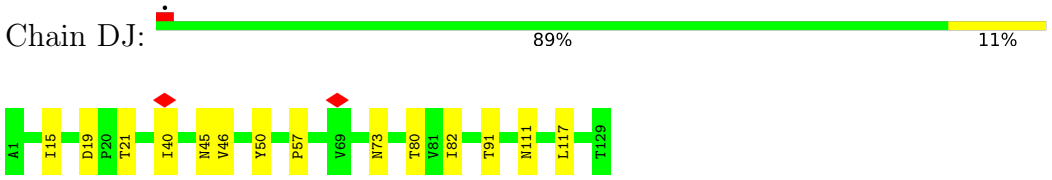
• Molecule 1: Coat protein

Chain DI:



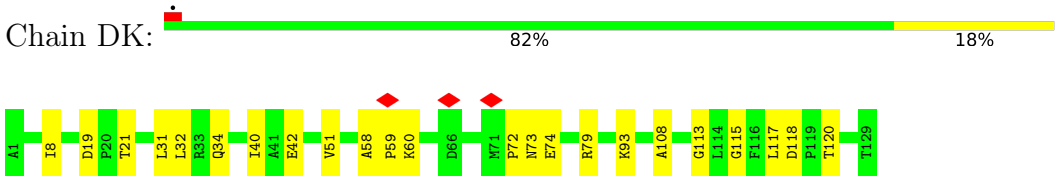
• Molecule 1: Coat protein

Chain DJ:



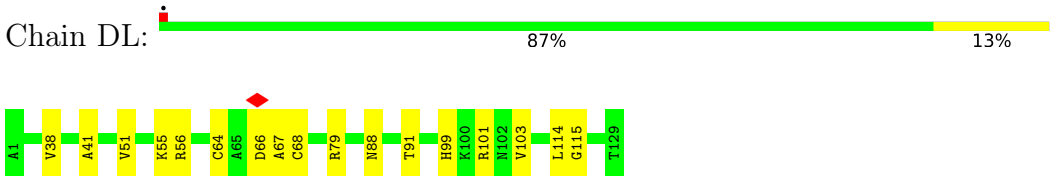
• Molecule 1: Coat protein

Chain DK:



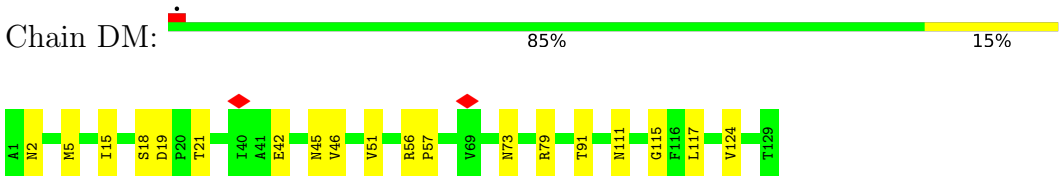
• Molecule 1: Coat protein

Chain DL:



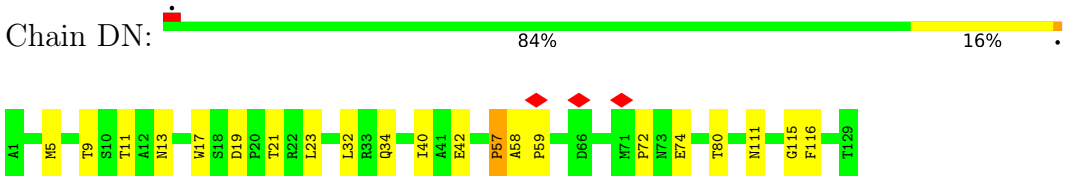
• Molecule 1: Coat protein

Chain DM:



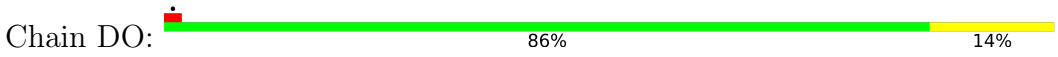
• Molecule 1: Coat protein

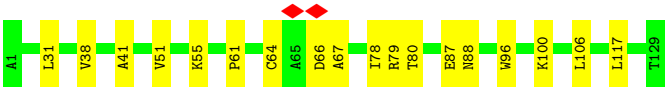
Chain DN:



• Molecule 1: Coat protein

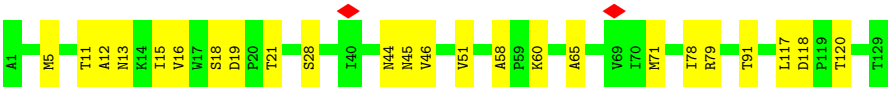
Chain DO:





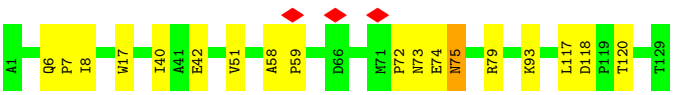
• Molecule 1: Coat protein

Chain DP:



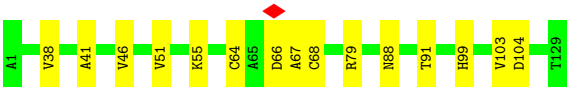
• Molecule 1: Coat protein

Chain DQ:



• Molecule 1: Coat protein

Chain DR:

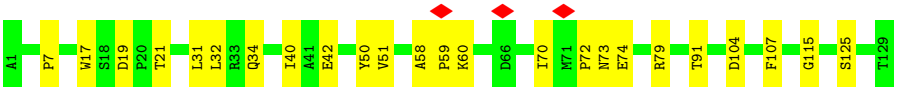


• Molecule 1: Coat protein

Chain DS:

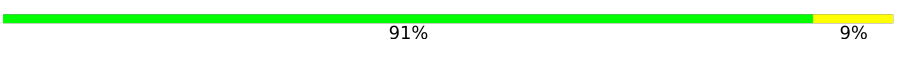
• Molecule 1: Coat protein

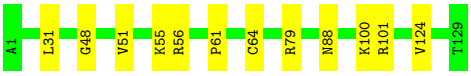
Chain DT:



• Molecule 1: Coat protein

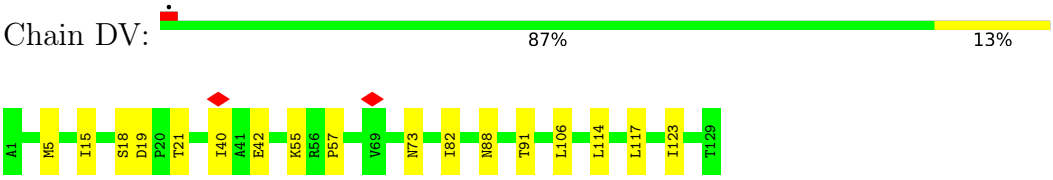
Chain DU:





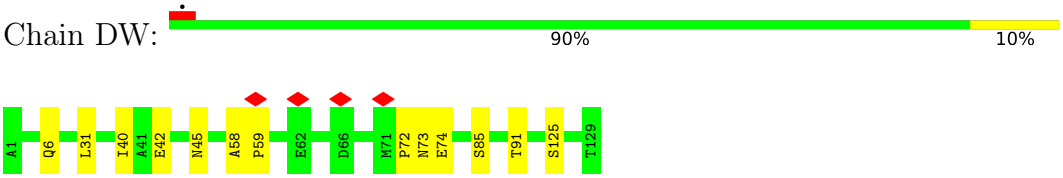
• Molecule 1: Coat protein

Chain DV:



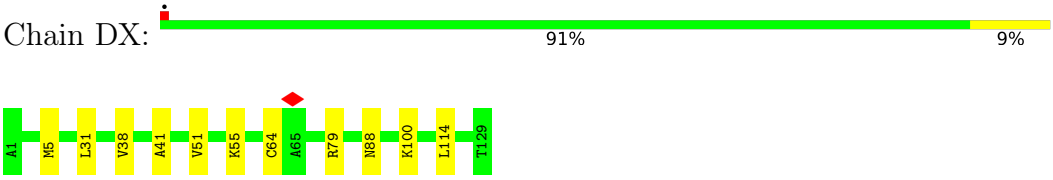
• Molecule 1: Coat protein

Chain DW:



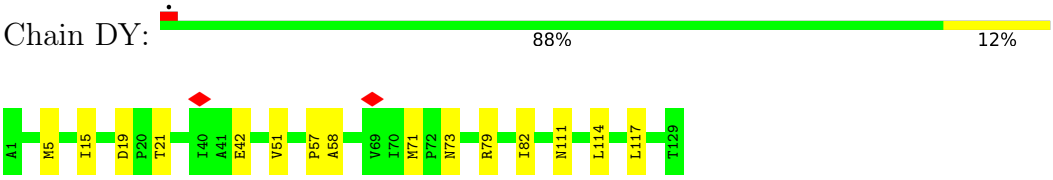
• Molecule 1: Coat protein

Chain DX:



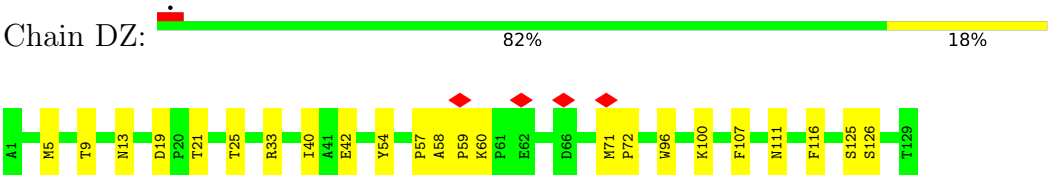
• Molecule 1: Coat protein

Chain DY:



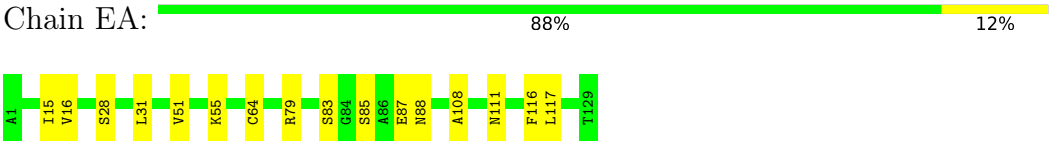
• Molecule 1: Coat protein

Chain DZ:



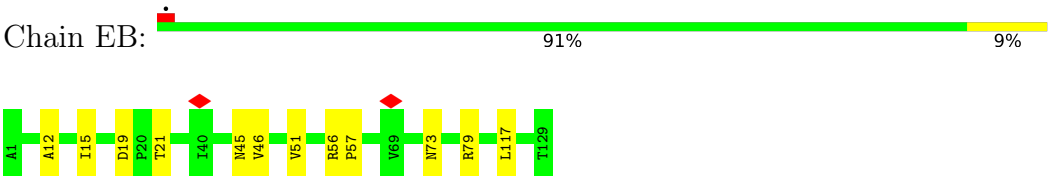
• Molecule 1: Coat protein

Chain EA:



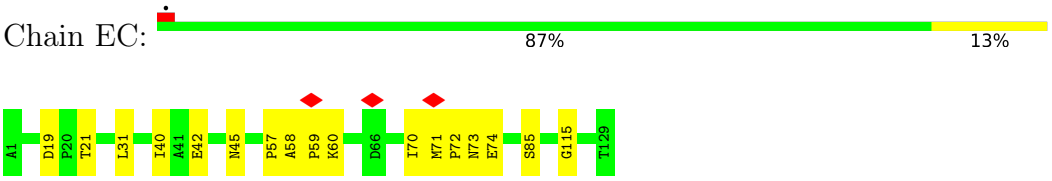
• Molecule 1: Coat protein

Chain EB:



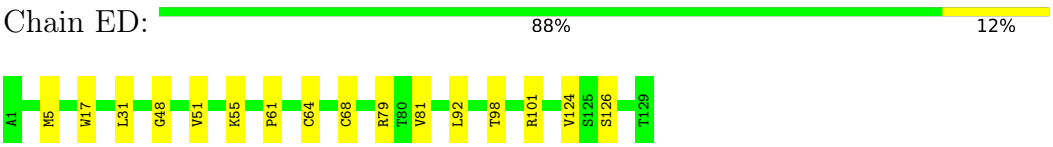
• Molecule 1: Coat protein

Chain EC:



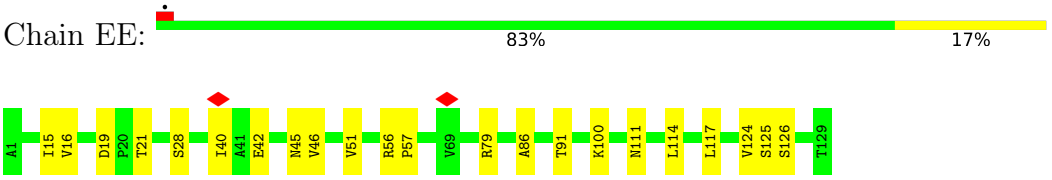
• Molecule 1: Coat protein

Chain ED:



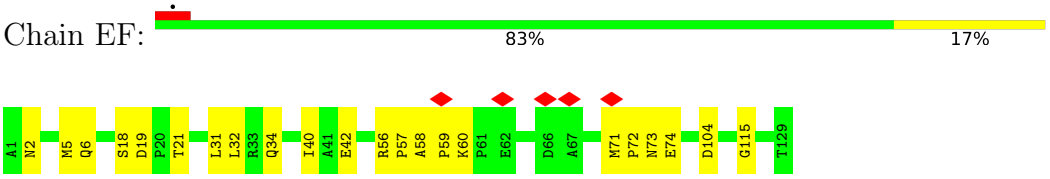
• Molecule 1: Coat protein

Chain EE:



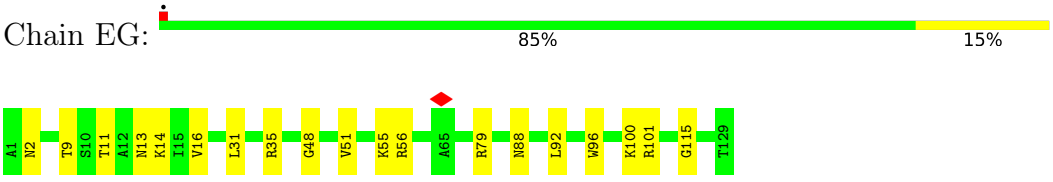
• Molecule 1: Coat protein

Chain EF:



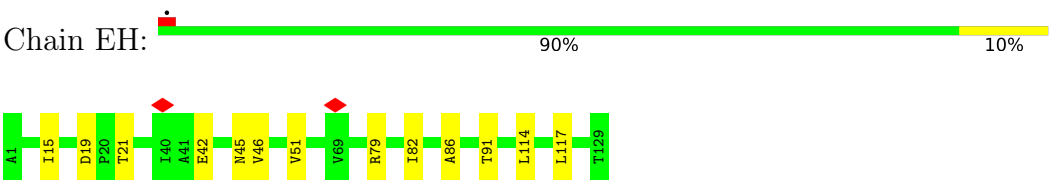
• Molecule 1: Coat protein

Chain EG:



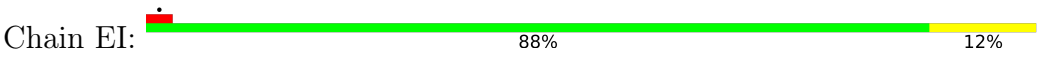
• Molecule 1: Coat protein

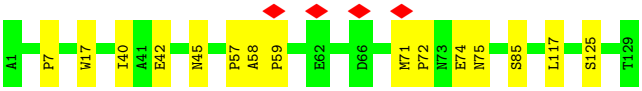
Chain EH:



• Molecule 1: Coat protein

Chain EI:



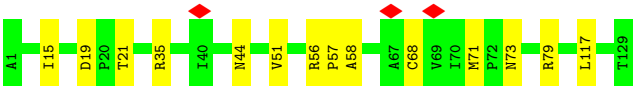


• Molecule 1: Coat protein

Chain EJ:

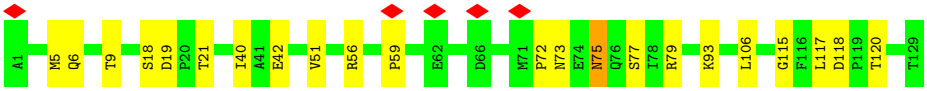
• Molecule 1: Coat protein

Chain EK:



• Molecule 1: Coat protein

Chain EL:

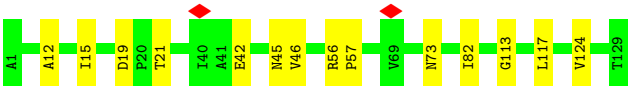


• Molecule 1: Coat protein

Chain EM:

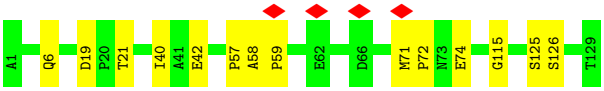
• Molecule 1: Coat protein

Chain EN:



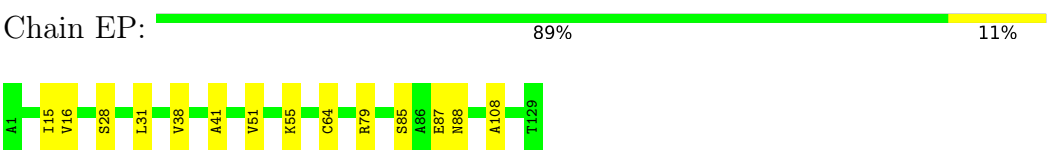
• Molecule 1: Coat protein

Chain EO:



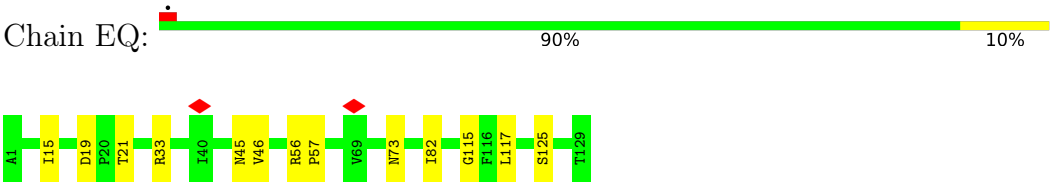
• Molecule 1: Coat protein

Chain EP:



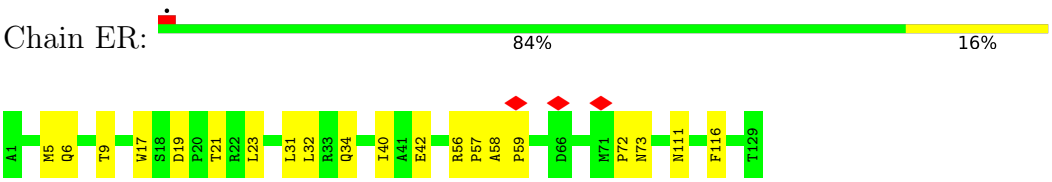
• Molecule 1: Coat protein

Chain EQ:



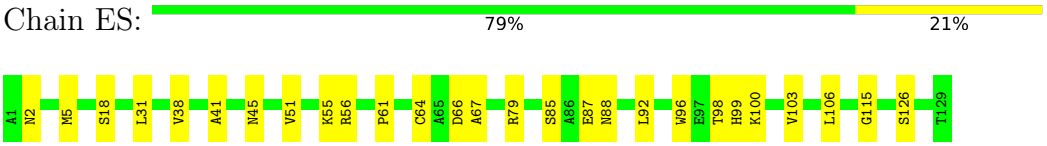
• Molecule 1: Coat protein

Chain ER:



• Molecule 1: Coat protein

Chain ES:



• Molecule 1: Coat protein

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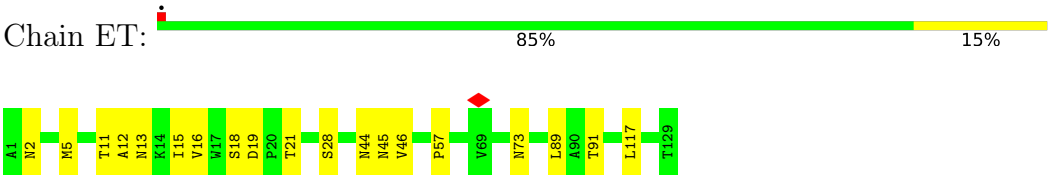

• Molecule 1: Coat protein

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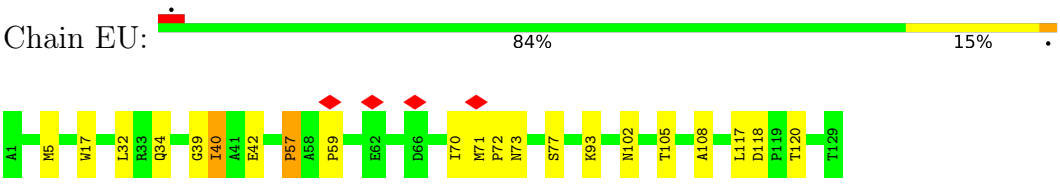
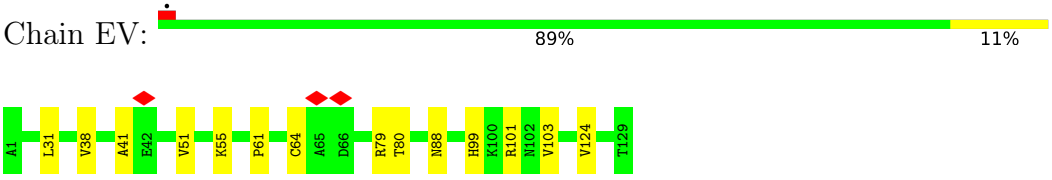


• Molecule 1: Coat protein

Chain EV:



• Molecule 1: Coat protein

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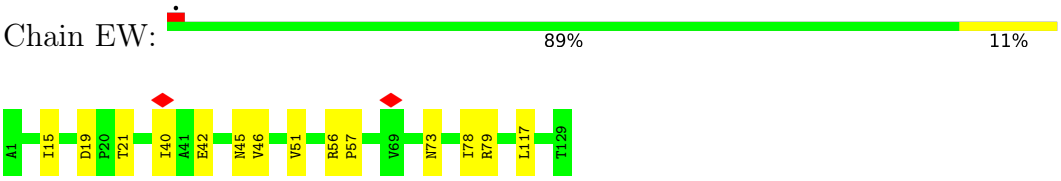
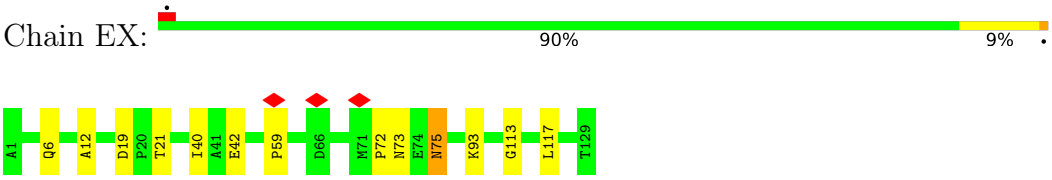


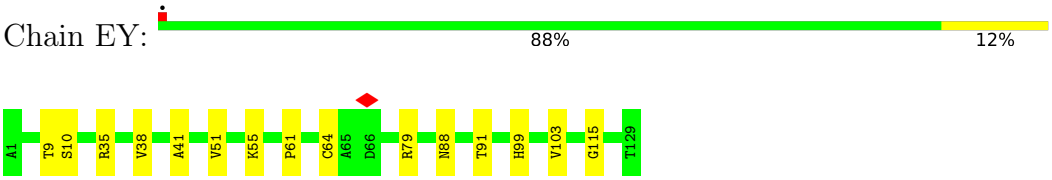
• Molecule 1: Coat protein

Chain EX:



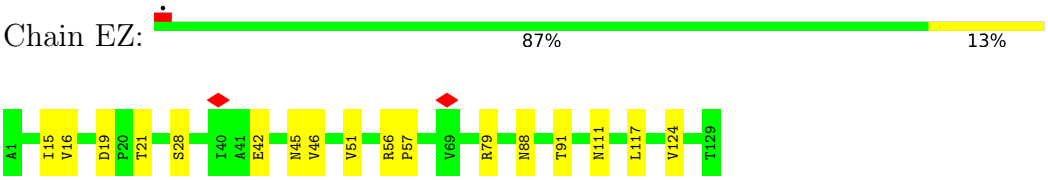
• Molecule 1: Coat protein

Chain EY:



• Molecule 1: Coat protein

Chain EZ:



• Molecule 1: Coat protein

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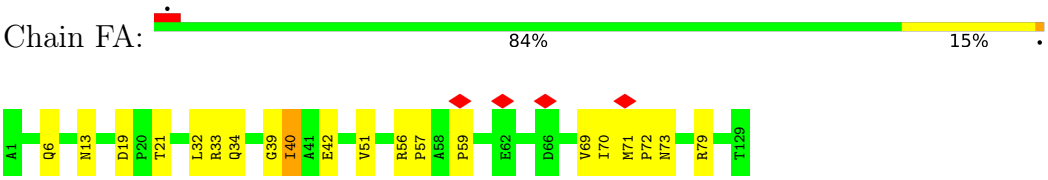
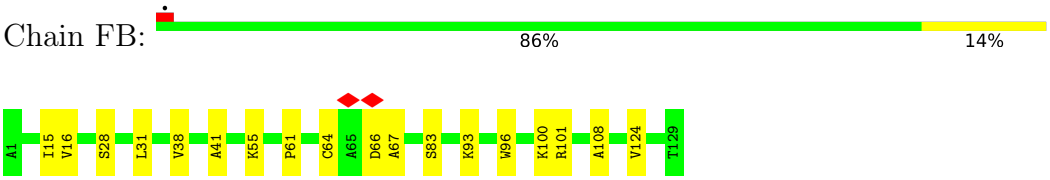


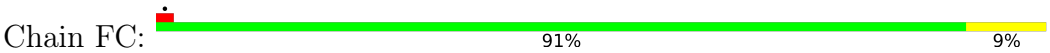
• Molecule 1: Coat protein

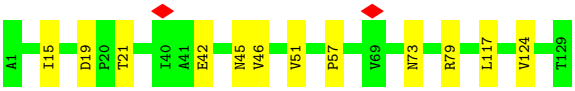
Chain FB:



• Molecule 1: Coat protein

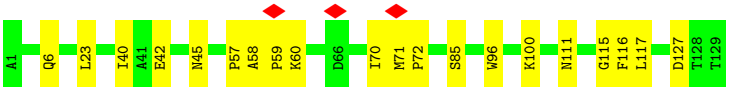
Chain FC:





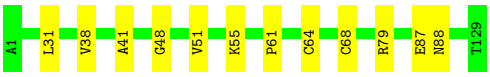
• Molecule 1: Coat protein

Chain FD:



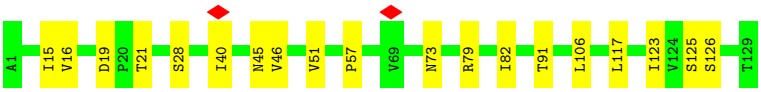
• Molecule 1: Coat protein

Chain FE:



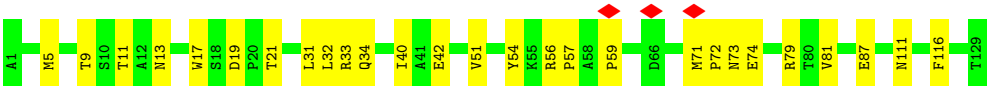
• Molecule 1: Coat protein

Chain FF:



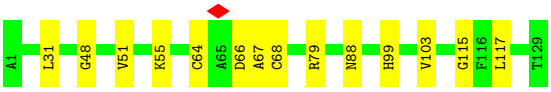
• Molecule 1: Coat protein

Chain FG:



• Molecule 1: Coat protein

Chain FH:

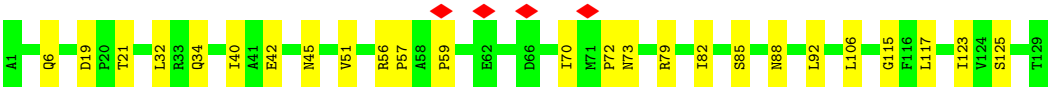


• Molecule 1: Coat protein

Chain FI:

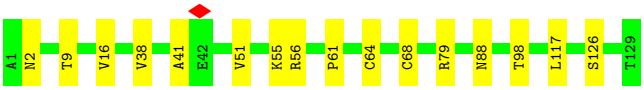
• Molecule 1: Coat protein

Chain FJ:



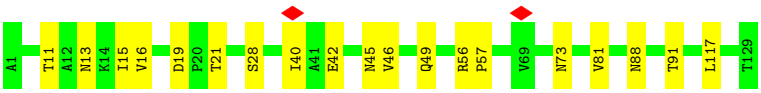
• Molecule 1: Coat protein

Chain FK:



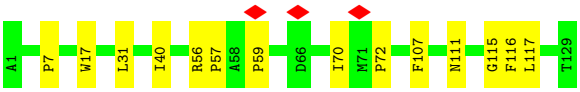
• Molecule 1: Coat protein

Chain FL:



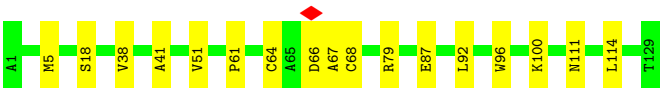
• Molecule 1: Coat protein

Chain FM:



• Molecule 1: Coat protein

Chain FN:

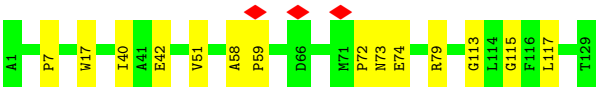


• Molecule 1: Coat protein

Chain FO:

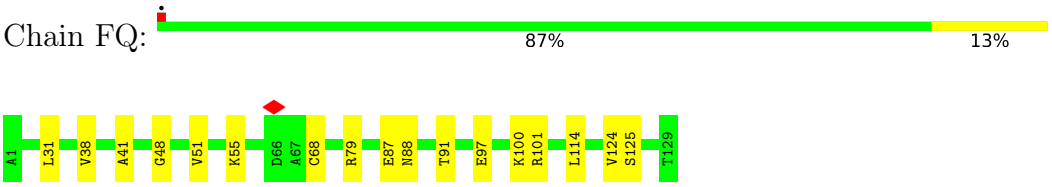
• Molecule 1: Coat protein

Chain FP:



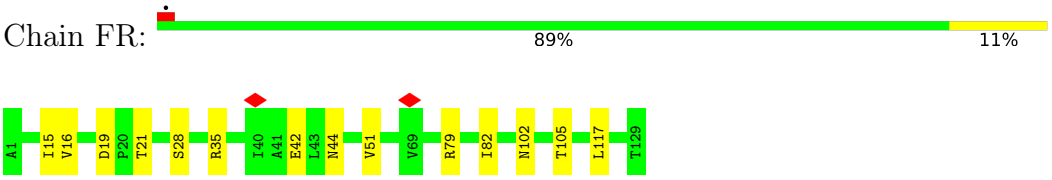
• Molecule 1: Coat protein

Chain FQ:



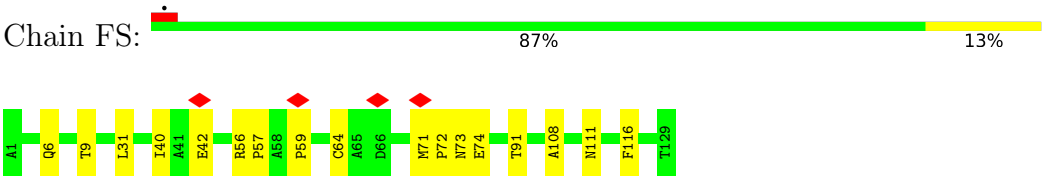
• Molecule 1: Coat protein

Chain FR:



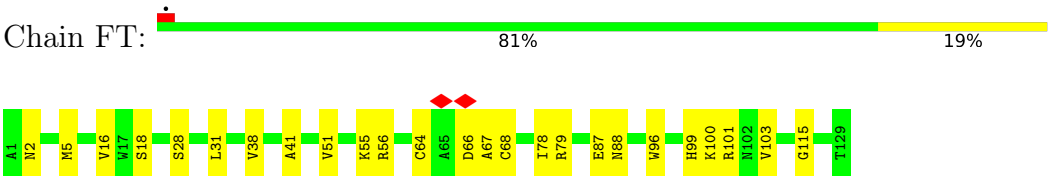
• Molecule 1: Coat protein

Chain FS:



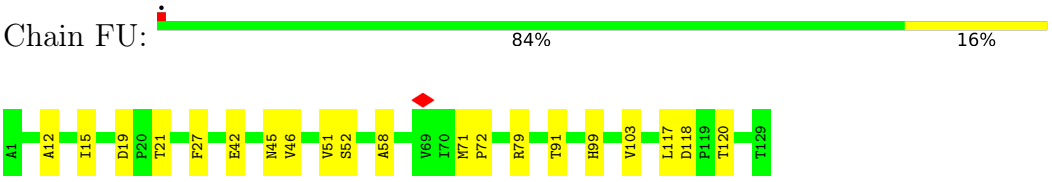
• Molecule 1: Coat protein

Chain FT:



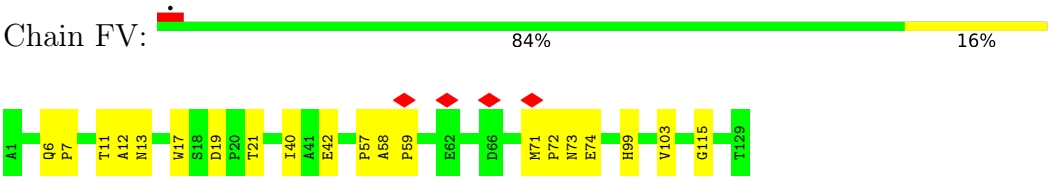
• Molecule 1: Coat protein

Chain FU:



• Molecule 1: Coat protein

Chain FV:

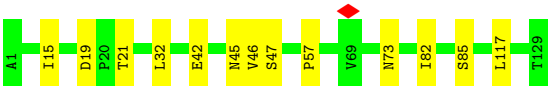


• Molecule 1: Coat protein

Chain FW:

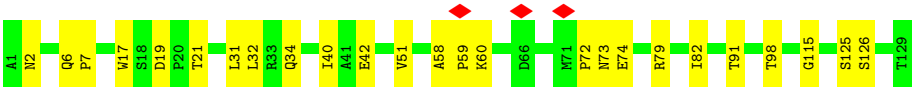
• Molecule 1: Coat protein

Chain FX:



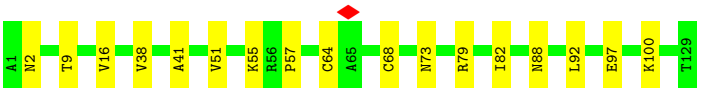
• Molecule 1: Coat protein

Chain FY:



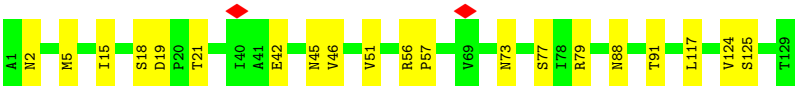
• Molecule 1: Coat protein

Chain FZ:



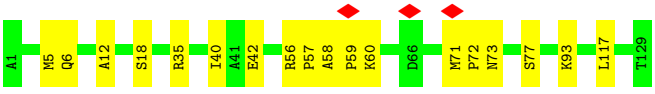
• Molecule 1: Coat protein

Chain GA:



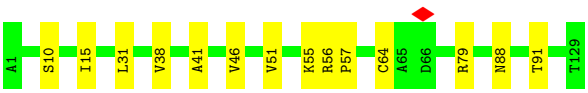
• Molecule 1: Coat protein

Chain GB:



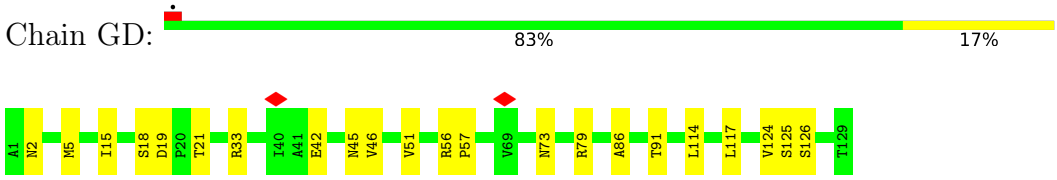
• Molecule 1: Coat protein

Chain GC:



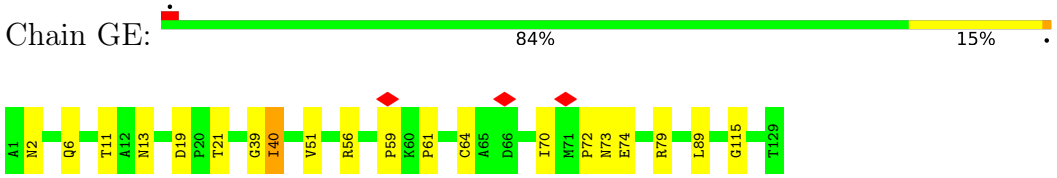
• Molecule 1: Coat protein

Chain GD:



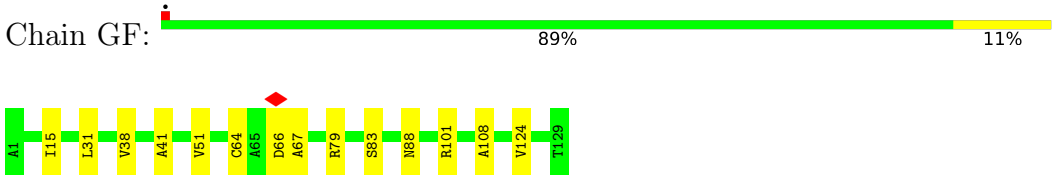
• Molecule 1: Coat protein

Chain GE:



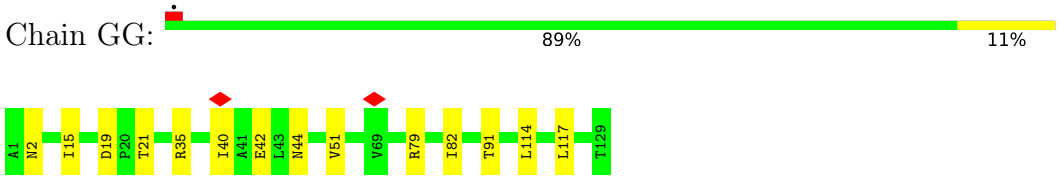
• Molecule 1: Coat protein

Chain GF:



• Molecule 1: Coat protein

Chain GG:



• Molecule 1: Coat protein

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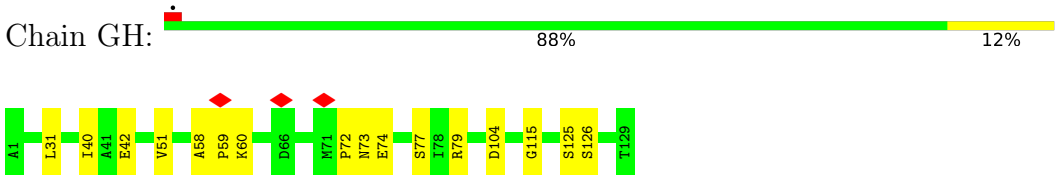
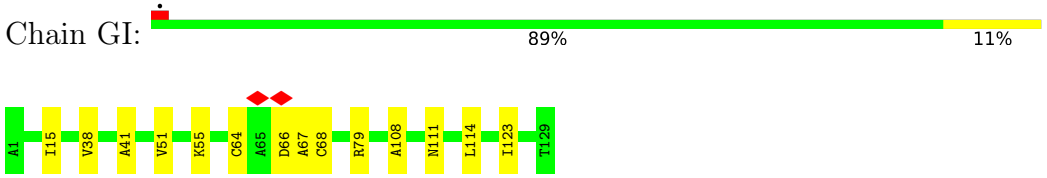


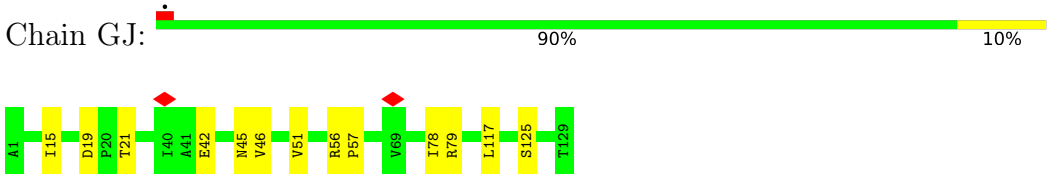
• Molecule 1: Coat protein

Chain GI:



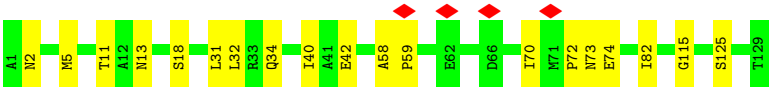
• Molecule 1: Coat protein

Chain GJ:



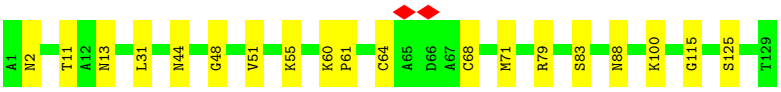
• Molecule 1: Coat protein

Chain GK:



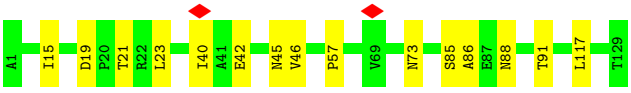
• Molecule 1: Coat protein

Chain GL:



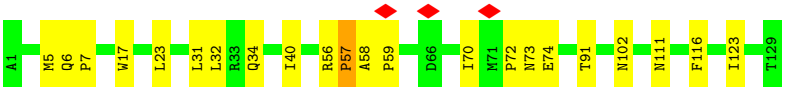
• Molecule 1: Coat protein

Chain GM:



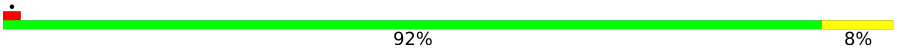
• Molecule 1: Coat protein

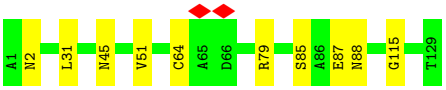
Chain GN:



• Molecule 1: Coat protein

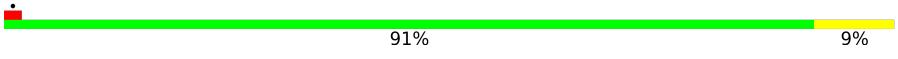
Chain GO:

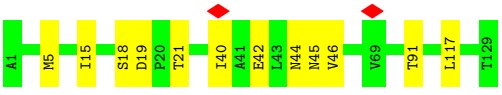




• Molecule 1: Coat protein

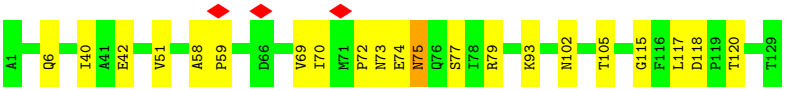
Chain GP:





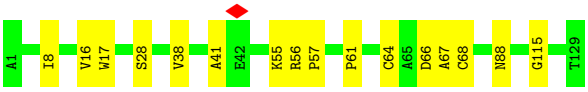
• Molecule 1: Coat protein

Chain GQ:



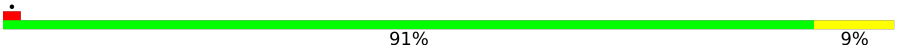
• Molecule 1: Coat protein

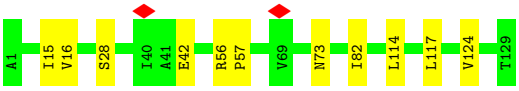
Chain GR:



• Molecule 1: Coat protein

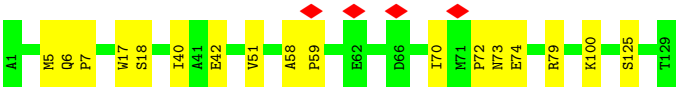
Chain GS:





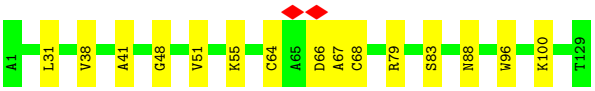
• Molecule 1: Coat protein

Chain GT:



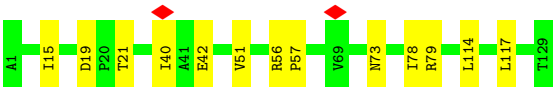
• Molecule 1: Coat protein

Chain GU:



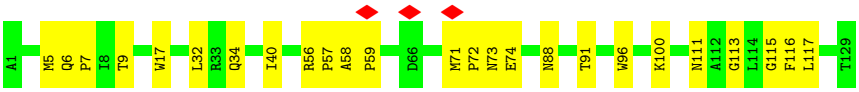
• Molecule 1: Coat protein

Chain GV:



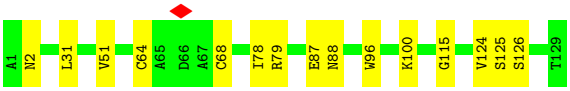
• Molecule 1: Coat protein

Chain GW:



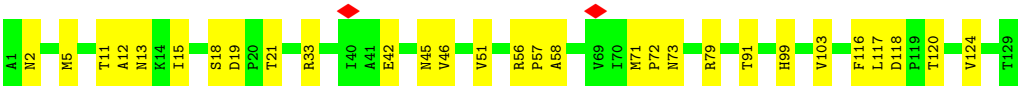
• Molecule 1: Coat protein

Chain GX:



• Molecule 1: Coat protein

Chain GY:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10000	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 ($e^-/Å^2$)	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	1.909	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	457.91998, 457.91998, 457.91998	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	AB	0.24	0/985	0.49	0/1342
1	AC	0.25	0/985	0.49	0/1342
1	AD	0.25	0/985	0.48	0/1342
1	AE	0.25	0/985	0.50	0/1342
1	AF	0.25	0/985	0.49	0/1342
1	AG	0.25	0/985	0.49	0/1342
1	AH	0.25	0/985	0.50	0/1342
1	AI	0.25	0/985	0.50	0/1342
1	AJ	0.25	0/985	0.49	0/1342
1	AK	0.24	0/985	0.51	0/1342
1	AL	0.26	0/985	0.52	0/1342
1	AM	0.25	0/985	0.50	0/1342
1	AN	0.26	0/985	0.53	1/1342 (0.1%)
1	AO	0.25	0/985	0.48	0/1342
1	AP	0.24	0/985	0.49	0/1342
1	AQ	0.25	0/985	0.51	0/1342
1	AR	0.25	0/985	0.49	0/1342
1	AS	0.25	0/985	0.49	0/1342
1	AT	0.25	0/985	0.50	0/1342
1	AU	0.24	0/985	0.49	0/1342
1	AV	0.24	0/985	0.49	0/1342
1	AW	0.25	0/985	0.51	0/1342
1	AX	0.24	0/985	0.48	0/1342
1	AY	0.25	0/985	0.49	0/1342
1	AZ	0.25	0/985	0.52	0/1342
1	BA	0.25	0/985	0.49	0/1342
1	BB	0.25	0/985	0.49	0/1342
1	BC	0.25	0/985	0.51	0/1342
1	BD	0.24	0/985	0.49	0/1342
1	BE	0.25	0/985	0.49	0/1342
1	BF	0.25	0/985	0.50	0/1342
1	BG	0.25	0/985	0.48	0/1342
1	BH	0.25	0/985	0.50	0/1342
1	BI	0.27	0/985	0.58	1/1342 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	BJ	0.25	0/985	0.49	0/1342
1	BK	0.25	0/985	0.49	0/1342
1	BL	0.25	0/985	0.50	0/1342
1	BM	0.25	0/985	0.49	0/1342
1	BN	0.26	0/985	0.51	0/1342
1	BO	0.25	0/985	0.51	0/1342
1	BP	0.25	0/985	0.49	0/1342
1	BQ	0.25	0/985	0.50	0/1342
1	BR	0.25	0/985	0.51	0/1342
1	BS	0.25	0/985	0.50	0/1342
1	BT	0.25	0/985	0.49	0/1342
1	BU	0.25	0/985	0.51	0/1342
1	BV	0.25	0/985	0.49	0/1342
1	BW	0.25	0/985	0.49	0/1342
1	BX	0.25	0/985	0.51	0/1342
1	BY	0.25	0/985	0.49	0/1342
1	BZ	0.24	0/985	0.47	0/1342
1	CA	0.25	0/985	0.51	0/1342
1	CB	0.25	0/985	0.49	0/1342
1	CC	0.24	0/985	0.50	0/1342
1	CD	0.25	0/985	0.51	0/1342
1	CE	0.25	0/985	0.49	0/1342
1	CF	0.24	0/985	0.49	0/1342
1	CG	0.24	0/985	0.49	0/1342
1	CH	0.24	0/985	0.48	0/1342
1	CI	0.25	0/985	0.50	0/1342
1	CJ	0.25	0/985	0.51	0/1342
1	CK	0.25	0/985	0.49	0/1342
1	CL	0.25	0/985	0.49	0/1342
1	CM	0.26	0/985	0.52	0/1342
1	CN	0.25	0/985	0.48	0/1342
1	CO	0.25	0/985	0.48	0/1342
1	CP	0.25	0/985	0.50	0/1342
1	CQ	0.25	0/985	0.50	0/1342
1	CR	0.25	0/985	0.50	0/1342
1	CS	0.25	0/985	0.50	0/1342
1	CT	0.25	0/985	0.48	0/1342
1	CU	0.25	0/985	0.49	0/1342
1	CV	0.26	0/985	0.53	1/1342 (0.1%)
1	CW	0.25	0/985	0.49	0/1342
1	CX	0.25	0/985	0.49	0/1342
1	CY	0.25	0/985	0.50	0/1342
1	CZ	0.24	0/985	0.49	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	DA	0.25	0/985	0.48	0/1342
1	DB	0.25	0/985	0.50	0/1342
1	DC	0.25	0/985	0.50	0/1342
1	DD	0.25	0/985	0.48	0/1342
1	DE	0.24	0/985	0.49	0/1342
1	DF	0.25	0/985	0.49	0/1342
1	DG	0.25	0/985	0.49	0/1342
1	DH	0.25	0/985	0.51	0/1342
1	DI	0.25	0/985	0.48	0/1342
1	DJ	0.25	0/985	0.48	0/1342
1	DK	0.26	0/985	0.52	0/1342
1	DL	0.25	0/985	0.49	0/1342
1	DM	0.25	0/985	0.49	0/1342
1	DN	0.27	0/985	0.57	1/1342 (0.1%)
1	DO	0.25	0/985	0.49	0/1342
1	DP	0.25	0/985	0.49	0/1342
1	DQ	0.25	0/985	0.50	0/1342
1	DR	0.25	0/985	0.49	0/1342
1	DS	0.25	0/985	0.49	0/1342
1	DT	0.25	0/985	0.52	0/1342
1	DU	0.25	0/985	0.49	0/1342
1	DV	0.24	0/985	0.48	0/1342
1	DW	0.25	0/985	0.52	0/1342
1	DX	0.25	0/985	0.48	0/1342
1	DY	0.25	0/985	0.48	0/1342
1	DZ	0.25	0/985	0.51	0/1342
1	EA	0.25	0/985	0.49	0/1342
1	EB	0.25	0/985	0.49	0/1342
1	EC	0.25	0/985	0.51	0/1342
1	ED	0.25	0/985	0.49	0/1342
1	EE	0.25	0/985	0.48	0/1342
1	EF	0.25	0/985	0.51	0/1342
1	EG	0.25	0/985	0.49	0/1342
1	EH	0.25	0/985	0.49	0/1342
1	EI	0.25	0/985	0.51	0/1342
1	EJ	0.25	0/985	0.48	0/1342
1	EK	0.24	0/985	0.49	0/1342
1	EL	0.24	0/985	0.51	0/1342
1	EM	0.24	0/985	0.49	0/1342
1	EN	0.25	0/985	0.50	0/1342
1	EO	0.24	0/985	0.51	0/1342
1	EP	0.25	0/985	0.51	0/1342
1	EQ	0.25	0/985	0.49	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	ER	0.25	0/985	0.51	0/1342
1	ES	0.25	0/985	0.50	0/1342
1	ET	0.25	0/985	0.49	0/1342
1	EU	0.26	0/985	0.54	1/1342 (0.1%)
1	EV	0.25	0/985	0.48	0/1342
1	EW	0.25	0/985	0.50	0/1342
1	EX	0.24	0/985	0.50	0/1342
1	EY	0.25	0/985	0.49	0/1342
1	EZ	0.25	0/985	0.49	0/1342
1	FA	0.24	0/985	0.51	0/1342
1	FB	0.25	0/985	0.49	0/1342
1	FC	0.24	0/985	0.49	0/1342
1	FD	0.25	0/985	0.52	0/1342
1	FE	0.25	0/985	0.49	0/1342
1	FF	0.25	0/985	0.51	0/1342
1	FG	0.25	0/985	0.50	0/1342
1	FH	0.25	0/985	0.50	0/1342
1	FI	0.25	0/985	0.50	0/1342
1	FJ	0.25	0/985	0.51	0/1342
1	FK	0.25	0/985	0.49	0/1342
1	FL	0.24	0/985	0.48	0/1342
1	FM	0.25	0/985	0.51	0/1342
1	FN	0.25	0/985	0.49	0/1342
1	FO	0.25	0/985	0.49	0/1342
1	FP	0.25	0/985	0.49	0/1342
1	FQ	0.25	0/985	0.49	0/1342
1	FR	0.25	0/985	0.48	0/1342
1	FS	0.25	0/985	0.51	0/1342
1	FT	0.25	0/985	0.49	0/1342
1	FU	0.25	0/985	0.49	0/1342
1	FV	0.24	0/985	0.51	0/1342
1	FW	0.25	0/985	0.50	0/1342
1	FX	0.25	0/985	0.49	0/1342
1	FY	0.25	0/985	0.51	0/1342
1	FZ	0.24	0/985	0.49	0/1342
1	GA	0.24	0/985	0.48	0/1342
1	GB	0.25	0/985	0.50	0/1342
1	GC	0.24	0/985	0.48	0/1342
1	GD	0.25	0/985	0.50	0/1342
1	GE	0.25	0/985	0.51	0/1342
1	GF	0.25	0/985	0.50	0/1342
1	GG	0.25	0/985	0.50	0/1342
1	GH	0.26	0/985	0.53	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	GI	0.25	0/985	0.49	0/1342
1	GJ	0.25	0/985	0.48	0/1342
1	GK	0.26	0/985	0.52	0/1342
1	GL	0.24	0/985	0.49	0/1342
1	GM	0.25	0/985	0.50	0/1342
1	GN	0.27	0/985	0.59	1/1342 (0.1%)
1	GO	0.25	0/985	0.49	0/1342
1	GP	0.25	0/985	0.49	0/1342
1	GQ	0.25	0/985	0.50	0/1342
1	GR	0.25	0/985	0.50	0/1342
1	GS	0.25	0/985	0.50	0/1342
1	GT	0.24	0/985	0.51	0/1342
1	GU	0.24	0/985	0.48	0/1342
1	GV	0.25	0/985	0.48	0/1342
1	GW	0.25	0/985	0.51	0/1342
1	GX	0.25	0/985	0.49	0/1342
1	GY	0.26	0/985	0.51	0/1342
All	All	0.25	0/177300	0.50	6/241560 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	GN	57	PRO	CA-N-CD	-9.16	98.67	111.50
1	BI	57	PRO	CA-N-CD	-8.85	99.12	111.50
1	DN	57	PRO	CA-N-CD	-8.59	99.48	111.50
1	EU	57	PRO	CA-N-CD	-6.38	102.58	111.50
1	CV	57	PRO	CA-N-CD	-5.61	103.64	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	968	0	973	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AC	968	0	973	16	0
1	AD	968	0	973	12	0
1	AE	968	0	973	16	0
1	AF	968	0	973	18	0
1	AG	968	0	973	21	0
1	AH	968	0	973	15	0
1	AI	968	0	973	13	0
1	AJ	968	0	973	10	0
1	AK	968	0	973	15	0
1	AL	968	0	973	9	0
1	AM	968	0	973	14	0
1	AN	968	0	973	9	0
1	AO	968	0	973	6	0
1	AP	968	0	973	8	0
1	AQ	968	0	973	21	0
1	AR	968	0	973	16	0
1	AS	968	0	973	17	0
1	AT	968	0	973	20	0
1	AU	968	0	973	9	0
1	AV	968	0	973	15	0
1	AW	968	0	973	13	0
1	AX	968	0	973	12	0
1	AY	968	0	973	10	0
1	AZ	968	0	973	22	0
1	BA	968	0	973	16	0
1	BB	968	0	973	15	0
1	BC	968	0	973	16	0
1	BD	968	0	973	12	0
1	BE	968	0	973	14	0
1	BF	968	0	973	16	0
1	BG	968	0	973	11	0
1	BH	968	0	973	20	0
1	BI	968	0	973	19	0
1	BJ	968	0	973	15	0
1	BK	968	0	973	15	0
1	BL	968	0	973	20	0
1	BM	968	0	973	11	0
1	BN	968	0	973	13	0
1	BO	968	0	973	15	0
1	BP	968	0	973	8	0
1	BQ	968	0	973	13	0
1	BR	968	0	973	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BS	968	0	973	10	0
1	BT	968	0	973	13	0
1	BU	968	0	973	14	0
1	BV	968	0	973	13	0
1	BW	968	0	973	17	0
1	BX	968	0	973	16	0
1	BY	968	0	973	19	0
1	BZ	968	0	973	7	0
1	CA	968	0	973	9	0
1	CB	968	0	973	14	0
1	CC	968	0	973	11	0
1	CD	968	0	973	11	0
1	CE	968	0	973	18	0
1	CF	968	0	973	8	0
1	CG	968	0	973	17	0
1	CH	968	0	973	14	0
1	CI	968	0	973	12	0
1	CJ	968	0	973	14	0
1	CK	968	0	973	12	0
1	CL	968	0	973	15	0
1	CM	968	0	973	12	0
1	CN	968	0	973	11	0
1	CO	968	0	973	16	0
1	CP	968	0	973	20	0
1	CQ	968	0	973	17	0
1	CR	968	0	973	21	0
1	CS	968	0	973	12	0
1	CT	968	0	973	15	0
1	CU	968	0	973	17	0
1	CV	968	0	973	14	0
1	CW	968	0	973	9	0
1	CX	968	0	973	7	0
1	CY	968	0	973	11	0
1	CZ	968	0	973	15	0
1	DA	968	0	973	8	0
1	DB	968	0	973	10	0
1	DC	968	0	973	11	0
1	DD	968	0	973	11	0
1	DE	968	0	973	18	0
1	DF	968	0	973	12	0
1	DG	968	0	973	12	0
1	DH	968	0	973	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DI	968	0	973	12	0
1	DJ	968	0	973	10	0
1	DK	968	0	973	18	0
1	DL	968	0	973	15	0
1	DM	968	0	973	18	0
1	DN	968	0	973	15	0
1	DO	968	0	973	15	0
1	DP	968	0	973	17	0
1	DQ	968	0	973	14	0
1	DR	968	0	973	13	0
1	DS	968	0	973	17	0
1	DT	968	0	973	20	0
1	DU	968	0	973	12	0
1	DV	968	0	973	14	0
1	DW	968	0	973	10	0
1	DX	968	0	973	10	0
1	DY	968	0	973	11	0
1	DZ	968	0	973	14	0
1	EA	968	0	973	15	0
1	EB	968	0	973	9	0
1	EC	968	0	973	13	0
1	ED	968	0	973	14	0
1	EE	968	0	973	18	0
1	EF	968	0	973	18	0
1	EG	968	0	973	17	0
1	EH	968	0	973	10	0
1	EI	968	0	973	11	0
1	EJ	968	0	973	11	0
1	EK	968	0	973	13	0
1	EL	968	0	973	20	0
1	EM	968	0	973	14	0
1	EN	968	0	973	13	0
1	EO	968	0	973	10	0
1	EP	968	0	973	12	0
1	EQ	968	0	973	11	0
1	ER	968	0	973	17	0
1	ES	968	0	973	21	0
1	ET	968	0	973	15	0
1	EU	968	0	973	18	0
1	EV	968	0	973	10	0
1	EW	968	0	973	13	0
1	EX	968	0	973	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EY	968	0	973	12	0
1	EZ	968	0	973	12	0
1	FA	968	0	973	14	0
1	FB	968	0	973	12	0
1	FC	968	0	973	8	0
1	FD	968	0	973	13	0
1	FE	968	0	973	11	0
1	FF	968	0	973	12	0
1	FG	968	0	973	23	0
1	FH	968	0	973	12	0
1	FI	968	0	973	18	0
1	FJ	968	0	973	21	0
1	FK	968	0	973	12	0
1	FL	968	0	973	12	0
1	FM	968	0	973	10	0
1	FN	968	0	973	10	0
1	FO	968	0	973	15	0
1	FP	968	0	973	10	0
1	FQ	968	0	973	14	0
1	FR	968	0	973	9	0
1	FS	968	0	973	13	0
1	FT	968	0	973	20	0
1	FU	968	0	973	13	0
1	FV	968	0	973	15	0
1	FW	968	0	973	14	0
1	FX	968	0	973	9	0
1	FY	968	0	973	21	0
1	FZ	968	0	973	13	0
1	GA	968	0	973	15	0
1	GB	968	0	973	13	0
1	GC	968	0	973	12	0
1	GD	968	0	973	20	0
1	GE	968	0	973	14	0
1	GF	968	0	973	12	0
1	GG	968	0	973	12	0
1	GH	968	0	973	12	0
1	GI	968	0	973	10	0
1	GJ	968	0	973	9	0
1	GK	968	0	973	15	0
1	GL	968	0	973	17	0
1	GM	968	0	973	11	0
1	GN	968	0	973	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GO	968	0	973	9	0
1	GP	968	0	973	9	0
1	GQ	968	0	973	15	0
1	GR	968	0	973	14	0
1	GS	968	0	973	11	0
1	GT	968	0	973	13	0
1	GU	968	0	973	13	0
1	GV	968	0	973	11	0
1	GW	968	0	973	21	0
1	GX	968	0	973	13	0
1	GY	968	0	973	23	0
All	All	174240	0	175140	1772	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1772 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CV:59:PRO:HG3	1:CV:72:PRO:HD2	1.58	0.86
1:FM:59:PRO:HG3	1:FM:72:PRO:HD2	1.59	0.83
1:BO:59:PRO:HG3	1:BO:72:PRO:HD2	1.62	0.82
1:FV:59:PRO:HG3	1:FV:72:PRO:HD2	1.61	0.82
1:CP:59:PRO:HG3	1:CP:72:PRO:HD2	1.62	0.82

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
1	AB	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AD	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AE	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	AF	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	AG	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AH	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	AI	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	AJ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AK	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	AL	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AM	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AN	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	AO	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	AP	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AQ	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	AR	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	AS	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	AT	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	AU	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	AV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AW	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	AX	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AY	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AZ	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	BA	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BB	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	BC	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	BD	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BE	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	BF	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	BG	127/129 (98%)	124 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BH	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	BI	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	BJ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BK	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	BL	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	BM	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	BN	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	BO	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	BP	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BQ	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	BR	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	57
1	BS	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BT	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	BU	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	BV	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	BW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BX	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	BY	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	BZ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CA	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	57
1	CB	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	CC	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	CD	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	57
1	CE	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	CF	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CG	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	CH	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	CI	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CJ	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	57
1	CK	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	CL	127/129 (98%)	122 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	CM	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19 57
1	CN	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	CO	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	CP	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19 57
1	CQ	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	CR	127/129 (98%)	120 (94%)	7 (6%)	0	100 100
1	CS	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19 57
1	CT	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	CU	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	CV	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19 57
1	CW	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	CX	127/129 (98%)	123 (97%)	4 (3%)	0	100 100
1	CY	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19 57
1	CZ	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	DA	127/129 (98%)	123 (97%)	4 (3%)	0	100 100
1	DB	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19 57
1	DC	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	DD	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	DE	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19 57
1	DF	127/129 (98%)	123 (97%)	4 (3%)	0	100 100
1	DG	127/129 (98%)	121 (95%)	6 (5%)	0	100 100
1	DH	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19 57
1	DI	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	DJ	127/129 (98%)	123 (97%)	4 (3%)	0	100 100
1	DK	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19 57
1	DL	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	DM	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	DN	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19 57
1	DO	127/129 (98%)	123 (97%)	4 (3%)	0	100 100
1	DP	127/129 (98%)	123 (97%)	4 (3%)	0	100 100
1	DQ	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DR	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	DS	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DT	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	57
1	DU	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	DV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DW	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	DX	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	DY	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	DZ	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	57
1	EA	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	EB	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	EC	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	ED	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	EE	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	EF	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	57
1	EG	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	EH	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	EI	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	EJ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	EK	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	EL	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	EM	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	EN	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	EO	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	EP	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	EQ	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	ER	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	ES	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	ET	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	EU	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	57
1	EV	127/129 (98%)	124 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	EX	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	EY	127/129 (98%)	125 (98%)	2 (2%)	0	100	100
1	EZ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	FA	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19	57
1	FB	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	FC	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	FD	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	FE	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	FF	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	FG	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	FH	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	FI	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
1	FJ	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19	57
1	FK	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	FL	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	FM	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	FN	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	FO	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	FP	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	FQ	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	FR	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	FS	127/129 (98%)	121 (95%)	5 (4%)	1 (1%)	19	57
1	FT	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	FU	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	FV	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19	57
1	FW	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
1	FX	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	FY	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19	57
1	FZ	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
1	GA	127/129 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	GB	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	19 57
1	GC	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	GD	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	GE	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19 57
1	GF	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	GG	127/129 (98%)	123 (97%)	4 (3%)	0	100 100
1	GH	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19 57
1	GI	127/129 (98%)	123 (97%)	4 (3%)	0	100 100
1	GJ	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	GK	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19 57
1	GL	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	GM	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	GN	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	19 57
1	GO	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	GP	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	GQ	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19 57
1	GR	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	GS	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	GT	127/129 (98%)	125 (98%)	1 (1%)	1 (1%)	19 57
1	GU	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	GV	127/129 (98%)	122 (96%)	5 (4%)	0	100 100
1	GW	127/129 (98%)	124 (98%)	2 (2%)	1 (1%)	19 57
1	GX	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
1	GY	127/129 (98%)	121 (95%)	6 (5%)	0	100 100
All	All	22860/23220 (98%)	22165 (97%)	635 (3%)	60 (0%)	44 76

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	ER	40	ILE
1	GE	40	ILE
1	GN	40	ILE
1	GT	40	ILE
1	AB	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	
1	AB	108/108 (100%)	108 (100%)	0	100	100
1	AC	108/108 (100%)	108 (100%)	0	100	100
1	AD	108/108 (100%)	108 (100%)	0	100	100
1	AE	108/108 (100%)	108 (100%)	0	100	100
1	AF	108/108 (100%)	108 (100%)	0	100	100
1	AG	108/108 (100%)	108 (100%)	0	100	100
1	AH	108/108 (100%)	108 (100%)	0	100	100
1	AI	108/108 (100%)	108 (100%)	0	100	100
1	AJ	108/108 (100%)	108 (100%)	0	100	100
1	AK	108/108 (100%)	108 (100%)	0	100	100
1	AL	108/108 (100%)	108 (100%)	0	100	100
1	AM	108/108 (100%)	108 (100%)	0	100	100
1	AN	108/108 (100%)	108 (100%)	0	100	100
1	AO	108/108 (100%)	108 (100%)	0	100	100
1	AP	108/108 (100%)	108 (100%)	0	100	100
1	AQ	108/108 (100%)	108 (100%)	0	100	100
1	AR	108/108 (100%)	108 (100%)	0	100	100
1	AS	108/108 (100%)	108 (100%)	0	100	100
1	AT	108/108 (100%)	108 (100%)	0	100	100
1	AU	108/108 (100%)	108 (100%)	0	100	100
1	AV	108/108 (100%)	108 (100%)	0	100	100
1	AW	108/108 (100%)	108 (100%)	0	100	100
1	AX	108/108 (100%)	108 (100%)	0	100	100
1	AY	108/108 (100%)	108 (100%)	0	100	100
1	AZ	108/108 (100%)	108 (100%)	0	100	100
1	BA	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BB	108/108 (100%)	108 (100%)	0	100	100
1	BC	108/108 (100%)	108 (100%)	0	100	100
1	BD	108/108 (100%)	108 (100%)	0	100	100
1	BE	108/108 (100%)	108 (100%)	0	100	100
1	BF	108/108 (100%)	106 (98%)	2 (2%)	57	84
1	BG	108/108 (100%)	108 (100%)	0	100	100
1	BH	108/108 (100%)	108 (100%)	0	100	100
1	BI	108/108 (100%)	108 (100%)	0	100	100
1	BJ	108/108 (100%)	108 (100%)	0	100	100
1	BK	108/108 (100%)	108 (100%)	0	100	100
1	BL	108/108 (100%)	107 (99%)	1 (1%)	78	92
1	BM	108/108 (100%)	108 (100%)	0	100	100
1	BN	108/108 (100%)	108 (100%)	0	100	100
1	BO	108/108 (100%)	108 (100%)	0	100	100
1	BP	108/108 (100%)	108 (100%)	0	100	100
1	BQ	108/108 (100%)	108 (100%)	0	100	100
1	BR	108/108 (100%)	108 (100%)	0	100	100
1	BS	108/108 (100%)	108 (100%)	0	100	100
1	BT	108/108 (100%)	108 (100%)	0	100	100
1	BU	108/108 (100%)	106 (98%)	2 (2%)	57	84
1	BV	108/108 (100%)	108 (100%)	0	100	100
1	BW	108/108 (100%)	108 (100%)	0	100	100
1	BX	108/108 (100%)	108 (100%)	0	100	100
1	BY	108/108 (100%)	108 (100%)	0	100	100
1	BZ	108/108 (100%)	108 (100%)	0	100	100
1	CA	108/108 (100%)	108 (100%)	0	100	100
1	CB	108/108 (100%)	108 (100%)	0	100	100
1	CC	108/108 (100%)	108 (100%)	0	100	100
1	CD	108/108 (100%)	108 (100%)	0	100	100
1	CE	108/108 (100%)	108 (100%)	0	100	100
1	CF	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	CG	108/108 (100%)	106 (98%)	2 (2%)	57 84
1	CH	108/108 (100%)	108 (100%)	0	100 100
1	CI	108/108 (100%)	108 (100%)	0	100 100
1	CJ	108/108 (100%)	108 (100%)	0	100 100
1	CK	108/108 (100%)	108 (100%)	0	100 100
1	CL	108/108 (100%)	108 (100%)	0	100 100
1	CM	108/108 (100%)	108 (100%)	0	100 100
1	CN	108/108 (100%)	108 (100%)	0	100 100
1	CO	108/108 (100%)	108 (100%)	0	100 100
1	CP	108/108 (100%)	108 (100%)	0	100 100
1	CQ	108/108 (100%)	108 (100%)	0	100 100
1	CR	108/108 (100%)	108 (100%)	0	100 100
1	CS	108/108 (100%)	108 (100%)	0	100 100
1	CT	108/108 (100%)	108 (100%)	0	100 100
1	CU	108/108 (100%)	108 (100%)	0	100 100
1	CV	108/108 (100%)	108 (100%)	0	100 100
1	CW	108/108 (100%)	108 (100%)	0	100 100
1	CX	108/108 (100%)	108 (100%)	0	100 100
1	CY	108/108 (100%)	108 (100%)	0	100 100
1	CZ	108/108 (100%)	108 (100%)	0	100 100
1	DA	108/108 (100%)	108 (100%)	0	100 100
1	DB	108/108 (100%)	107 (99%)	1 (1%)	78 92
1	DC	108/108 (100%)	108 (100%)	0	100 100
1	DD	108/108 (100%)	108 (100%)	0	100 100
1	DE	108/108 (100%)	108 (100%)	0	100 100
1	DF	108/108 (100%)	108 (100%)	0	100 100
1	DG	108/108 (100%)	108 (100%)	0	100 100
1	DH	108/108 (100%)	108 (100%)	0	100 100
1	DI	108/108 (100%)	108 (100%)	0	100 100
1	DJ	108/108 (100%)	108 (100%)	0	100 100
1	DK	108/108 (100%)	108 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	DL	108/108 (100%)	108 (100%)	0	100	100
1	DM	108/108 (100%)	108 (100%)	0	100	100
1	DN	108/108 (100%)	108 (100%)	0	100	100
1	DO	108/108 (100%)	108 (100%)	0	100	100
1	DP	108/108 (100%)	108 (100%)	0	100	100
1	DQ	108/108 (100%)	107 (99%)	1 (1%)	78	92
1	DR	108/108 (100%)	108 (100%)	0	100	100
1	DS	108/108 (100%)	108 (100%)	0	100	100
1	DT	108/108 (100%)	108 (100%)	0	100	100
1	DU	108/108 (100%)	108 (100%)	0	100	100
1	DV	108/108 (100%)	108 (100%)	0	100	100
1	DW	108/108 (100%)	108 (100%)	0	100	100
1	DX	108/108 (100%)	108 (100%)	0	100	100
1	DY	108/108 (100%)	108 (100%)	0	100	100
1	DZ	108/108 (100%)	108 (100%)	0	100	100
1	EA	108/108 (100%)	108 (100%)	0	100	100
1	EB	108/108 (100%)	108 (100%)	0	100	100
1	EC	108/108 (100%)	108 (100%)	0	100	100
1	ED	108/108 (100%)	108 (100%)	0	100	100
1	EE	108/108 (100%)	108 (100%)	0	100	100
1	EF	108/108 (100%)	108 (100%)	0	100	100
1	EG	108/108 (100%)	108 (100%)	0	100	100
1	EH	108/108 (100%)	108 (100%)	0	100	100
1	EI	108/108 (100%)	108 (100%)	0	100	100
1	EJ	108/108 (100%)	108 (100%)	0	100	100
1	EK	108/108 (100%)	108 (100%)	0	100	100
1	EL	108/108 (100%)	107 (99%)	1 (1%)	78	92
1	EM	108/108 (100%)	108 (100%)	0	100	100
1	EN	108/108 (100%)	108 (100%)	0	100	100
1	EO	108/108 (100%)	108 (100%)	0	100	100
1	EP	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	EQ	108/108 (100%)	108 (100%)	0	100	100
1	ER	108/108 (100%)	108 (100%)	0	100	100
1	ES	108/108 (100%)	108 (100%)	0	100	100
1	ET	108/108 (100%)	108 (100%)	0	100	100
1	EU	108/108 (100%)	108 (100%)	0	100	100
1	EV	108/108 (100%)	108 (100%)	0	100	100
1	EW	108/108 (100%)	108 (100%)	0	100	100
1	EX	108/108 (100%)	107 (99%)	1 (1%)	78	92
1	EY	108/108 (100%)	108 (100%)	0	100	100
1	EZ	108/108 (100%)	108 (100%)	0	100	100
1	FA	108/108 (100%)	108 (100%)	0	100	100
1	FB	108/108 (100%)	108 (100%)	0	100	100
1	FC	108/108 (100%)	108 (100%)	0	100	100
1	FD	108/108 (100%)	108 (100%)	0	100	100
1	FE	108/108 (100%)	108 (100%)	0	100	100
1	FF	108/108 (100%)	108 (100%)	0	100	100
1	FG	108/108 (100%)	108 (100%)	0	100	100
1	FH	108/108 (100%)	108 (100%)	0	100	100
1	FI	108/108 (100%)	108 (100%)	0	100	100
1	FJ	108/108 (100%)	108 (100%)	0	100	100
1	FK	108/108 (100%)	108 (100%)	0	100	100
1	FL	108/108 (100%)	108 (100%)	0	100	100
1	FM	108/108 (100%)	108 (100%)	0	100	100
1	FN	108/108 (100%)	108 (100%)	0	100	100
1	FO	108/108 (100%)	108 (100%)	0	100	100
1	FP	108/108 (100%)	108 (100%)	0	100	100
1	FQ	108/108 (100%)	108 (100%)	0	100	100
1	FR	108/108 (100%)	108 (100%)	0	100	100
1	FS	108/108 (100%)	107 (99%)	1 (1%)	78	92
1	FT	108/108 (100%)	108 (100%)	0	100	100
1	FU	108/108 (100%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FV	108/108 (100%)	108 (100%)	0	100	100
1	FW	108/108 (100%)	108 (100%)	0	100	100
1	FX	108/108 (100%)	108 (100%)	0	100	100
1	FY	108/108 (100%)	108 (100%)	0	100	100
1	FZ	108/108 (100%)	108 (100%)	0	100	100
1	GA	108/108 (100%)	108 (100%)	0	100	100
1	GB	108/108 (100%)	107 (99%)	1 (1%)	78	92
1	GC	108/108 (100%)	108 (100%)	0	100	100
1	GD	108/108 (100%)	108 (100%)	0	100	100
1	GE	108/108 (100%)	108 (100%)	0	100	100
1	GF	108/108 (100%)	108 (100%)	0	100	100
1	GG	108/108 (100%)	108 (100%)	0	100	100
1	GH	108/108 (100%)	108 (100%)	0	100	100
1	GI	108/108 (100%)	108 (100%)	0	100	100
1	GJ	108/108 (100%)	108 (100%)	0	100	100
1	GK	108/108 (100%)	108 (100%)	0	100	100
1	GL	108/108 (100%)	108 (100%)	0	100	100
1	GM	108/108 (100%)	108 (100%)	0	100	100
1	GN	108/108 (100%)	108 (100%)	0	100	100
1	GO	108/108 (100%)	108 (100%)	0	100	100
1	GP	108/108 (100%)	108 (100%)	0	100	100
1	GQ	108/108 (100%)	106 (98%)	2 (2%)	57	84
1	GR	108/108 (100%)	108 (100%)	0	100	100
1	GS	108/108 (100%)	108 (100%)	0	100	100
1	GT	108/108 (100%)	108 (100%)	0	100	100
1	GU	108/108 (100%)	108 (100%)	0	100	100
1	GV	108/108 (100%)	108 (100%)	0	100	100
1	GW	108/108 (100%)	108 (100%)	0	100	100
1	GX	108/108 (100%)	108 (100%)	0	100	100
1	GY	108/108 (100%)	108 (100%)	0	100	100
All	All	19440/19440 (100%)	19425 (100%)	15 (0%)	93	98

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DB	6	GLN
1	GQ	6	GLN
1	DQ	75	ASN
1	GQ	75	ASN
1	FS	6	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	ER	73	ASN
1	FV	6	GLN
1	ES	88	ASN
1	FA	34	GLN
1	GQ	75	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

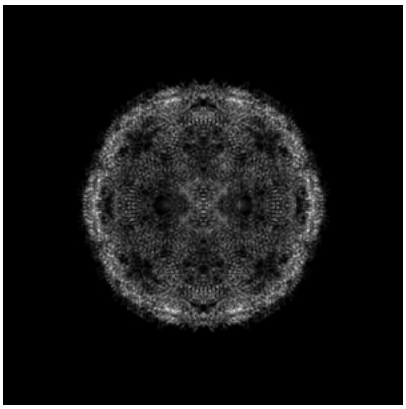
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41666. These allow visual inspection of the internal detail of the map and identification of artifacts.

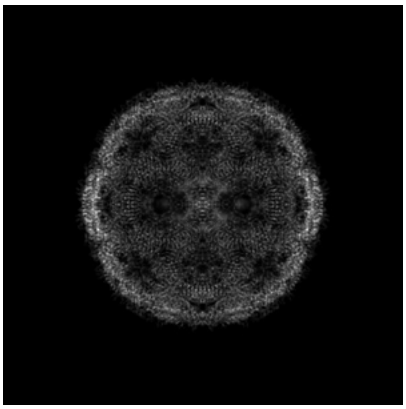
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

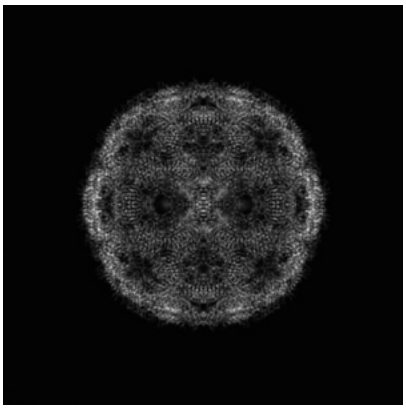
6.1.1 Primary map



X

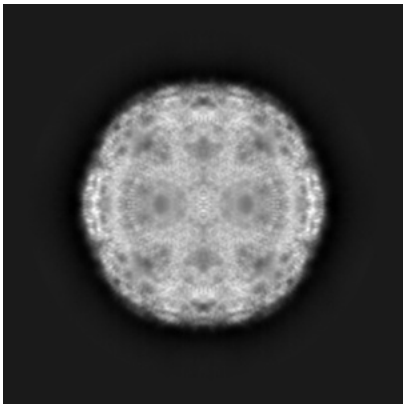


Y

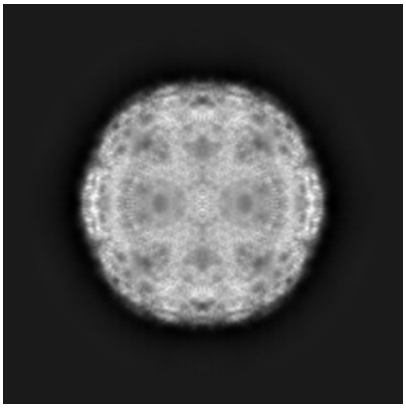


Z

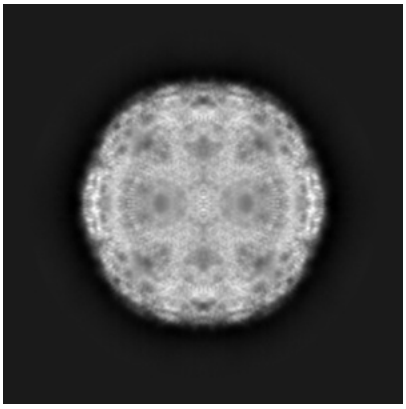
6.1.2 Raw map



X



Y

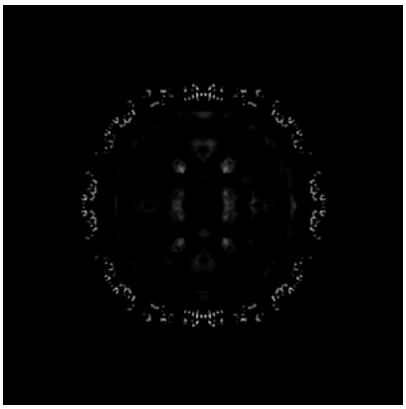


Z

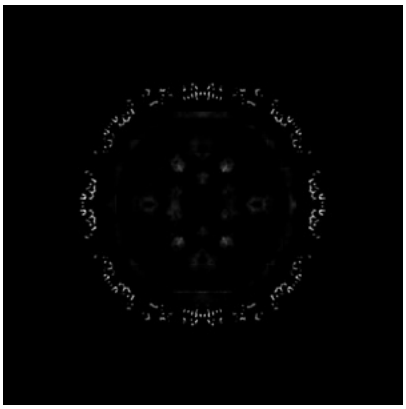
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

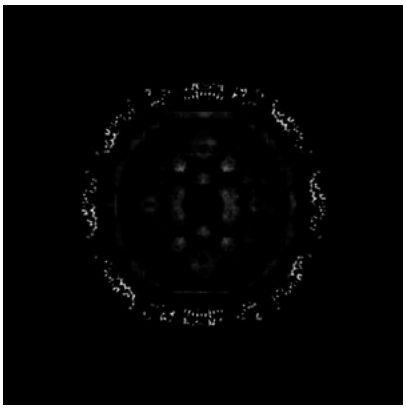
6.2.1 Primary map



X Index: 216

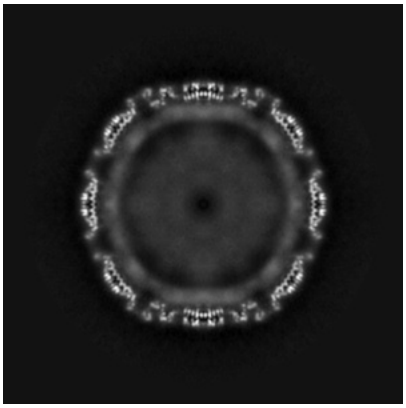


Y Index: 216

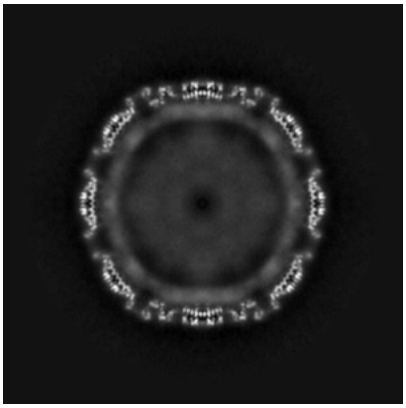


Z Index: 216

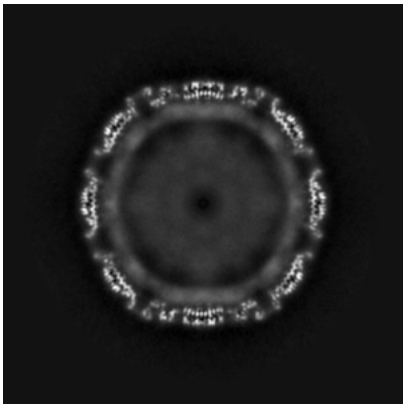
6.2.2 Raw map



X Index: 216



Y Index: 216

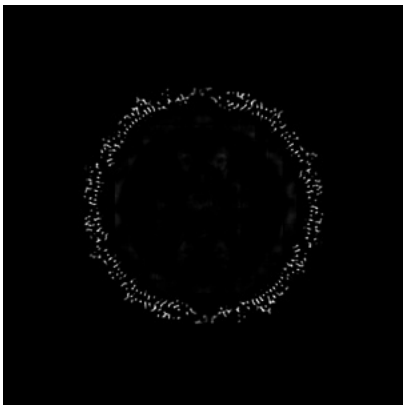


Z Index: 216

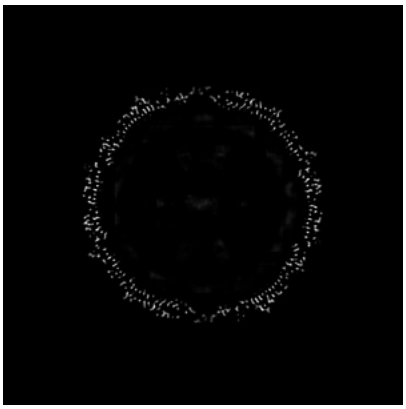
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

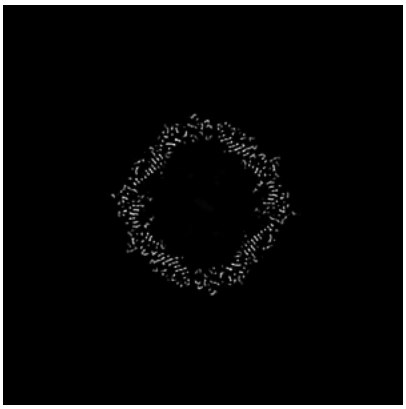
6.3.1 Primary map



X Index: 183

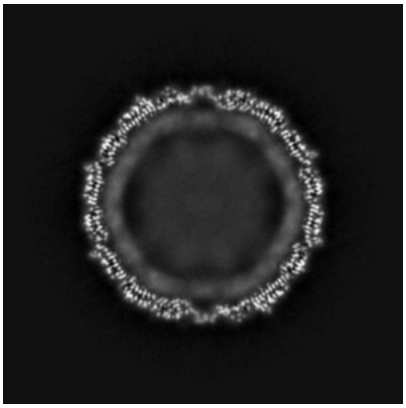


Y Index: 183

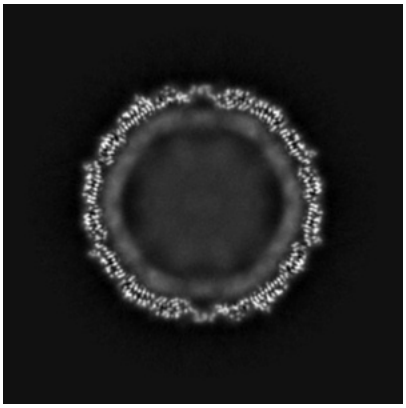


Z Index: 118

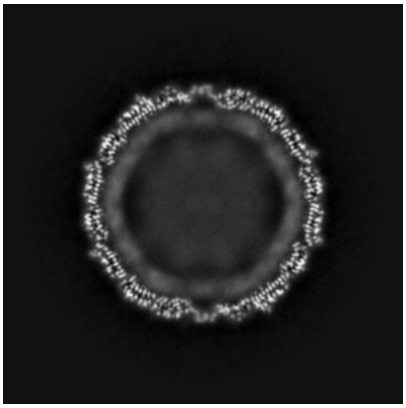
6.3.2 Raw map



X Index: 182



Y Index: 182

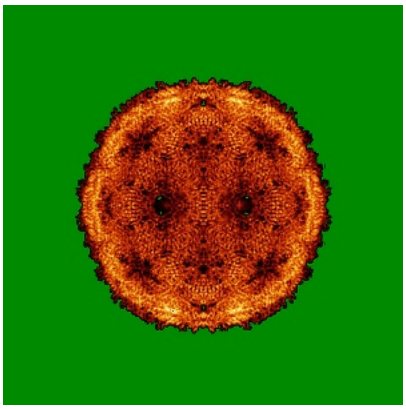


Z Index: 181

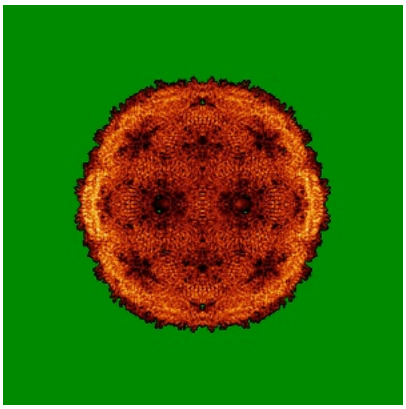
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

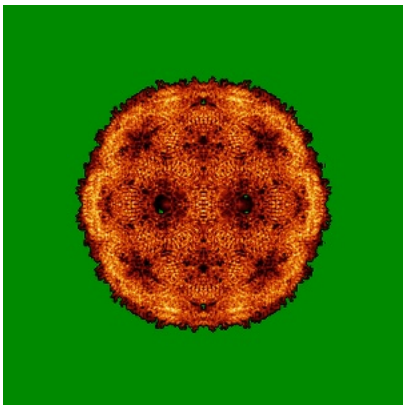
6.4.1 Primary map



X

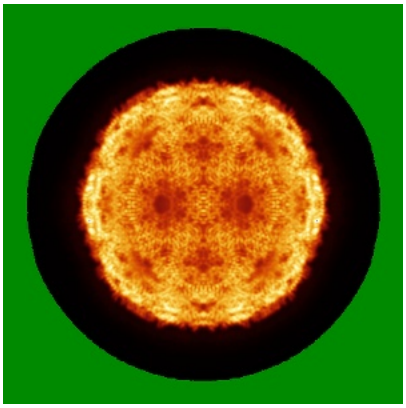


Y

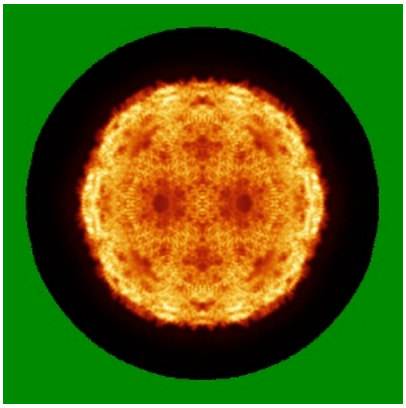


Z

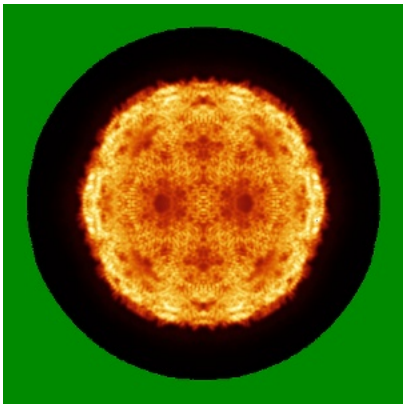
6.4.2 Raw map



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.

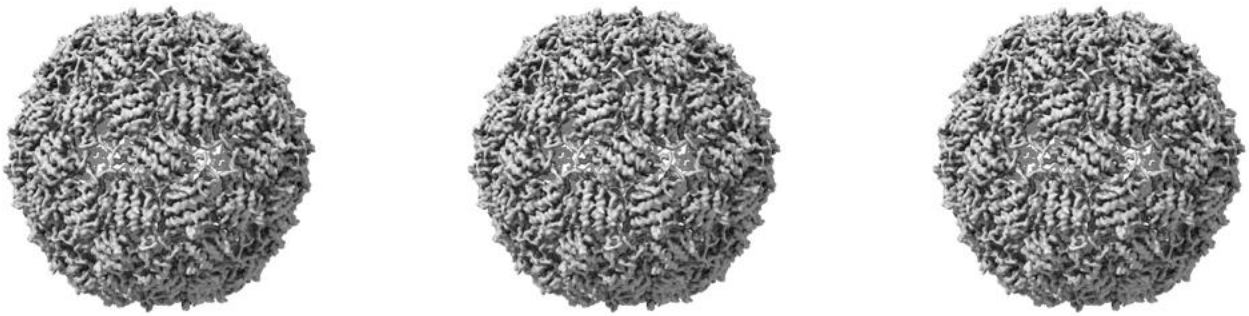
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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



X Y Z

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.

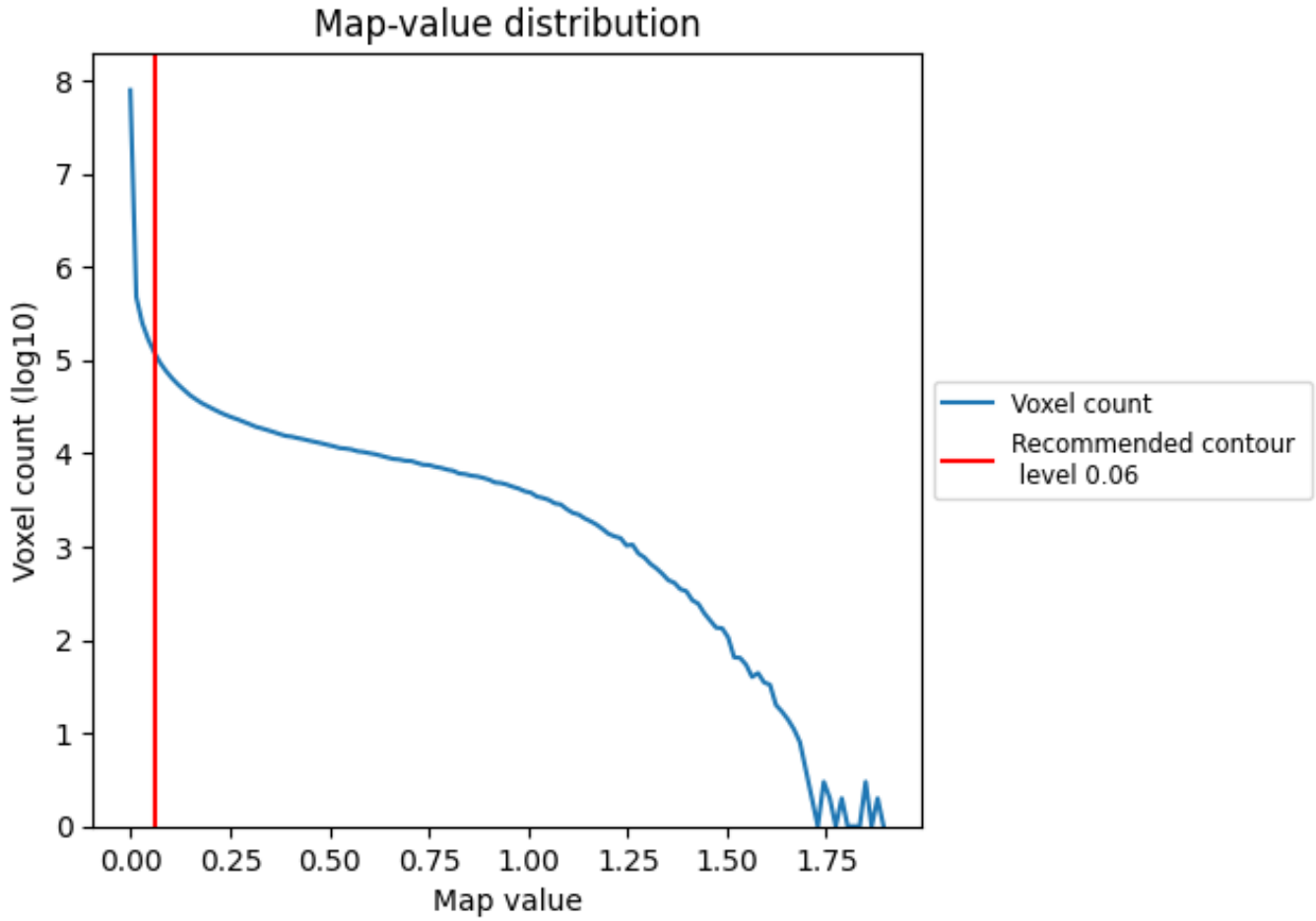
6.6 Mask visualisation (i)

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

7 Map analysis

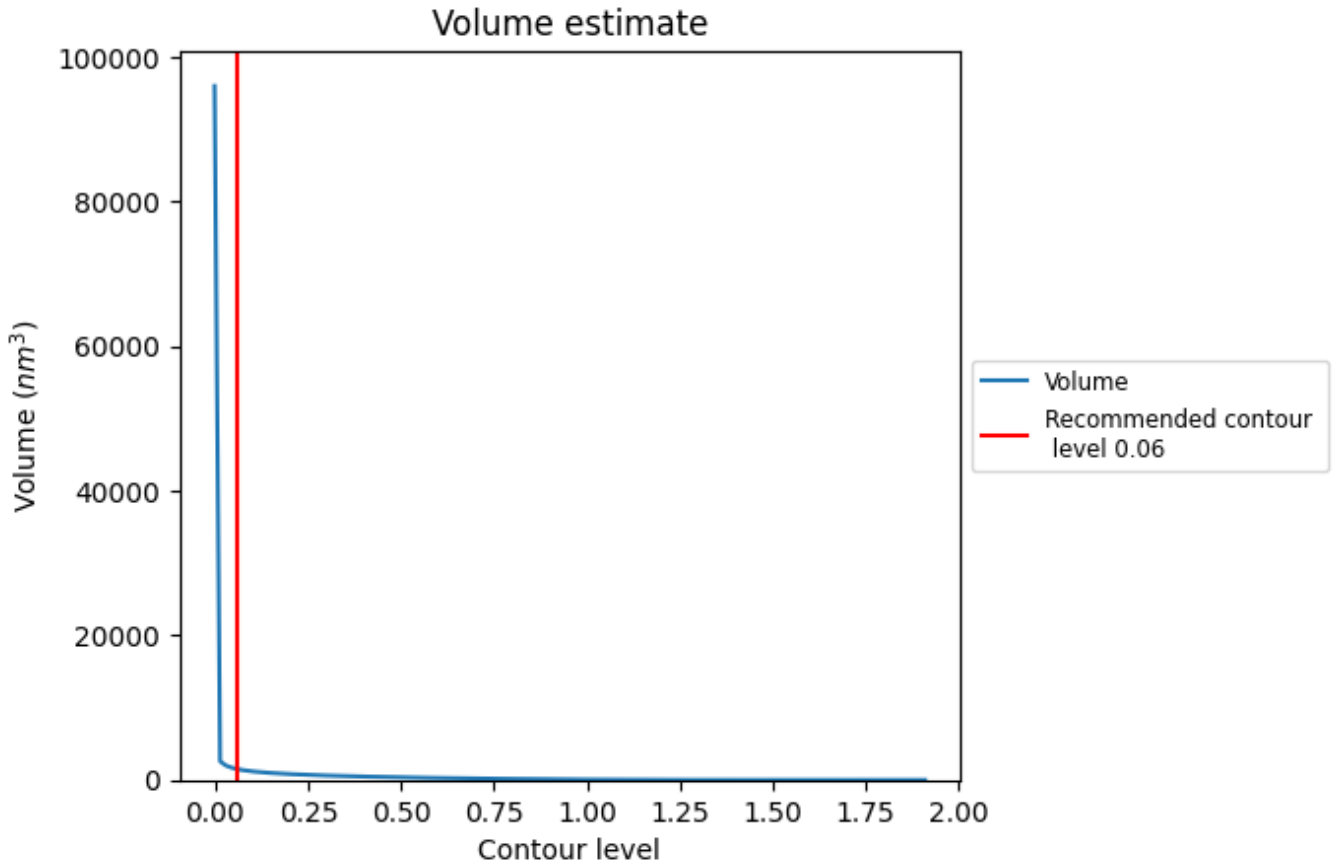
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

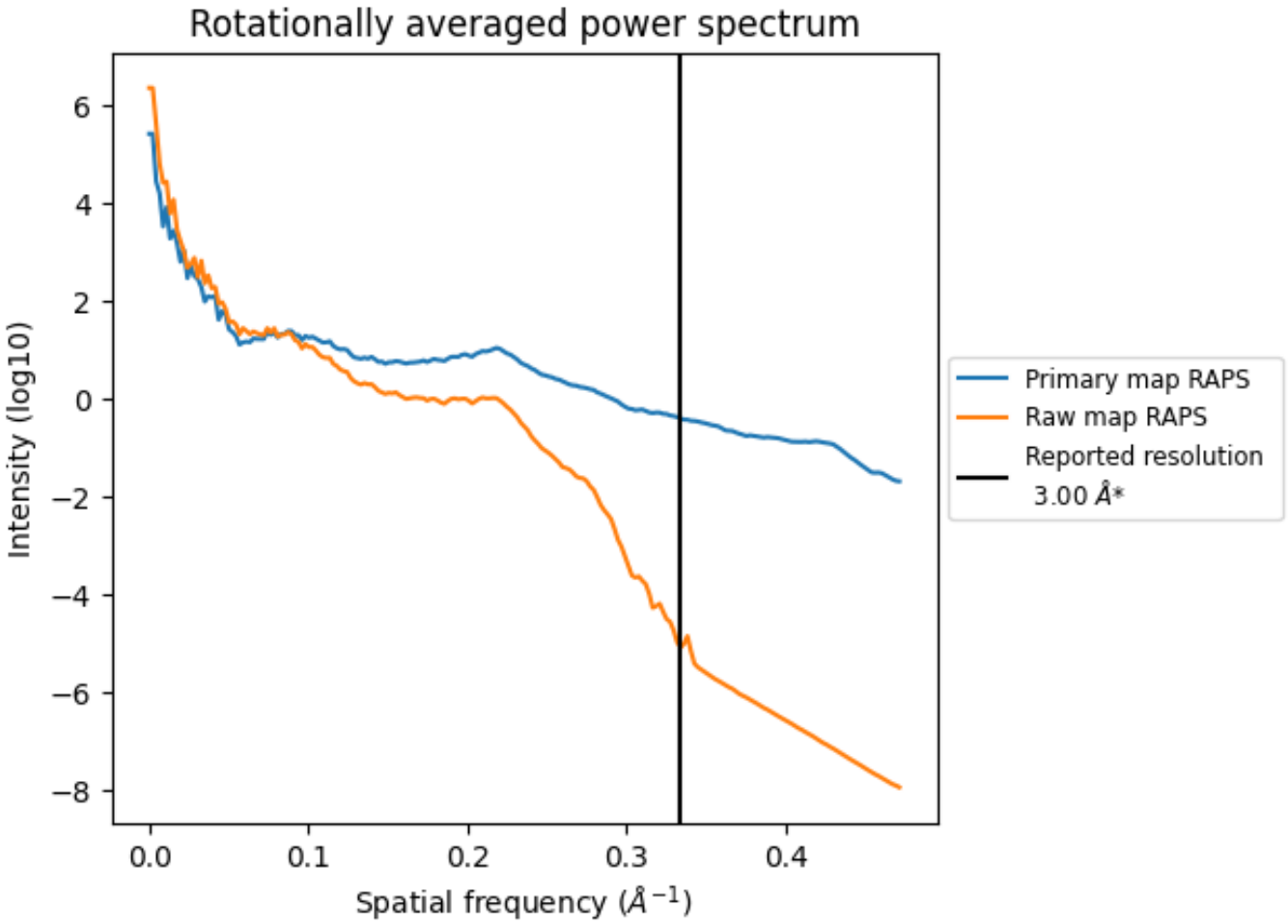
7.2 Volume estimate (i)



The volume at the recommended contour level is 1500 nm^3; this corresponds to an approximate mass of 1355 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)

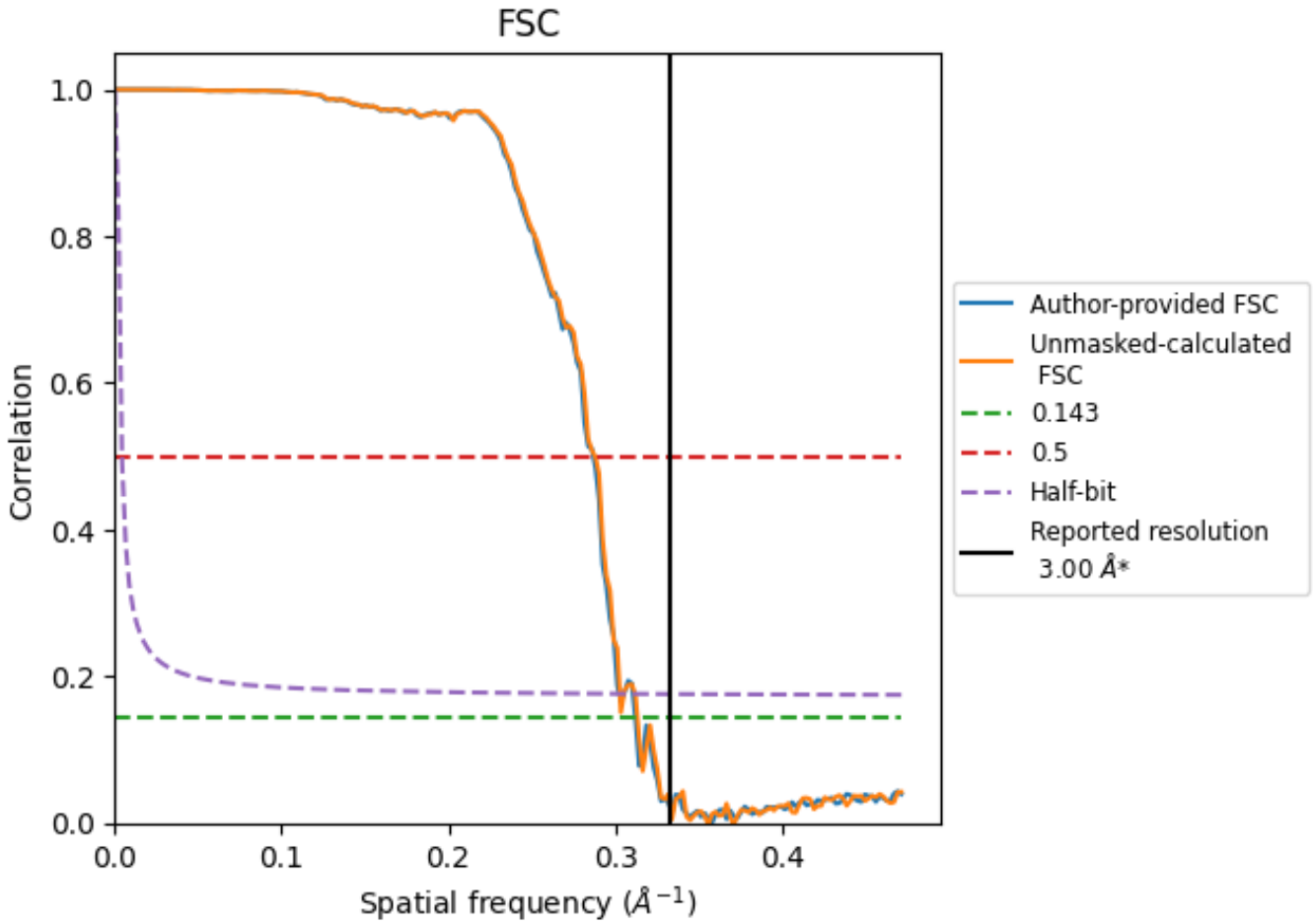


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

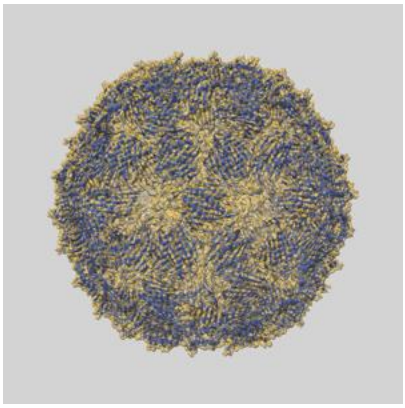
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.20	3.49	3.31
Unmasked-calculated*	3.19	3.47	3.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

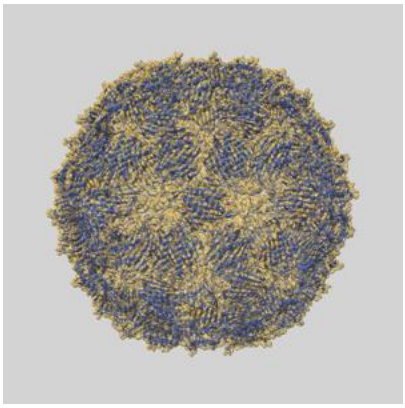
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41666 and PDB model 8TWC. Per-residue inclusion information can be found in section 3 on page 19.

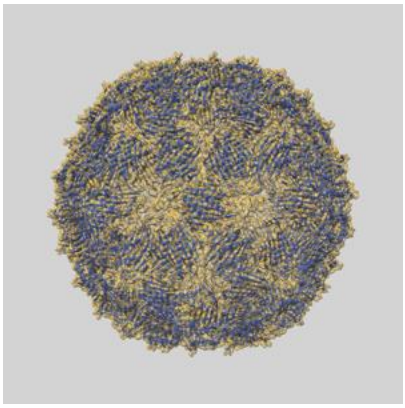
9.1 Map-model overlay



X



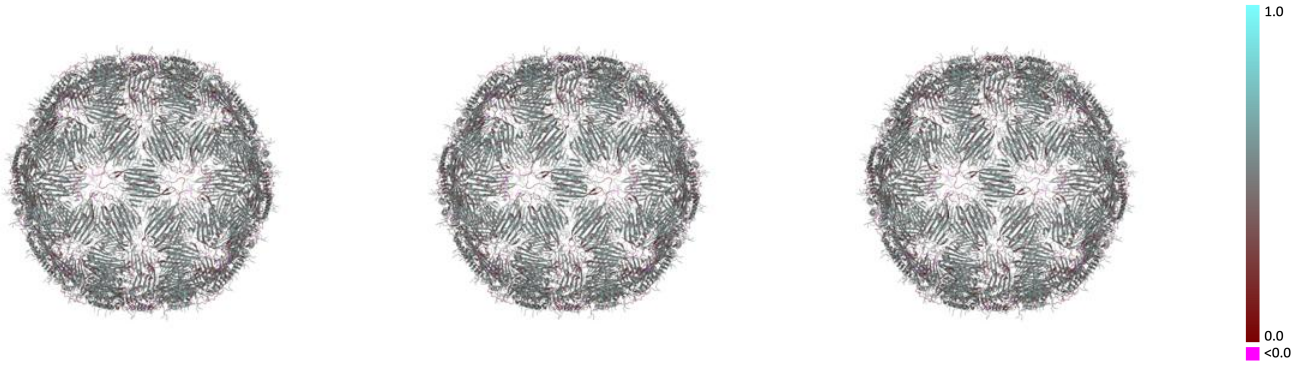
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

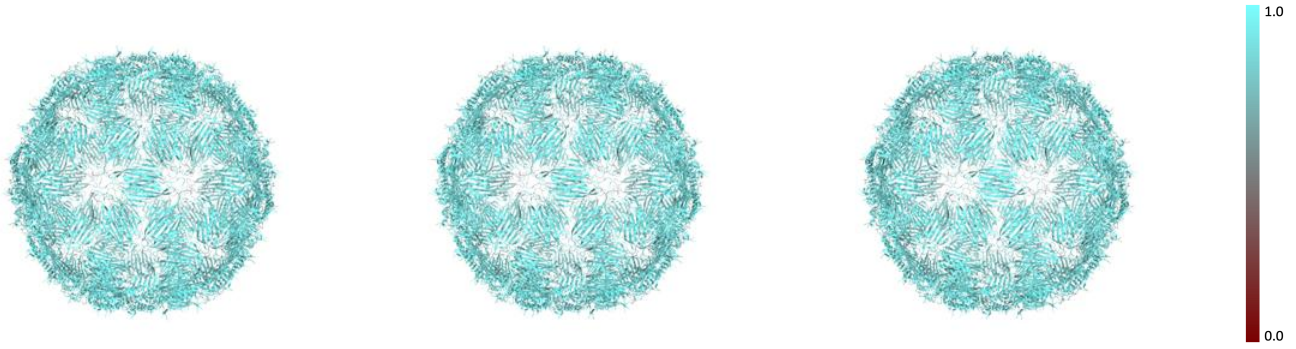
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

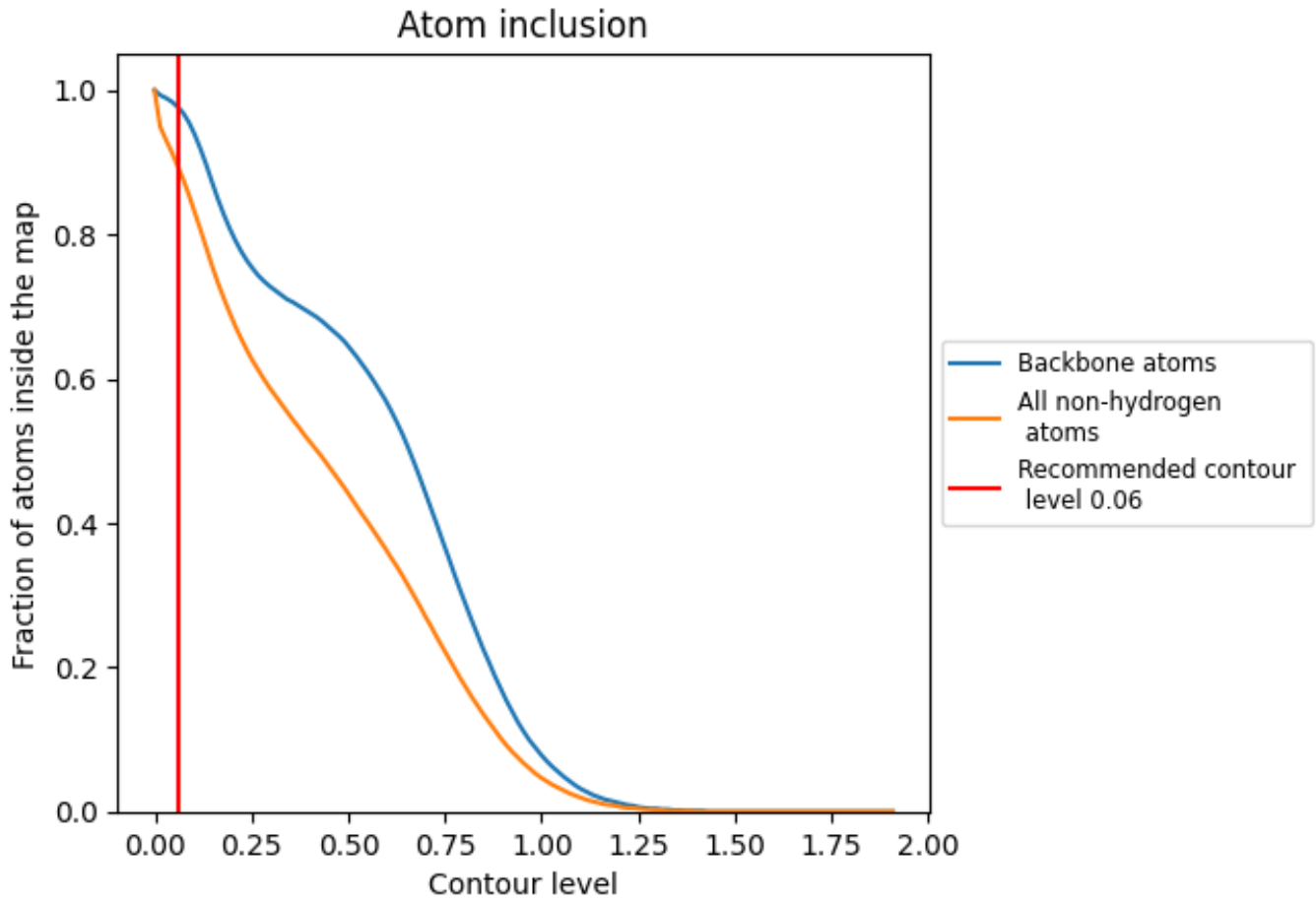
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 89% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8930	0.4600
AB	0.8790	0.4530
AC	0.8990	0.4590
AD	0.9080	0.4680
AE	0.8810	0.4540
AF	0.8960	0.4610
AG	0.9010	0.4710
AH	0.8950	0.4580
AI	0.8960	0.4570
AJ	0.9040	0.4580
AK	0.8800	0.4520
AL	0.8870	0.4600
AM	0.9030	0.4680
AN	0.8920	0.4550
AO	0.8900	0.4630
AP	0.8990	0.4720
AQ	0.9050	0.4590
AR	0.9090	0.4630
AS	0.9040	0.4590
AT	0.8870	0.4540
AU	0.8830	0.4560
AV	0.8990	0.4700
AW	0.8770	0.4460
AX	0.8830	0.4580
AY	0.8980	0.4650
AZ	0.8840	0.4510
BA	0.8840	0.4510
BB	0.8890	0.4670
BC	0.8760	0.4460
BD	0.8780	0.4570
BE	0.9010	0.4690
BF	0.8930	0.4560
BG	0.8960	0.4570
BH	0.9050	0.4680
BI	0.8870	0.4590

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BJ	0.8870	0.4580
BK	0.9040	0.4720
BL	0.8760	0.4470
BM	0.8800	0.4590
BN	0.9000	0.4650
BO	0.8880	0.4570
BP	0.8920	0.4610
BQ	0.8980	0.4640
BR	0.8870	0.4530
BS	0.8830	0.4560
BT	0.9080	0.4660
BU	0.8870	0.4530
BV	0.8930	0.4600
BW	0.9030	0.4680
BX	0.8750	0.4560
BY	0.8830	0.4590
BZ	0.8820	0.4640
CA	0.8970	0.4570
CB	0.8920	0.4570
CC	0.9100	0.4670
CD	0.8880	0.4530
CE	0.8940	0.4610
CF	0.8980	0.4700
CG	0.8840	0.4620
CH	0.8930	0.4580
CI	0.9090	0.4690
CJ	0.9010	0.4470
CK	0.9000	0.4600
CL	0.9120	0.4670
CM	0.8820	0.4520
CN	0.8990	0.4620
CO	0.8850	0.4650
CP	0.8890	0.4550
CQ	0.9110	0.4580
CR	0.9090	0.4700
CS	0.8940	0.4510
CT	0.8880	0.4580
CU	0.8960	0.4650
CV	0.8890	0.4520
CW	0.8910	0.4570
CX	0.8980	0.4700
CY	0.8880	0.4570

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Chain	Atom inclusion	Q-score
CZ	0.8950	0.4660
DA	0.8990	0.4690
DB	0.8800	0.4540
DC	0.8830	0.4490
DD	0.8970	0.4590
DE	0.8850	0.4550
DF	0.9000	0.4590
DG	0.8940	0.4620
DH	0.8980	0.4500
DI	0.8900	0.4550
DJ	0.9020	0.4650
DK	0.8910	0.4580
DL	0.8940	0.4620
DM	0.9060	0.4680
DN	0.8790	0.4490
DO	0.8900	0.4620
DP	0.9010	0.4690
DQ	0.8830	0.4500
DR	0.8940	0.4590
DS	0.9000	0.4700
DT	0.8920	0.4500
DU	0.9000	0.4620
DV	0.9080	0.4640
DW	0.8870	0.4540
DX	0.8850	0.4540
DY	0.9050	0.4730
DZ	0.8920	0.4570
EA	0.8950	0.4590
EB	0.9110	0.4650
EC	0.8930	0.4600
ED	0.9110	0.4630
EE	0.9060	0.4660
EF	0.8830	0.4510
EG	0.8840	0.4550
EH	0.9020	0.4720
EI	0.8810	0.4510
EJ	0.8850	0.4530
EK	0.8800	0.4620
EL	0.8770	0.4480
EM	0.8740	0.4540
EN	0.8970	0.4670
EO	0.8840	0.4530

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Chain	Atom inclusion	Q-score
EP	0.8950	0.4540
EQ	0.9050	0.4670
ER	0.8950	0.4550
ES	0.9060	0.4560
ET	0.9030	0.4660
EU	0.8940	0.4590
EV	0.8870	0.4600
EW	0.9110	0.4680
EX	0.8810	0.4530
EY	0.8890	0.4570
EZ	0.9010	0.4640
FA	0.8900	0.4570
FB	0.8870	0.4560
FC	0.9080	0.4660
FD	0.9060	0.4580
FE	0.8920	0.4570
FF	0.9020	0.4670
FG	0.8890	0.4560
FH	0.9130	0.4640
FI	0.8980	0.4680
FJ	0.8840	0.4600
FK	0.8970	0.4660
FL	0.8930	0.4640
FM	0.8920	0.4520
FN	0.8990	0.4540
FO	0.9010	0.4610
FP	0.8840	0.4500
FQ	0.8900	0.4600
FR	0.8970	0.4690
FS	0.8840	0.4510
FT	0.8790	0.4530
FU	0.9000	0.4700
FV	0.8930	0.4530
FW	0.9020	0.4550
FX	0.9140	0.4700
FY	0.8730	0.4490
FZ	0.8950	0.4580
GA	0.8870	0.4630
GB	0.8970	0.4520
GC	0.8940	0.4610
GD	0.9100	0.4690
GE	0.8940	0.4560

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Chain	Atom inclusion	Q-score
GF	0.8910	0.4570
GG	0.9000	0.4690
GH	0.8770	0.4460
GI	0.8830	0.4580
GJ	0.9050	0.4700
GK	0.8910	0.4580
GL	0.8930	0.4610
GM	0.8990	0.4650
GN	0.8910	0.4560
GO	0.8870	0.4640
GP	0.8910	0.4670
GQ	0.8840	0.4450
GR	0.8940	0.4560
GS	0.9010	0.4640
GT	0.8800	0.4540
GU	0.8830	0.4510
GV	0.8950	0.4630
GW	0.8890	0.4580
GX	0.8900	0.4640
GY	0.8980	0.4670