



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 10:36 AM UTC

PDB ID : 8PSQ / pdb_00008psq
EMDB ID : EMD-17860
Title : Tilapia Lake Virus polymerase in cRNA pre-initiation state mode A (core only)
Authors : Arragain, B.; Cusack, S.
Deposited on : 2023-07-13
Resolution : 2.65 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

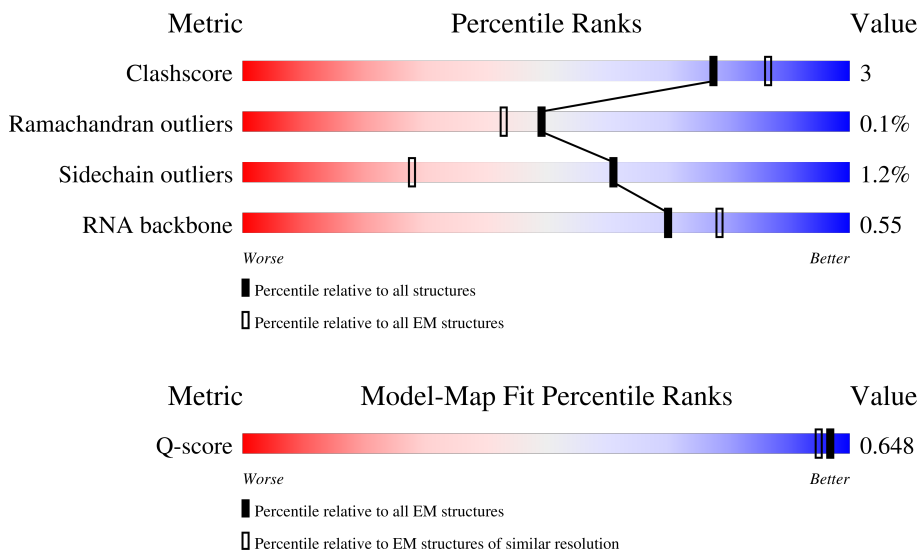
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.65 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.



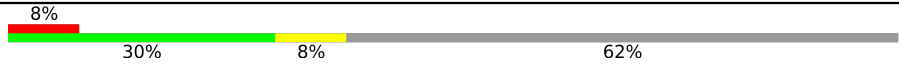

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9050 (2.15 - 3.15)

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	419	
2	B	519	
3	C	478	

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Mol	Chain	Length	Quality of chain
4	S	40	 8% 30% 8% 62%
4	V	40	 12% 15% 18% 68%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16079 atoms, of which 7898 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 Polymerase acidic protein (PA-like).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	315	5030	1582	2522	458	456	12	0	0

- Molecule 2 is a protein called Putative PB1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	515	7973	2490	4000	694	759	30	0	0

- Molecule 3 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	139	2221	693	1119	200	207	2	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	391	LYS	ARG	conflict	UNP A0A7G3S745
C	458	GLY	-	expression tag	UNP A0A7G3S745
C	459	SER	-	expression tag	UNP A0A7G3S745
C	460	GLY	-	expression tag	UNP A0A7G3S745
C	461	SER	-	expression tag	UNP A0A7G3S745
C	462	GLU	-	expression tag	UNP A0A7G3S745
C	463	ASN	-	expression tag	UNP A0A7G3S745
C	464	LEU	-	expression tag	UNP A0A7G3S745
C	465	TYR	-	expression tag	UNP A0A7G3S745
C	466	PHE	-	expression tag	UNP A0A7G3S745
C	467	GLN	-	expression tag	UNP A0A7G3S745
C	468	GLY	-	expression tag	UNP A0A7G3S745
C	469	HIS	-	expression tag	UNP A0A7G3S745
C	470	HIS	-	expression tag	UNP A0A7G3S745
C	471	HIS	-	expression tag	UNP A0A7G3S745

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Chain	Residue	Modelled	Actual	Comment	Reference
C	472	HIS	-	expression tag	UNP A0A7G3S745
C	473	HIS	-	expression tag	UNP A0A7G3S745
C	474	HIS	-	expression tag	UNP A0A7G3S745
C	475	HIS	-	expression tag	UNP A0A7G3S745
C	476	HIS	-	expression tag	UNP A0A7G3S745
C	477	HIS	-	expression tag	UNP A0A7G3S745
C	478	HIS	-	expression tag	UNP A0A7G3S745

- Molecule 4 is a RNA chain called 5' cRNA end - cRNA loop (40-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
4	V	13	386	122	116	44	91	13	0	0
4	S	15	466	145	141	61	104	15	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	B	1	Total	Mg	0
			1	1	

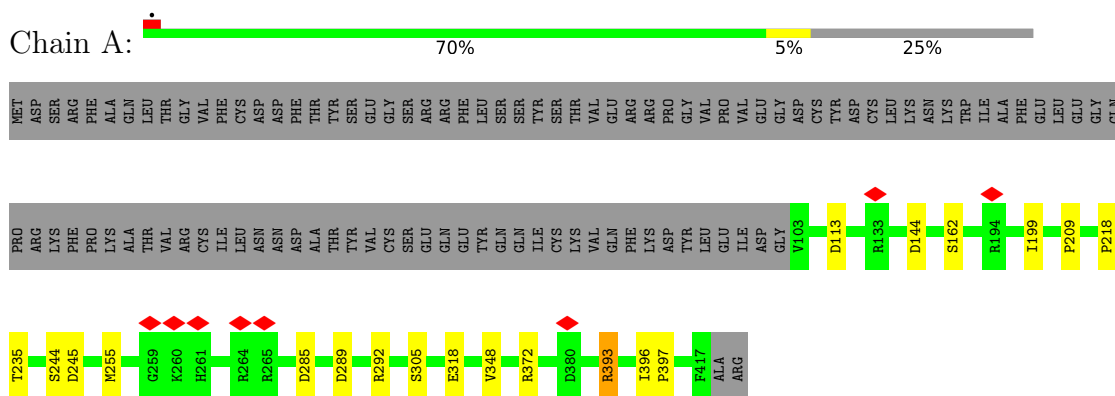
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	O	0
			1	1	

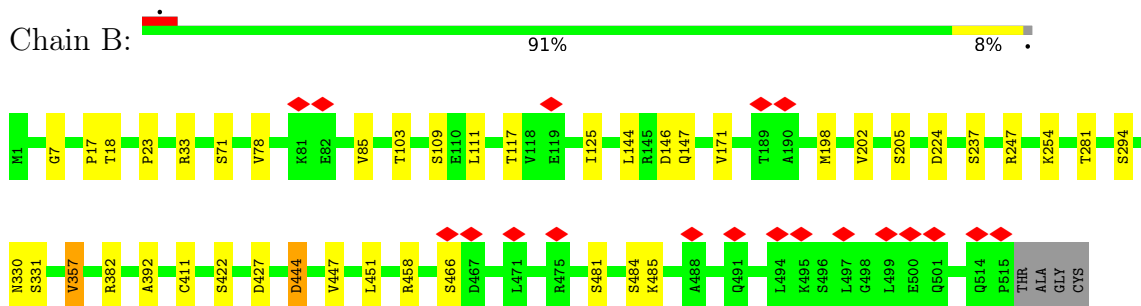
3 Residue-property plots [i](#)

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

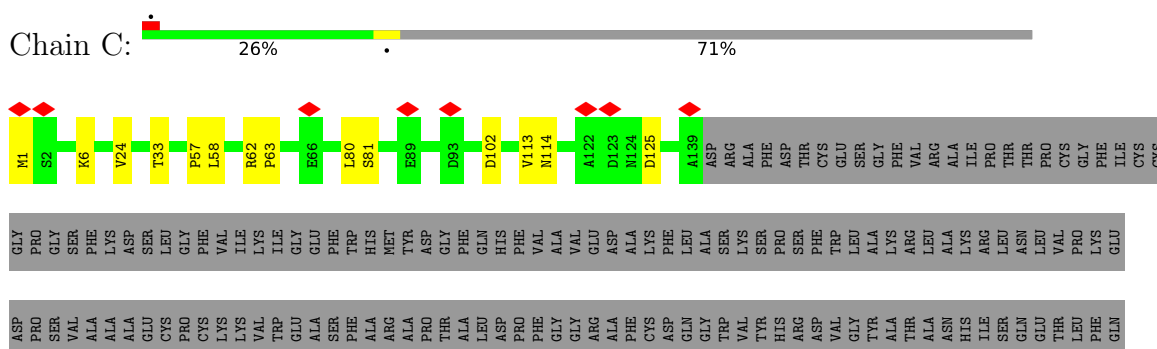
- Molecule 1: Polymerase acidic protein (PA-like)



- Molecule 2: Putative PB1



- Molecule 3: RNA-dependent RNA polymerase

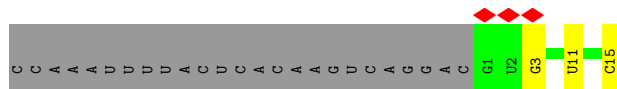


GLN	ASP	GLY	TYR
ALA	LYS	THR	PHE
LEU	ARG	PHE	GLN
SER	LYS	TYR	GLY
VAL	LEU	CYS	HIS
ARG	ASN	HIS	HIS
ASN	ILE	HIS	HIS
LEU	LYS	ARG	HIS
GLY	ALA	LYS	HIS
PRO	LEU	ALA	HIS
GLN	ARG	MET	HIS
GLY	SER	LEU	HIS
SER	PRO	LEU	HIS
ALA	GLU	ILE	HIS
ASN	ARG	SER	HIS
VAL	TYR	CYS	
GLY	ILE	SER	
SER	THR	PRO	
ILE	ILE	GLY	
ILE	GLU	THR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

● Molecule 4: 5' cRNA end - cRNA loop (40-mer)



● Molecule 4: 5' cRNA end - cRNA loop (40-mer)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107798	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	251.99998, 251.99998, 251.99998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/2564	0.27	0/3465
2	B	0.12	0/4045	0.26	0/5474
3	C	0.12	0/1121	0.27	0/1507
4	S	0.09	0/364	0.16	0/566
4	V	0.11	0/300	0.20	0/463
All	All	0.12	0/8394	0.26	0/11475

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	2508	2522	2520	13	0
2	B	3973	4000	4000	24	0
3	C	1102	1119	1119	10	0
4	S	325	141	162	3	0
4	V	270	116	139	4	0
5	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
All	All	8181	7898	7940	46	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 46 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:A:113:ASP:OD2	2:B:237:SER:OG	1.93	0.85
4:V:13:C:O2	4:S:3:G:N2	2.14	0.80
2:B:117:THR:O	2:B:117:THR:HG22	1.88	0.72
1:A:235:THR:HG21	1:A:305:SER:HB2	1.70	0.72
2:B:18:THR:OG1	2:B:146:ASP:OD2	2.09	0.68

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	313/419 (75%)	310 (99%)	3 (1%)	0	100	100
2	B	513/519 (99%)	502 (98%)	10 (2%)	1 (0%)	43	60
3	C	137/478 (29%)	131 (96%)	6 (4%)	0	100	100
All	All	963/1416 (68%)	943 (98%)	19 (2%)	1 (0%)	49	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	254	LYS

5.3.2 Protein sidechains [i](#)

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	272/365 (74%)	270 (99%)	2 (1%)	76	86
2	B	445/447 (100%)	437 (98%)	8 (2%)	51	72
3	C	121/405 (30%)	121 (100%)	0	100	100
All	All	838/1217 (69%)	828 (99%)	10 (1%)	61	79

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	294	SER
2	B	357	VAL
2	B	444	ASP
2	B	109	SER
2	B	171	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
2	B	296	ASN
2	B	474	HIS
3	C	28	HIS
3	C	88	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	S	14/40 (35%)	1 (7%)	0
4	V	12/40 (30%)	4 (33%)	0
All	All	26/80 (32%)	5 (19%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	V	5	A
4	V	7	U
4	V	10	A
4	V	11	C

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Mol	Chain	Res	Type
4	S	15	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

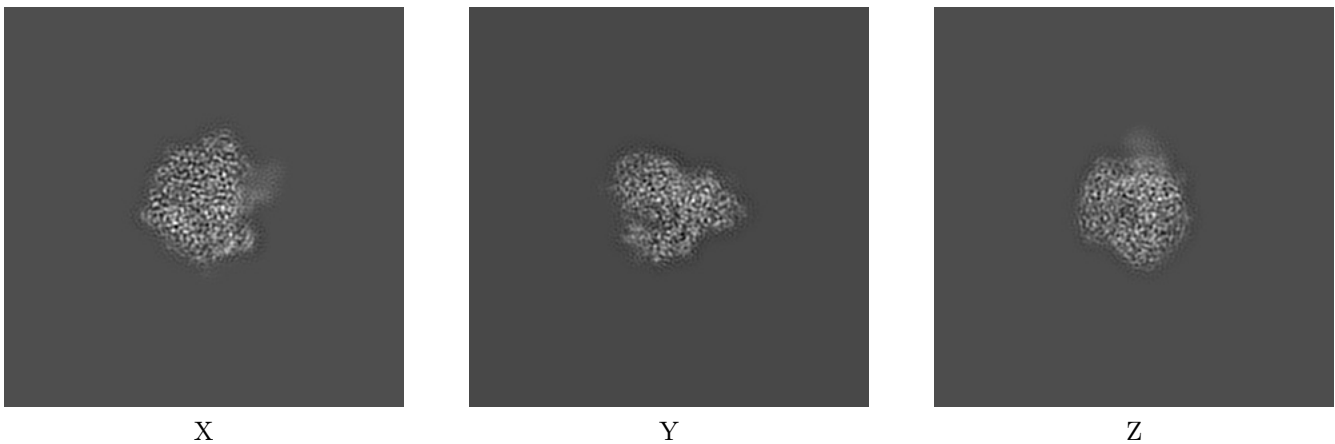
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17860. These allow visual inspection of the internal detail of the map and identification of artifacts.

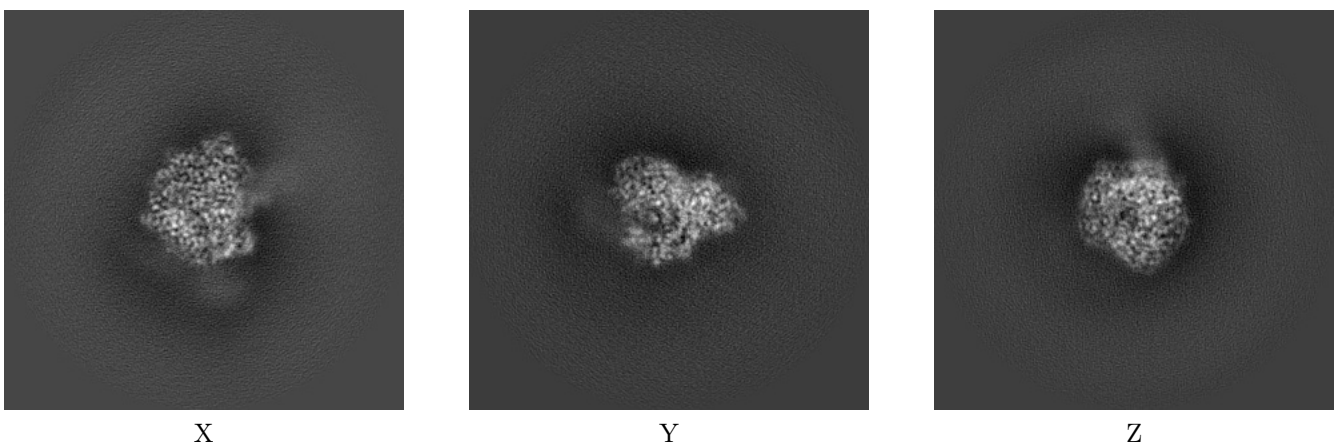
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



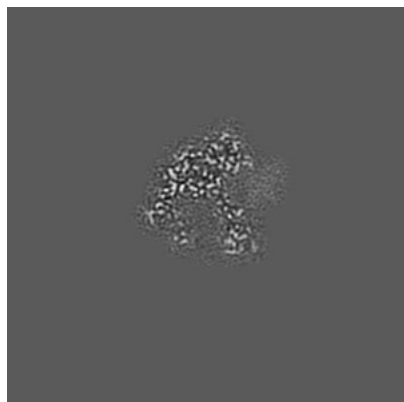
6.1.2 Raw map



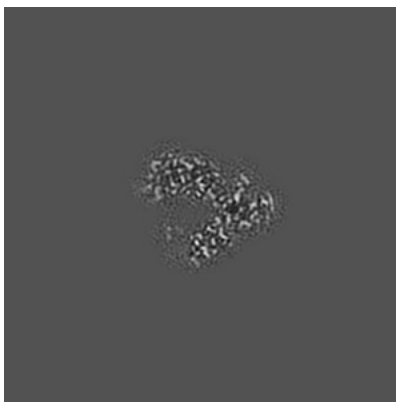
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

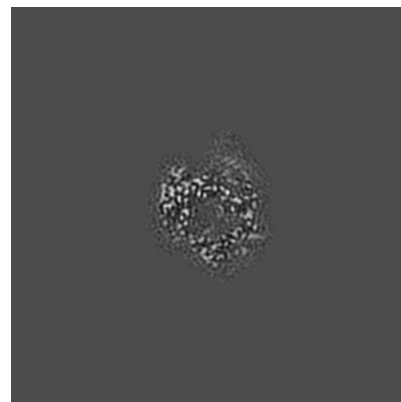
6.2.1 Primary map



X Index: 150

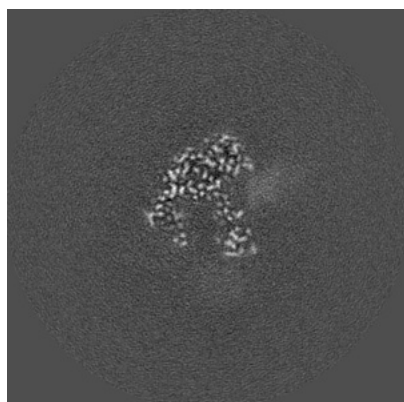


Y Index: 150

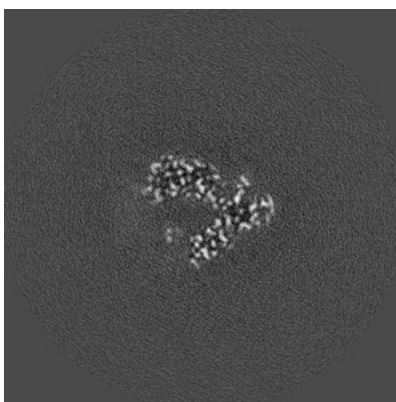


Z Index: 150

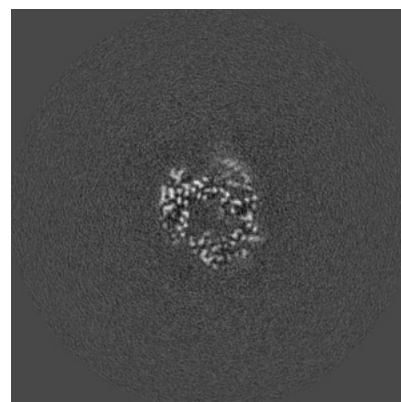
6.2.2 Raw map



X Index: 150



Y Index: 150

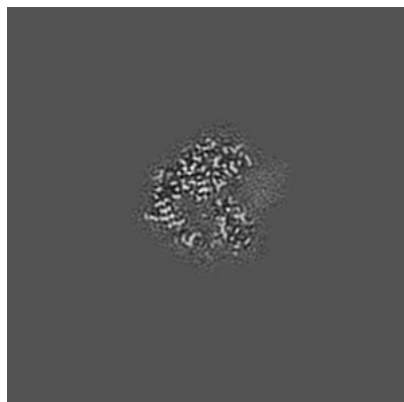


Z Index: 150

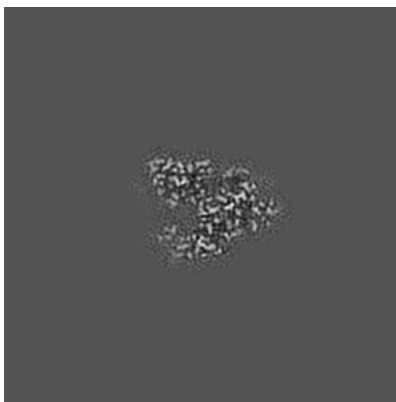
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

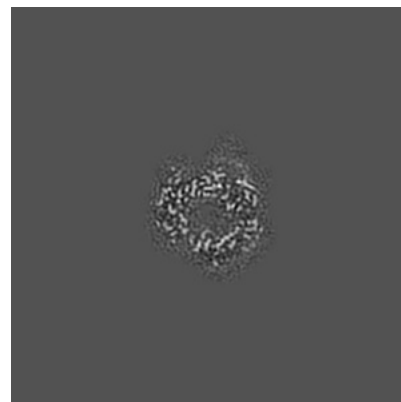
6.3.1 Primary map



X Index: 155

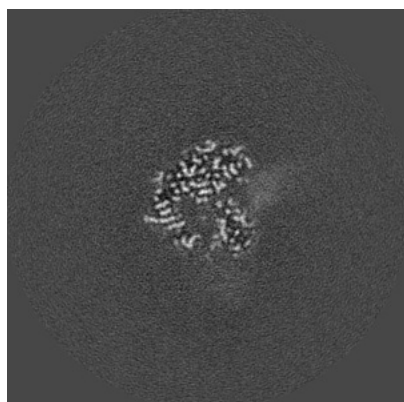


Y Index: 158

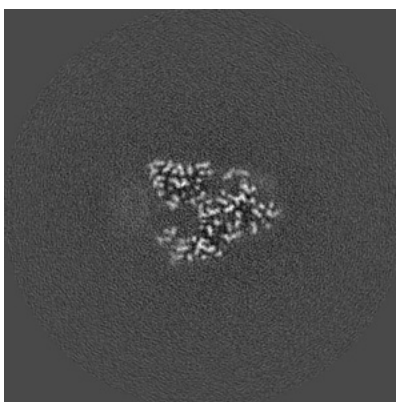


Z Index: 148

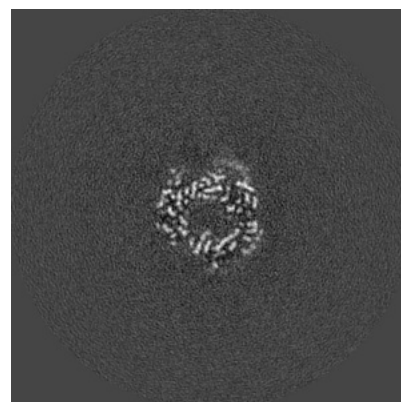
6.3.2 Raw map



X Index: 155



Y Index: 158

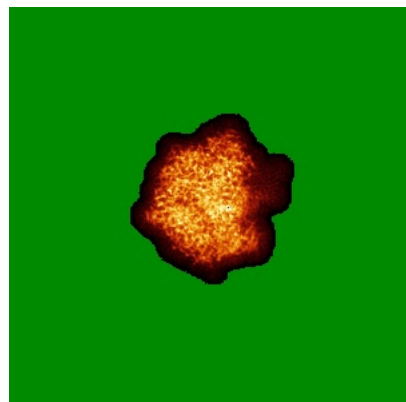


Z Index: 148

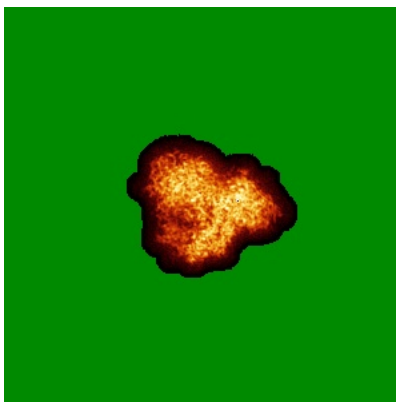
The images above show the largest variance slices of the map in three orthogonal directions.

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

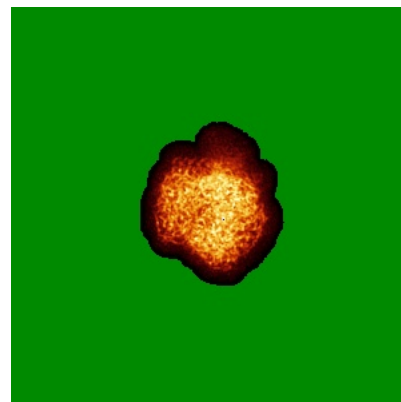
6.4.1 Primary map



X

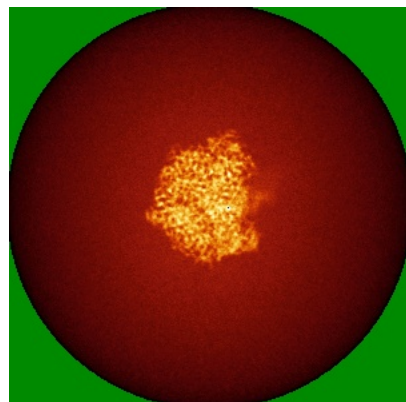


Y

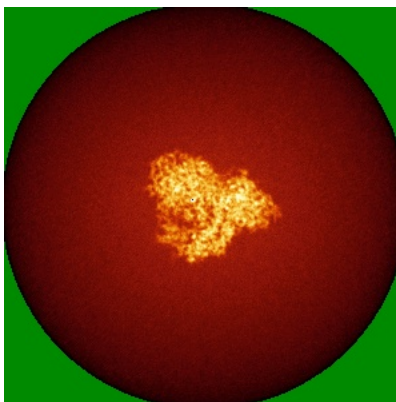


Z

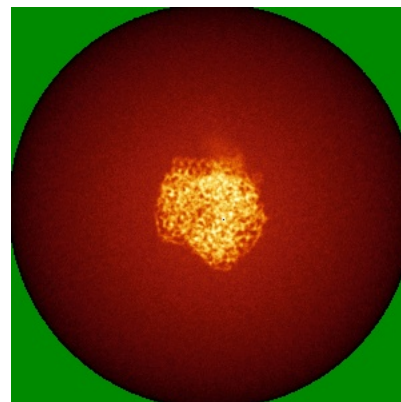
6.4.2 Raw map



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](#)

This section was not generated.

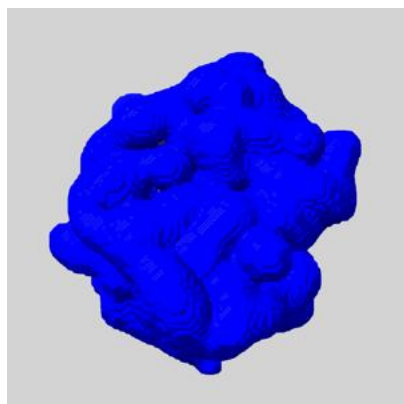
6.6 Mask visualisation [i](#)

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

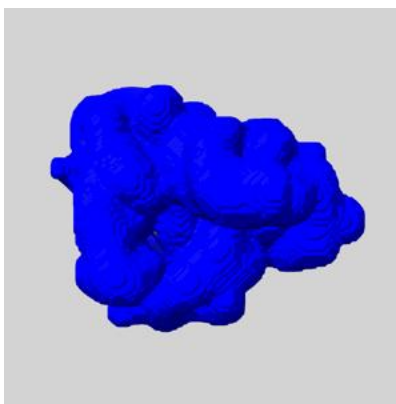
A mask typically either:

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

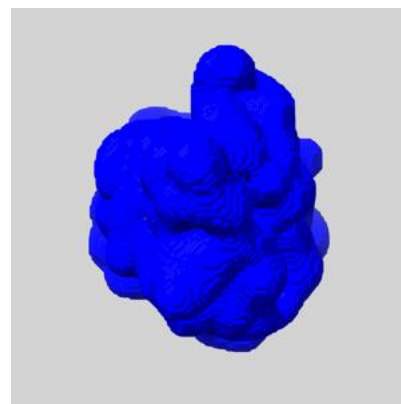
6.6.1 emd_17860_msk_1.map [i](#)



X



Y

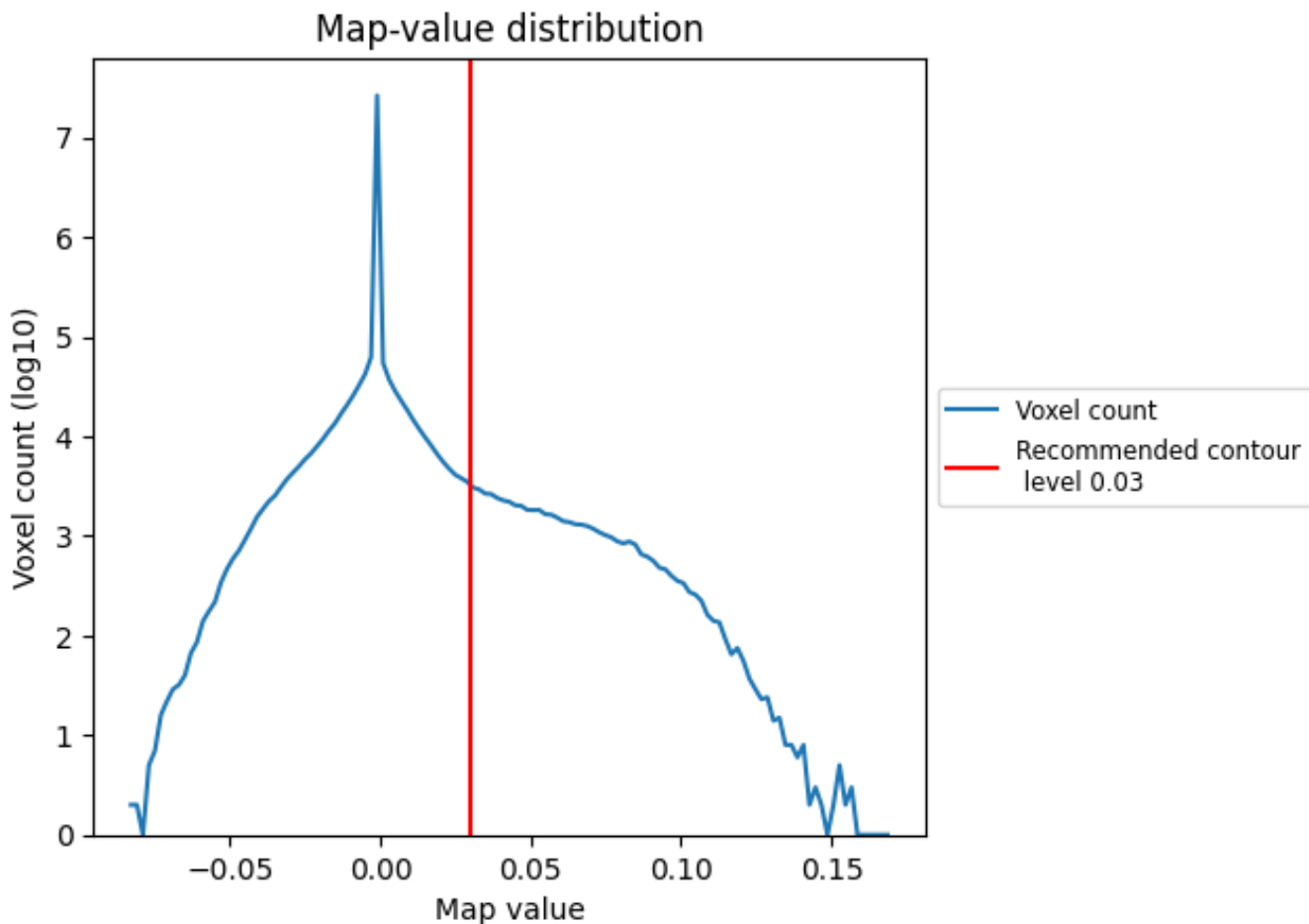


Z

7 Map analysis [i](#)

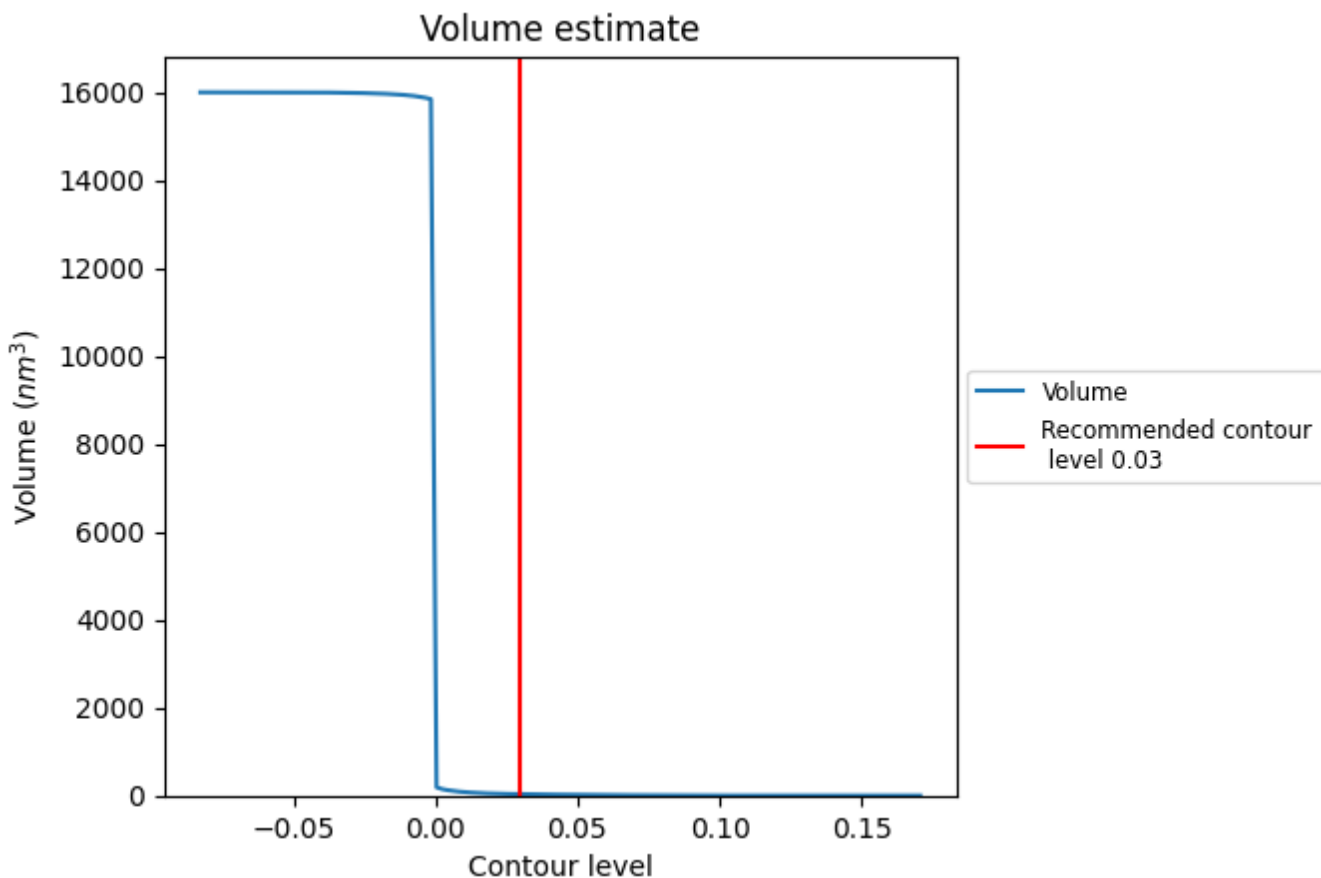
This section contains the results of statistical analysis of the map.

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.

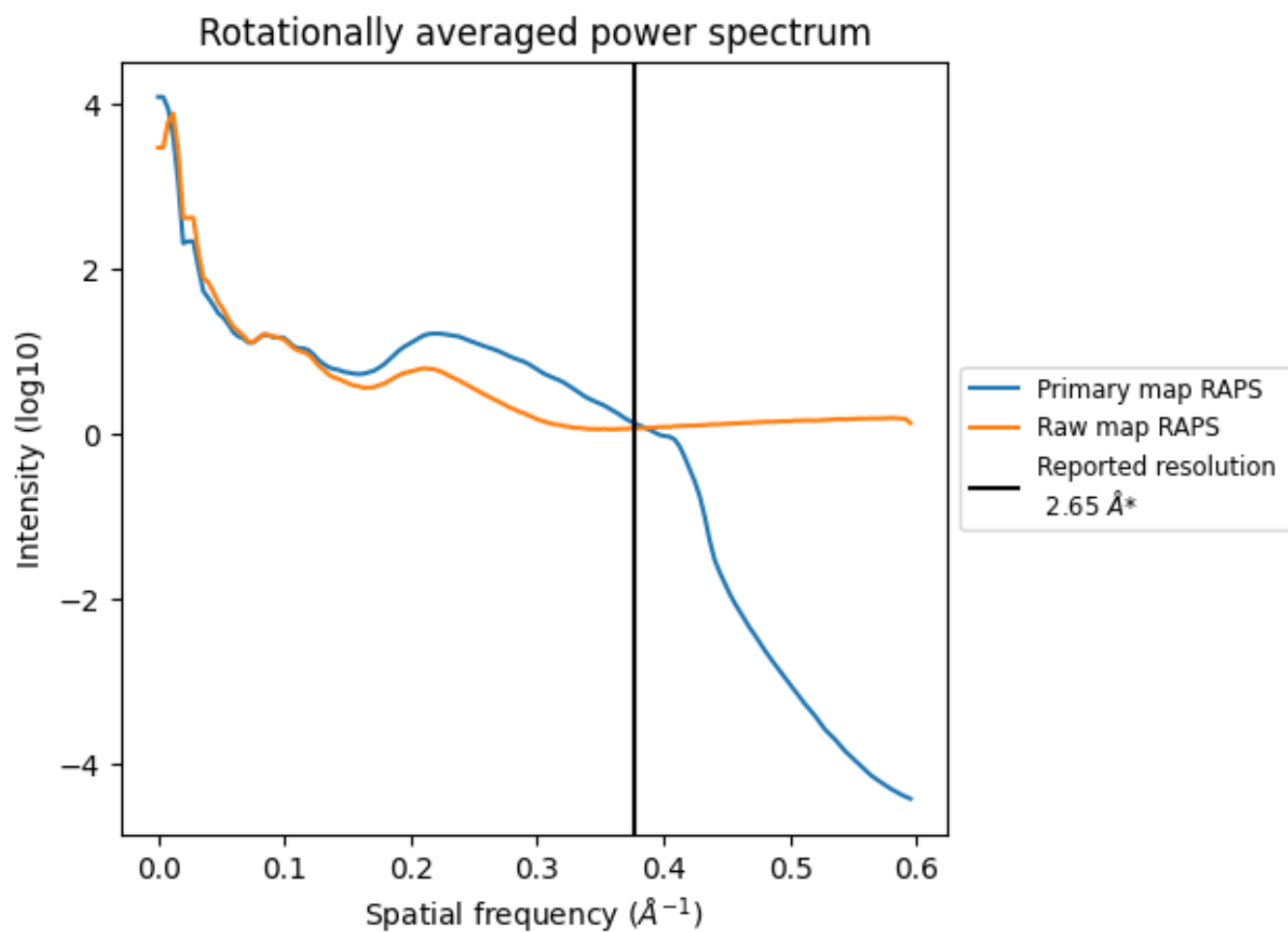
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 32 nm³; this corresponds to an approximate mass of 29 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

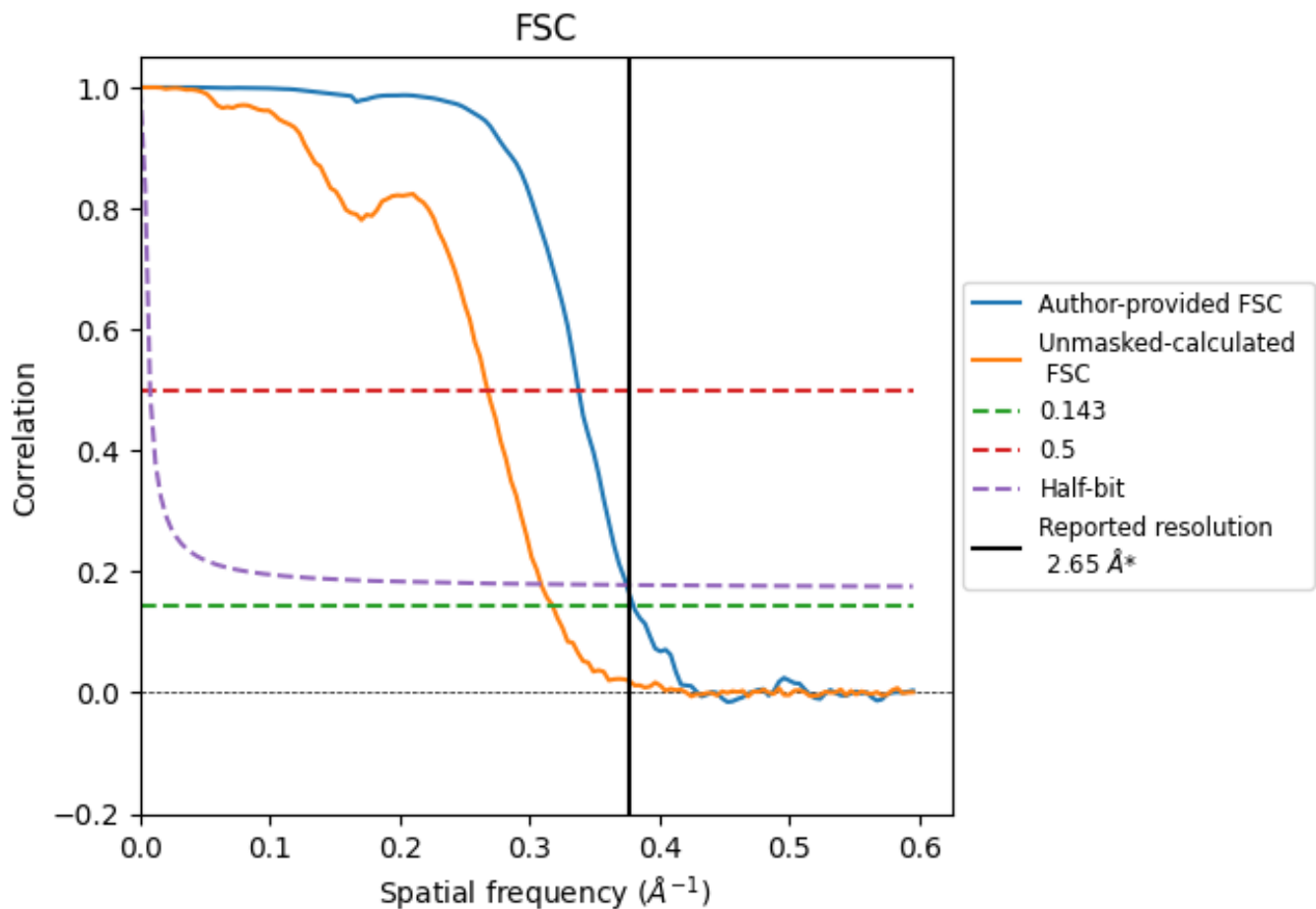


*Reported resolution corresponds to spatial frequency of 0.377 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.63	2.96	2.67
Unmasked-calculated*	3.15	3.74	3.24

*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 3.15 differs from the reported value 2.65 by more than 10 %

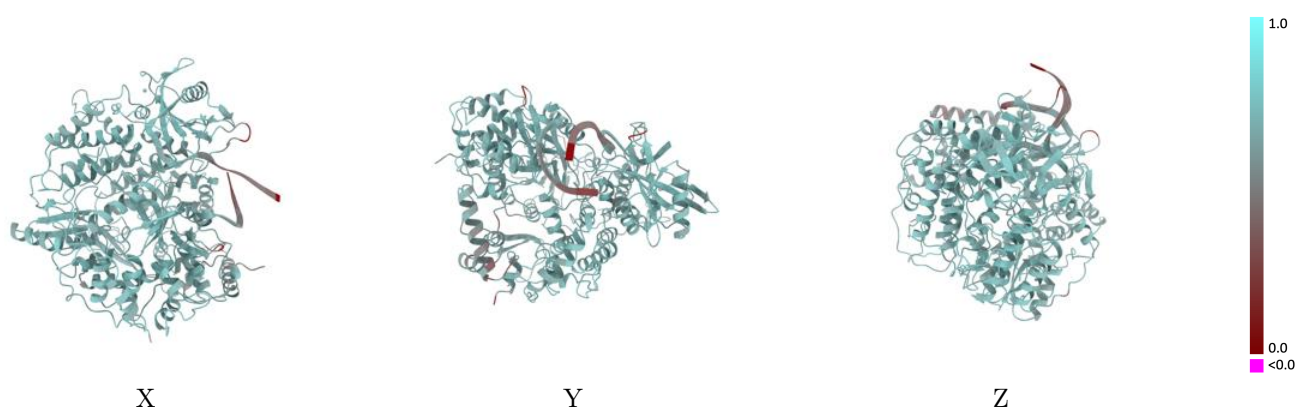
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-17860 and PDB model 8PSQ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)

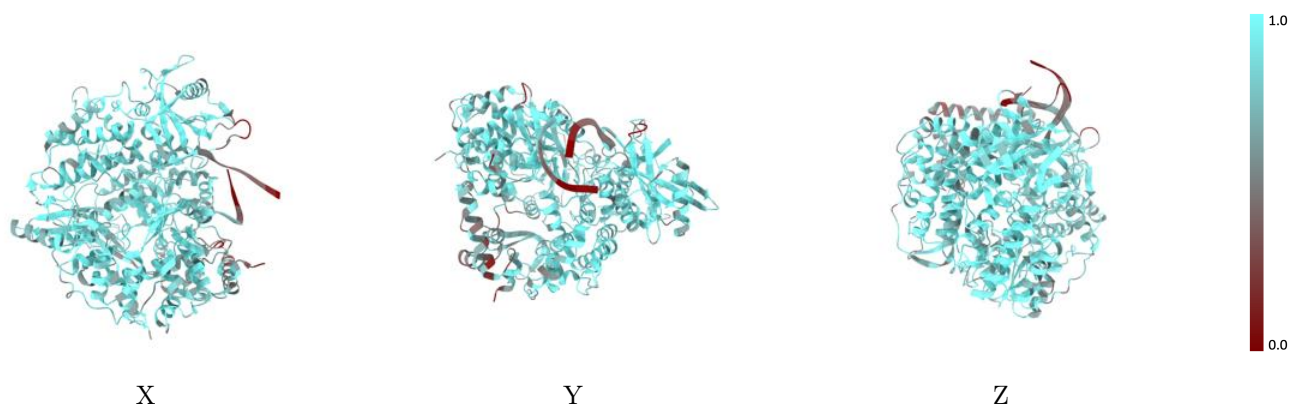
This section was not generated.

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



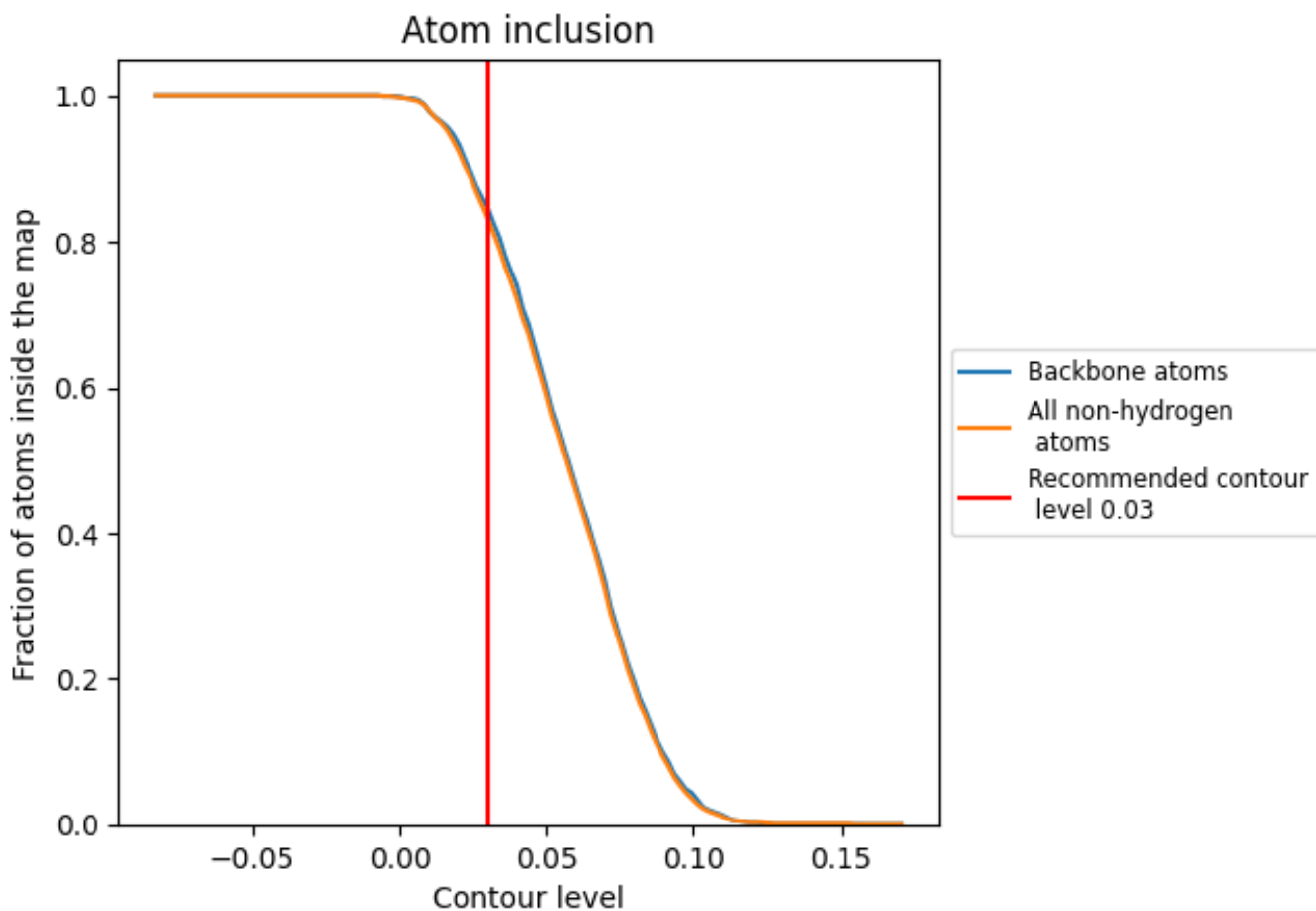
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).













9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.6480
A	 0.8670	 0.6600
B	 0.8510	 0.6590
C	 0.7760	 0.6380
S	 0.6650	 0.5620
V	 0.6300	 0.5200

