



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 02:27 PM JST

PDB ID : 9K2V / pdb_00009k2v
EMDB ID : EMD-61998
Title : Cyanophage A4 pre-ejectosome
Authors : Hou, P.; Li, Q.; Zhou, C.Z.
Deposited on : 2024-10-18
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

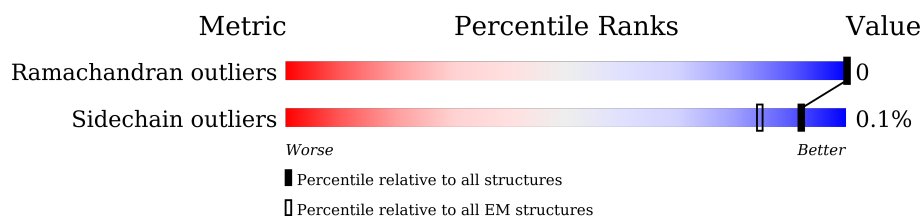
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


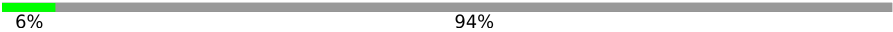
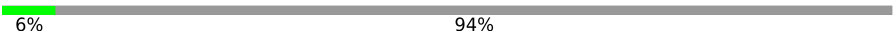
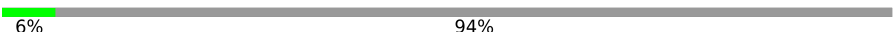
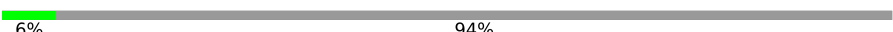
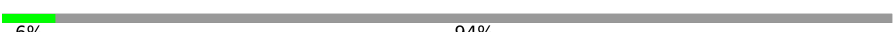



The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



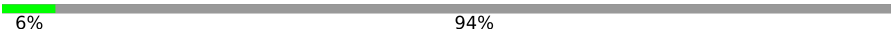













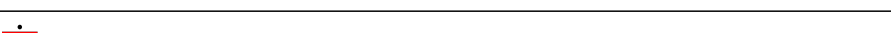
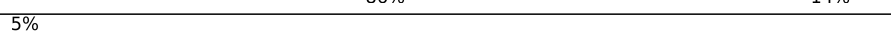





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	F	653	 6% 94%
1	G	653	 6% 94%
1	H	653	 6% 94%
1	I	653	 6% 94%
1	J	653	 6% 94%
1	K	653	 6% 94%
1	L	653	 6% 94%
1	M	653	 6% 94%
1	N	653	 6% 94%

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Mol	Chain	Length	Quality of chain
1	O	653	 6% 94%
2	V	380	 24% 76%
2	W	380	 24% 76%
2	X	380	 24% 76%
2	Y	380	 24% 76%
2	Z	380	 24% 76%
2	v	380	 24% 76%
2	w	380	 24% 76%
2	x	380	 24% 76%
2	y	380	 24% 76%
2	z	380	 24% 76%
3	A	1058	 5% 86% 14%
3	B	1058	 5% 85% 14%
3	C	1058	 5% 86% 14%
3	D	1058	 5% 86% 14%
3	E	1058	 5% 86% 14%
3	a	1058	 44% 56%
3	b	1058	 43% 56%
3	c	1058	 43% 56%
3	d	1058	 43% 56%
3	e	1058	 44% 56%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 63405 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 Portal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	K	40	Total	C	N	O	0	0
			290	178	50	62		
1	M	40	Total	C	N	O	0	0
			290	178	50	62		
1	O	40	Total	C	N	O	0	0
			290	178	50	62		
1	G	40	Total	C	N	O	0	0
			290	178	50	62		
1	I	40	Total	C	N	O	0	0
			290	178	50	62		
1	F	40	Total	C	N	O	0	0
			290	178	50	62		
1	H	40	Total	C	N	O	0	0
			290	178	50	62		
1	J	40	Total	C	N	O	0	0
			290	178	50	62		
1	L	40	Total	C	N	O	0	0
			290	178	50	62		
1	N	40	Total	C	N	O	0	0
			290	178	50	62		

- Molecule 2 is a protein called Internal virion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	92	Total 706	C 422	N 138	O 142	S 4	0	0
2	W	92	Total 706	C 422	N 138	O 142	S 4	0	0
2	X	92	Total 706	C 422	N 138	O 142	S 4	0	0
2	Y	92	Total 706	C 422	N 138	O 142	S 4	0	0
2	Z	92	Total 706	C 422	N 138	O 142	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	v	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	w	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	x	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	y	92	Total	C	N	O	S	0	0
			706	422	138	142	4		
2	z	92	Total	C	N	O	S	0	0
			706	422	138	142	4		

- Molecule 3 is a protein called Internal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	907	Total	C	N	O	S	0	0
			7028	4342	1304	1361	21		
3	d	462	Total	C	N	O	S	0	0
			3660	2236	682	732	10		
3	A	907	Total	C	N	O	S	0	0
			7028	4342	1304	1361	21		
3	e	462	Total	C	N	O	S	0	0
			3660	2236	682	732	10		
3	B	907	Total	C	N	O	S	0	0
			7028	4342	1304	1361	21		
3	a	462	Total	C	N	O	S	0	0
			3660	2236	682	732	10		
3	C	907	Total	C	N	O	S	0	0
			7028	4342	1304	1361	21		
3	b	462	Total	C	N	O	S	0	0
			3660	2236	682	732	10		
3	D	907	Total	C	N	O	S	0	0
			7028	4342	1304	1361	21		
3	c	462	Total	C	N	O	S	0	0
			3660	2236	682	732	10		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	E	1	Total	Zn	0
			1	1	
4	A	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Zn 1	0
4	C	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0



GLU	PRO	GLN	THR	GLY	GLN	ALA	PRO	ASP	GLU	Q612	T613	A651	ASP	GLN	TYR	VAL	ARG	GLN	ARG	LEU	GLY	ARG	MET	VAL	ASP	PHE	ILE	ALA	PHE	GLN	SER	GLN	ILE	PRO	GLN	GLU	ALA	GLY	GLU	MET	GLU	ALA	GLY	ASN	LEU	ARG	ILE	MET	PRO	THR	VAL	PHE	GLN	ALA	SER	THR	VAL	ARG	TYR	VAL	ASP	MET	GLN	ARG	ILE	MET																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																

● Molecule 1: Portal protein

Chain G: 6% 94%

GLU	PRO	GLN	THR	GLY	GLN	ALA	PRO	PRO	ASP	GLU	Q612	T613	A651	ASP	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
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● Molecule 1: Portal protein

Chain I: 6% 94%

MET	ILE	ARG	ILE	LYS	ASP	PHE	ASN	HIS	VAL	THR	ILE	GLY	GLY	GLU	GLU	GLU	PRO	ASP	LEU	ASP	ASP	ILE	ASN	GLU	GLU	THR	THR	ILE	ALA	ALA	GLY	TYR	TYR	ILE	ILE	THR	THR	THR	ARG	ARG	ALA	ALA	GLU	GLU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
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[illegible]



PHE ALA GLY LEU LEU SER SER GLY VAL ASN ASN ALA PHE ASN THR TYR GLN GLN VAL LEU GLY GLN GLN ASN ASN LEU ASN GLN GLN GLN LYS MET GLN THR TYR LEU LEU ASN SER SER LEU LEU SER ASN ASN GLY ALA THR THR ASN ASN PHE LYS GLY TYR ASN

- Molecule 2: Internal virion protein



SER	GLN	GLN	LEU	THR	GLY	ALA	GLU	ASP	ALA	THR	LYS	GLU	LEU	GLN	ARG	LEU	ASP	THR	ARG	ASP	VAL	LEU	ALA	ALA	MET	ALA	SER	GLY	VAL	GLY	LEU	GLY	SER	SER	THR	SER	SER	GLN	GLN	GLN	ASN	ALA	ASP	LEU	LEU	GLY	THR	ILE	ASP	LYS	VAL	LYS	VAL	LEU	GLN	GLY	THR	THR
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VAL	GLY	MET	GLU	VAL	GLN	GLN	ARG	MET	THR	GLU	LEU	ALA	SER	ALA	SER	ASN	GLY	TYR	SER	LEU	GLU	GLU	ARG	ASN	LYS	LEU	SER	LEU	GLY	ASP	ASP	PHE	MET	ASN	ASN	ALA	ASN	ILE	GLN	ALA	ALA	SER	ALA	THR	THR	ASN	GLN	ASN	VAL	ASP	SER	THR	MET	GLY	VAL	ASN
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ALA	ALA	ALA	ALA	ARG	GLU	THR	VAL	ALA	ASN	ALA	ALA	ASP	MET	MET	ASN	ARG	GLN	THR	THR	THR	VAL	ASN	ASN	ASP	ASP	LEU	ALA	ALA	GLU	MET	GLY	TYR	GLN	VAL	GLN	GLN	THR	SER	ALA	ALA	ASN	ASN	ASN	ASN	SER	SER	GLY	ILE	ILE	ALA	ALA	GLN	TYR	GLY	SER	SER	ILE	GLY	GLY
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ASN	THR	PHE	ALA	GLY	LEU	SER	SER	GLY	VAL	ASN	ALA	PHE	ASN	THR	THR	GLN	GLY	VAL	LEU	GLY	GLN	ASN	ALA	ALA	LEU	ASN	ASN	GLN	GLN	GLN	LYS	GLN	GLN	THR	THR	TYR	LEU	ASN	ASN	SER	GLY	ILE	LEU	SER	ASN	GLY	ALA	ALA	ASN	ASN	THR	PHE	LYS	GLY	TYR
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- Molecule 2: Internal virion protein



M1	E87	Q88	M89	D90	A91	E92	THR	THR	LYS	GLN	GLN	ALA	ALA	GLU	GLN	GLN	ARG	ARG	LEU	GLN	THR	MET	SER	GLY	ILE	GLU	GLN	LYS	ASP	ARG	ASP	GLN	THR	GLU	GLN	GLN	MET	VAL	GLY	ALA	GLU	VAL	ASN	ASN	PHE	GLN	GLN	THR	LEU	GLN	GLN	LEU	ALA	GLN	GLN	LEU	VAL	VAL	ASN	ALA
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SER	GLN	GLN	LEU	THR	GLY	ALA	GLU	ASP	THR	ALA	LYS	GLU	GLY	GLN	ARG	LEU	ASP	THR	ARG	ASP	VAL	LEU	ALA	MET	ALA	ALA	GLY	VAL	GLY	LEU	GLY	SER	SER	THR	SER	SER	GLN	GLN	ASN	ALA	ASP	LEU	LEU	GLY	THR	THR	ILE	ASP	LYS	VAL	ALA	LYS	VAL	LEU	GLN	THR	GLY	THR
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M E T
G L U
V A L
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ASN	ALA	ALA	ALA	ALA	ARG	GLU	THR	ALA	ASN	ASN	VAL	ASN	ASN	ILE	ALA	ASN	ALA	ALA	ALA	ASP	ASP	ASP	ASP	LEU	GLU	GLY	GLY	GLN	GLN	VAL	GLN	THR	SER	SER	SER	ALA	ALA	ALA	VAL	VAL	ASN	ASN	ASN	ALA	ASN	MET	SER	GLY	ILE	ILE	ALA	ALA	GLN	TYR	GLY	SER	GLY	ILE	ILE	TYR
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GLY	ASN	THR	PHE	ALA	ALA	LEU	LEU	SER	SER	GLY	VAL	ASN	ALA	PHE	ASN	THR	TYR	GLN	GLN	GLY	VAL	LEU	GLY	GLN	GLN	ALA	LEU	ASN	GLN	GLN	LYS	GLN	GLN	MET	THR	TYR	LEU	ASN	SER	SER	GLY	ILE	LEU	SER	ASN	GLY	ALA	THR	ASN	ASN	ASN	THR	PHE	LYS	GLY	TYR
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- Molecule 2: Internal virion protein



 M1
 E87
 Q88
 M89
 E92
 THR THR LYS GLN GLN GLN GLN ALA ALA GLU GLN GLN GLN ARG ARG LEU LEU GLN THR MET MET SER SER GLY GLY ILE ILE GLU GLU GLN LYS ASP ASP ARG ARG GLN GLN THR THR GLU GLU GLN GLN MET MET MET VAL VAL GLY GLY ALA ALA GLU GLU VAL VAL ASN ASN PHE PHE GLN GLN GLN THR THR LEU LEU GLN GLN LEU LEU ALA ALA GLN GLN LEU LEU GLY GLY VAL VAL VAL VAL ASN ASN ALA ALA GLN GLN THR THR

[illegible]

ASN	THR	PHE	GLY	LEU	LEU	SER	SER	GLY	VAL	ASN	ASN	ALA	PHE	ASN	THR	TYR	GLN	GLY	VAL	LEU	LEU	GLN	GLN	ASN	ALA	LEU	ASN	ASN	GLN	GLN	LYS	GLN	GLN	THR	THR	TYR	LEU	ASN	GLY	ILE	SER	ASN	GLY	ALA	THR	ASN	ASN	THR	PHE	LYS	GLY	TYR	ASN
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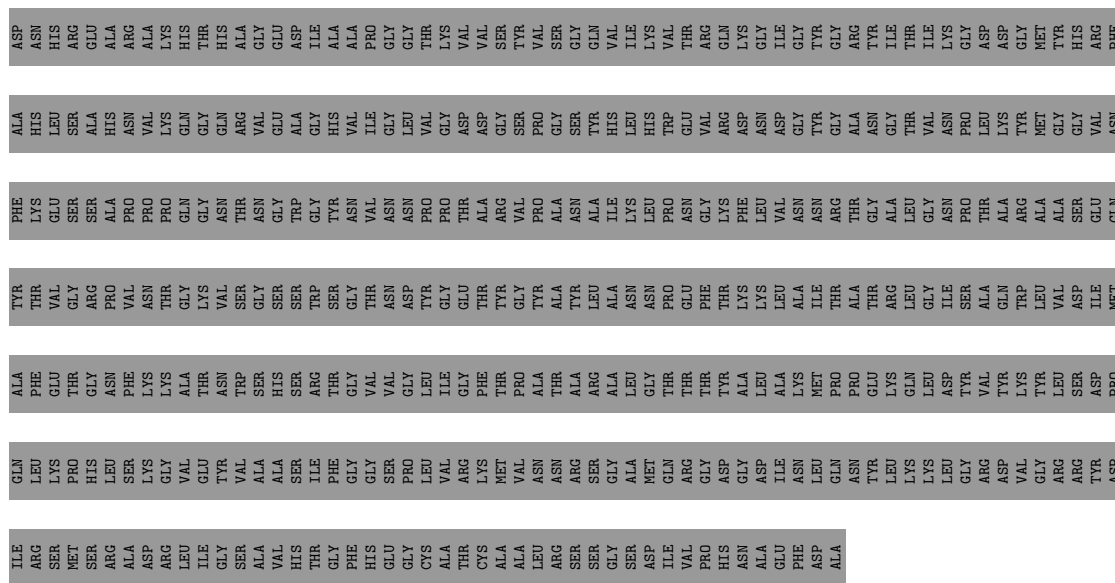
Chain x: 24% 76%

ASN	THR	PHE	ALA	GLY	LEU	LEU	SER	SER	GLY	VAL	ASN	ALA	ASN	PHE	ASN	THR	THR	GLN	GLY	VAL	LEU	GLY	GLN	GLN	ASN	ASN	ALA	LEU	ALA	ASN	ASN	GLN	GLN	LYS	GLN	GLN	THR	THR	THR	TYR	LEU	ASN	SER	GLY	ILE	LEU	LEU	SER	ASN	ASN	ASN	THR	THR	PHE	LYS	GLY	TYR	ASN
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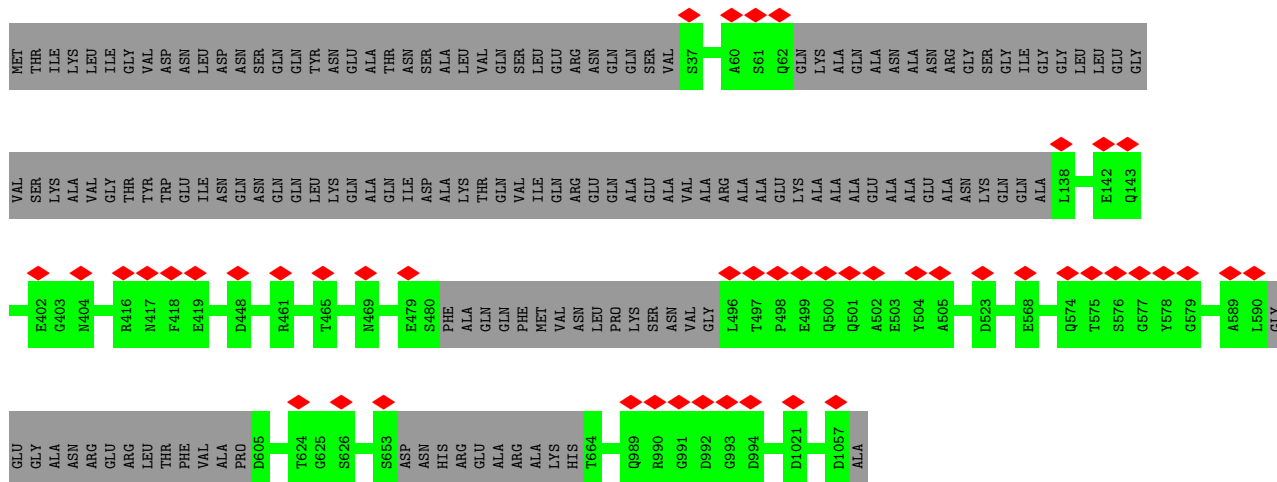
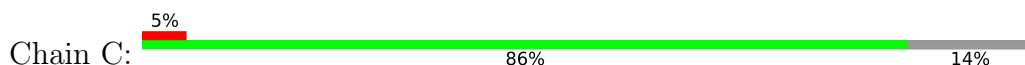
Chain γ : 

	GLY	ASN	THR	THR	PHE	ALA	GLY	LEU	LEU	SER	VAL	ASN	ALA	ASN	THR	THR	TYR	GLN	GLY	GLY	VAL	LEU	LEU	GLY	GLN	GLN	GLN	LYS	LYS	MET	THR	THR	TYR	LEU	ASN	ASN	ASN	GLY	ILE	LEU	SER	ASN	ASN	THR	THR	THR	THR	THR	GLY	GLY	ALA	ALA	ASN	ASN	LYS	GLY	TYR	ASN
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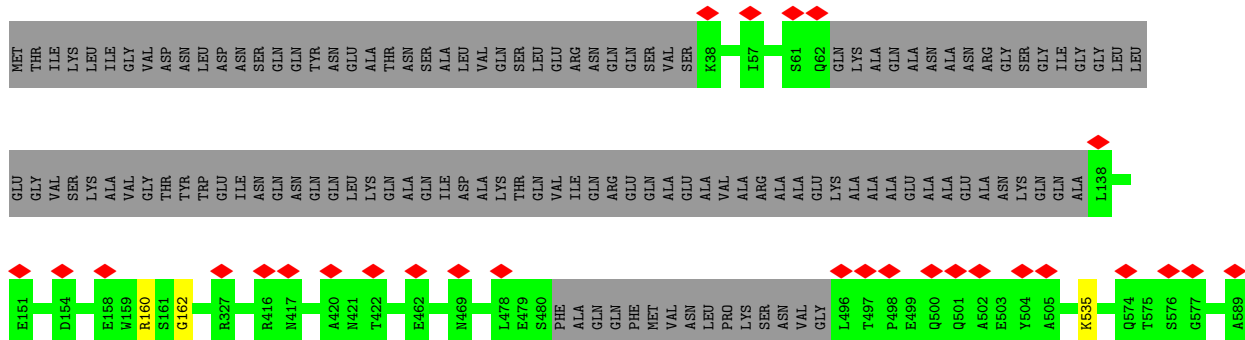
Chain z:  24% 76%



- Molecule 3: Internal protein



- Molecule 3: Internal protein



[illegible]

- Molecule 3: Internal protein

Chain D: 86% 14%

The diagram illustrates the mapping of amino acid sequences to a 3D protein structure. It is divided into two main horizontal sections. The top section shows a sequence of amino acids (MET, THR, ILE, LEU, LYS, LEU, ILE, GLY, VAL, ASP, ASN, LEU, ASP, ASN, SER, GLN, GLN, TYR, ASN, GLU, ALA, THR, ASN, SER, ALA, LEU, VAL, GLN, SER, LEU, GLU, ARG, ASN, GLN, GLN, SER, VAL) with corresponding 3D models of the protein structure. The bottom section shows a sequence of amino acids (LEU, GLU, GLY, VAL, SER, LYS, ALA, VAL, GLY, THR, TRP, GLU, ILE, ASN, ASN, GLN, GLN, LEU, LYS, GLN, ALA, GLN, ALA, ILE, ASP, ASP, ALA, LYS, THR, GLN, VAL, ILE, GLN, ARG, GLU, GLN, ALA, ALA, ARG, VAL, ASN, LYS, LEU, PRO, LYS, SER, ASN, VAL, GLY, L496, T497, P498, E499, Q500, Q501, A502, E503, Y504, A505, D523, Q527, E568, Q574, T576, S576, G577, N578) with corresponding 3D models of the protein structure. The diagram uses color coding to highlight specific regions and amino acids.

- Molecule 3: Internal protein

Chain c: 43% 56%

[illegible]

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	Depositor
Map size (\AA)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	F	0.25	0/293	0.43	0/400
1	G	0.25	0/293	0.44	0/400
1	H	0.24	0/293	0.43	0/400
1	I	0.25	0/293	0.44	0/400
1	J	0.24	0/293	0.44	0/400
1	K	0.24	0/293	0.44	0/400
1	L	0.24	0/293	0.43	0/400
1	M	0.25	0/293	0.43	0/400
1	N	0.24	0/293	0.43	0/400
1	O	0.25	0/293	0.42	0/400
2	V	0.24	0/708	0.48	0/949
2	W	0.24	0/708	0.48	0/949
2	X	0.25	0/708	0.47	0/949
2	Y	0.24	0/708	0.48	0/949
2	Z	0.24	0/708	0.49	0/949
2	v	0.26	0/708	0.47	0/949
2	w	0.27	0/708	0.50	0/949
2	x	0.26	0/708	0.48	0/949
2	y	0.26	0/708	0.46	0/949
2	z	0.26	0/708	0.50	0/949
3	A	0.25	0/7146	0.50	3/9662 (0.0%)
3	B	0.25	0/7146	0.51	4/9662 (0.0%)
3	C	0.25	0/7146	0.49	0/9662
3	D	0.25	0/7146	0.49	0/9662
3	E	0.25	0/7146	0.51	3/9662 (0.0%)
3	a	0.26	0/3701	0.49	0/4993
3	b	0.26	0/3701	0.51	1/4993 (0.0%)
3	c	0.26	0/3701	0.59	4/4993 (0.1%)
3	d	0.26	0/3701	0.48	0/4993
3	e	0.26	0/3701	0.50	0/4993
All	All	0.25	0/64245	0.50	15/86765 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	a	0	1
3	b	0	1
3	c	0	1
3	d	0	1
3	e	0	1
All	All	0	5

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	162	GLY	N-CA-C	-15.49	74.37	113.10
3	c	161	SER	CB-CA-C	12.46	133.76	110.10
3	A	579	GLY	N-CA-C	-9.90	88.35	113.10
3	B	579	GLY	N-CA-C	-9.38	89.64	113.10
3	E	579	GLY	N-CA-C	-9.35	89.73	113.10
3	c	139	THR	N-CA-CB	8.13	125.76	110.30
3	b	162	GLY	N-CA-C	-8.05	92.97	113.10
3	c	138	LEU	CB-CA-C	-6.86	97.17	110.20
3	A	580	GLN	N-CA-CB	6.41	122.13	110.60
3	E	580	GLN	N-CA-CB	5.75	120.95	110.60
3	B	580	GLN	N-CA-CB	5.72	120.90	110.60
3	A	580	GLN	N-CA-C	-5.65	95.75	111.00
3	B	580	GLN	N-CA-C	-5.34	96.58	111.00
3	E	580	GLN	N-CA-C	-5.33	96.62	111.00
3	B	633	PRO	CA-N-CD	-5.24	104.17	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	a	160	ARG	Sidechain
3	b	160	ARG	Sidechain
3	c	160	ARG	Sidechain
3	d	160	ARG	Sidechain
3	e	160	ARG	Sidechain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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	F	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	G	38/653 (6%)	37 (97%)	1 (3%)	0	100	100
1	H	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	I	38/653 (6%)	37 (97%)	1 (3%)	0	100	100
1	J	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	K	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	L	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	M	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	N	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
1	O	38/653 (6%)	36 (95%)	2 (5%)	0	100	100
2	V	90/380 (24%)	90 (100%)	0	0	100	100
2	W	90/380 (24%)	90 (100%)	0	0	100	100
2	X	90/380 (24%)	90 (100%)	0	0	100	100
2	Y	90/380 (24%)	90 (100%)	0	0	100	100
2	Z	90/380 (24%)	90 (100%)	0	0	100	100
2	v	90/380 (24%)	90 (100%)	0	0	100	100
2	w	90/380 (24%)	90 (100%)	0	0	100	100
2	x	90/380 (24%)	90 (100%)	0	0	100	100
2	y	90/380 (24%)	90 (100%)	0	0	100	100
2	z	90/380 (24%)	90 (100%)	0	0	100	100
3	A	897/1058 (85%)	873 (97%)	24 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	897/1058 (85%)	870 (97%)	27 (3%)	0	100	100
3	C	897/1058 (85%)	869 (97%)	28 (3%)	0	100	100
3	D	897/1058 (85%)	869 (97%)	28 (3%)	0	100	100
3	E	897/1058 (85%)	868 (97%)	29 (3%)	0	100	100
3	a	456/1058 (43%)	451 (99%)	5 (1%)	0	100	100
3	b	456/1058 (43%)	452 (99%)	4 (1%)	0	100	100
3	c	456/1058 (43%)	451 (99%)	5 (1%)	0	100	100
3	d	456/1058 (43%)	449 (98%)	7 (2%)	0	100	100
3	e	456/1058 (43%)	451 (99%)	5 (1%)	0	100	100
All	All	8045/20910 (38%)	7865 (98%)	180 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	F	30/572 (5%)	30 (100%)	0	100	100
1	G	30/572 (5%)	30 (100%)	0	100	100
1	H	30/572 (5%)	30 (100%)	0	100	100
1	I	30/572 (5%)	30 (100%)	0	100	100
1	J	30/572 (5%)	30 (100%)	0	100	100
1	K	30/572 (5%)	30 (100%)	0	100	100
1	L	30/572 (5%)	30 (100%)	0	100	100
1	M	30/572 (5%)	30 (100%)	0	100	100
1	N	30/572 (5%)	30 (100%)	0	100	100
1	O	30/572 (5%)	30 (100%)	0	100	100
2	V	73/306 (24%)	73 (100%)	0	100	100
2	W	73/306 (24%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	73/306 (24%)	73 (100%)	0	100	100
2	Y	73/306 (24%)	73 (100%)	0	100	100
2	Z	73/306 (24%)	73 (100%)	0	100	100
2	v	73/306 (24%)	73 (100%)	0	100	100
2	w	73/306 (24%)	73 (100%)	0	100	100
2	x	73/306 (24%)	73 (100%)	0	100	100
2	y	73/306 (24%)	73 (100%)	0	100	100
2	z	73/306 (24%)	73 (100%)	0	100	100
3	A	735/850 (86%)	735 (100%)	0	100	100
3	B	735/850 (86%)	735 (100%)	0	100	100
3	C	735/850 (86%)	735 (100%)	0	100	100
3	D	735/850 (86%)	734 (100%)	1 (0%)	92	97
3	E	735/850 (86%)	735 (100%)	0	100	100
3	a	386/850 (45%)	386 (100%)	0	100	100
3	b	386/850 (45%)	385 (100%)	1 (0%)	91	95
3	c	386/850 (45%)	385 (100%)	1 (0%)	91	95
3	d	386/850 (45%)	385 (100%)	1 (0%)	91	95
3	e	386/850 (45%)	386 (100%)	0	100	100
All	All	6635/17280 (38%)	6631 (100%)	4 (0%)	92	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	d	535	LYS
3	b	535	LYS
3	D	527	GLN
3	c	140	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	625	GLN
2	V	25	GLN
2	V	61	ASN
2	W	25	GLN

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Mol	Chain	Res	Type
2	W	61	ASN
2	X	25	GLN
2	X	61	ASN
2	Y	25	GLN
2	Y	61	ASN
2	Z	25	GLN
2	Z	61	ASN
2	w	21	GLN
2	y	21	GLN
3	E	982	ASN
3	d	40	GLN
3	d	282	ASN
3	d	336	GLN
3	e	40	GLN
3	e	52	GLN
3	e	282	ASN
3	e	336	GLN
3	e	548	ASN
3	B	453	GLN
3	B	982	ASN
3	a	40	GLN
3	a	225	GLN
3	a	282	ASN
3	a	336	GLN
3	a	363	GLN
3	C	335	GLN
3	C	417	ASN
3	C	453	GLN
3	C	982	ASN
3	b	40	GLN
3	b	146	ASN
3	b	225	GLN
3	b	336	GLN
3	D	41	GLN
3	D	282	ASN
3	D	335	GLN
3	D	665	HIS
3	c	40	GLN
3	c	336	GLN
3	c	524	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

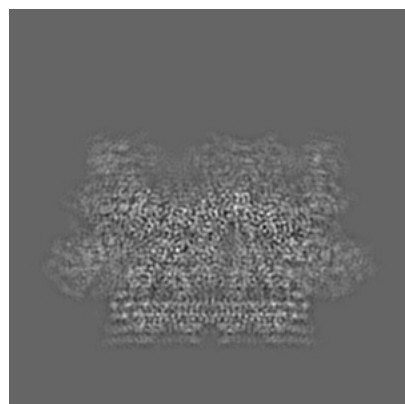
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61998. These allow visual inspection of the internal detail of the map and identification of artifacts.

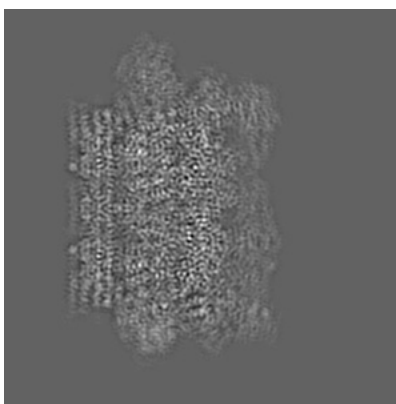
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

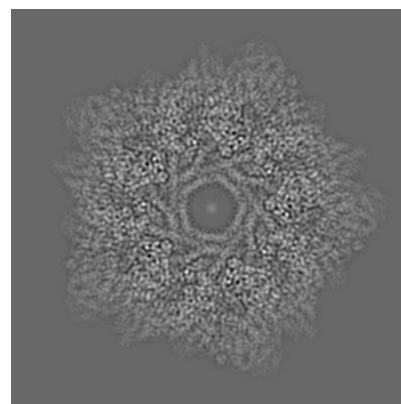
6.1.1 Primary map



X

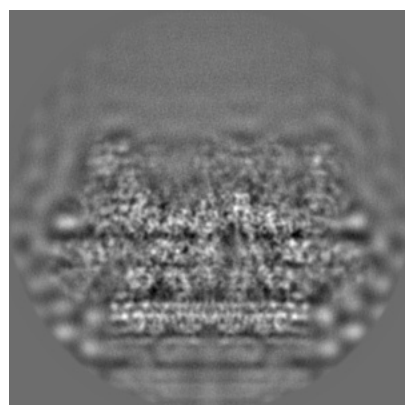


Y

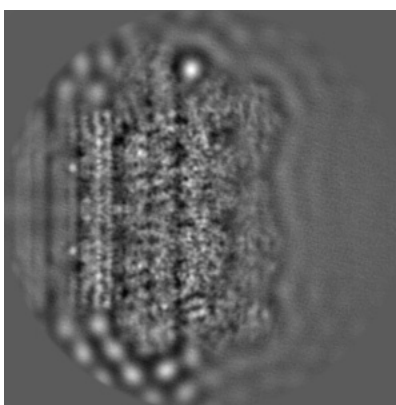


Z

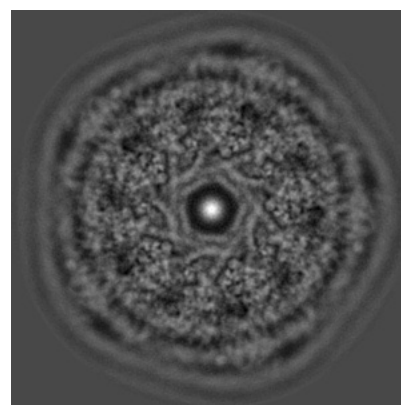
6.1.2 Raw map



X



Y

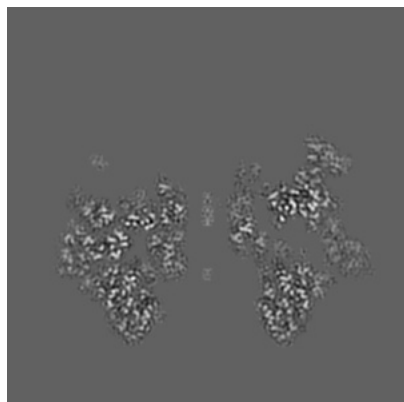


Z

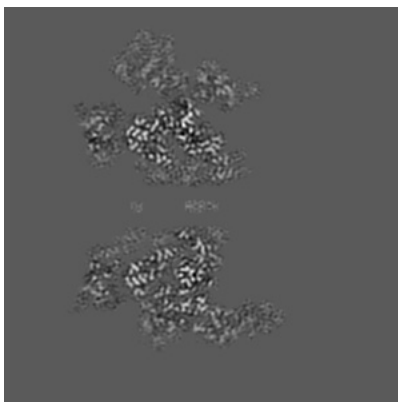
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

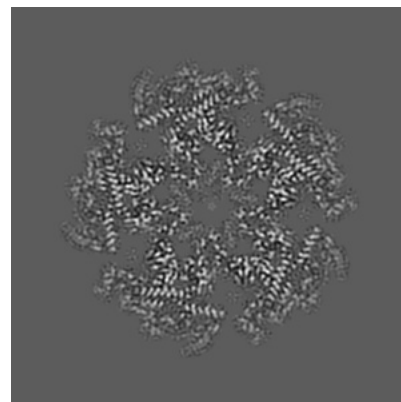
6.2.1 Primary map



X Index: 150

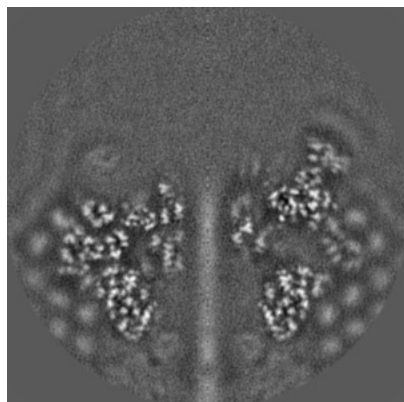


Y Index: 150

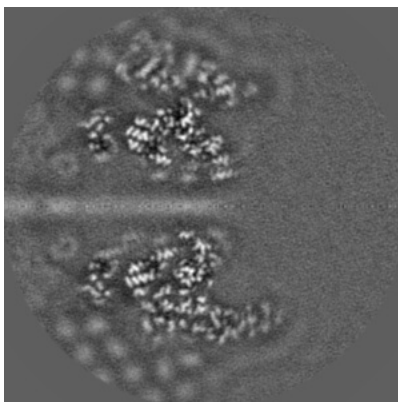


Z Index: 150

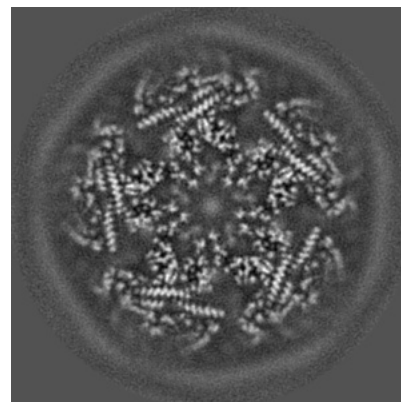
6.2.2 Raw map



X Index: 150



Y Index: 150

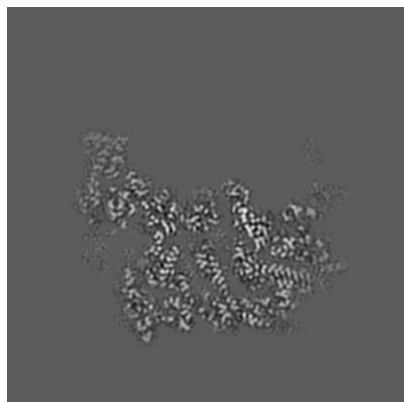


Z Index: 150

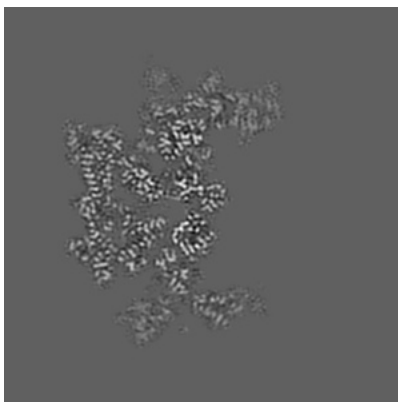
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

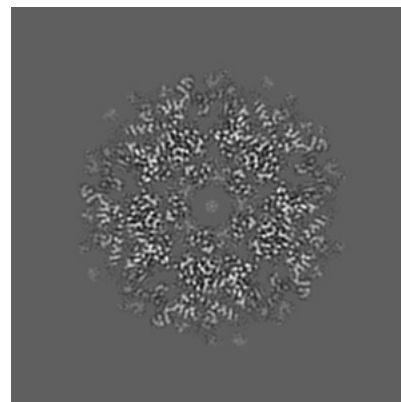
6.3.1 Primary map



X Index: 108

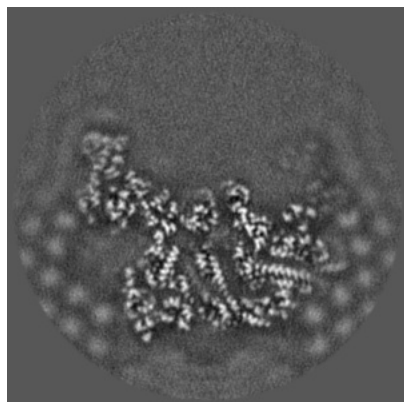


Y Index: 199

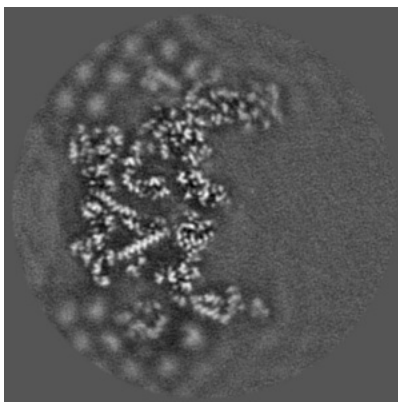


Z Index: 139

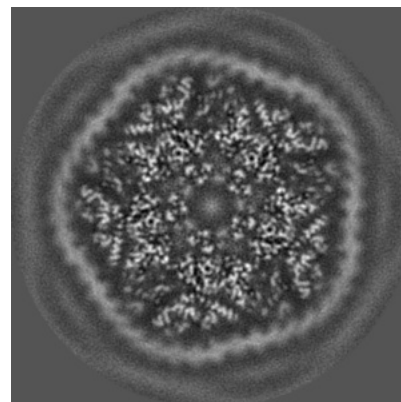
6.3.2 Raw map



X Index: 108



Y Index: 196

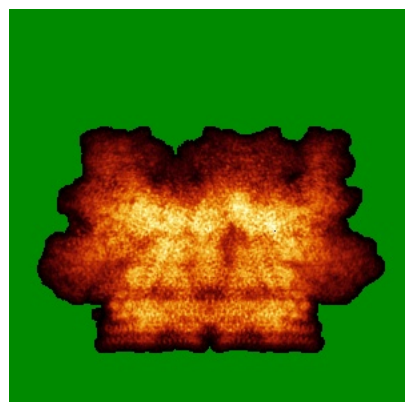


Z Index: 139

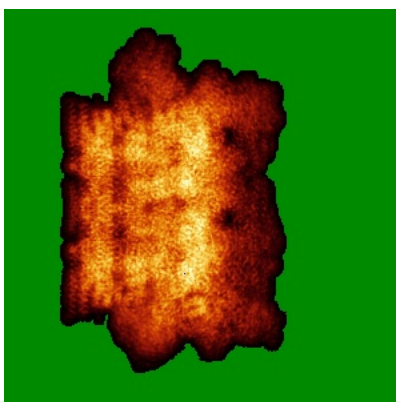
The images above show the largest variance slices of the map in three orthogonal directions.

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

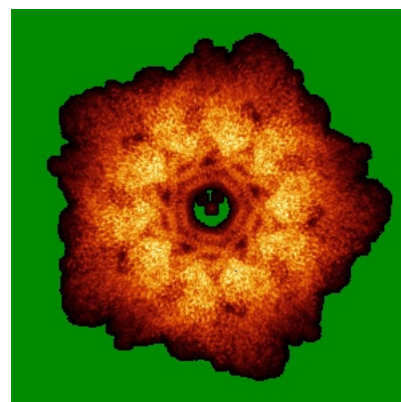
6.4.1 Primary map



X

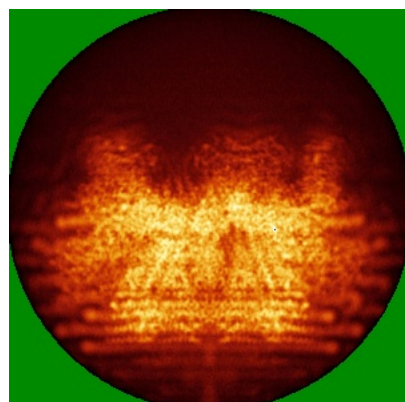


Y

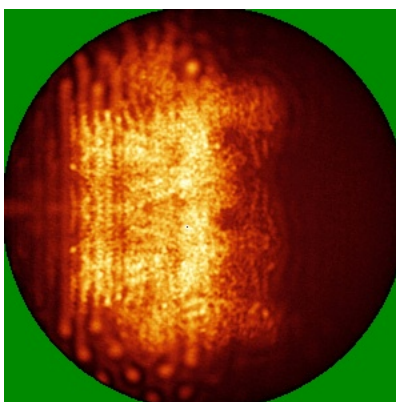


Z

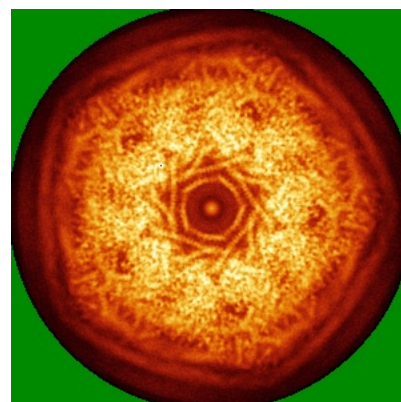
6.4.2 Raw map



X



Y

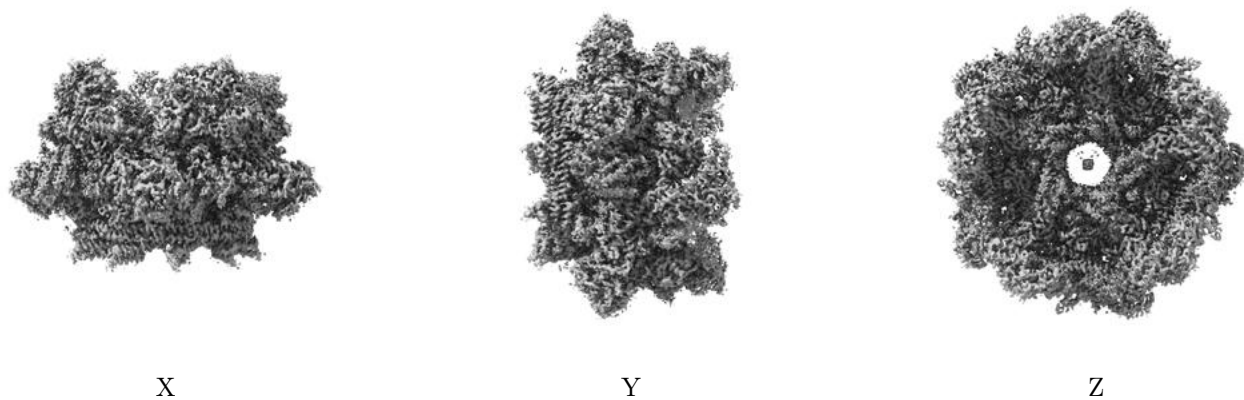


Z

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

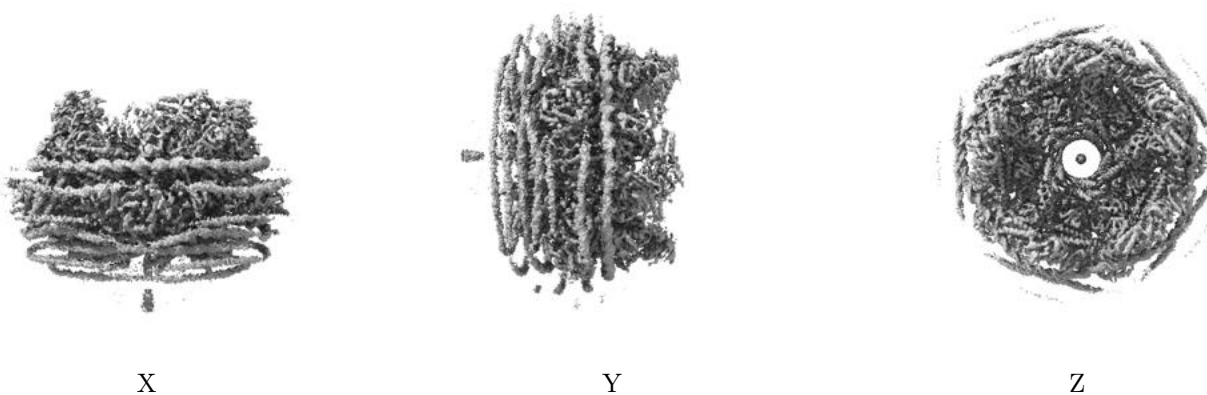
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

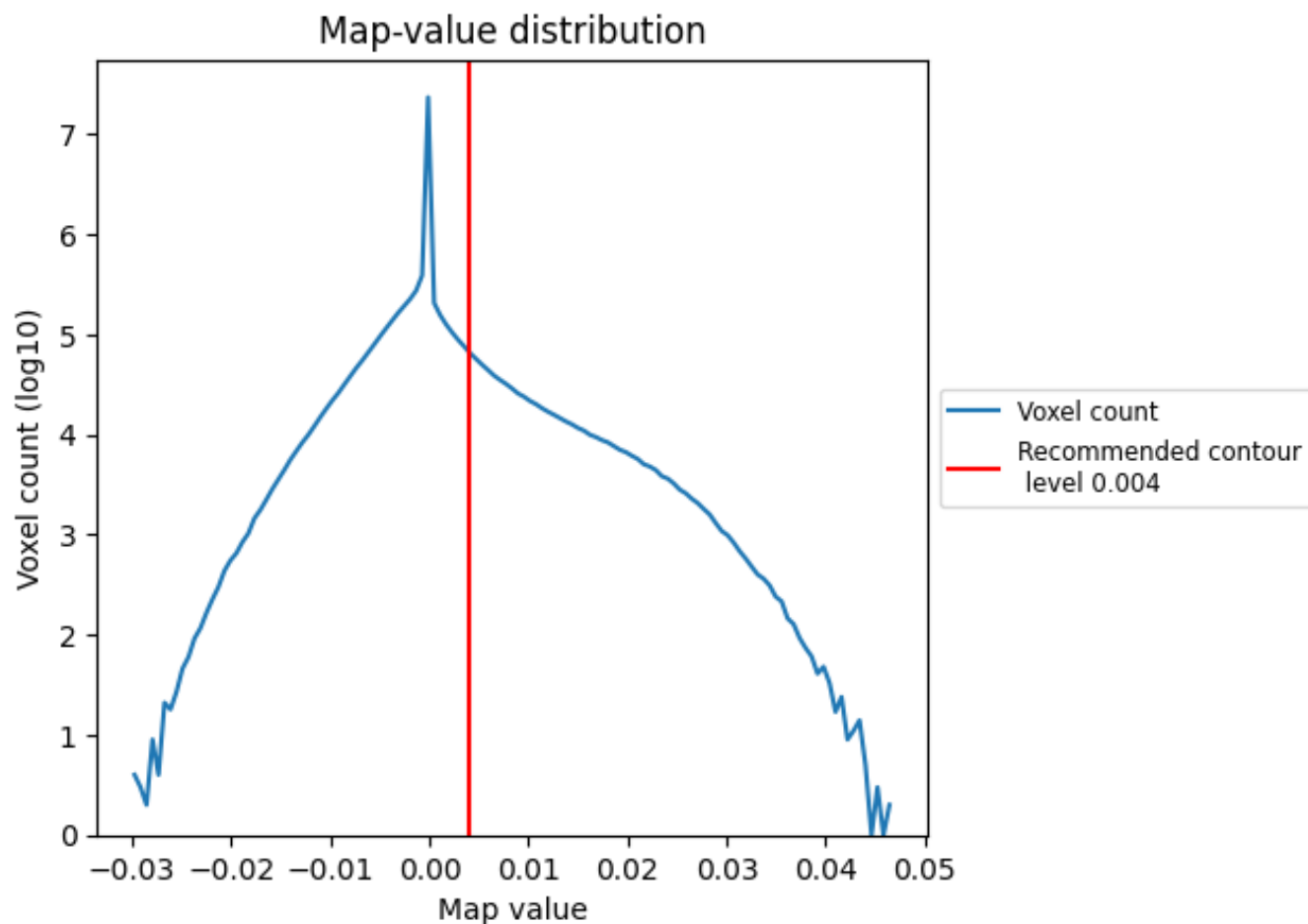
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

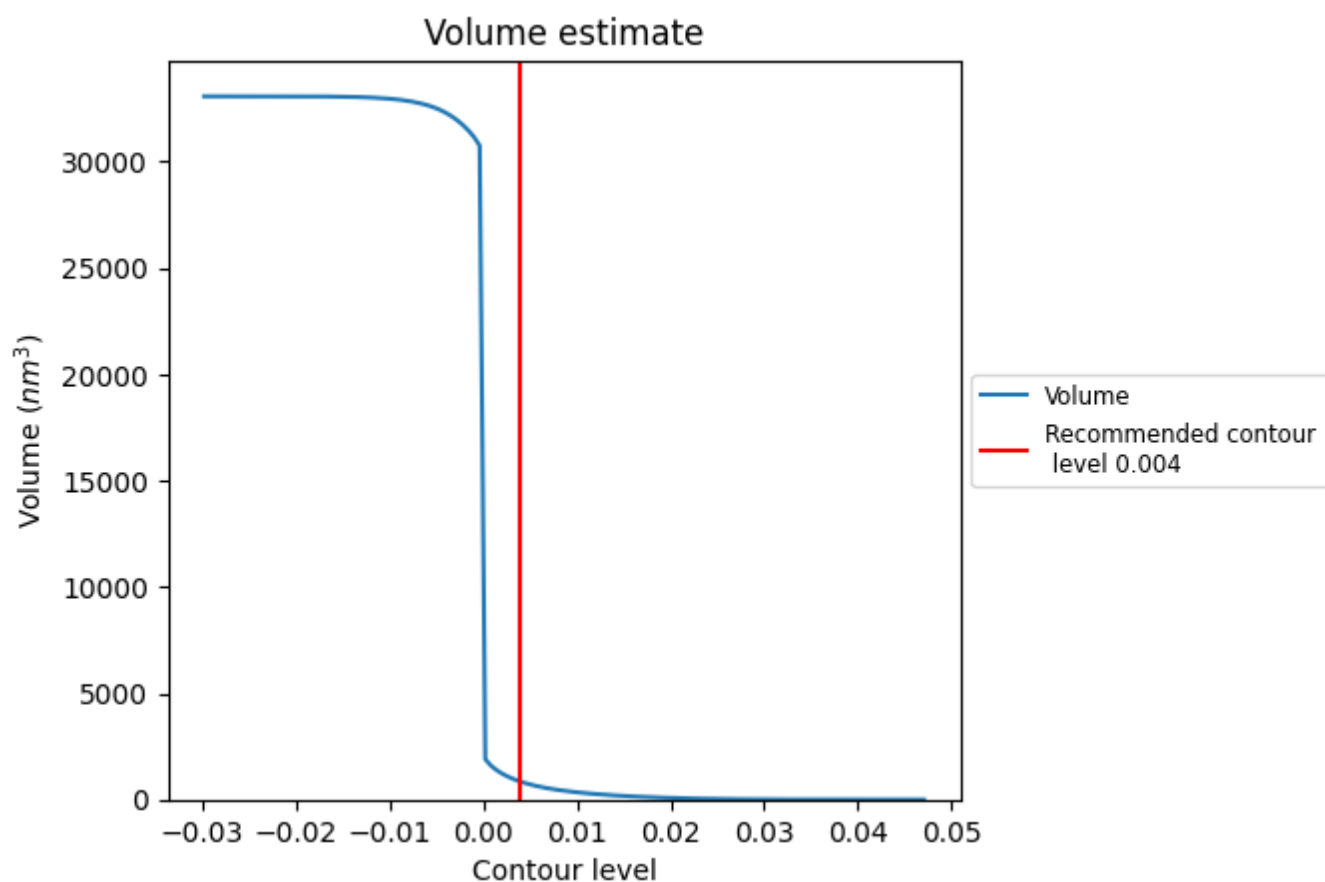
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

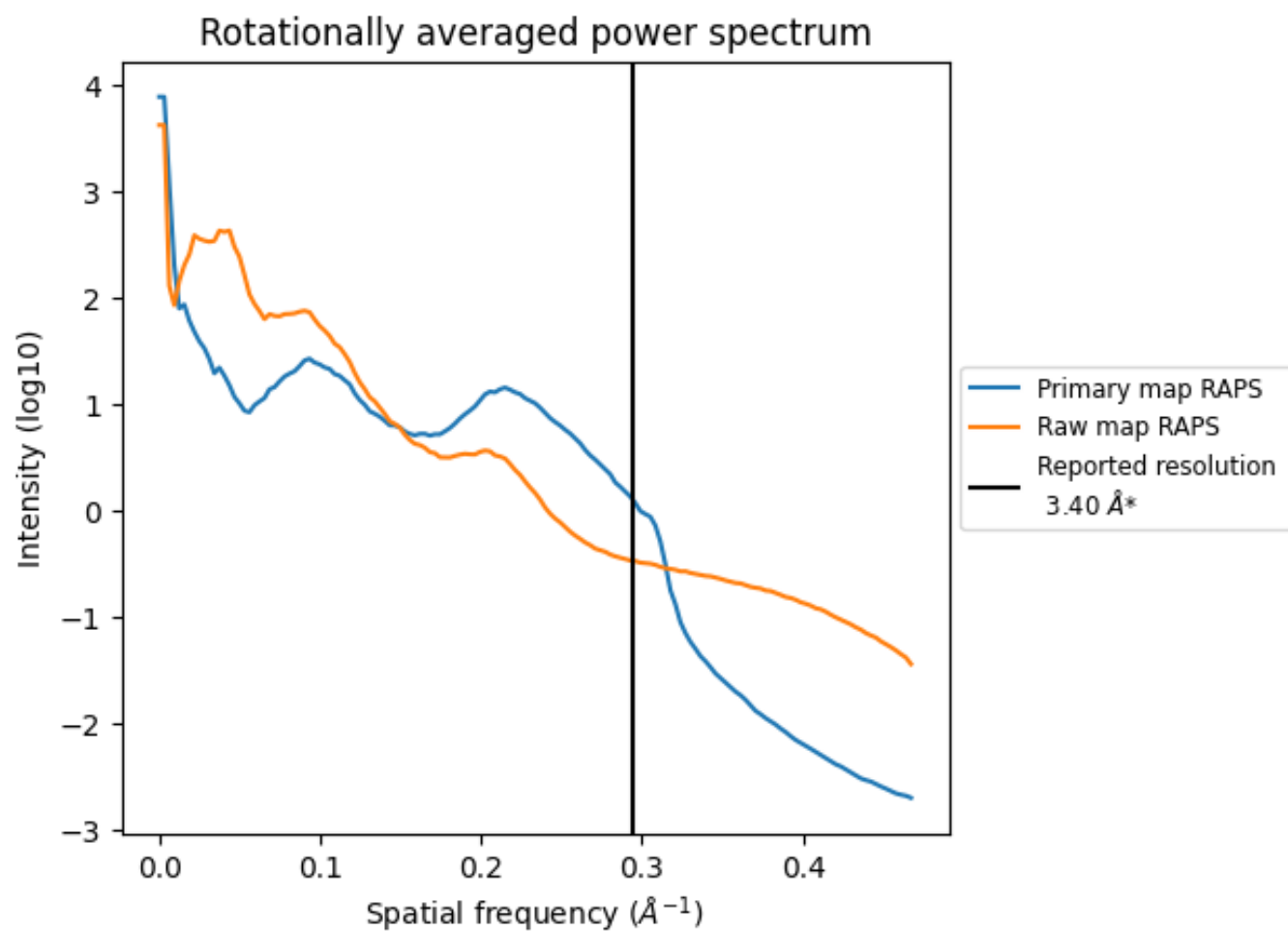
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 843 nm³; this corresponds to an approximate mass of 761 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 ⓘ

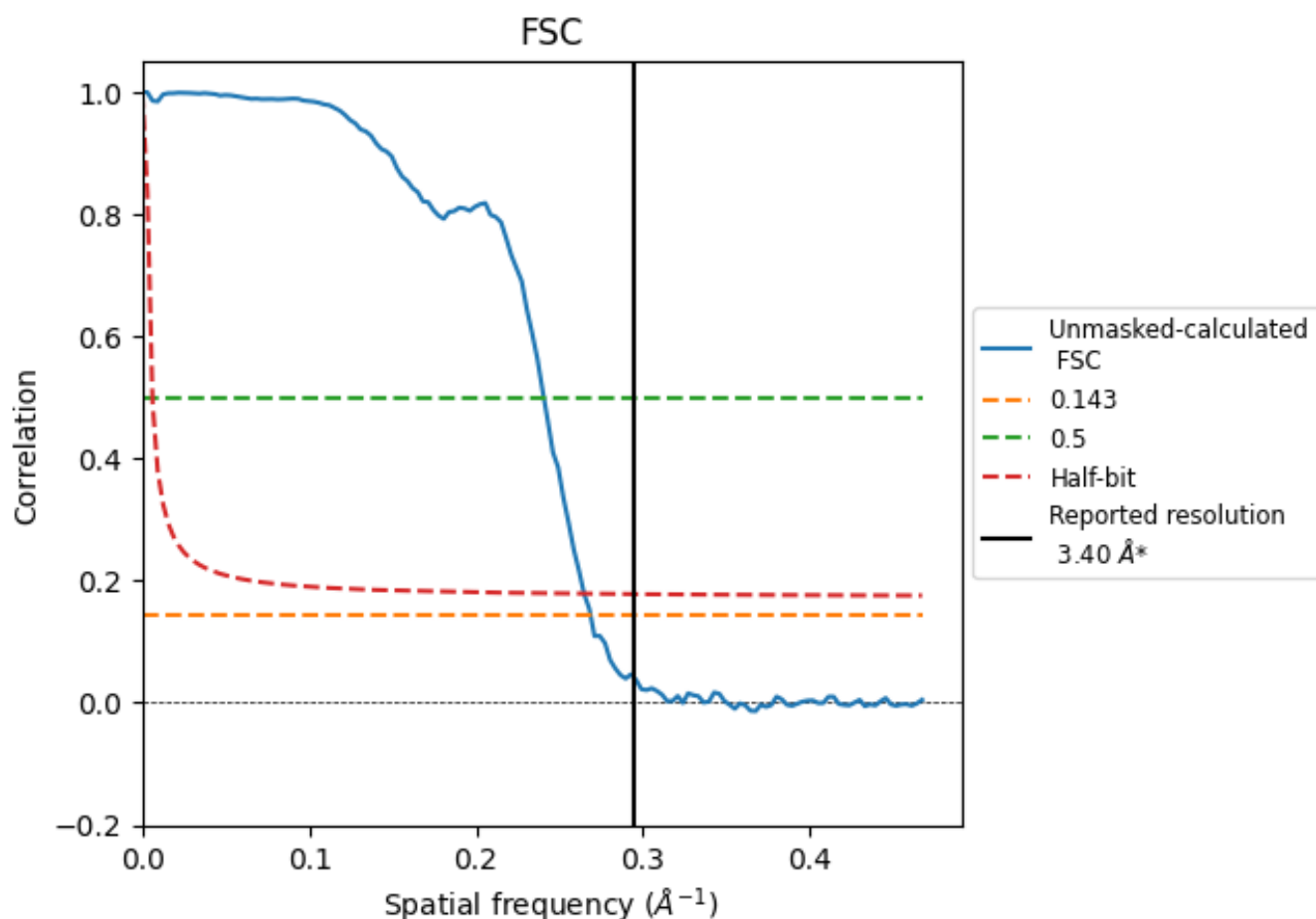


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

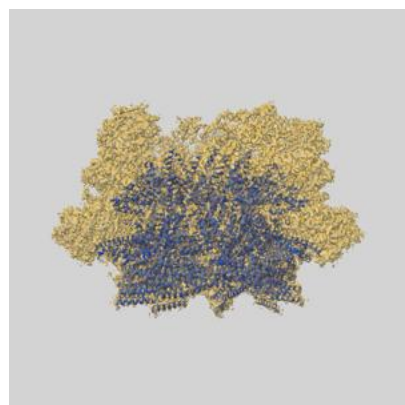
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	4.16	3.78

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

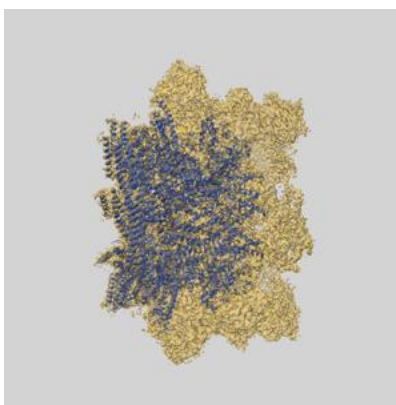
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61998 and PDB model 9K2V. Per-residue inclusion information can be found in section [3](#) on page [7](#).

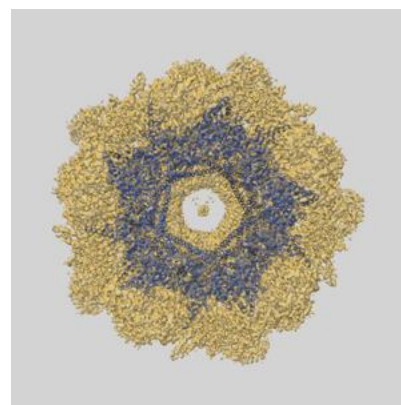
9.1 Map-model overlay [i](#)



X



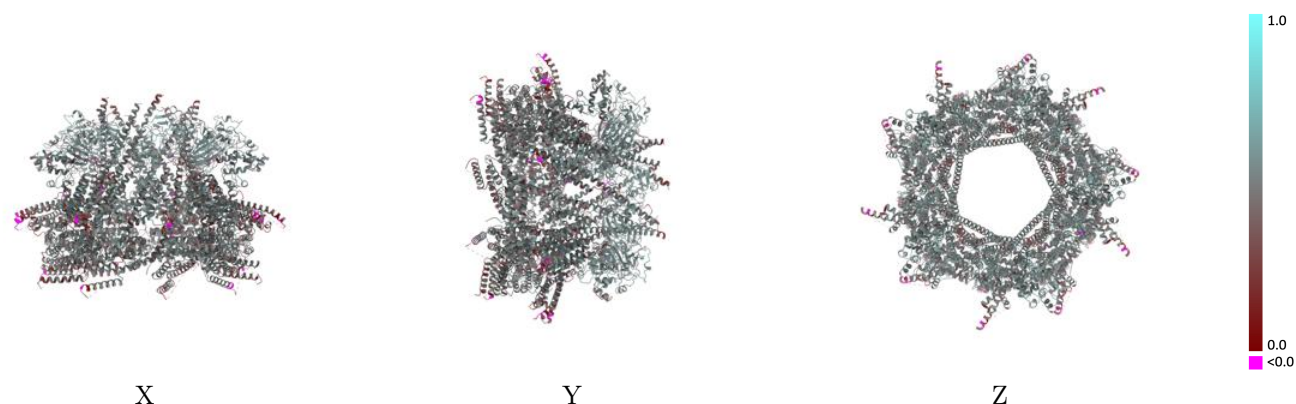
Y



Z

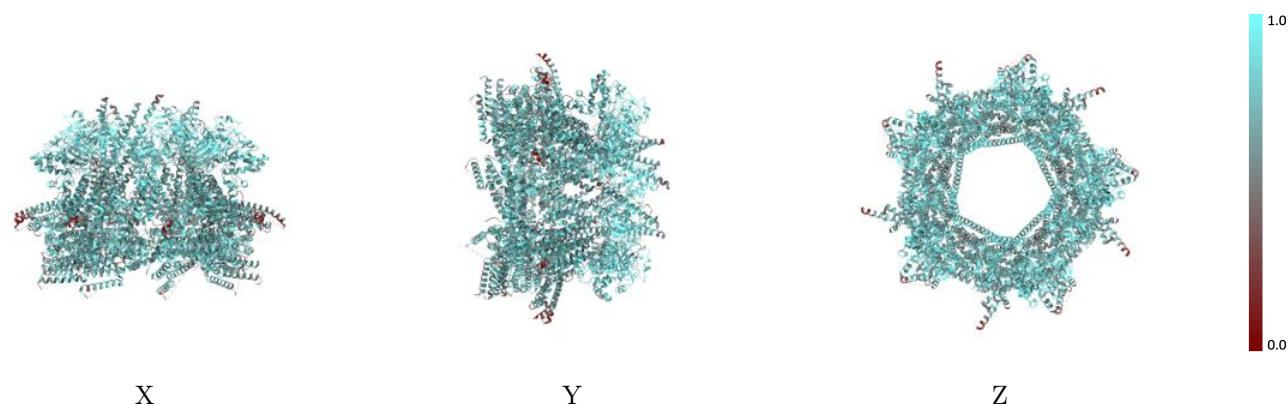
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



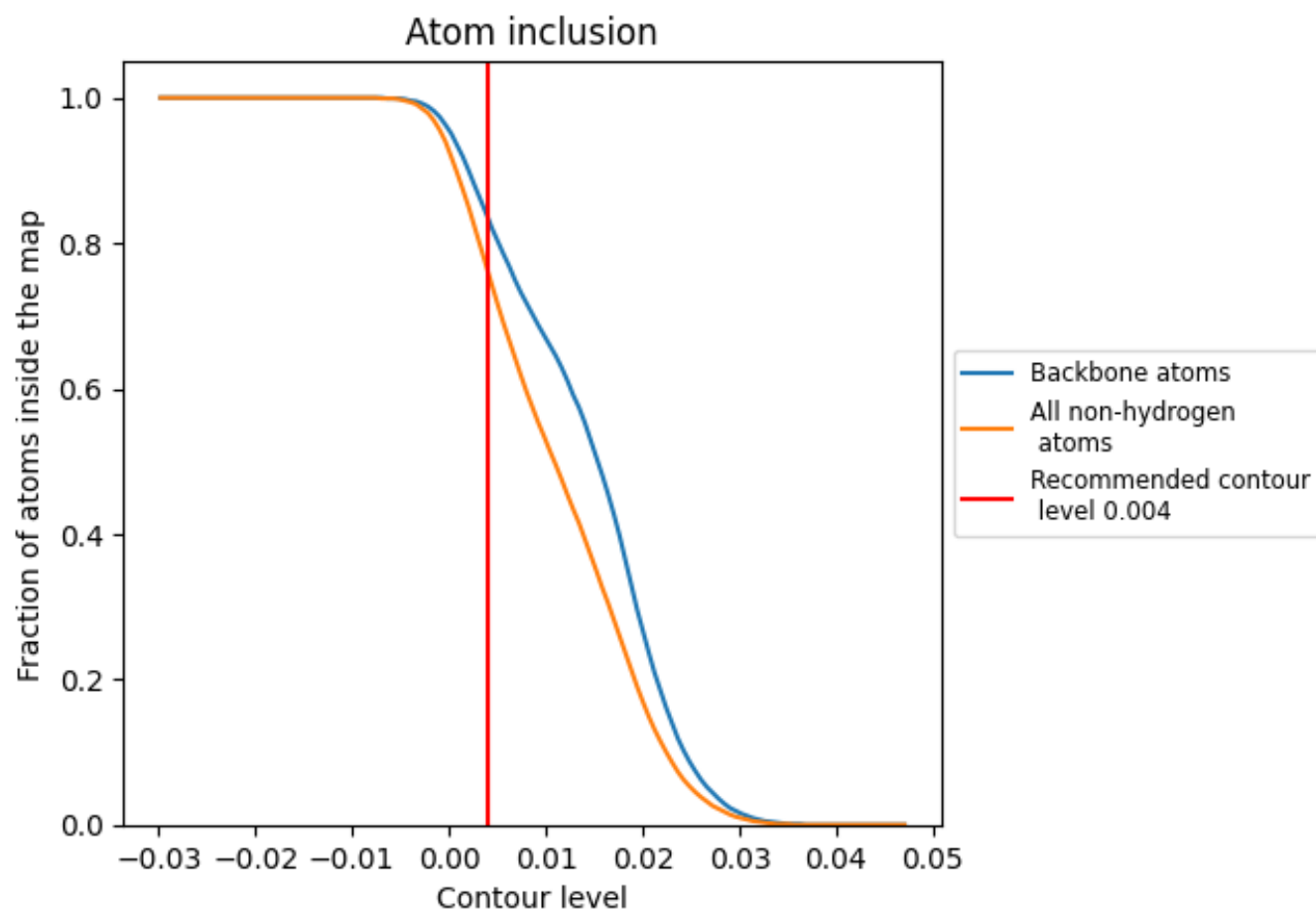
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7620	 0.4800
A	 0.7770	 0.4950
B	 0.7800	 0.4950
C	 0.7780	 0.4940
D	 0.7810	 0.4940
E	 0.7770	 0.4960
F	 0.7680	 0.4950
G	 0.7610	 0.4510
H	 0.7820	 0.4910
I	 0.7580	 0.4570
J	 0.7850	 0.4990
K	 0.7510	 0.4640
L	 0.7850	 0.4980
M	 0.7650	 0.4680
N	 0.7960	 0.4990
O	 0.7470	 0.4550
V	 0.7580	 0.4870
W	 0.7630	 0.4760
X	 0.7510	 0.4750
Y	 0.7700	 0.4780
Z	 0.7630	 0.4830
a	 0.7260	 0.4560
b	 0.7300	 0.4580
c	 0.7350	 0.4610
d	 0.7290	 0.4560
e	 0.7310	 0.4590
v	 0.7510	 0.4550
w	 0.7440	 0.4510
x	 0.7570	 0.4620
y	 0.7440	 0.4520
z	 0.7470	 0.4560

