



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 10:04 PM UTC

PDB ID : 6ZH8 / pdb_00006zh8
EMDB ID : EMD-11216
Title : Cryo-EM structure of DNA-PKcs:DNA
Authors : Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2020-06-21
Resolution : 4.14 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

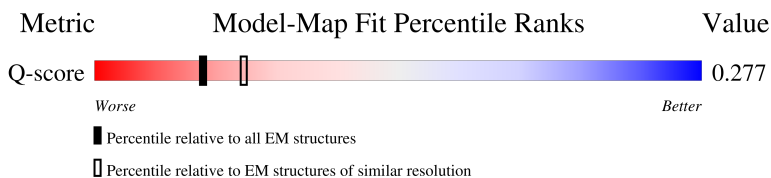
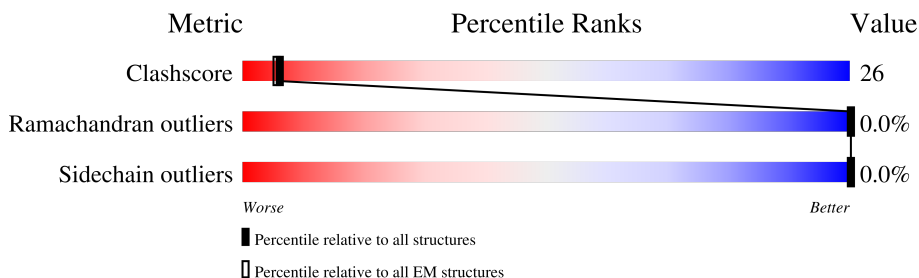
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.14 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	5577 (3.64 - 4.64)

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	4156	 47% 42% 11%
2	B	11	 27% 73%
3	C	8	 25% 75%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29506 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 DNA-dependent protein kinase catalytic subunit,DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3694	Total	C	N	O	S	0	0
			29120	18668	4926	5333	193		

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*TP*TP*TP*TP*TP*AP*GP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	11	Total	C	N	O	P	0	0
			222	106	34	71	11		

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*CP*TP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	8	Total	C	N	O	P	0	0
			164	78	35	43	8		





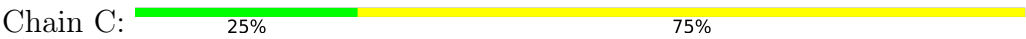
V4080	V4081	K4085	D4086	H4087	H4088	I4089	R4090	A4091	Q4092	E4095	S4096	E4100	E4101	T4102	Q4103	V4104	K4105	C4106	L4107	M4108	P4114	L4117	G4118	R4119	W4124	E4125	P4126	W4127	M4128	X6005	X6009	X6015	X6019	X6023	UNK	UNK												
R3874	E3875	V3878	P3879	L3882	R3885	A3886	F3887	V3888	R3889	R3901	R3910	I3911	L3918	D3922	R3923	H3924	L3925	N3926	N3927	M3928	M3929	V3937	H3944	A3945	F3946	G3947	S3948	Q3951	P3956	R3962	R3965	N3969	L3970	M3971	L3972	F3973	M3974	K3975	E3976	T3977	Y3981	L3988	R3989					
R3718	I3719	F3722	D3723	E3724	R3726	V3727	V3728	M3729	A3730	S3731	L3732	R3733	R3734	P3735	K3736	R3737	R3741	G3742	H3743	P3749	K3753	G3754	G3755	L3758	R3759	Q3766	L3767	F3768	Q3769	V3770	M3771	N3772	I3774	D3778	S3779	A3780	C3781	S3782	A3785	L3786	Q3787	L3788	V3793	V3794	P3795	M3796	L3800	
G3801	L3802	E3803	V3805	L3806	E3807	N3808	L3809	T3811	L3812	K3813	D3814	L3815	L3816	L3817	L3818	T3819	M3820	K3825	R3826	A3827	D3831	R3832	R3833	A3834	P3835	R3836	C3837	E3838	W3842	L3843	T3844	K3845	M3846	S3847	H3850	G3853	M3856	L3857	N3858	M3859	L3860	R3864	T3867	V3868	S3870	F3871	R3872	K3873
R3874	E3875	V3878	P3879	L3882	R3885	A3886	F3887	V3888	R3889	R3901	R3910	I3911	L3918	D3922	R3923	H3924	L3925	N3926	N3927	M3928	M3929	V3937	H3944	A3945	F3946	G3947	S3948	Q3951	P3956	R3962	R3965	N3969	L3970	M3971	L3972	F3973	M3974	K3975	E3976	T3977	Y3981	L3988	R3989					
R3718	I3719	F3722	D3723	E3724	R3726	V3727	V3728	M3729	A3730	S3731	L3732	R3733	R3734	P3735	K3736	R3737	R3741	G3742	H3743	P3749	K3753	G3754	G3755	L3758	R3759	Q3766	L3767	F3768	Q3769	V3770	M3771	N3772	I3774	D3778	S3779	A3780	C3781	S3782	A3785	L3786	Q3787	L3788	V3793	V3794	P3795	M3796	L3800	
G3801	L3802	E3803	V3805	L3806	E3807	N3808	L3809	T3811	L3812	K3813	D3814	L3815	L3816	L3817	L3818	T3819	M3820	K3825	R3826	A3827	D3831	R3832	R3833	A3834	P3835	R3836	C3837	E3838	W3842	L3843	T3844	K3845	M3846	S3847	H3850	G3853	M3856	L3857	N3858	M3859	L3860	R3864	T3867	V3868	S3870	F3871	R3872	K3873
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G3801	L3802	E3803	V3805	L3806	E3807	N3808	L3809	T3811	L3812	K3813	D3814	L3815	L3816	L3817	L3818	T3819	M3820	K3825	R3826	A3827	D3831	R3832	R3833	A3834	P3835	R3836	C3837	E3838	W3842	L3843	T3844	K3845	M3846	S3847	H3850	G3853	M3856	L3857	N3858	M3859	L3860	R3864	T3867	V3868	S3870	F3871	R3872	K3873
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R3874	E3875	V3878	P3879	L3882	R3885	A3886	F3887	V3888	R3889	R3901	R3910	I3911	L3918	D3922	R3923	H3924	L3925	N3926	N3927	M3928	M3929	V3937	H3944	A3945	F3946	G3947	S3948	Q3951	P3956	R3962	R3965	N3969	L3970	M3971	L3972	F3973	M3974	K3975	E3976	T3977	Y3981	L3988	R3989					
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G3801	L3802	E3803	V3805	L3806	E3807	N3808	L3809	T3811	L3812	K3813	D3814	L3815	L3816	L3817	L3818	T3819	M3820	K3825	R3826	A3827	D3831	R3832	R3833	A3834	P3835	R3836	C3837	E3838	W3842	L3843	T3844	K3845	M3846	S3847	H3850	G3853	M3856	L3857	N3858	M3859	L3860	R3864	T3867	V3868	S3870	F3871	R3872	K3873
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R3718	I3719	F3722	D3723	E3724	R3726	V3727																																										

- Molecule 2: DNA (5'-D(P*AP*GP*TP*TP*TP*TP*TP*AP*GP*TP*T)-3')

Chain B:  27% 73%

T21	T22	T23	T24	T25	T26	T27	T28	T29	T30	T31
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- Molecule 3: DNA (5'-D(P*AP*CP*TP*AP*AP*AP*AP*A)-3')



A26
C27
T28
A29
A30
A31
A32
A33

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31881	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 ($e^-/\text{\AA}^2$)	52.97	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.445	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	356.99997, 356.99997, 356.99997	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	0.26	0/29582	0.44	2/40029 (0.0%)
2	B	0.23	0/247	0.44	0/378
3	C	0.24	0/185	0.37	0/282
All	All	0.26	0/30014	0.44	2/40689 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3030	ILE	N-CA-C	-5.57	108.42	113.71
1	A	553	VAL	N-CA-C	-5.22	107.26	111.91

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	29120	0	29078	1434	0
2	B	222	0	117	10	0
3	C	164	0	87	6	0
All	All	29506	0	29282	1450	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 26.

The worst 5 of 1450 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:3472:ILE:HG21	1:A:3483:MET:CE	1.65	1.25
1:A:3472:ILE:CG2	1:A:3483:MET:HE3	1.79	1.11
1:A:3472:ILE:CG2	1:A:3483:MET:CE	2.32	1.06
1:A:1351:THR:HG22	1:A:1353:PRO:HD2	1.48	0.95
1:A:3472:ILE:HG21	1:A:3483:MET:HE1	1.48	0.92

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	3634/4156 (87%)	3246 (89%)	387 (11%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1895	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	3172/3671 (86%)	3171 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3483	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3569	GLN
1	A	3573	ASN
1	A	4015	ASN
1	A	1465	HIS
1	A	1459	HIS

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	5011:UNK	N	92.87
1	A	5016:UNK	C	6004:UNK	N	47.75

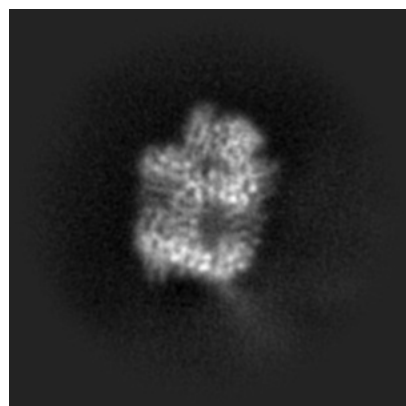
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11216. These allow visual inspection of the internal detail of the map and identification of artifacts.

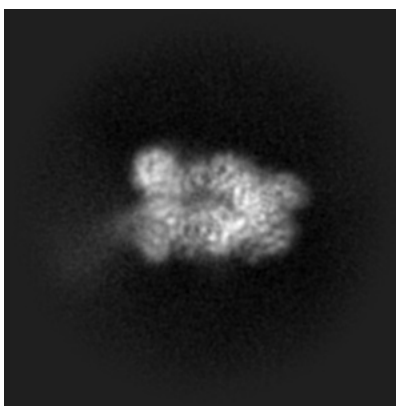
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

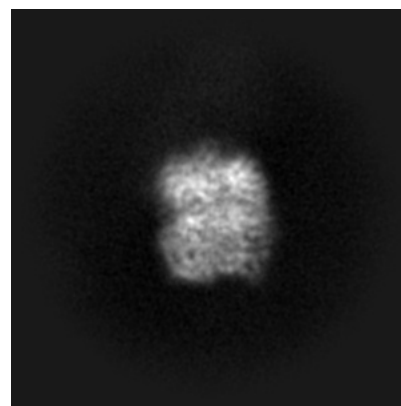
6.1.1 Primary map



X

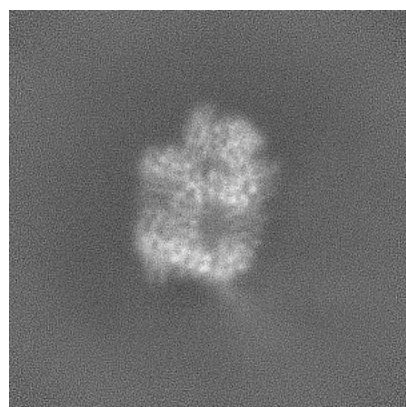


Y

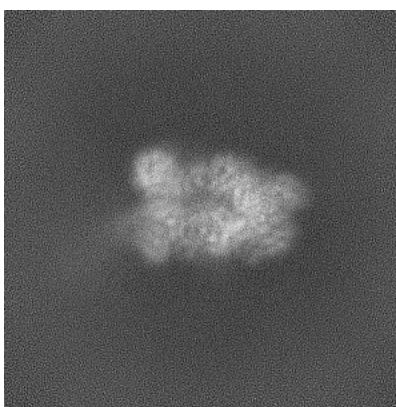


Z

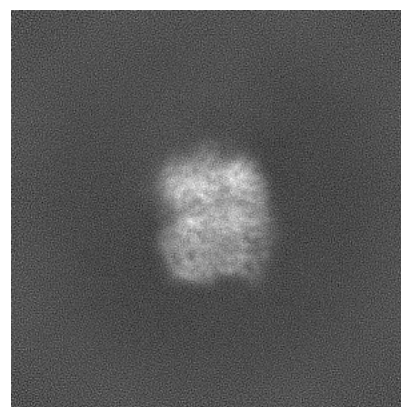
6.1.2 Raw map



X



Y

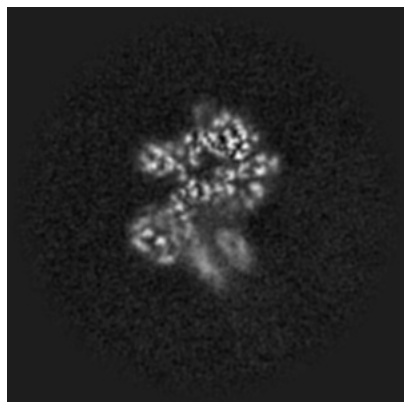


Z

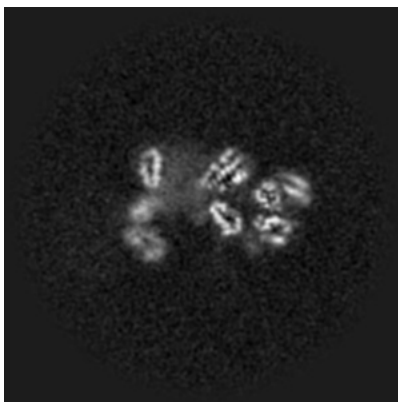
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

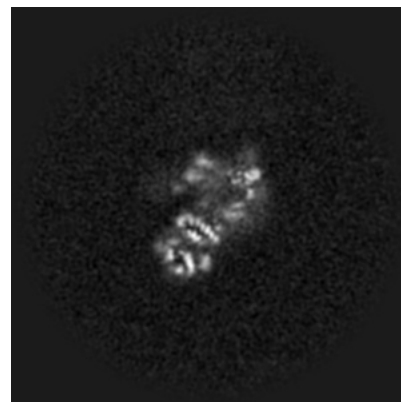
6.2.1 Primary map



X Index: 170

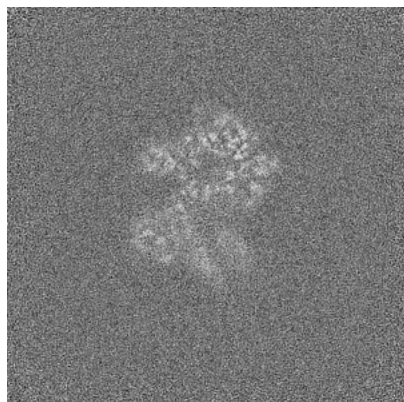


Y Index: 170

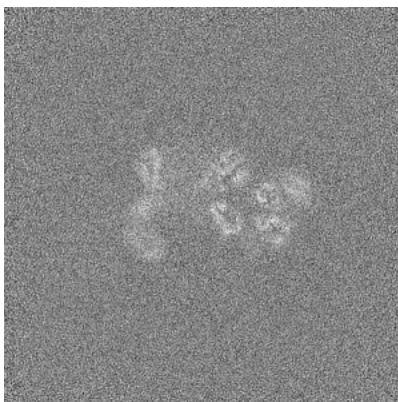


Z Index: 170

6.2.2 Raw map



X Index: 170



Y Index: 170

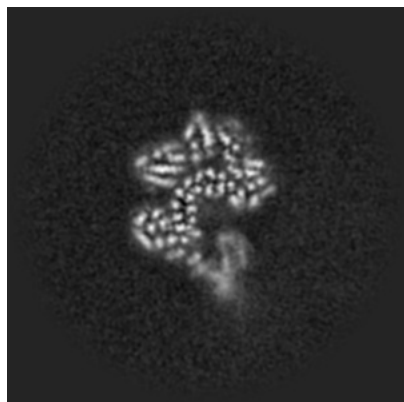


Z Index: 170

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

6.3 Largest variance slices [i](#)

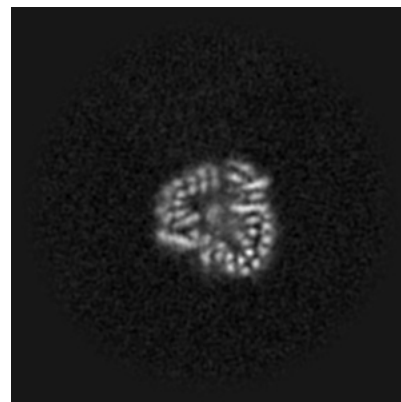
6.3.1 Primary map



X Index: 158

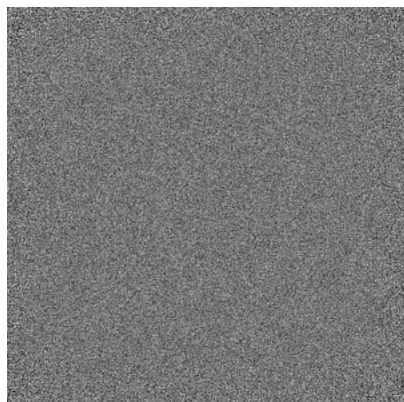


Y Index: 190

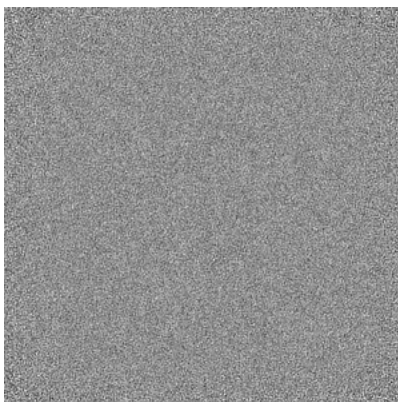


Z Index: 129

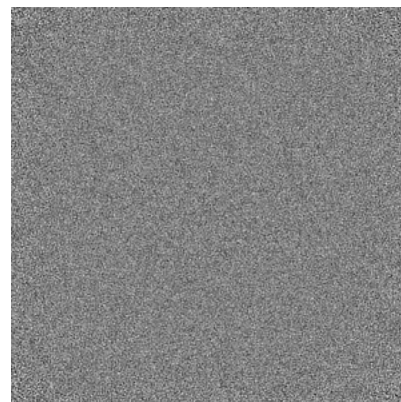
6.3.2 Raw map



X Index: 0



Y Index: 0

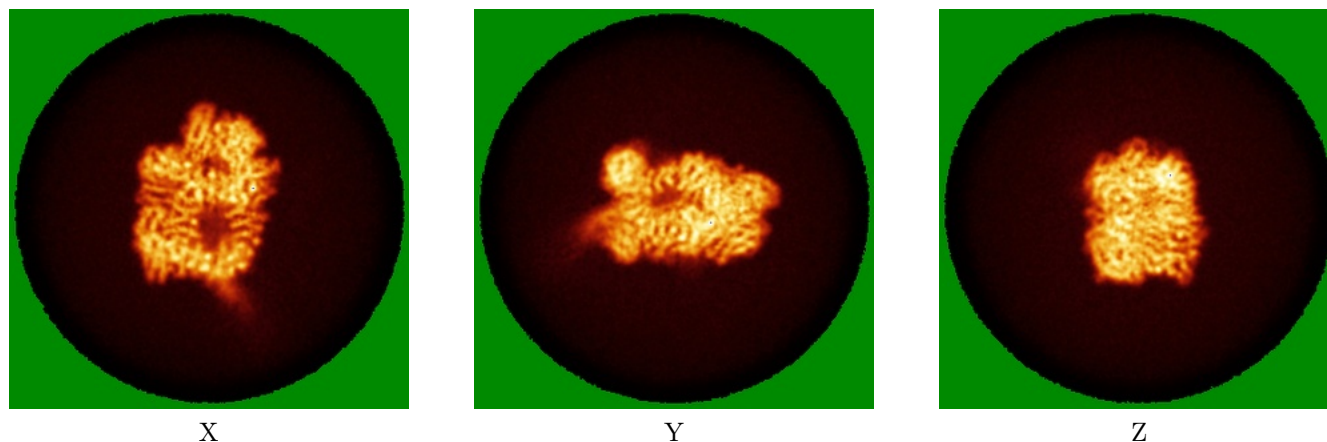


Z Index: 0

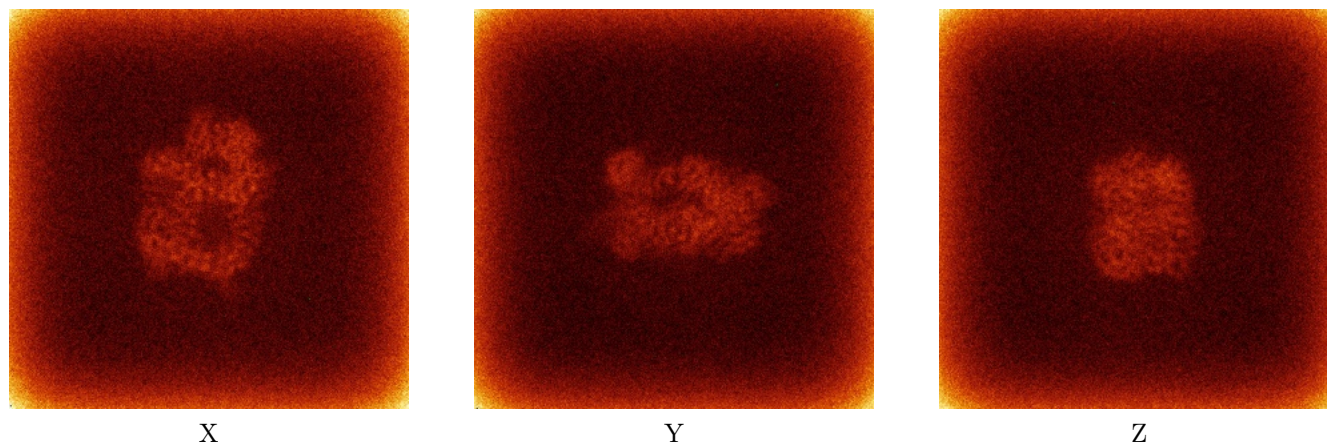
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



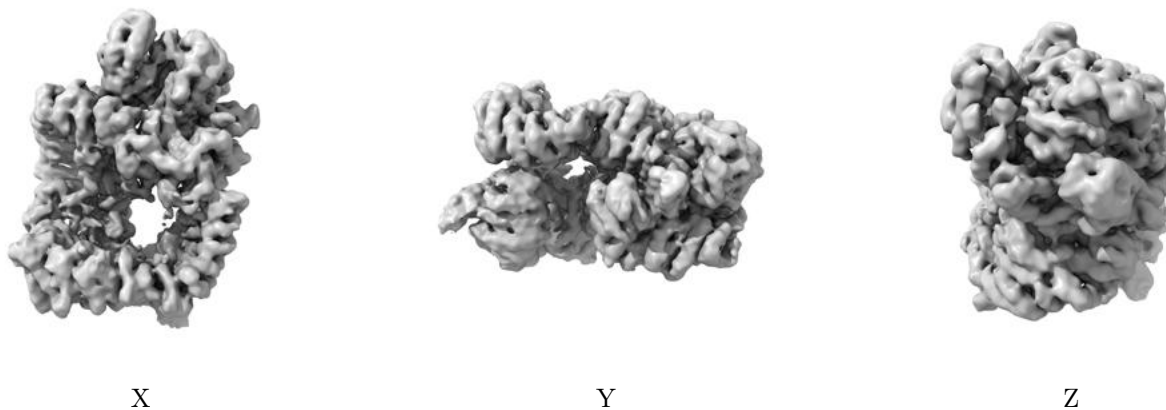
6.4.2 Raw map



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.

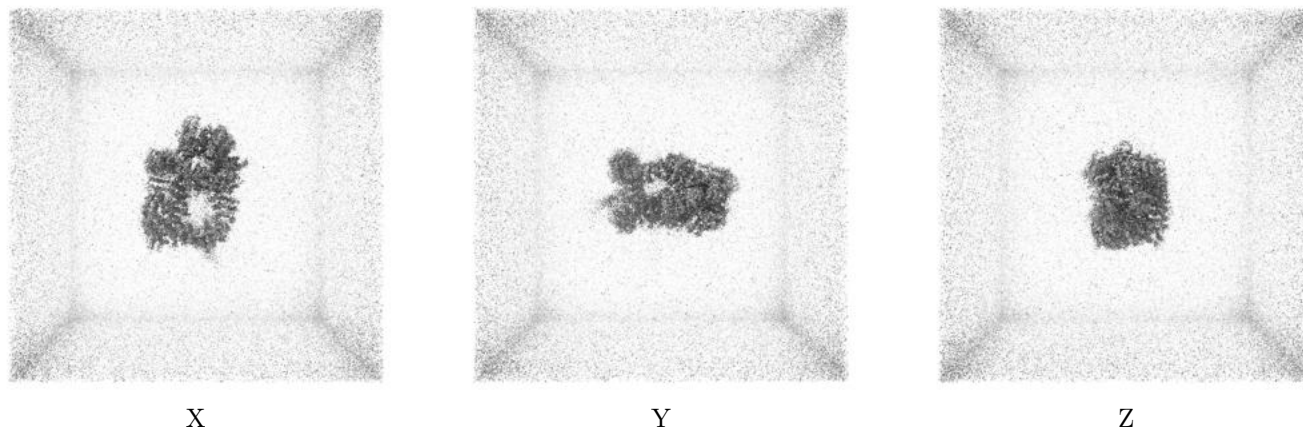
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.125. 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.

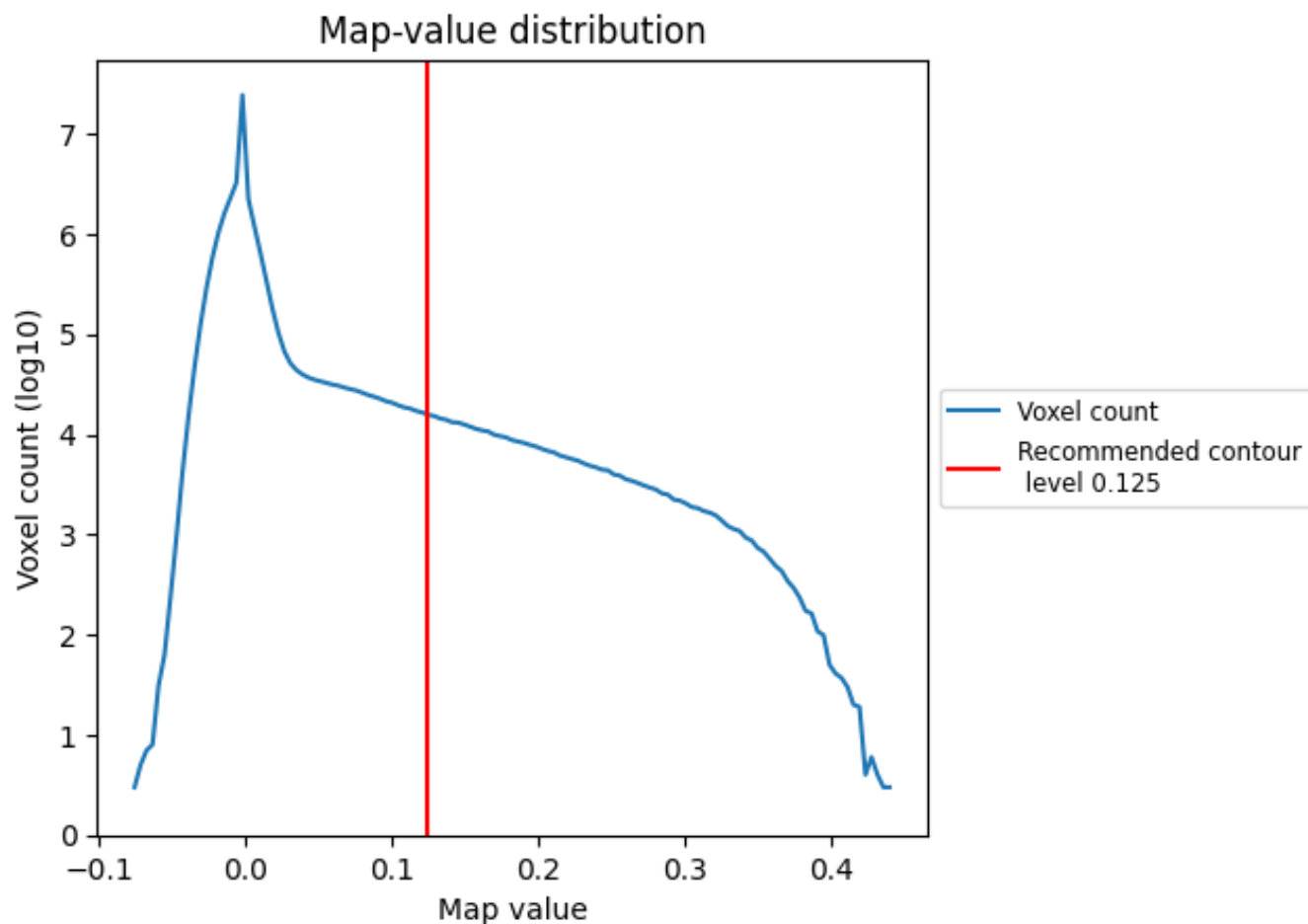
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

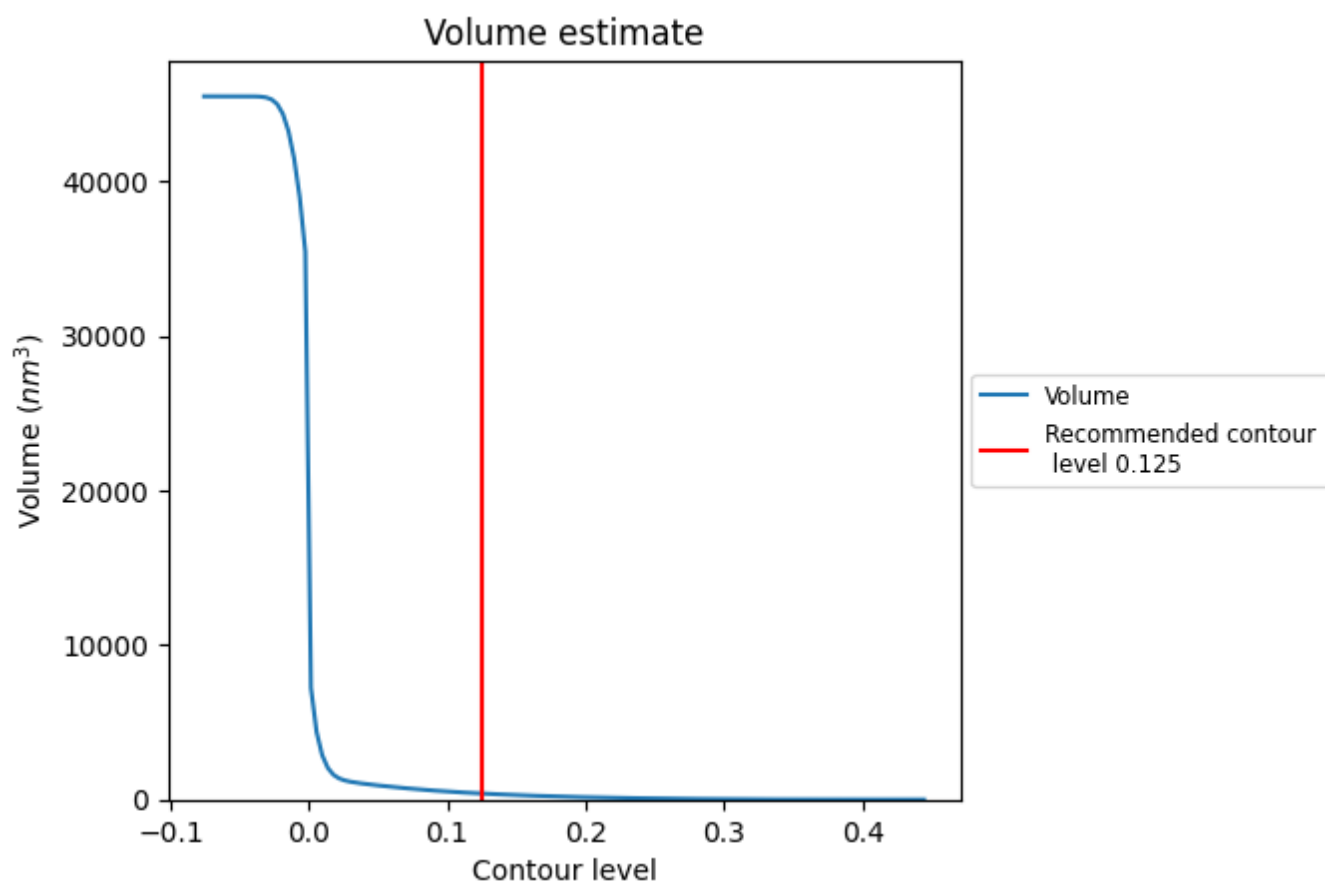
This section contains the results of statistical analysis of the map.

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.

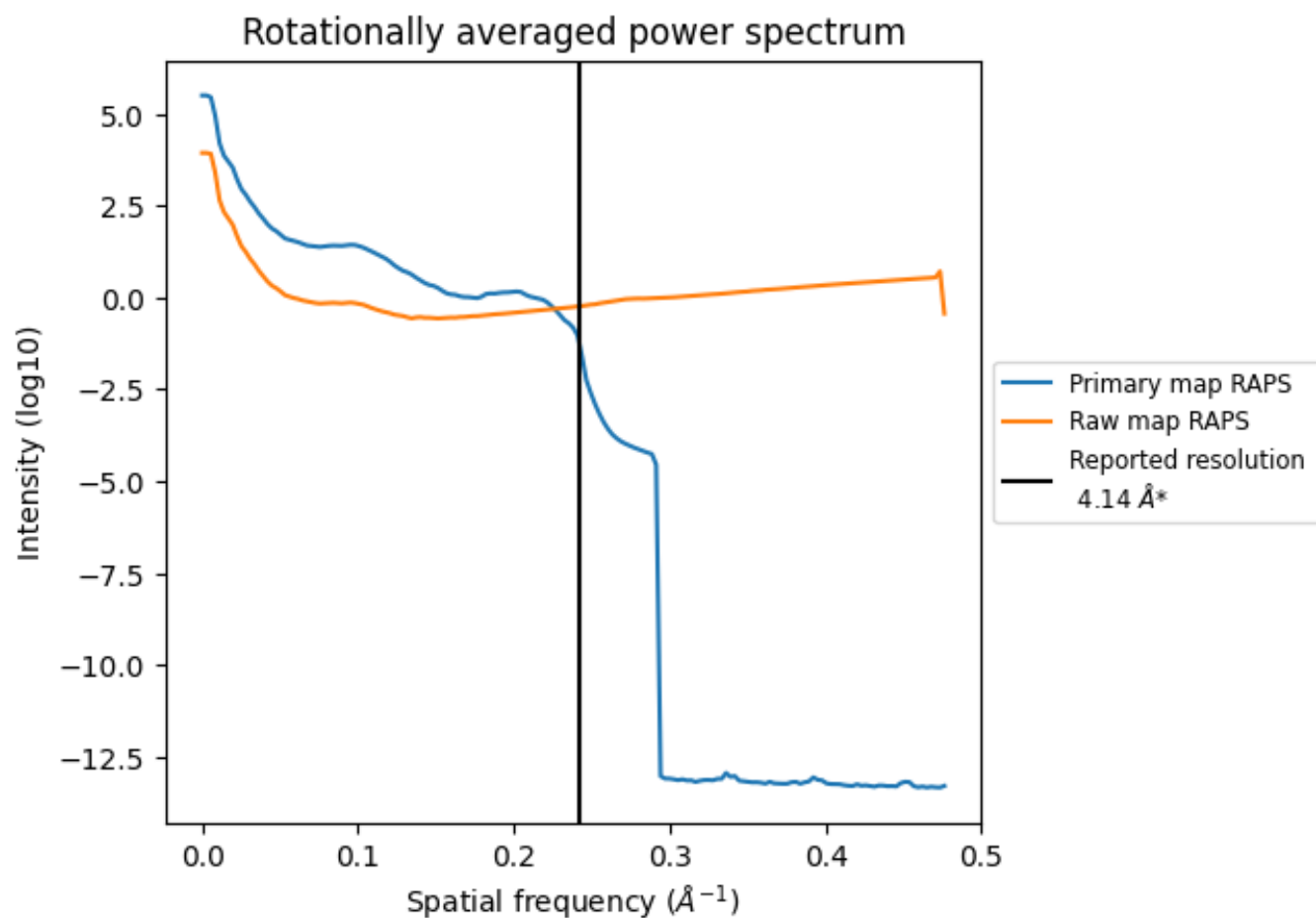
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 392 nm³; this corresponds to an approximate mass of 354 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 ⓘ

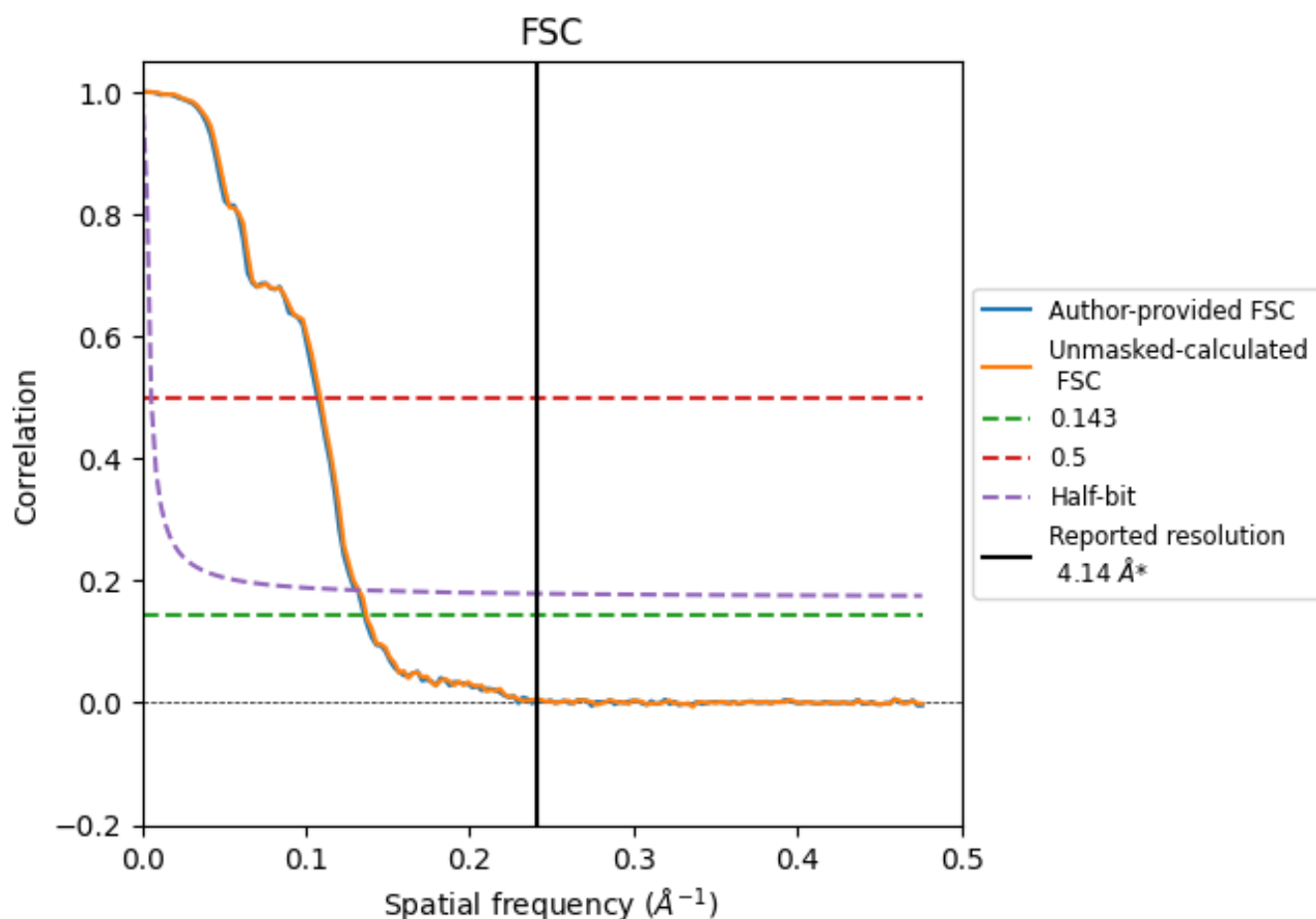


*Reported resolution corresponds to spatial frequency of 0.242 $\text{\AA}^{-1}$

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 $0.242 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.14	-	-
Author-provided FSC curve	7.37	9.34	7.59
Unmasked-calculated*	7.31	9.20	7.56

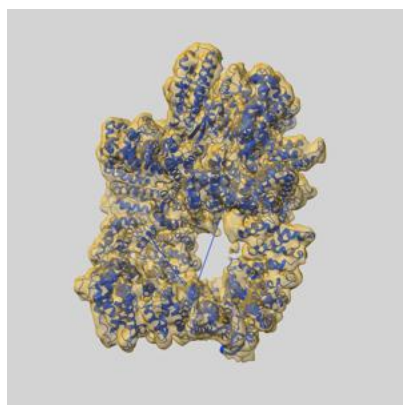
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.37 differs from the reported value 4.14 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.31 differs from the reported value 4.14 by more than 10 %

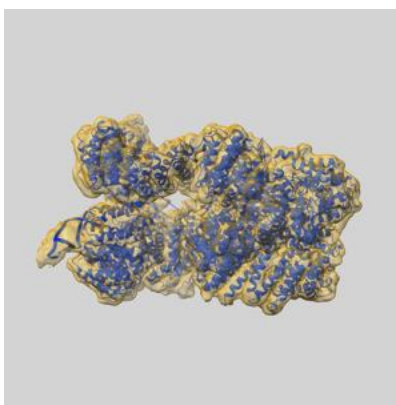
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11216 and PDB model 6ZH8. Per-residue inclusion information can be found in section [3](#) on page [4](#).

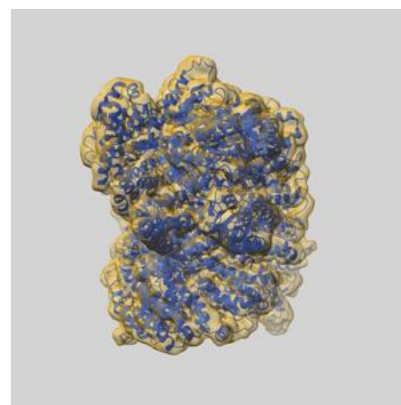
9.1 Map-model overlay [i](#)



X



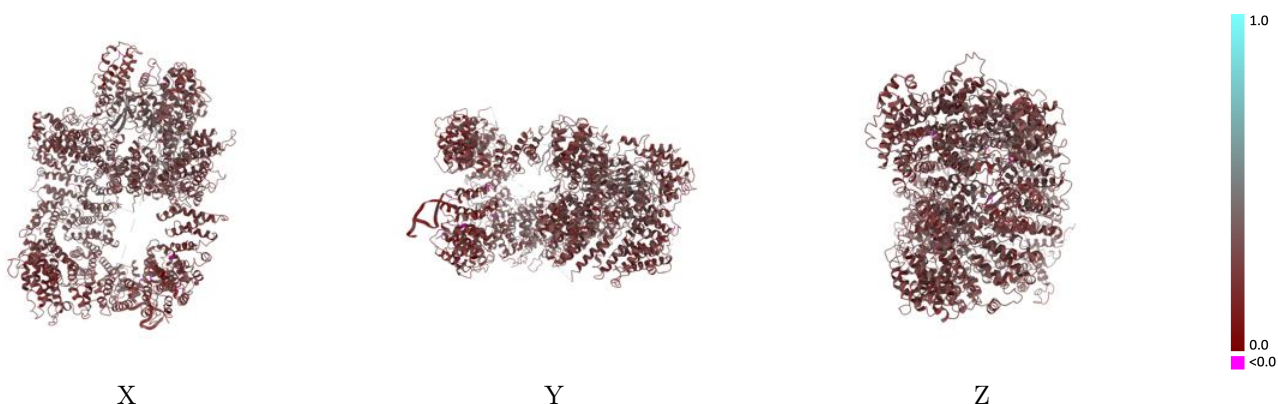
Y



Z

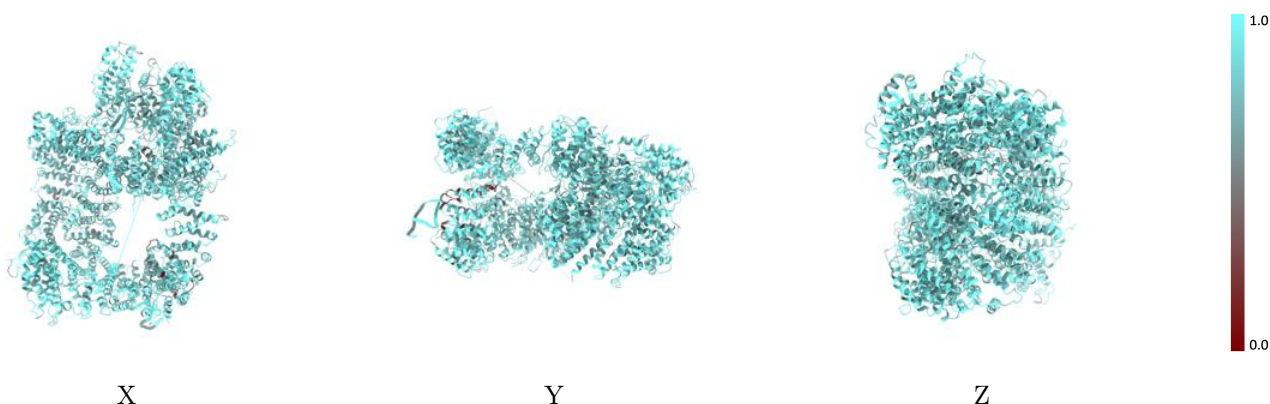
The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



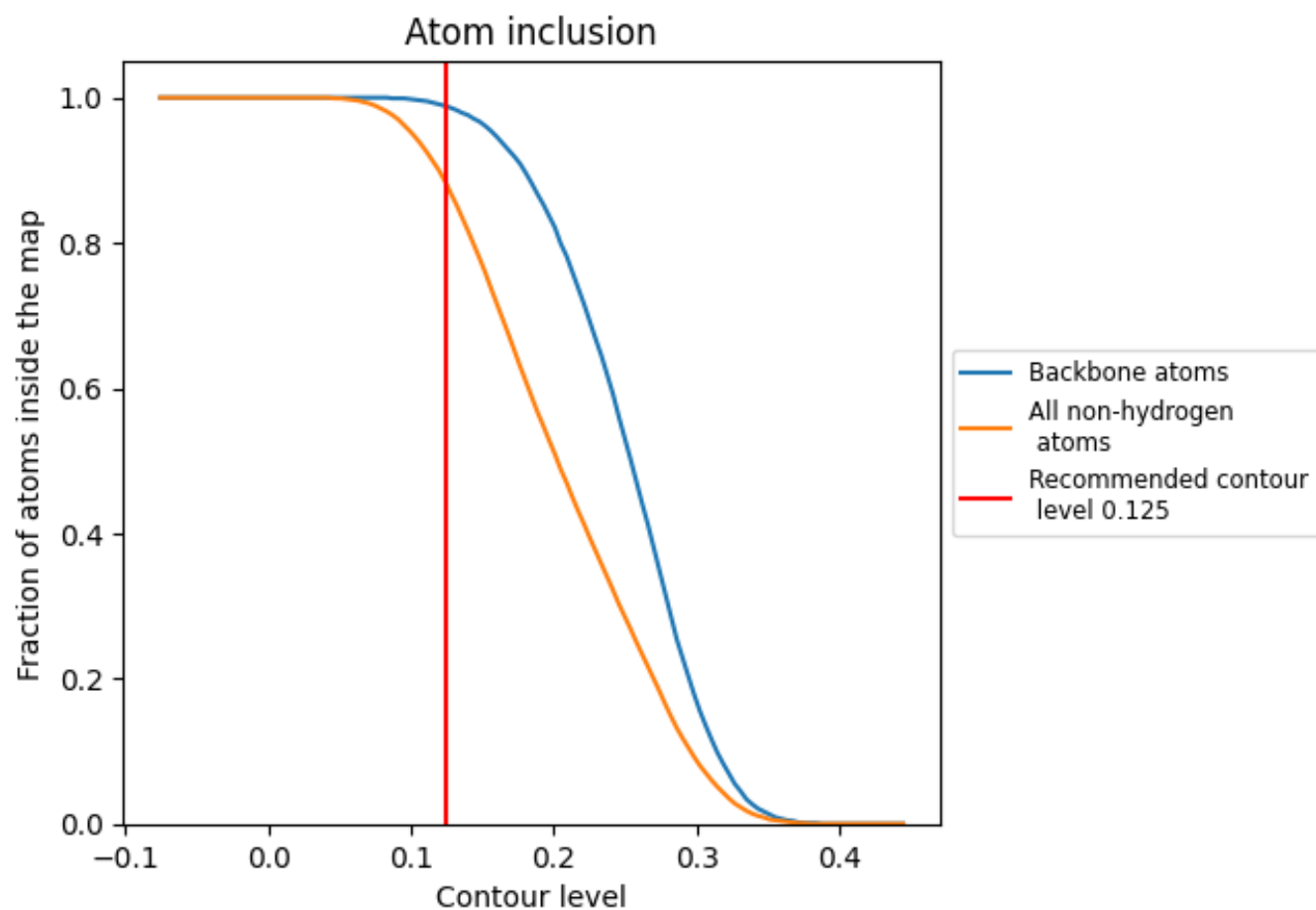
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 88% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8800	0.2770
A	0.8800	0.2780
B	0.8290	0.2110
C	0.9760	0.2030

