



## wwPDB EM Validation Summary Report ⓘ

May 11, 2026 – 10:27 pm BST

PDB ID : 9TIO / pdb\_00009tio  
EMDB ID : EMD-55963  
Title : Phage 812 baseplate in the pre-contraction state - upper arm (segment B)  
Authors : Binovsky, J.; Plevka, P.  
Deposited on : 2025-12-05  
Resolution : 3.90 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](mailto: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



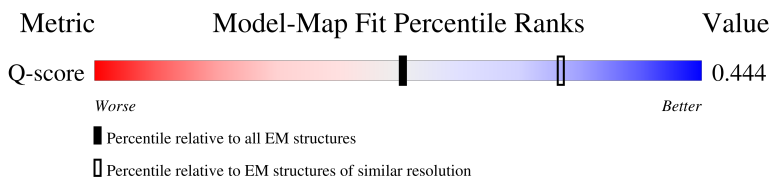
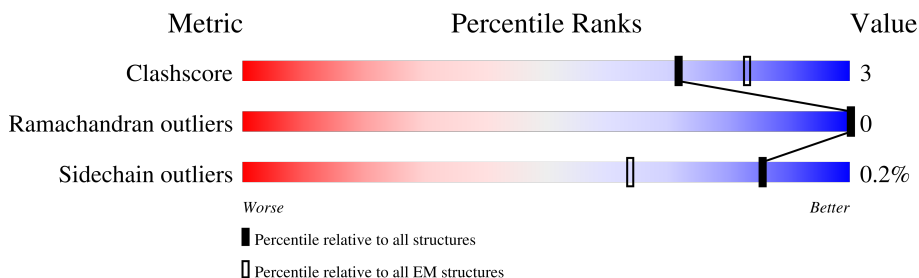
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.90 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	8855 ( 3.40 - 4.40 )

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  $\geq 3$ , 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	1152	 27% 70%
1	B	1152	 13% 86%
1	D	1152	 13% 86%
2	C	173	 6% 60% 36%

*Continued on next page...*



Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	173	<div><div><div></div><div></div><div></div></div><div>89%10%</div></div>
2	F	173	<div><div><div></div><div></div><div></div></div><div>87%7%6%</div></div>
2	K	173	<div><div><div></div><div></div><div></div></div><div>14%76%11%12%</div></div>
3	G	1019	<div><div><div></div><div></div><div></div></div><div>22%75%</div></div>
4	H	640	<div><div><div></div><div></div><div></div></div><div>21%77%</div></div>
4	I	640	<div><div><div></div><div></div><div></div></div><div>21%75%</div></div>
4	J	640	<div><div><div></div><div></div><div></div></div><div>22%76%</div></div>



## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15828 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 ORF65.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	342	Total	C	N	O	S	0	0
			2695	1692	441	554	8		
1	B	165	Total	C	N	O	S	0	0
			1306	823	211	269	3		
1	D	166	Total	C	N	O	S	0	0
			1314	829	212	270	3		

- Molecule 2 is a protein called ORF64.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	111	Total	C	N	O	S	0	0
			889	578	145	165	1		
2	E	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
2	F	163	Total	C	N	O	S	0	0
			1277	817	208	251	1		
2	K	152	Total	C	N	O	S	0	0
			1199	769	196	233	1		

- Molecule 3 is a protein called ORF63.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	257	Total	C	N	O	S	0	0
			2138	1364	339	428	7		

- Molecule 4 is a protein called CBM-cenC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	145	Total	C	N	O	S	0	0
			1193	760	192	239	2		
4	I	157	Total	C	N	O	S	0	0
			1259	798	205	254	2		

*Continued on next page...*



*Continued from previous page...*

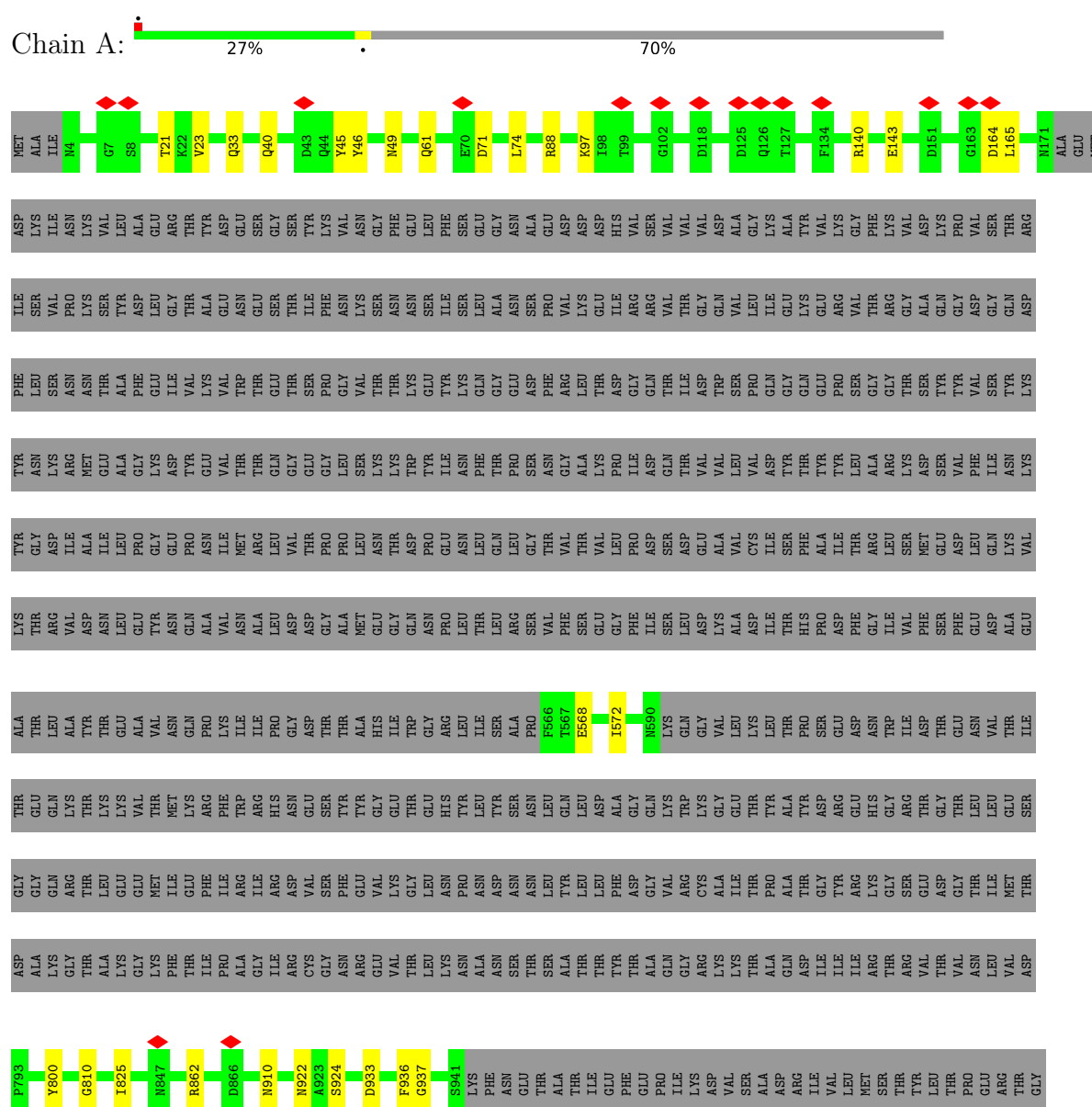
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	151	1209	768	198	241	2	0	0



### 3 Residue-property plots

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

#### • Molecule 1: ORF65





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

- Molecule 1: ORF65

Chain B:  13% 86%

[illegible]

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

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

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

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

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

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

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

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

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

GLY	SER	GLU	ASP	GLY	THR	ILE	MET	THR	THR	ASP	ALA	LYS	LYS	PHE	THR	ALA	LYS	LYS	THR	PRO	ARG	CYS	GLY	ASN	ARG	GLU	VAL	LEU	THR	LYS	ASN	ALA	ALA	ASN	SER	SER	SER	ALA	THR	THR	Tyr	THR	THR	THR	ALA	GLN	GLY	ARG	Lys	Lys	Thr	Lys	Thr	Ala	Ala	Gln	Asn	Arg	Ile	Ile	Ile	Ile	Ile	Ile
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

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

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

LEU MET SER THR TYR LEU THR PRO GLU ARG ALG THR GLY CYS THR TRP TRP GLU MET LYS LEU LEU LEU ASP ASP MET MET SER SER SER THR THR PHE ASP ASP GLN LEU LEU LYS TYR TYR GLN ASP LEU LEU ASP VAL VAL LEU LEU LEU ALA ARG ALA LYS LEU LEU ALA ARG ALA THR THR PHE

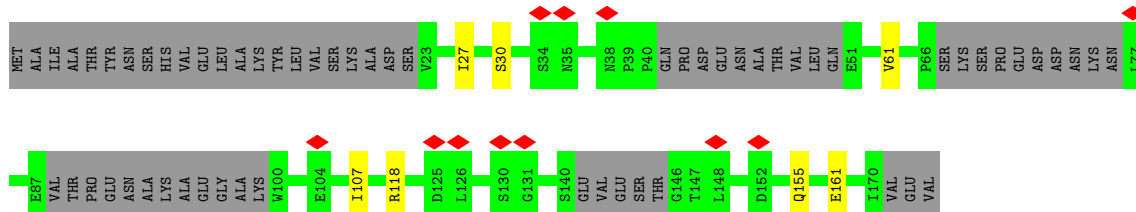


- Molecule 1: ORF65

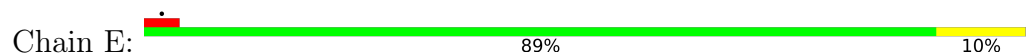
[illegible]



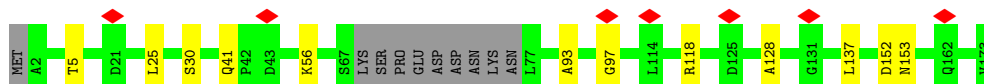
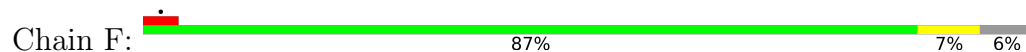
- Molecule 2: ORF64



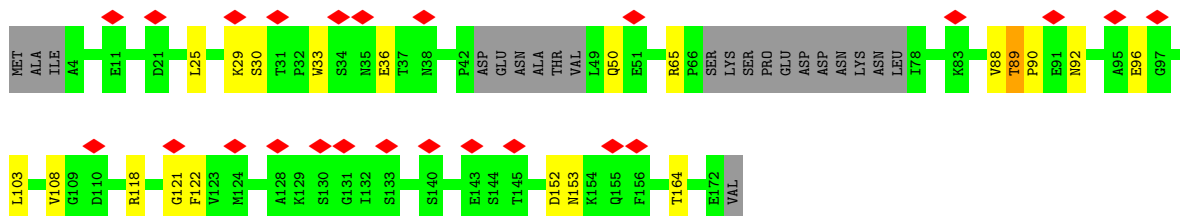
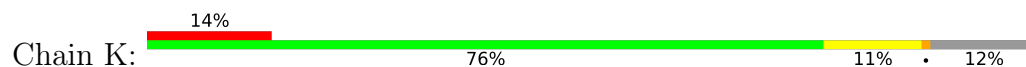
- Molecule 2: ORF64



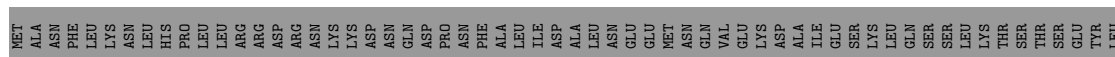
- Molecule 2: ORF64



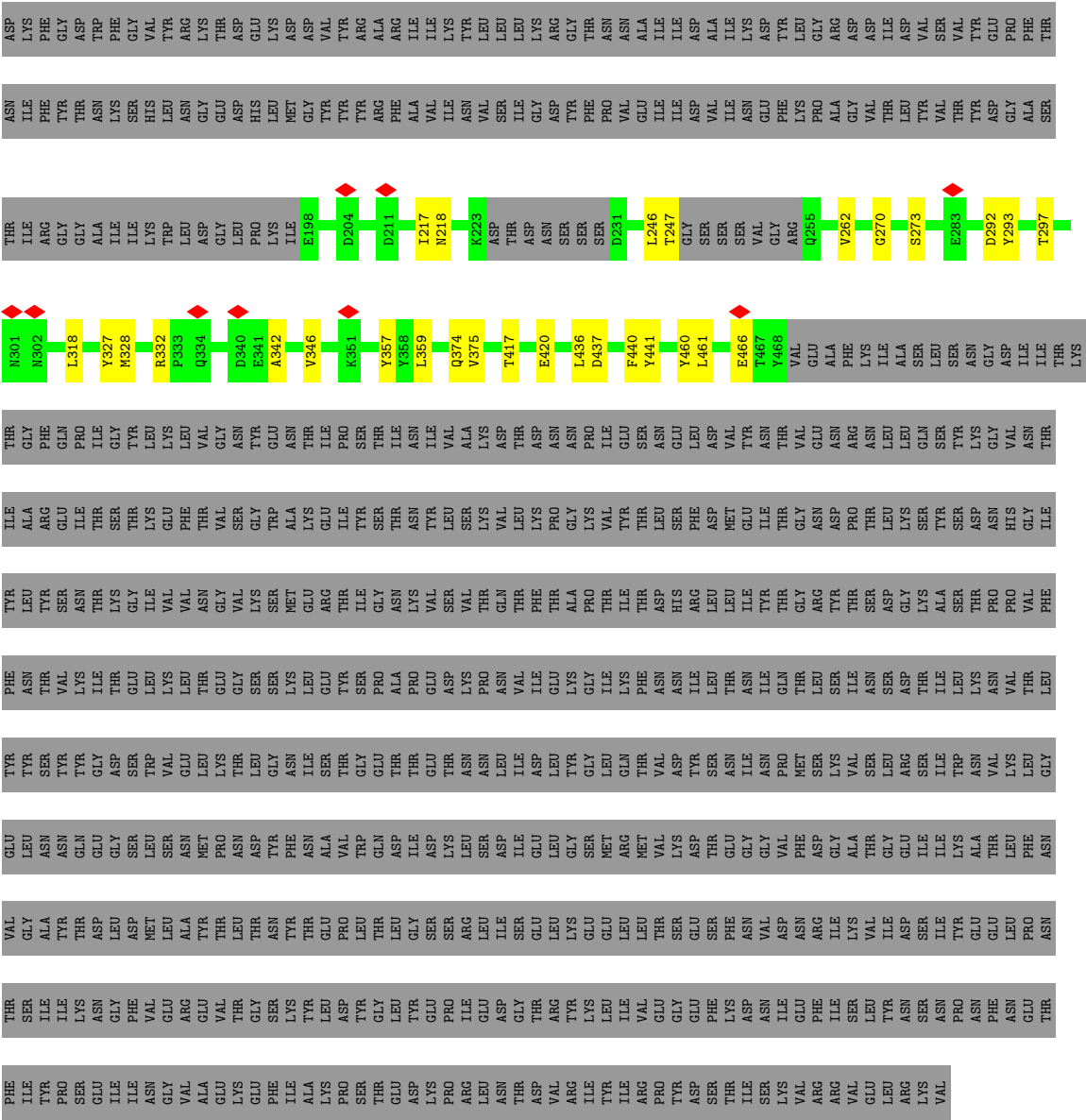
- Molecule 2: ORF64



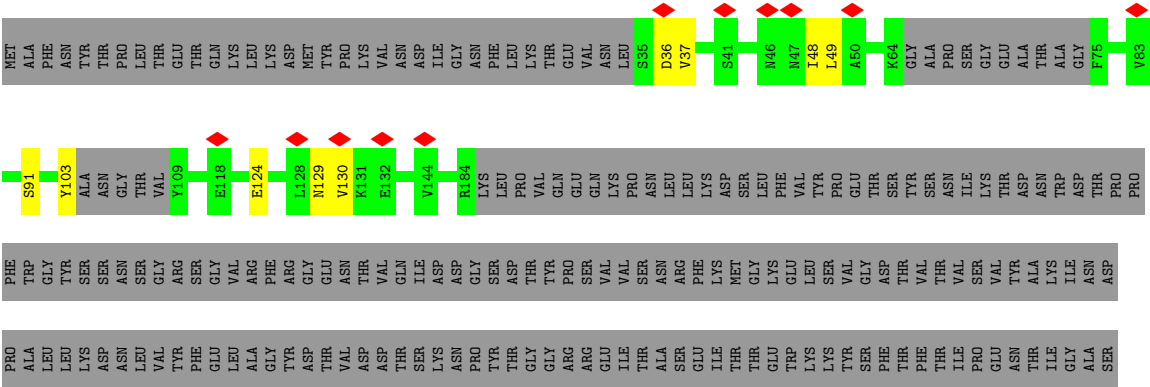
- Molecule 3: ORF63



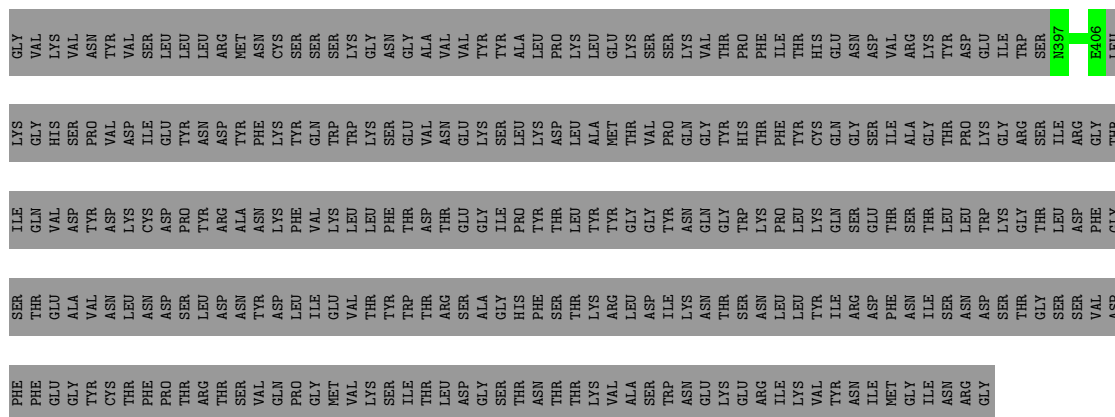




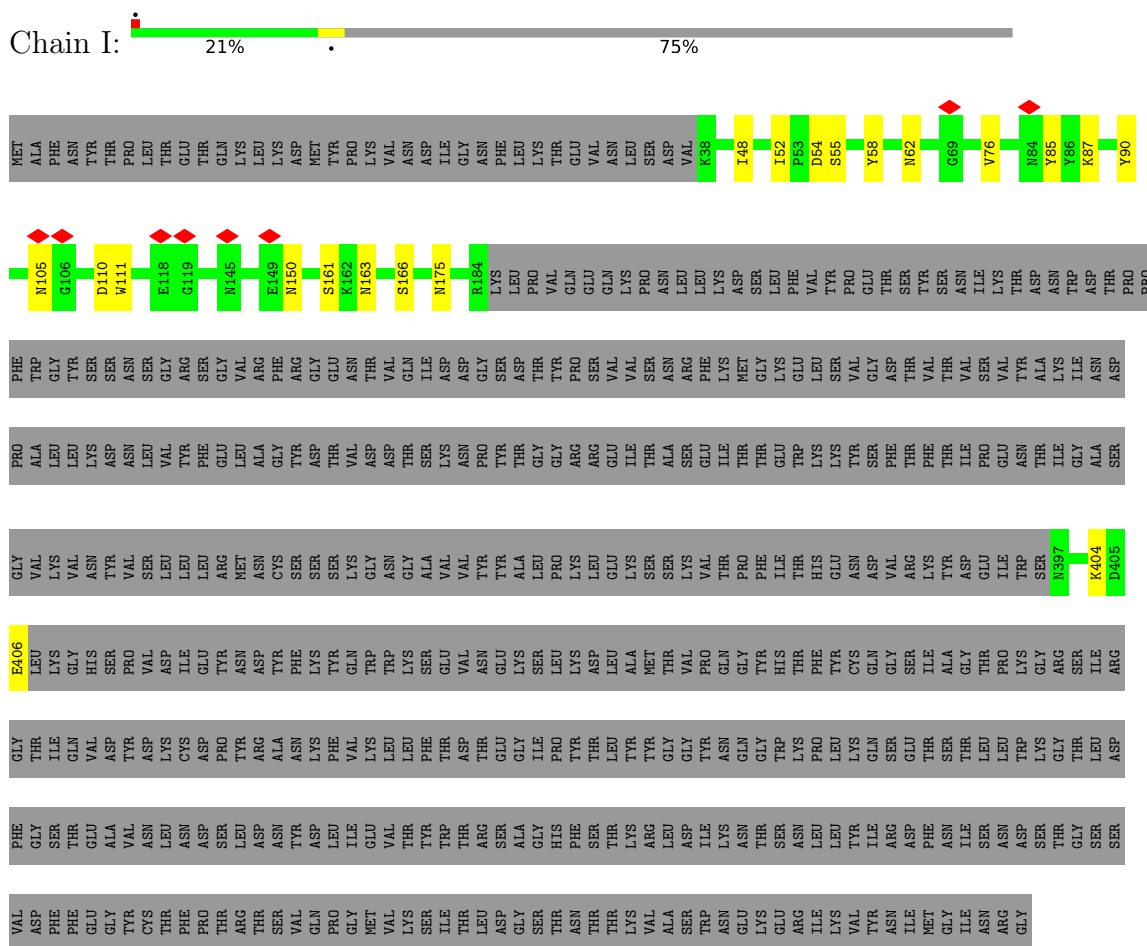
● Molecule 4: CBM-cenC domain-containing protein



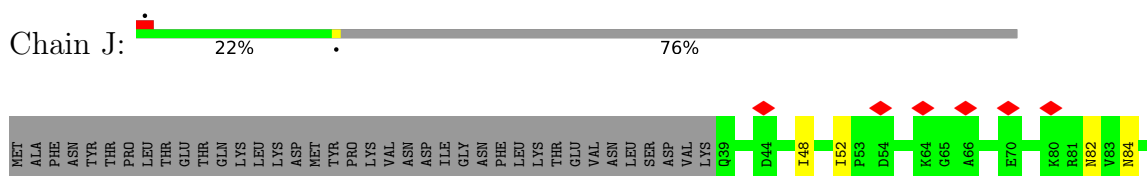




- Molecule 4: CBM-cenC domain-containing protein



- Molecule 4: CBM-cenC domain-containing protein





WORLDWIDE  
**PDB**  
PROTEIN DATA BANK



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19727	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 ( $e^-/\text{\AA}^2$ )	40.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.221	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	300.096, 300.096, 300.096	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.6672001, 1.6672001, 1.6672001	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	A	0.11	0/2748	0.30	0/3725
1	B	0.10	0/1330	0.31	0/1800
1	D	0.12	0/1338	0.33	0/1811
2	C	0.11	0/907	0.29	0/1225
2	E	0.11	0/1377	0.32	0/1872
2	F	0.11	0/1303	0.28	0/1771
2	K	0.12	0/1224	0.30	0/1660
3	G	0.10	0/2185	0.29	0/2961
4	H	0.11	0/1219	0.30	0/1651
4	I	0.11	0/1288	0.27	0/1749
4	J	0.11	0/1236	0.32	0/1678
All	All	0.11	0/16155	0.30	0/21903

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	A	2695	0	2590	17	0
1	B	1306	0	1267	10	0
1	D	1314	0	1278	14	0
2	C	889	0	893	5	0
2	E	1349	0	1339	13	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1277	0	1274	7	0
2	K	1199	0	1195	12	0
3	G	2138	0	2032	18	0
4	H	1193	0	1144	5	0
4	I	1259	0	1207	13	0
4	J	1209	0	1164	5	0
All	All	15828	0	15383	105	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 3.

The worst 5 of 105 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:B:83:ILE:O	1:B:88:ARG:NH1	2.18	0.77
1:B:69:SER:OG	1:B:71:ASP:OD1	2.05	0.75
1:A:88:ARG:NH2	1:A:143:GLU:OE1	2.20	0.74
2:F:30:SER:O	2:F:118:ARG:NH1	2.25	0.70
4:I:85:TYR:OH	4:I:105:ASN:OD1	2.05	0.69

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	336/1152 (29%)	333 (99%)	3 (1%)	0	100	100
1	B	163/1152 (14%)	162 (99%)	1 (1%)	0	100	100
1	D	164/1152 (14%)	162 (99%)	2 (1%)	0	100	100
2	C	101/173 (58%)	98 (97%)	3 (3%)	0	100	100
2	E	170/173 (98%)	164 (96%)	6 (4%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	159/173 (92%)	157 (99%)	2 (1%)	0	100	100
2	K	146/173 (84%)	142 (97%)	4 (3%)	0	100	100
3	G	251/1019 (25%)	247 (98%)	4 (2%)	0	100	100
4	H	137/640 (21%)	133 (97%)	4 (3%)	0	100	100
4	I	153/640 (24%)	153 (100%)	0	0	100	100
4	J	145/640 (23%)	141 (97%)	4 (3%)	0	100	100
All	All	1925/7087 (27%)	1892 (98%)	33 (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	A	302/1010 (30%)	301 (100%)	1 (0%)	86	85
1	B	147/1010 (15%)	147 (100%)	0	100	100
1	D	148/1010 (15%)	147 (99%)	1 (1%)	76	78
2	C	100/153 (65%)	100 (100%)	0	100	100
2	E	152/153 (99%)	152 (100%)	0	100	100
2	F	143/153 (94%)	143 (100%)	0	100	100
2	K	134/153 (88%)	133 (99%)	1 (1%)	76	78
3	G	241/928 (26%)	241 (100%)	0	100	100
4	H	138/577 (24%)	137 (99%)	1 (1%)	76	78
4	I	142/577 (25%)	142 (100%)	0	100	100
4	J	136/577 (24%)	136 (100%)	0	100	100
All	All	1783/6301 (28%)	1779 (100%)	4 (0%)	85	87

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



Mol	Chain	Res	Type
1	A	936	PHE
1	D	92	ASN
4	H	103	TYR
2	K	89	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	157	GLN
3	G	201	GLN
4	J	397	ASN
4	J	42	GLN
4	J	172	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.



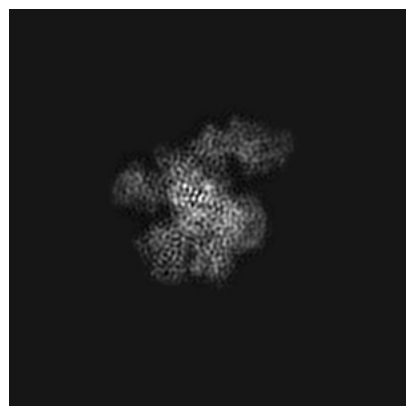
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55963. These allow visual inspection of the internal detail of the map and identification of artifacts.

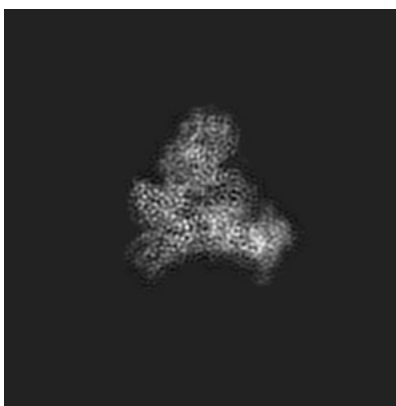
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

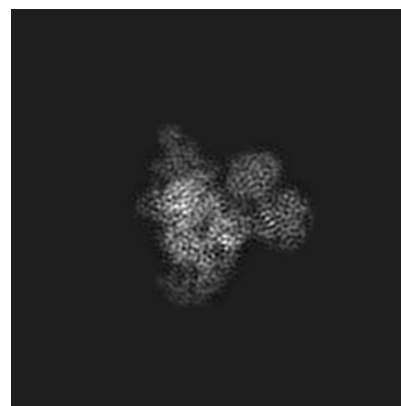
#### 6.1.1 Primary map



X

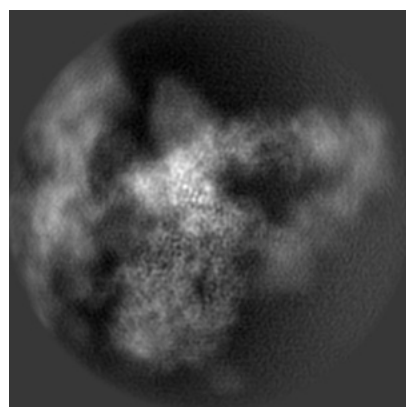


Y

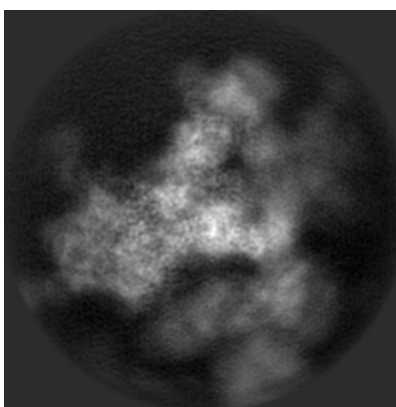


Z

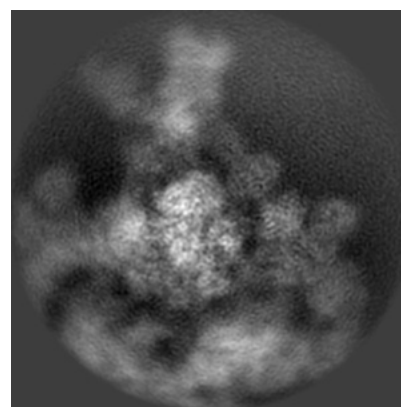
#### 6.1.2 Raw map



X



Y



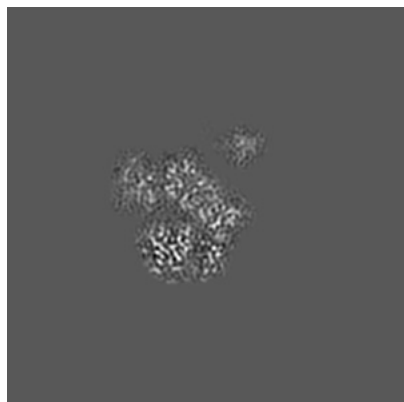
Z

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

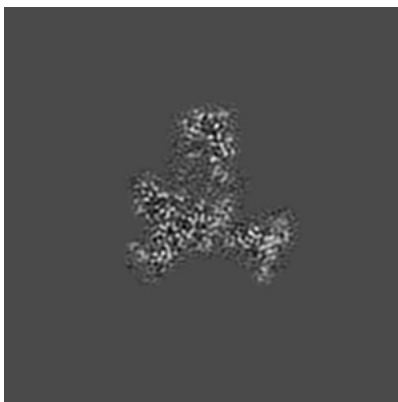


## 6.2 Central slices [i](#)

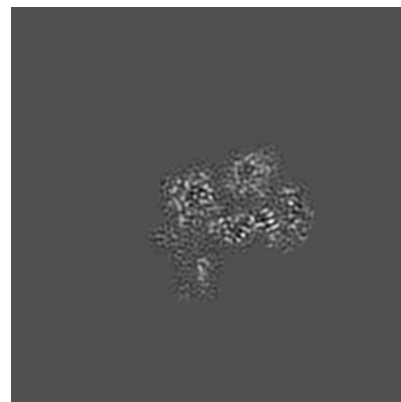
### 6.2.1 Primary map



X Index: 90

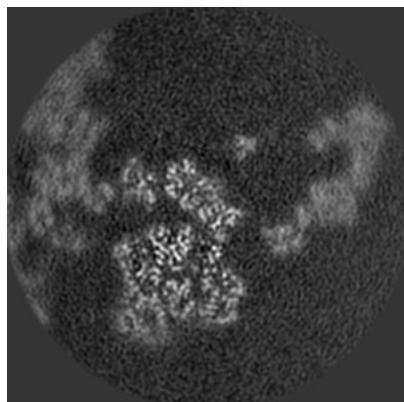


Y Index: 90

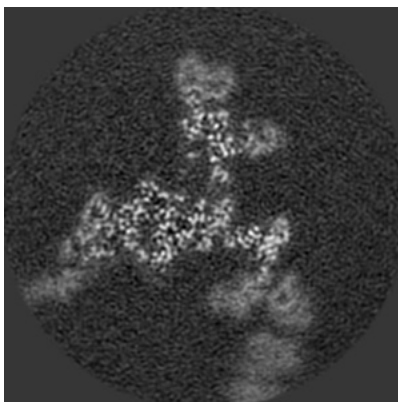


Z Index: 90

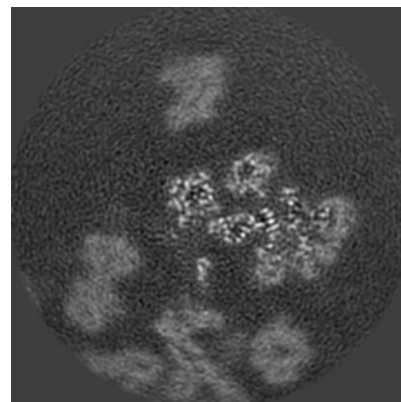
### 6.2.2 Raw map



X Index: 90



Y Index: 90



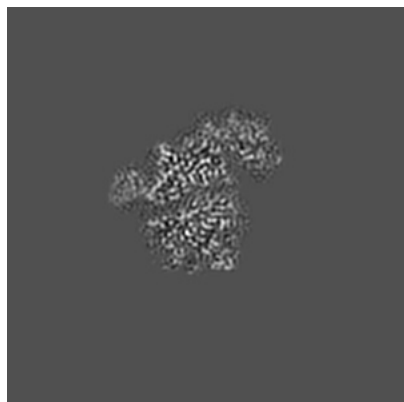
Z Index: 90

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

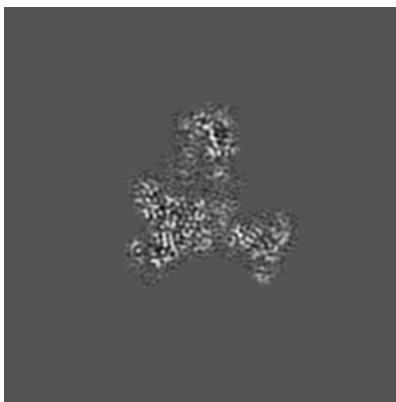


## 6.3 Largest variance slices [i](#)

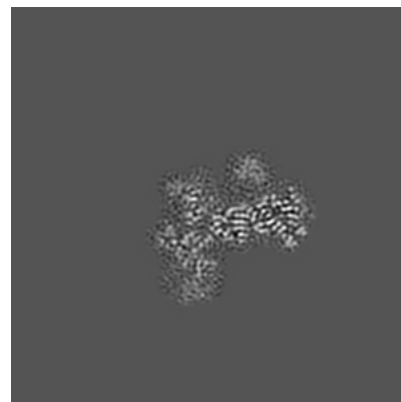
### 6.3.1 Primary map



X Index: 78

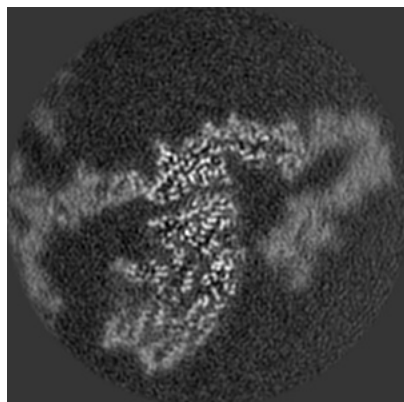


Y Index: 91

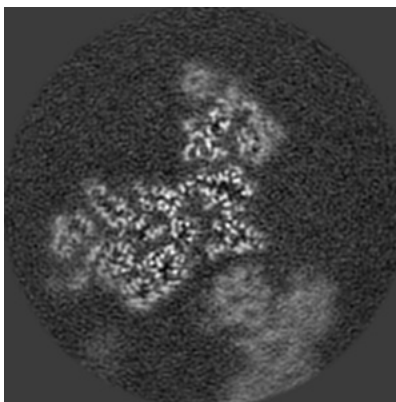


Z Index: 94

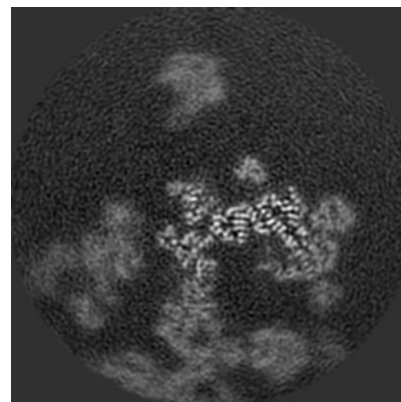
### 6.3.2 Raw map



X Index: 78



Y Index: 78



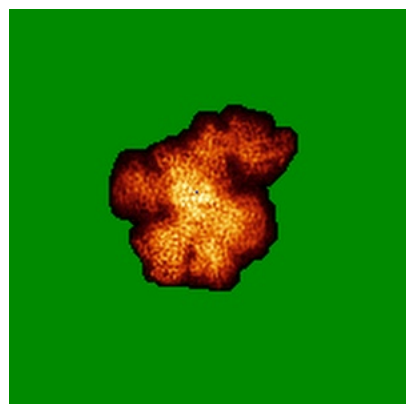
Z Index: 94

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

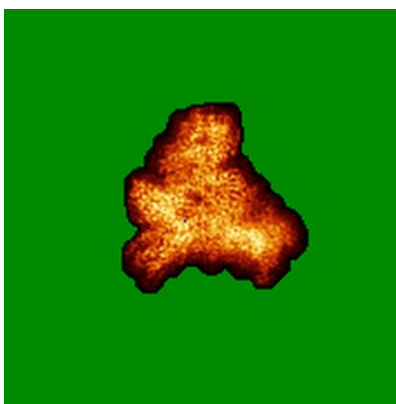


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

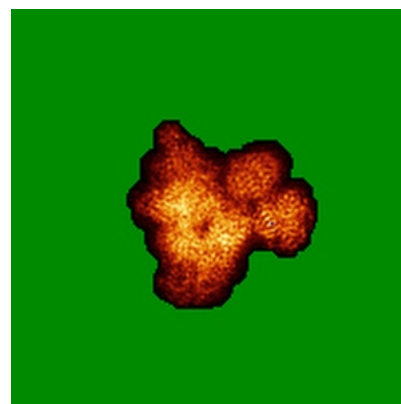
### 6.4.1 Primary map



X

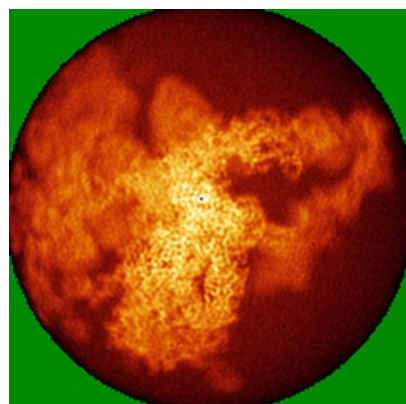


Y

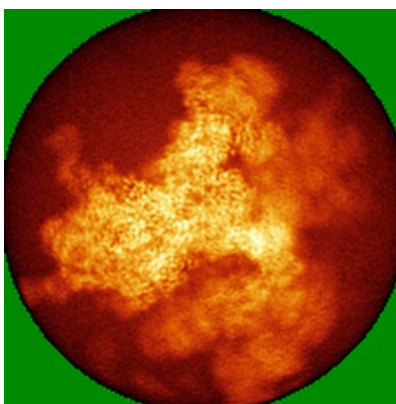


Z

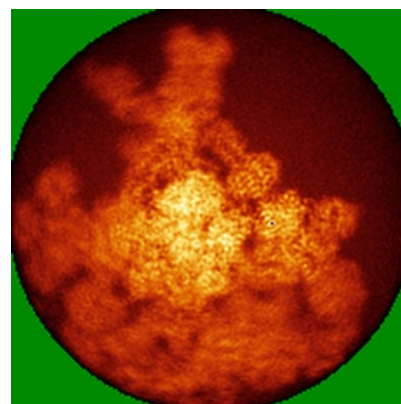
### 6.4.2 Raw map



X



Y



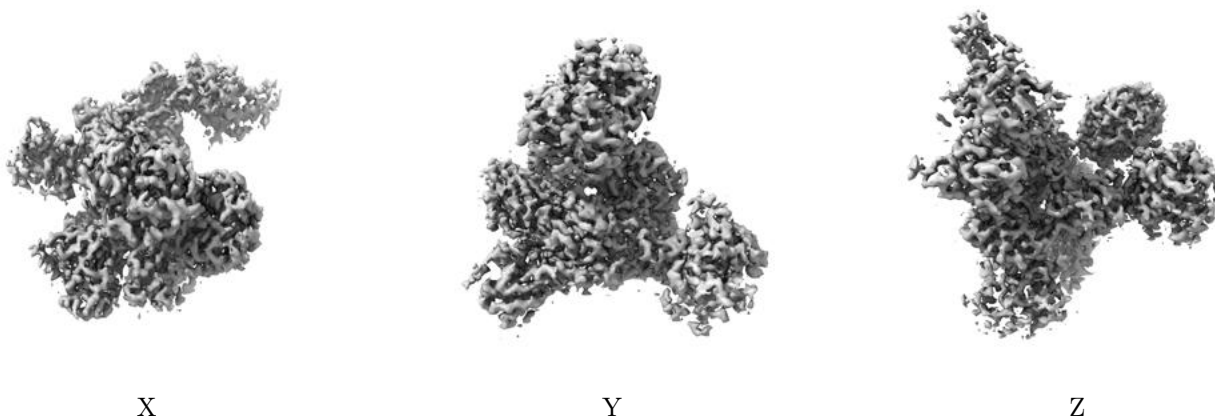
Z

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 0.04. 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.



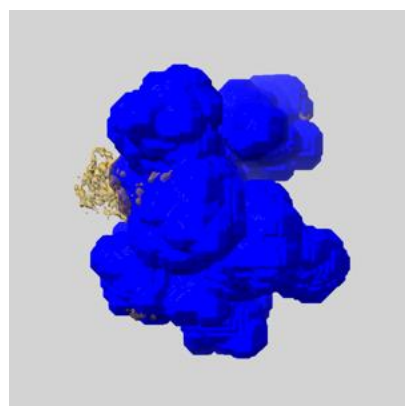
## 6.6 Mask visualisation [i](#)

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

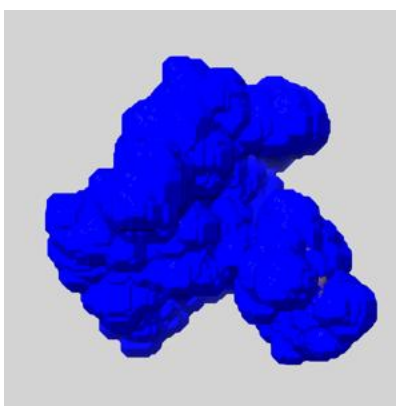
A mask typically either:

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

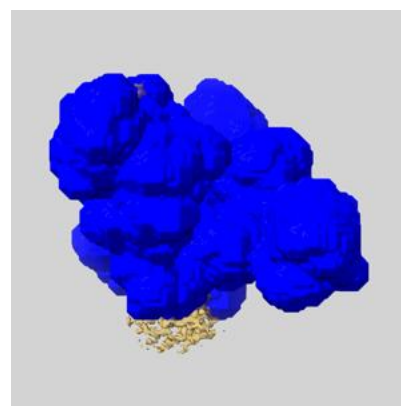
### 6.6.1 emd\_55963\_msk\_1.map [i](#)



X



Y



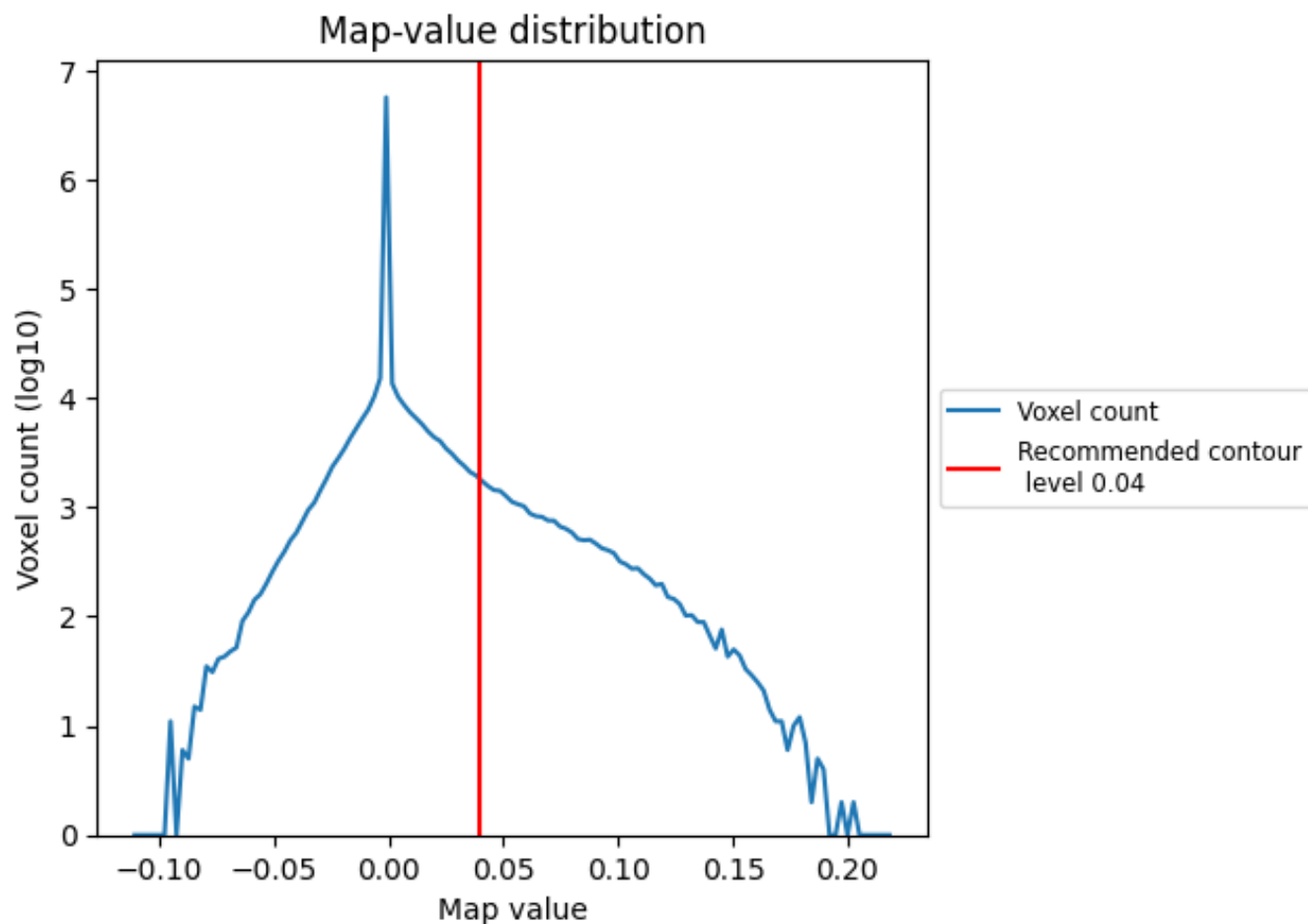
Z



## 7 Map analysis [i](#)

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

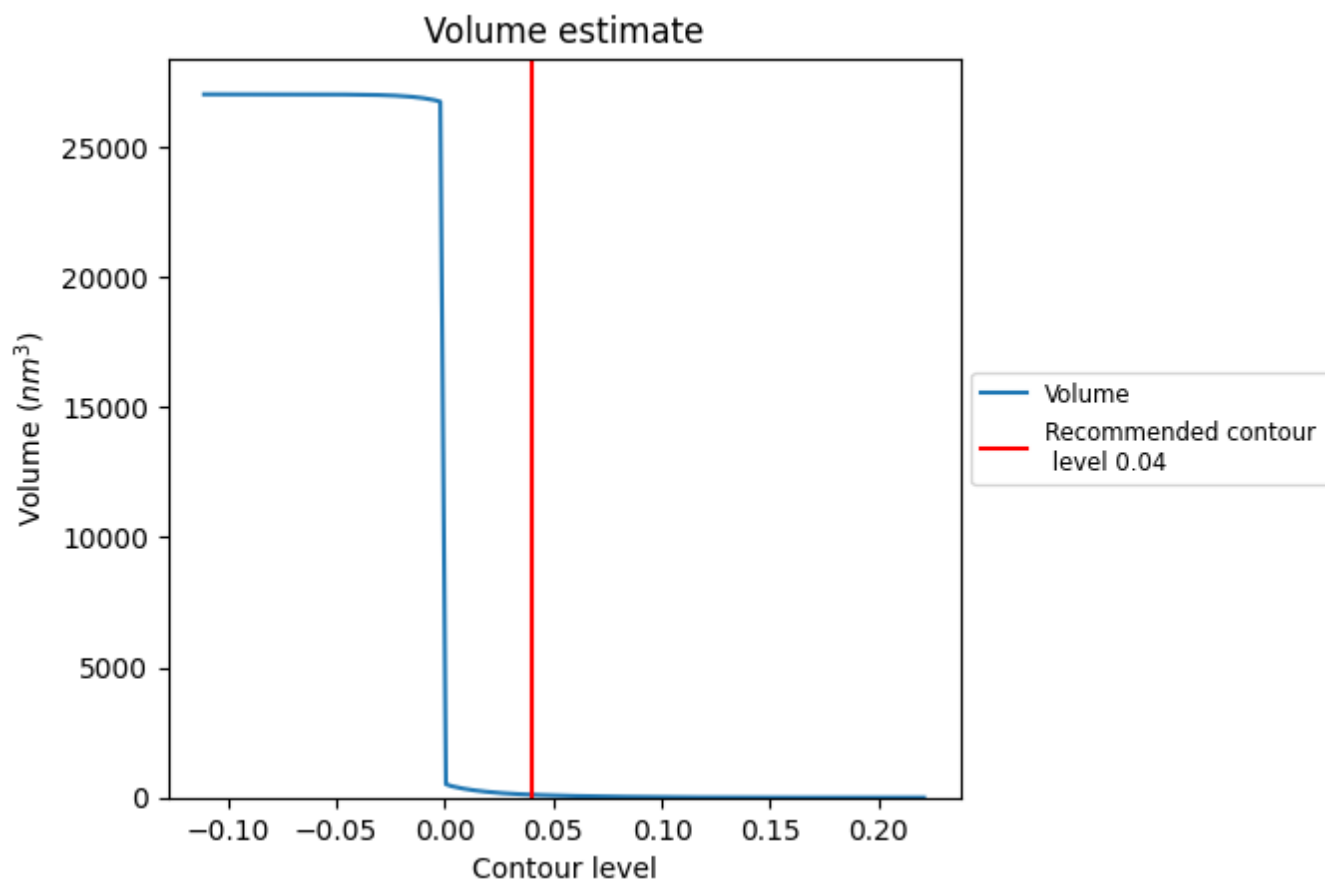
### 7.1 Map-value distribution [i](#)



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](#)

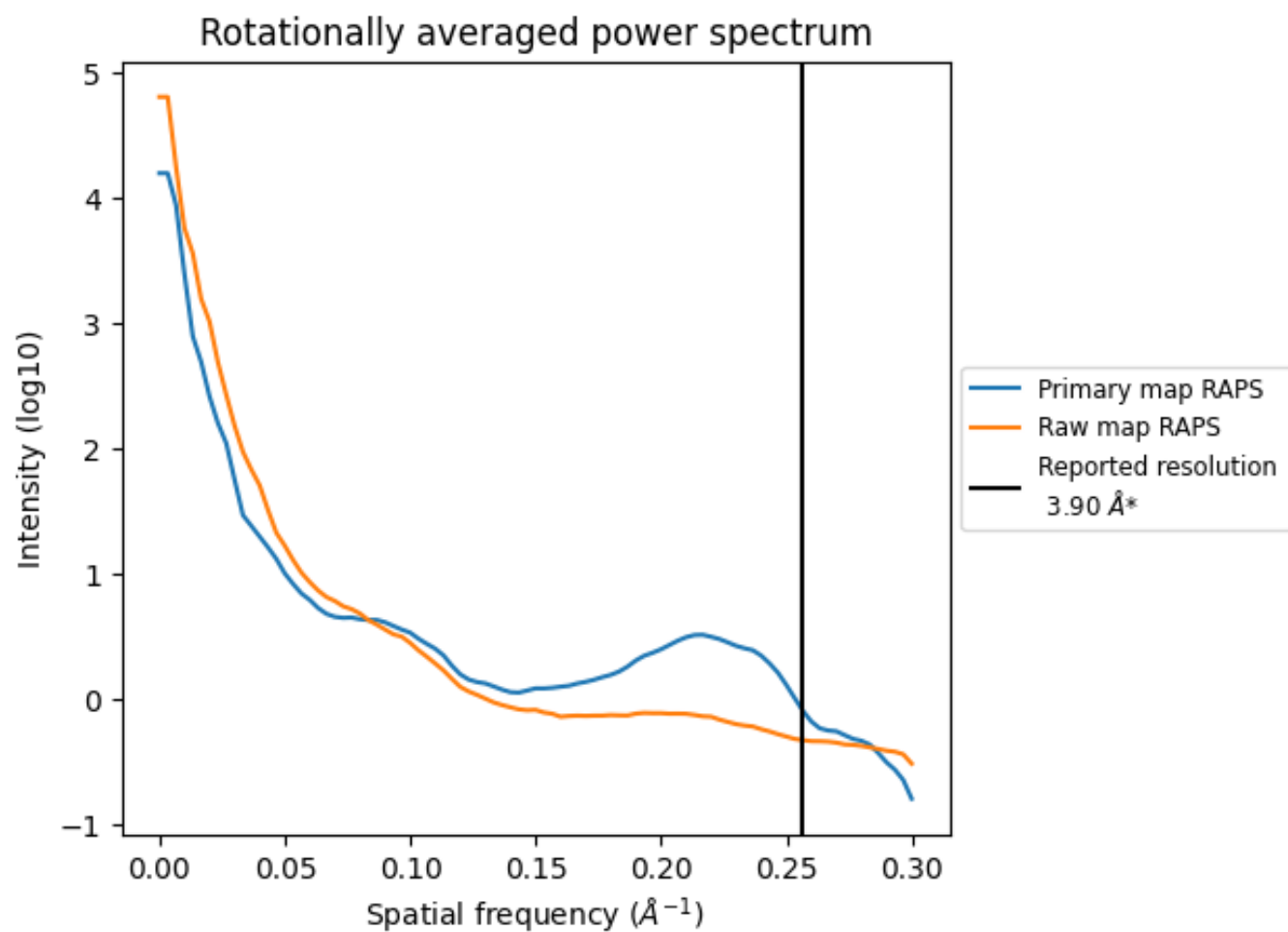


The volume at the recommended contour level is 109 nm<sup>3</sup>; this corresponds to an approximate mass of 99 kDa.

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 ⓘ



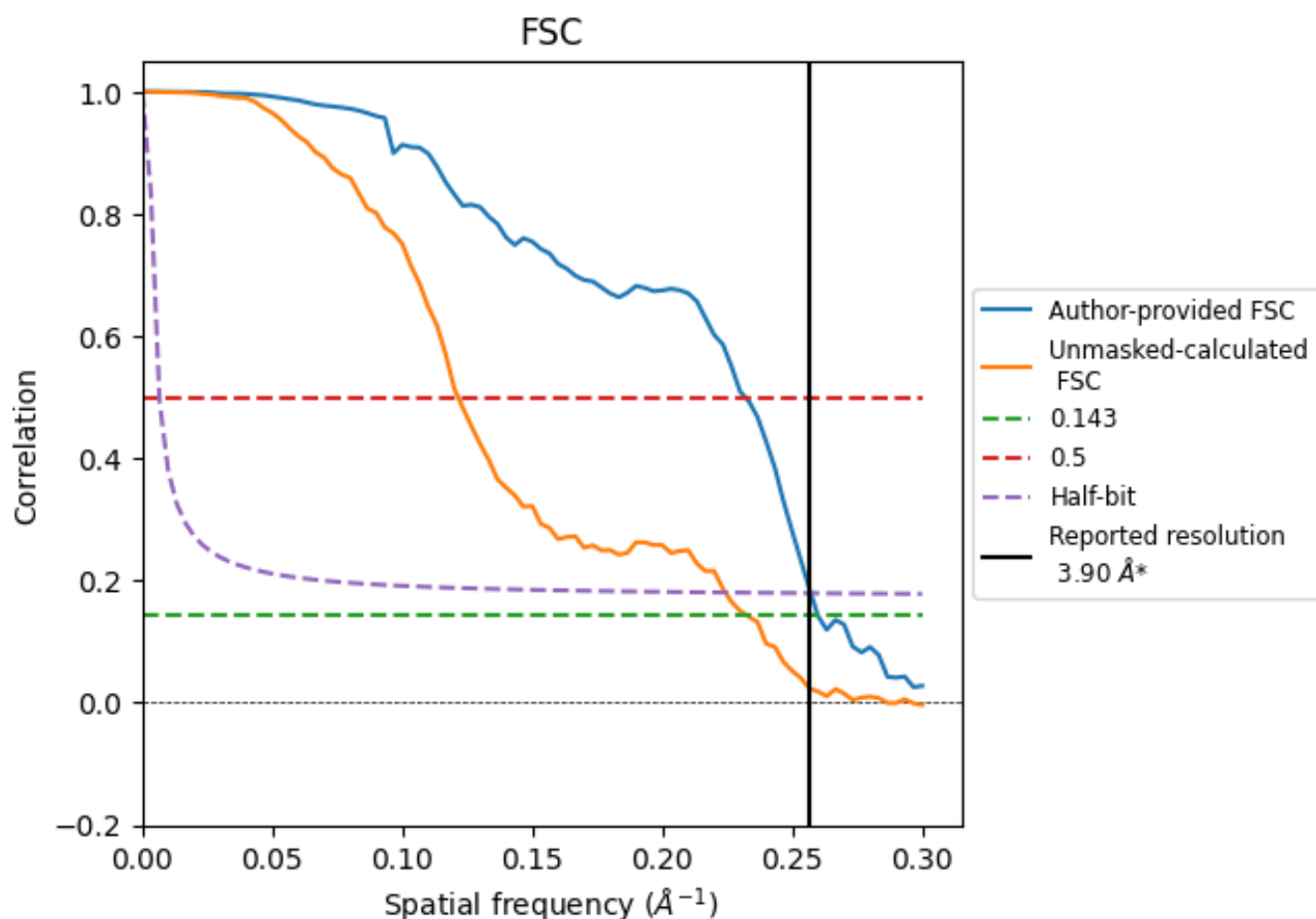
\*Reported resolution corresponds to spatial frequency of 0.256 Å<sup>-1</sup>



## 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 0.256  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.85	4.31	3.89
Unmasked-calculated*	4.30	8.24	4.46

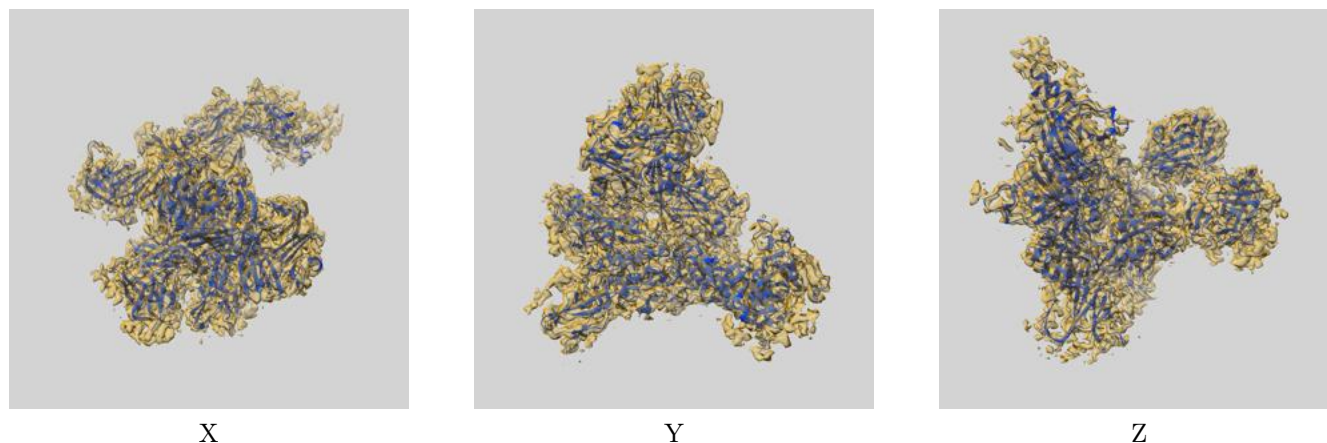
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.9 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55963 and PDB model 9TIO. Per-residue inclusion information can be found in section [3](#) on page [6](#).

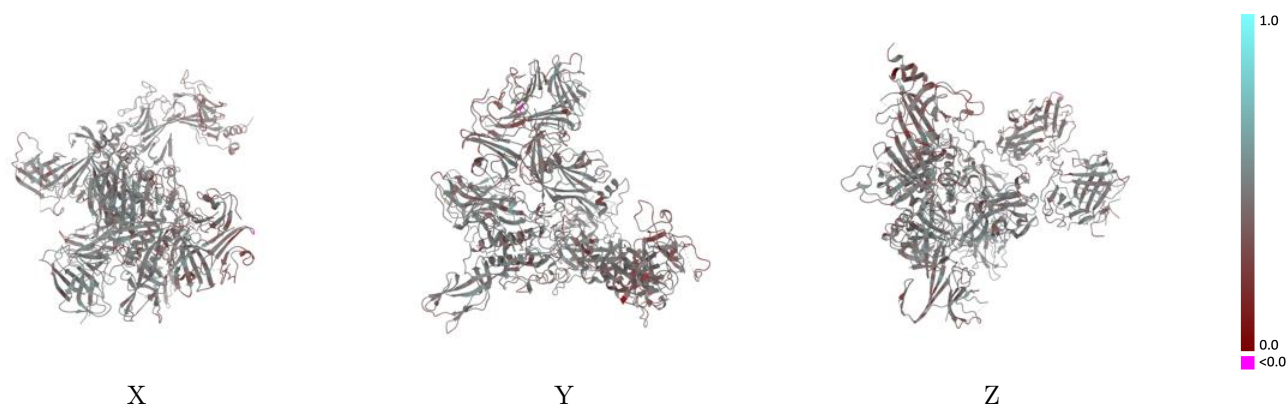
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

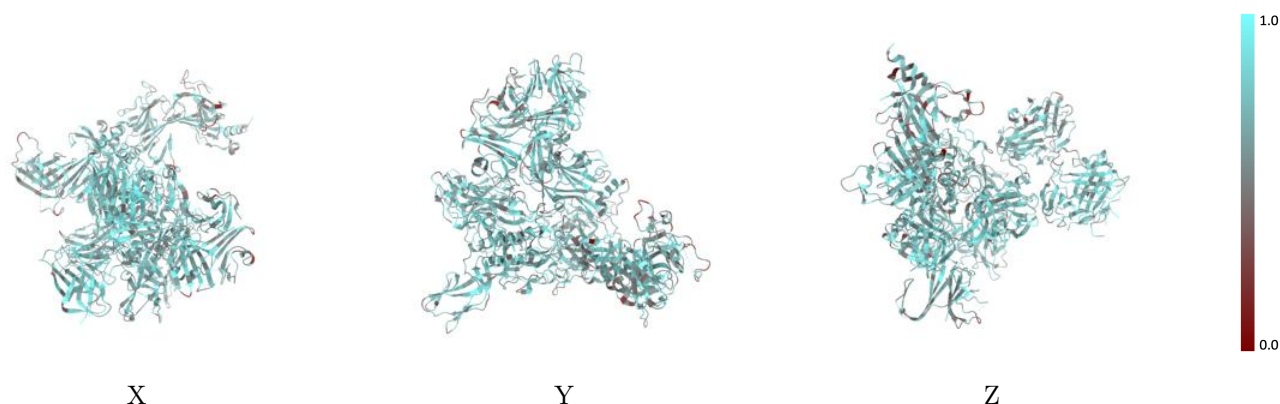


## 9.2 Q-score mapped to coordinate model [i](#)



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.

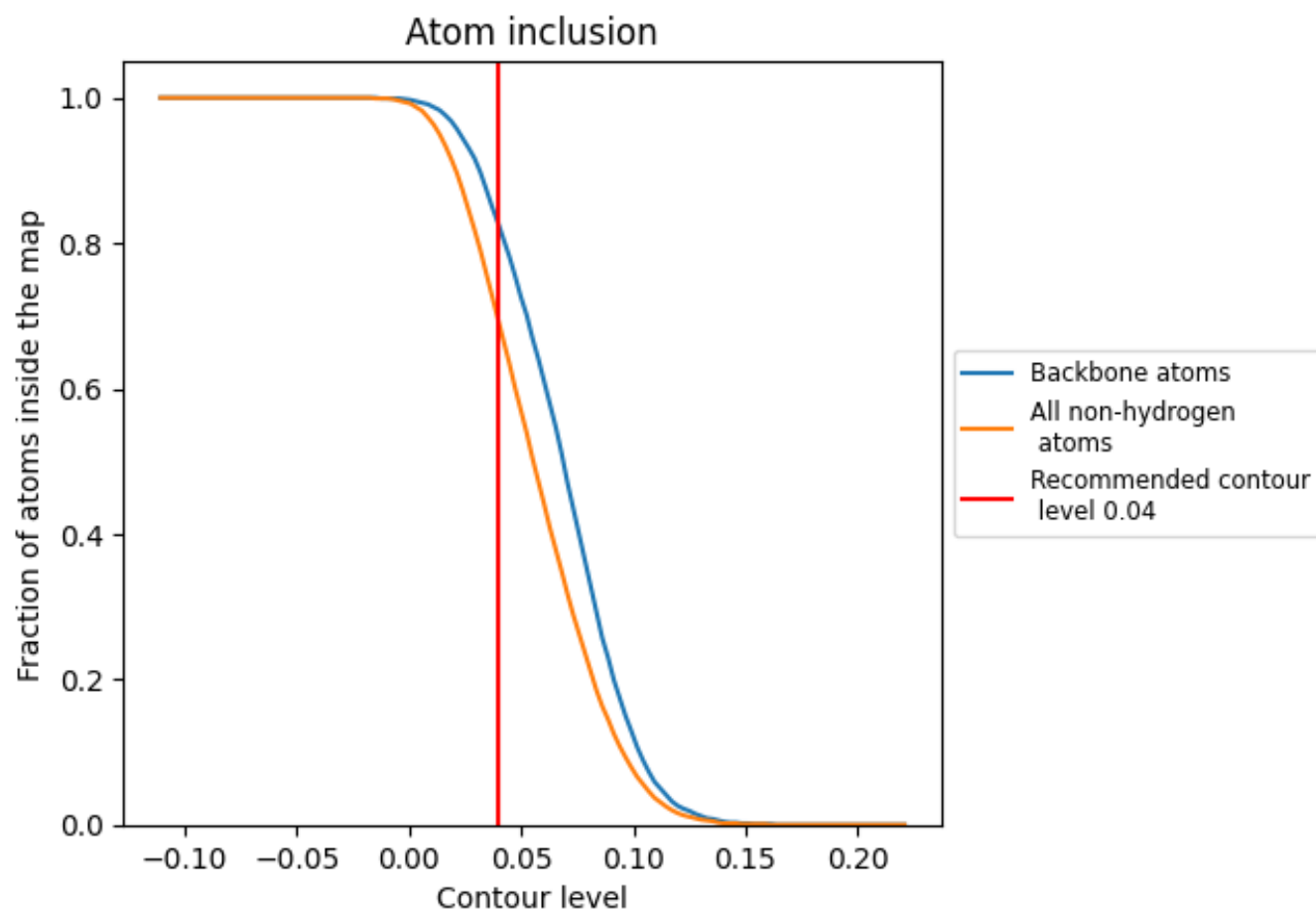
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.04).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6910	<div></div> 0.4440
A	<div></div> 0.7120	<div></div> 0.4670
B	<div></div> 0.6950	<div></div> 0.4550
C	<div></div> 0.6220	<div></div> 0.4270
D	<div></div> 0.7020	<div></div> 0.4600
E	<div></div> 0.6810	<div></div> 0.4400
F	<div></div> 0.7060	<div></div> 0.4500
G	<div></div> 0.7320	<div></div> 0.4620
H	<div></div> 0.6750	<div></div> 0.4120
I	<div></div> 0.7150	<div></div> 0.4500
J	<div></div> 0.6850	<div></div> 0.4250
K	<div></div> 0.5980	<div></div> 0.3920

1.0

0.0

<0.0