



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 08:09 PM UTC

PDB ID : 9OPB / pdb_00009opb
EMDB ID : EMD-70687
Title : Herpes simplex virus type 1 (HSV-1) D-capsid pUL6 portal protein turrets, decamer
Authors : Crofut, E.H.; Kashyap, S.; Stevens, A.; Jih, J.; Liu, Y.-T.; Zhou, Z.H.
Deposited on : 2025-05-17
Resolution : 3.60 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:

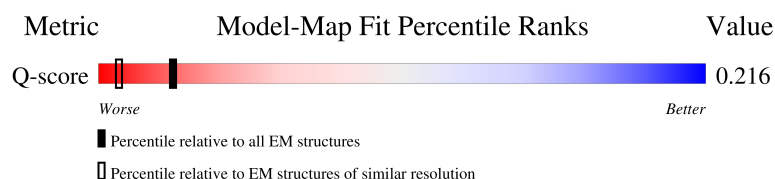
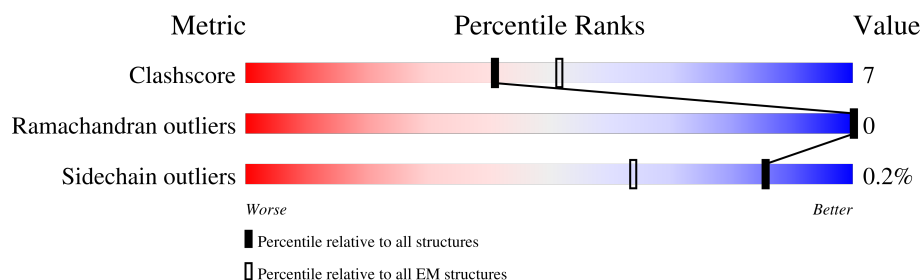
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.60 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	12797 (3.10 - 4.10)

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	M	676	 6% 9% 5% 80%
1	N	676	 6% 9% 5% 80%
1	O	676	 6% 9% 5% 80%
1	P	676	 6% 10% 5% 79%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Q	676	5% 9% . 89%
1	R	676	5% 11% . 88%
1	S	676	6% 9% . 89%
1	T	676	5% 9% . 88%
1	U	676	5% 10% . 89%
1	V	676	9% . 88%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6145 atoms, of which 0 are hydrogens and 0 are deuteriums.

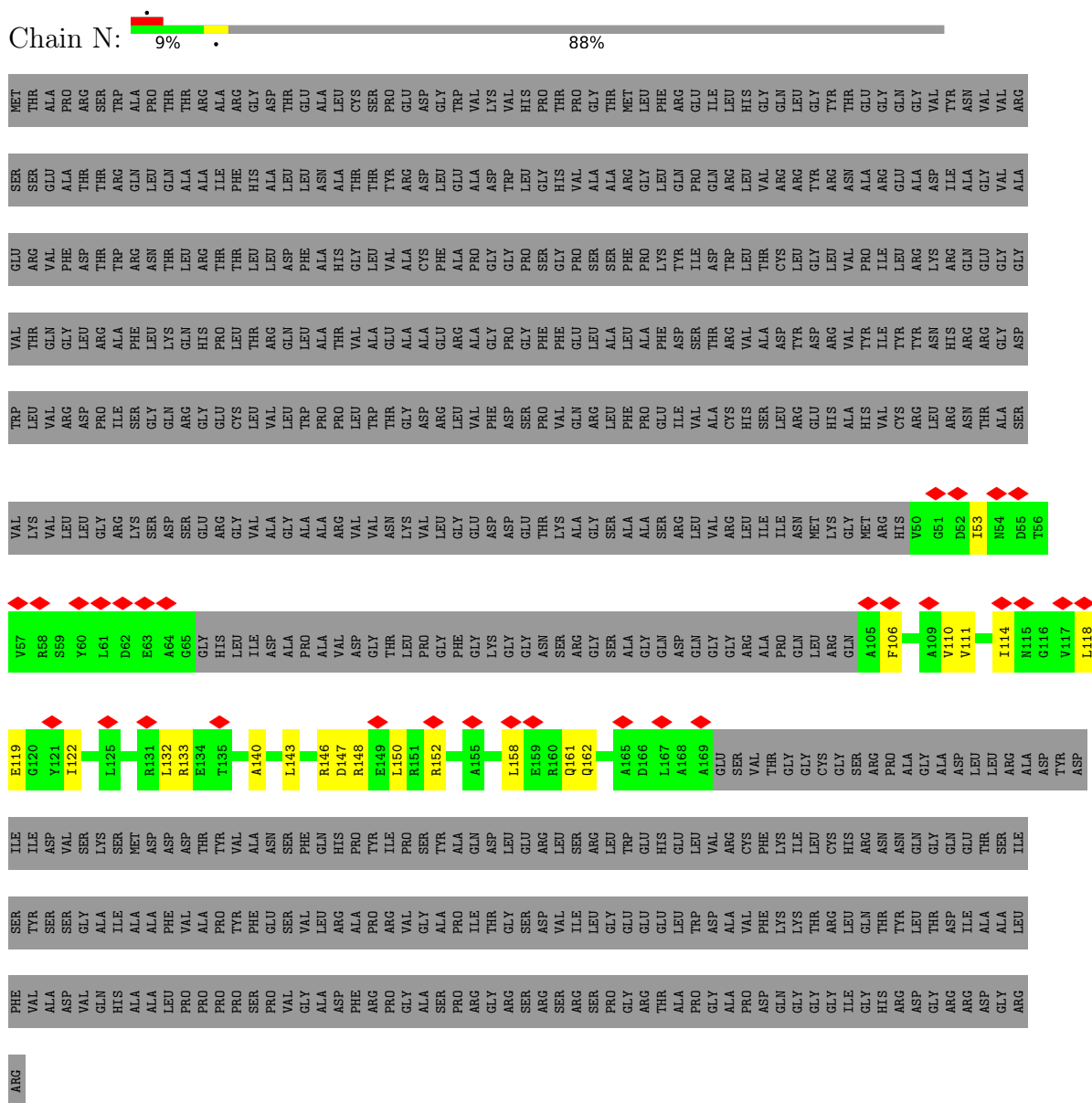
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid portal protein.

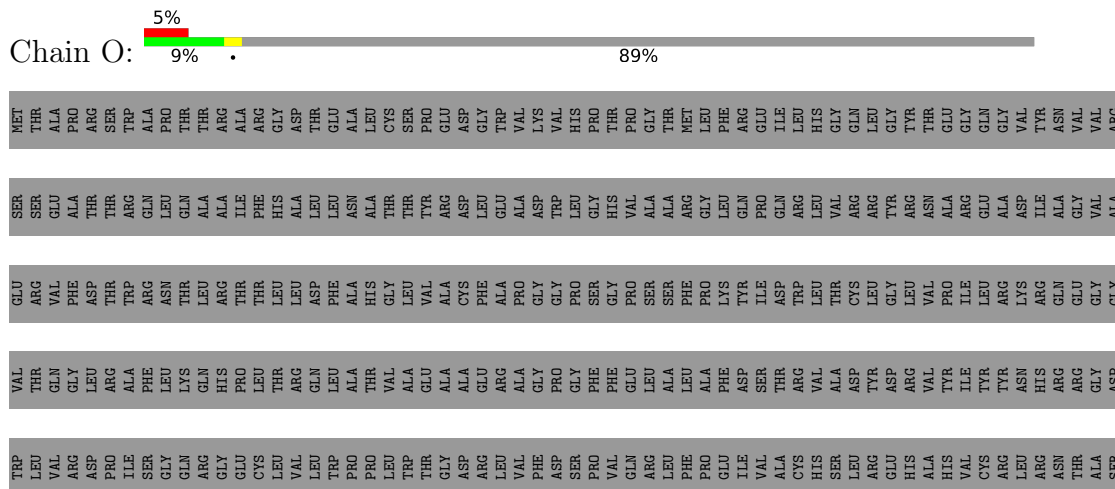
Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	75	Total	C	N	O	S	0	0
			603	369	119	114	1		
1	N	81	Total	C	N	O		0	0
			626	379	122	125			
1	O	75	Total	C	N	O	S	0	0
			603	369	119	114	1		
1	P	81	Total	C	N	O		0	0
			626	379	122	125			
1	Q	75	Total	C	N	O	S	0	0
			603	369	119	114	1		
1	R	81	Total	C	N	O		0	0
			626	379	122	125			
1	S	75	Total	C	N	O	S	0	0
			603	369	119	114	1		
1	T	81	Total	C	N	O		0	0
			626	379	122	125			
1	U	75	Total	C	N	O	S	0	0
			603	369	119	114	1		
1	V	81	Total	C	N	O		0	0
			626	379	122	125			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	59	SER	ALA	conflict	UNP H9E912
N	59	SER	ALA	conflict	UNP H9E912
O	59	SER	ALA	conflict	UNP H9E912
P	59	SER	ALA	conflict	UNP H9E912
Q	59	SER	ALA	conflict	UNP H9E912
R	59	SER	ALA	conflict	UNP H9E912
S	59	SER	ALA	conflict	UNP H9E912
T	59	SER	ALA	conflict	UNP H9E912
U	59	SER	ALA	conflict	UNP H9E912
V	59	SER	ALA	conflict	UNP H9E912



- Molecule 1: Capsid portal protein





ASP	GLN	HIS	ALA	LEU	PRO	PRO	PRO	SER	PRO	VAL	GLY	ARG	PHE	ARG	THR	ARG	ASP	GLN	GLY	GLY	ILE	GLY	HIS	ARG	ASP	GLY	ARG
SER	GLY	ILE	ALA	PHE	VAL	ALA	TYR	PHE	GLU	SER	VAL	ARG	ALA	PRO	ARG	THR	ASP	VAL	ILE	LEU	GLY	THR	TRP	LEU	GLU	GLY	ASP

- Molecule 1: Capsid portal protein

Chain Q:  5% 9% 89%

NET	THR	ALA	ALA	ARG	SER	TRP	ALA	ALA	PRO	THR	THR	THR	ARG	ALA	GLY	ASP	GLY	THR	GLU	ALA	LEU	CYS	SER	PRO	ASP	GLY	GLY	VAL	VAL	LYS	HIS	PRO	THR	PRO	GLY	THR	GLY	THR	NET	LEU	PHE	GLY	GLN	GLY	GLY	GLY	TYR	ASN	VAL	VAL	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	SER	GLU	ALA	THR	THR	ARG	GLN	LEU	GLN	ALA	ALA	ILE	PHE	HIS	LEU	LEU	LEU	ASN	ALA	THR	THR	TYR	ARG	ASP	LEU	GLU	ALA	ASP	TRP	LEU	GLY	HIS	VAL	ALA	ALA	ARG	GLY	LEU	GLN	GLN	PRO	GLN	ARG	LEU	VAL	ARG	ARG	TYR	ASN	ALA	ALA	ARG	GLU	ALA	VAL	GLY	VAL	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

VAL	THR	GLN	GLY	LEU	ARG	ALA	PHE	LEU	LEU	LYS	GLN	HIS	PRO	THR	THR	ARG	GLN	LEU	ALA	ALA	GLU	ALA	ALA	GLU	ARG	ALA	ALA	GLY	GLY	PRO	GLY	PHE	PHE	GLU	GLU	LEU	ALA	ALA	LEU	LEU	ALA	PHE	PHE	ASP	ASP	THR	THR	ARG	VAL	VAL	TYR	TYR	ILE	ILE	TYR	TYR	ASN	HIS	ARG	ARG	ARG	GLY	GLY	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

TRP	LEU	VAL	ARG	ASP	PRO	ILE	SER	GLY	GLN	ARG	GLY	GLU	CYS	LEU	VAL	LEU	TRP	PRO	PRO	LEU	THR	GLY	ASP	ARG	LEU	VAL	PHE	PHE	ASP	SER	PRO	PRO	GLU	ILE	VAL	ALA	CYS	HIS	HIS	SER	LEU	ARG	GLU	HIS	ALA	ASN	ARG	LEU	ARG	ASP	TRP	ALA	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL	LYS	VAL	LEU	LEU	GLY	ARG	LYS	SER	ASP	SER	GLU	ARG	GLY	VAL	ALA	GLY	ALA	ALA	ARG	VAL	VAL	ASN	LYS	VAL	LEU	GLY	GLU	ASP	ASP	GLU	THR	LYS	ALA	GLY	SER	A33	R36	L37	V38	R39	L40	L41	I42	N43	M44	LYS	GLY	MET	ARG	HIS	VAL	GLY	D62	I53	N54	D55		R58
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----

S59 Y60 D62 A109 G116 E119 G120
 R103 Q104 A105 F106 R107 T108 M112 M113

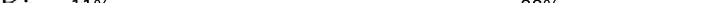
N123	N124	L125	A137	T141	Q142	L143	Q144	E145	R146	D147	F148	E149	L150	R151	R152	A153	T154	ALA	GLY	GLY	ALA	LEU	LEU	GLU	ARG	GLN	GLN	ARG	ALA	ALA	ASP	ASP	LEU	ALA	ALA	GLU	SER	VAL	THR	THR	GLY	GLY	CYS	GLY	SER	ARG	PRO	ALA	GLY	ALA	ASP	LEU	LEU	ARG	ALA	ASP	TYR	ASP	ILE	ILE	ASP
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

VAL	SER	SER	LYS	SER	MET	SER	ASP	ASP	ASP	THR	TYR	VAL	ALA	ALA	ASN	SER	SER	PHE	GLN	HIS	GLN	PRO	PRO	TYR	TYR	ILE	ILE	PRO	SER	SER	TYR	ALA	ALA	GLN	ASP	LEU	LEU	GLU	GLU	ARG	LEU	LEU	SER	GLU	HIS	GLY	TRP	TRP	TRP	LEU	LEU	VAL	VAL	ARG	ARG	CYS	CYS	PHE	LYS	ILE	ILE	LEU	LEU	CYS	CYS	HIS	ARG	ARG	ASN	ASN	GLN	GLN	GLY	GLY	GLN	GLN	GLU	GLU	THR	SER	SER	ILE	ILE	SER	SER	TYR	TYR	SER	SER	FER	FER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER GLY ALA ALA ILE ALA ALA PHE VAL VAL PRO TYR PHE GLU SER VAL LEU ARG ALA ALA PRO ARG VAL VAL GLY GLU ALA ALA PRO ILE THR GLY SER ASP VAL VAL LEU LEU GLY GLU GLU GLU LEU TRP ASP ALA ALA VAL PHE LYS THR ARG LEU GLN THR TYR LEU THR ASP ILE ALA ALA PHE VAL VAL

ASP VAL GLN HIS ALA LEU PRO PRO PRO PRO SER VAL GLY ALA ASP PHE ARG PRO PRO GLY GLY SER SER SER ARG ARG SER SER PRO PRO THR PRO GLY GLY GLY GLY ILE HIS HIS ASP ASP ASP ASP GLY GLY GLY GLY

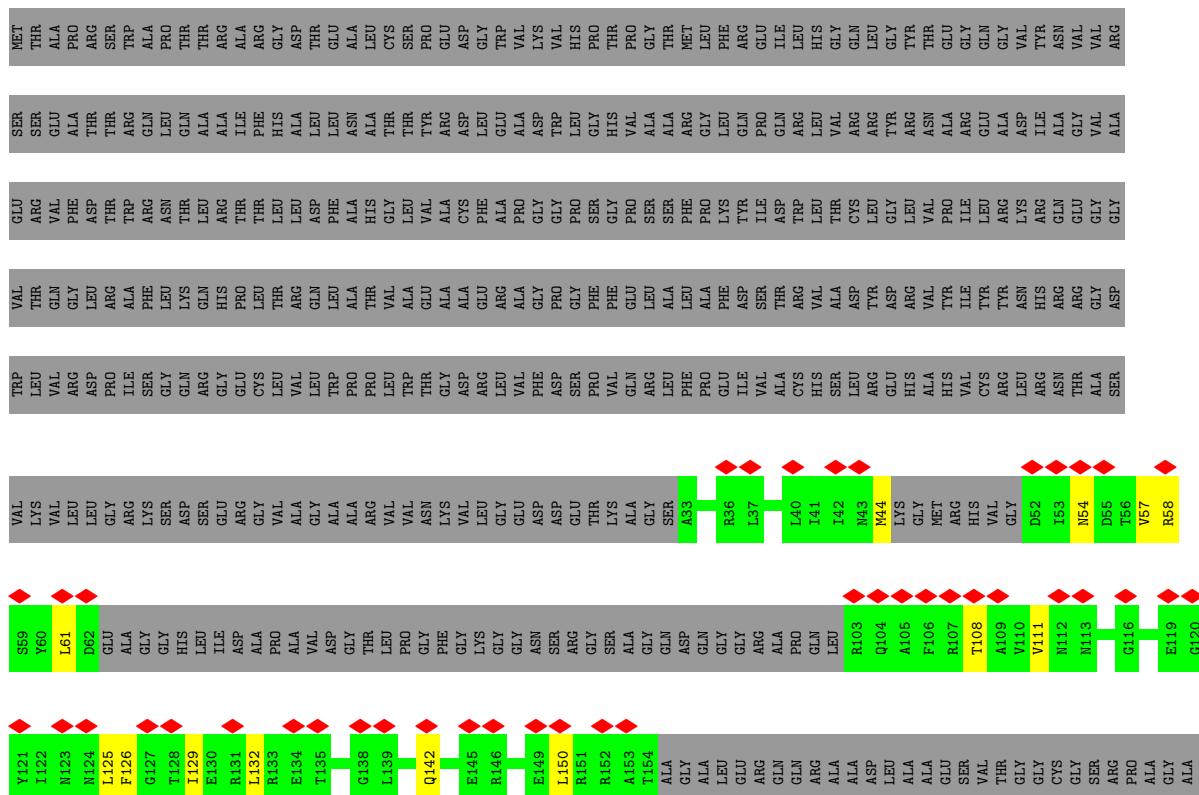
- Molecule 1: Capsid portal protein

Chain R:  5% 11% 88%

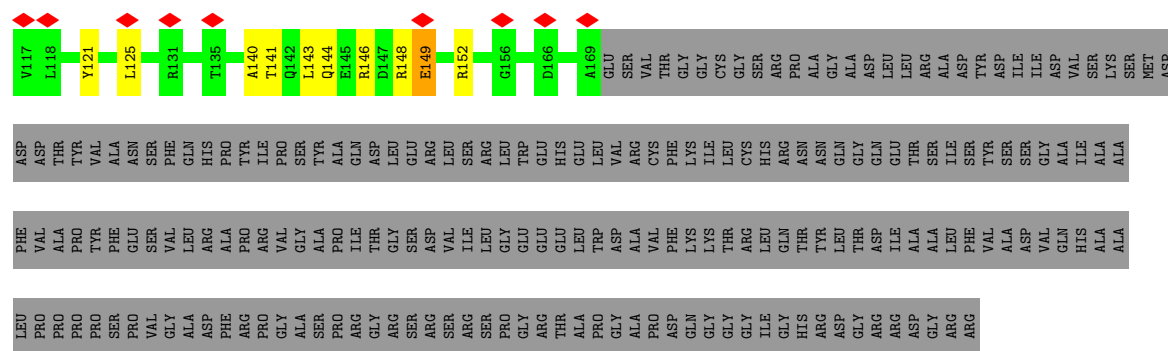
MET	THR	ALA	PRO	ARG	SER	TRP	ALA	PRO	THR	THR	ARG	ALA	ARG	GLY	ASP	THR	GLU	ALA	LEU	CYS	SER	PRO	GLU	ASP	GLY	TRP	VAL	LYS	VAL	HIS	PRO	THR	PRO	GLY	THR	MET	LEU	PHE	ARG	GLU	GLU	LEU	ILE	HIS	GLY	GLN	LEU	GLY	TYR	GLU	THR	GLY	VAL	ASN	VAL	VAL	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER SER GLU THR THR ARG GLN LEU GLN ALA ALA ILE PRE HIS LEU LEU LEU ASN ALA ALA THR THR TYR ARG ASP LEU LEU GLU GLU ALA ALA ASP TRP LEU GLY HIS VAL VAL ALA ALA ARG ARG GLY LEU LEU GLN GLN PRO PRO GLN ARG LEU LEU VAL VAL ARG ARG TYR ARG ASN ALA ALA ALA GLU ASP ILE ALA GLY VAL VAL

GLU ARG VAL ARG ASP THR TRP ARG ASN THR LEU ARG THR THR LEU LEU ASP PHE ALA HIS GLY LEU VAL ALA CYS PHE PHE PRO PRO GLY GLY PRO SER SER PHE PHE PRO LYS TYR TLE ASP ASP LEU LEU THR THR CYS CYS GLY LEU LEU VAL VAL PRO PRO TLE TLE ARG LYS ARG GLN GLU GLY GLY







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	135916	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.654	Depositor
Minimum map value	-0.304	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.096	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	M	0.10	0/604	0.24	0/811
1	N	0.16	0/628	0.27	0/846
1	O	0.10	0/604	0.23	0/811
1	P	0.12	0/628	0.25	0/846
1	Q	0.10	0/604	0.23	0/811
1	R	0.14	0/628	0.28	0/846
1	S	0.10	0/604	0.25	0/811
1	T	0.11	0/628	0.24	0/846
1	U	0.09	0/604	0.22	0/811
1	V	0.14	0/628	0.30	0/846
All	All	0.12	0/6160	0.25	0/8285

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	603	0	612	10	0
1	N	626	0	616	22	0
1	O	603	0	612	15	0
1	P	626	0	616	11	0
1	Q	603	0	612	10	0
1	R	626	0	616	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	603	0	612	9	0
1	T	626	0	616	14	0
1	U	603	0	612	6	0
1	V	626	0	616	9	0
All	All	6145	0	6140	85	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 7.

All (85) 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:N:53:ILE:HG23	1:O:58:ARG:HH12	1.57	0.70
1:M:147:ASP:HA	1:N:146:ARG:NH2	2.12	0.65
1:O:129:ILE:HD11	1:P:125:LEU:HG	1.78	0.65
1:V:146:ARG:HA	1:V:149:GLU:OE2	2.00	0.61
1:M:132:LEU:HD11	1:N:133:ARG:HH21	1.66	0.60
1:Q:125:LEU:HD22	1:R:125:LEU:HD13	1.85	0.58
1:N:147:ASP:HA	1:N:150:LEU:HD12	1.85	0.57
1:P:114:ILE:HA	1:P:117:VAL:HG22	1.89	0.55
1:T:129:ILE:O	1:T:133:ARG:HG2	2.09	0.53
1:S:150:LEU:HD12	1:T:150:LEU:HB2	1.91	0.53
1:N:111:VAL:HA	1:N:114:ILE:HG12	1.90	0.52
1:O:150:LEU:HD23	1:P:146:ARG:HH22	1.74	0.52
1:N:140:ALA:O	1:N:143:LEU:HG	2.10	0.52
1:T:53:ILE:HG23	1:U:58:ARG:HH22	1.75	0.52
1:S:142:GLN:HE22	1:T:143:LEU:HD11	1.75	0.52
1:O:125:LEU:HB3	1:P:125:LEU:HD21	1.92	0.52
1:S:54:ASN:HA	1:S:57:VAL:HG12	1.92	0.52
1:R:141:THR:O	1:R:144:GLN:HG3	2.11	0.51
1:T:148:ARG:HA	1:T:151:ARG:HD2	1.91	0.51
1:T:119:GLU:O	1:T:122:ILE:HG22	2.10	0.51
1:M:139:LEU:O	1:M:142:GLN:HG3	2.11	0.51
1:M:146:ARG:NH2	1:N:143:LEU:HB2	2.27	0.50
1:P:50:VAL:HG12	1:P:52:ASP:H	1.75	0.50
1:O:115:ASN:O	1:O:119:GLU:HG2	2.11	0.50
1:Q:125:LEU:HD21	1:R:125:LEU:HB3	1.93	0.50
1:N:53:ILE:HD12	1:O:58:ARG:NH1	2.27	0.49
1:N:110:VAL:HG22	1:O:60:TYR:OH	2.13	0.49
1:V:50:VAL:HG12	1:V:52:ASP:H	1.76	0.49
1:M:58:ARG:HH22	1:N:122:ILE:HG23	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:122:ILE:HD13	1:R:125:LEU:HD12	1.94	0.49
1:S:125:LEU:HD13	1:T:125:LEU:HD13	1.95	0.49
1:N:114:ILE:O	1:N:118:LEU:HG	2.14	0.48
1:O:122:ILE:HD13	1:P:118:LEU:HD22	1.96	0.48
1:S:132:LEU:HG	1:T:132:LEU:HD22	1.96	0.47
1:V:59:SER:O	1:V:63:GLU:HG2	2.15	0.47
1:Q:141:THR:O	1:Q:144:GLN:HG3	2.15	0.47
1:Q:55:ASP:HA	1:Q:58:ARG:HE	1.80	0.46
1:T:53:ILE:HA	1:U:58:ARG:NH2	2.30	0.46
1:N:161:GLN:NE2	1:N:162:GLN:HG2	2.30	0.46
1:M:133:ARG:HH12	1:N:132:LEU:HD22	1.80	0.46
1:T:128:THR:O	1:T:131:ARG:HG2	2.16	0.46
1:Q:58:ARG:HG3	1:R:119:GLU:HG3	1.98	0.45
1:M:131:ARG:O	1:M:134:GLU:HG2	2.17	0.45
1:Q:143:LEU:HG	1:R:143:LEU:HG	1.98	0.45
1:O:124:ASN:O	1:O:128:THR:HG23	2.16	0.45
1:S:58:ARG:HA	1:S:61:LEU:HB3	1.98	0.45
1:O:38:VAL:HA	1:O:41:ILE:HG22	1.99	0.45
1:O:139:LEU:HD22	1:P:139:LEU:HB3	1.98	0.45
1:R:121:TYR:CE2	1:R:125:LEU:HD21	2.52	0.45
1:N:119:GLU:O	1:N:122:ILE:HG22	2.18	0.44
1:T:50:VAL:HG12	1:T:52:ASP:H	1.81	0.44
1:P:158:LEU:HA	1:P:161:GLN:HG2	1.98	0.44
1:V:55:ASP:O	1:V:58:ARG:HG3	2.18	0.44
1:N:140:ALA:HA	1:N:143:LEU:HD23	1.99	0.44
1:U:60:TYR:HD1	1:U:61:LEU:HD23	1.83	0.44
1:U:142:GLN:O	1:U:146:ARG:HG2	2.18	0.44
1:S:126:PHE:HA	1:S:129:ILE:HG22	1.99	0.44
1:U:39:ARG:HA	1:U:42:ILE:HG22	2.00	0.44
1:V:141:THR:O	1:V:144:GLN:HG2	2.17	0.44
1:Q:149:GLU:HA	1:Q:152:ARG:HG2	2.00	0.43
1:R:50:VAL:HG12	1:R:52:ASP:OD1	2.18	0.43
1:T:148:ARG:HB3	1:T:152:ARG:HH12	1.82	0.43
1:N:106:PHE:O	1:N:110:VAL:HG23	2.19	0.43
1:N:53:ILE:HG23	1:O:58:ARG:NH1	2.31	0.42
1:N:110:VAL:O	1:N:114:ILE:HG23	2.19	0.42
1:M:139:LEU:HD11	1:N:143:LEU:CD2	2.49	0.42
1:P:56:THR:HG22	1:Q:61:LEU:HD21	2.01	0.42
1:V:140:ALA:O	1:V:143:LEU:HG	2.20	0.42
1:V:148:ARG:HG3	1:V:152:ARG:HH12	1.85	0.42
1:N:158:LEU:O	1:N:161:GLN:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:44:MET:HE2	1:S:44:MET:HB3	1.85	0.42
1:U:141:THR:HA	1:U:144:GLN:HG2	2.01	0.42
1:T:124:ASN:O	1:T:128:THR:HG23	2.19	0.41
1:V:121:TYR:O	1:V:125:LEU:HG	2.20	0.41
1:O:125:LEU:HD13	1:P:125:LEU:HD22	2.01	0.41
1:T:148:ARG:HB3	1:T:152:ARG:NH1	2.35	0.41
1:O:146:ARG:HH21	1:P:150:LEU:HB3	1.85	0.41
1:M:146:ARG:HG2	1:N:150:LEU:HD11	2.03	0.41
1:N:148:ARG:O	1:N:152:ARG:HG2	2.20	0.41
1:V:111:VAL:O	1:V:114:ILE:HG22	2.21	0.41
1:S:108:THR:HA	1:S:111:VAL:HG12	2.04	0.40
1:M:39:ARG:HA	1:M:42:ILE:HG22	2.03	0.40
1:Q:147:ASP:O	1:Q:151:ARG:HG3	2.21	0.40
1:O:128:THR:HG22	1:O:131:ARG:NH2	2.36	0.40
1:Q:142:GLN:O	1:Q:146:ARG:HG2	2.21	0.40

There are no symmetry-related clashes.

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	M	69/676 (10%)	69 (100%)	0	0	100	100
1	N	77/676 (11%)	77 (100%)	0	0	100	100
1	O	69/676 (10%)	69 (100%)	0	0	100	100
1	P	77/676 (11%)	77 (100%)	0	0	100	100
1	Q	69/676 (10%)	69 (100%)	0	0	100	100
1	R	77/676 (11%)	77 (100%)	0	0	100	100
1	S	69/676 (10%)	69 (100%)	0	0	100	100
1	T	77/676 (11%)	77 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	69/676 (10%)	69 (100%)	0	0	100	100
1	V	77/676 (11%)	77 (100%)	0	0	100	100
All	All	730/6760 (11%)	730 (100%)	0	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	M	64/535 (12%)	64 (100%)	0	100	100
1	N	62/535 (12%)	62 (100%)	0	100	100
1	O	64/535 (12%)	64 (100%)	0	100	100
1	P	62/535 (12%)	62 (100%)	0	100	100
1	Q	64/535 (12%)	64 (100%)	0	100	100
1	R	62/535 (12%)	62 (100%)	0	100	100
1	S	64/535 (12%)	64 (100%)	0	100	100
1	T	62/535 (12%)	62 (100%)	0	100	100
1	U	64/535 (12%)	64 (100%)	0	100	100
1	V	62/535 (12%)	61 (98%)	1 (2%)	55	69
All	All	630/5350 (12%)	629 (100%)	1 (0%)	85	85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V	149	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	112	ASN
1	P	144	GLN
1	Q	54	ASN
1	R	162	GLN
1	U	123	ASN
1	V	112	ASN
1	V	113	ASN
1	V	123	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 [i](#)

There are no chain breaks in this entry.

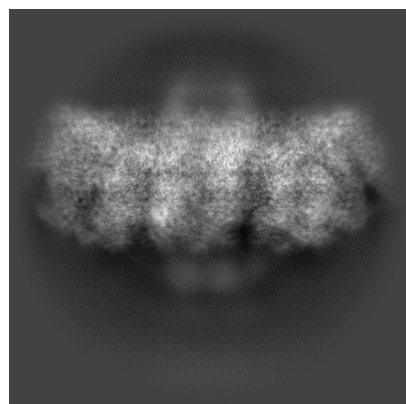
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70687. These allow visual inspection of the internal detail of the map and identification of artifacts.

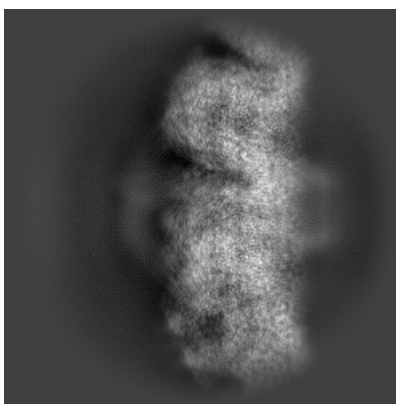
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

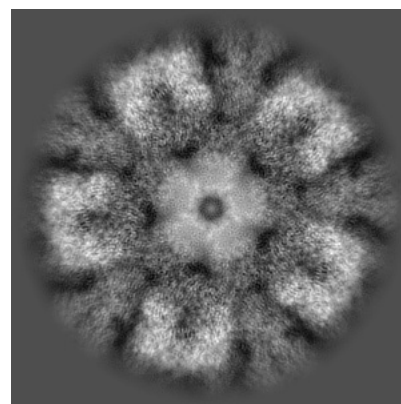
6.1.1 Primary map



X

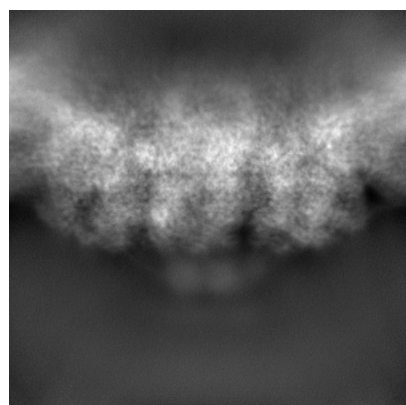


Y

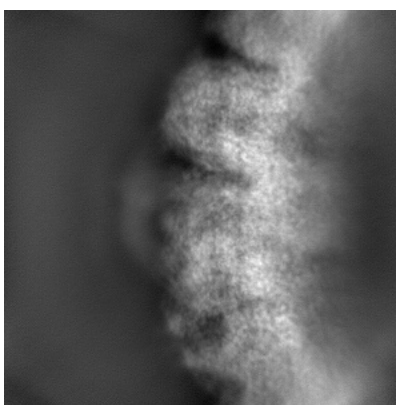


Z

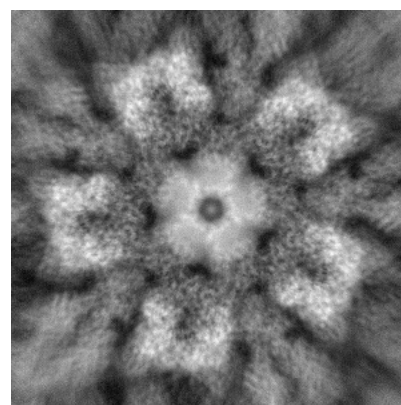
6.1.2 Raw map



X



Y

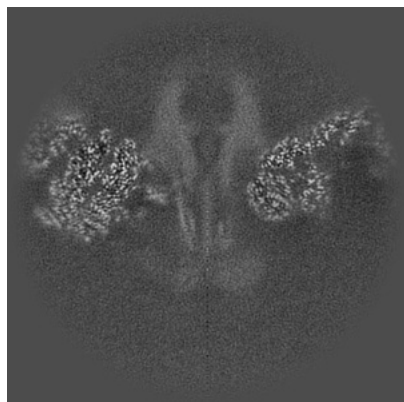


Z

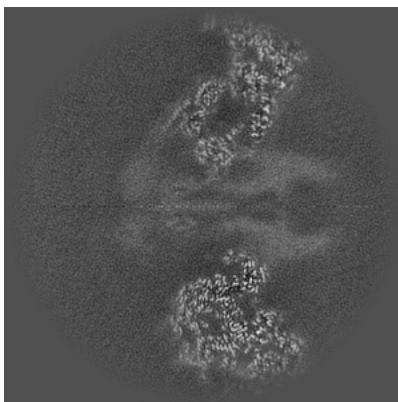
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

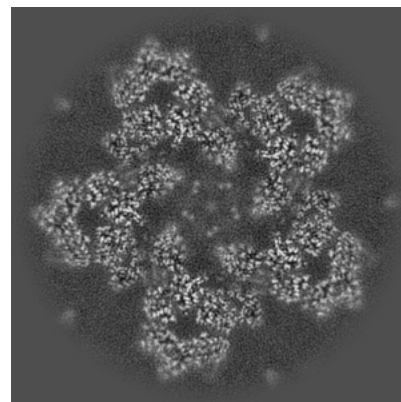
6.2.1 Primary map



X Index: 240

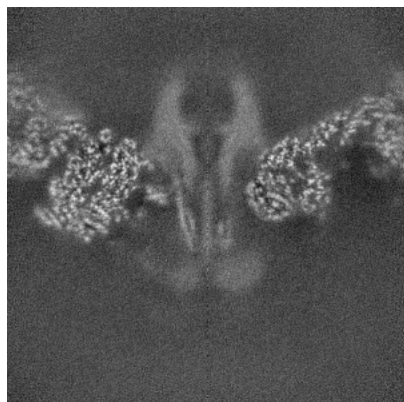


Y Index: 240

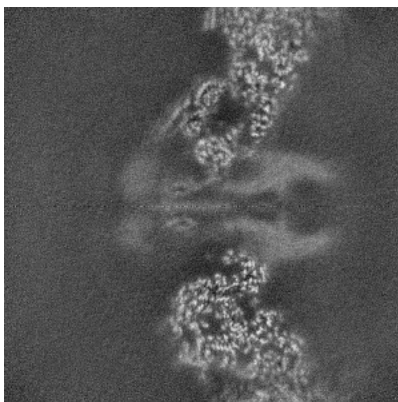


Z Index: 240

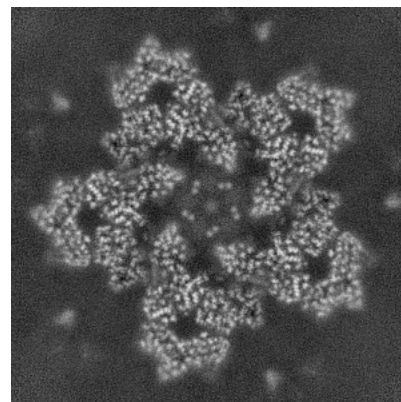
6.2.2 Raw map



X Index: 240



Y Index: 240

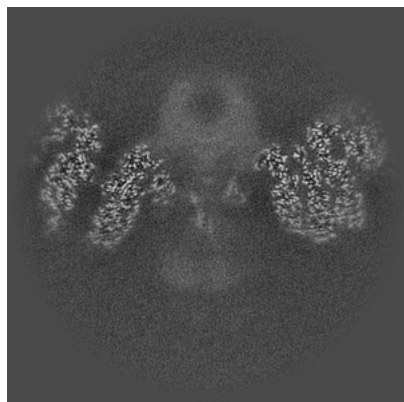


Z Index: 240

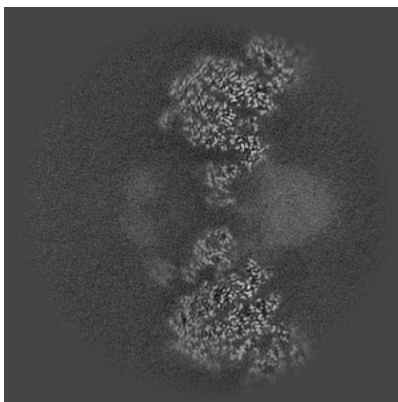
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

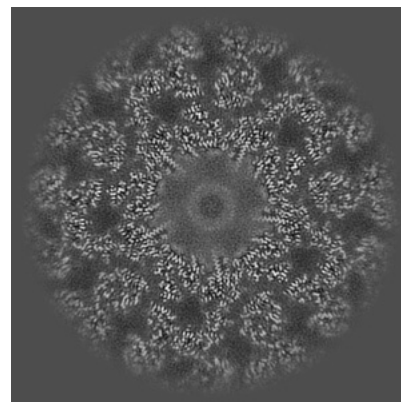
6.3.1 Primary map



X Index: 212

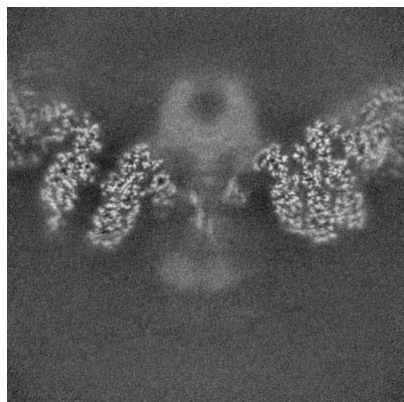


Y Index: 197

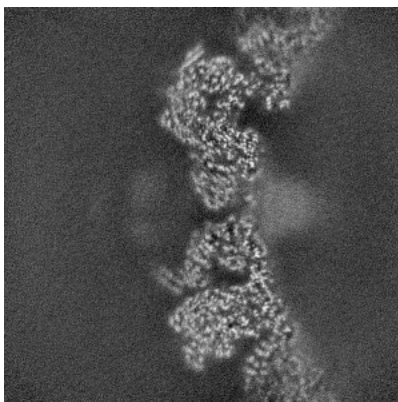


Z Index: 298

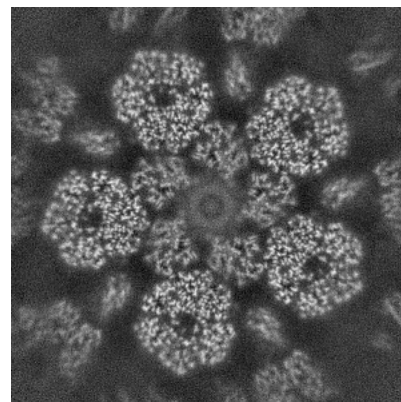
6.3.2 Raw map



X Index: 212



Y Index: 184

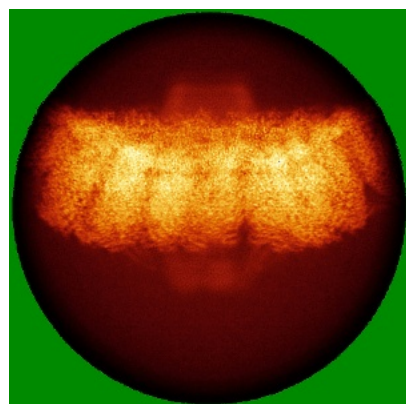


Z Index: 264

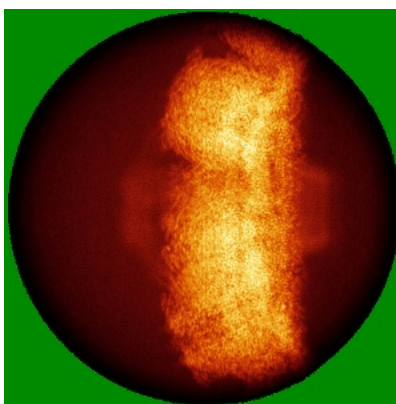
The images above show the largest variance slices of the map in three orthogonal directions.

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

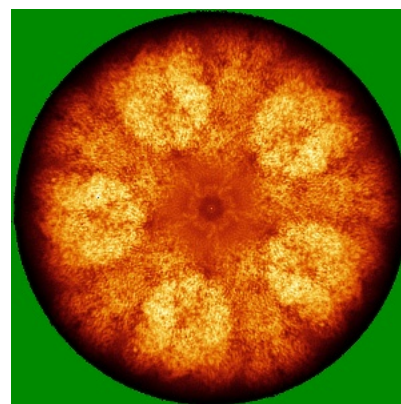
6.4.1 Primary map



X

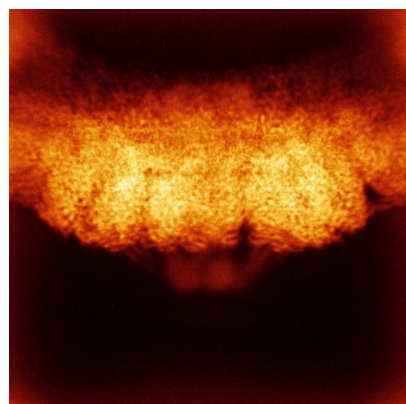


Y

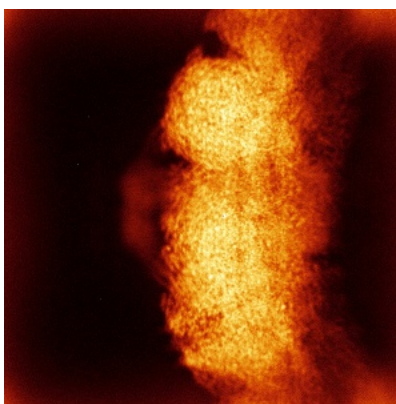


Z

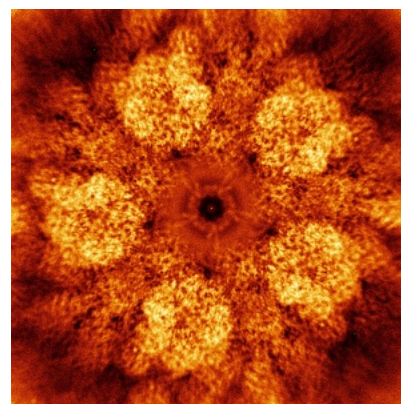
6.4.2 Raw map



X



Y

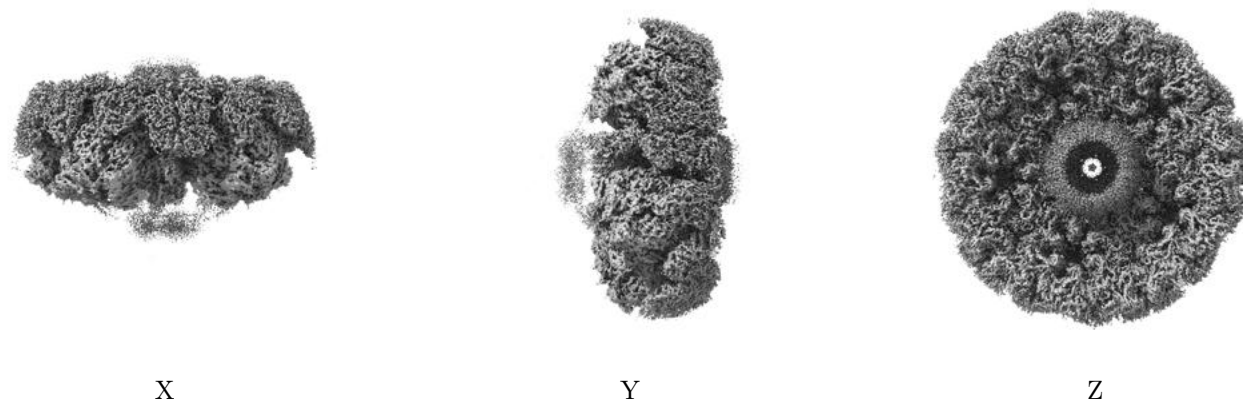


Z

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 0.096. 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.

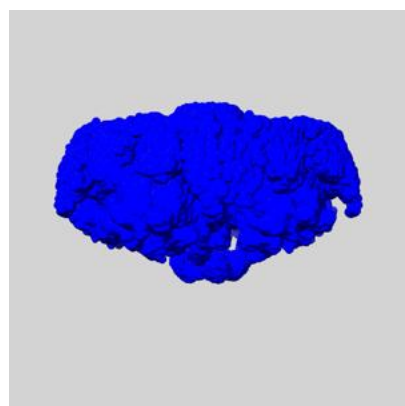
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

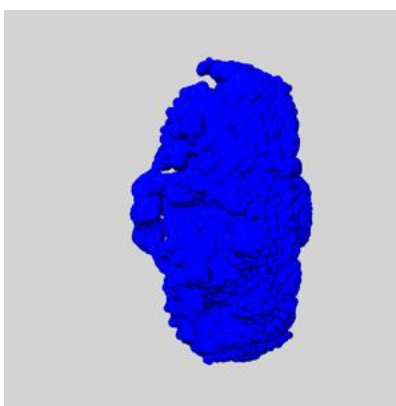
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

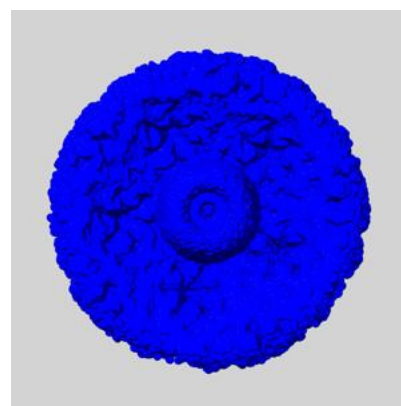
6.6.1 emd_70687_msk_1.map [i](#)



X



Y

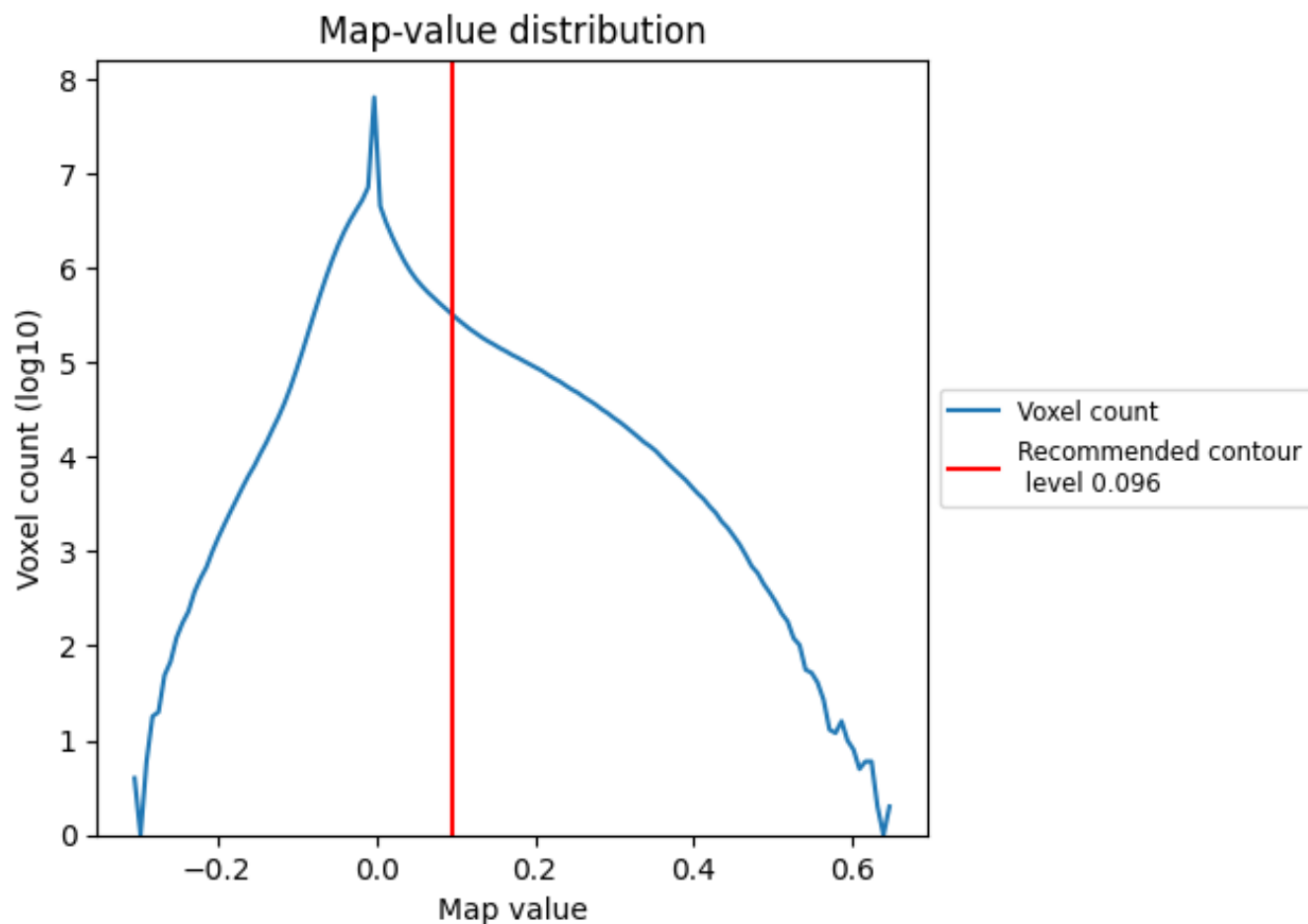


Z

7 Map analysis [i](#)

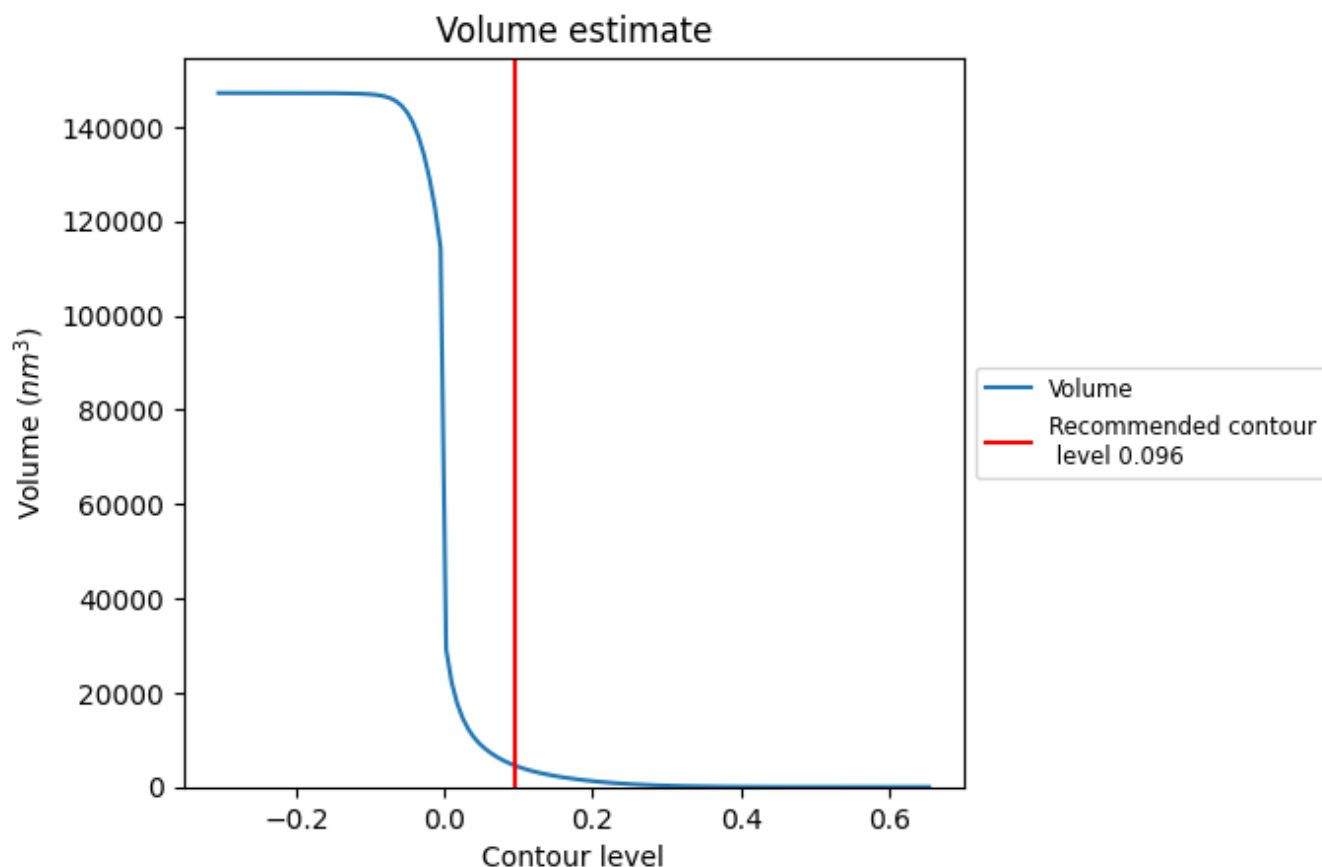
This section contains the results of statistical analysis of the map.

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.

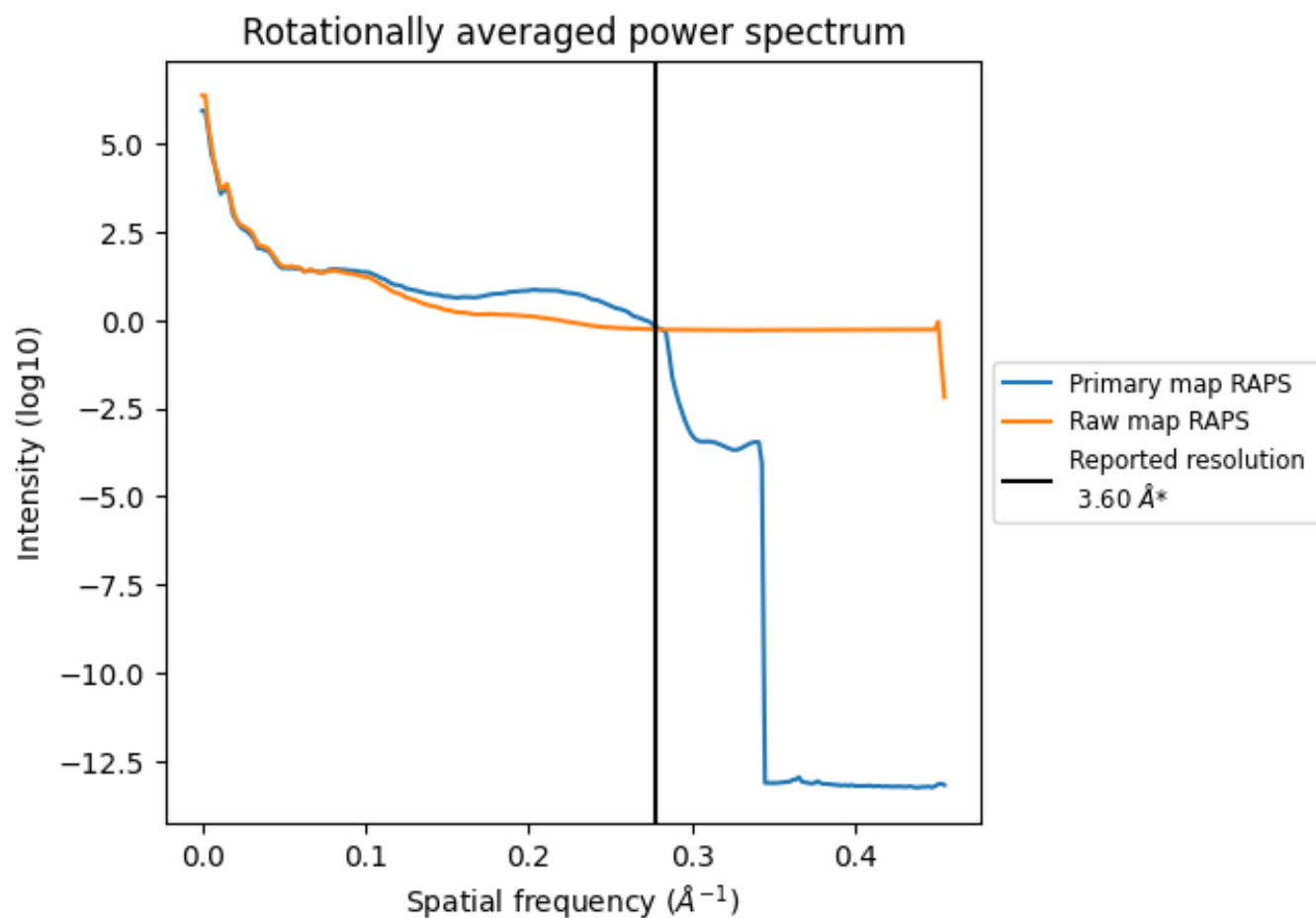
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4513 nm^3 ; this corresponds to an approximate mass of 4076 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 ⓘ

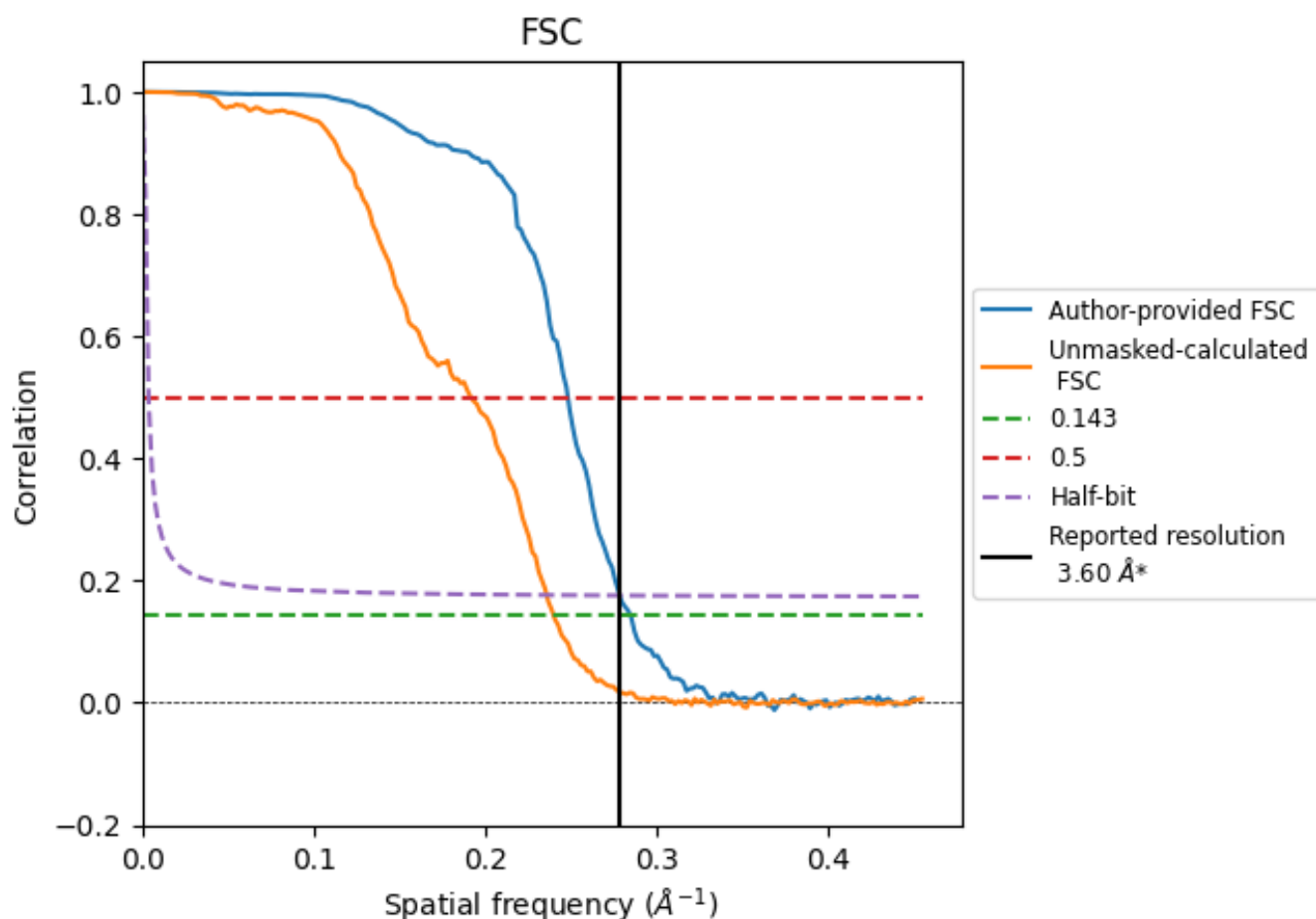


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

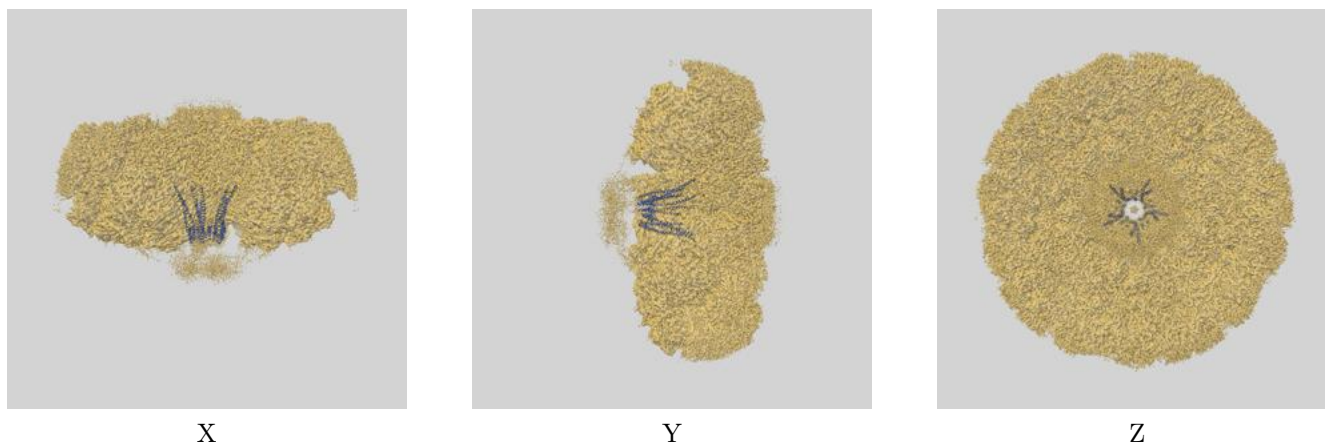
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.51	4.03	3.59
Unmasked-calculated*	4.17	5.22	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

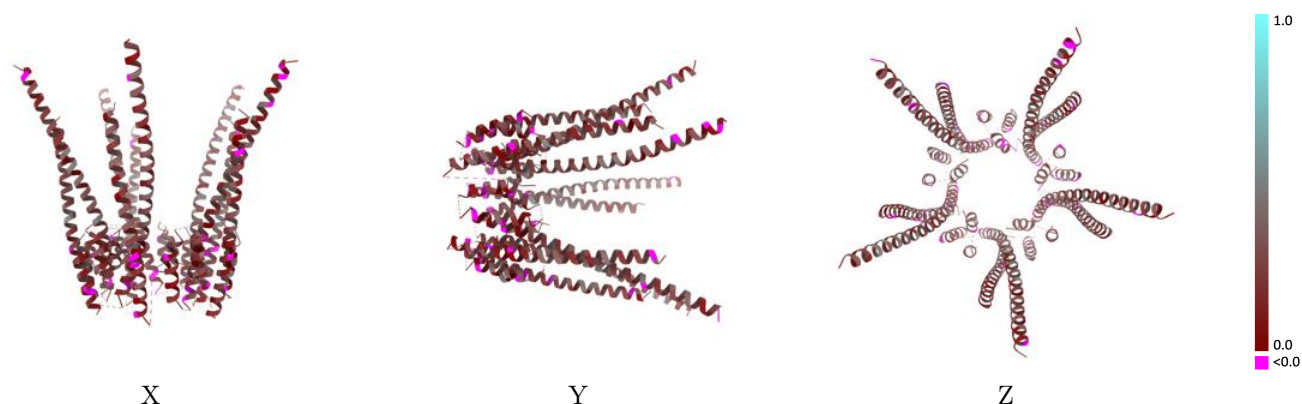
This section contains information regarding the fit between EMDB map EMD-70687 and PDB model 9OPB. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



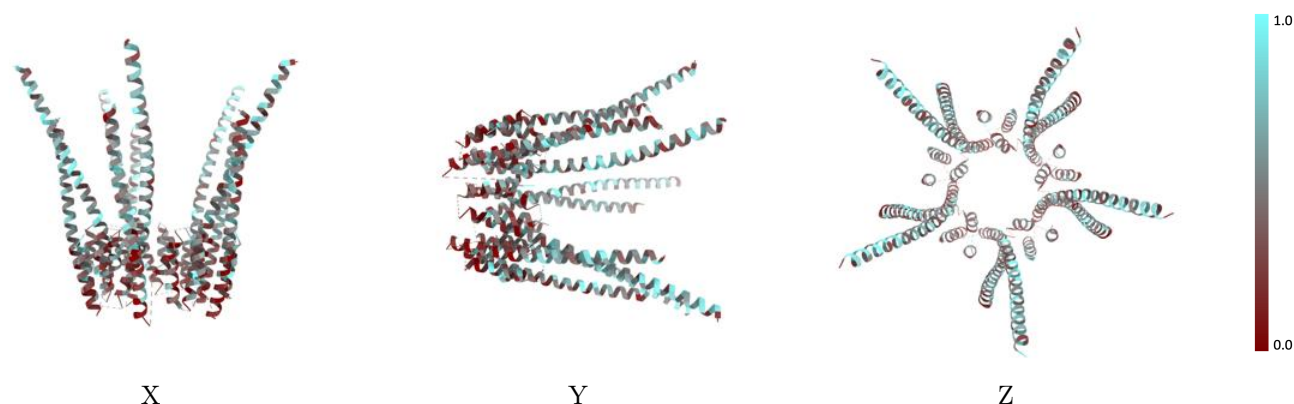
The images above show the 3D surface view of the map at the recommended contour level 0.096 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



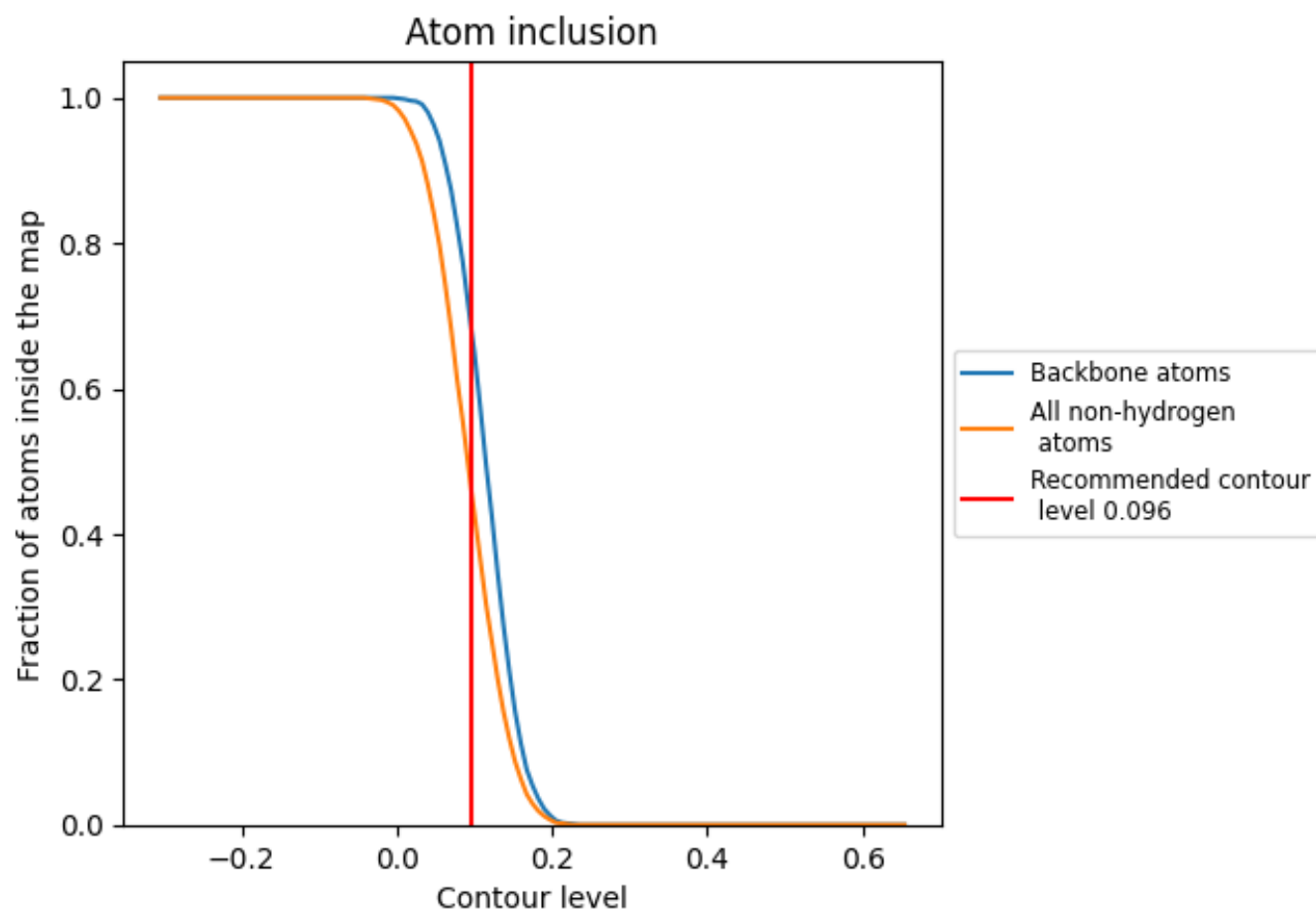
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.096).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 46% 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 (0.096) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4590	0.2160
M	0.4020	0.1930
N	0.4720	0.2130
O	0.4330	0.1970
P	0.4880	0.2190
Q	0.4420	0.2320
R	0.4880	0.2250
S	0.4270	0.2000
T	0.4770	0.2290
U	0.4660	0.2280
V	0.4870	0.2210

