



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 05:32 AM UTC

PDB ID : 5LQP / pdb_00005lqp
EMDB ID : EMD-4098
Title : Cryo-EM reconstruction of bacteriophage AP205 virus-like particles.
Authors : Diebolder, C.A.; Rumnieks, J.; Tars, K.; Koning, R.I.
Deposited on : 2016-08-17
Resolution : 6.00 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

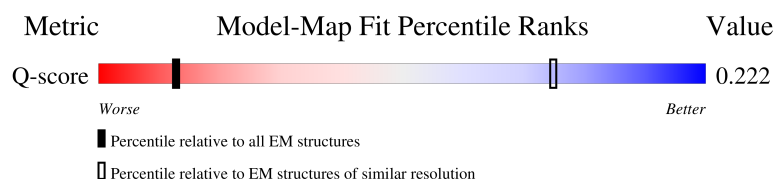
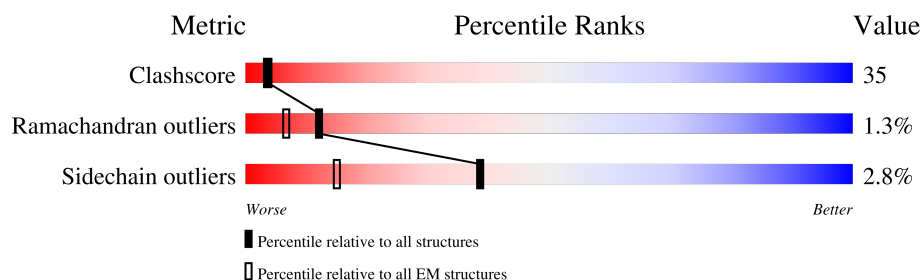
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 6.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	525 (5.50 - 6.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	129	
1	AC	129	
1	AD	129	
1	AE	129	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AF	129	
1	AG	129	
1	AH	129	
1	AI	129	
1	AJ	129	
1	AK	129	
1	AL	129	
1	AM	129	
1	AN	129	
1	AO	129	
1	AP	129	
1	AQ	129	
1	AR	129	
1	AS	129	
1	AT	129	
1	AU	129	
1	AV	129	
1	AW	129	
1	AX	129	
1	AY	129	
1	AZ	129	
1	BA	129	
1	BB	129	
1	BC	129	
1	BD	129	

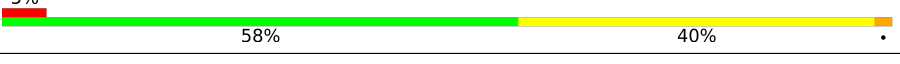
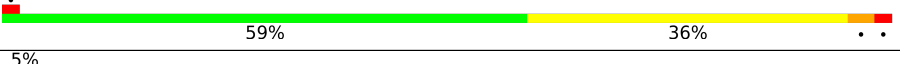
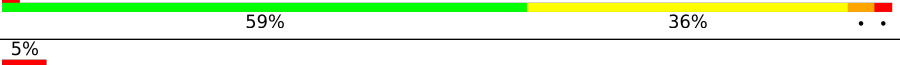
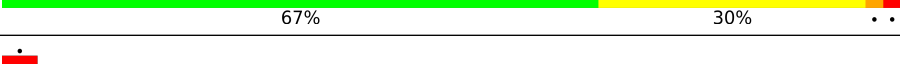
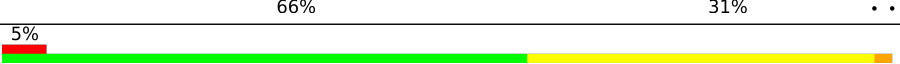
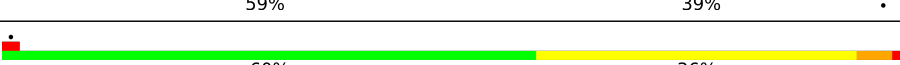
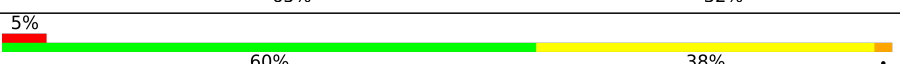
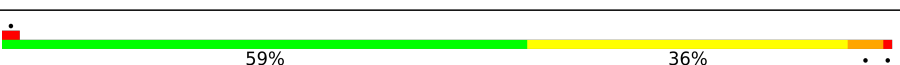
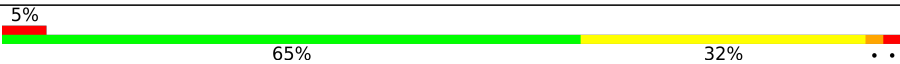
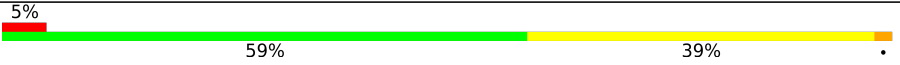
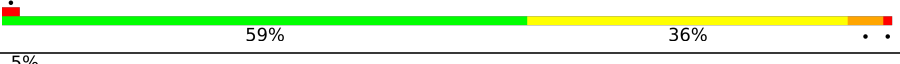
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	BE	129	
1	BF	129	
1	BG	129	
1	BH	129	
1	BI	129	
1	BJ	129	
1	BK	129	
1	BL	129	
1	BM	129	
1	BN	129	
1	BO	129	
1	BP	129	
1	BQ	129	
1	BR	129	
1	BS	129	
1	BT	129	
1	BU	129	
1	BV	129	
1	BW	129	
1	BX	129	
1	BY	129	
1	BZ	129	
1	CA	129	
1	CB	129	
1	CC	129	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	CD	129	
1	CE	129	
1	CF	129	
1	CG	129	
1	CH	129	
1	CI	129	
1	CJ	129	
1	CK	129	
1	CL	129	
1	CM	129	
1	CN	129	
1	CO	129	
1	CP	129	
1	CQ	129	
1	CR	129	
1	CS	129	
1	CT	129	
1	CU	129	
1	CV	129	
1	CW	129	
1	CX	129	
1	CY	129	
1	CZ	129	
1	DA	129	
1	DB	129	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	DC	129	
1	DD	129	
1	DE	129	
1	DF	129	
1	DG	129	
1	DH	129	
1	DI	129	
1	DJ	129	
1	DK	129	
1	DL	129	
1	DM	129	
1	DN	129	
1	DO	129	
1	DP	129	
1	DQ	129	
1	DR	129	
1	DS	129	
1	DT	129	
1	DU	129	
1	DV	129	
1	DW	129	
1	DX	129	
1	DY	129	
1	DZ	129	
1	EA	129	

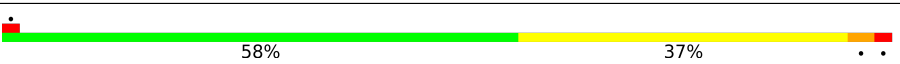
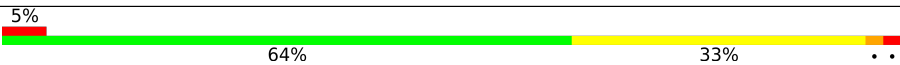
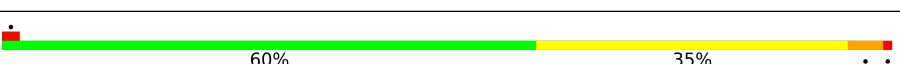
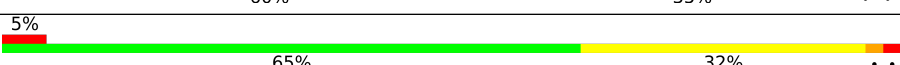
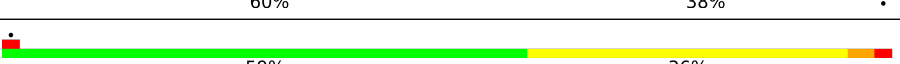
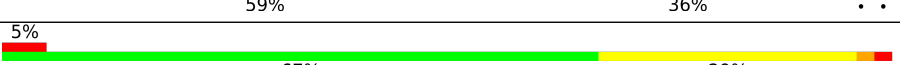
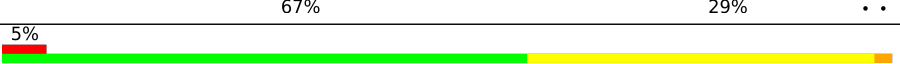
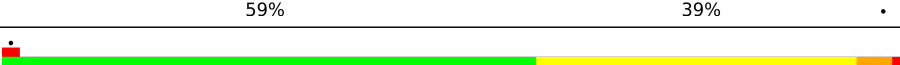
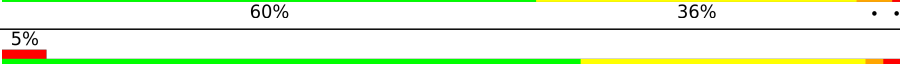
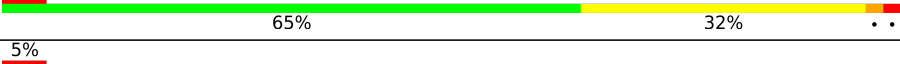
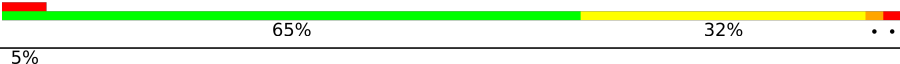
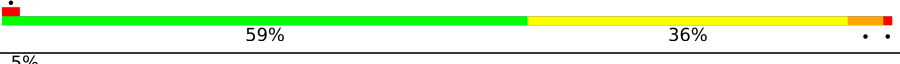
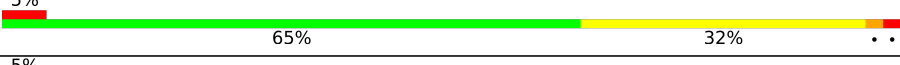
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	EB	129	
1	EC	129	
1	ED	129	
1	EE	129	
1	EF	129	
1	EG	129	
1	EH	129	
1	EI	129	
1	EJ	129	
1	EK	129	
1	EL	129	
1	EM	129	
1	EN	129	
1	EO	129	
1	EP	129	
1	EQ	129	
1	ER	129	
1	ES	129	
1	ET	129	
1	EU	129	
1	EV	129	
1	EW	129	
1	EX	129	
1	EY	129	
1	EZ	129	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FA	129	
1	FB	129	
1	FC	129	
1	FD	129	
1	FE	129	
1	FF	129	
1	FG	129	
1	FH	129	
1	FI	129	
1	FJ	129	
1	FK	129	
1	FL	129	
1	FM	129	
1	FN	129	
1	FO	129	
1	FP	129	
1	FQ	129	
1	FR	129	
1	FS	129	
1	FT	129	
1	FU	129	
1	FV	129	
1	FW	129	
1	FX	129	
1	FY	129	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	FZ	129	
1	GA	129	
1	GB	129	
1	GC	129	
1	GD	129	
1	GE	129	
1	GF	129	
1	GG	129	
1	GH	129	
1	GI	129	
1	GJ	129	
1	GK	129	
1	GL	129	
1	GM	129	
1	GN	129	
1	GO	129	
1	GP	129	
1	GQ	129	
1	GR	129	
1	GS	129	
1	GT	129	
1	GU	129	
1	GV	129	
1	GW	129	
1	GX	129	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	GY	129	5% 60% 38%

2 Entry composition

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

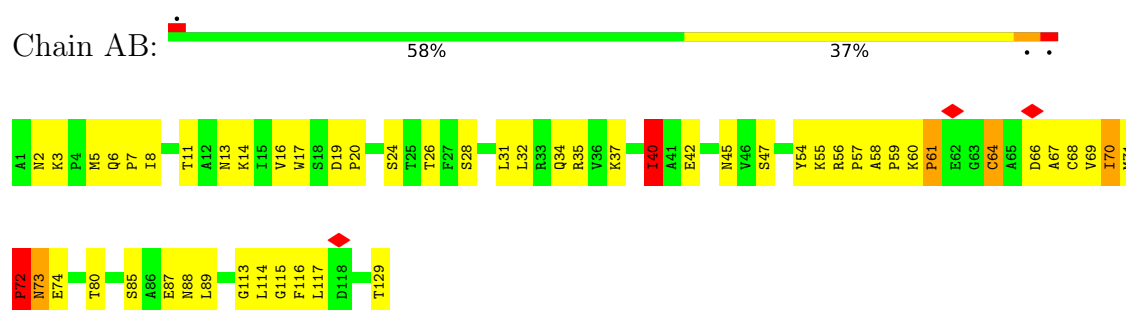
Continued from previous page...

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

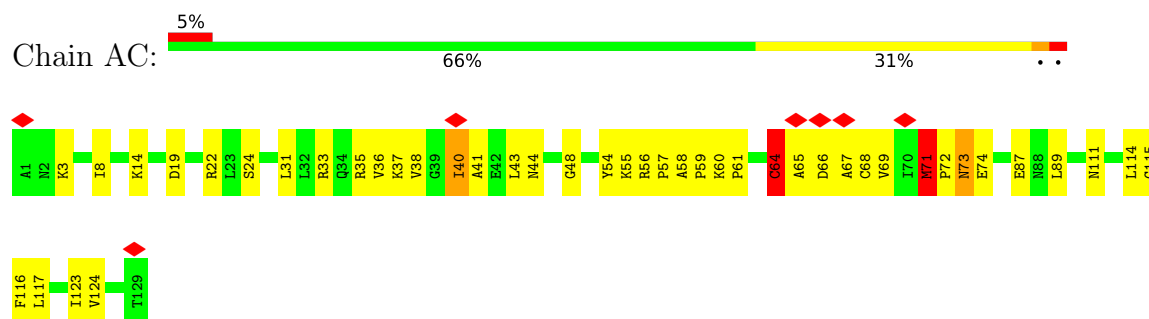
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

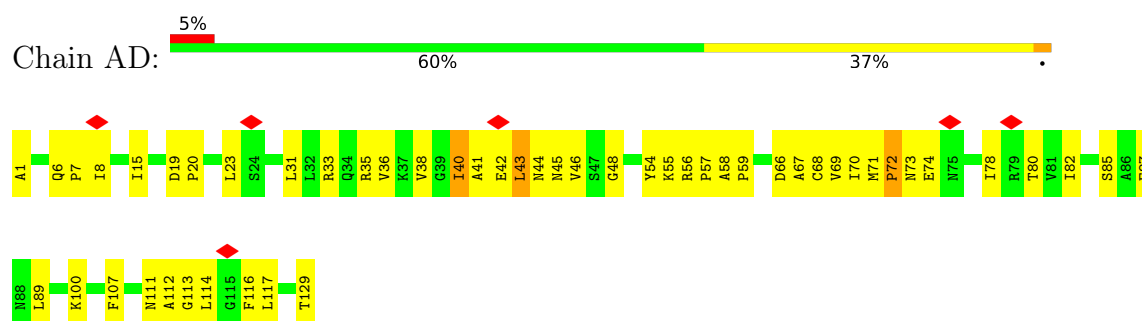
- Molecule 1: Coat protein



- Molecule 1: Coat protein

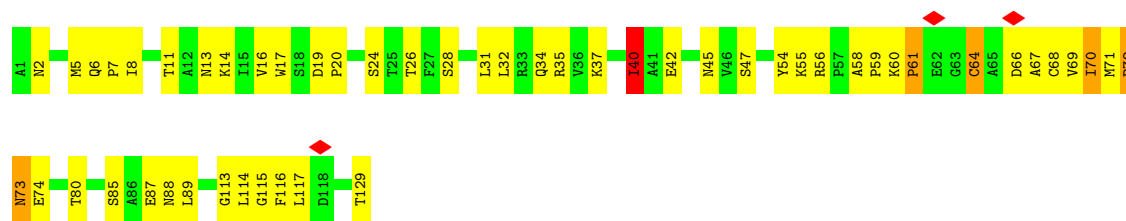


- Molecule 1: Coat protein



- Molecule 1: Coat protein

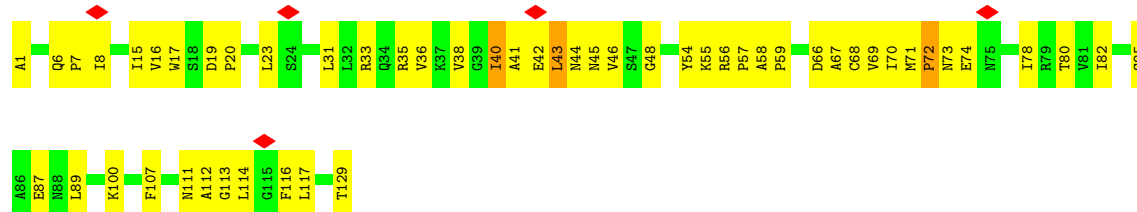




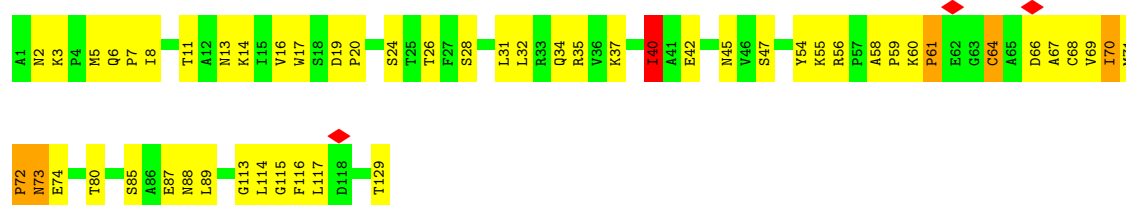
- Molecule 1: Coat protein



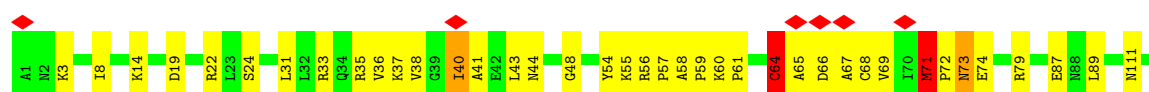
- Molecule 1: Coat protein

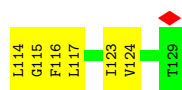


- Molecule 1: Coat protein

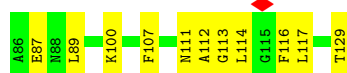


- Molecule 1: Coat protein

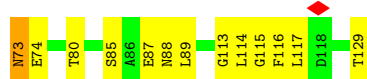




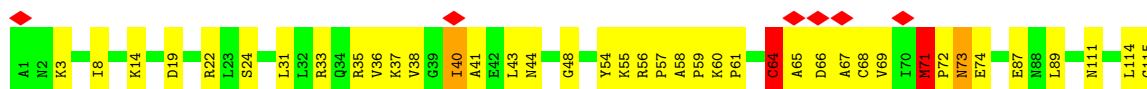
- Molecule 1: Coat protein



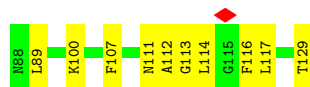
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



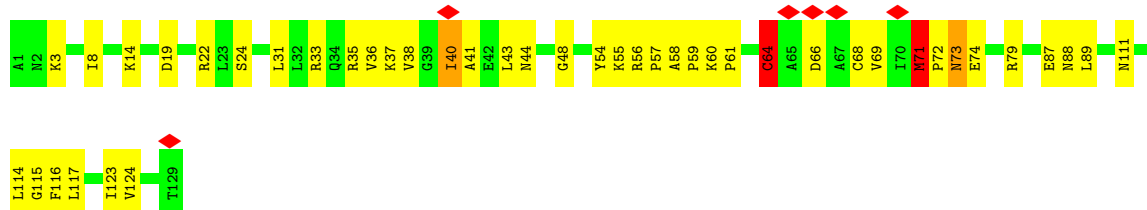
- Molecule 1: Coat protein

Chain AN:  60% 36%



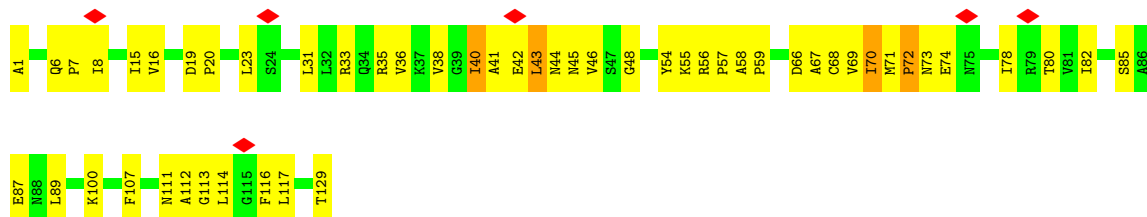
• Molecule 1: Coat protein

Chain AO:  5% 66% 31%



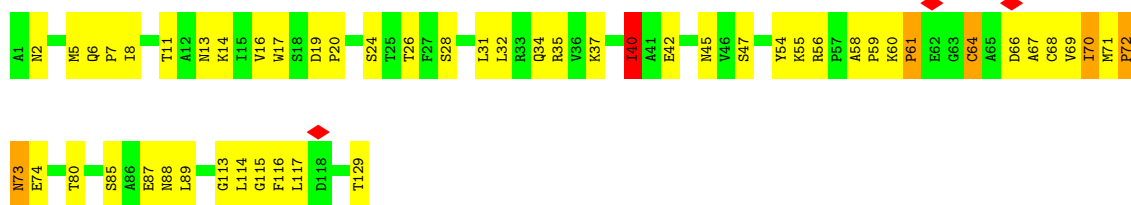
• Molecule 1: Coat protein

Chain AP:  5% 60% 37%



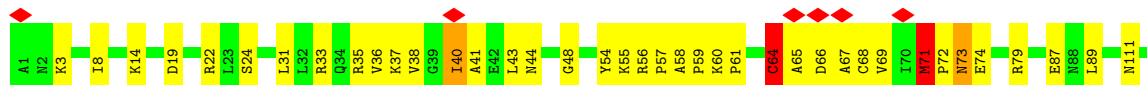
• Molecule 1: Coat protein

Chain AQ:  60% 36%



• Molecule 1: Coat protein

Chain AR:  5% 65% 32%

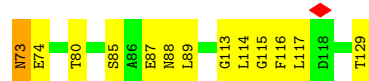




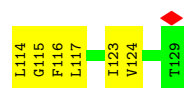
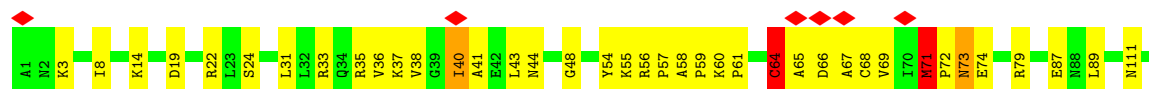
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein

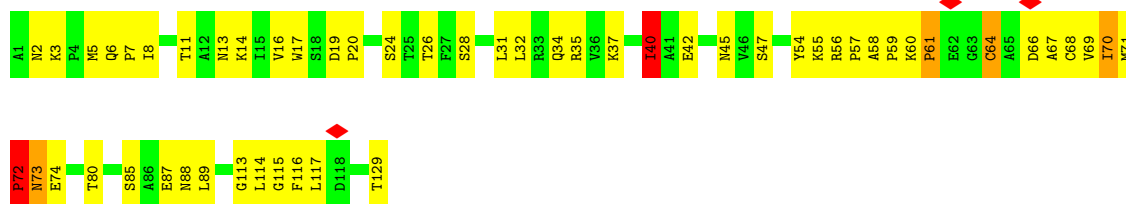


- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain AW:  58% 37%



• Molecule 1: Coat protein

Chain AX:  5% 64% 33%



Chain BF:  60% 36% . .



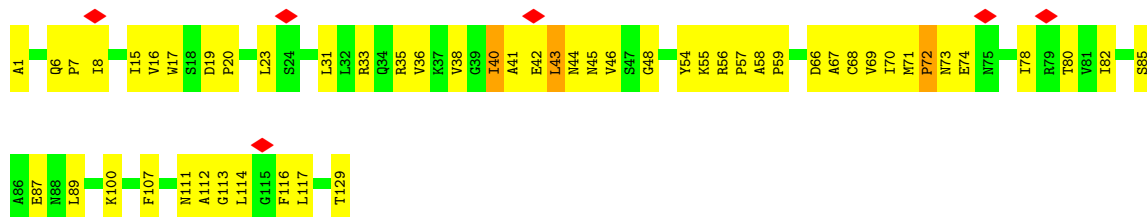
- Molecule 1: Coat protein

Chain BG:  5% 65% 32% . .



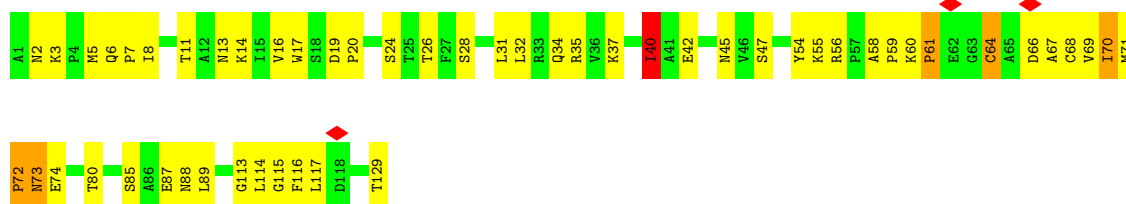
- Molecule 1: Coat protein

Chain BH:  5% 59% 39% .



- Molecule 1: Coat protein

Chain BI:  5% 59% 36% . .



- Molecule 1: Coat protein

Chain BJ:  5% 64% 33% . .





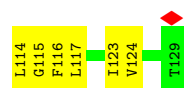
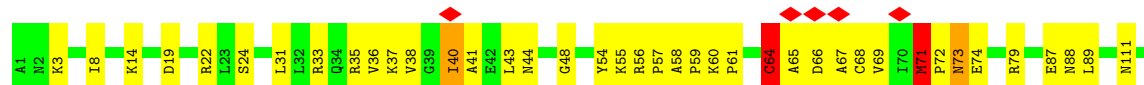
- Molecule 1: Coat protein



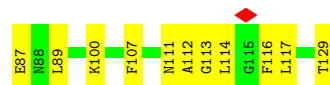
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



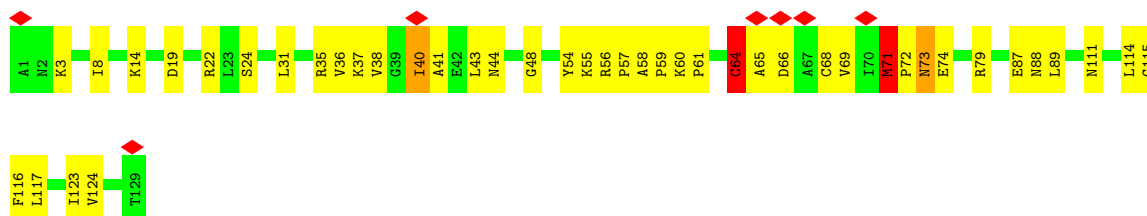
- Molecule 1: Coat protein

Chain BO:  59% 36%



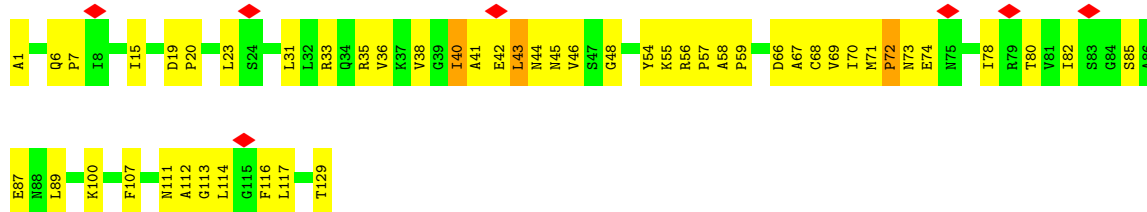
• Molecule 1: Coat protein

Chain BP:  5% 66% 31%



• Molecule 1: Coat protein

Chain BQ:  5% 61% 36%



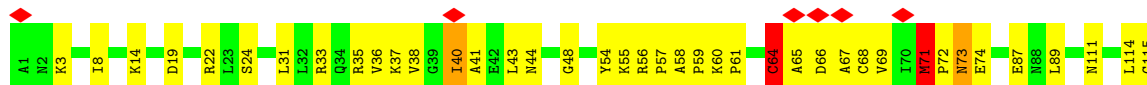
• Molecule 1: Coat protein

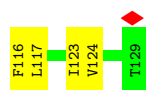
Chain BR:  60% 36%



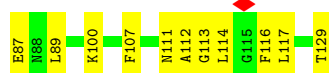
• Molecule 1: Coat protein

Chain BS:  5% 66% 31%

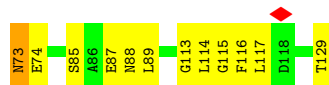




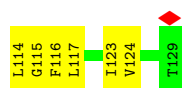
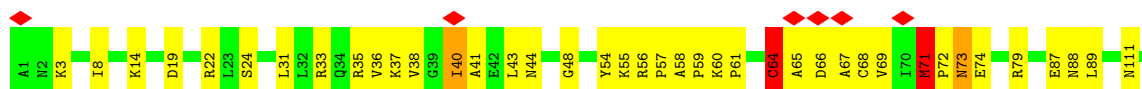
- Molecule 1: Coat protein



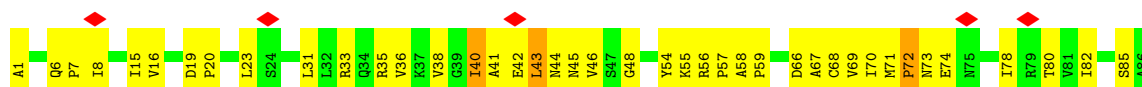
- Molecule 1: Coat protein



- Molecule 1: Coat protein

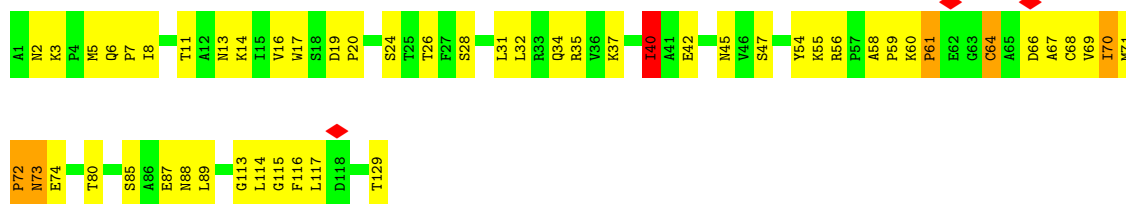


- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain BX: 



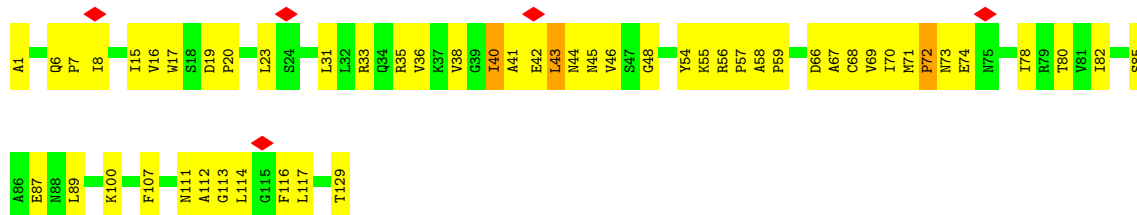
• Molecule 1: Coat protein

Chain BY: 



• Molecule 1: Coat protein

Chain BZ: 



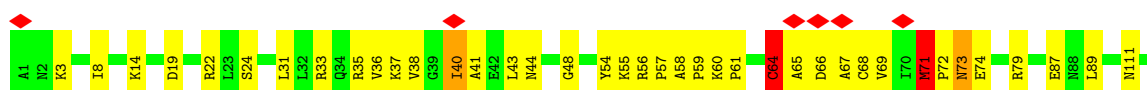
• Molecule 1: Coat protein

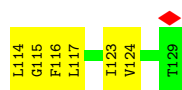
Chain CA: 



• Molecule 1: Coat protein

Chain CB: 





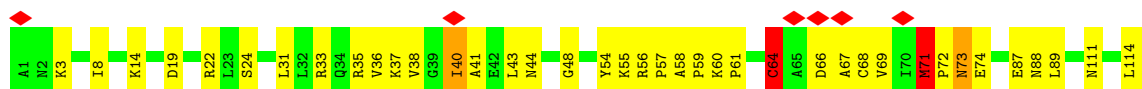
- Molecule 1: Coat protein



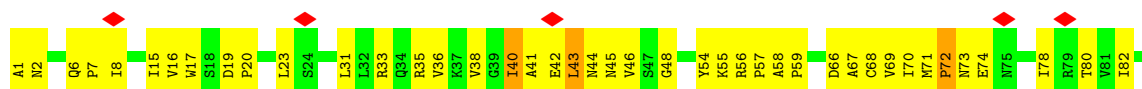
- Molecule 1: Coat protein



- Molecule 1: Coat protein

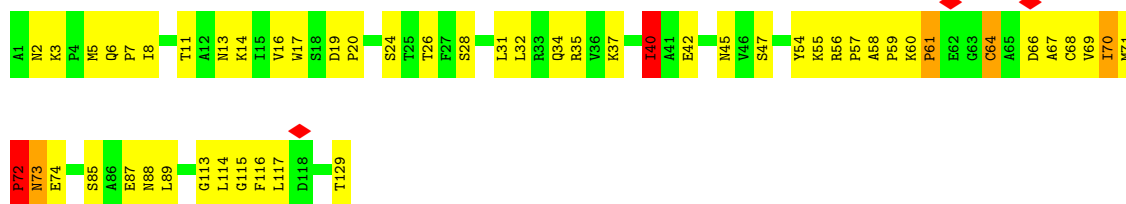


- Molecule 1: Coat protein



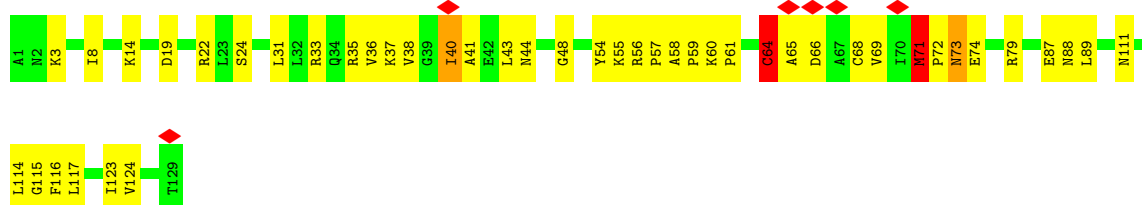
- Molecule 1: Coat protein

Chain CG:  59% 36%



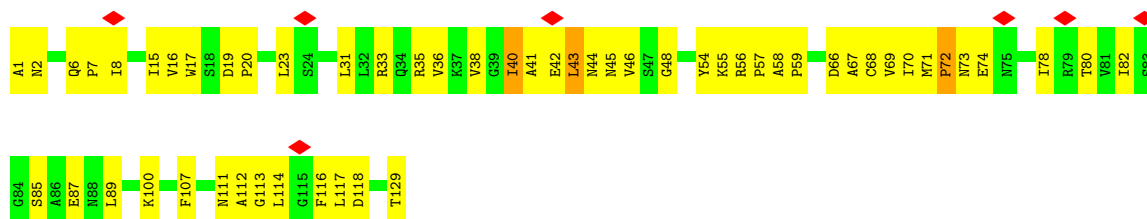
• Molecule 1: Coat protein

Chain CH:  5% 65% 32%



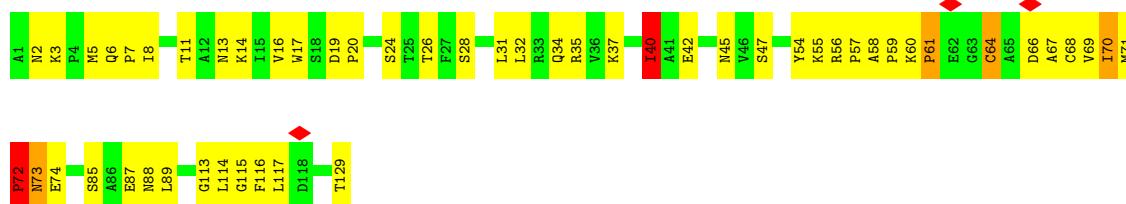
• Molecule 1: Coat protein

Chain CI:  5% 57% 40%



• Molecule 1: Coat protein

Chain CJ:  59% 36%



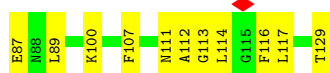
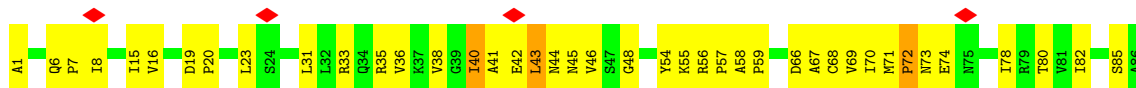
• Molecule 1: Coat protein

Chain CK:  5% 67% 30%

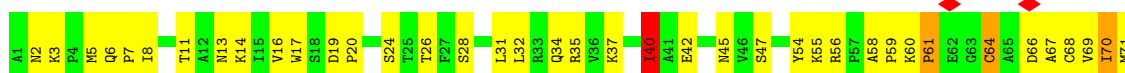




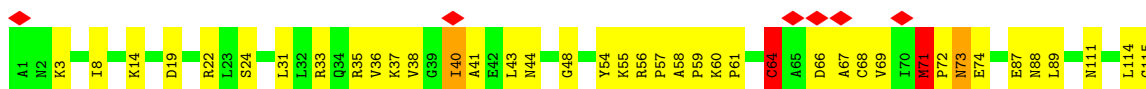
- Molecule 1: Coat protein



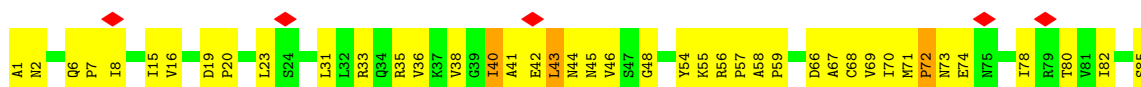
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



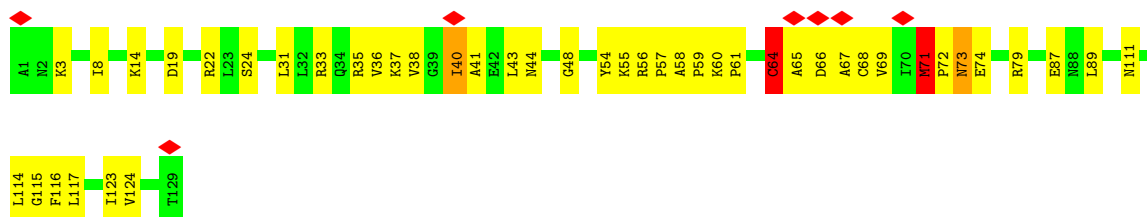
- Molecule 1: Coat protein

Chain CP:  60% 36%



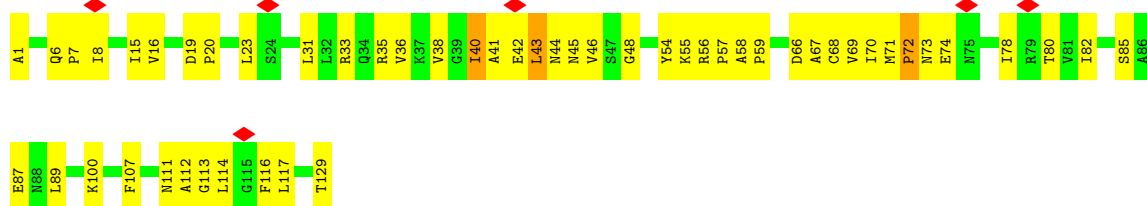
• Molecule 1: Coat protein

Chain CQ:  5% 65% 32%



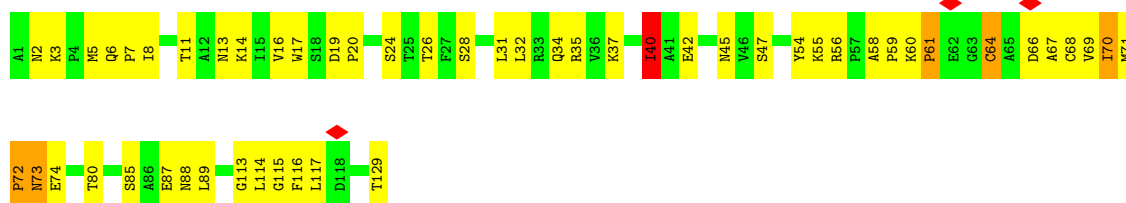
• Molecule 1: Coat protein

Chain CR:  5% 60% 38%



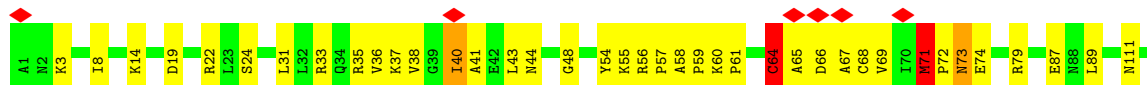
• Molecule 1: Coat protein

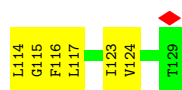
Chain CS:  59% 36%



• Molecule 1: Coat protein

Chain CT:  5% 65% 32%





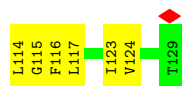
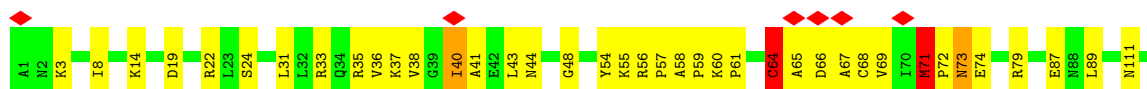
- Molecule 1: Coat protein



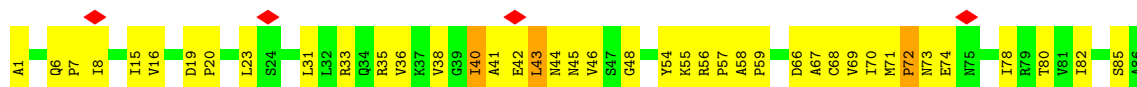
- Molecule 1: Coat protein



- Molecule 1: Coat protein

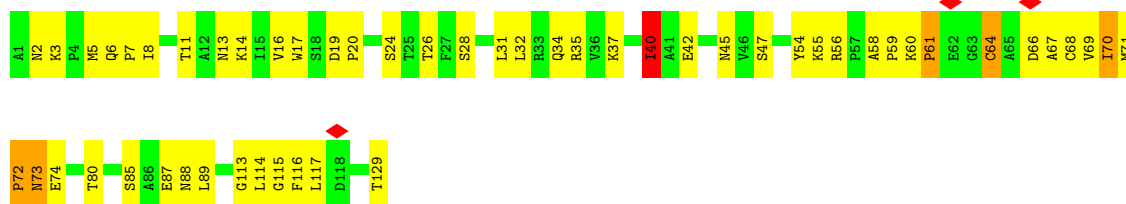


- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain CY:  59% 36%



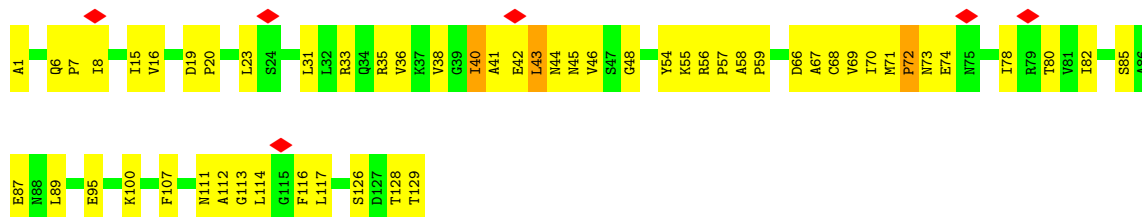
• Molecule 1: Coat protein

Chain CZ:  5% 65% 32%



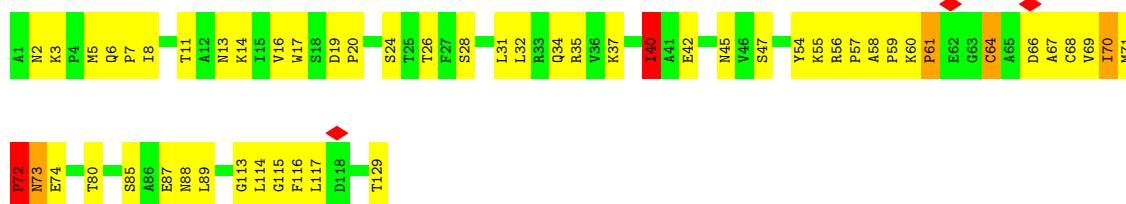
• Molecule 1: Coat protein

Chain DA:  5% 57% 40%



• Molecule 1: Coat protein

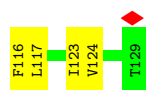
Chain DB:  58% 37%



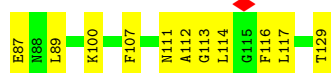
• Molecule 1: Coat protein

Chain DC:  5% 67% 30%





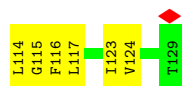
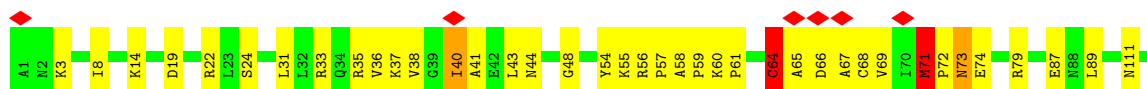
- Molecule 1: Coat protein



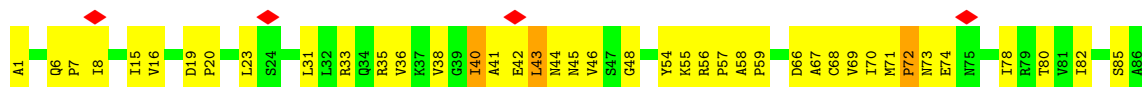
- Molecule 1: Coat protein



- Molecule 1: Coat protein

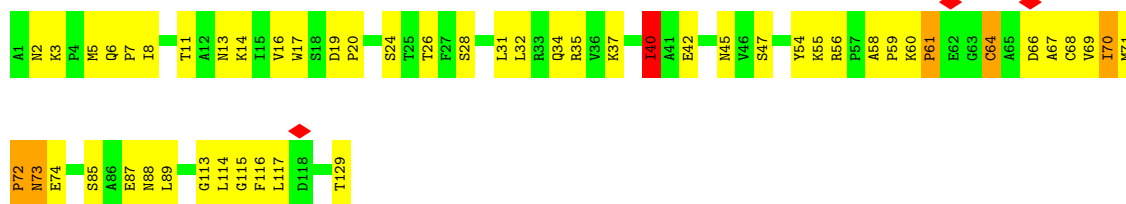


- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain DH:  60% 36% . .



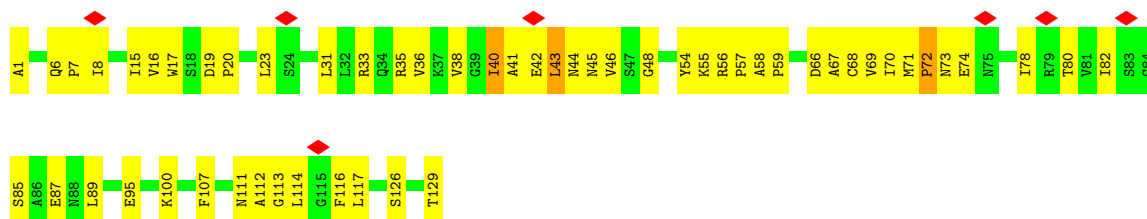
• Molecule 1: Coat protein

Chain DI:  5% 65% 32% . .



• Molecule 1: Coat protein

Chain DJ:  5% 57% 40% .



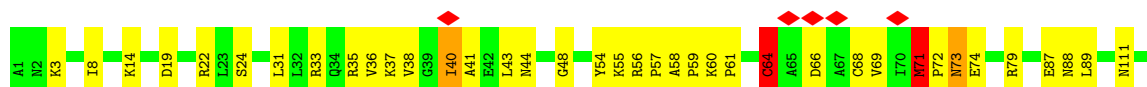
• Molecule 1: Coat protein

Chain DK:  60% 35% . .



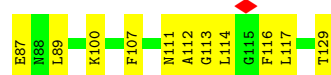
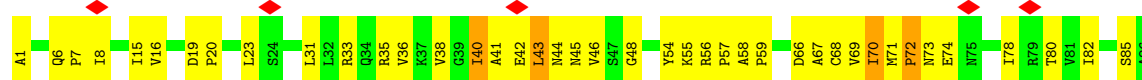
• Molecule 1: Coat protein

Chain DL:  5% 66% 31% . .





- Molecule 1: Coat protein



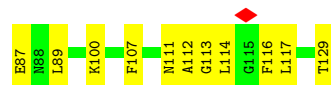
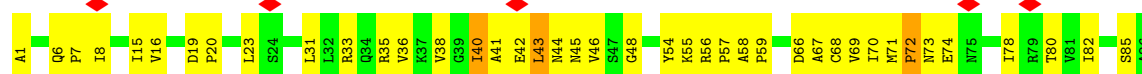
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



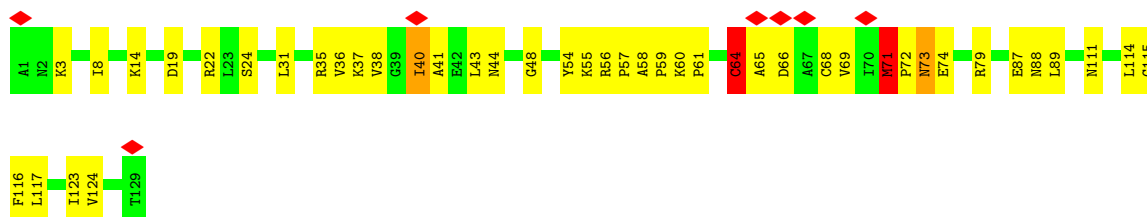
- Molecule 1: Coat protein

Chain DQ:  59% 36% ..



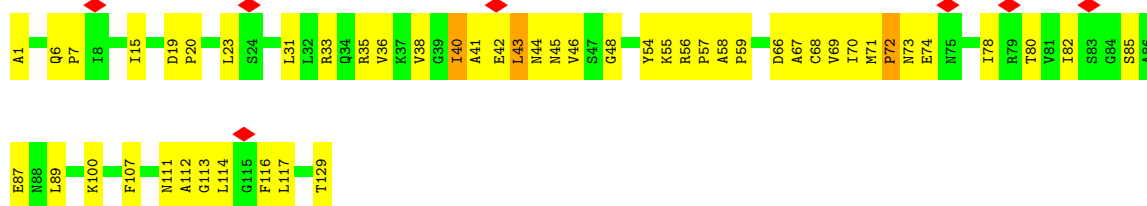
• Molecule 1: Coat protein

Chain DR:  5% 66% 31% ..



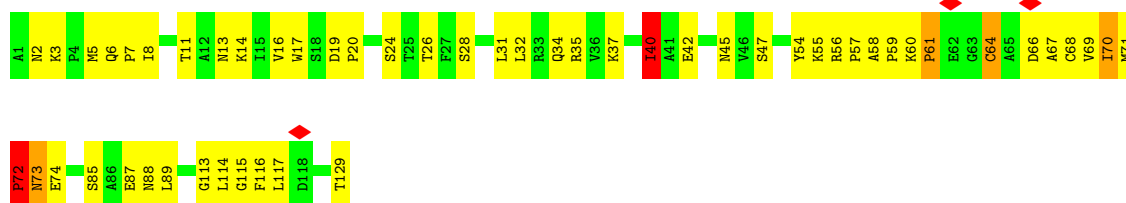
• Molecule 1: Coat protein

Chain DS:  5% 61% 36% .



• Molecule 1: Coat protein

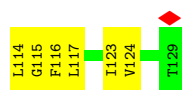
Chain DT:  59% 36% ..



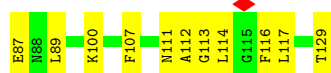
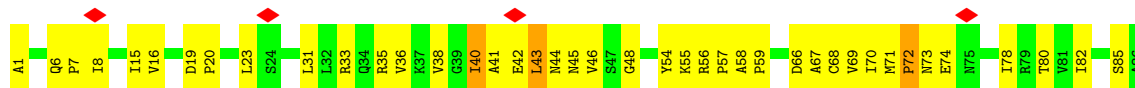
• Molecule 1: Coat protein

Chain DU:  5% 66% 31% ..

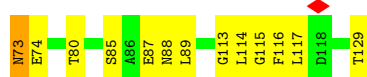




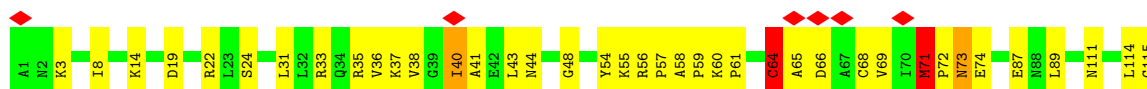
- Molecule 1: Coat protein



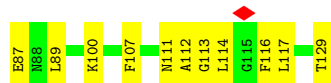
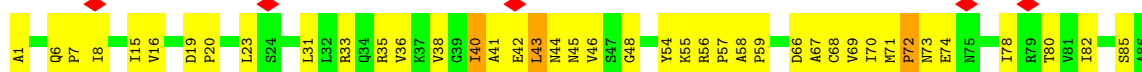
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain DZ:  60% 36%



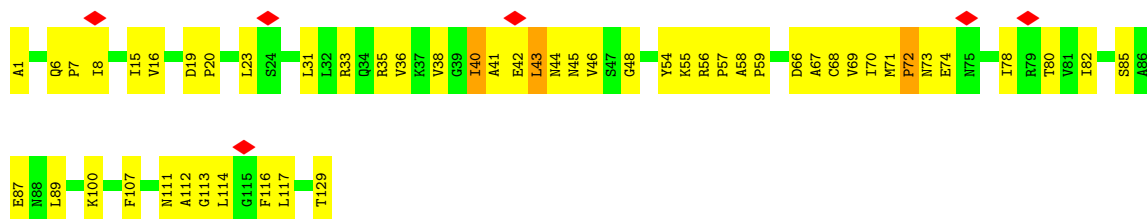
• Molecule 1: Coat protein

Chain EA:  5% 65% 32%



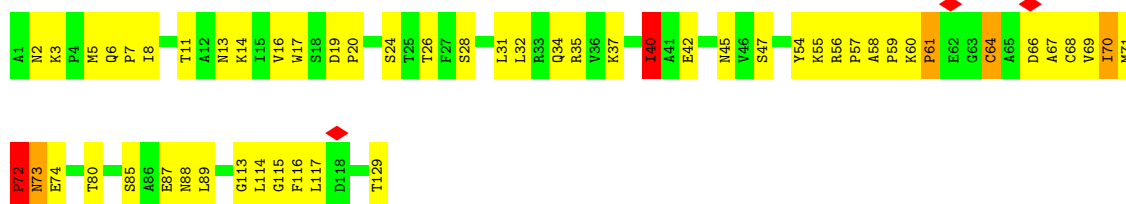
• Molecule 1: Coat protein

Chain EB:  5% 60% 38%



• Molecule 1: Coat protein

Chain EC:  58% 37%



• Molecule 1: Coat protein

Chain ED:  5% 67% 30%

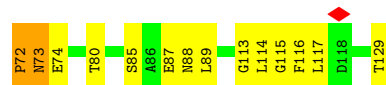
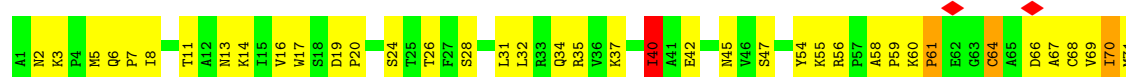




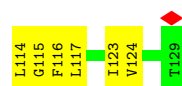
- Molecule 1: Coat protein



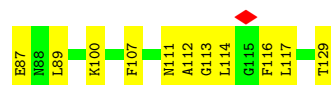
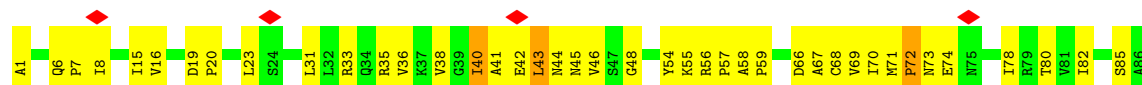
- Molecule 1: Coat protein



- Molecule 1: Coat protein

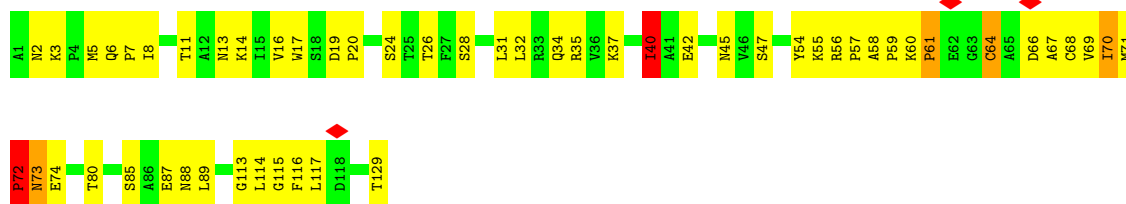


- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain EI:  58% 37%



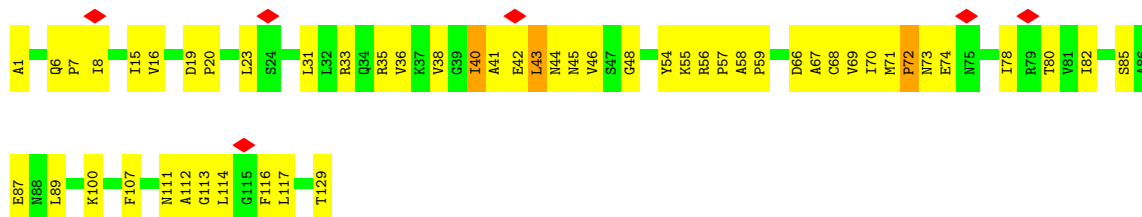
- Molecule 1: Coat protein

Chain EJ:  5% 64% 33%



- Molecule 1: Coat protein

Chain EK:  5% 60% 38%



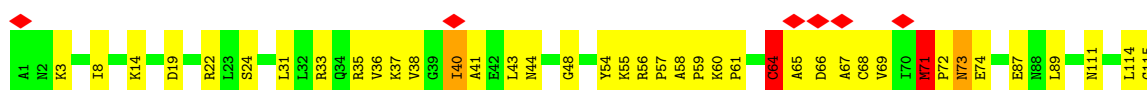
- Molecule 1: Coat protein

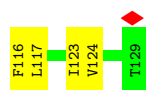
Chain EL:  60% 36%



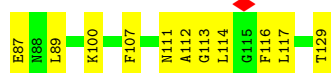
- Molecule 1: Coat protein

Chain EM:  5% 66% 31%





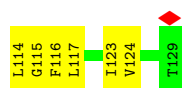
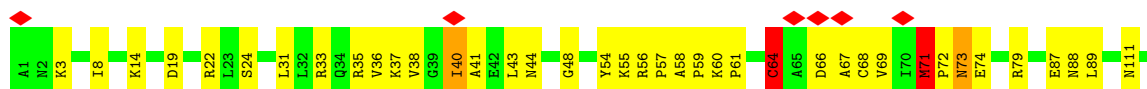
- Molecule 1: Coat protein



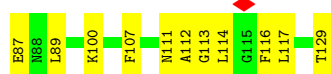
- Molecule 1: Coat protein



- Molecule 1: Coat protein

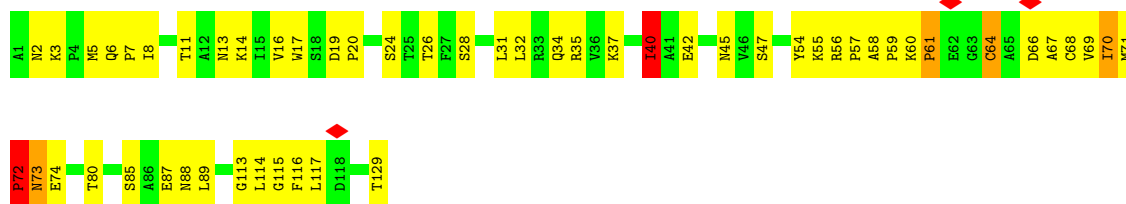


- Molecule 1: Coat protein



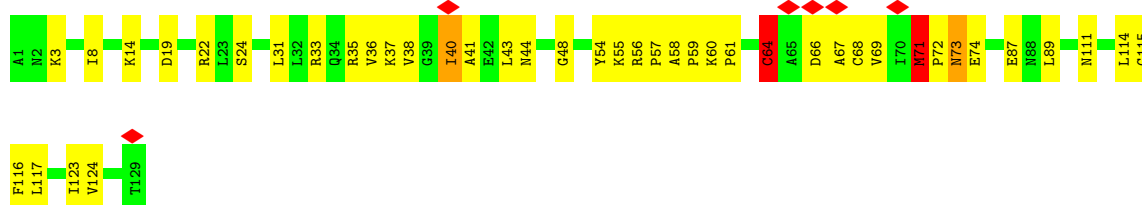
- Molecule 1: Coat protein

Chain ER:  58% 37% . .



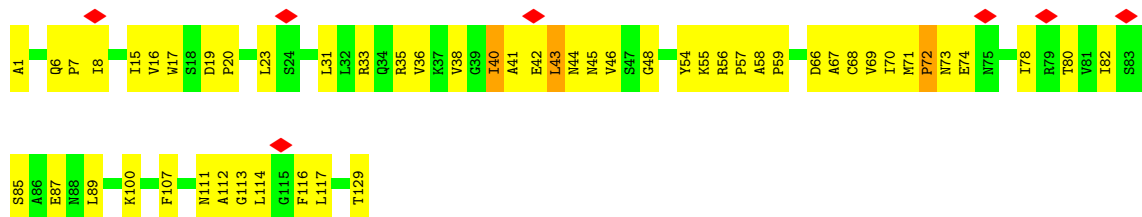
• Molecule 1: Coat protein

Chain ES:  5% 67% 30% . .



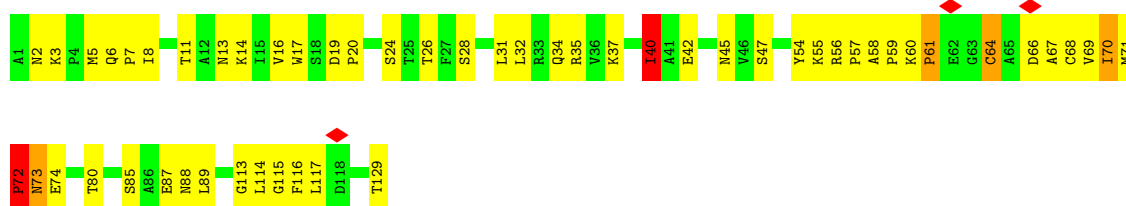
• Molecule 1: Coat protein

Chain ET:  5% 59% 39% .



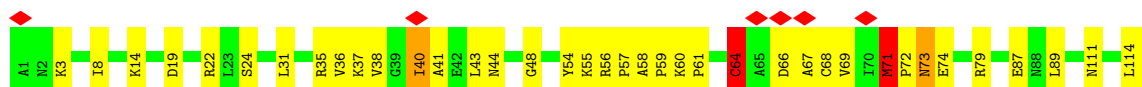
• Molecule 1: Coat protein

Chain EU:  58% 37% . .



• Molecule 1: Coat protein

Chain EV:  5% 67% 30% . .

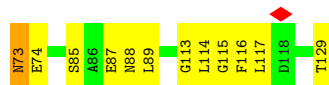




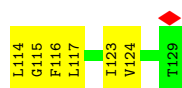
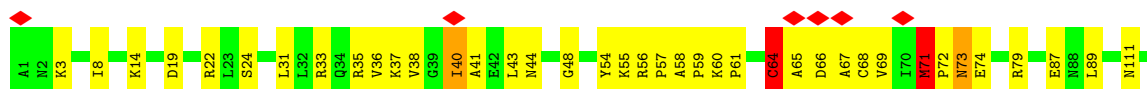
- Molecule 1: Coat protein



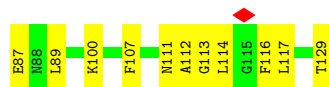
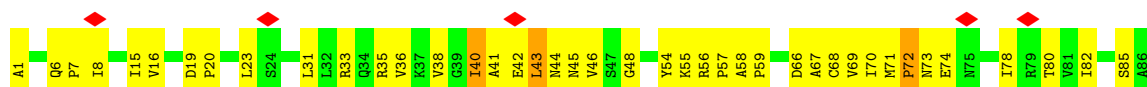
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain FA:  60% 36% . .



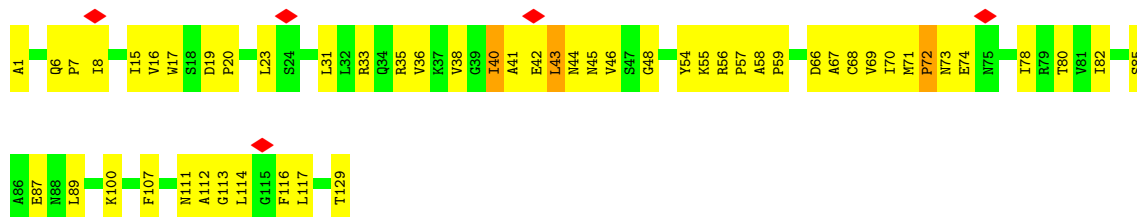
• Molecule 1: Coat protein

Chain FB:  5% 64% 33% . .



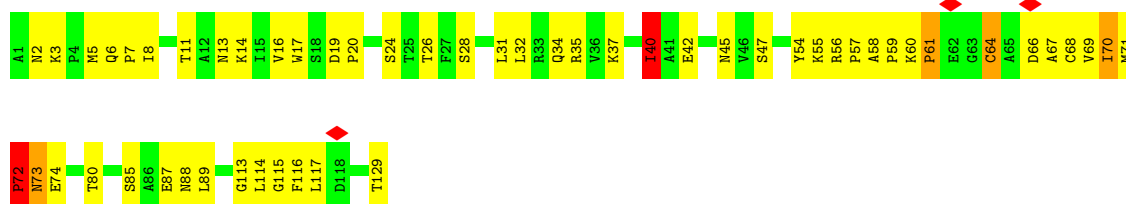
• Molecule 1: Coat protein

Chain FC:  59% 39% .



• Molecule 1: Coat protein

Chain FD:  58% 37% . .



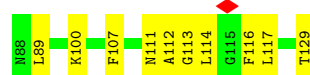
• Molecule 1: Coat protein

Chain FE:  5% 64% 33% . .





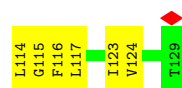
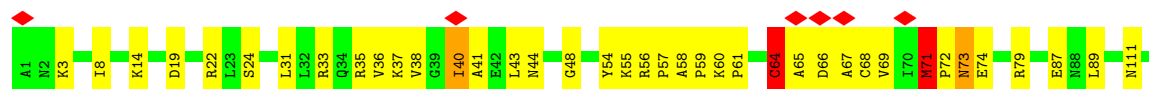
- Molecule 1: Coat protein



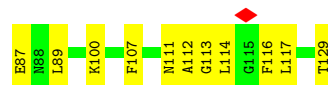
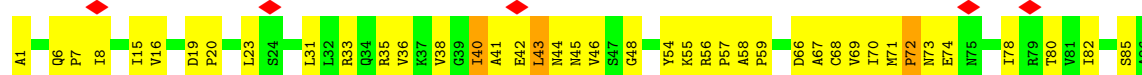
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



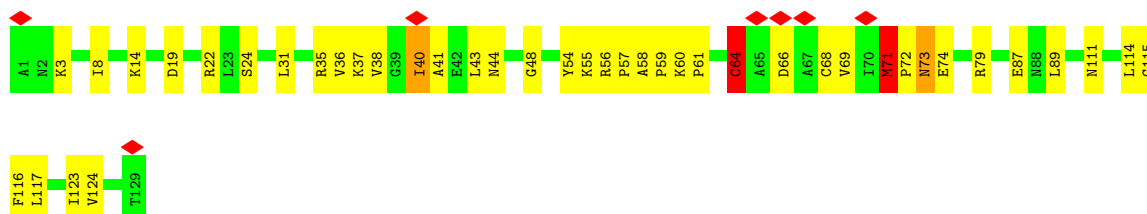
- Molecule 1: Coat protein

Chain FJ:  59% 36%



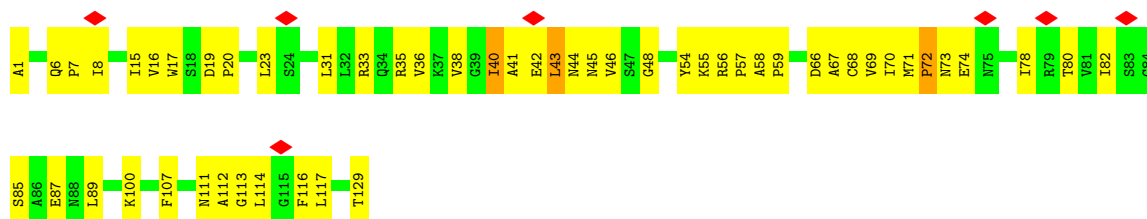
• Molecule 1: Coat protein

Chain FK:  5% 67% 29%



• Molecule 1: Coat protein

Chain FL:  5% 59% 39%



• Molecule 1: Coat protein

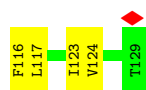
Chain FM:  60% 36%



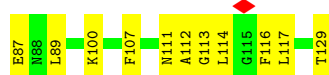
• Molecule 1: Coat protein

Chain FN:  5% 65% 32%

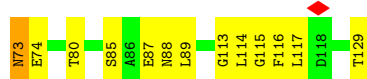




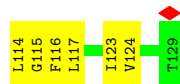
- Molecule 1: Coat protein



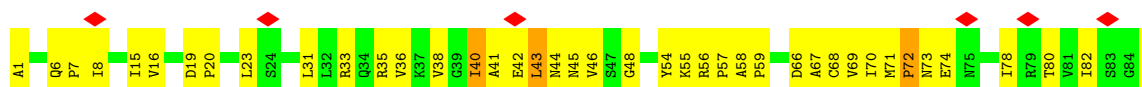
- Molecule 1: Coat protein



- Molecule 1: Coat protein

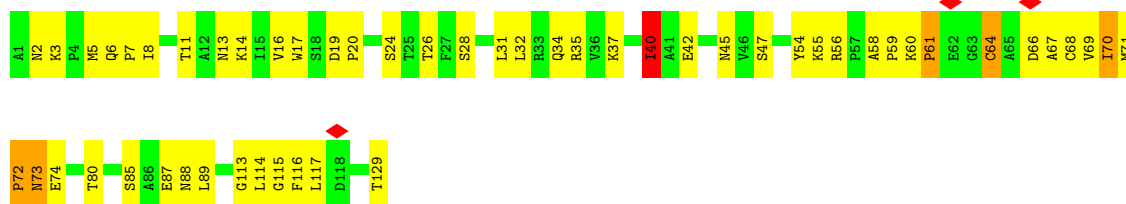


- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain FS:  59% 36% ..



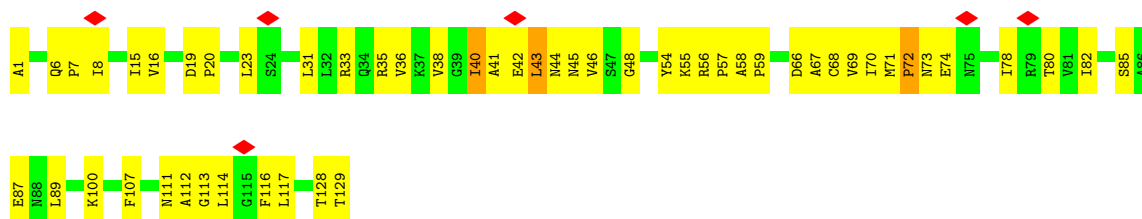
• Molecule 1: Coat protein

Chain FT:  5% 65% 32% ..



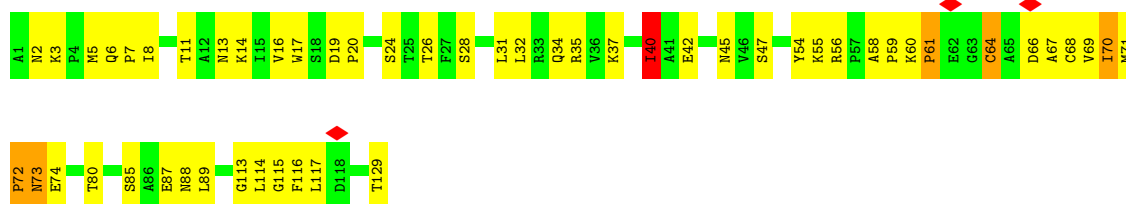
• Molecule 1: Coat protein

Chain FU:  5% 59% 39% .



• Molecule 1: Coat protein

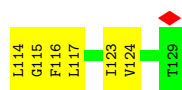
Chain FV:  59% 36% ..



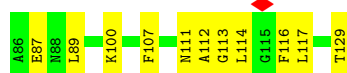
• Molecule 1: Coat protein

Chain FW:  5% 65% 32% ..





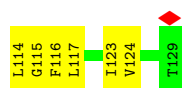
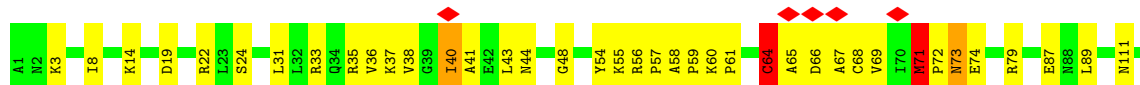
- Molecule 1: Coat protein



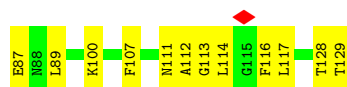
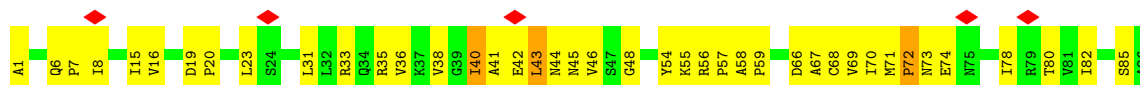
- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein



- Molecule 1: Coat protein

Chain GB:  60% 36% . .



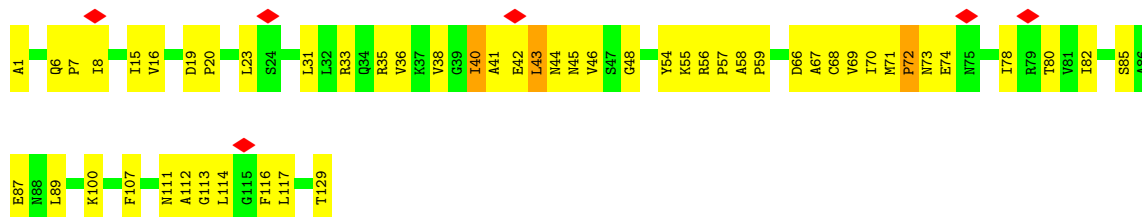
• Molecule 1: Coat protein

Chain GC:  5% 65% 32% . .



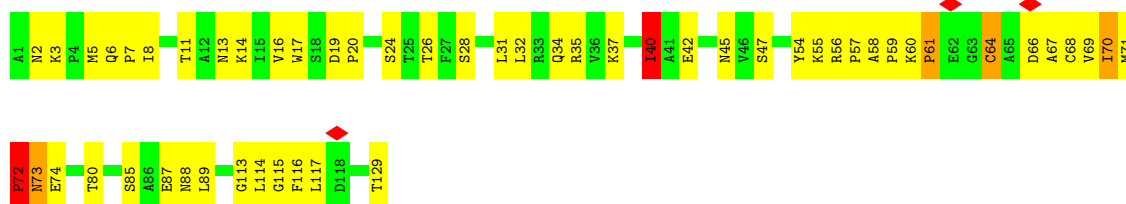
• Molecule 1: Coat protein

Chain GD:  5% 60% 38% .



• Molecule 1: Coat protein

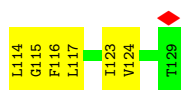
Chain GE:  58% 37% . .



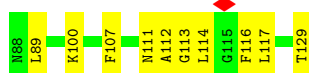
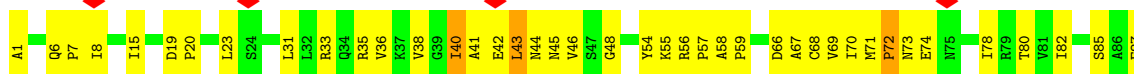
• Molecule 1: Coat protein

Chain GF:  5% 65% 32% . .





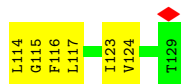
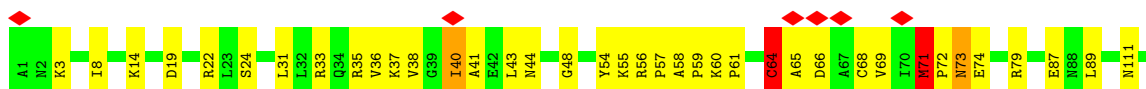
- Molecule 1: Coat protein



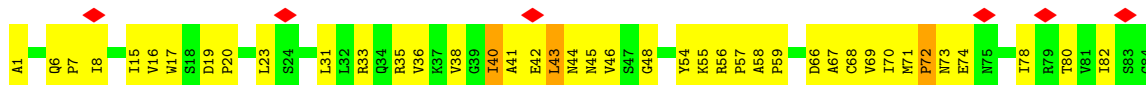
- Molecule 1: Coat protein



- Molecule 1: Coat protein

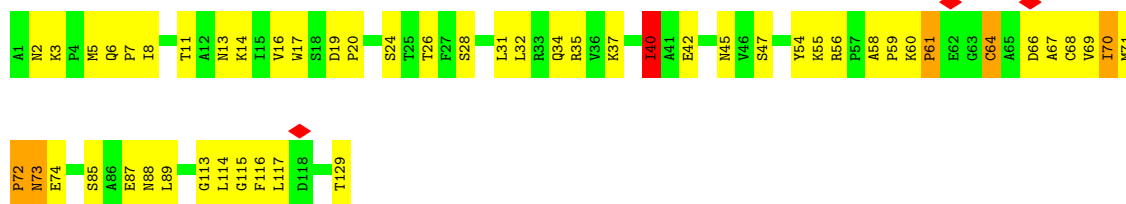


- Molecule 1: Coat protein



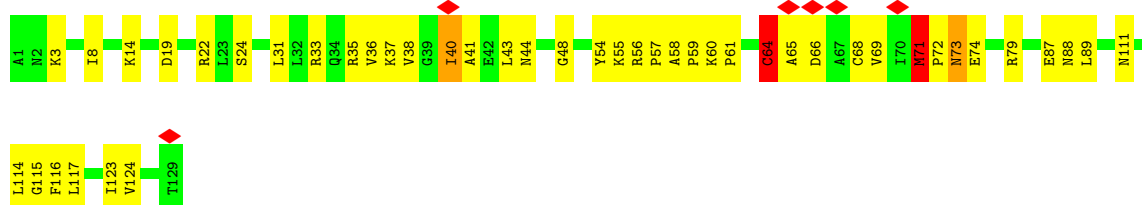
- Molecule 1: Coat protein

Chain GK:  60% 36%



• Molecule 1: Coat protein

Chain GL:  5% 65% 32%



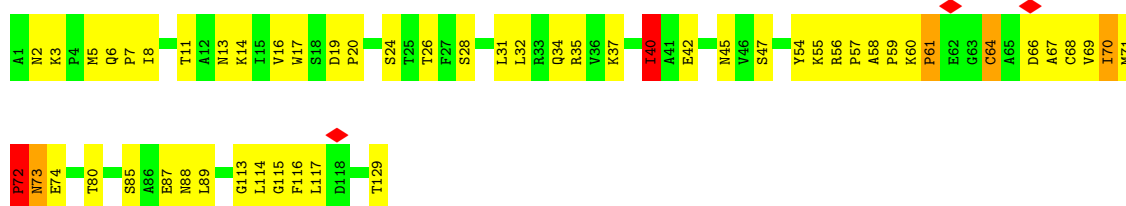
• Molecule 1: Coat protein

Chain GM:  5% 57% 40%



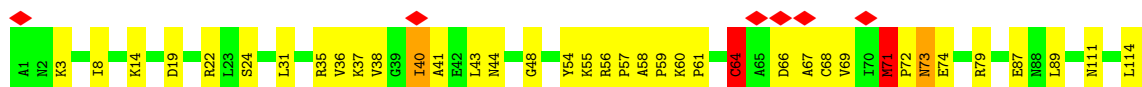
• Molecule 1: Coat protein

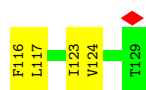
Chain GN:  58% 37%



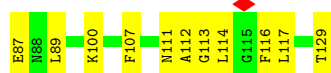
• Molecule 1: Coat protein

Chain GO:  5% 67% 30%

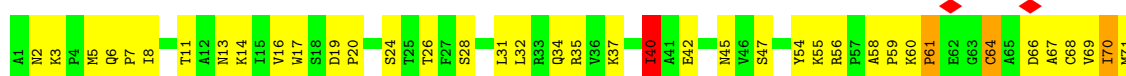




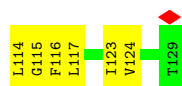
- Molecule 1: Coat protein



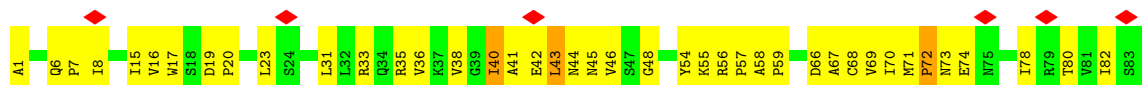
- Molecule 1: Coat protein



- Molecule 1: Coat protein

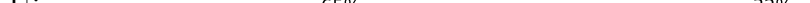


- Molecule 1: Coat protein



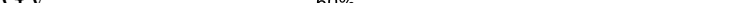
- Molecule 1: Coat protein

P72	N73	E74	T80	S85	A86	E87	N88	L89	G113	L114	G115	F116	L117	D118	T129	A1	N2	K3	P4	Q6	P7	I8	T11	A12	N13	K14	L15	V16	W17	S18	D19	P20	S24	T25	T26	F27	S28	L31	L32	R33	Q34	R35	V36	K37	T40	A41	E42	M45	V46	S47	Y54	K55	R56	P57	A58	P59	K60	P61	E62	G63	C64	A65	D66	A67	C68	V69	I70
-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain GU:  5% 65% 32% .

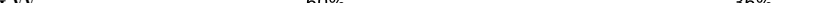
The chart displays 114 categories (A1 to N114) across 10 groups. The categories are color-coded: yellow for most, red for A64, A65, A71, and T129, and orange for A40, A41, and N73. Red diamonds are placed above the bars for A40, A64, A65, A71, and T129.

Category	Group	Color	Marker
A1	1	Yellow	
A2	1	Yellow	
A3	1	Yellow	
T8	1	Yellow	
K14	1	Yellow	
D19	1	Yellow	
R22	1	Yellow	
L23	1	Yellow	
S24	1	Yellow	
L31	1	Yellow	
L32	1	Yellow	
R33	1	Yellow	
Q34	1	Yellow	
R35	1	Yellow	
V36	1	Yellow	
K37	1	Yellow	
V38	1	Yellow	
G39	1	Yellow	
A40	1	Orange	Yes
A41	1	Orange	Yes
E42	1	Yellow	
L43	1	Yellow	
N44	1	Yellow	
G48	1	Yellow	
Y64	2	Yellow	
X65	2	Yellow	
R56	2	Yellow	
P57	2	Yellow	
A58	2	Yellow	
P59	2	Yellow	
K60	2	Yellow	
P61	2	Yellow	
G64	2	Red	Yes
A65	2	Red	Yes
D66	2	Yellow	
A67	2	Yellow	
C68	2	Yellow	
V69	2	Yellow	
L70	2	Yellow	
A71	2	Red	Yes
P72	2	Yellow	
N73	2	Orange	Yes
E74	2	Yellow	
R79	2	Yellow	
E87	2	Yellow	
N88	2	Yellow	
L89	2	Yellow	
N111	2	Yellow	
L114	3	Yellow	
G115	3	Yellow	
F116	3	Yellow	
L117	3	Yellow	
I123	3	Yellow	
V124	3	Yellow	
T129	3	Red	Yes

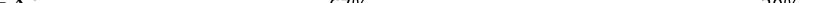
- Chain GV: 

The chart displays the distribution of 1000 samples across 100 categories. The categories are labeled A1 through A86 on the top row and N88 through T129 on the bottom row. The bars are color-coded: yellow for categories with 1 sample, green for 2 samples, orange for 3 samples, and red for 4 samples. Red diamonds are placed above the bars for categories A1, A8, A24, A41, A58, A75, A82, and A86.

Category	Count
A1	1
A6	2
A7	1
A8	1
A15	2
A16	1
A19	1
A20	1
A21	1
A22	1
A23	1
A24	1
A25	2
A31	1
A32	2
A33	2
A34	2
A35	2
A36	2
A37	2
A38	2
A39	2
A40	3
A41	1
A42	2
A43	3
A44	2
A45	2
A46	2
A47	2
A48	2
A54	2
A55	2
A56	2
A57	2
A58	1
A59	2
A66	2
A67	2
A68	2
A69	2
A70	2
A71	2
A72	3
A73	2
A74	2
A75	1
A78	2
A79	2
A80	2
A81	2
A82	1
A85	2
A86	2
N88	2
N89	2
K100	2
F107	2
M111	2
A112	2
G113	2
L114	2
G115	2
F116	2
L117	2
T129	2

- Chain GW: 

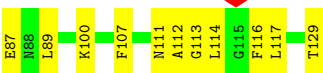
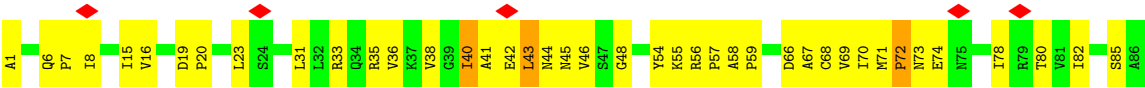
N73	E74	S85	A86	E87	M88	L89	G113	L114	G115	F116	L117	D118	T129	A1	N2	M5	Q6	P7	I8	T11	A12	M13	K14	I15	V16	M17	S18	D19	P20	S24	T25	T26	F27	S28	L31	L32	R33	Q34	R35	V36	K37	I40	A41	E42	M45	V46	S47	Y54	K55	R56	P57	A58	P59	K60	E62	G63	C64	A65	D66	A67	C68	V69	I70	M71
-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain GX: 

Category	Count
A1	100
A2	80
A3	60
A4	40
A5	20
A6	10
A7	5
A8	3
A9	2
A10	1
A11	1
A12	1
A13	1
A14	1
A15	1
A16	1
A17	1
A18	1
A19	1
A20	1
A21	1
A22	1
A23	1
A24	1
A25	1
A26	1
A27	1
A28	1
A29	1
A30	1
A31	1
A32	1
A33	1
A34	1
A35	1
A36	1
A37	1
A38	1
A39	1
A40	1
A41	1
A42	1
A43	1
A44	1
A45	1
A46	1
A47	1
A48	1
A49	1
A50	1
A51	1
A52	1
A53	1
A54	1
A55	1
A56	1
A57	1
A58	1
A59	1
A60	1
A61	1
A62	1
A63	1
A64	1
A65	1
A66	1
A67	1
A68	1
A69	1
A70	1
A71	1
A72	1
A73	1
A74	1
A75	1
A76	1
A77	1
A78	1
A79	1
A80	1
A81	1
A82	1
A83	1
A84	1
A85	1
A86	1
A87	1
A88	1
A89	1
A90	1
A91	1
A92	1
A93	1
A94	1
A95	1
A96	1
A97	1
A98	1
A99	1
A100	1
A101	1
A102	1
A103	1
A104	1
A105	1
A106	1
A107	1
A108	1
A109	1
A110	1
A111	1



● Molecule 1: Coat protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	2215	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AB	0.66	0/985	1.01	8/1342 (0.6%)
1	AC	0.60	0/985	0.95	5/1342 (0.4%)
1	AD	0.69	0/985	0.91	0/1342
1	AE	0.66	0/985	1.01	8/1342 (0.6%)
1	AF	0.60	0/985	0.95	5/1342 (0.4%)
1	AG	0.69	0/985	0.91	0/1342
1	AH	0.66	0/985	1.01	8/1342 (0.6%)
1	AI	0.60	0/985	0.95	5/1342 (0.4%)
1	AJ	0.69	0/985	0.92	0/1342
1	AK	0.66	0/985	1.01	8/1342 (0.6%)
1	AL	0.60	0/985	0.95	5/1342 (0.4%)
1	AM	0.69	0/985	0.91	0/1342
1	AN	0.66	0/985	1.01	8/1342 (0.6%)
1	AO	0.60	0/985	0.95	5/1342 (0.4%)
1	AP	0.69	0/985	0.92	0/1342
1	AQ	0.67	0/985	1.01	8/1342 (0.6%)
1	AR	0.60	0/985	0.95	5/1342 (0.4%)
1	AS	0.69	0/985	0.92	0/1342
1	AT	0.66	0/985	1.01	8/1342 (0.6%)
1	AU	0.60	0/985	0.95	5/1342 (0.4%)
1	AV	0.69	0/985	0.92	0/1342
1	AW	0.66	0/985	1.01	8/1342 (0.6%)
1	AX	0.60	0/985	0.95	5/1342 (0.4%)
1	AY	0.69	0/985	0.91	0/1342
1	AZ	0.66	0/985	1.01	8/1342 (0.6%)
1	BA	0.60	0/985	0.95	5/1342 (0.4%)
1	BB	0.69	0/985	0.92	0/1342
1	BC	0.66	0/985	1.01	8/1342 (0.6%)
1	BD	0.60	0/985	0.95	5/1342 (0.4%)
1	BE	0.69	0/985	0.92	0/1342
1	BF	0.67	0/985	1.01	8/1342 (0.6%)
1	BG	0.60	0/985	0.95	5/1342 (0.4%)
1	BH	0.69	0/985	0.92	0/1342
1	BI	0.66	0/985	1.01	8/1342 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BJ	0.60	0/985	0.95	5/1342 (0.4%)
1	BK	0.69	0/985	0.91	0/1342
1	BL	0.66	0/985	1.01	8/1342 (0.6%)
1	BM	0.60	0/985	0.95	5/1342 (0.4%)
1	BN	0.69	0/985	0.92	0/1342
1	BO	0.66	0/985	1.01	8/1342 (0.6%)
1	BP	0.60	0/985	0.95	5/1342 (0.4%)
1	BQ	0.69	0/985	0.92	0/1342
1	BR	0.67	0/985	1.01	8/1342 (0.6%)
1	BS	0.60	0/985	0.95	5/1342 (0.4%)
1	BT	0.69	0/985	0.92	0/1342
1	BU	0.66	0/985	1.01	8/1342 (0.6%)
1	BV	0.60	0/985	0.95	5/1342 (0.4%)
1	BW	0.69	0/985	0.92	0/1342
1	BX	0.66	0/985	1.01	8/1342 (0.6%)
1	BY	0.60	0/985	0.95	5/1342 (0.4%)
1	BZ	0.69	0/985	0.91	0/1342
1	CA	0.66	0/985	1.01	8/1342 (0.6%)
1	CB	0.60	0/985	0.95	5/1342 (0.4%)
1	CC	0.69	0/985	0.91	0/1342
1	CD	0.67	0/985	1.01	8/1342 (0.6%)
1	CE	0.60	0/985	0.95	5/1342 (0.4%)
1	CF	0.69	0/985	0.92	0/1342
1	CG	0.66	0/985	1.01	8/1342 (0.6%)
1	CH	0.60	0/985	0.95	5/1342 (0.4%)
1	CI	0.69	0/985	0.92	0/1342
1	CJ	0.66	0/985	1.01	8/1342 (0.6%)
1	CK	0.60	0/985	0.95	5/1342 (0.4%)
1	CL	0.69	0/985	0.91	0/1342
1	CM	0.67	0/985	1.01	8/1342 (0.6%)
1	CN	0.60	0/985	0.95	5/1342 (0.4%)
1	CO	0.69	0/985	0.92	0/1342
1	CP	0.66	0/985	1.01	8/1342 (0.6%)
1	CQ	0.60	0/985	0.95	5/1342 (0.4%)
1	CR	0.69	0/985	0.91	0/1342
1	CS	0.66	0/985	1.01	8/1342 (0.6%)
1	CT	0.60	0/985	0.95	5/1342 (0.4%)
1	CU	0.69	0/985	0.92	0/1342
1	CV	0.66	0/985	1.01	8/1342 (0.6%)
1	CW	0.60	0/985	0.95	5/1342 (0.4%)
1	CX	0.69	0/985	0.91	0/1342
1	CY	0.67	0/985	1.01	8/1342 (0.6%)
1	CZ	0.60	0/985	0.95	5/1342 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	DA	0.69	0/985	0.92	0/1342
1	DB	0.66	0/985	1.01	8/1342 (0.6%)
1	DC	0.60	0/985	0.95	5/1342 (0.4%)
1	DD	0.69	0/985	0.91	0/1342
1	DE	0.66	0/985	1.01	8/1342 (0.6%)
1	DF	0.60	0/985	0.95	5/1342 (0.4%)
1	DG	0.69	0/985	0.91	0/1342
1	DH	0.66	0/985	1.01	8/1342 (0.6%)
1	DI	0.60	0/985	0.95	5/1342 (0.4%)
1	DJ	0.69	0/985	0.92	0/1342
1	DK	0.66	0/985	1.01	8/1342 (0.6%)
1	DL	0.60	0/985	0.95	5/1342 (0.4%)
1	DM	0.69	0/985	0.92	0/1342
1	DN	0.66	0/985	1.01	8/1342 (0.6%)
1	DO	0.60	0/985	0.95	5/1342 (0.4%)
1	DP	0.69	0/985	0.91	0/1342
1	DQ	0.66	0/985	1.01	8/1342 (0.6%)
1	DR	0.60	0/985	0.95	5/1342 (0.4%)
1	DS	0.69	0/985	0.92	0/1342
1	DT	0.66	0/985	1.01	8/1342 (0.6%)
1	DU	0.60	0/985	0.95	5/1342 (0.4%)
1	DV	0.69	0/985	0.91	0/1342
1	DW	0.66	0/985	1.01	8/1342 (0.6%)
1	DX	0.60	0/985	0.95	5/1342 (0.4%)
1	DY	0.69	0/985	0.91	0/1342
1	DZ	0.67	0/985	1.01	8/1342 (0.6%)
1	EA	0.60	0/985	0.95	5/1342 (0.4%)
1	EB	0.69	0/985	0.92	0/1342
1	EC	0.66	0/985	1.01	8/1342 (0.6%)
1	ED	0.60	0/985	0.95	5/1342 (0.4%)
1	EE	0.69	0/985	0.92	0/1342
1	EF	0.66	0/985	1.01	8/1342 (0.6%)
1	EG	0.60	0/985	0.95	5/1342 (0.4%)
1	EH	0.69	0/985	0.91	0/1342
1	EI	0.66	0/985	1.01	8/1342 (0.6%)
1	EJ	0.60	0/985	0.95	5/1342 (0.4%)
1	EK	0.69	0/985	0.91	0/1342
1	EL	0.67	0/985	1.01	8/1342 (0.6%)
1	EM	0.60	0/985	0.95	5/1342 (0.4%)
1	EN	0.69	0/985	0.92	0/1342
1	EO	0.66	0/985	1.01	8/1342 (0.6%)
1	EP	0.60	0/985	0.95	5/1342 (0.4%)
1	EQ	0.69	0/985	0.91	0/1342

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	ER	0.66	0/985	1.01	8/1342 (0.6%)
1	ES	0.60	0/985	0.95	5/1342 (0.4%)
1	ET	0.69	0/985	0.92	0/1342
1	EU	0.66	0/985	1.01	8/1342 (0.6%)
1	EV	0.60	0/985	0.95	5/1342 (0.4%)
1	EW	0.69	0/985	0.92	0/1342
1	EX	0.67	0/985	1.01	8/1342 (0.6%)
1	EY	0.60	0/985	0.95	5/1342 (0.4%)
1	EZ	0.69	0/985	0.92	0/1342
1	FA	0.66	0/985	1.01	8/1342 (0.6%)
1	FB	0.60	0/985	0.95	5/1342 (0.4%)
1	FC	0.69	0/985	0.91	0/1342
1	FD	0.66	0/985	1.01	8/1342 (0.6%)
1	FE	0.60	0/985	0.95	5/1342 (0.4%)
1	FF	0.69	0/985	0.91	0/1342
1	FG	0.67	0/985	1.01	8/1342 (0.6%)
1	FH	0.60	0/985	0.95	5/1342 (0.4%)
1	FI	0.69	0/985	0.92	0/1342
1	FJ	0.66	0/985	1.01	8/1342 (0.6%)
1	FK	0.60	0/985	0.95	5/1342 (0.4%)
1	FL	0.69	0/985	0.92	0/1342
1	FM	0.66	0/985	1.01	8/1342 (0.6%)
1	FN	0.60	0/985	0.95	5/1342 (0.4%)
1	FO	0.69	0/985	0.91	0/1342
1	FP	0.66	0/985	1.01	8/1342 (0.6%)
1	FQ	0.60	0/985	0.95	5/1342 (0.4%)
1	FR	0.69	0/985	0.92	0/1342
1	FS	0.67	0/985	1.01	8/1342 (0.6%)
1	FT	0.60	0/985	0.95	5/1342 (0.4%)
1	FU	0.69	0/985	0.92	0/1342
1	FV	0.66	0/985	1.01	8/1342 (0.6%)
1	FW	0.60	0/985	0.95	5/1342 (0.4%)
1	FX	0.69	0/985	0.92	0/1342
1	FY	0.66	0/985	1.01	8/1342 (0.6%)
1	FZ	0.60	0/985	0.95	5/1342 (0.4%)
1	GA	0.69	0/985	0.92	0/1342
1	GB	0.66	0/985	1.01	8/1342 (0.6%)
1	GC	0.60	0/985	0.95	5/1342 (0.4%)
1	GD	0.69	0/985	0.91	0/1342
1	GE	0.66	0/985	1.01	8/1342 (0.6%)
1	GF	0.60	0/985	0.95	5/1342 (0.4%)
1	GG	0.69	0/985	0.91	0/1342
1	GH	0.66	0/985	1.01	8/1342 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GI	0.60	0/985	0.95	5/1342 (0.4%)
1	GJ	0.69	0/985	0.92	0/1342
1	GK	0.66	0/985	1.01	8/1342 (0.6%)
1	GL	0.60	0/985	0.95	5/1342 (0.4%)
1	GM	0.69	0/985	0.92	0/1342
1	GN	0.66	0/985	1.01	8/1342 (0.6%)
1	GO	0.60	0/985	0.95	5/1342 (0.4%)
1	GP	0.69	0/985	0.91	0/1342
1	GQ	0.66	0/985	1.01	8/1342 (0.6%)
1	GR	0.60	0/985	0.95	5/1342 (0.4%)
1	GS	0.69	0/985	0.92	0/1342
1	GT	0.66	0/985	1.01	8/1342 (0.6%)
1	GU	0.60	0/985	0.95	5/1342 (0.4%)
1	GV	0.69	0/985	0.91	0/1342
1	GW	0.67	0/985	1.01	8/1342 (0.6%)
1	GX	0.60	0/985	0.95	5/1342 (0.4%)
1	GY	0.69	0/985	0.92	0/1342
All	All	0.65	0/177300	0.96	780/241560 (0.3%)

There are no bond length outliers.

The worst 5 of 780 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AF	73	ASN	N-CA-C	10.41	123.96	110.53
1	BJ	73	ASN	N-CA-C	10.41	123.96	110.53
1	BY	73	ASN	N-CA-C	10.41	123.96	110.53
1	CK	73	ASN	N-CA-C	10.41	123.96	110.53
1	CW	73	ASN	N-CA-C	10.41	123.96	110.53

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	968	0	973	80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AC	968	0	973	67	0
1	AD	968	0	973	97	0
1	AE	968	0	973	79	0
1	AF	968	0	973	67	0
1	AG	968	0	973	100	0
1	AH	968	0	973	79	0
1	AI	968	0	973	67	0
1	AJ	968	0	973	100	0
1	AK	968	0	973	79	0
1	AL	968	0	973	66	0
1	AM	968	0	973	96	0
1	AN	968	0	973	78	0
1	AO	968	0	973	68	0
1	AP	968	0	973	100	0
1	AQ	968	0	973	79	0
1	AR	968	0	973	69	0
1	AS	968	0	973	100	0
1	AT	968	0	973	79	0
1	AU	968	0	973	68	0
1	AV	968	0	973	100	0
1	AW	968	0	973	81	0
1	AX	968	0	973	68	0
1	AY	968	0	973	101	0
1	AZ	968	0	973	81	0
1	BA	968	0	973	70	0
1	BB	968	0	973	101	0
1	BC	968	0	973	79	0
1	BD	968	0	973	68	0
1	BE	968	0	973	100	0
1	BF	968	0	973	79	0
1	BG	968	0	973	70	0
1	BH	968	0	973	99	0
1	BI	968	0	973	81	0
1	BJ	968	0	973	70	0
1	BK	968	0	973	101	0
1	BL	968	0	973	78	0
1	BM	968	0	973	69	0
1	BN	968	0	973	98	0
1	BO	968	0	973	81	0
1	BP	968	0	973	68	0
1	BQ	968	0	973	99	0
1	BR	968	0	973	79	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BS	968	0	973	67	0
1	BT	968	0	973	99	0
1	BU	968	0	973	78	0
1	BV	968	0	973	69	0
1	BW	968	0	973	98	0
1	BX	968	0	973	81	0
1	BY	968	0	973	70	0
1	BZ	968	0	973	101	0
1	CA	968	0	973	79	0
1	CB	968	0	973	68	0
1	CC	968	0	973	99	0
1	CD	968	0	973	79	0
1	CE	968	0	973	69	0
1	CF	968	0	973	98	0
1	CG	968	0	973	80	0
1	CH	968	0	973	69	0
1	CI	968	0	973	103	0
1	CJ	968	0	973	78	0
1	CK	968	0	973	67	0
1	CL	968	0	973	102	0
1	CM	968	0	973	78	0
1	CN	968	0	973	68	0
1	CO	968	0	973	98	0
1	CP	968	0	973	78	0
1	CQ	968	0	973	68	0
1	CR	968	0	973	100	0
1	CS	968	0	973	80	0
1	CT	968	0	973	68	0
1	CU	968	0	973	99	0
1	CV	968	0	973	81	0
1	CW	968	0	973	70	0
1	CX	968	0	973	99	0
1	CY	968	0	973	80	0
1	CZ	968	0	973	69	0
1	DA	968	0	973	101	0
1	DB	968	0	973	80	0
1	DC	968	0	973	69	0
1	DD	968	0	973	100	0
1	DE	968	0	973	81	0
1	DF	968	0	973	70	0
1	DG	968	0	973	100	0
1	DH	968	0	973	79	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	DI	968	0	973	69	0
1	DJ	968	0	973	100	0
1	DK	968	0	973	76	0
1	DL	968	0	973	68	0
1	DM	968	0	973	100	0
1	DN	968	0	973	80	0
1	DO	968	0	973	66	0
1	DP	968	0	973	97	0
1	DQ	968	0	973	81	0
1	DR	968	0	973	69	0
1	DS	968	0	973	99	0
1	DT	968	0	973	78	0
1	DU	968	0	973	70	0
1	DV	968	0	973	102	0
1	DW	968	0	973	79	0
1	DX	968	0	973	66	0
1	DY	968	0	973	97	0
1	DZ	968	0	973	80	0
1	EA	968	0	973	69	0
1	EB	968	0	973	100	0
1	EC	968	0	973	80	0
1	ED	968	0	973	68	0
1	EE	968	0	973	99	0
1	EF	968	0	973	78	0
1	EG	968	0	973	67	0
1	EH	968	0	973	101	0
1	EI	968	0	973	81	0
1	EJ	968	0	973	69	0
1	EK	968	0	973	101	0
1	EL	968	0	973	79	0
1	EM	968	0	973	67	0
1	EN	968	0	973	98	0
1	EO	968	0	973	79	0
1	EP	968	0	973	67	0
1	EQ	968	0	973	100	0
1	ER	968	0	973	79	0
1	ES	968	0	973	67	0
1	ET	968	0	973	100	0
1	EU	968	0	973	82	0
1	EV	968	0	973	67	0
1	EW	968	0	973	100	0
1	EX	968	0	973	78	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	EY	968	0	973	69	0
1	EZ	968	0	973	99	0
1	FA	968	0	973	79	0
1	FB	968	0	973	70	0
1	FC	968	0	973	100	0
1	FD	968	0	973	81	0
1	FE	968	0	973	72	0
1	FF	968	0	973	100	0
1	FG	968	0	973	78	0
1	FH	968	0	973	69	0
1	FI	968	0	973	99	0
1	FJ	968	0	973	81	0
1	FK	968	0	973	67	0
1	FL	968	0	973	99	0
1	FM	968	0	973	79	0
1	FN	968	0	973	69	0
1	FO	968	0	973	103	0
1	FP	968	0	973	81	0
1	FQ	968	0	973	68	0
1	FR	968	0	973	100	0
1	FS	968	0	973	80	0
1	FT	968	0	973	70	0
1	FU	968	0	973	101	0
1	FV	968	0	973	79	0
1	FW	968	0	973	67	0
1	FX	968	0	973	99	0
1	FY	968	0	973	82	0
1	FZ	968	0	973	68	0
1	GA	968	0	973	100	0
1	GB	968	0	973	79	0
1	GC	968	0	973	69	0
1	GD	968	0	973	103	0
1	GE	968	0	973	79	0
1	GF	968	0	973	69	0
1	GG	968	0	973	97	0
1	GH	968	0	973	81	0
1	GI	968	0	973	69	0
1	GJ	968	0	973	101	0
1	GK	968	0	973	79	0
1	GL	968	0	973	68	0
1	GM	968	0	973	104	0
1	GN	968	0	973	80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	GO	968	0	973	68	0
1	GP	968	0	973	100	0
1	GQ	968	0	973	81	0
1	GR	968	0	973	69	0
1	GS	968	0	973	102	0
1	GT	968	0	973	80	0
1	GU	968	0	973	69	0
1	GV	968	0	973	99	0
1	GW	968	0	973	79	0
1	GX	968	0	973	68	0
1	GY	968	0	973	99	0
All	All	174240	0	175140	12064	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 35.

The worst 5 of 12064 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:DG:107:PHE:HA	1:DG:112:ALA:CB	1.43	1.49
1:CX:107:PHE:HA	1:CX:112:ALA:CB	1.43	1.49
1:AV:107:PHE:HA	1:AV:112:ALA:CB	1.43	1.48
1:BE:107:PHE:HA	1:BE:112:ALA:CB	1.43	1.48
1:BW:107:PHE:HA	1:BW:112:ALA:CB	1.43	1.48

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%)	116 (91%)	8 (6%)	3 (2%)	4 27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AC	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	AD	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	AE	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	AF	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	AG	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	AH	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	AI	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	AJ	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	AK	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	AL	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	AM	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	AN	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	AO	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	AP	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	AQ	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	AR	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	AS	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	AT	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	AU	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	AV	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	AW	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	AX	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	AY	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	AZ	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	BA	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	BB	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	BC	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	BD	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	BE	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	BF	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	BG	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BH	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	BI	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	BJ	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	BK	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	BL	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	BM	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	BN	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	BO	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	BP	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	BQ	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	BR	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	BS	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	BT	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	BU	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	BV	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	BW	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	BX	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	BY	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	BZ	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	CA	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	CB	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	CC	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	CD	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	CE	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	CF	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	CG	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	CH	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	CI	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	CJ	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	CK	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	CL	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CM	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	CN	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	CO	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	CP	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	CQ	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	CR	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	CS	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	CT	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	CU	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	CV	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	CW	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	CX	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	CY	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	CZ	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	DA	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	DB	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	DC	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	DD	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	DE	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	DF	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	DG	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	DH	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	DI	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	DJ	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	DK	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	DL	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	DM	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	DN	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	DO	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	DP	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	DQ	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DR	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	DS	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	DT	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	DU	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	DV	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	DW	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	DX	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	DY	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	DZ	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	EA	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	EB	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	EC	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	ED	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	EE	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	EF	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	EG	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	EH	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	EI	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	EJ	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	EK	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	EL	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	EM	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	EN	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	EO	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	EP	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	EQ	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	ER	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	ES	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	ET	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	EU	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	EV	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EW	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	EX	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	EY	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	EZ	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	FA	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	FB	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	FC	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	FD	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	FE	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	FF	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	FG	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	FH	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	FI	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	FJ	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	FK	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	FL	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	FM	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	FN	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	FO	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	FP	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	FQ	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	FR	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	FS	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	FT	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	FU	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	FV	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	FW	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	FX	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	FY	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	FZ	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	GA	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	GB	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	GC	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	GD	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	GE	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	GF	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	GG	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	GH	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	GI	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	GJ	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	GK	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	GL	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	GM	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	GN	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	GO	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	GP	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	GQ	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	GR	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	GS	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	GT	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	GU	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	GV	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
1	GW	127/129 (98%)	116 (91%)	8 (6%)	3 (2%)	4	27
1	GX	127/129 (98%)	122 (96%)	4 (3%)	1 (1%)	16	54
1	GY	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	54
All	All	22860/23220 (98%)	21420 (94%)	1140 (5%)	300 (1%)	12	42

5 of 300 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	40	ILE
1	AE	40	ILE
1	AH	40	ILE
1	AK	40	ILE
1	AN	40	ILE

5.3.2 Protein sidechains ⓘ

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%)	107 (99%)	1 (1%)	70	78
1	AC	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	AD	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	AE	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	AF	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	AG	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	AH	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	AI	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	AJ	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	AK	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	AL	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	AM	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	AN	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	AO	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	AP	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	AQ	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	AR	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	AS	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	AT	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	AU	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	AV	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	AW	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	AX	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	AY	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	AZ	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	BA	108/108 (100%)	103 (95%)	5 (5%)	24	45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	BB	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	BC	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	BD	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	BE	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	BF	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	BG	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	BH	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	BI	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	BJ	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	BK	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	BL	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	BM	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	BN	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	BO	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	BP	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	BQ	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	BR	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	BS	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	BT	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	BU	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	BV	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	BW	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	BX	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	BY	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	BZ	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	CA	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	CB	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	CC	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	CD	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	CE	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	CF	108/108 (100%)	105 (97%)	3 (3%)	38	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CG	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	CH	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	CI	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	CJ	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	CK	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	CL	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	CM	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	CN	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	CO	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	CP	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	CQ	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	CR	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	CS	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	CT	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	CU	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	CV	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	CW	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	CX	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	CY	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	CZ	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	DA	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	DB	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	DC	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	DD	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	DE	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	DF	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	DG	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	DH	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	DI	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	DJ	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	DK	108/108 (100%)	107 (99%)	1 (1%)	70	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	DL	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	DM	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	DN	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	DO	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	DP	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	DQ	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	DR	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	DS	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	DT	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	DU	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	DV	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	DW	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	DX	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	DY	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	DZ	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	EA	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	EB	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	EC	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	ED	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	EE	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	EF	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	EG	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	EH	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	EI	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	EJ	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	EK	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	EL	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	EM	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	EN	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	EO	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	EP	108/108 (100%)	103 (95%)	5 (5%)	24	45	

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	EQ	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	ER	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	ES	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	ET	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	EU	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	EV	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	EW	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	EX	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	EY	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	EZ	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	FA	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	FB	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	FC	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	FD	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	FE	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	FF	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	FG	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	FH	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	FI	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	FJ	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	FK	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	FL	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	FM	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	FN	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	FO	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	FP	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	FQ	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	FR	108/108 (100%)	105 (97%)	3 (3%)	38	60	
1	FS	108/108 (100%)	107 (99%)	1 (1%)	70	78	
1	FT	108/108 (100%)	103 (95%)	5 (5%)	24	45	
1	FU	108/108 (100%)	105 (97%)	3 (3%)	38	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	FV	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	FW	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	FX	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	FY	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	FZ	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	GA	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	GB	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	GC	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	GD	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	GE	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	GF	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	GG	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	GH	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	GI	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	GJ	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	GK	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	GL	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	GM	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	GN	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	GO	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	GP	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	GQ	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	GR	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	GS	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	GT	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	GU	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	GV	108/108 (100%)	105 (97%)	3 (3%)	38	60
1	GW	108/108 (100%)	107 (99%)	1 (1%)	70	78
1	GX	108/108 (100%)	103 (95%)	5 (5%)	24	45
1	GY	108/108 (100%)	105 (97%)	3 (3%)	38	60
All	All	19440/19440 (100%)	18900 (97%)	540 (3%)	38	60

5 of 540 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	FZ	69	VAL
1	GD	70	ILE
1	FZ	64	CYS
1	GS	43	LEU
1	CN	71	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 576 such sidechains are listed below:

Mol	Chain	Res	Type
1	FP	45	ASN
1	GY	44	ASN
1	FT	73	ASN
1	FP	34	GLN
1	GH	88	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 oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

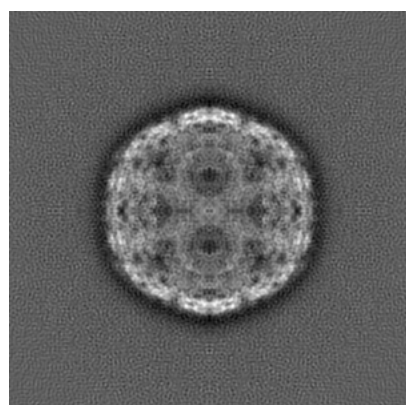
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4098. These allow visual inspection of the internal detail of the map and identification of artifacts.

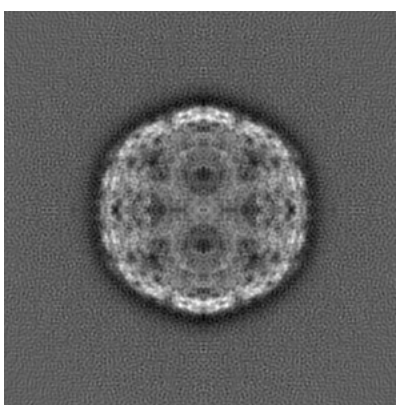
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

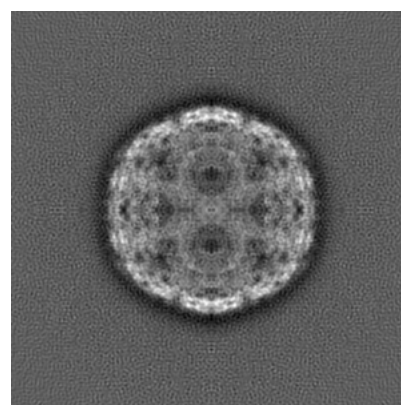
6.1.1 Primary map



X



Y

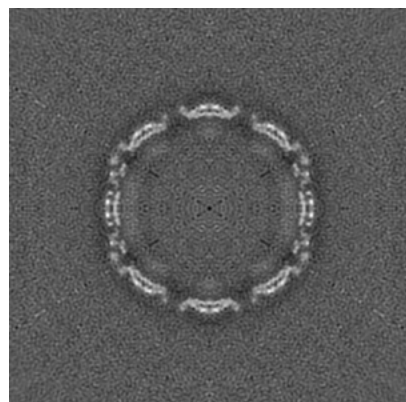


Z

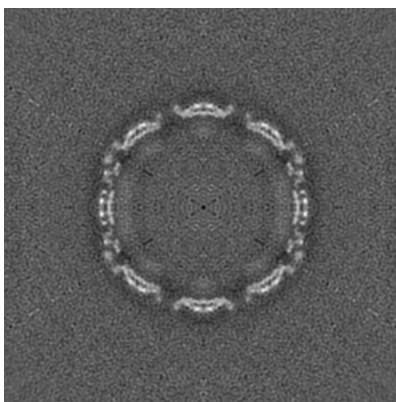
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

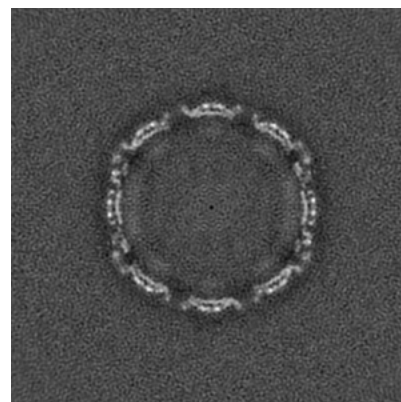
6.2.1 Primary map



X Index: 200



Y Index: 200

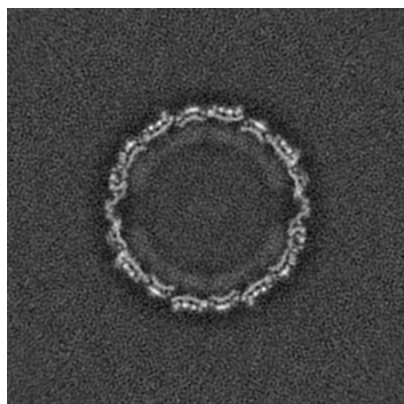


Z Index: 200

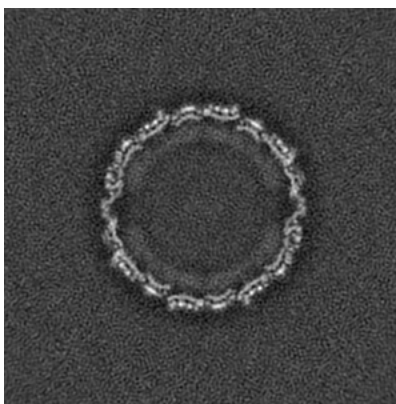
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

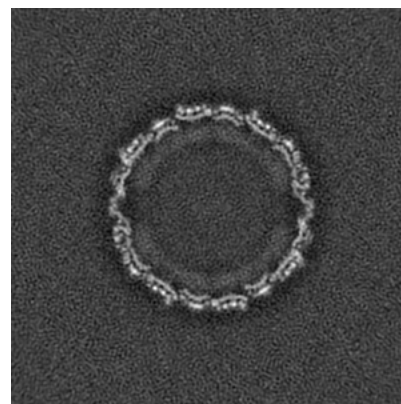
6.3.1 Primary map



X Index: 173



Y Index: 173

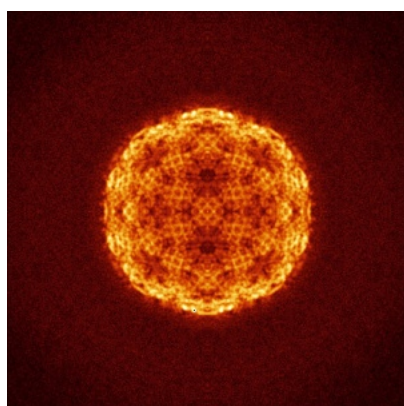


Z Index: 226

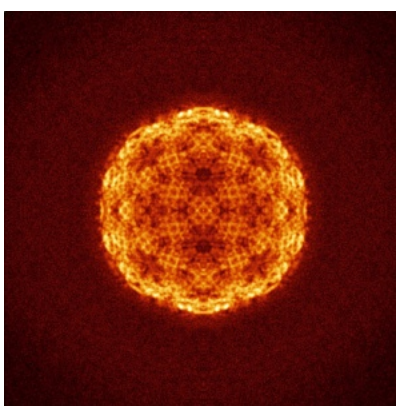
The images above show the largest variance slices of the map in three orthogonal directions.

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

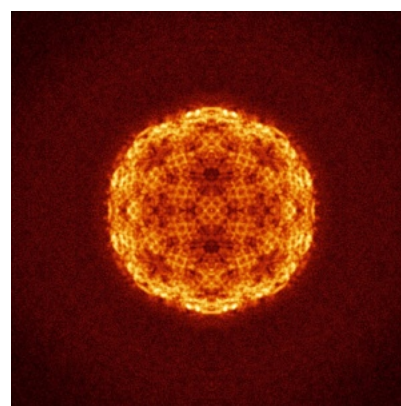
6.4.1 Primary map



X



Y

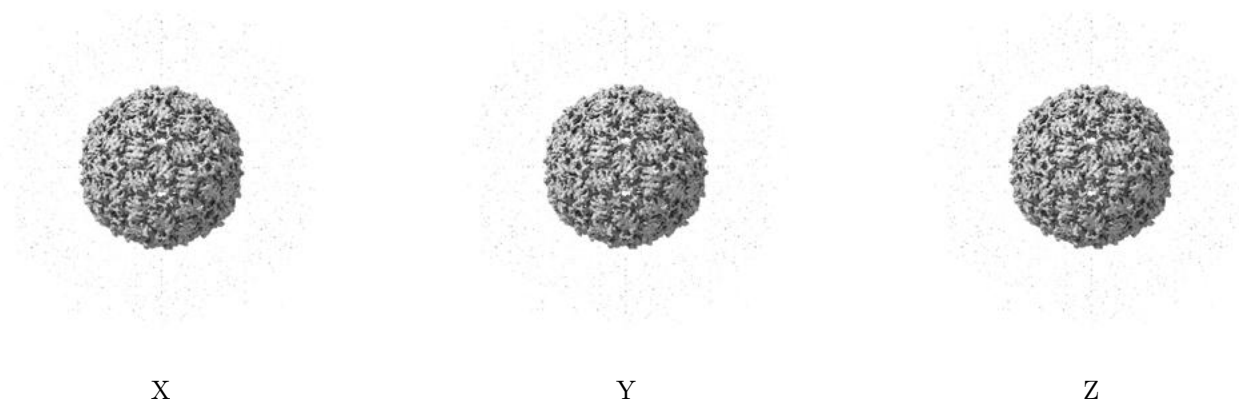


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

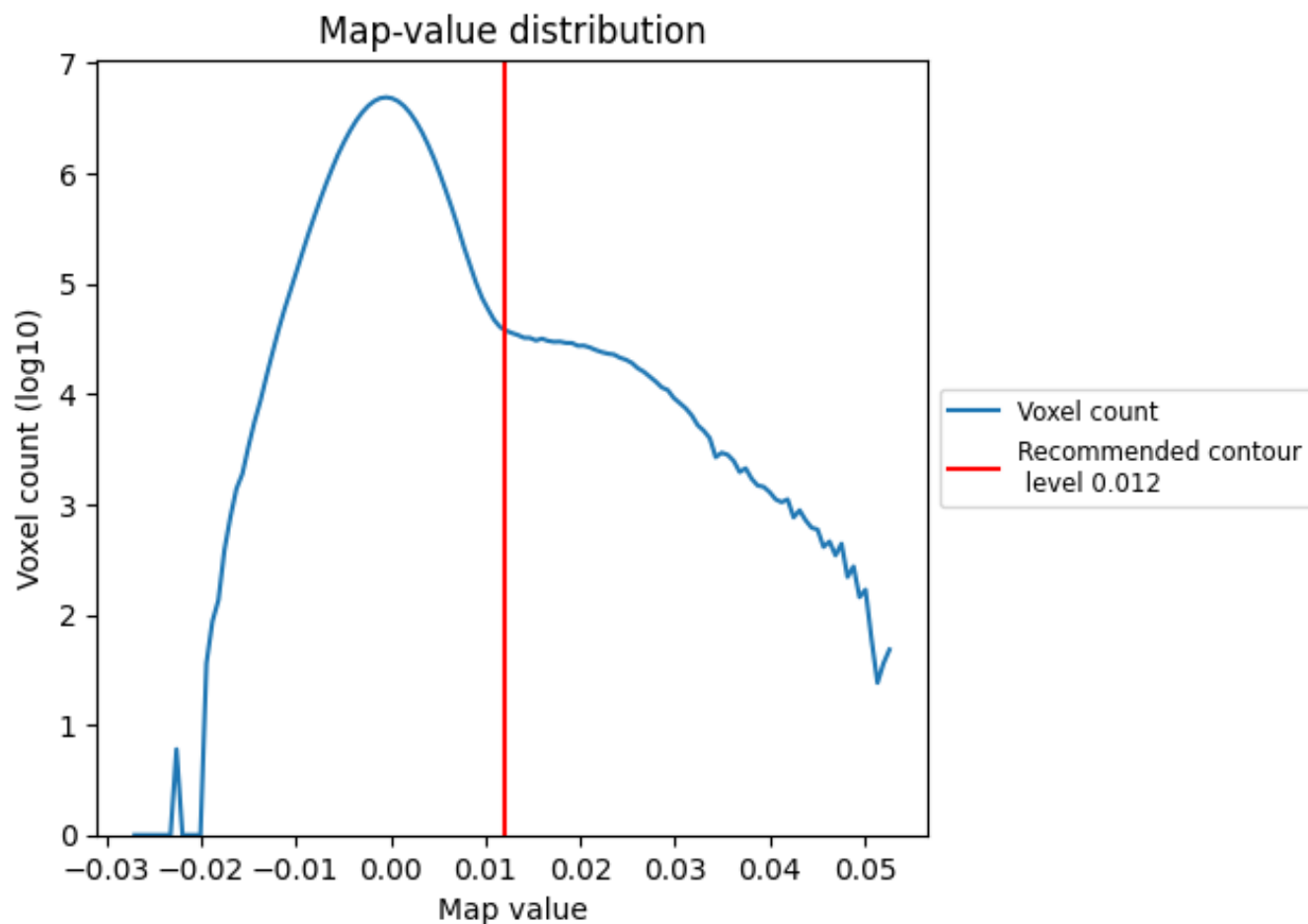
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

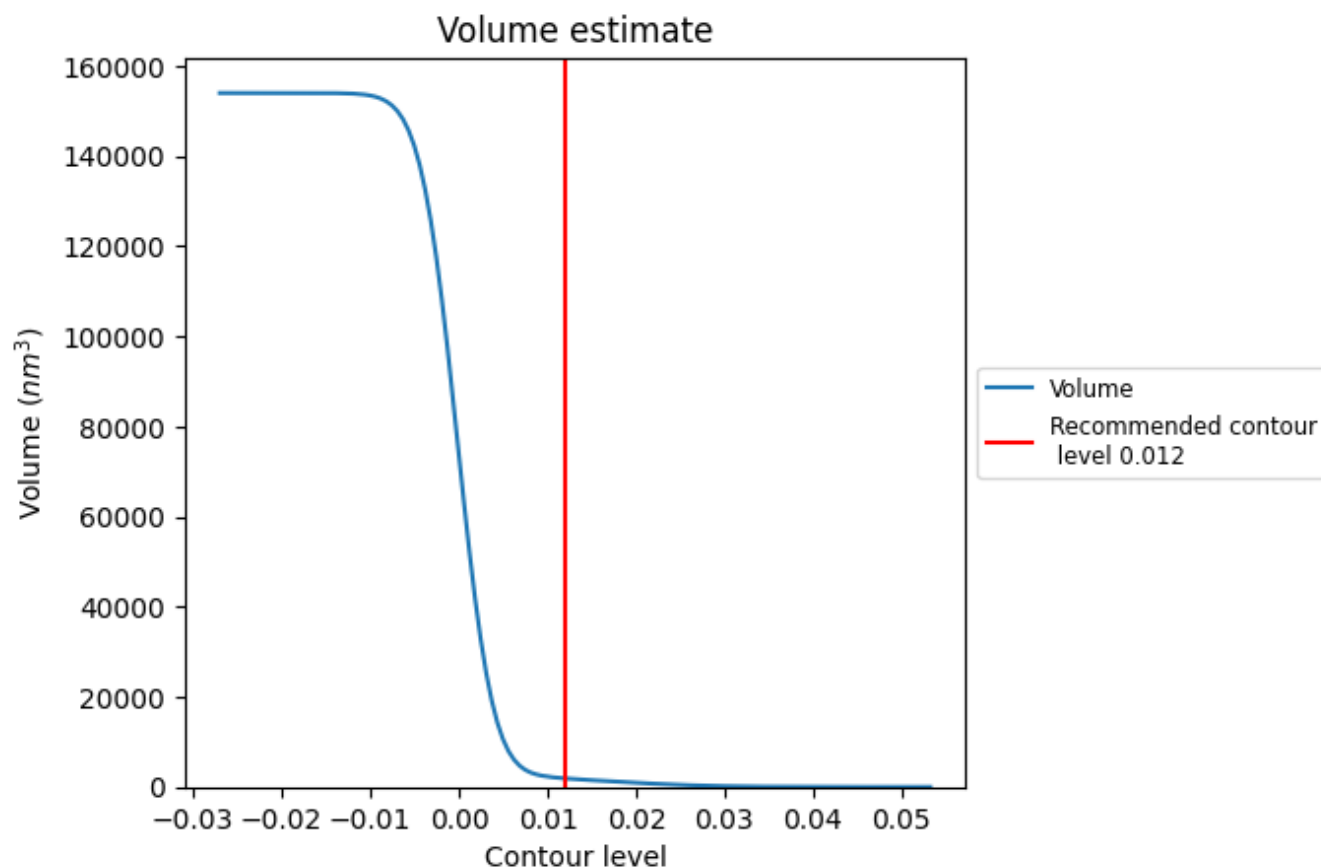
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

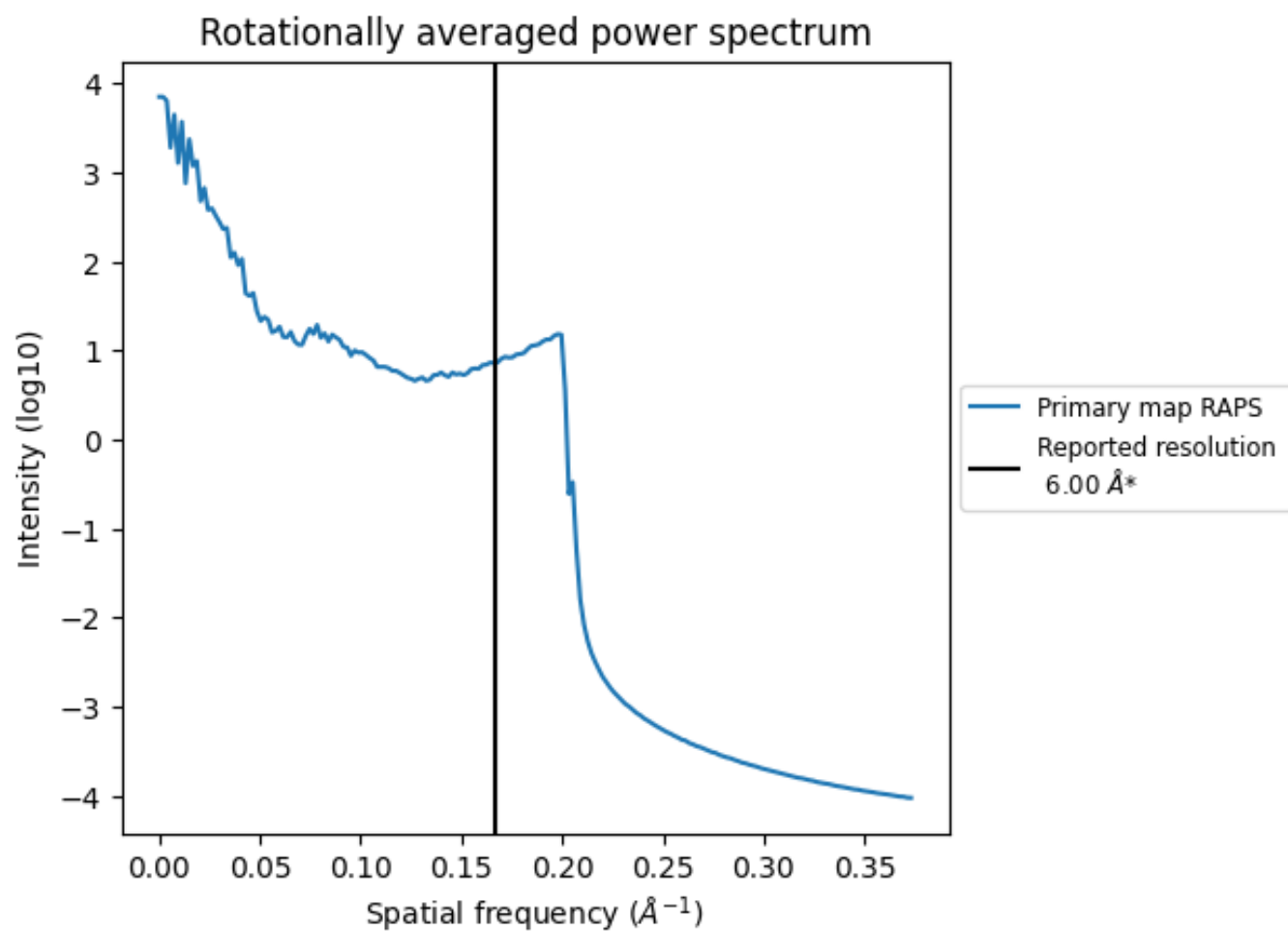
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1899 nm³; this corresponds to an approximate mass of 1715 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](#)

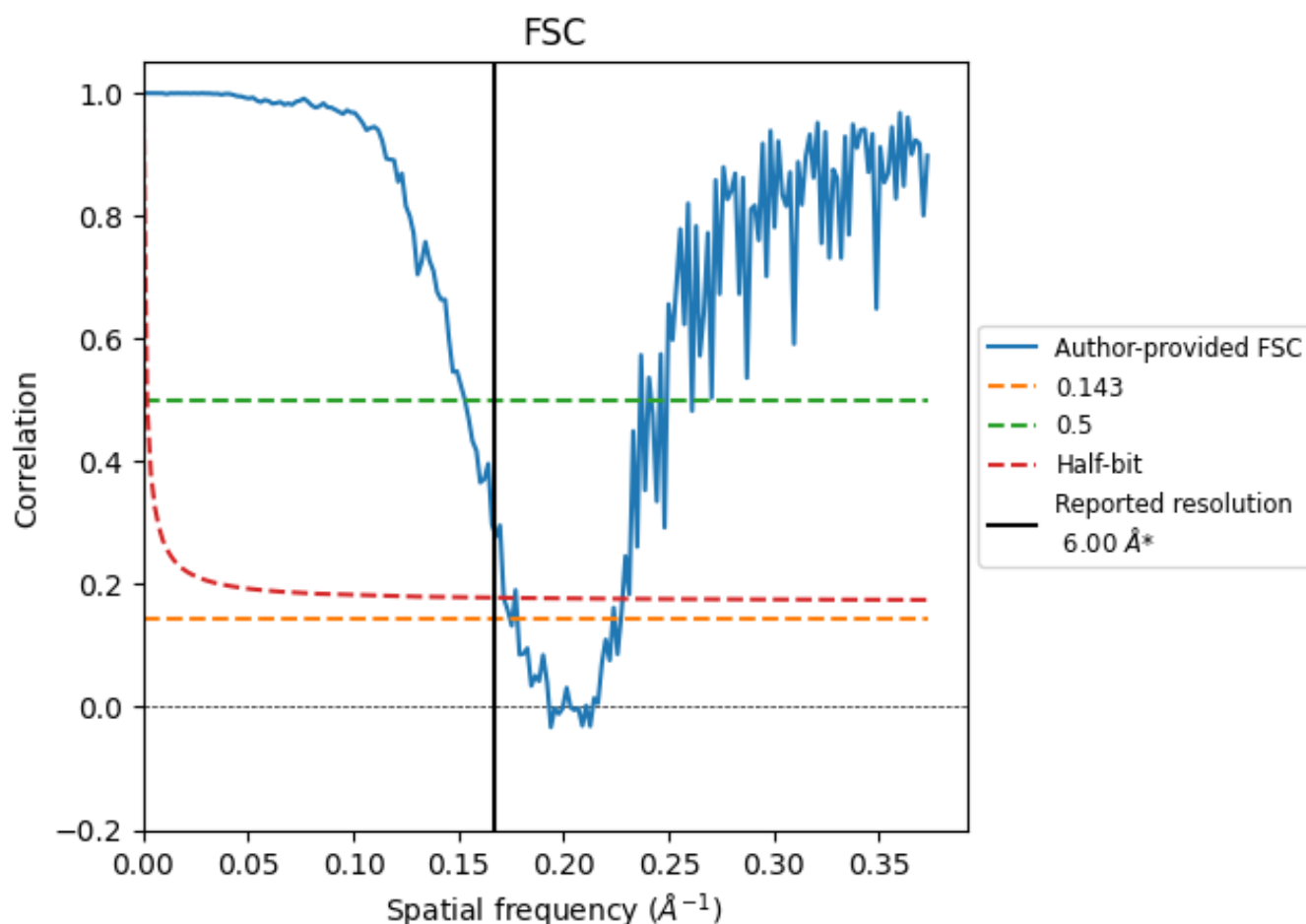


*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

8.2 Resolution estimates [i](#)

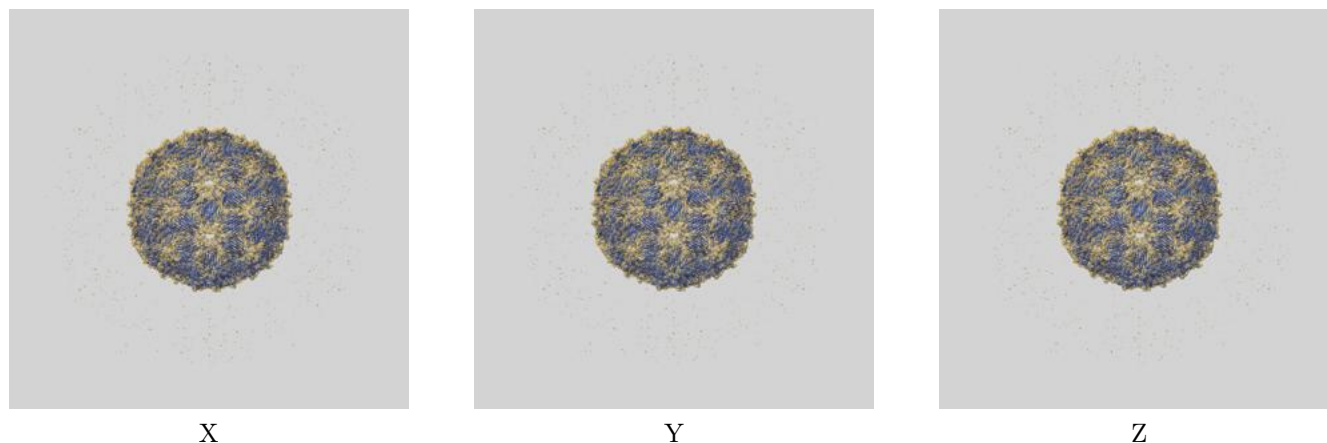
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	5.73	6.53	5.83
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

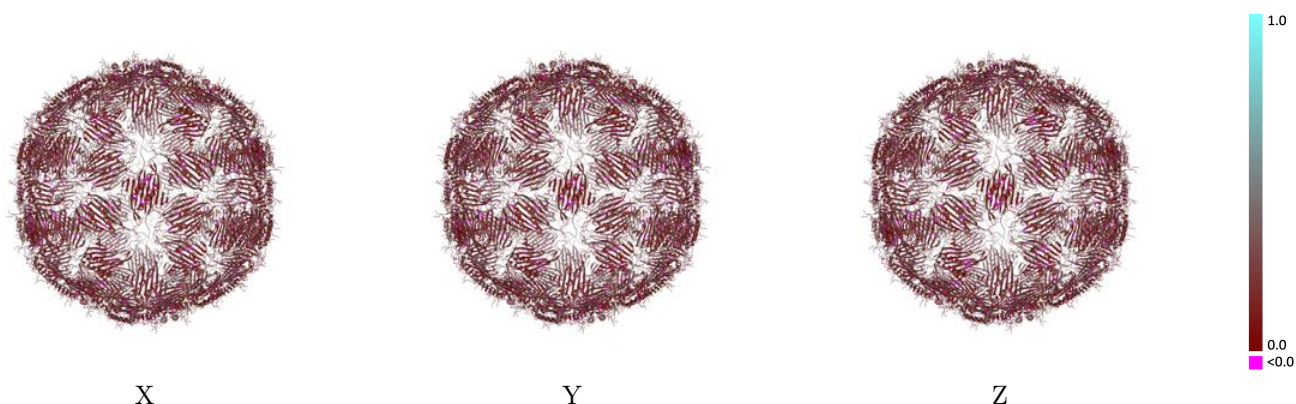
This section contains information regarding the fit between EMDB map EMD-4098 and PDB model 5LQP. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



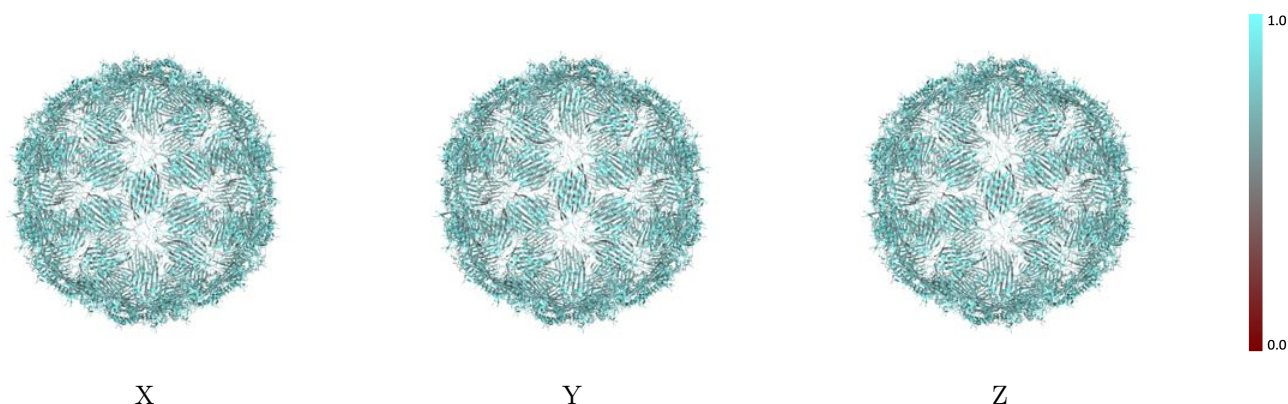
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



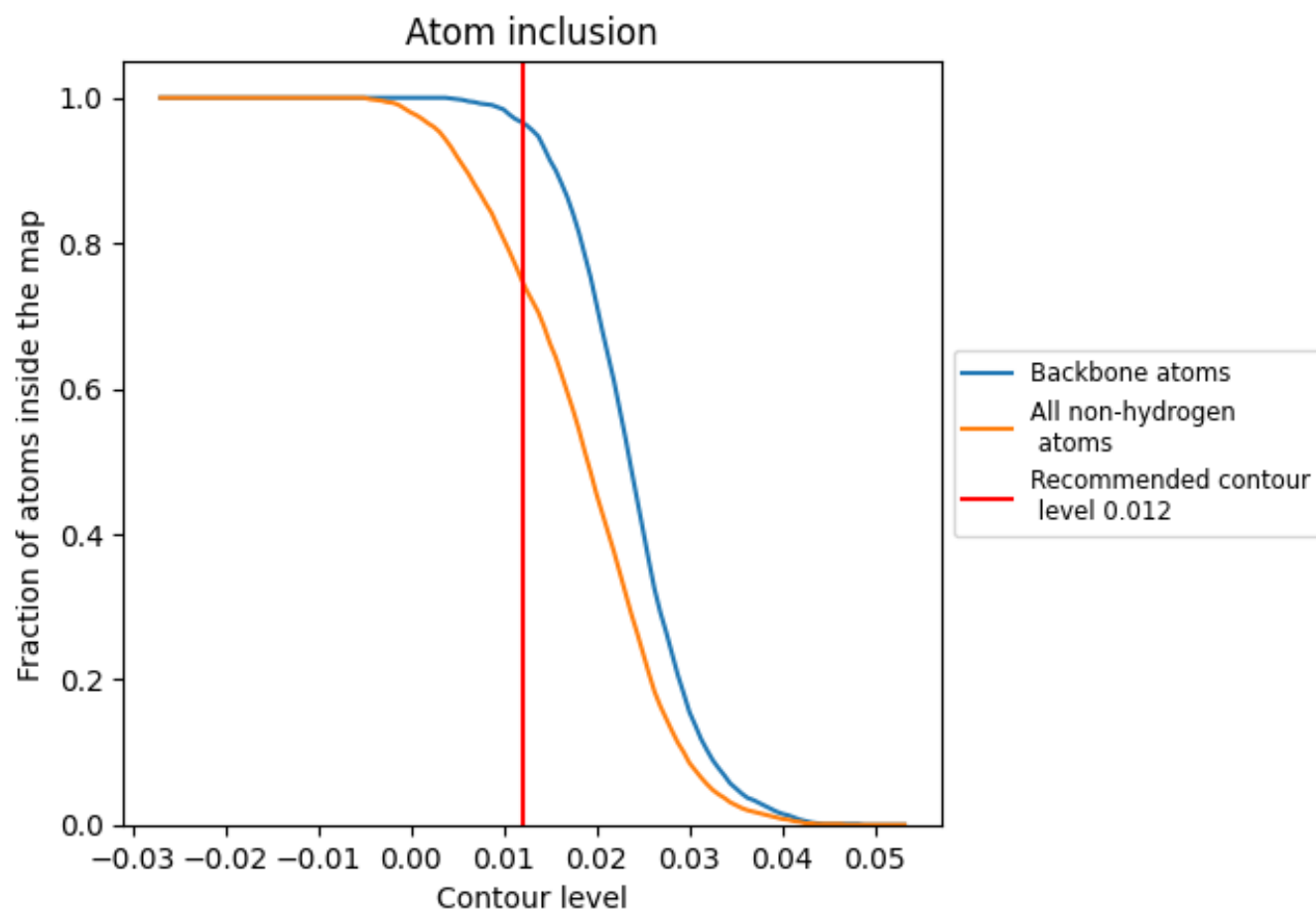
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 75% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7480	 0.2220
AB	 0.7590	 0.2400
AC	 0.7430	 0.2240
AD	 0.7440	 0.2020
AE	 0.7620	 0.2430
AF	 0.7400	 0.2190
AG	 0.7440	 0.2040
AH	 0.7620	 0.2430
AI	 0.7400	 0.2260
AJ	 0.7440	 0.2010
AK	 0.7590	 0.2380
AL	 0.7420	 0.2220
AM	 0.7440	 0.2000
AN	 0.7590	 0.2430
AO	 0.7420	 0.2240
AP	 0.7440	 0.2010
AQ	 0.7580	 0.2430
AR	 0.7470	 0.2210
AS	 0.7430	 0.2080
AT	 0.7620	 0.2430
AU	 0.7400	 0.2220
AV	 0.7440	 0.2010
AW	 0.7580	 0.2410
AX	 0.7430	 0.2220
AY	 0.7440	 0.2030
AZ	 0.7590	 0.2420
BA	 0.7430	 0.2220
BB	 0.7440	 0.2040
BC	 0.7620	 0.2390
BD	 0.7380	 0.2210
BE	 0.7440	 0.2020
BF	 0.7580	 0.2450
BG	 0.7450	 0.2240
BH	 0.7430	 0.2020
BI	 0.7620	 0.2430



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BJ	 0.7400	 0.2230
BK	 0.7440	 0.2030
BL	 0.7590	 0.2440
BM	 0.7420	 0.2200
BN	 0.7440	 0.2010
BO	 0.7620	 0.2470
BP	 0.7400	 0.2240
BQ	 0.7440	 0.2010
BR	 0.7580	 0.2410
BS	 0.7470	 0.2190
BT	 0.7430	 0.2050
BU	 0.7590	 0.2400
BV	 0.7420	 0.2190
BW	 0.7450	 0.2030
BX	 0.7620	 0.2410
BY	 0.7380	 0.2170
BZ	 0.7440	 0.2010
CA	 0.7590	 0.2460
CB	 0.7430	 0.2230
CC	 0.7440	 0.2010
CD	 0.7580	 0.2430
CE	 0.7450	 0.2210
CF	 0.7430	 0.2010
CG	 0.7590	 0.2400
CH	 0.7430	 0.2230
CI	 0.7440	 0.1990
CJ	 0.7620	 0.2450
CK	 0.7400	 0.2210
CL	 0.7440	 0.2040
CM	 0.7580	 0.2420
CN	 0.7470	 0.2220
CO	 0.7430	 0.2010
CP	 0.7590	 0.2430
CQ	 0.7430	 0.2220
CR	 0.7440	 0.2050
CS	 0.7620	 0.2420
CT	 0.7400	 0.2200
CU	 0.7440	 0.2010
CV	 0.7620	 0.2450
CW	 0.7380	 0.2200
CX	 0.7440	 0.2020
CY	 0.7580	 0.2430

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
CZ	 0.7470	 0.2220
DA	 0.7430	 0.2010
DB	 0.7590	 0.2410
DC	 0.7430	 0.2230
DD	 0.7440	 0.2020
DE	 0.7620	 0.2440
DF	 0.7380	 0.2230
DG	 0.7440	 0.1970
DH	 0.7620	 0.2430
DI	 0.7400	 0.2210
DJ	 0.7440	 0.2050
DK	 0.7590	 0.2420
DL	 0.7430	 0.2210
DM	 0.7440	 0.2040
DN	 0.7580	 0.2360
DO	 0.7430	 0.2210
DP	 0.7440	 0.2030
DQ	 0.7620	 0.2450
DR	 0.7400	 0.2210
DS	 0.7440	 0.2050
DT	 0.7620	 0.2450
DU	 0.7380	 0.2200
DV	 0.7440	 0.2000
DW	 0.7590	 0.2400
DX	 0.7430	 0.2230
DY	 0.7440	 0.2010
DZ	 0.7580	 0.2440
EA	 0.7470	 0.2240
EB	 0.7430	 0.2010
EC	 0.7590	 0.2400
ED	 0.7420	 0.2220
EE	 0.7450	 0.2080
EF	 0.7620	 0.2420
EG	 0.7400	 0.2220
EH	 0.7440	 0.2020
EI	 0.7590	 0.2390
EJ	 0.7430	 0.2220
EK	 0.7440	 0.2030
EL	 0.7580	 0.2440
EM	 0.7470	 0.2240
EN	 0.7430	 0.2000
EO	 0.7620	 0.2410

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
EP	 0.7400	 0.2200
EQ	 0.7440	 0.2070
ER	 0.7590	 0.2440
ES	 0.7430	 0.2250
ET	 0.7440	 0.2030
EU	 0.7620	 0.2420
EV	 0.7380	 0.2210
EW	 0.7440	 0.2010
EX	 0.7580	 0.2460
EY	 0.7470	 0.2220
EZ	 0.7430	 0.2010
FA	 0.7620	 0.2440
FB	 0.7380	 0.2230
FC	 0.7440	 0.1990
FD	 0.7590	 0.2390
FE	 0.7420	 0.2200
FF	 0.7450	 0.2070
FG	 0.7580	 0.2420
FH	 0.7470	 0.2210
FI	 0.7430	 0.2030
FJ	 0.7620	 0.2420
FK	 0.7400	 0.2220
FL	 0.7440	 0.2050
FM	 0.7590	 0.2420
FN	 0.7420	 0.2250
FO	 0.7440	 0.1980
FP	 0.7590	 0.2410
FQ	 0.7430	 0.2200
FR	 0.7440	 0.2010
FS	 0.7580	 0.2430
FT	 0.7450	 0.2210
FU	 0.7430	 0.2000
FV	 0.7620	 0.2430
FW	 0.7380	 0.2210
FX	 0.7440	 0.2040
FY	 0.7590	 0.2410
FZ	 0.7430	 0.2200
GA	 0.7440	 0.1980
GB	 0.7580	 0.2420
GC	 0.7430	 0.2220
GD	 0.7440	 0.2070
GE	 0.7620	 0.2410

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
GF	 0.7380	 0.2240
GG	 0.7440	 0.2010
GH	 0.7620	 0.2410
GI	 0.7400	 0.2230
GJ	 0.7440	 0.2040
GK	 0.7590	 0.2440
GL	 0.7420	 0.2230
GM	 0.7440	 0.2040
GN	 0.7590	 0.2390
GO	 0.7420	 0.2230
GP	 0.7440	 0.1970
GQ	 0.7620	 0.2410
GR	 0.7400	 0.2230
GS	 0.7440	 0.2000
GT	 0.7620	 0.2410
GU	 0.7400	 0.2210
GV	 0.7440	 0.2030
GW	 0.7580	 0.2440
GX	 0.7470	 0.2240
GY	 0.7430	 0.2070