wwPDB EM Validation Summary Report

Mar 6, 2026 – 09:31 AM UTC

PDB ID	:	7QFW / pdb_00007qfw
EMDB ID	:	EMD-13950
Title	:	S.c. Condensin peripheral Ycg1 subcomplex bound to DNA
Authors	:	Lecomte, L.; Hassler, M.; Haering, C.; Eustermann, S.
Deposited on	:	2021-12-06
Resolution	:	3.86 Å(reported)
Based on initial model	:	5OQN

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:

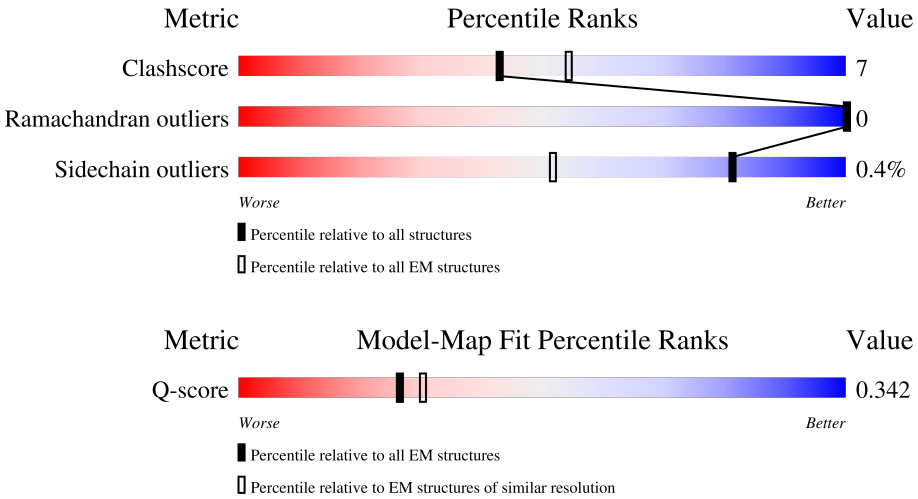
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.86 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	8889 (3.36 - 4.35)

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 <=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	1035	65% 15% 20%
2	B	811	9% 88%
3	C	50	10% 50% 14% 36%
4	D	50	52% 12% 36%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8765 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 Condensin complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	823	Total	C	N	O	S	0	0
			6643	4236	1125	1253	29		

- Molecule 2 is a protein called Condensin complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	94	Total	C	N	O	S	0	0
			810	519	143	145	3		

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	517	ALA	GLY	conflict	UNP P38170
B	755	LEU	-	expression tag	UNP P38170
B	756	VAL	-	expression tag	UNP P38170
B	757	GLY	-	expression tag	UNP P38170
B	758	GLY	-	expression tag	UNP P38170
B	759	GLY	-	expression tag	UNP P38170
B	760	HIS	-	expression tag	UNP P38170
B	761	HIS	-	expression tag	UNP P38170
B	762	ARG	-	expression tag	UNP P38170
B	763	PRO	-	expression tag	UNP P38170
B	764	HIS	-	expression tag	UNP P38170
B	765	HIS	-	expression tag	UNP P38170
B	766	GLY	-	expression tag	UNP P38170
B	767	GLY	-	expression tag	UNP P38170
B	768	HIS	-	expression tag	UNP P38170
B	769	HIS	-	expression tag	UNP P38170
B	770	HIS	-	expression tag	UNP P38170
B	771	HIS	-	expression tag	UNP P38170
B	772	HIS	-	expression tag	UNP P38170
B	773	HIS	-	expression tag	UNP P38170
B	774	GLY	-	expression tag	UNP P38170

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Chain	Residue	Modelled	Actual	Comment	Reference
B	775	GLY	-	expression tag	UNP P38170
B	776	ARG	-	expression tag	UNP P38170
B	777	ILE	-	expression tag	UNP P38170
B	778	PHE	-	expression tag	UNP P38170
B	779	TYR	-	expression tag	UNP P38170
B	780	PRO	-	expression tag	UNP P38170
B	781	TYR	-	expression tag	UNP P38170
B	782	ASP	-	expression tag	UNP P38170
B	783	VAL	-	expression tag	UNP P38170
B	784	PRO	-	expression tag	UNP P38170
B	785	ASP	-	expression tag	UNP P38170
B	786	TYR	-	expression tag	UNP P38170
B	787	ALA	-	expression tag	UNP P38170
B	788	GLY	-	expression tag	UNP P38170
B	789	TYR	-	expression tag	UNP P38170
B	790	PRO	-	expression tag	UNP P38170
B	791	TYR	-	expression tag	UNP P38170
B	792	ASP	-	expression tag	UNP P38170
B	793	VAL	-	expression tag	UNP P38170
B	794	PRO	-	expression tag	UNP P38170
B	795	ASP	-	expression tag	UNP P38170
B	796	TYR	-	expression tag	UNP P38170
B	797	ALA	-	expression tag	UNP P38170
B	798	GLY	-	expression tag	UNP P38170
B	799	SER	-	expression tag	UNP P38170
B	800	TYR	-	expression tag	UNP P38170
B	801	PRO	-	expression tag	UNP P38170
B	802	TYR	-	expression tag	UNP P38170
B	803	ASP	-	expression tag	UNP P38170
B	804	VAL	-	expression tag	UNP P38170
B	805	PRO	-	expression tag	UNP P38170
B	806	ASN	-	expression tag	UNP P38170
B	807	TYR	-	expression tag	UNP P38170
B	808	ALA	-	expression tag	UNP P38170
B	809	ALA	-	expression tag	UNP P38170
B	810	GLY	-	expression tag	UNP P38170
B	811	HIS	-	expression tag	UNP P38170

- Molecule 3 is a DNA chain called Synthetic DNA ligand.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	32	Total	C	N	O	P	0	0
			672	320	160	160	32		

- Molecule 4 is a DNA chain called synthetic DNA ligand.

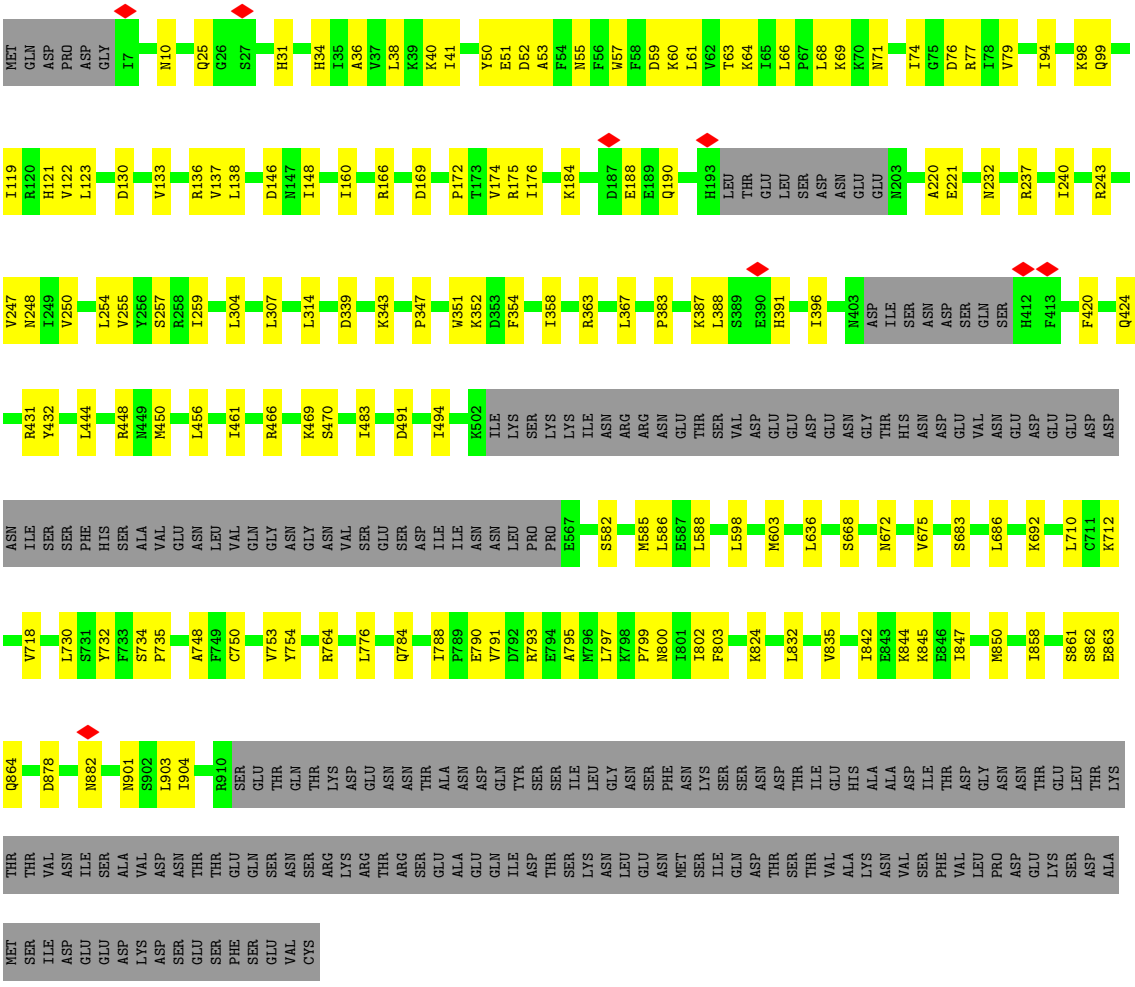
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	32	640	320	64	224	32	0	0

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.

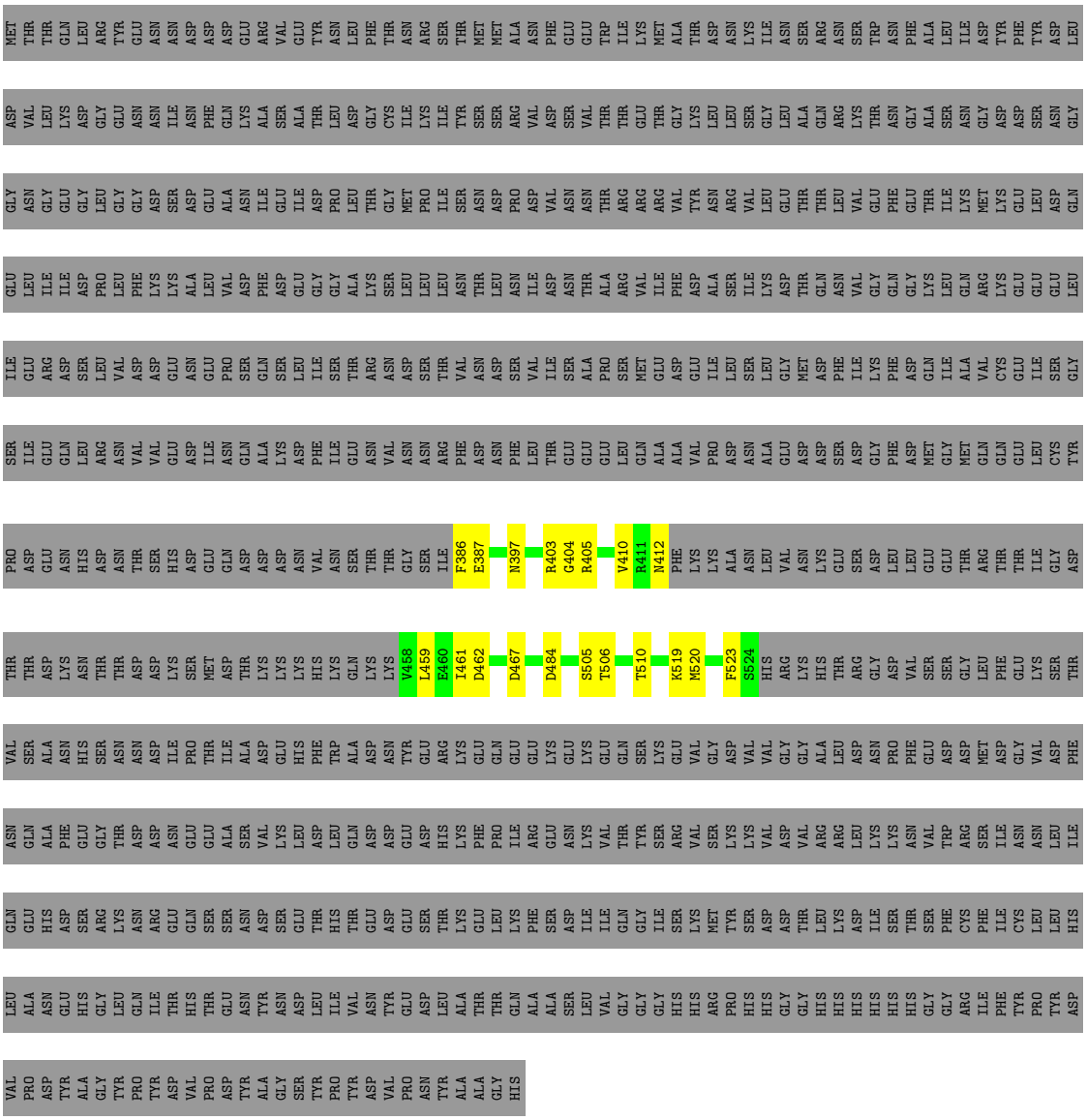
• Molecule 1: Condensin complex subunit 3

Chain A:

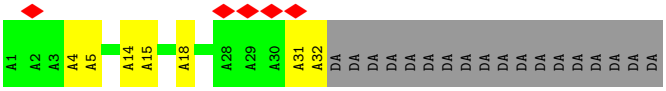


• Molecule 2: Condensin complex subunit 2

Chain B:



• Molecule 3: Synthetic DNA ligand



• Molecule 4: synthetic DNA ligand

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27701	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 ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.238	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	0.27	0/6746	0.61	0/9119
2	B	0.25	0/830	0.67	0/1111
3	C	0.33	0/767	0.45	0/1180
4	D	0.40	0/703	0.71	0/1084
All	All	0.29	0/9046	0.61	0/12494

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

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	6643	0	6749	99	0
2	B	810	0	787	18	0
3	C	672	0	353	4	0
4	D	640	0	385	4	0
All	All	8765	0	8274	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 113 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:71:ASN:HD21	3:C:18:DA:H3'	1.58	0.69
1:A:240:ILE:O	1:A:243:ARG:HB2	2.01	0.60
1:A:69:LYS:O	1:A:136:ARG:NH1	2.36	0.59
1:A:25:GLN:NE2	2:B:462:ASP:OD1	2.36	0.59
1:A:732:TYR:O	2:B:405:ARG:NH1	2.36	0.58

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	815/1035 (79%)	786 (96%)	29 (4%)	0	100	100
2	B	90/811 (11%)	84 (93%)	6 (7%)	0	100	100
All	All	905/1846 (49%)	870 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	749/947 (79%)	747 (100%)	2 (0%)	86	85
2	B	89/731 (12%)	88 (99%)	1 (1%)	65	73
All	All	838/1678 (50%)	835 (100%)	3 (0%)	81	83

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ILE
1	A	304	LEU
2	B	410	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	499	GLN
2	B	401	ASN
1	A	613	ASN
2	B	495	HIS
1	A	884	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.

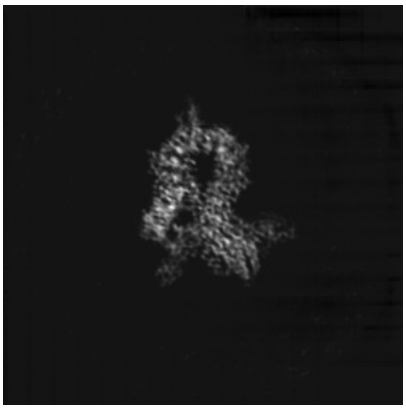
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13950. 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

6.1.1 Primary map



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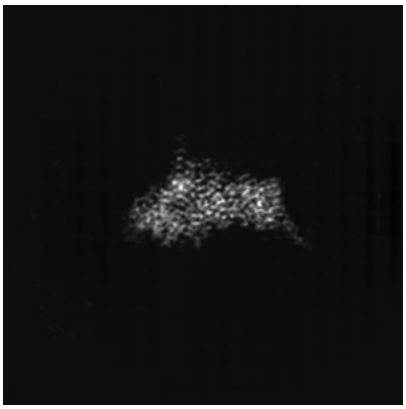

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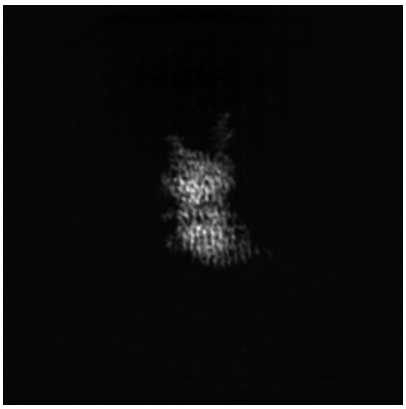
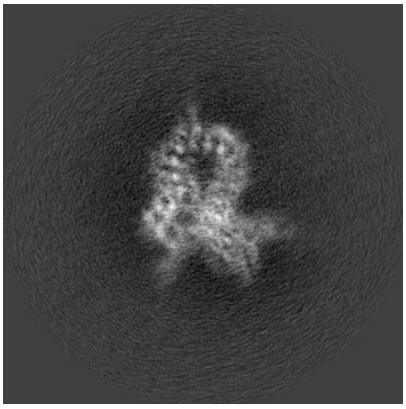
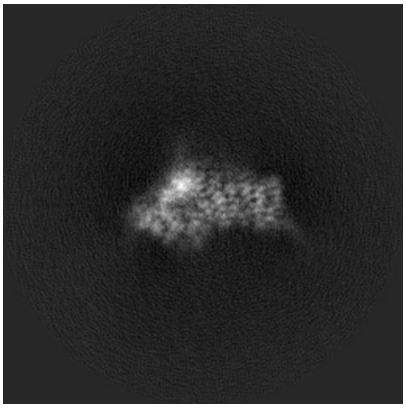


Z

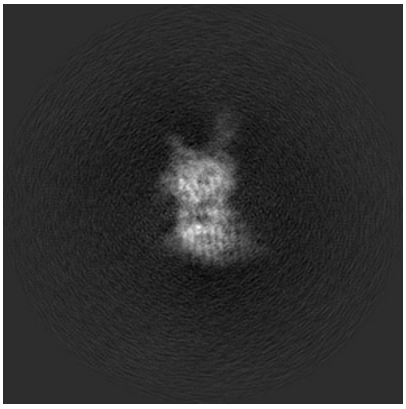
6.1.2 Raw map



X



Y

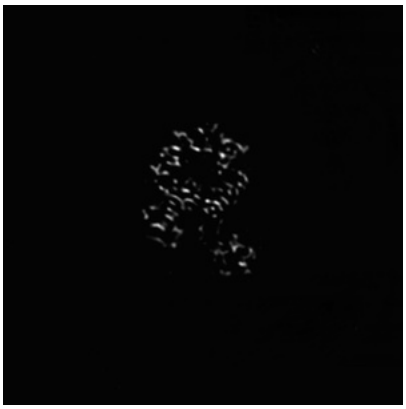


Z

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

6.2 Central slices (i)

6.2.1 Primary map

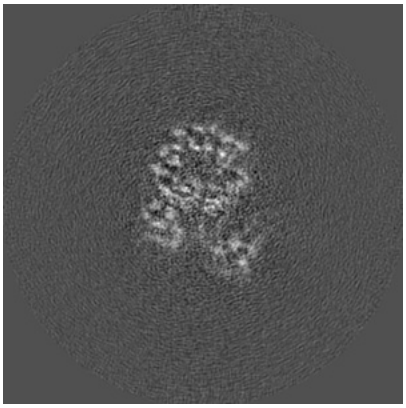


X Index: 128

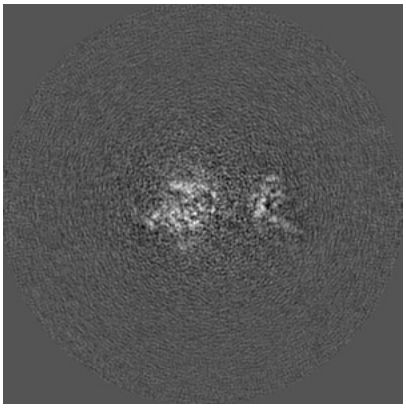
Y Index: 128

Z Index: 128

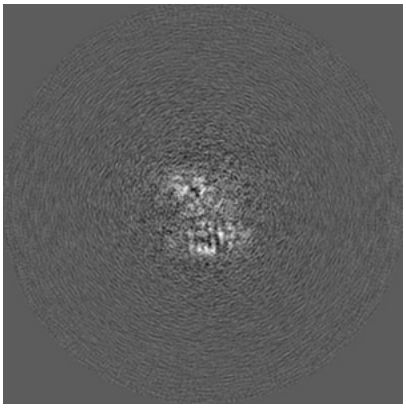
6.2.2 Raw map



X Index: 128



Y Index: 128



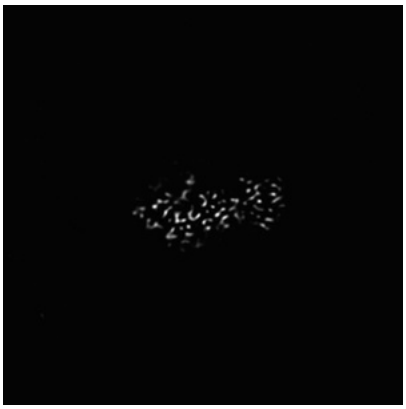
Z Index: 128

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

6.3 Largest variance slices (i)

6.3.1 Primary map

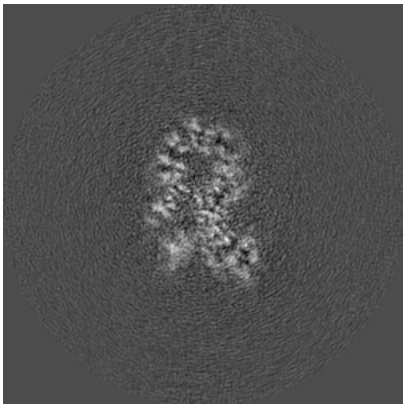
X Index: 121



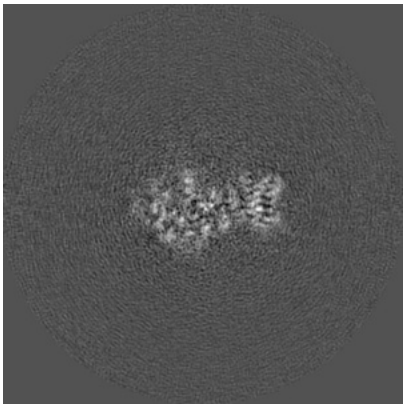
Y Index: 137

Z Index: 163

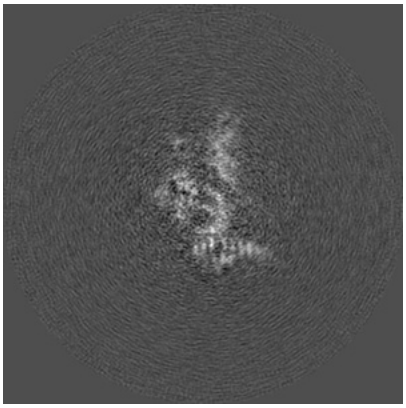
6.3.2 Raw map



X Index: 121



Y Index: 139

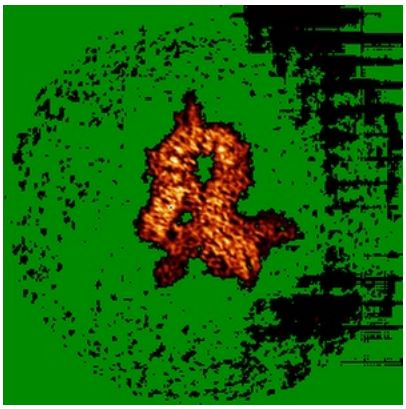


Z Index: 113

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



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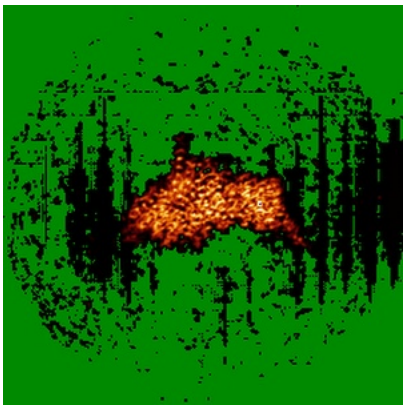
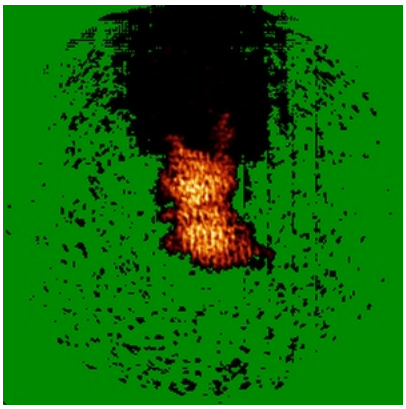
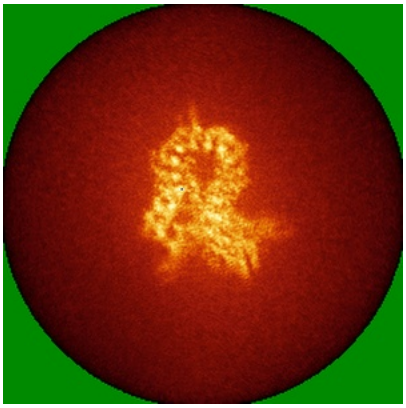


Y



Z

6.4.2 Raw map



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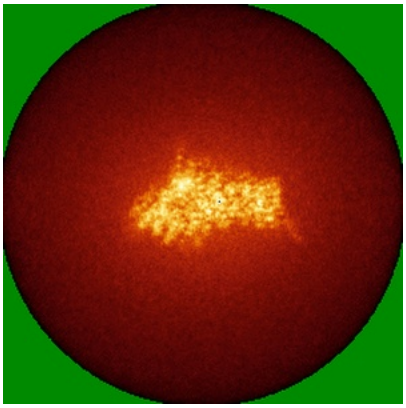

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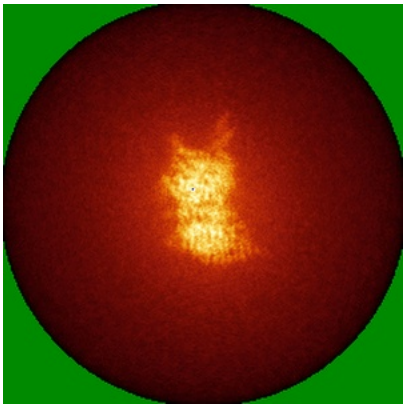


Z

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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. 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

X Y Z

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.

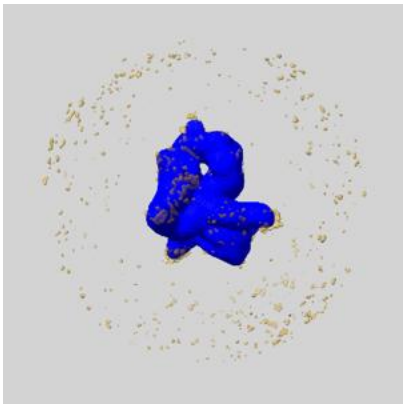
6.6 Mask visualisation (i)

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

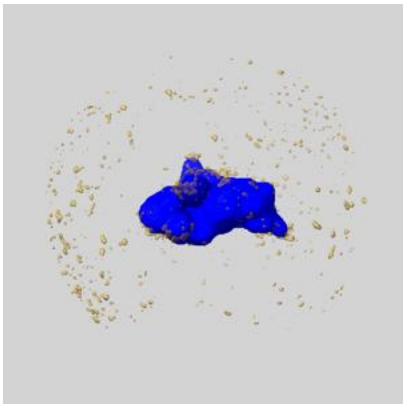
A mask typically either:

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

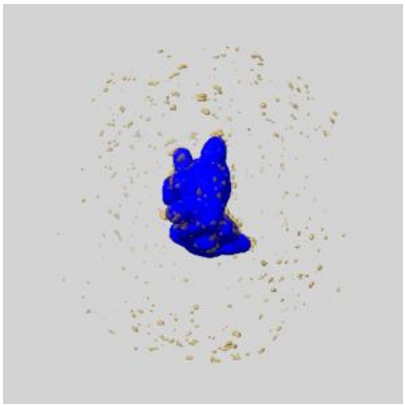
6.6.1 emd_13950_msk_1.map (i)



X



Y

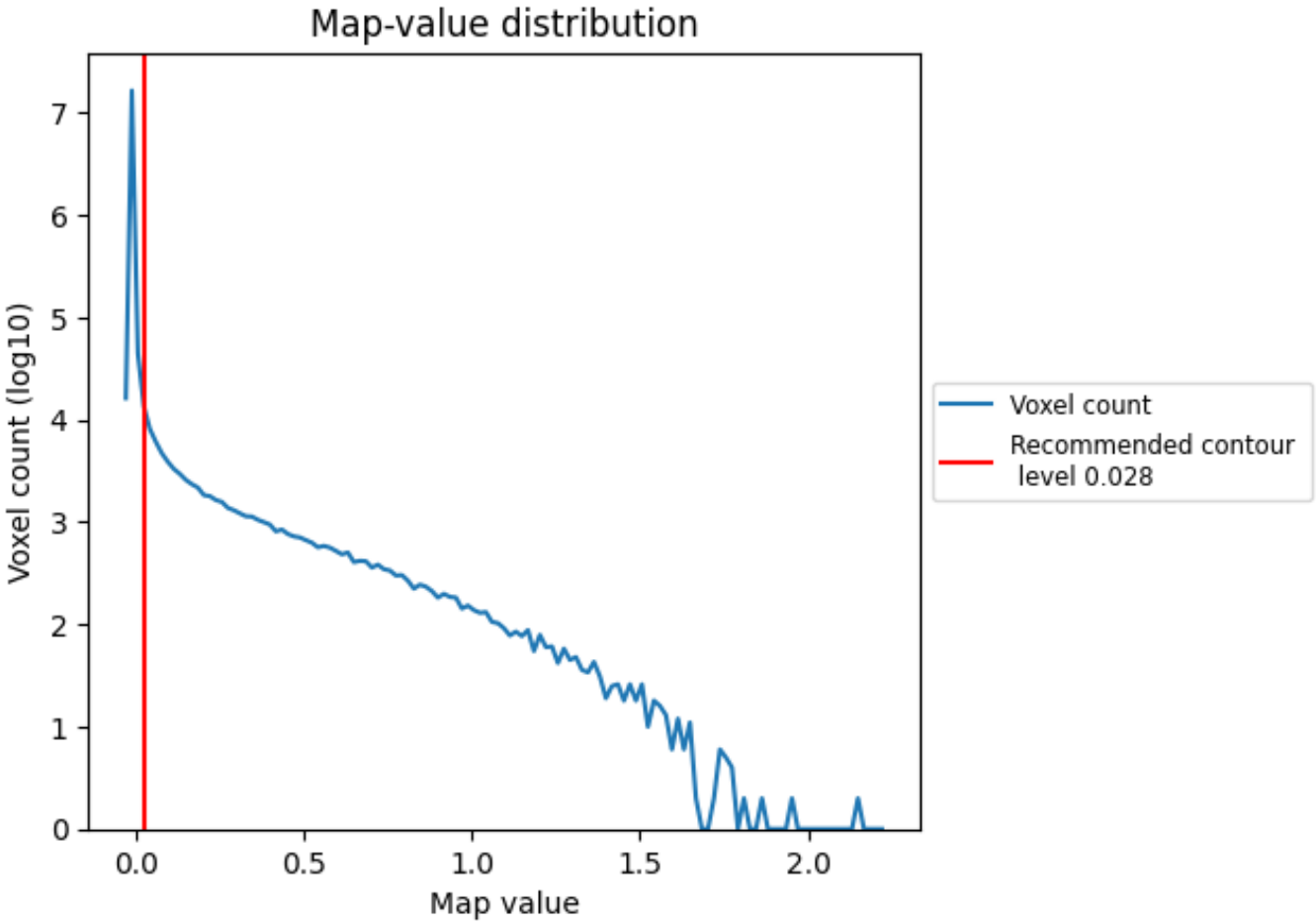


Z

7 Map analysis

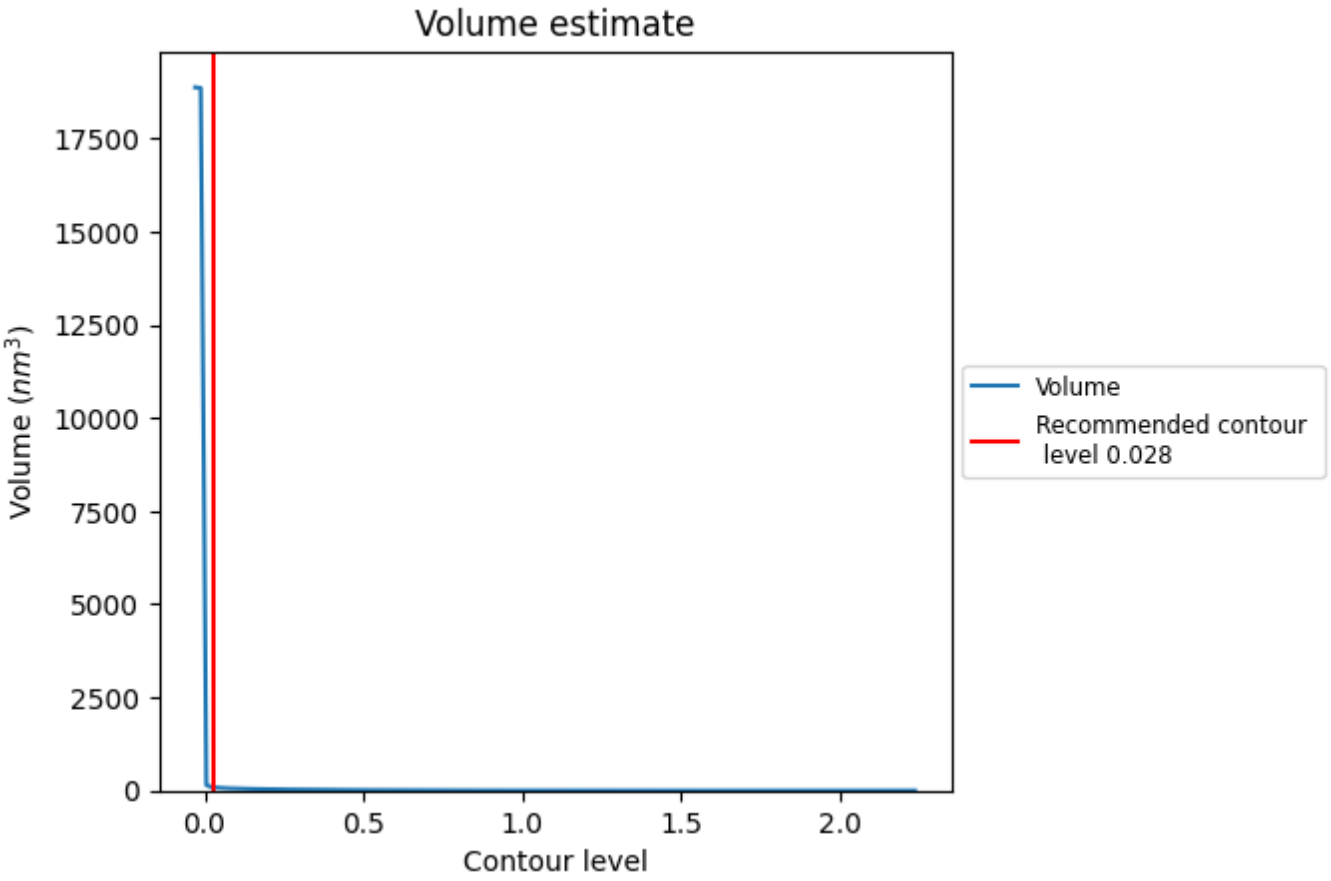
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

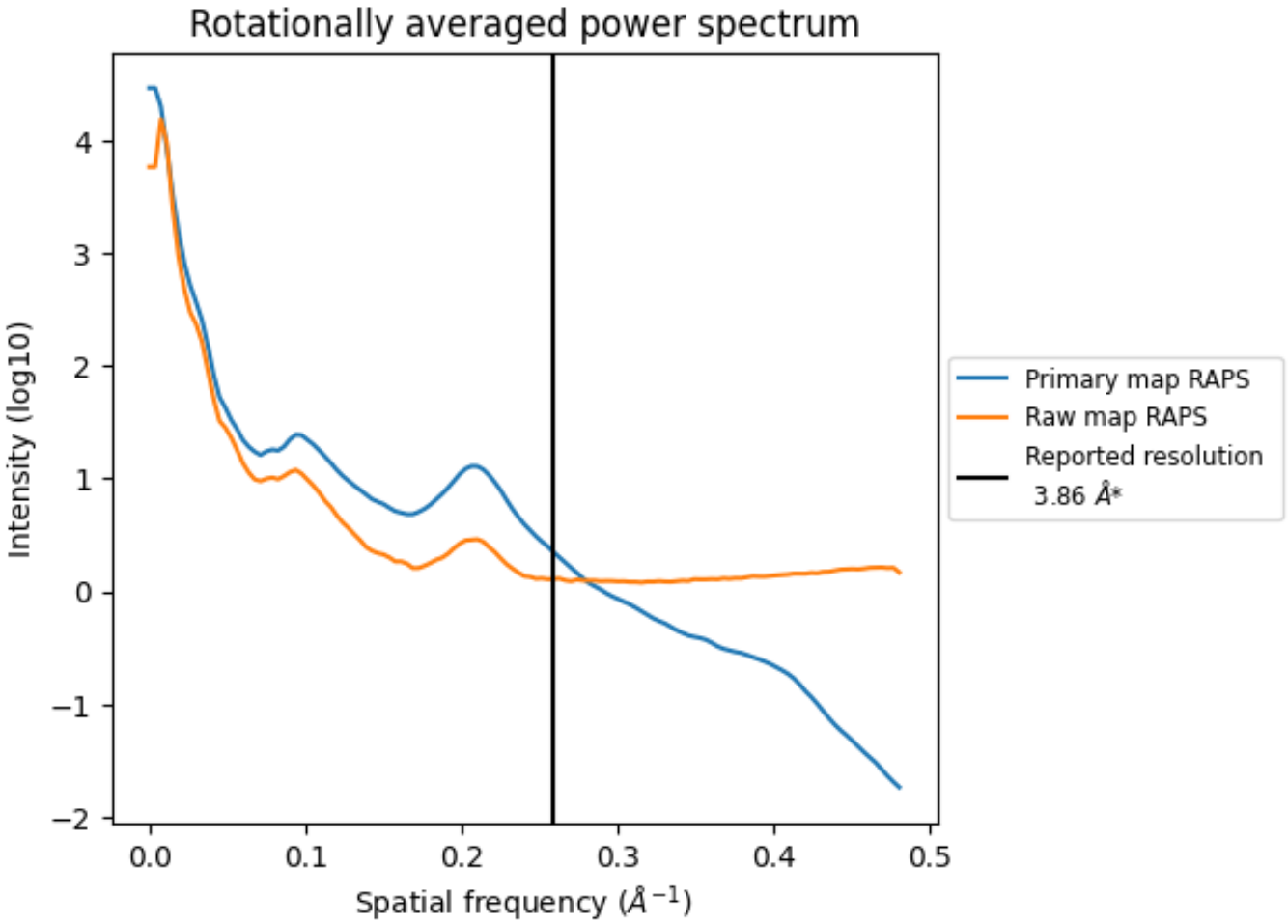
7.2 Volume estimate (i)



The volume at the recommended contour level is 88 nm^3; this corresponds to an approximate mass of 80 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)

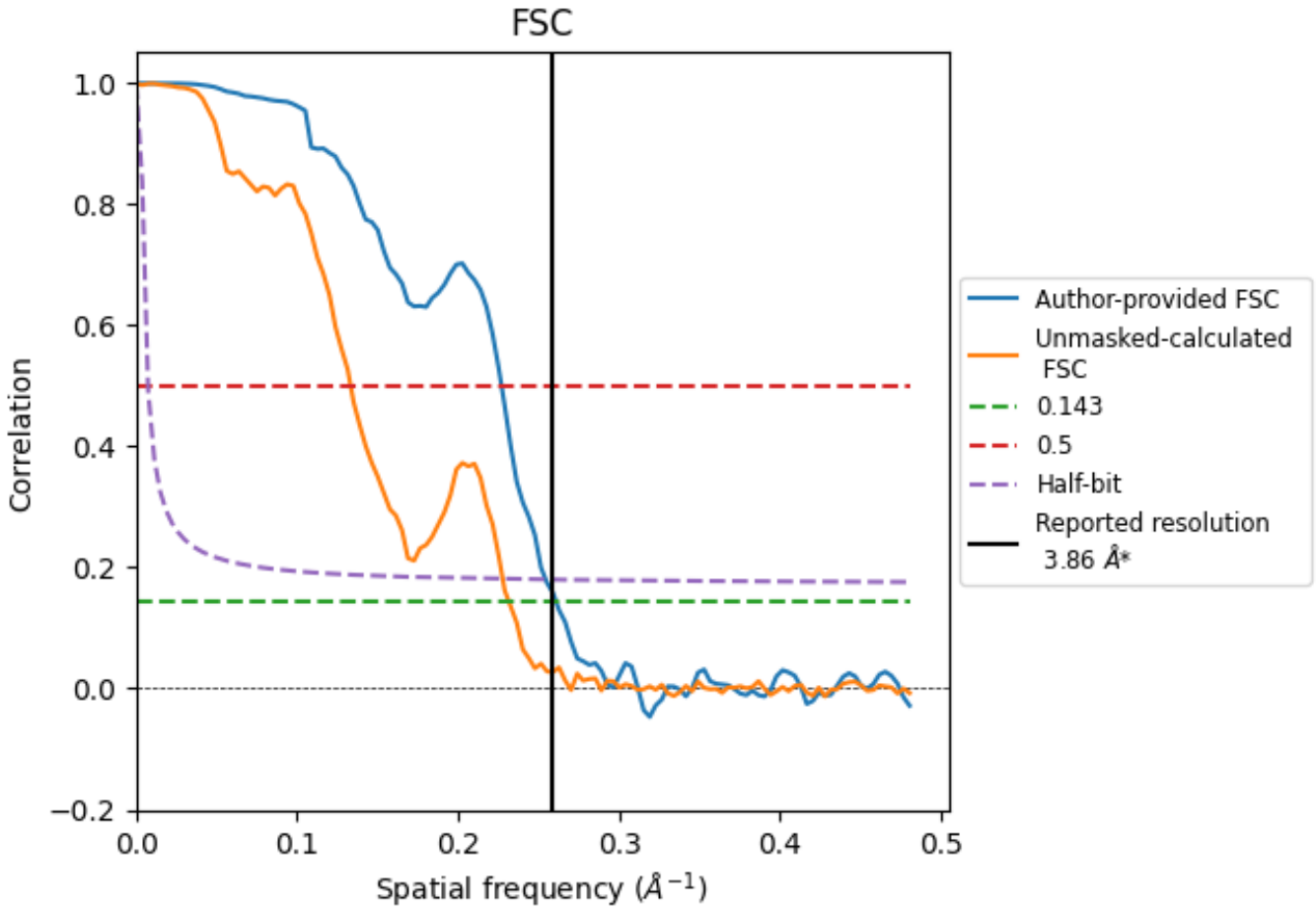


*Reported resolution corresponds to spatial frequency of 0.259 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.259 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.86	-	-
Author-provided FSC curve	3.83	4.40	3.93
Unmasked-calculated*	4.31	7.50	4.39

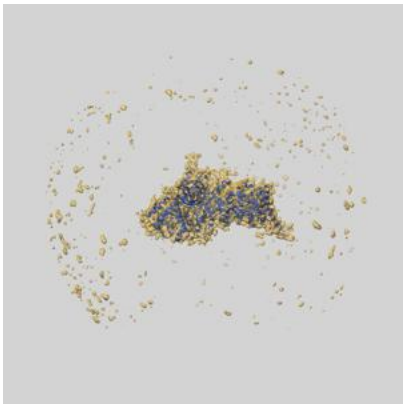
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.86 by more than 10 %

9 Map-model fit

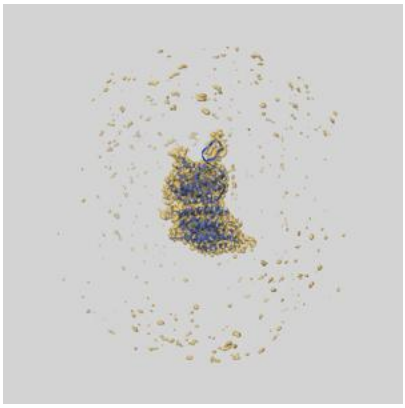
This section contains information regarding the fit between EMDB map EMD-13950 and PDB model 7QFW. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay

X



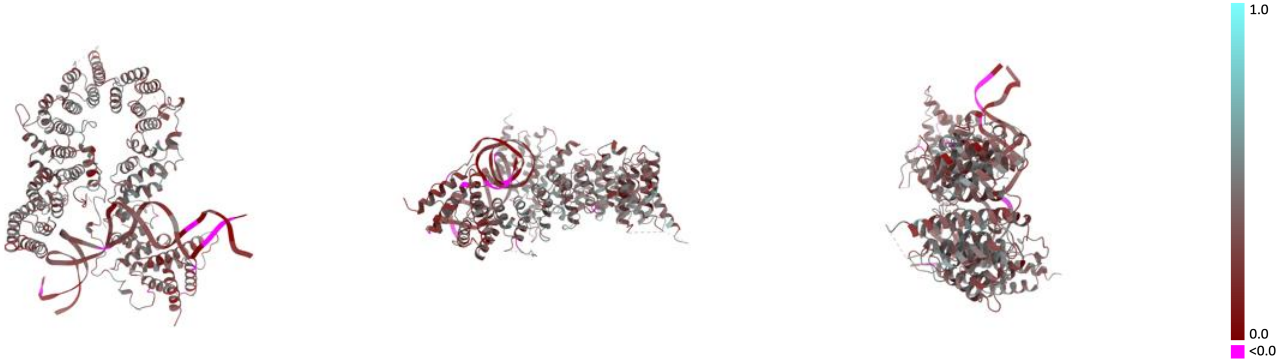
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.028 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.

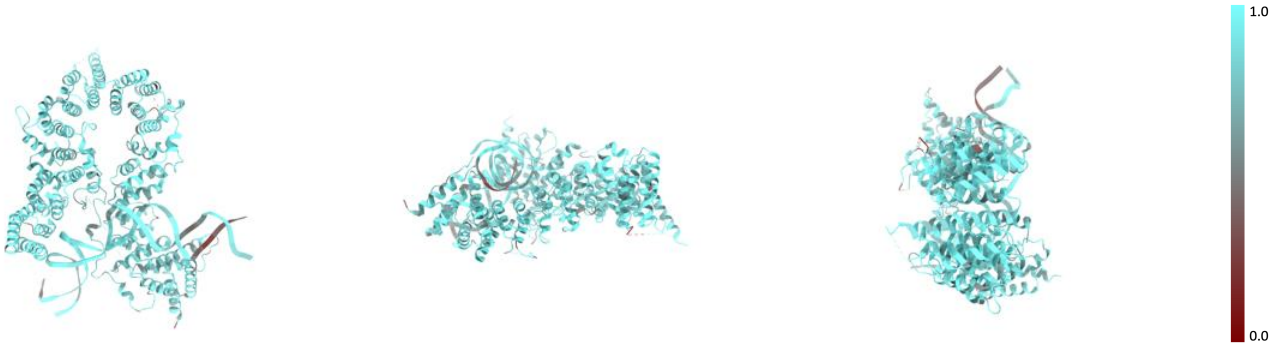
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

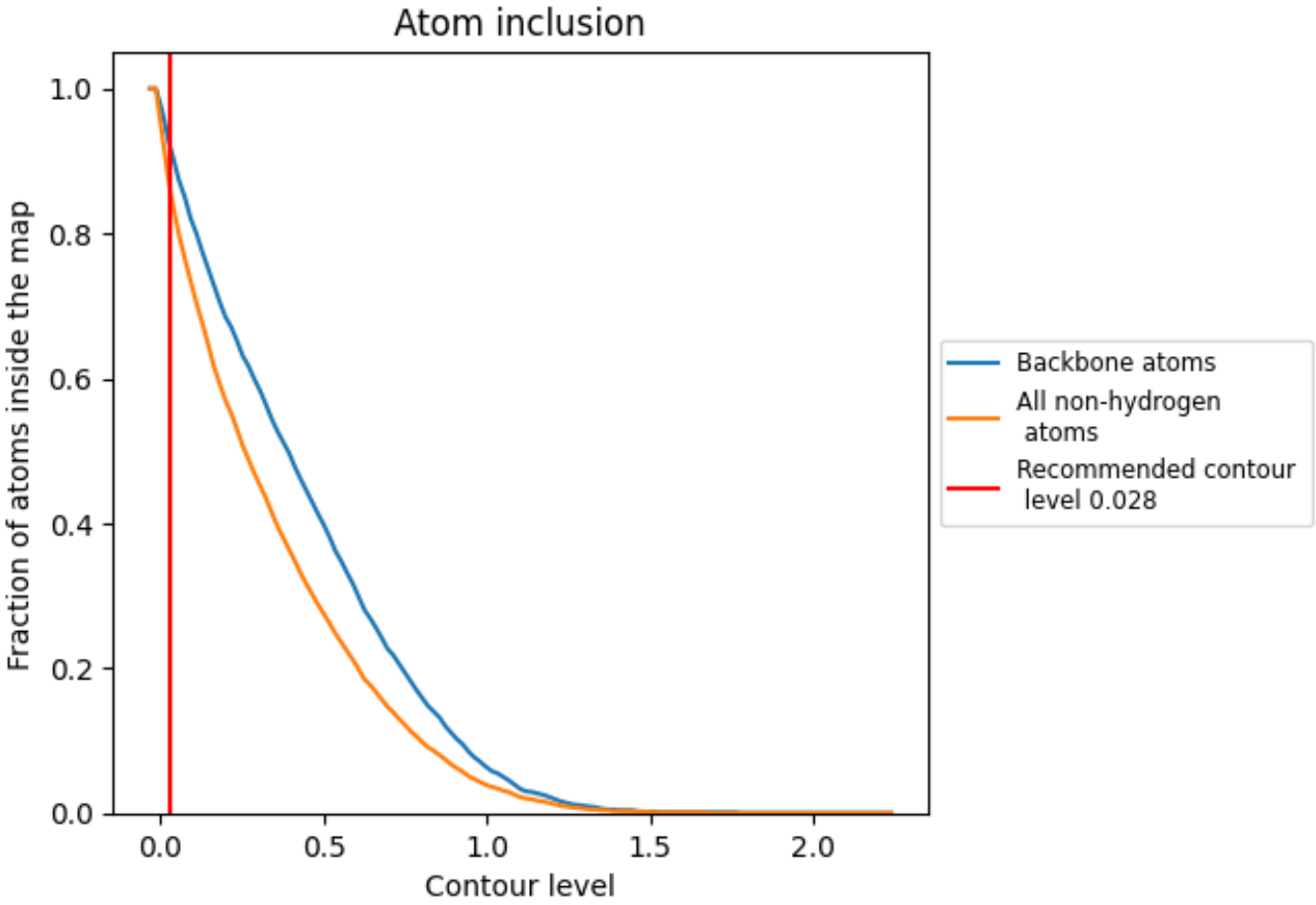
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.028).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8690	0.3420
A	0.8910	0.3700
B	0.8490	0.3610
C	0.7620	0.1880
D	0.7800	0.1990