



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 02:45 PM UTC

PDB ID : 9GW2 / pdb_00009gw2
EMDB ID : EMD-51643
Title : State 2 MAP 1 SETD2 bound to proximal H3 of upstream nucleosome
Authors : Walshe, J.L.; Ochmann, M.; Dienemann, C.; Cramer, P.
Deposited on : 2024-09-26
Resolution : 4.84 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:

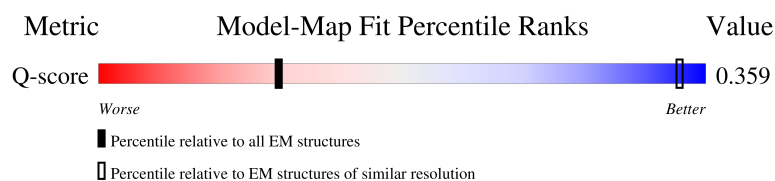
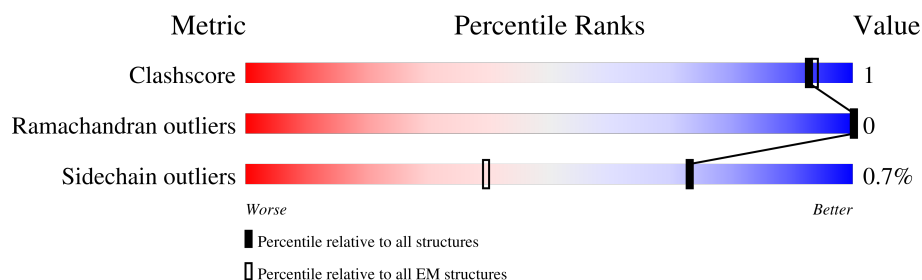
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.84 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.









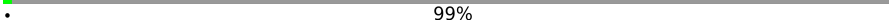
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1298 (4.34 - 5.34)

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	N	182	
2	O	1133	
3	T	182	
4	a	136	

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Mol	Chain	Length	Quality of chain
4	e	136	 68% 30%
5	b	103	 71% 5% 24%
5	f	103	 75% 24%
6	c	135	 75% 21%
6	g	135	 73% 24%
7	d	126	 70% 27%
7	h	126	 69% 29%
8	j	1049	 99%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24125 atoms, of which 11011 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 DNA chain called Non-Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	N	125	Total	C	H	N	O	P	0	0
			3982	1221	1403	483	750	125		

- Molecule 2 is a protein called Histone-lysine N-methyltransferase SETD2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	O	245	Total	C	H	N	O	S	0	0
			3923	1234	1930	364	374	21		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	1432	SER	-	expression tag	UNP Q9BYW2
O	1433	ASN	-	expression tag	UNP Q9BYW2
O	1434	ALA	-	expression tag	UNP Q9BYW2
O	1962	LEU	PRO	variant	UNP Q9BYW2

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	T	125	Total	C	H	N	O	P	0	0
			3949	1210	1403	461	750	125		

- Molecule 4 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	a	101	Total	C	H	N	O	S	0	0
			1684	519	863	157	142	3		
4	e	95	Total	C	H	N	O	S	0	0
			1601	494	819	150	136	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	37	MET	LYS	engineered mutation	UNP Q71DI3
a	111	ALA	CYS	engineered mutation	UNP Q71DI3
e	37	MET	LYS	engineered mutation	UNP Q71DI3
e	111	ALA	CYS	engineered mutation	UNP Q71DI3

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	b	78	Total	C	H	N	O	S	0	0
			1283	393	661	120	108	1		
5	f	78	Total	C	H	N	O	S	0	0
			1283	393	661	120	108	1		

- Molecule 6 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	c	107	Total	C	H	N	O		0	0
			1711	520	885	163	143			
6	g	103	Total	C	H	N	O		0	0
			1645	502	849	155	139			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-4	SER	-	expression tag	UNP P04908
c	-3	ASN	-	expression tag	UNP P04908
c	-2	ALA	-	expression tag	UNP P04908
c	-1	PRO	-	expression tag	UNP P04908
c	0	TRP	-	expression tag	UNP P04908
g	-4	SER	-	expression tag	UNP P04908
g	-3	ASN	-	expression tag	UNP P04908
g	-2	ALA	-	expression tag	UNP P04908
g	-1	PRO	-	expression tag	UNP P04908
g	0	TRP	-	expression tag	UNP P04908

- Molecule 7 is a protein called Histone H2B type 1-K.

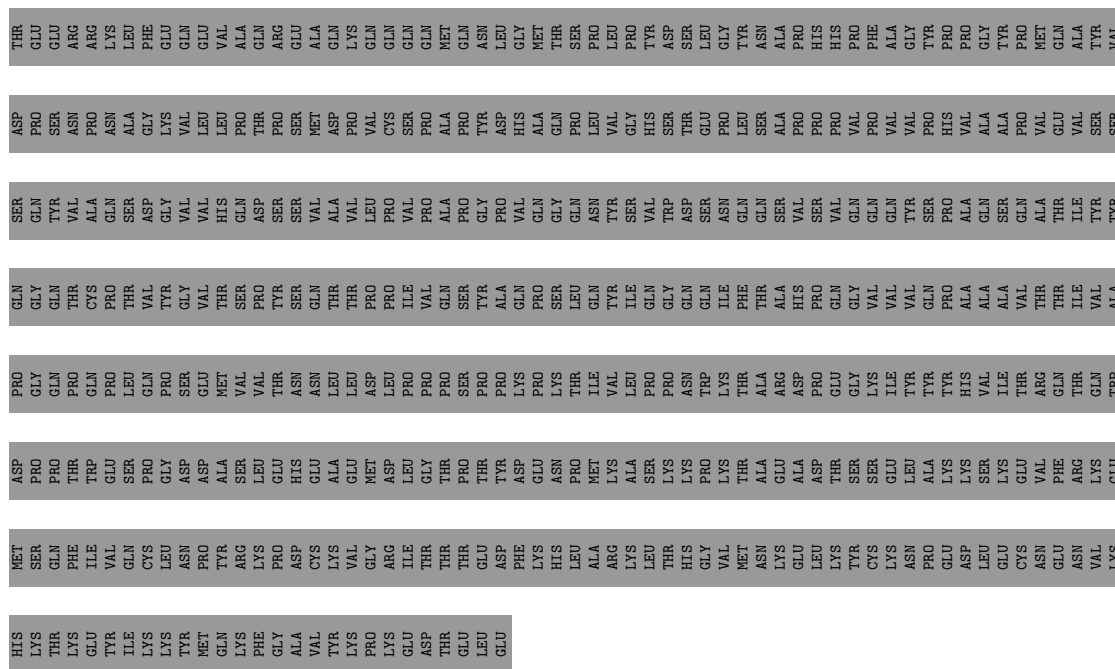
Mol	Chain	Residues	Atoms						AltConf	Trace
7	d	92	Total	C	H	N	O	S	0	0
			1458	452	739	129	136	2		
7	h	89	Total	C	H	N	O	S	0	0
			1401	437	708	122	132	2		

- Molecule 8 is a protein called FACT complex subunit SPT16.

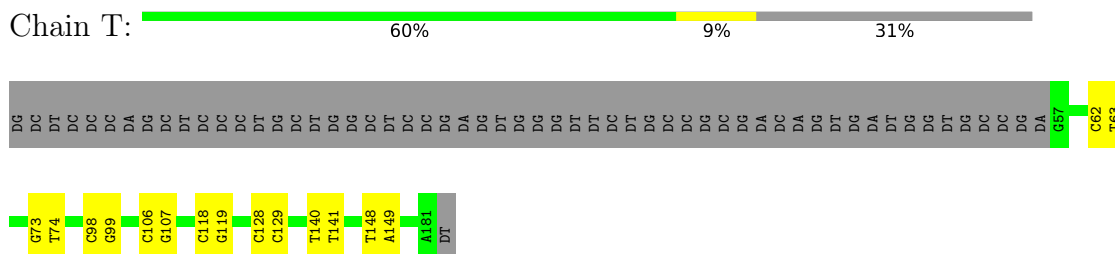
Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	15	Total	C	H	N	O	0	0
			205	67	90	16	32		

There are 2 discrepancies between the modelled and reference sequences:

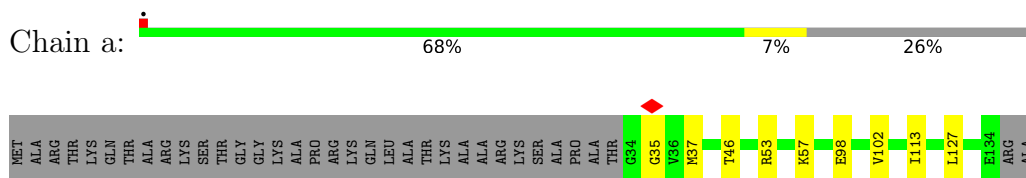
Chain	Residue	Modelled	Actual	Comment	Reference
j	-1	SER	-	expression tag	UNP Q9Y5B9
j	0	ASN	-	expression tag	UNP Q9Y5B9



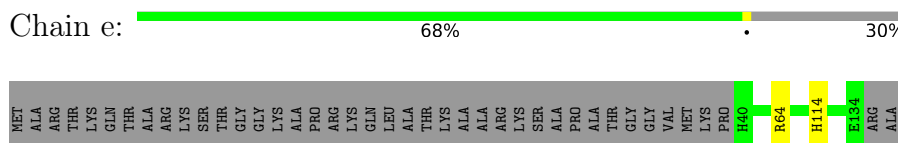
- Molecule 3: Template DNA



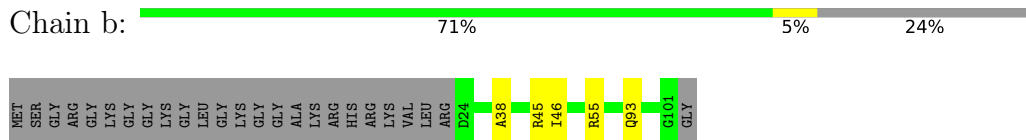
- Molecule 4: Histone H3.2



- Molecule 4: Histone H3.2

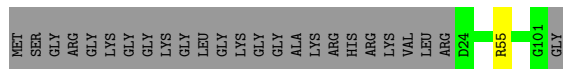


- Molecule 5: Histone H4



- Molecule 5: Histone H4

Chain f: 75% . 24%



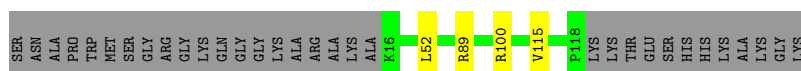
- Molecule 6: Histone H2A type 1-B/E

Chain c:  75% 21%



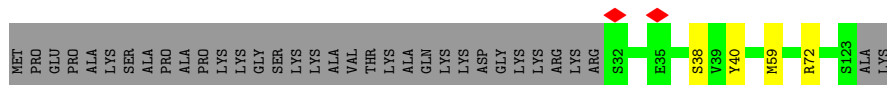
- Molecule 6: Histone H2A type 1-B/E

Chain g: 73% . 24%



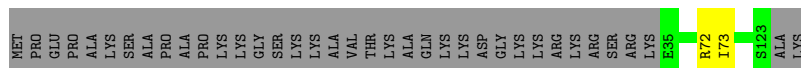
- Molecule 7: Histone H2B type 1-K

Chain d:  70% 27%



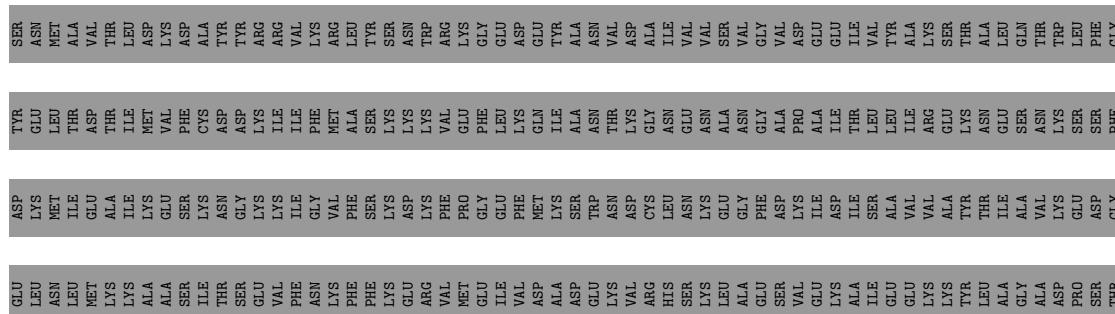
- Molecule 7: Histone H2B type 1-K

Chain h:  69% 29%



- Molecule 8: FACT complex subunit SPT16

Chain j:  99%



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.83	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	315.0, 315.0, 315.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	N	0.34	0/2896	1.16	4/4472 (0.1%)
2	O	0.29	0/2032	0.76	0/2722
3	T	0.31	0/2852	1.04	0/4395
4	a	0.23	0/833	0.60	0/1117
4	e	0.25	0/793	0.67	0/1064
5	b	0.26	0/629	0.63	0/843
5	f	0.24	0/629	0.63	0/843
6	c	0.24	0/836	0.61	0/1128
6	g	0.22	0/806	0.63	0/1089
7	d	0.25	0/730	0.61	0/982
7	h	0.28	0/704	0.60	0/949
8	j	0.32	0/116	0.94	0/156
All	All	0.29	0/13856	0.89	4/19760 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	e	0	1
5	b	0	1
5	f	0	1
6	c	0	3
6	g	0	1
7	d	0	1
7	h	0	1
All	All	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	48	DC	OP1-P-O3'	-26.53	28.42	108.00
1	N	48	DC	P-O3'-C3'	8.46	132.89	120.20
1	N	48	DC	C2'-C3'-O3'	5.67	120.01	111.50
1	N	3	DC	O4'-C1'-N1	5.12	116.07	108.40

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	b	55	ARG	Sidechain
6	c	33	ARG	Sidechain
6	c	43	ARG	Sidechain
6	c	82	ARG	Sidechain
7	d	72	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	2579	1403	1404	11	0
2	O	1993	1930	1929	5	0
3	T	2546	1403	1404	9	0
4	a	821	863	862	7	0
4	e	782	819	818	1	0
5	b	622	661	660	1	0
5	f	622	661	660	0	0
6	c	826	885	884	2	0
6	g	796	849	848	2	0
7	d	719	739	738	2	0
7	h	693	708	707	1	0
8	j	115	90	89	0	0
All	All	13114	11011	11003	33	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 1.

The worst 5 of 33 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:48:DC:H2'	1:N:49:DT:H72	1.68	0.75
1:N:109:DA:H1'	1:N:110:DC:C6	2.30	0.66
3:T:62:DC:H2''	3:T:63:DT:C6	2.44	0.53
1:N:77:DG:H1'	1:N:78:DT:C6	2.44	0.53
1:N:78:DT:H2''	1:N:79:DA:C8	2.49	0.48

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	
2	O	243/1133 (21%)	230 (95%)	13 (5%)	0	100	100
4	a	99/136 (73%)	98 (99%)	1 (1%)	0	100	100
4	e	93/136 (68%)	92 (99%)	1 (1%)	0	100	100
5	b	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
5	f	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
6	c	105/135 (78%)	104 (99%)	1 (1%)	0	100	100
6	g	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
7	d	90/126 (71%)	89 (99%)	1 (1%)	0	100	100
7	h	87/126 (69%)	86 (99%)	1 (1%)	0	100	100
8	j	13/1049 (1%)	12 (92%)	1 (8%)	0	100	100
All	All	983/3182 (31%)	961 (98%)	22 (2%)	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	
2	O	217/1017 (21%)	217 (100%)	0	100	100
4	a	86/110 (78%)	84 (98%)	2 (2%)	44	64
4	e	82/110 (74%)	82 (100%)	0	100	100
5	b	64/79 (81%)	62 (97%)	2 (3%)	35	56
5	f	64/79 (81%)	64 (100%)	0	100	100
6	c	84/104 (81%)	84 (100%)	0	100	100
6	g	82/104 (79%)	81 (99%)	1 (1%)	63	74
7	d	79/105 (75%)	79 (100%)	0	100	100
7	h	76/105 (72%)	76 (100%)	0	100	100
8	j	14/929 (2%)	13 (93%)	1 (7%)	13	35
All	All	848/2742 (31%)	842 (99%)	6 (1%)	73	79

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	b	93	GLN
6	g	100	ARG
8	j	946	GLU
4	a	57	LYS
4	a	37	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
7	d	84	ASN
6	g	25	GLN
7	h	84	ASN
2	O	1548	GLN
2	O	1479	ASN

5.3.3 RNA ⓘ

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.

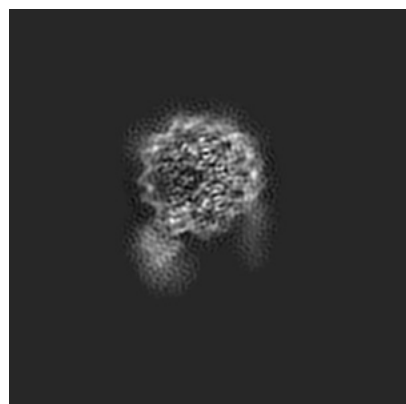
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51643. These allow visual inspection of the internal detail of the map and identification of artifacts.

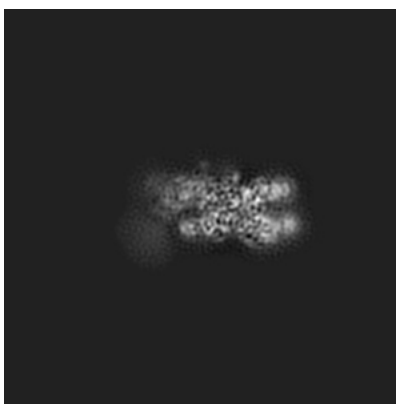
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

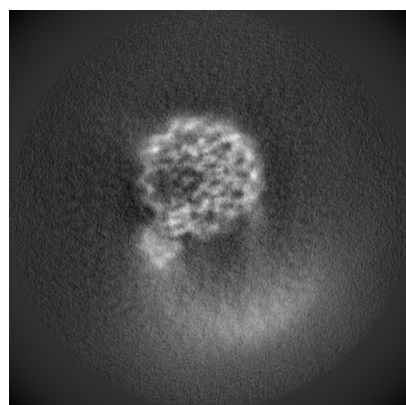


Y

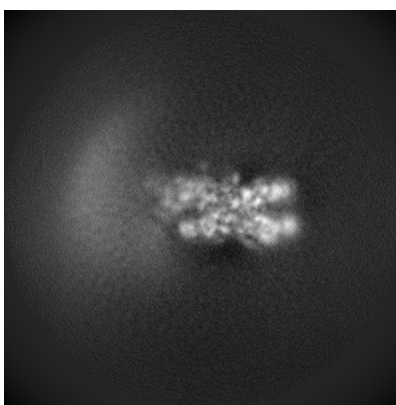


Z

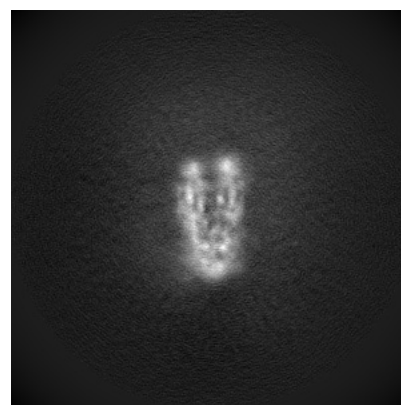
6.1.2 Raw map



X



Y



Z

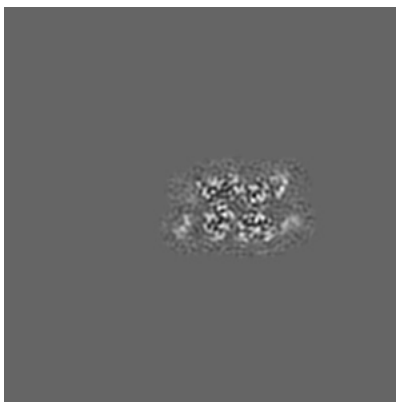
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

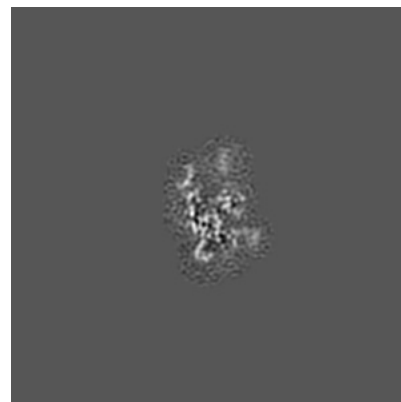
6.2.1 Primary map



X Index: 150

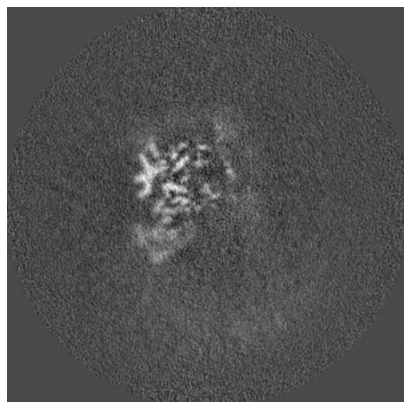


Y Index: 150

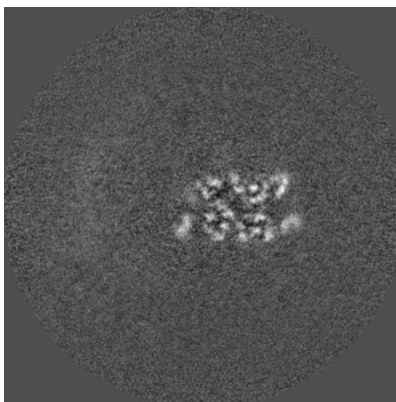


Z Index: 150

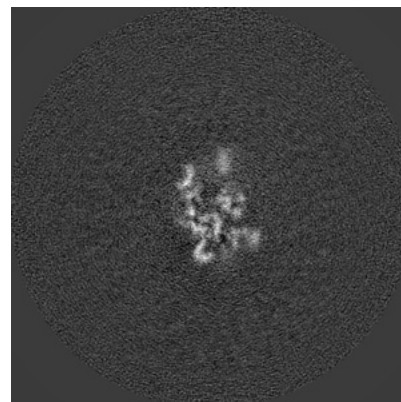
6.2.2 Raw map



X Index: 150



Y Index: 150

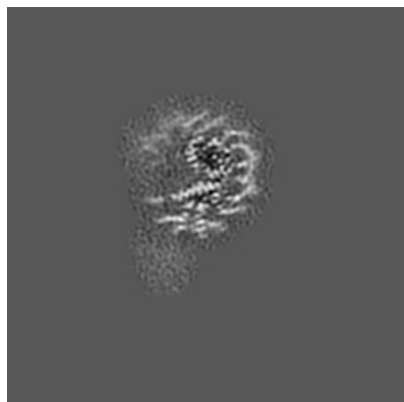


Z Index: 150

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

6.3 Largest variance slices [i](#)

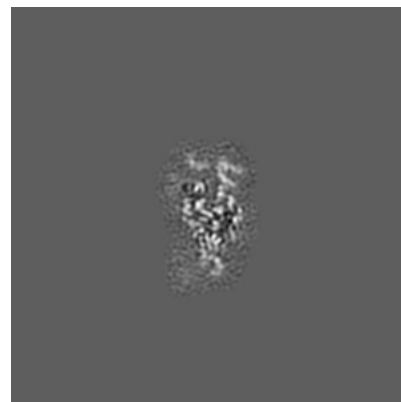
6.3.1 Primary map



X Index: 136

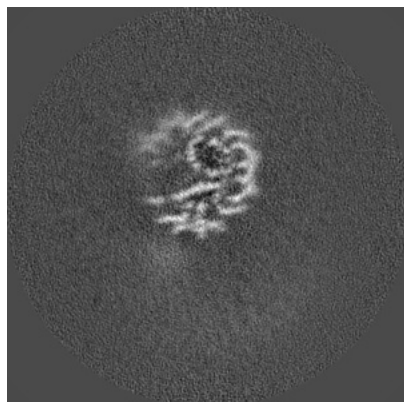


Y Index: 155

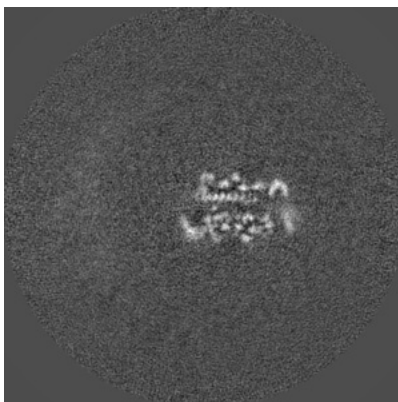


Z Index: 189

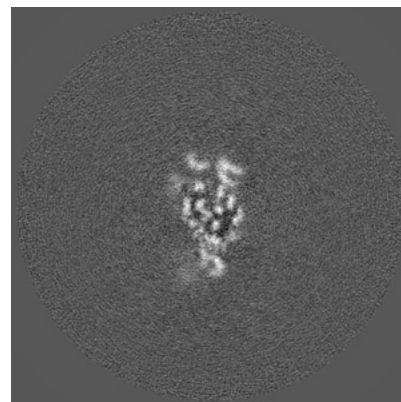
6.3.2 Raw map



X Index: 136



Y Index: 156

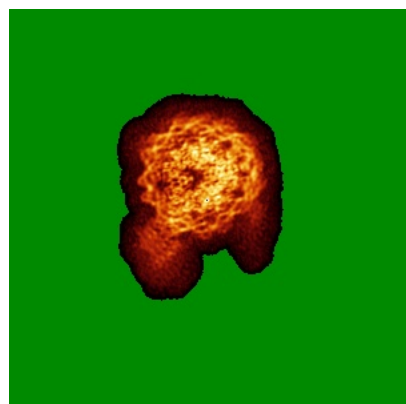


Z Index: 189

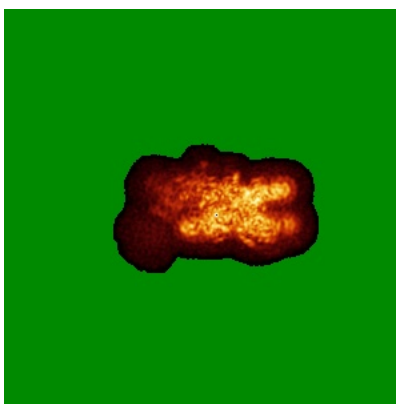
The images above show the largest variance slices of the map in three orthogonal directions.

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

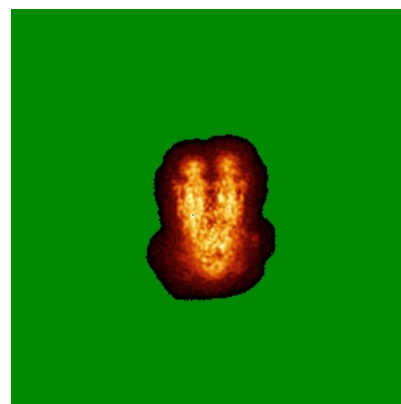
6.4.1 Primary map



X

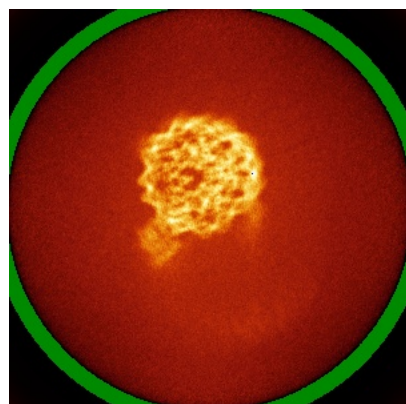


Y

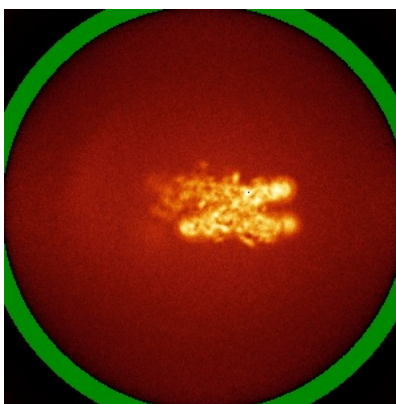


Z

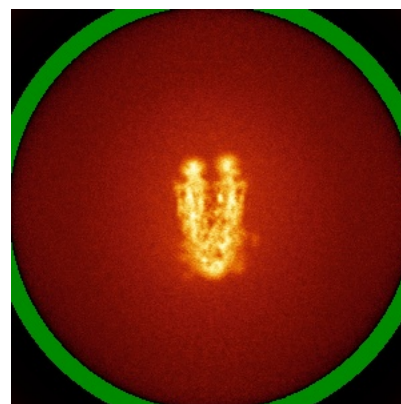
6.4.2 Raw map



X



Y

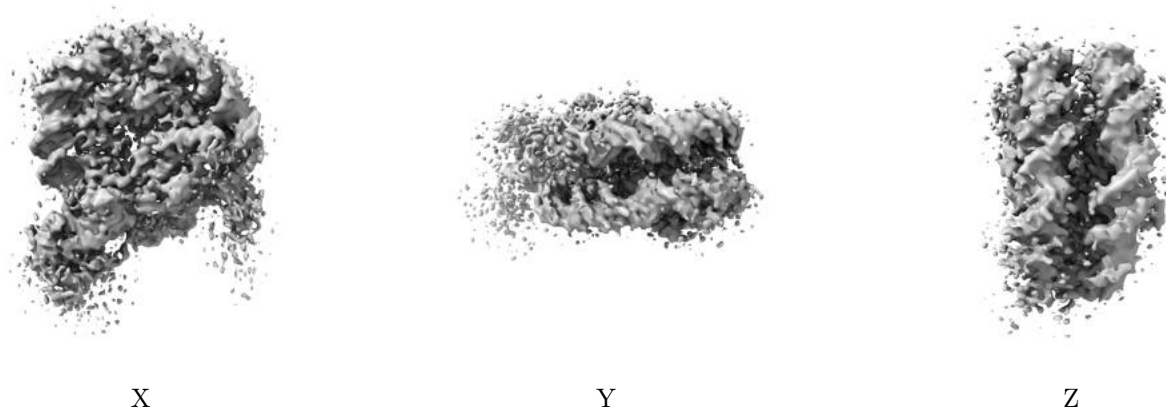


Z

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 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

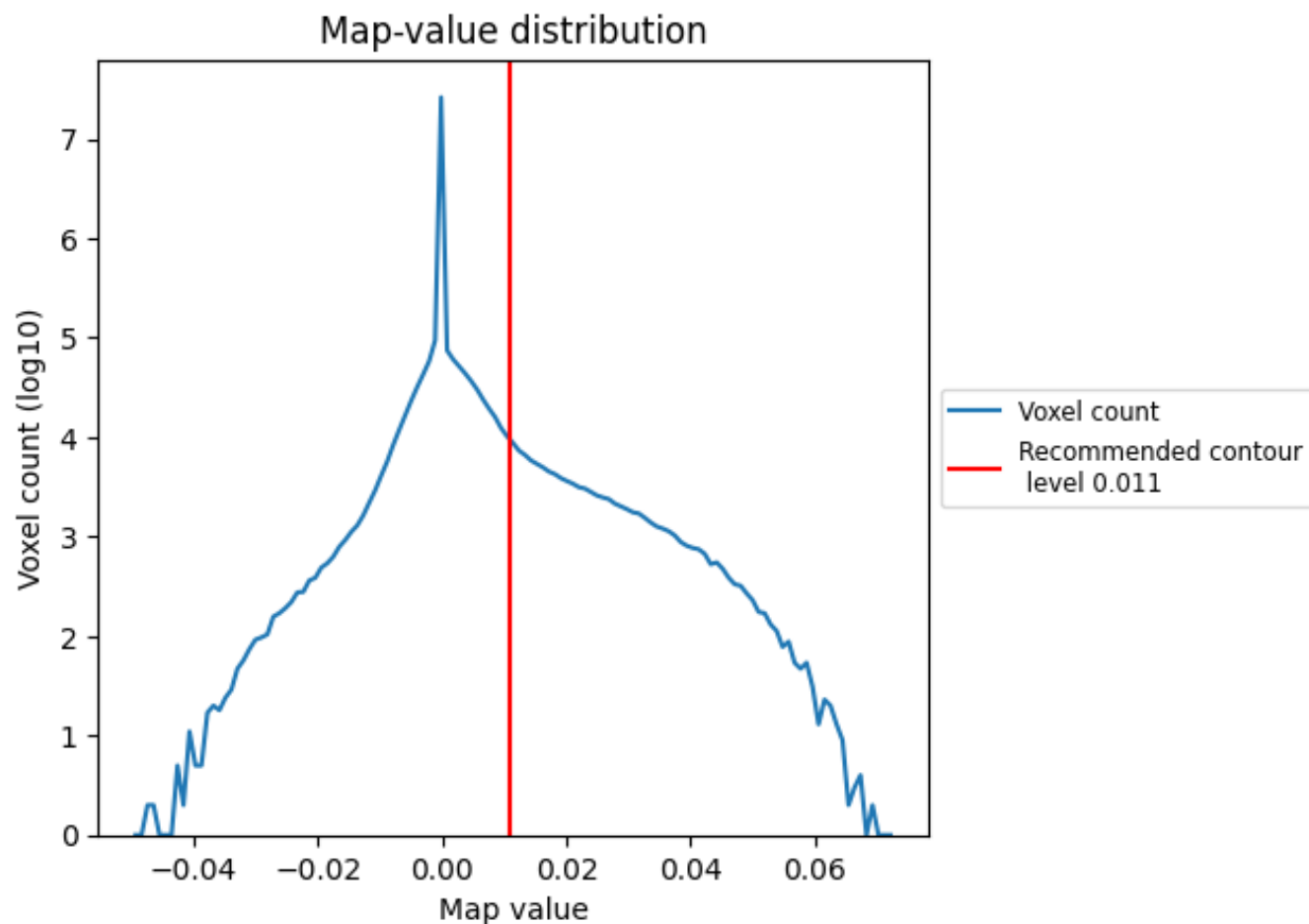
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

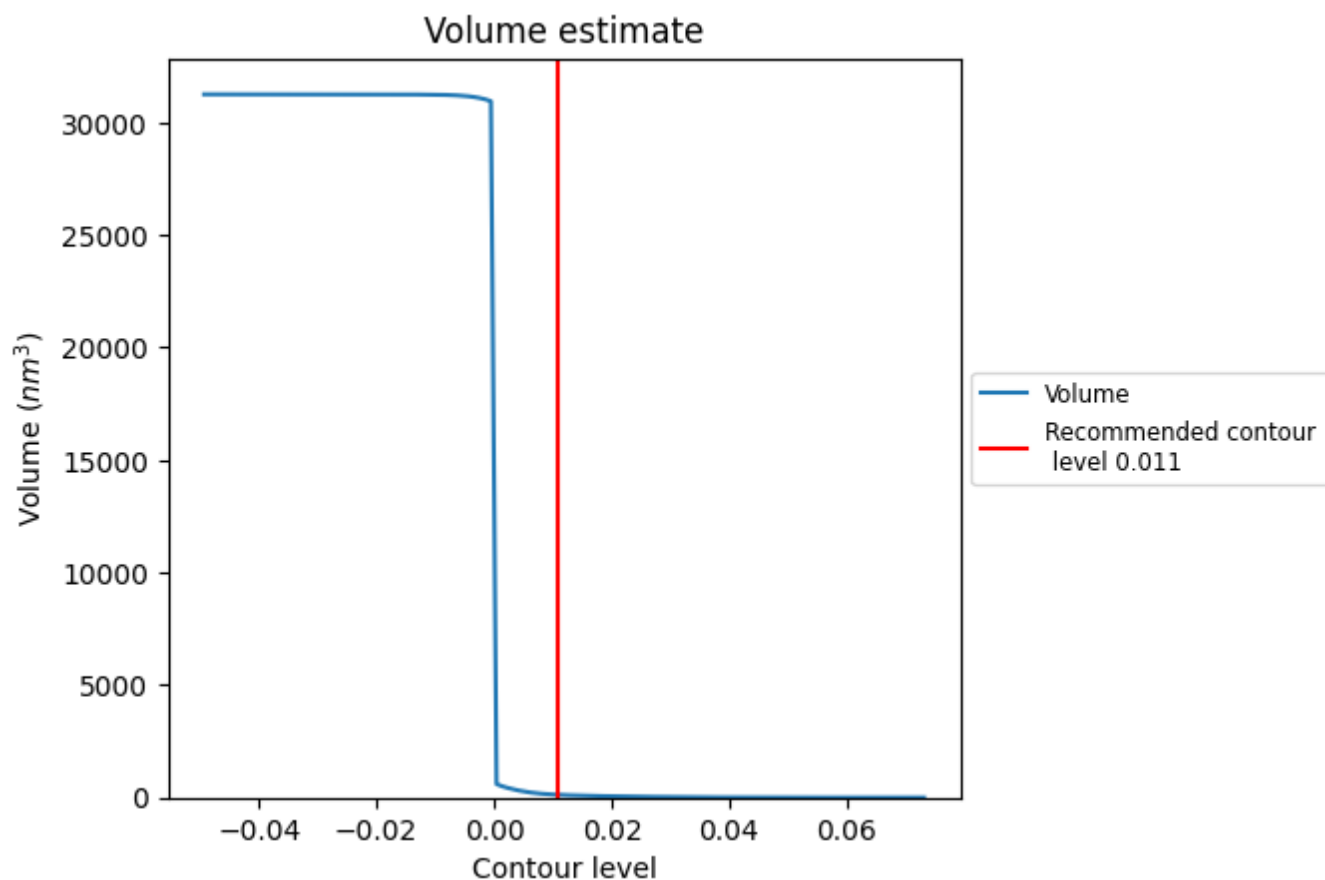
This section contains the results of statistical analysis of the map.

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.

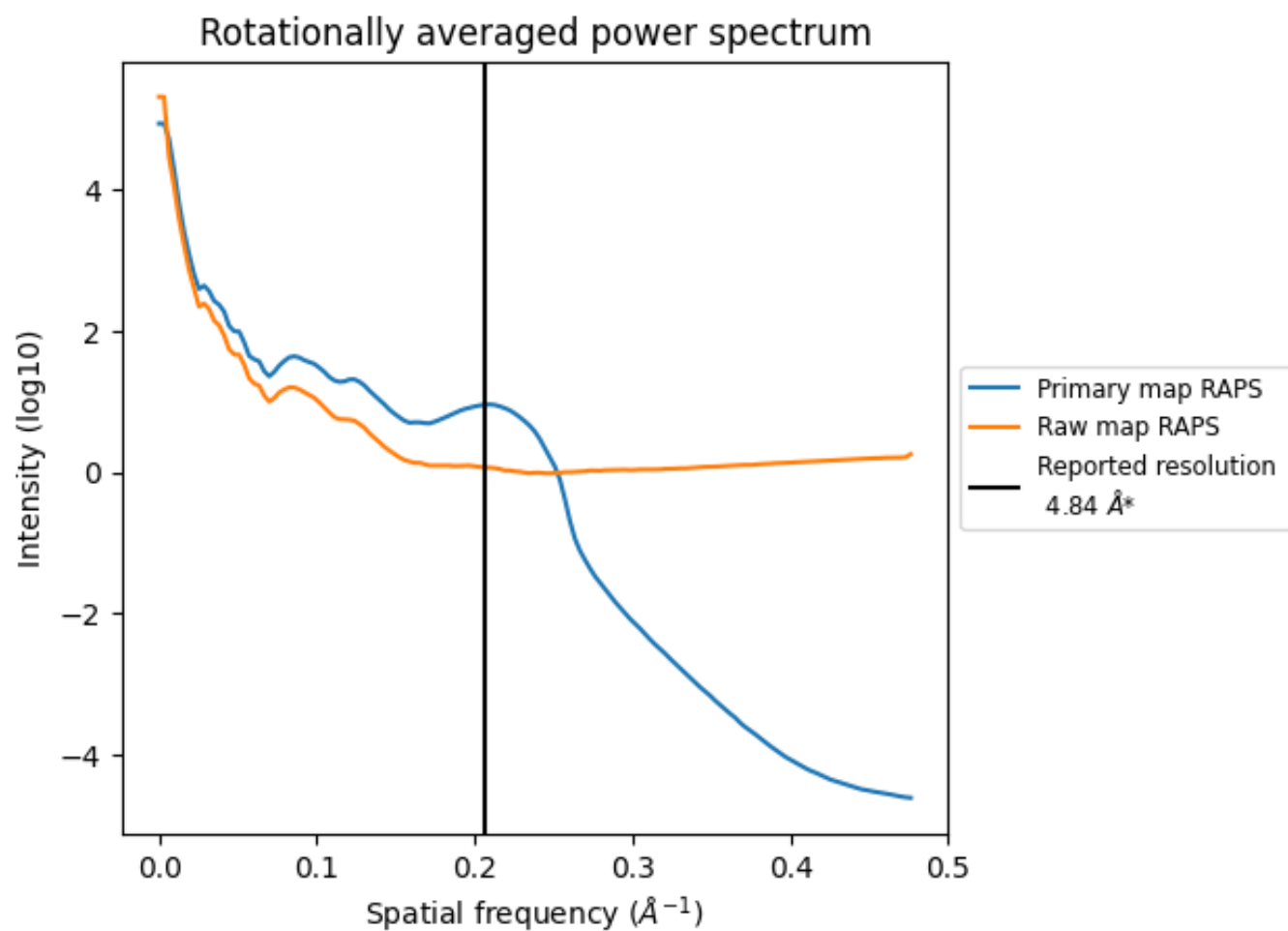
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm³; this corresponds to an approximate mass of 109 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 ⓘ

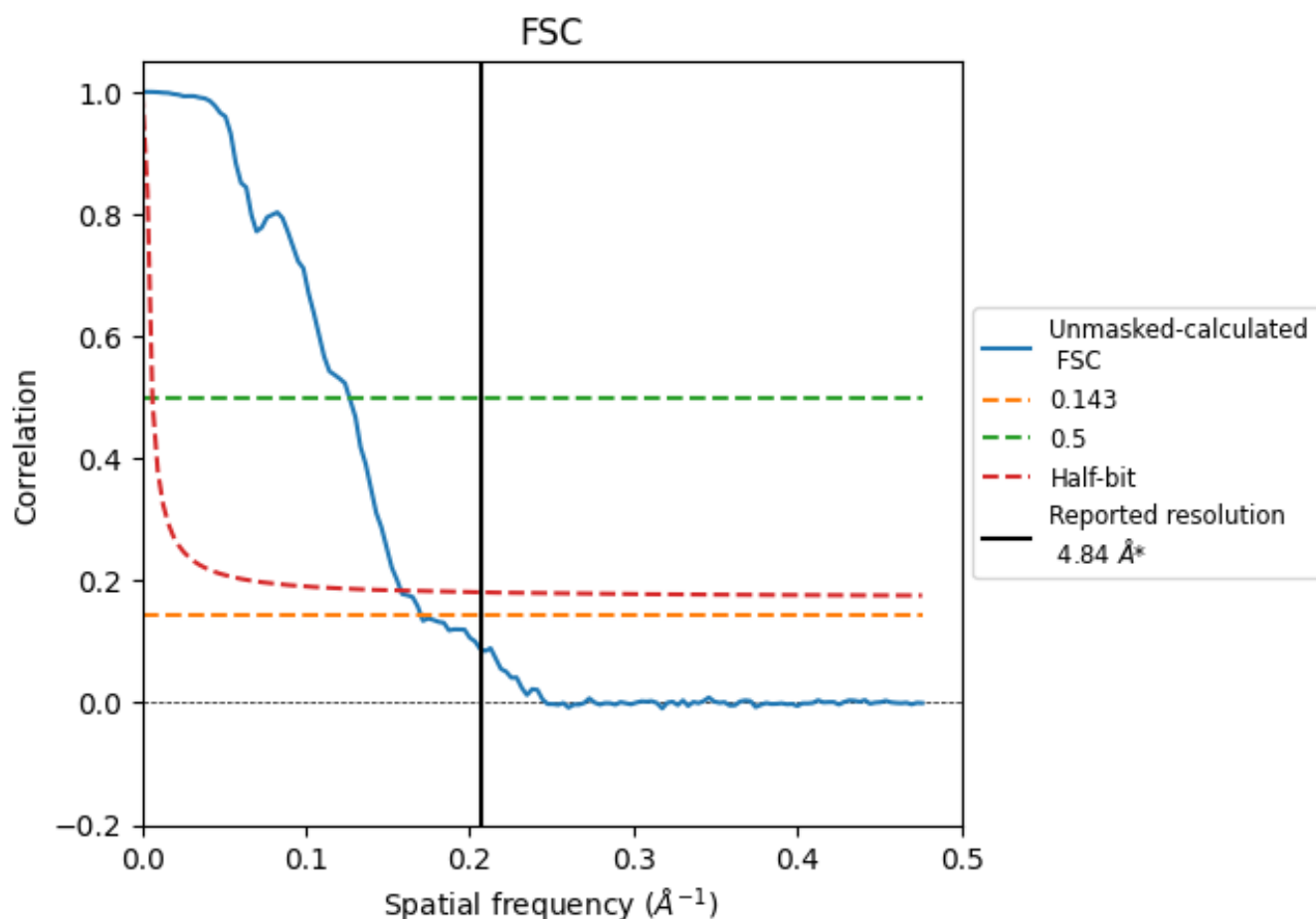


*Reported resolution corresponds to spatial frequency of 0.207 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.207 Å⁻¹

8.2 Resolution estimates [i](#)

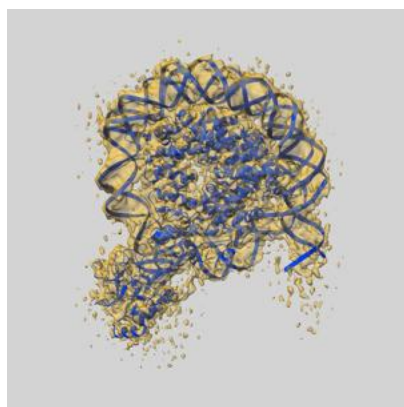
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.88	7.91	6.33

*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 5.88 differs from the reported value 4.84 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51643 and PDB model 9GW2. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

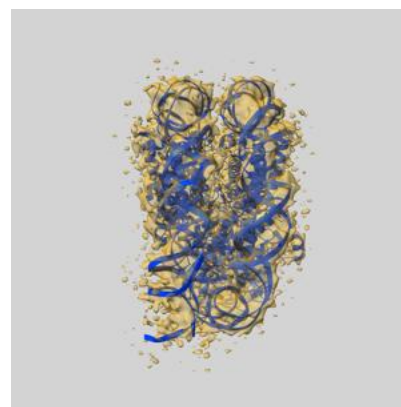
9.1 Map-model overlay [i](#)



X



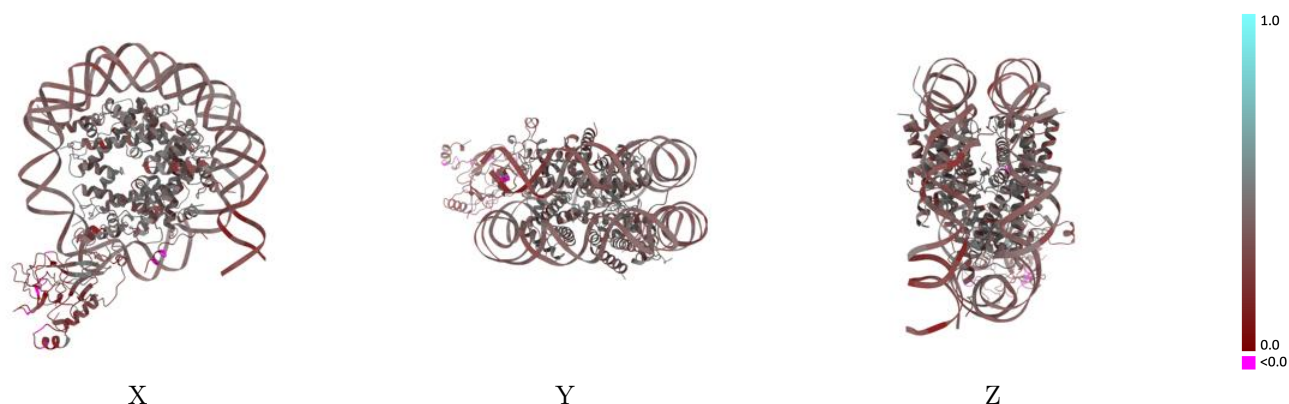
Y



Z

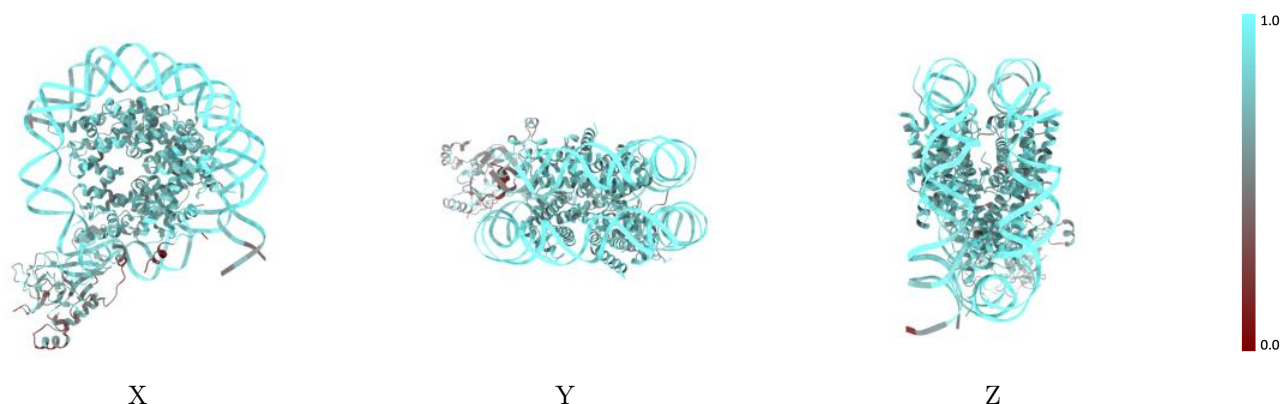
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



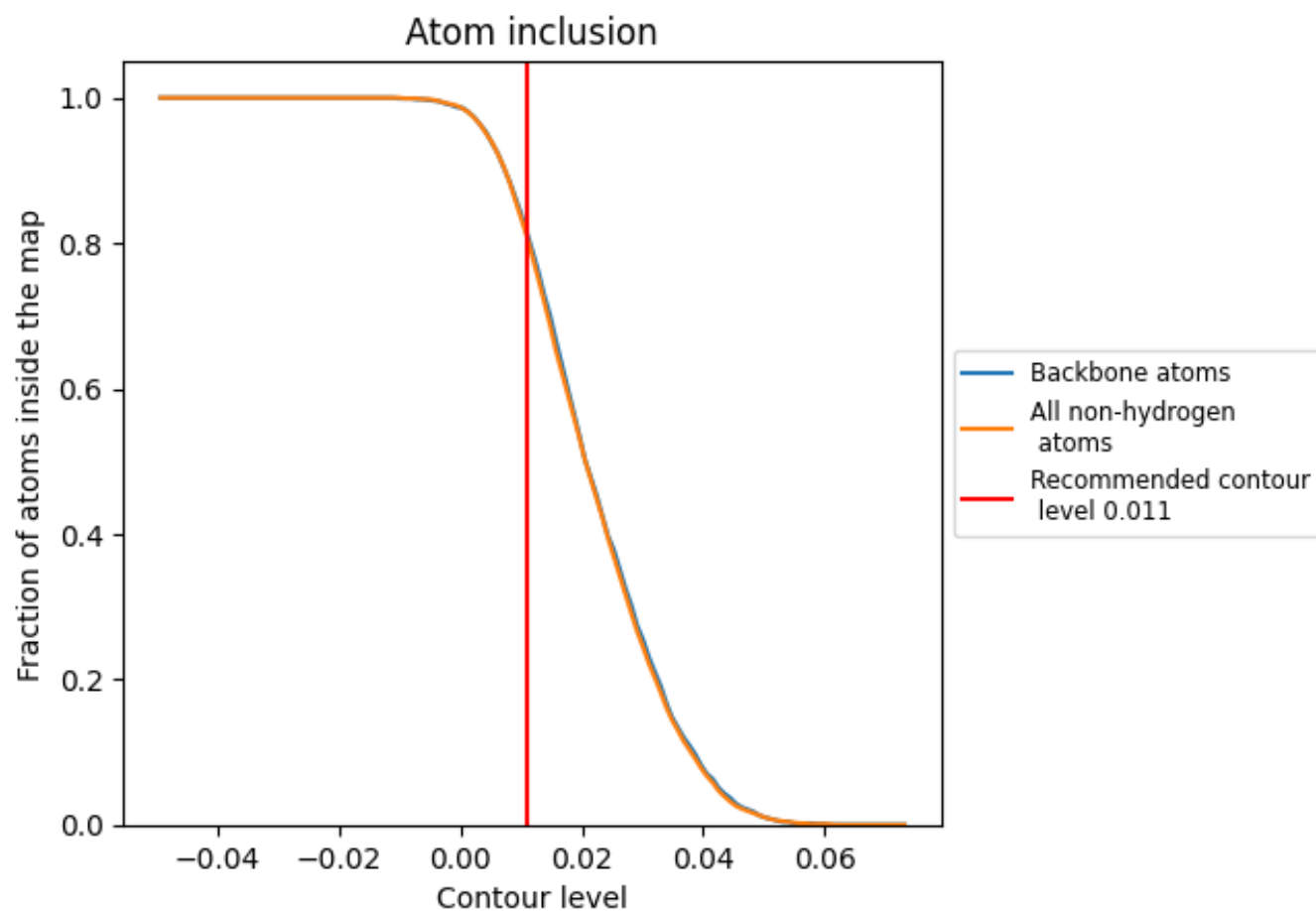
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8090	<div></div> 0.3590
N	<div></div> 0.9200	<div></div> 0.3380
O	<div></div> 0.5940	<div></div> 0.2680
T	<div></div> 0.9130	<div></div> 0.3430
a	<div></div> 0.8070	<div></div> 0.4030
b	<div></div> 0.8410	<div></div> 0.4180
c	<div></div> 0.8100	<div></div> 0.4170
d	<div></div> 0.8130	<div></div> 0.3970
e	<div></div> 0.8170	<div></div> 0.4150
f	<div></div> 0.8310	<div></div> 0.4260
g	<div></div> 0.8070	<div></div> 0.4110
h	<div></div> 0.8300	<div></div> 0.3930
j	<div></div> 0.3830	<div></div> 0.1890

