



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 08:57 am BST

PDB ID : 9TIR / pdb_00009tir
EMDB ID : EMD-55967
Title : Phage 812 baseplate in the post-contraction state (C6)
Authors : Binovsky, J.; Plevka, P.
Deposited on : 2025-12-05
Resolution : 4.40 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:

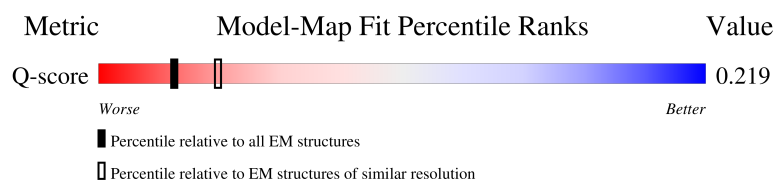
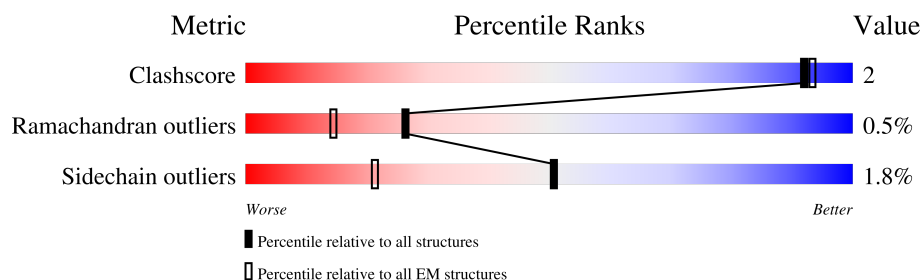
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 4.40 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.



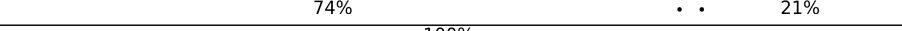
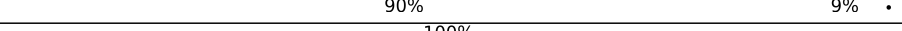
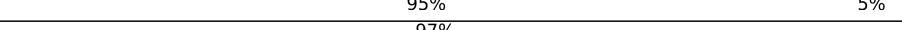
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	A	234	95% .
2	B	348	97% .
2	C	348	95% 5%
3	D	1019	39% 5% . 55%

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Mol	Chain	Length	Quality of chain
4	E	173	 87% 10% ...
4	F	173	 85% 11% ...
4	G	173	 7% 91% 6% ..
4	H	173	 25% 86% 9% ...
4	I	173	 96% 83% 12% ..
4	J	173	 99% 86% 12% ...
5	K	1152	 75% . 21%
5	L	1152	 75% . 21%
5	M	1152	 75% . 21%
5	N	1152	 73% 5% . 21%
5	O	1152	 10% 73% 5% . 21%
5	P	1152	 7% 74% . . 21%
6	Q	458	 100% 90% 9% .
6	R	458	 100% 95% 5%
6	S	458	 97% 91% 7% .
7	T	587	 86% 6% 8%
7	U	587	 89% 5% 6%
7	V	587	 6% 90% 5% 6%
7	W	587	 90% . 6%
7	X	587	 88% 5% . 6%
7	Y	587	 90% . 6%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 98678 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 ORF61.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	234	Total	C	N	O	S	0	0
			1871	1174	314	377	6		

- Molecule 2 is a protein called ORF62.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
2	C	347	Total	C	N	O	S	0	0
			2752	1729	458	559	6		

- Molecule 3 is a protein called ORF63.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	457	Total	C	N	O	S	0	0
			3769	2412	610	738	9		

- Molecule 4 is a protein called ORF64.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	170	Total	C	N	O	S	0	0
			1336	849	219	267	1		
4	F	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
4	G	170	Total	C	N	O	S	0	0
			1336	849	219	267	1		
4	H	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
4	I	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
4	J	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		

- Molecule 5 is a protein called ORF65.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
5	L	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
5	M	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
5	N	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
5	O	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
5	P	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		

- Molecule 6 is a protein called ORF68.

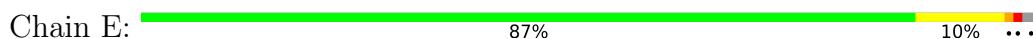
Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
6	R	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
6	S	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		

- Molecule 7 is a protein called ORF49.

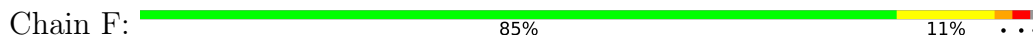
Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	540	Total	C	N	O	S	0	0
			4213	2653	714	839	7		
7	U	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
7	V	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
7	W	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
7	X	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
7	Y	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		

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

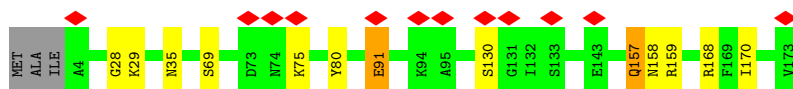
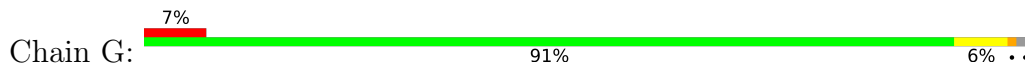
- Molecule 4: ORF64



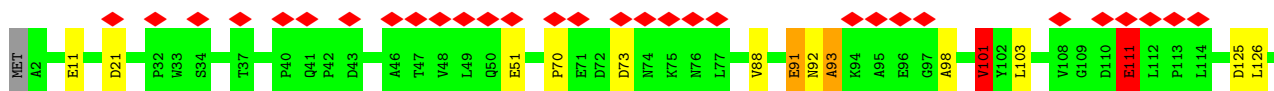
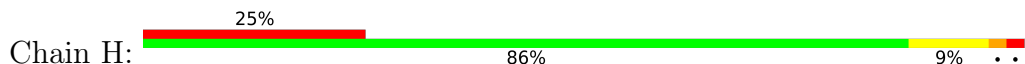
- Molecule 4: ORF64



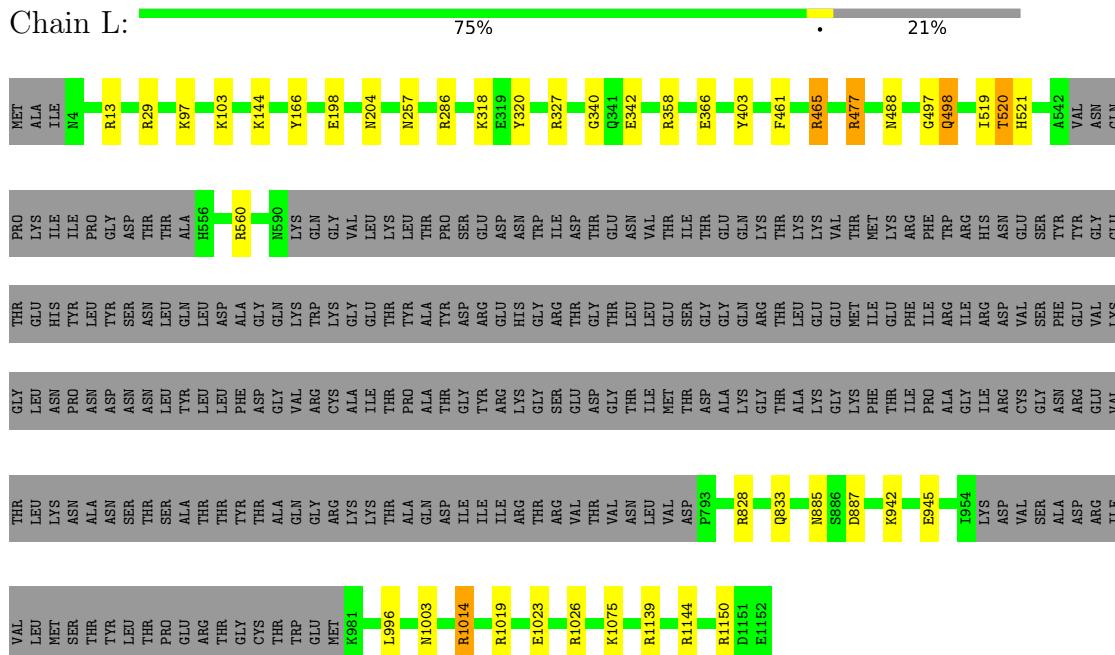
- Molecule 4: ORF64



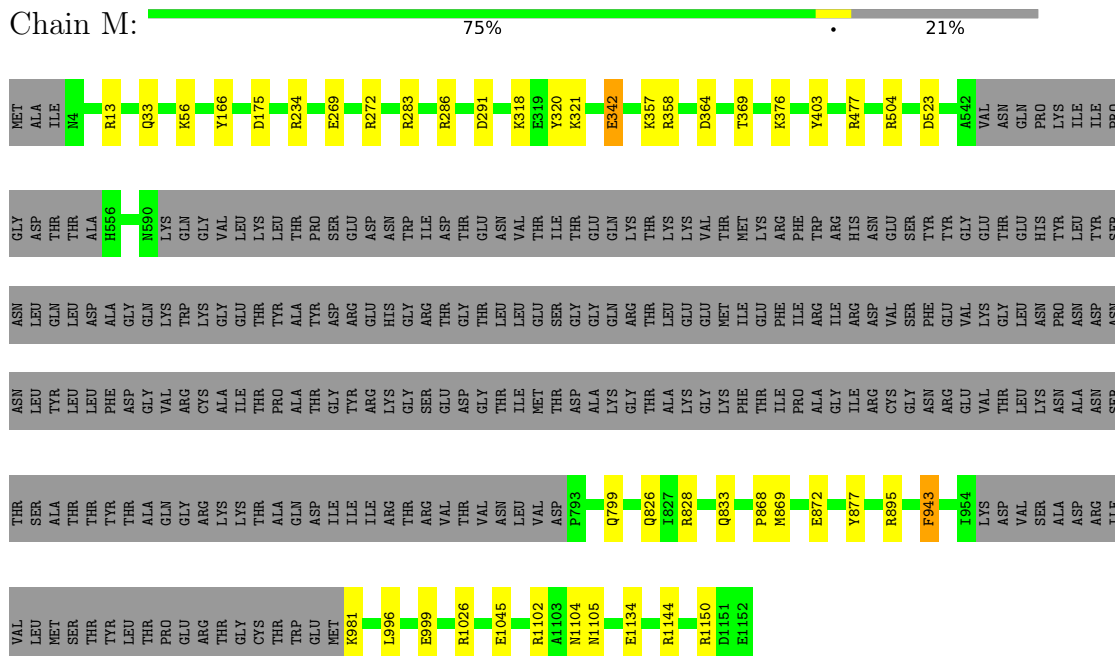
- Molecule 4: ORF64



- Molecule 5: ORF65



- Molecule 5: ORF65

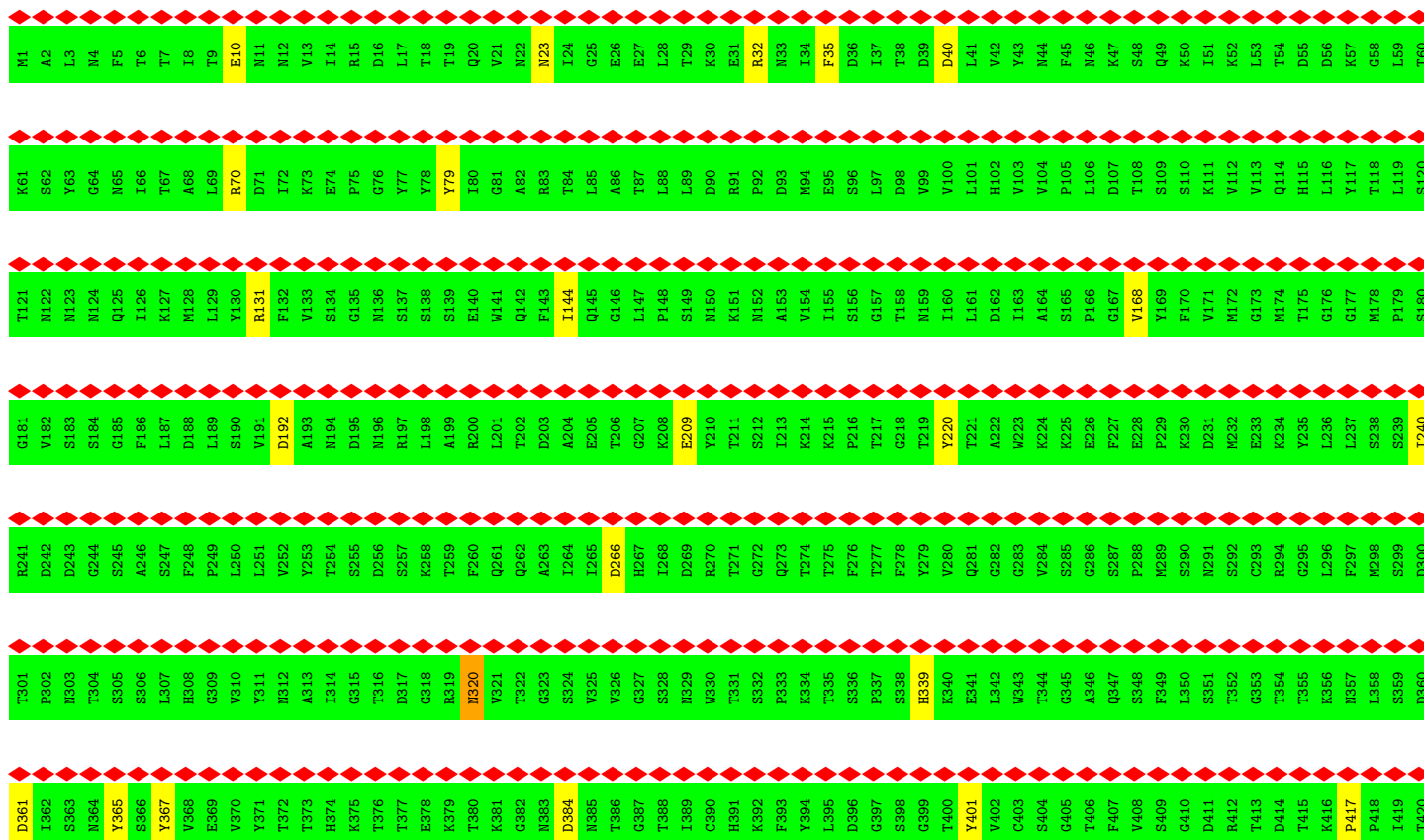


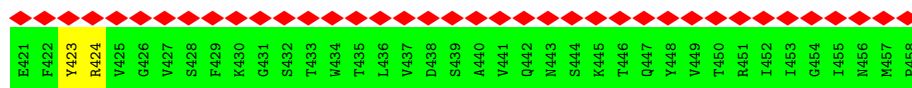
- Molecule 5: ORF65



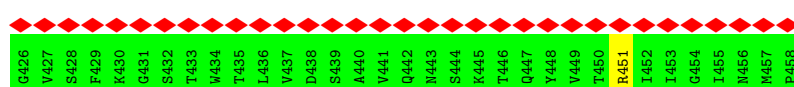
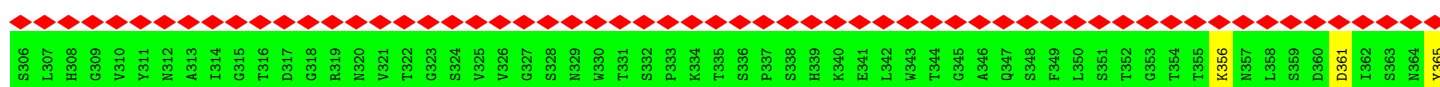
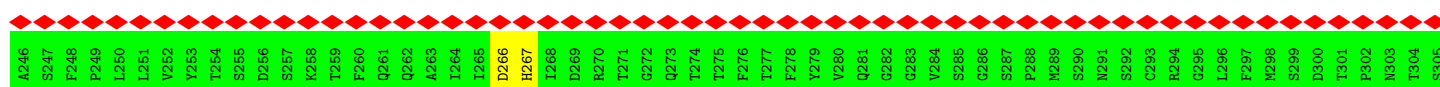
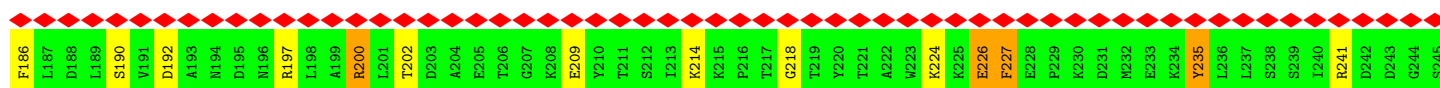
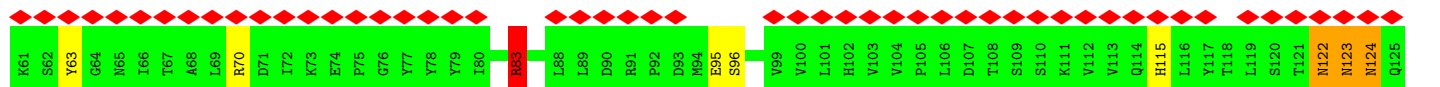
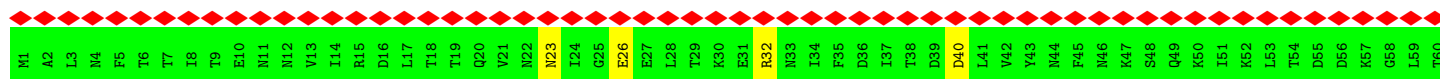
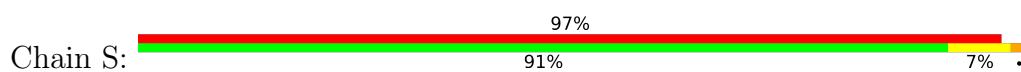


- Molecule 6: ORF68

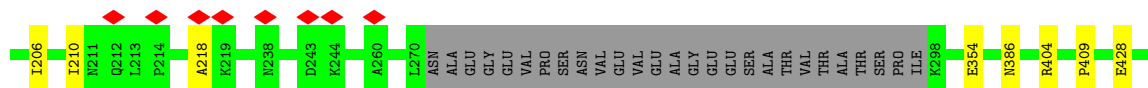
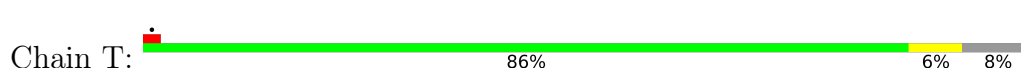




• Molecule 6: ORF68

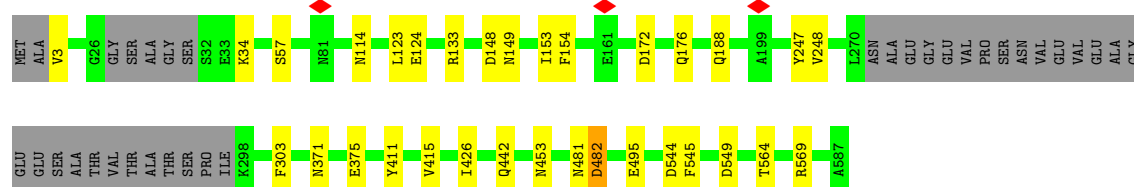


• Molecule 7: ORF49



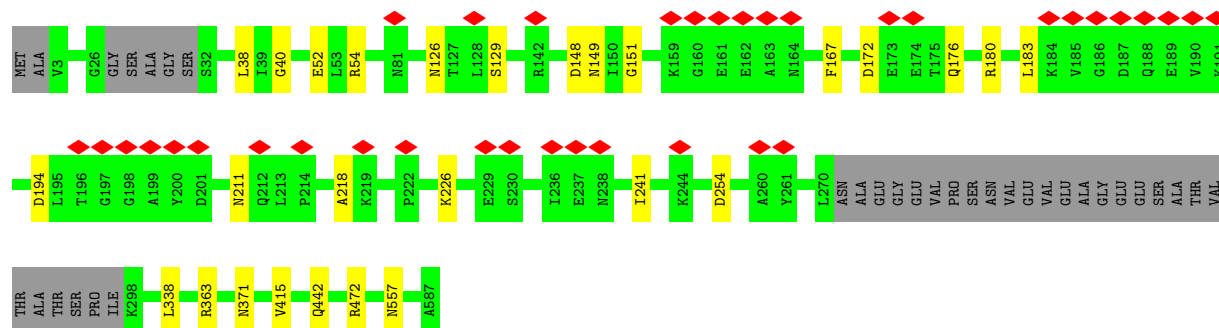
- Molecule 7: ORF49

Chain U: 

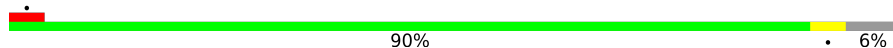


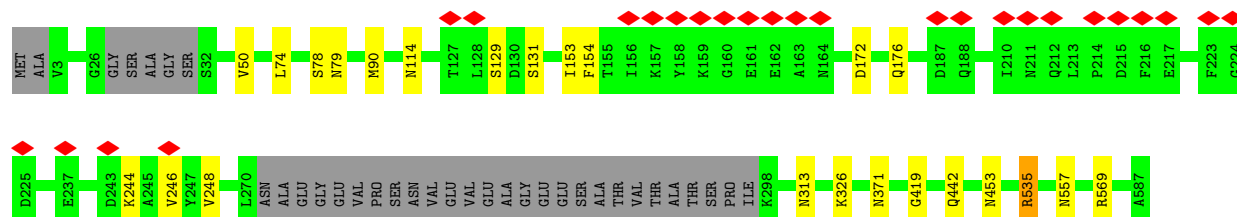
- Molecule 7: ORF49

Chain V: 



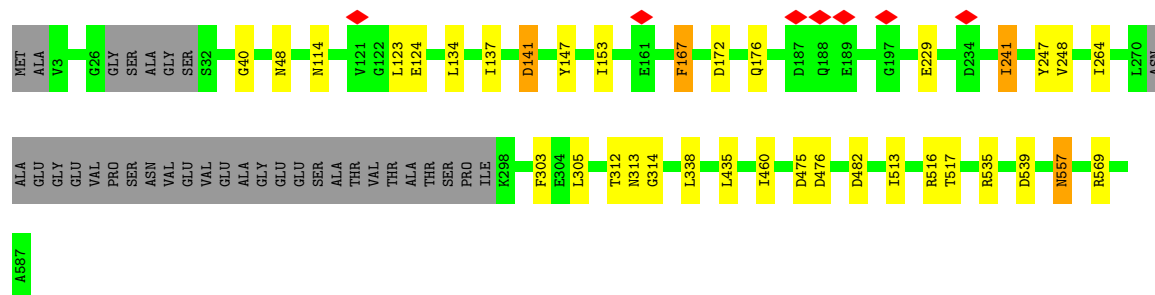
- Molecule 7: ORF49

Chain W: 

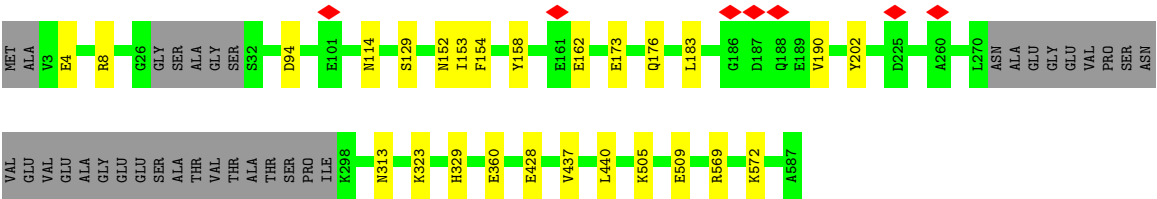
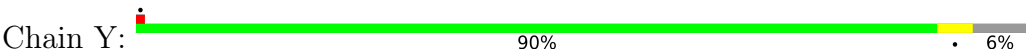


- Molecule 7: ORF49

Chain X: 



- Molecule 7: ORF49



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	21264	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 ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	1352.9601, 1352.9601, 1352.9601	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.114, 2.114, 2.114	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.23	0/1902	0.49	0/2572
2	B	0.41	0/2803	0.74	0/3794
2	C	0.21	0/2795	0.44	0/3784
3	D	0.70	1/3852 (0.0%)	1.30	30/5218 (0.6%)
4	E	0.72	0/1364	1.40	7/1854 (0.4%)
4	F	0.79	0/1377	1.44	7/1872 (0.4%)
4	G	0.72	0/1364	1.36	5/1854 (0.3%)
4	H	0.72	0/1377	1.39	8/1872 (0.4%)
4	I	0.73	0/1377	1.41	11/1872 (0.6%)
4	J	0.75	0/1377	1.42	6/1872 (0.3%)
5	K	0.71	0/7308	1.26	17/9911 (0.2%)
5	L	0.71	0/7308	1.27	18/9911 (0.2%)
5	M	0.71	0/7308	1.25	16/9911 (0.2%)
5	N	0.71	0/7308	1.28	29/9911 (0.3%)
5	O	0.75	0/7308	1.31	27/9911 (0.3%)
5	P	0.72	0/7308	1.29	23/9911 (0.2%)
6	Q	0.77	0/3619	1.34	18/4913 (0.4%)
6	R	0.76	0/3619	1.29	13/4913 (0.3%)
6	S	0.78	0/3619	1.34	17/4913 (0.3%)
7	T	0.24	0/4280	0.48	0/5777
7	U	0.33	0/4392	0.63	0/5930
7	V	0.35	0/4392	0.64	1/5930 (0.0%)
7	W	0.32	0/4392	0.62	1/5930 (0.0%)
7	X	0.28	0/4392	0.56	0/5930
7	Y	0.21	0/4392	0.45	0/5930
All	All	0.62	1/100533 (0.0%)	1.11	254/136196 (0.2%)

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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
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Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	7
4	E	0	2
4	F	0	3
4	G	0	2
4	H	0	1
4	I	0	1
4	J	0	1
5	K	0	10
5	L	0	6
5	M	0	7
5	N	0	8
5	O	0	13
5	P	0	5
6	Q	0	7
6	R	0	6
6	S	0	7
7	V	0	1
7	W	0	1
All	All	0	88

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	364	PRO	CA-C	5.34	1.54	1.51

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	227	PHE	N-CA-C	11.22	126.72	108.55
3	D	462	ASP	CA-CB-CG	11.11	123.71	112.60
3	D	191	LEU	N-CA-C	10.90	125.94	112.87
5	N	311	THR	CA-CB-CG2	9.89	127.31	110.50
3	D	280	ALA	CB-CA-C	9.55	131.02	110.19

There are no chirality outliers.

5 of 88 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	176	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	D	203	PHE	Sidechain
3	D	216	HIS	Sidechain
3	D	418	ARG	Sidechain
3	D	426	ARG	Sidechain

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	A	1871	0	1828	9	0
2	B	2760	0	2729	6	0
2	C	2752	0	2717	8	0
3	D	3769	0	3640	64	0
4	E	1336	0	1323	14	0
4	F	1349	0	1339	26	0
4	G	1336	0	1323	5	0
4	H	1349	0	1339	7	0
4	I	1349	0	1339	5	0
4	J	1349	0	1339	6	0
5	K	7166	0	6971	6	0
5	L	7166	0	6971	16	0
5	M	7166	0	6971	16	0
5	N	7166	0	6971	30	0
5	O	7166	0	6971	24	0
5	P	7166	0	6971	23	0
6	Q	3548	0	3468	9	0
6	R	3548	0	3468	3	0
6	S	3548	0	3468	23	0
7	T	4213	0	4167	21	0
7	U	4321	0	4280	17	0
7	V	4321	0	4280	16	0
7	W	4321	0	4280	14	0
7	X	4321	0	4280	22	0
7	Y	4321	0	4280	14	0
All	All	98678	0	96713	295	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 2.

The worst 5 of 295 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)
5:O:314:GLY:CA	6:S:122:ASN:HD21	1.27	1.44
5:O:314:GLY:CA	6:S:122:ASN:ND2	2.01	1.24
3:D:280:ALA:HB3	5:P:130:VAL:HG21	1.31	1.08
5:O:314:GLY:N	6:S:122:ASN:ND2	2.07	1.00
5:O:314:GLY:HA3	6:S:122:ASN:HD21	0.87	1.00

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	A	232/234 (99%)	223 (96%)	9 (4%)	0	100	100
2	B	346/348 (99%)	341 (99%)	5 (1%)	0	100	100
2	C	345/348 (99%)	339 (98%)	6 (2%)	0	100	100
3	D	451/1019 (44%)	407 (90%)	41 (9%)	3 (1%)	18	55
4	E	168/173 (97%)	156 (93%)	9 (5%)	3 (2%)	6	33
4	F	170/173 (98%)	160 (94%)	10 (6%)	0	100	100
4	G	168/173 (97%)	156 (93%)	9 (5%)	3 (2%)	6	33
4	H	170/173 (98%)	152 (89%)	11 (6%)	7 (4%)	2	18
4	I	170/173 (98%)	152 (89%)	13 (8%)	5 (3%)	3	23
4	J	170/173 (98%)	156 (92%)	10 (6%)	4 (2%)	4	27
5	K	900/1152 (78%)	851 (95%)	49 (5%)	0	100	100
5	L	900/1152 (78%)	846 (94%)	52 (6%)	2 (0%)	43	77
5	M	900/1152 (78%)	856 (95%)	43 (5%)	1 (0%)	48	83
5	N	900/1152 (78%)	845 (94%)	46 (5%)	9 (1%)	12	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	O	900/1152 (78%)	834 (93%)	58 (6%)	8 (1%)	14	49
5	P	900/1152 (78%)	842 (94%)	52 (6%)	6 (1%)	18	55
6	Q	456/458 (100%)	431 (94%)	23 (5%)	2 (0%)	30	66
6	R	456/458 (100%)	431 (94%)	25 (6%)	0	100	100
6	S	456/458 (100%)	428 (94%)	26 (6%)	2 (0%)	30	66
7	T	534/587 (91%)	502 (94%)	31 (6%)	1 (0%)	43	77
7	U	547/587 (93%)	516 (94%)	31 (6%)	0	100	100
7	V	547/587 (93%)	521 (95%)	26 (5%)	0	100	100
7	W	547/587 (93%)	524 (96%)	23 (4%)	0	100	100
7	X	547/587 (93%)	526 (96%)	21 (4%)	0	100	100
7	Y	547/587 (93%)	522 (95%)	25 (5%)	0	100	100
All	All	12427/14795 (84%)	11717 (94%)	654 (5%)	56 (0%)	26	62

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	70	PRO
4	H	93	ALA
4	I	93	ALA
4	J	93	ALA
4	J	111	GLU

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	A	209/209 (100%)	208 (100%)	1 (0%)	81	81
2	B	311/311 (100%)	310 (100%)	1 (0%)	86	84
2	C	310/311 (100%)	309 (100%)	1 (0%)	86	84
3	D	417/928 (45%)	406 (97%)	11 (3%)	40	60
4	E	151/153 (99%)	144 (95%)	7 (5%)	24	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	152/153 (99%)	142 (93%)	10 (7%)	15	37
4	G	151/153 (99%)	149 (99%)	2 (1%)	61	72
4	H	152/153 (99%)	141 (93%)	11 (7%)	13	35
4	I	152/153 (99%)	137 (90%)	15 (10%)	7	24
4	J	152/153 (99%)	142 (93%)	10 (7%)	15	37
5	K	800/1010 (79%)	790 (99%)	10 (1%)	61	72
5	L	800/1010 (79%)	786 (98%)	14 (2%)	51	67
5	M	800/1010 (79%)	791 (99%)	9 (1%)	65	74
5	N	800/1010 (79%)	781 (98%)	19 (2%)	43	63
5	O	800/1010 (79%)	785 (98%)	15 (2%)	50	66
5	P	800/1010 (79%)	781 (98%)	19 (2%)	43	63
6	Q	405/405 (100%)	396 (98%)	9 (2%)	45	64
6	R	405/405 (100%)	400 (99%)	5 (1%)	63	73
6	S	405/405 (100%)	394 (97%)	11 (3%)	39	59
7	T	459/495 (93%)	456 (99%)	3 (1%)	76	79
7	U	471/495 (95%)	464 (98%)	7 (2%)	57	70
7	V	471/495 (95%)	471 (100%)	0	100	100
7	W	471/495 (95%)	470 (100%)	1 (0%)	87	85
7	X	471/495 (95%)	464 (98%)	7 (2%)	57	70
7	Y	471/495 (95%)	470 (100%)	1 (0%)	87	85
All	All	10986/12922 (85%)	10787 (98%)	199 (2%)	51	67

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	N	1045	GLU
5	P	869	MET
5	N	1087	ASP
5	O	526	ILE
5	P	1045	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
5	N	356	ASN
5	O	590	ASN
7	X	171	HIS
5	N	799	GLN
5	O	276	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](#)

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.

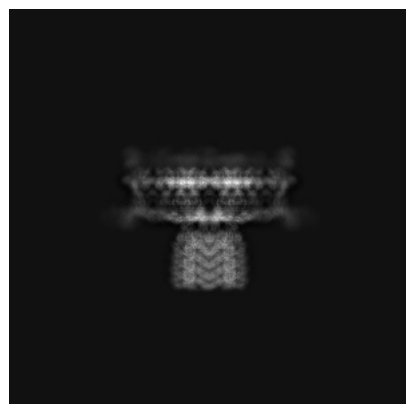
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55967. These allow visual inspection of the internal detail of the map and identification of artifacts.

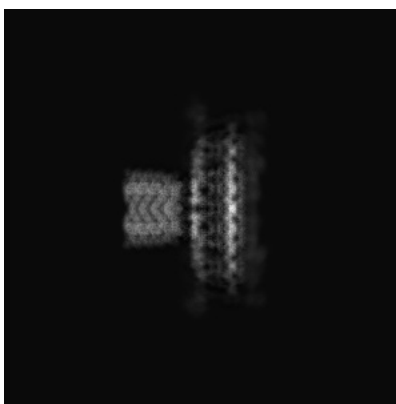
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

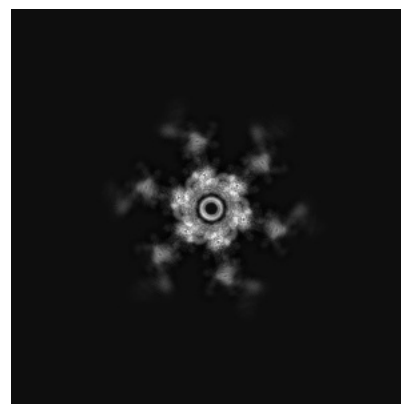
6.1.1 Primary map



X

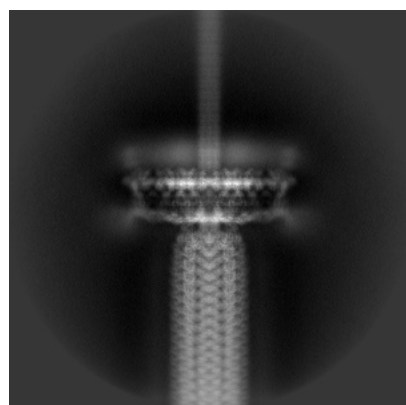


Y

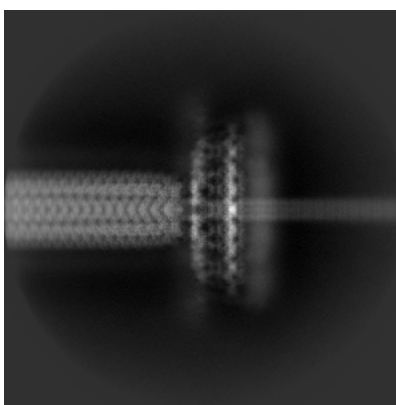


Z

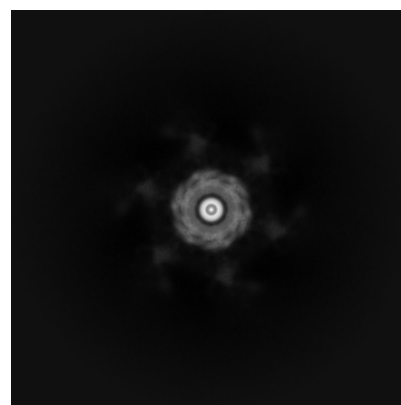
6.1.2 Raw map



X



Y



Z

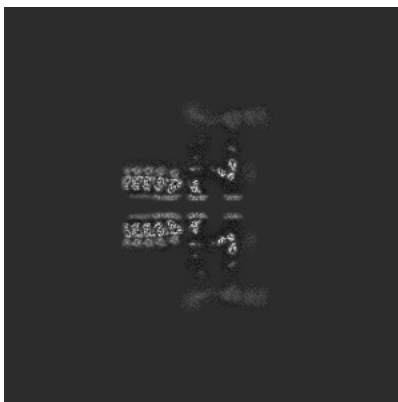
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

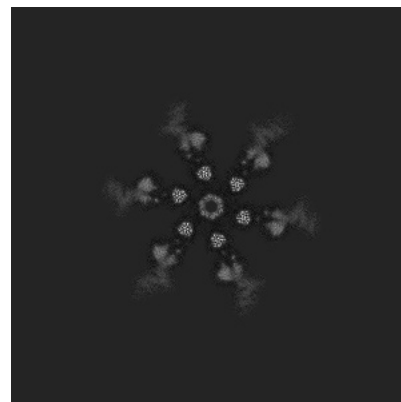
6.2.1 Primary map



X Index: 320

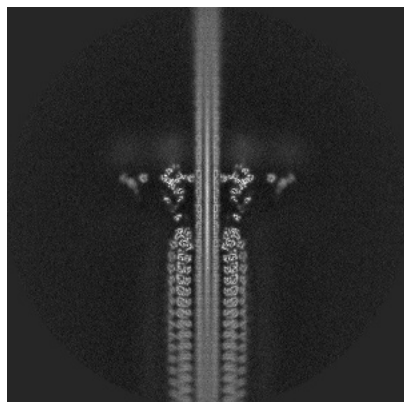


Y Index: 320

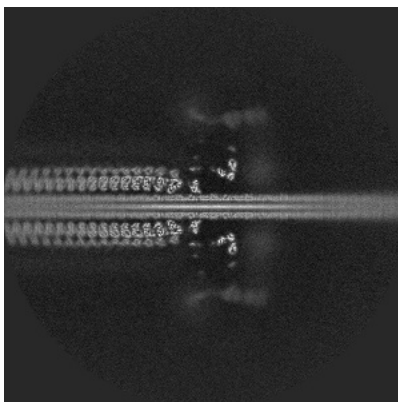


Z Index: 320

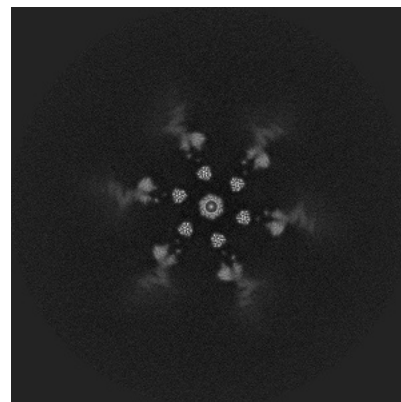
6.2.2 Raw map



X Index: 320



Y Index: 320

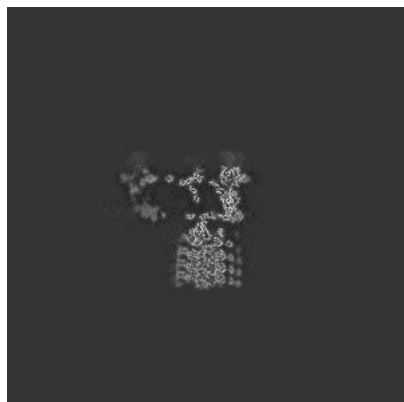


Z Index: 320

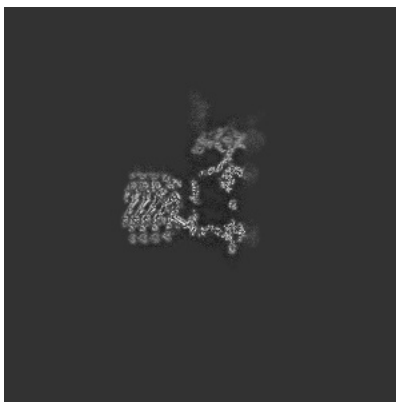
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

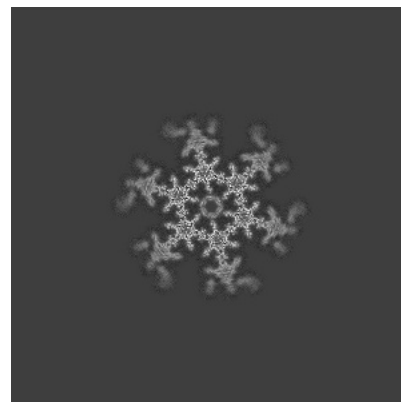
6.3.1 Primary map



X Index: 357

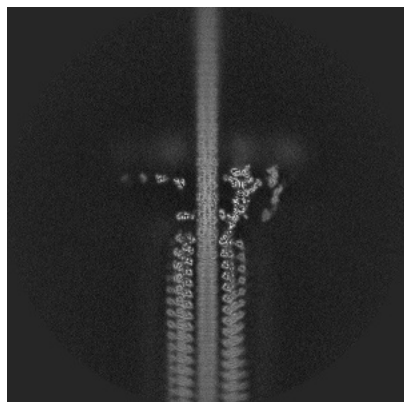


Y Index: 292

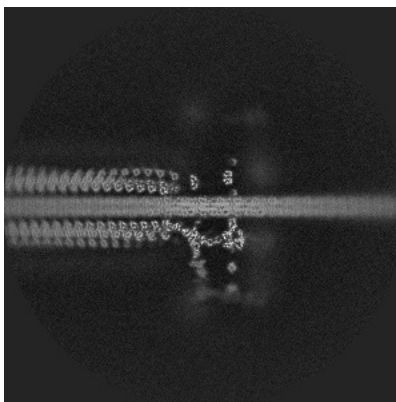


Z Index: 361

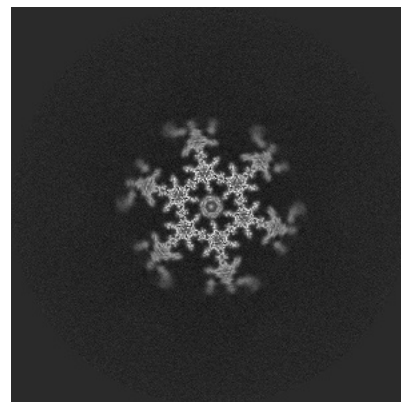
6.3.2 Raw map



X Index: 310



Y Index: 330

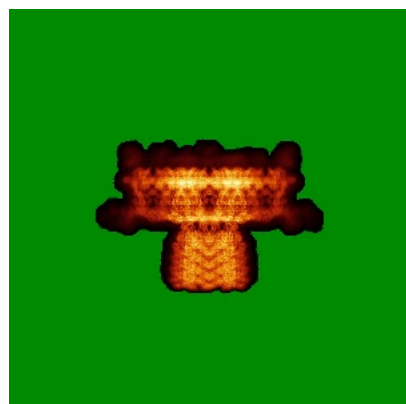


Z Index: 361

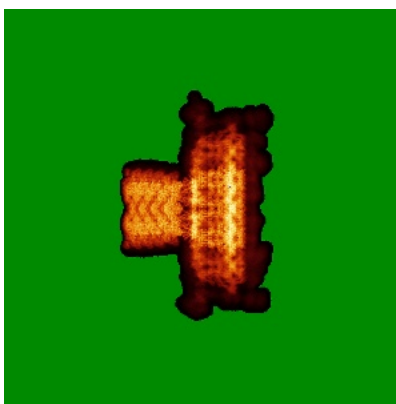
The images above show the largest variance slices of the map in three orthogonal directions.

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

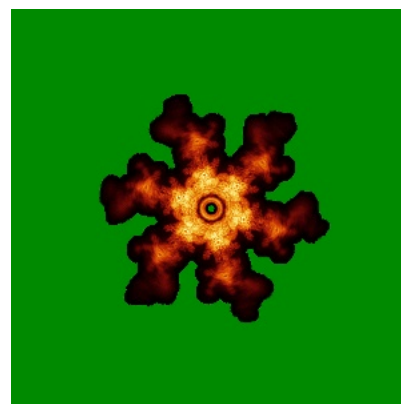
6.4.1 Primary map



X

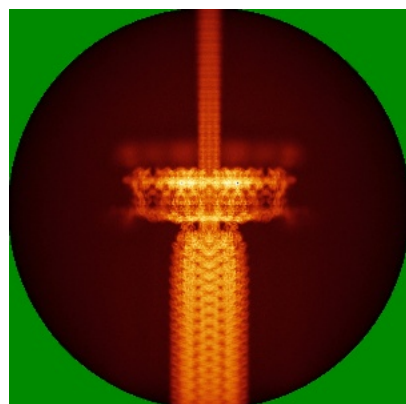


Y

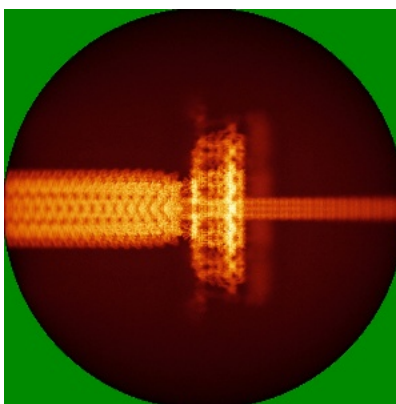


Z

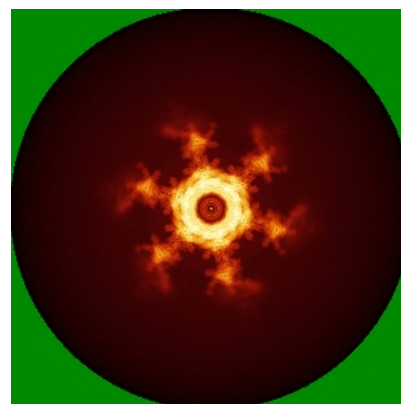
6.4.2 Raw map



X



Y

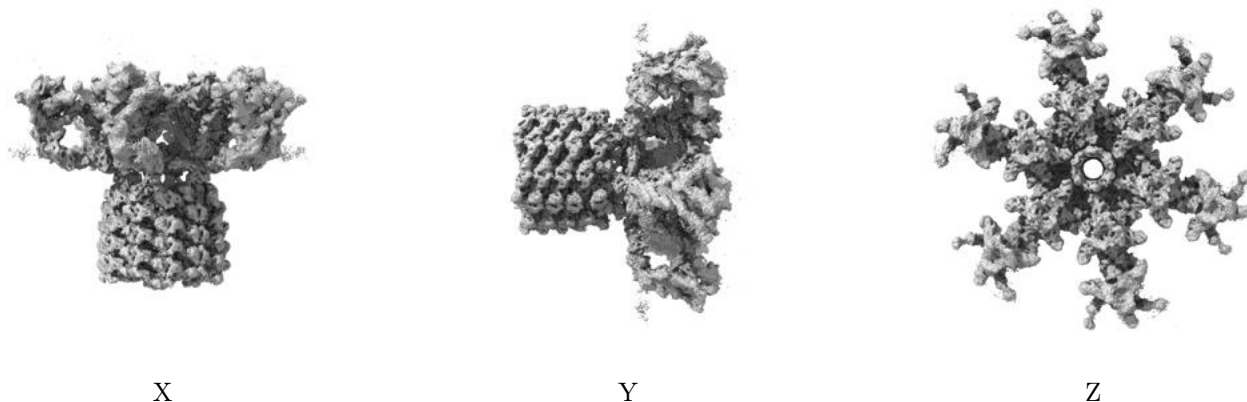


Z

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.

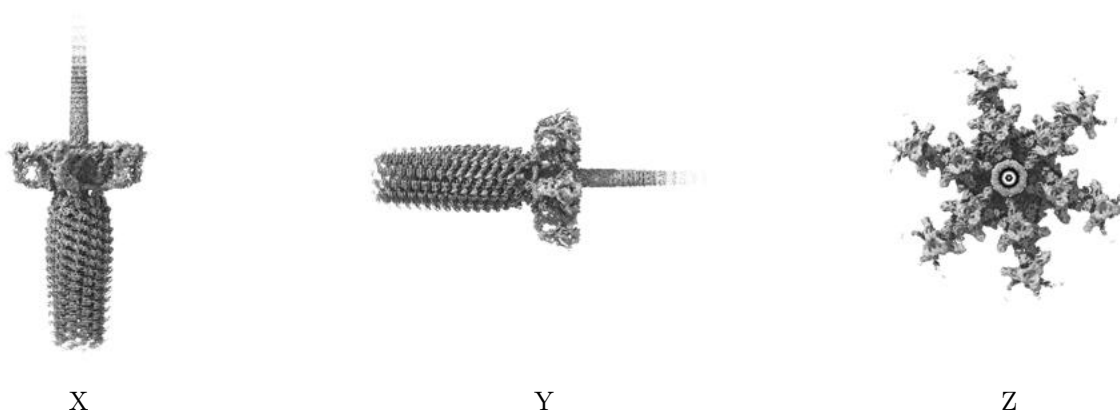
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

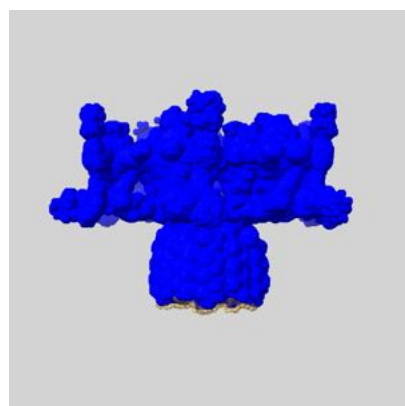
6.6 Mask visualisation [i](#)

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

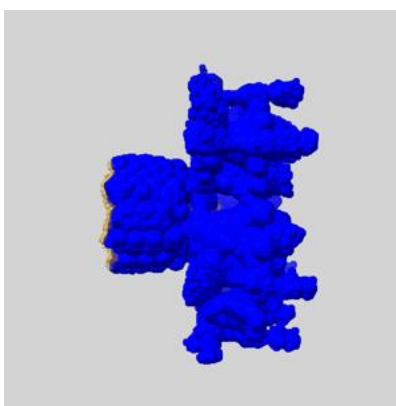
A mask typically either:

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

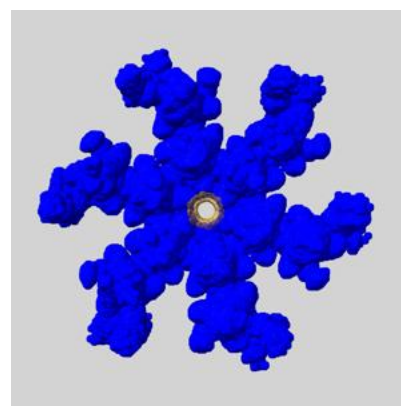
6.6.1 emd_55967_msk_1.map [i](#)



X



Y

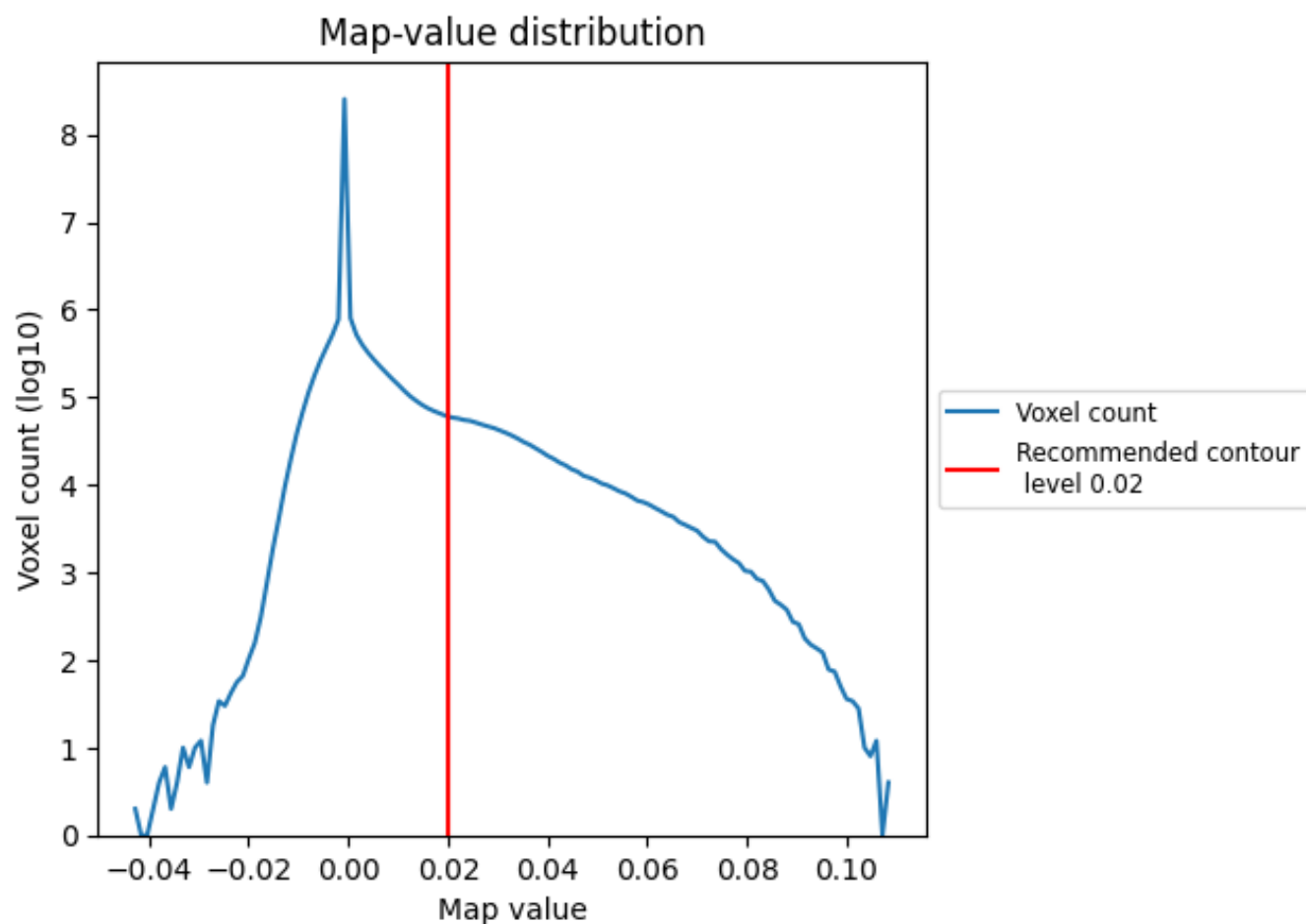


Z

7 Map analysis [i](#)

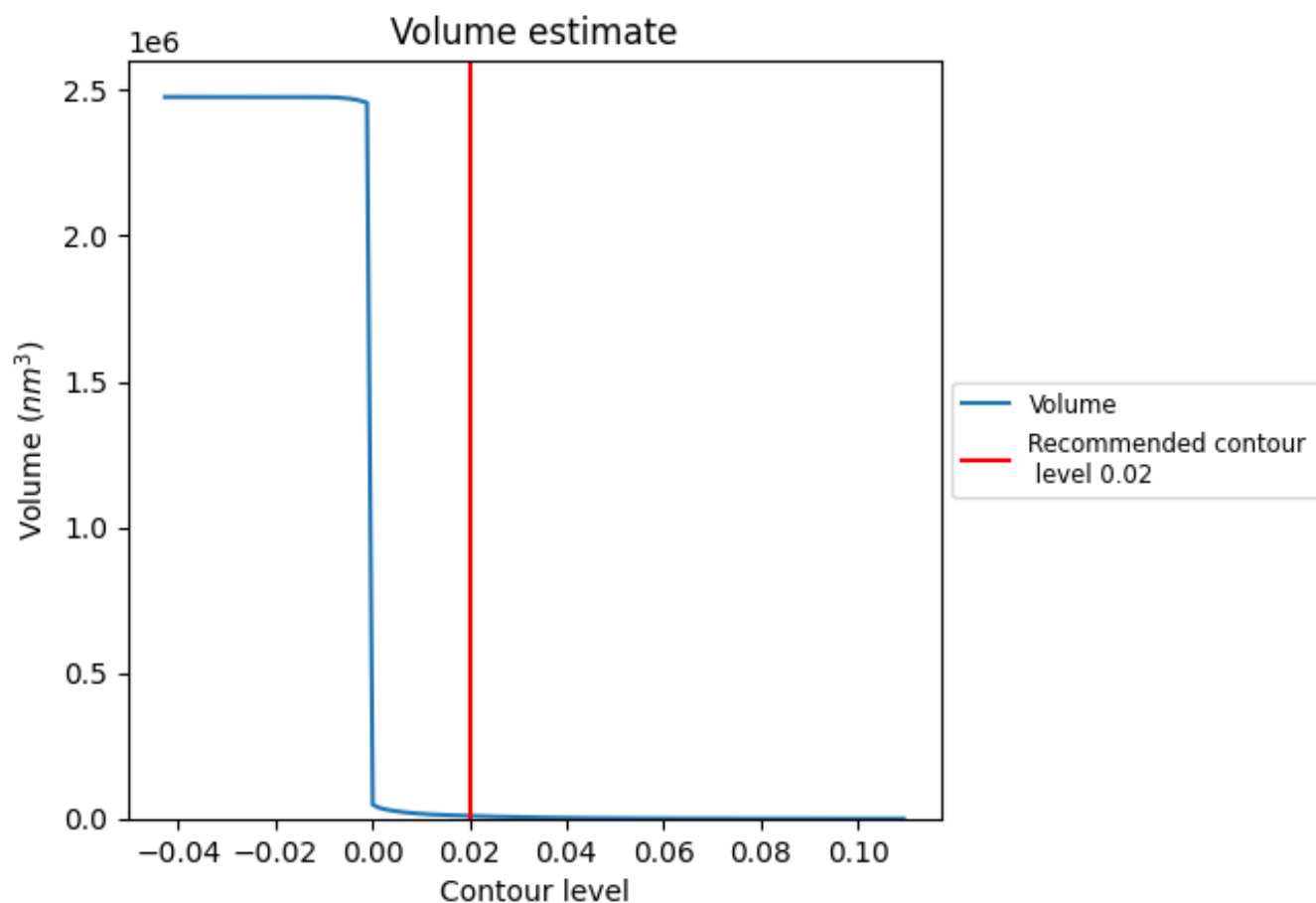
This section contains the results of statistical analysis of the map.

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.

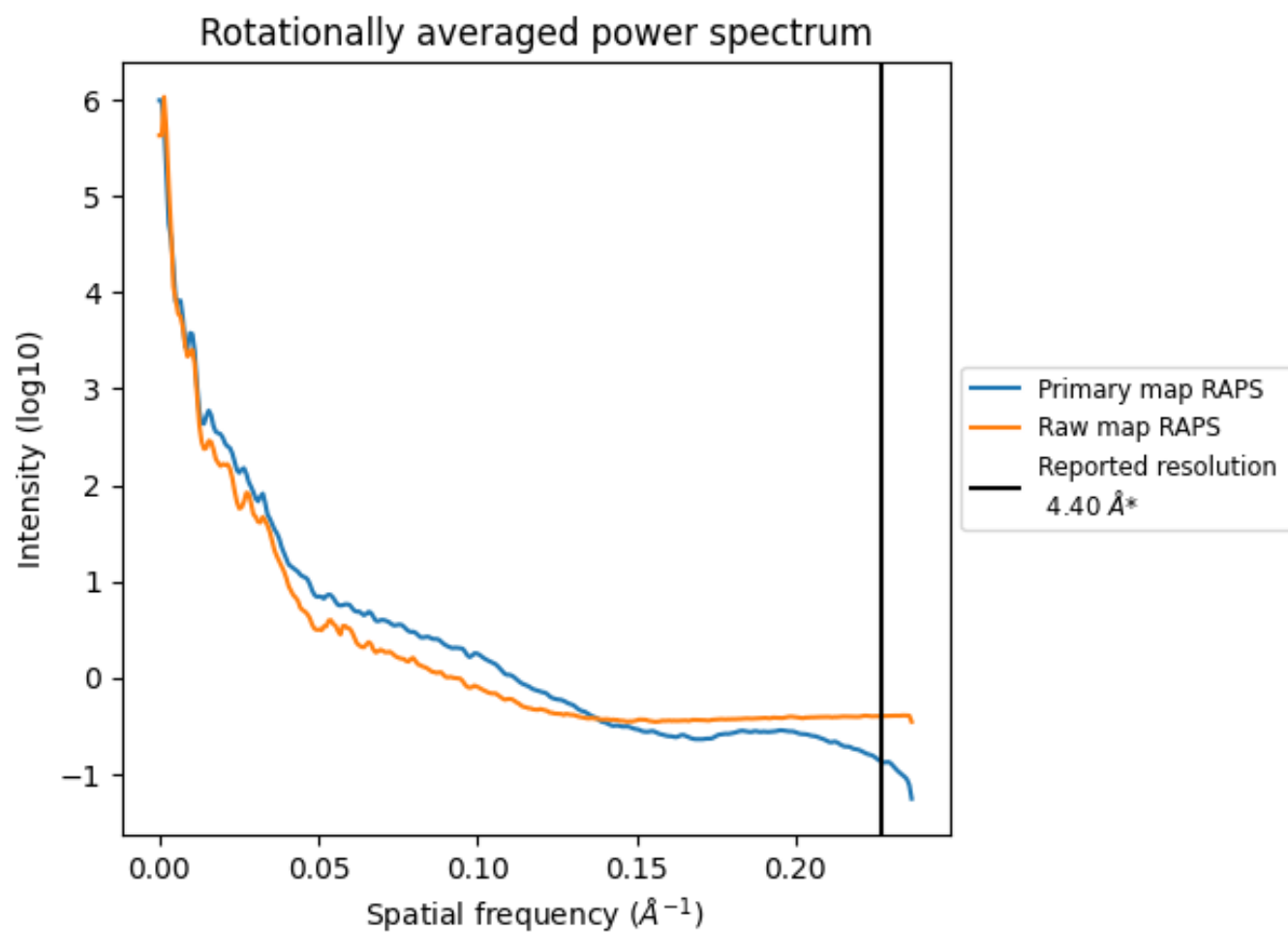
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 9334 nm^3 ; this corresponds to an approximate mass of 8431 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 ⓘ

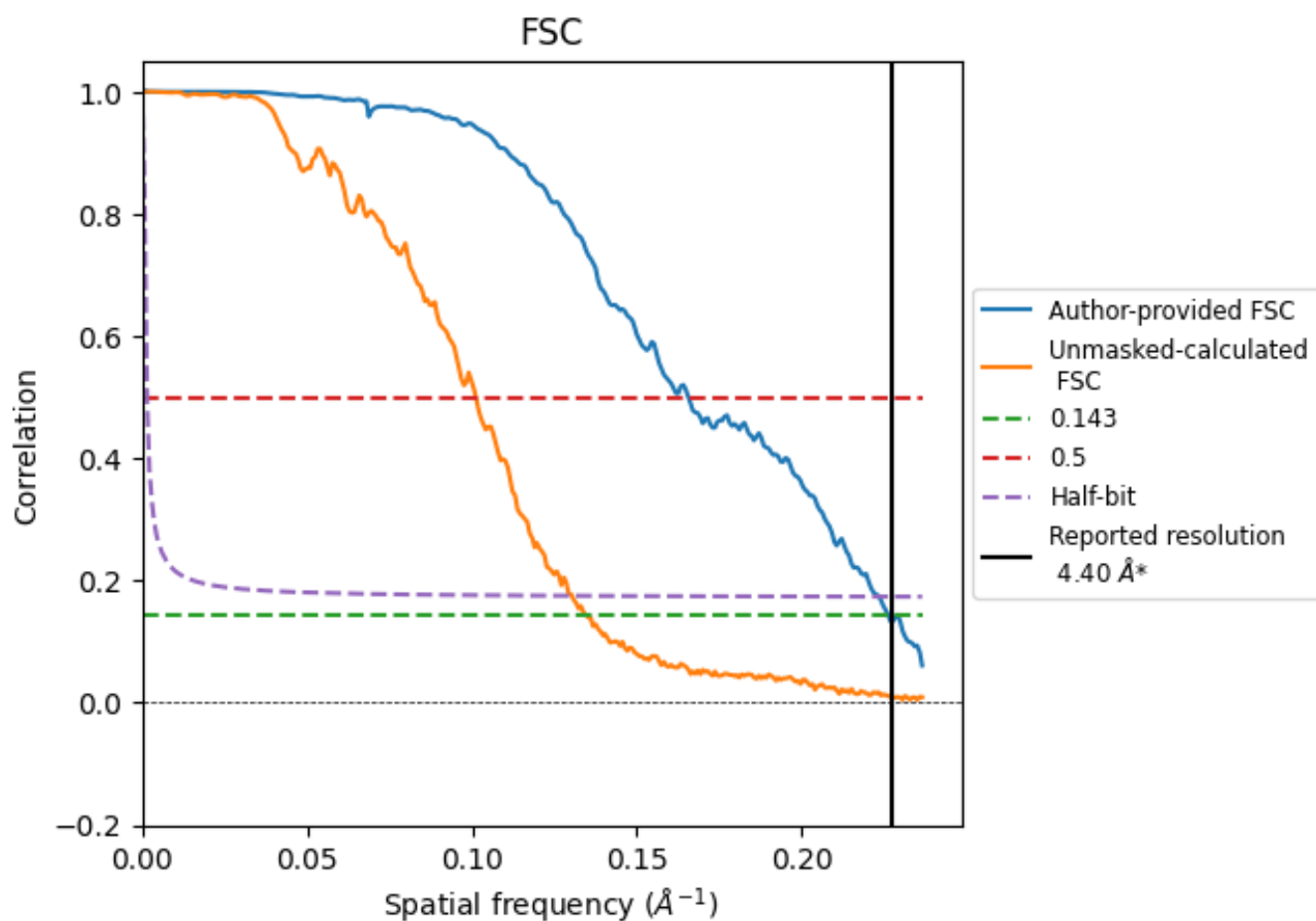


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 $0.227 \text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.42	6.04	4.48
Unmasked-calculated*	7.43	9.88	7.67

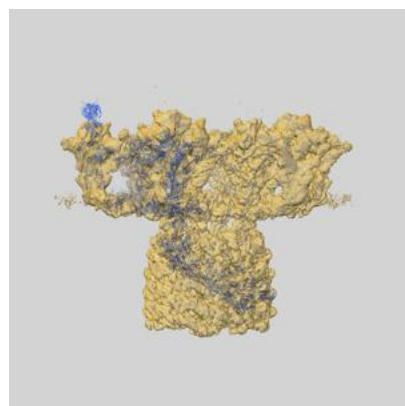
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.43 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

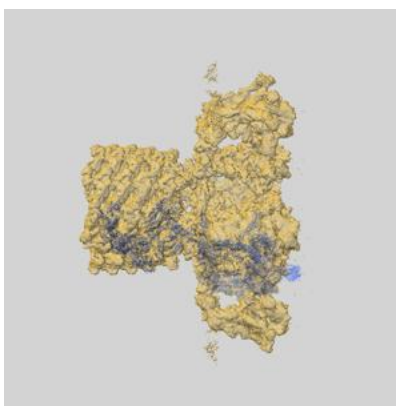
This section contains information regarding the fit between EMDB map EMD-55967 and PDB model 9TIR. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

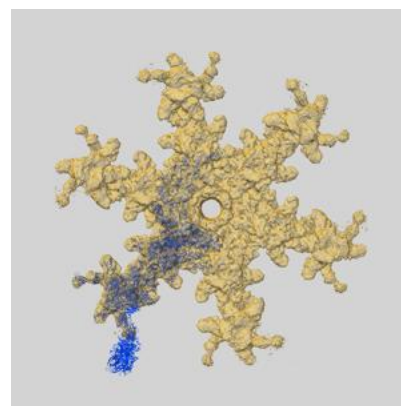
9.1.1 Map-model overlay [i](#)



X

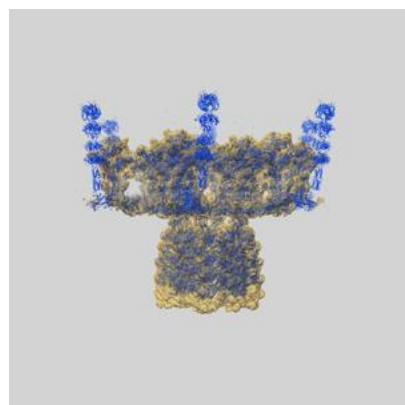


Y

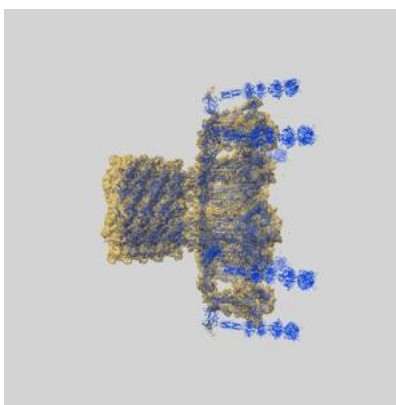


Z

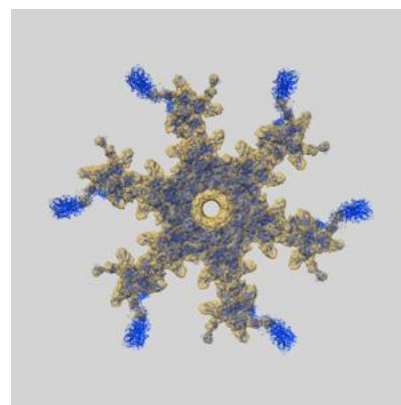
9.1.2 Map-model assembly overlay [i](#)



X



Y



Z

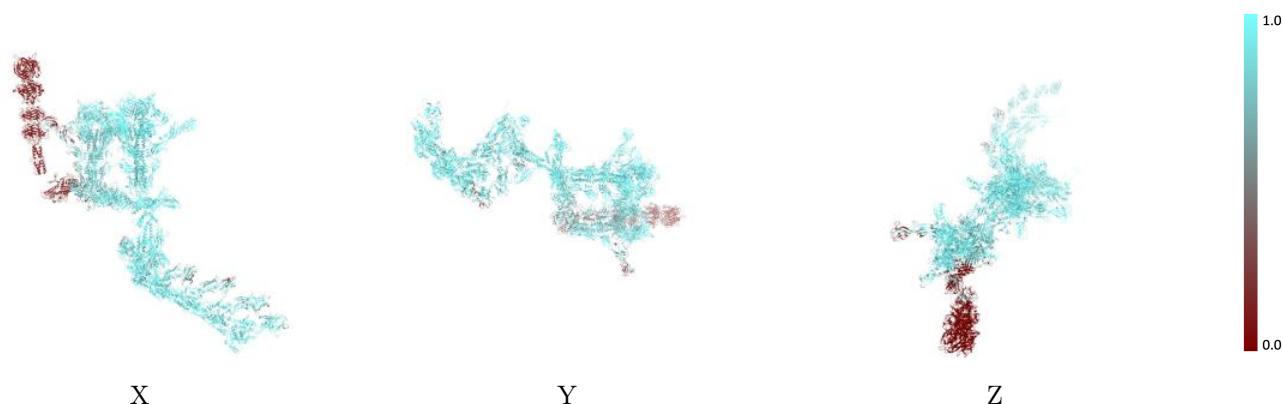
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



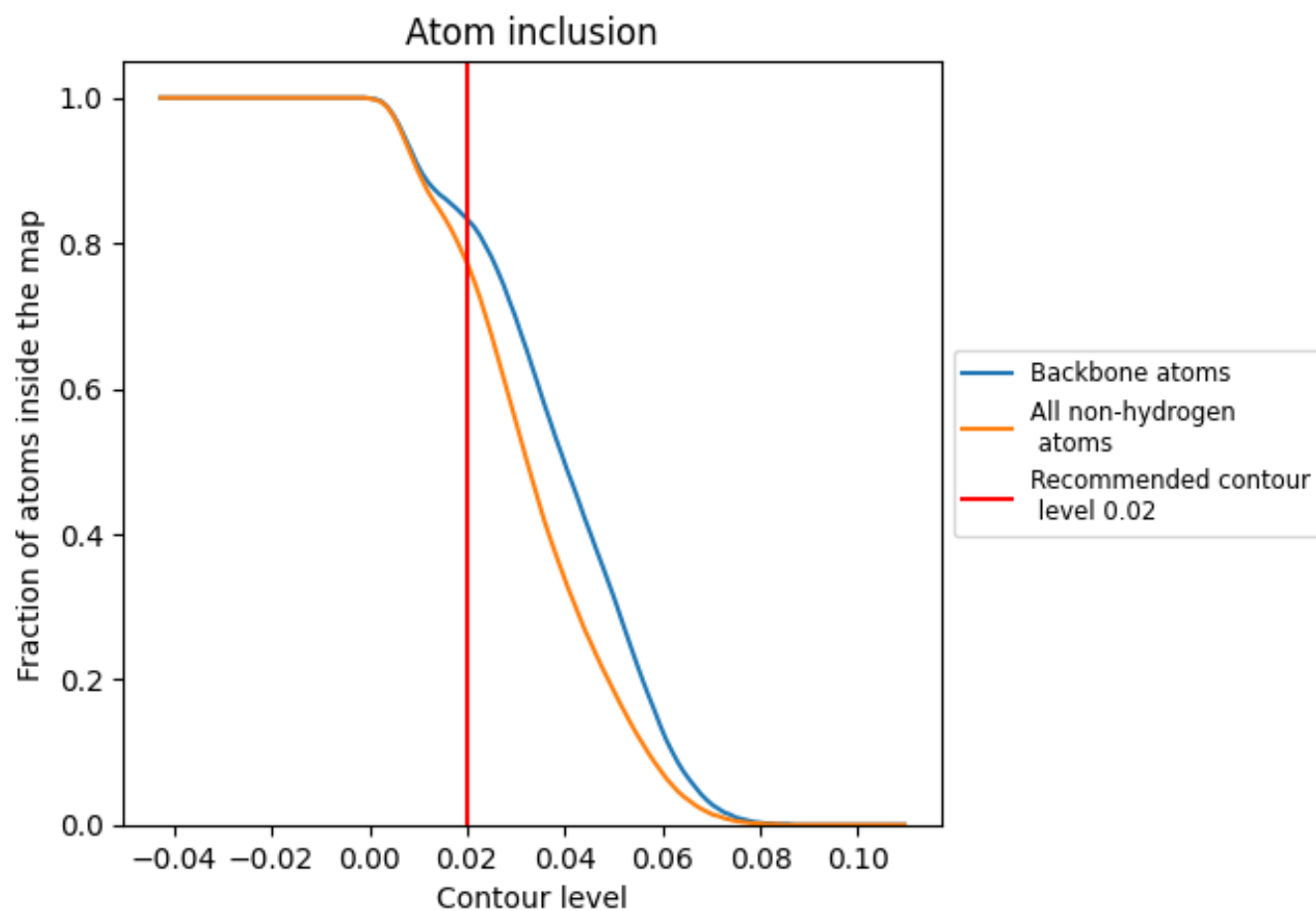
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.2190
A	 0.9240	 0.3200
B	 0.9360	 0.3200
C	 0.9410	 0.3320
D	 0.8400	 0.2060
E	 0.9410	 0.2920
F	 0.9340	 0.2140
G	 0.8070	 0.1600
H	 0.6440	 0.1270
I	 0.0440	 0.0340
J	 0.0110	 0.0390
K	 0.9480	 0.3330
L	 0.9500	 0.3430
M	 0.9510	 0.3430
N	 0.9100	 0.1620
O	 0.8080	 0.1270
P	 0.8560	 0.1270
Q	 0.0000	 0.0220
R	 0.0000	 0.0190
S	 0.0220	 0.0100
T	 0.8820	 0.2860
U	 0.9050	 0.2850
V	 0.8640	 0.2520
W	 0.8640	 0.2540
X	 0.8870	 0.2560
Y	 0.8940	 0.2520

