



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 12:58 PM UTC

PDB ID : 6ZH4 / pdb_00006zh4
EMDB ID : EMD-11213
Title : Cryo-EM structure of DNA-PKcs (State 3)
Authors : Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2020-06-20
Resolution : 3.62 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

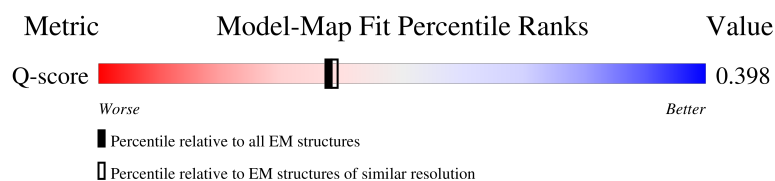
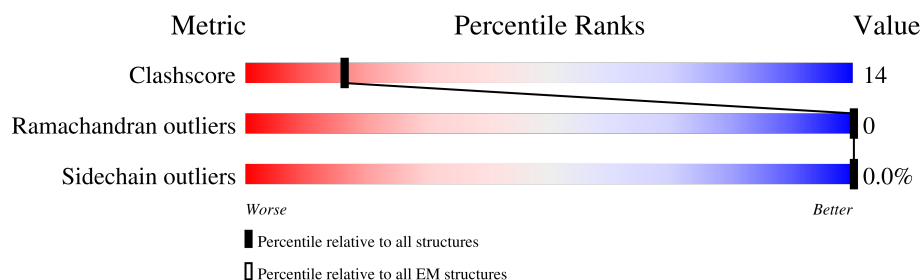
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.62 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	11773 (3.12 - 4.12)

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	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29352 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
			Total	C	N	O	S		
1	A	3698	29352	18827	4960	5372	193	0	0

3 Residue-property plots

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

- Molecule 1: DNA-dependent protein kinase catalytic subunit,DNA-PKCs







V4038	D3922	L3786	W3686	S3539	P3405	V3315
Y4039	R3923	V3793	M3687	K3543	TRP	L3316
R4049	M3932	R3799	F3690	T3547	SER	N3319
K4050	D3941	L3800	E3693	G3548	SER	I3320
G4053	H3944	G3801	F3694	H3549	CYS	L3321
A4054		L3802	L3695	K3550	GLY	F3323
I4059	A3949	L3803	R3696	N3551		
		V3810	R3697	K3552		N3327
D4062	L3953	T3819	E3698	E3553		I3328
E4063	P3954	E3823	Y3705	F3554		L3329
L4064	V3955	A3827	D3706	V3555		L3341
L4065	P3956	A3827	G3707	A3556		A3346
E4069	E3957	R3833	K3710	R3557		C3347
K4070	L3958	A3834	L3711	I3558		L3348
A4071	M3959	Y3839	L3712	K3559		A3349
P4072	R3965		R3718	S3560	ALA	E3350
A4073	N3969	M3842	F3722	K3561	SER	
F4074	L3970	L3843	D3723	L3562	VAL	I3351
R4075	M3974	M3846	E3724	L3578	ILE	E3352
D4076	K3975	Y3855	V3728	E3582	ASP	I3353
Y4077	I3983	M3856	S3731	F3585	SER	E3353
A4081	M3984	M3857	R3734	D3586	ALA	D3354
S4084		L3857	R3735	K3587		R3357
H4087	L3988	Y3858	K3736	S3589		R3358
H4088	R3989	M3859		N3590		I3359
I4089	R3992	K3860		D3591		L3360
R4090	S3993	N3863	R3741	V3592		E3361
A4091	D3994	R3864	G3742	K3593		L3362
Q4092			H3743	A3594		S3363
S4096	V4004	T3867	D3744	E3595		S3364
G4097	W4013	F3871	E3745	A3597		S3365
Q4103	K4014	E3874	R3746	K3598		S3366
V4104	E4017	E3875	E3747	T3599		
L4107	K4022	V3878	L3751	P3600		D3369
M4108	K4023	P3879	W3752	V3601		S3370
D4113	G4024	A3880	K3753	N3602		V3373
R4119	G4025	A3886	G3754	K3603		I3374
E4125	S4026		E3755	K3604		A3375
M4128	I4028	M3890	D3756	N3605		G3376
X5009	Q4029	R3901	L3758	T3606		Q3379
	E4030		R3759	E3607		R3380
	I4031	A3909	D3761	M3608		V3373
	N4032	L3910	A3780	K3609		I3374
	V4033	M3916	C3781	Y3610		A3375
	A4034		S3782	E3611		G3376
	E4035		R3784	R3612		Q3379
	K4036		A3785	M3613		R3380
	N4037			S3684		V3373
				P3685		A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
						Q3379
						R3380
						V3373
						I3374
						A3375
						G3376
		</				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47183	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 ($e^-/\text{\AA}^2$)	53.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.195	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	280.36002, 280.36002, 280.36002	wwPDB
Map dimensions	430, 430, 430	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.652, 0.652, 0.652	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	0.22	0/29811	0.40	1/40307 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3547	THR	N-CA-C	-5.71	107.31	114.56

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	29352	0	29489	830	0
All	All	29352	0	29489	830	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 14.

The worst 5 of 830 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:3628:PHE:H	1:A:3684:SER:HB3	1.42	0.85
1:A:1712:ARG:HH12	1:A:1716:GLN:HB2	1.44	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3282:ARG:HE	1:A:3329:LEU:HD21	1.46	0.80
1:A:1351:THR:HG22	1:A:1353:PRO:HD2	1.61	0.80
1:A:3482:LEU:HD12	1:A:3482:LEU:O	1.81	0.80

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	3632/4156 (87%)	3357 (92%)	275 (8%)	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	3229/3671 (88%)	3228 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	3482	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2543	ASN
1	A	2954	GLN
1	A	3634	GLN
1	A	2865	HIS
1	A	3154	GLN

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	5009:UNK	N	96.48

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	5016:UNK	C	6001:UNK	N	49.88

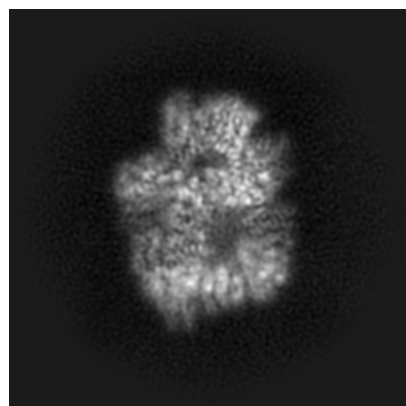
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11213. These allow visual inspection of the internal detail of the map and identification of artifacts.

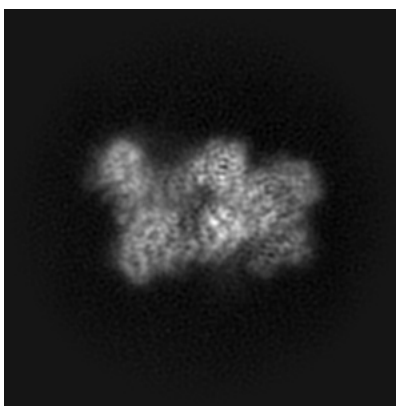
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

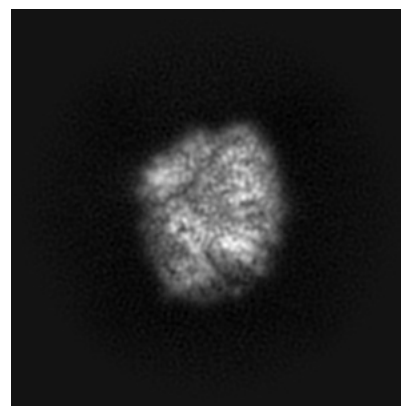
6.1.1 Primary map



X

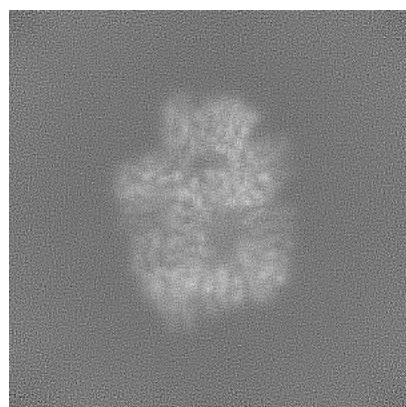


Y

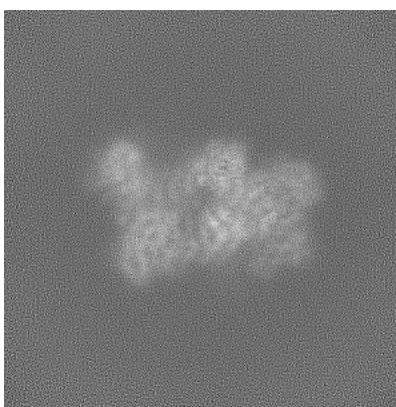


Z

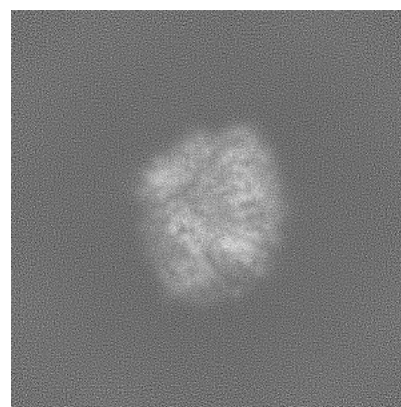
6.1.2 Raw map



X



Y

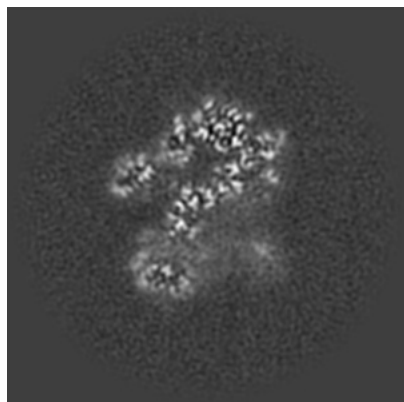


Z

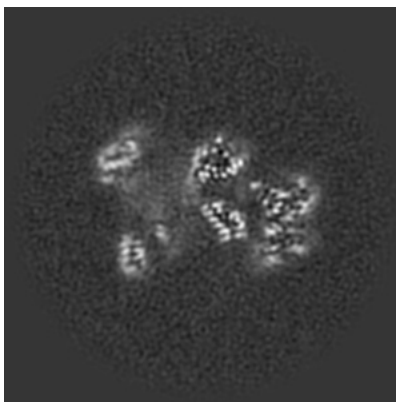
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 215

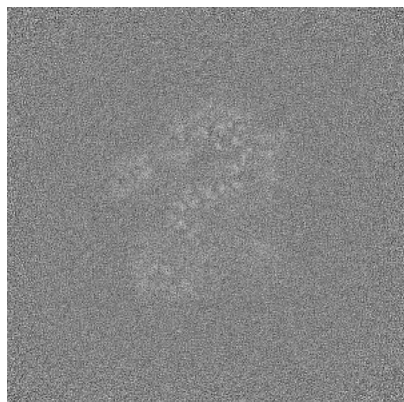


Y Index: 215

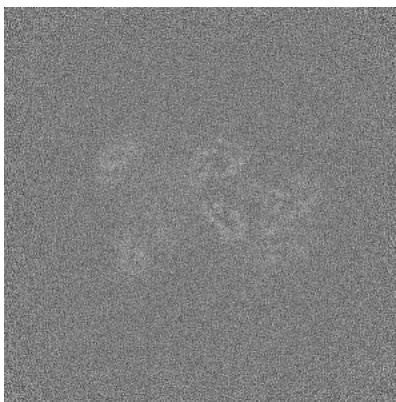


Z Index: 215

6.2.2 Raw map



X Index: 215



Y Index: 215

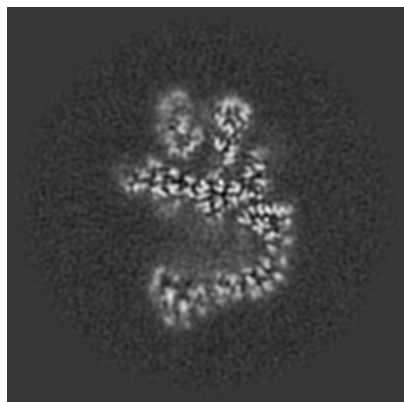


Z Index: 215

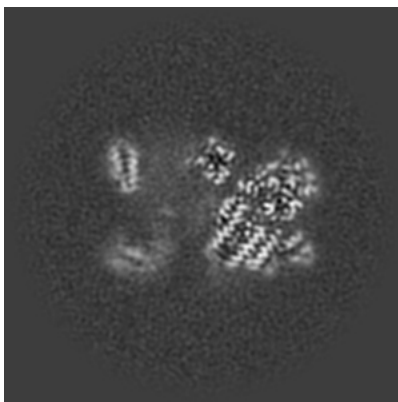
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

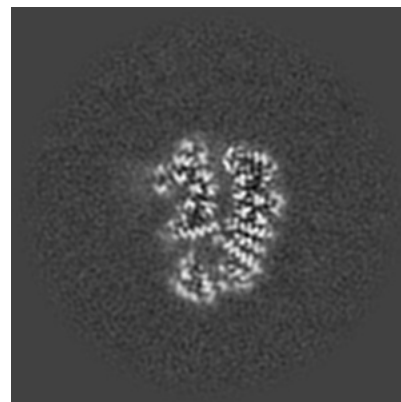
6.3.1 Primary map



X Index: 249

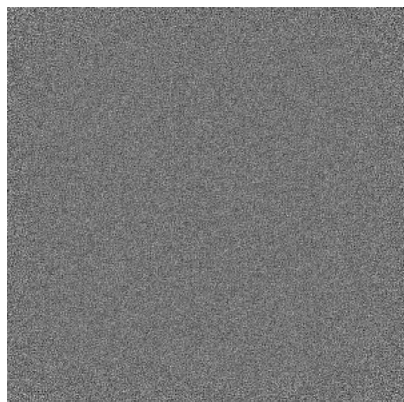


Y Index: 245

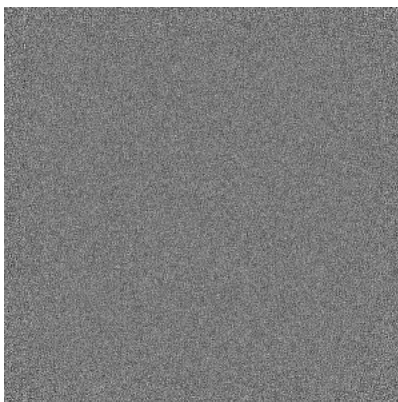


Z Index: 233

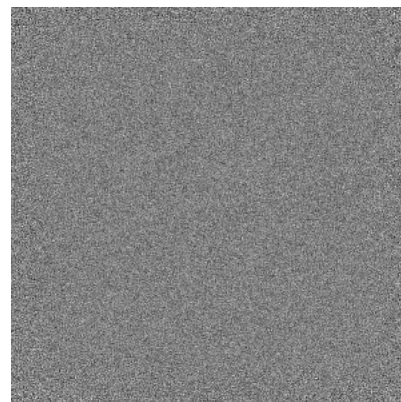
6.3.2 Raw map



X Index: 0



Y Index: 0

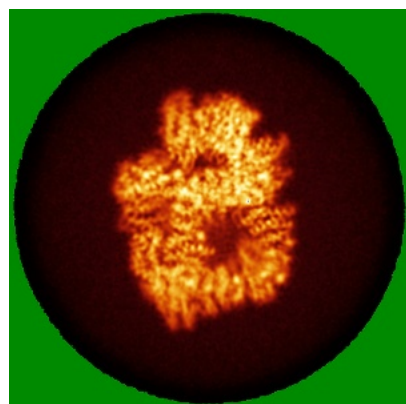


Z Index: 0

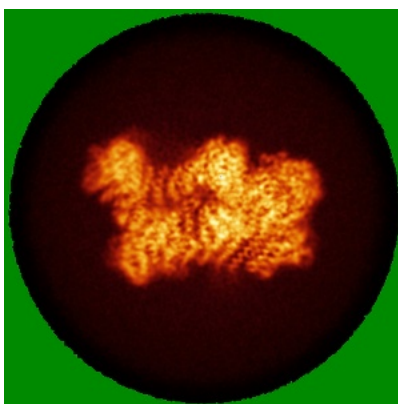
The images above show the largest variance slices of the map in three orthogonal directions.

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

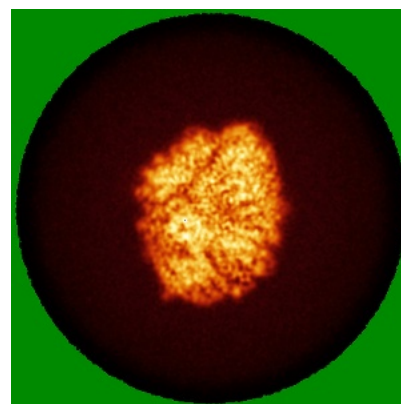
6.4.1 Primary map



X

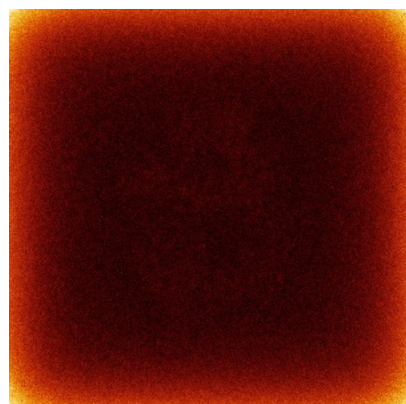


Y

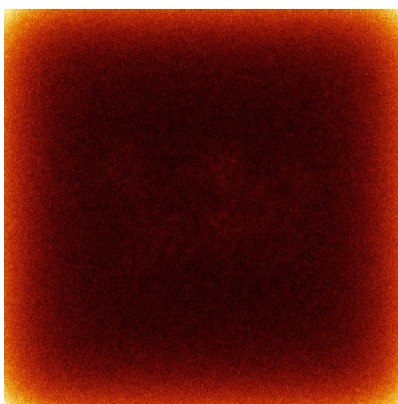


Z

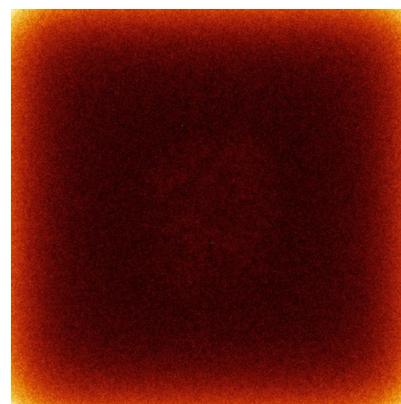
6.4.2 Raw map



X



Y

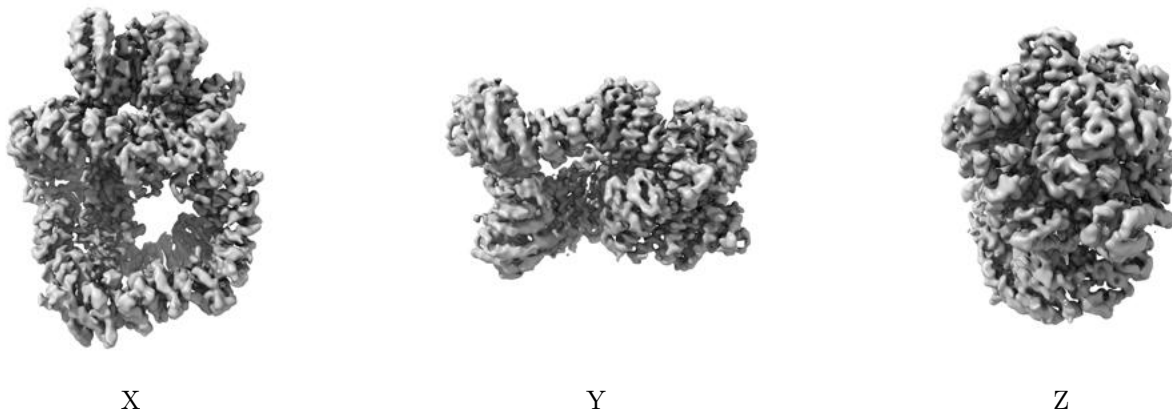


Z

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.

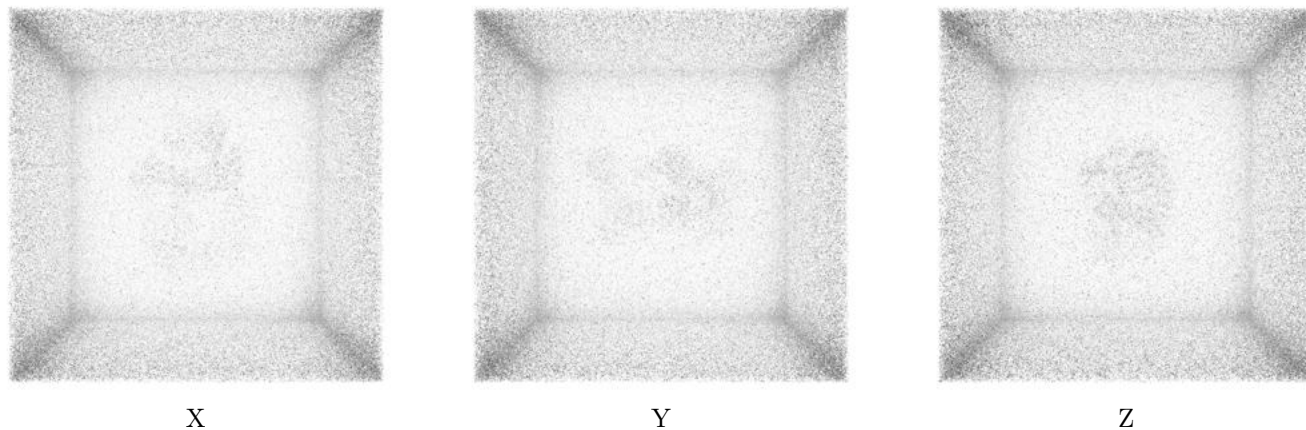
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. 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.

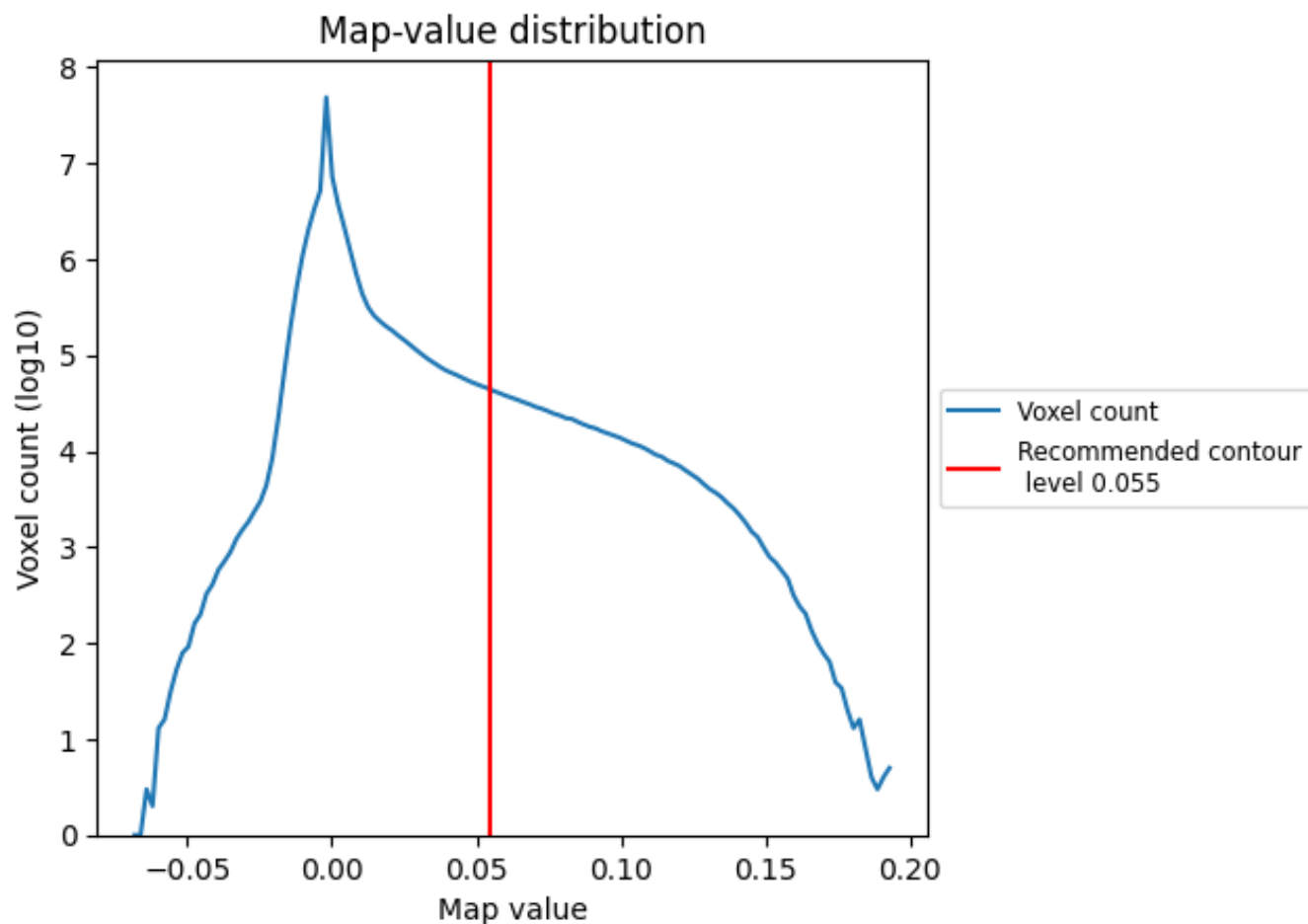
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

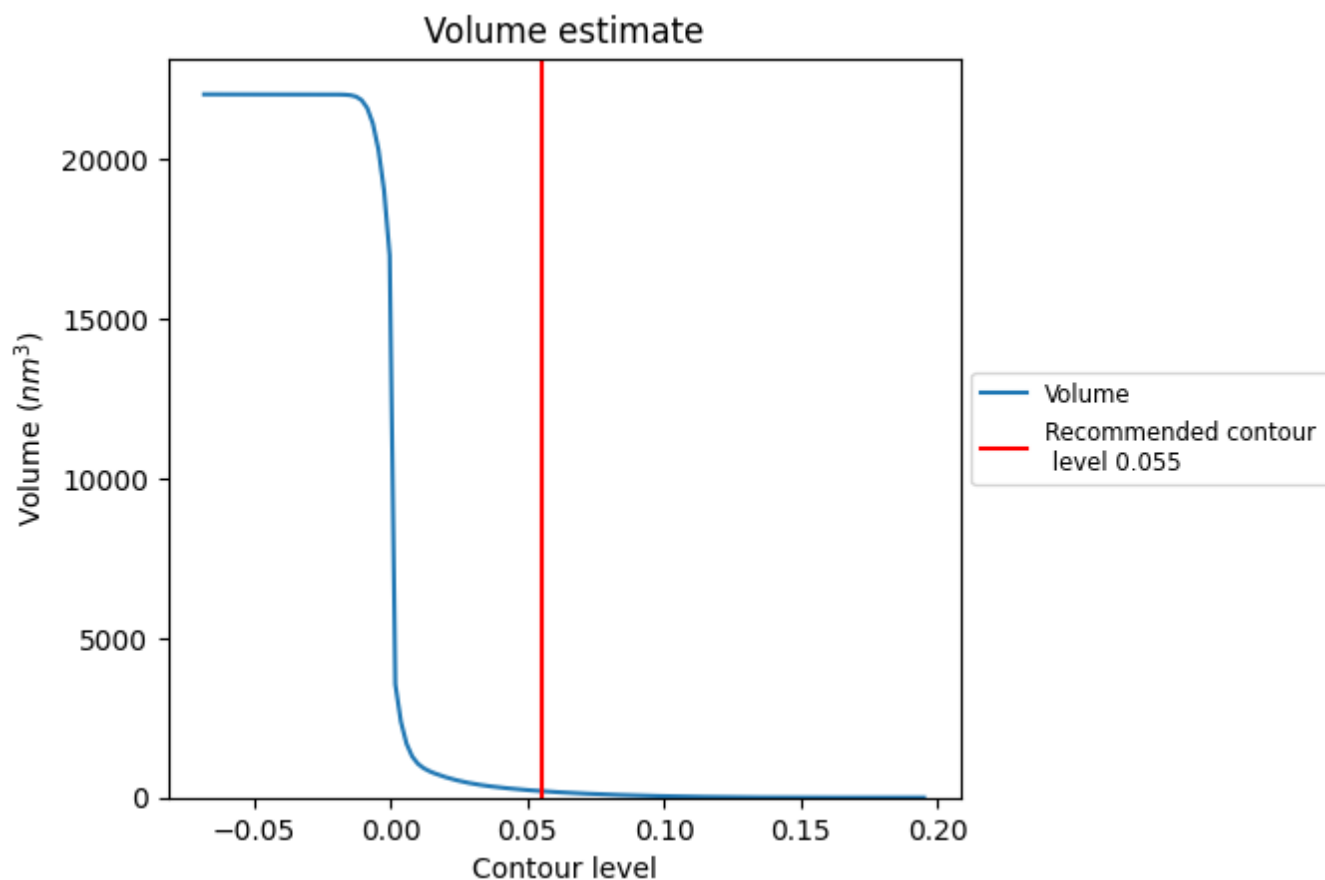
This section contains the results of statistical analysis of the map.

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.

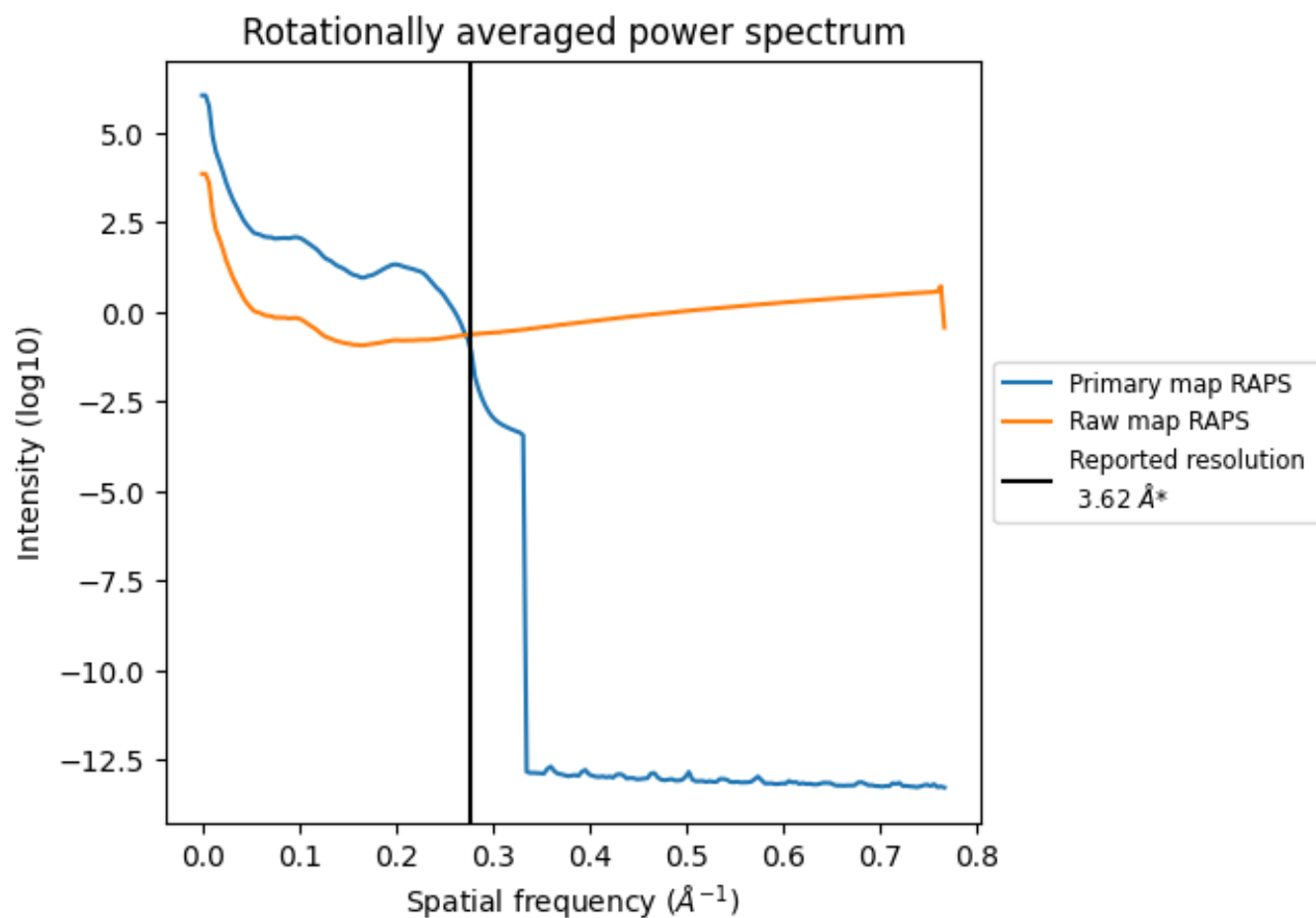
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 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](#)

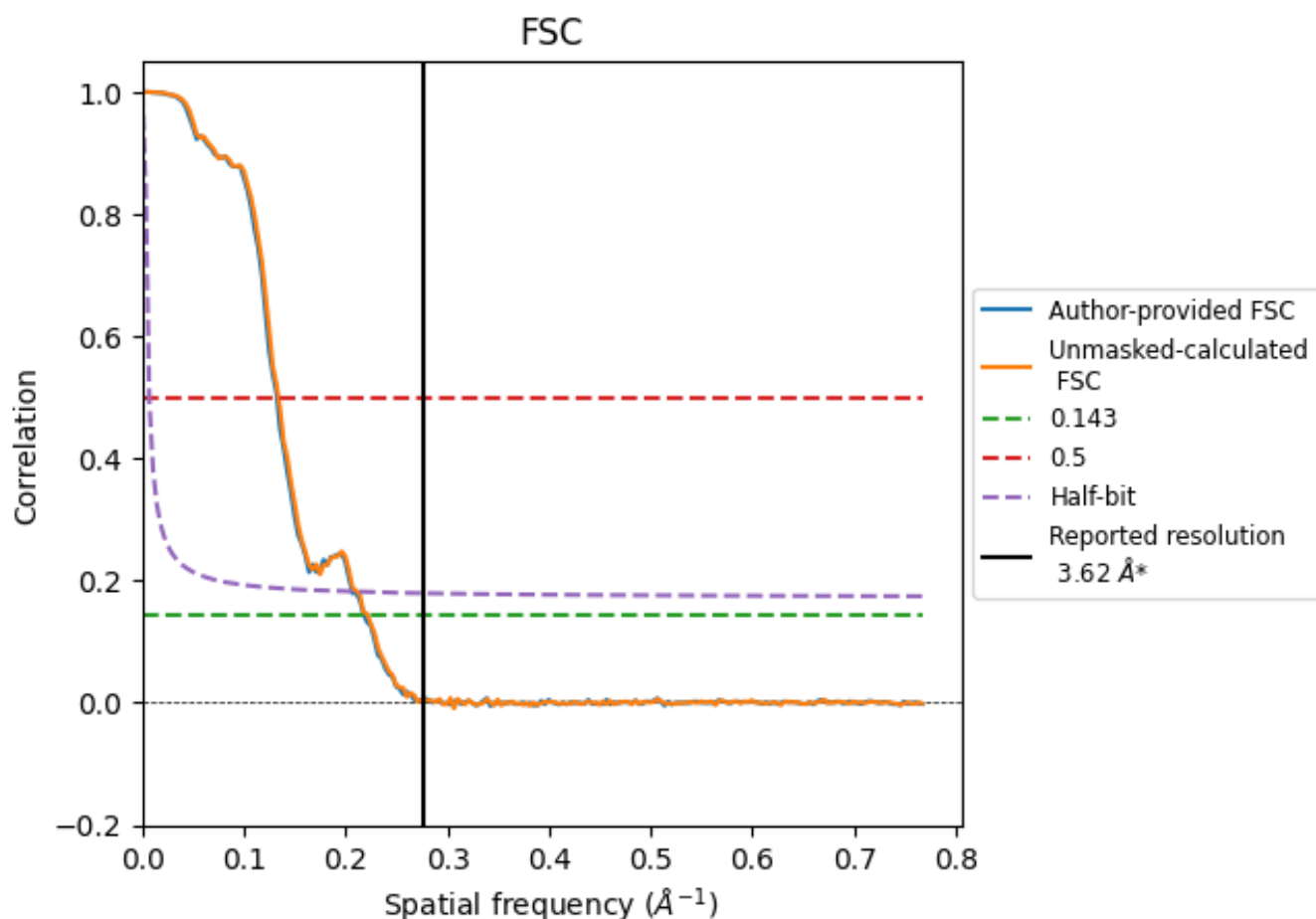


*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

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 $0.276 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	4.58	7.55	4.84
Unmasked-calculated*	4.51	7.47	4.73

*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 4.58 differs from the reported value 3.62 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 3.62 by more than 10 %

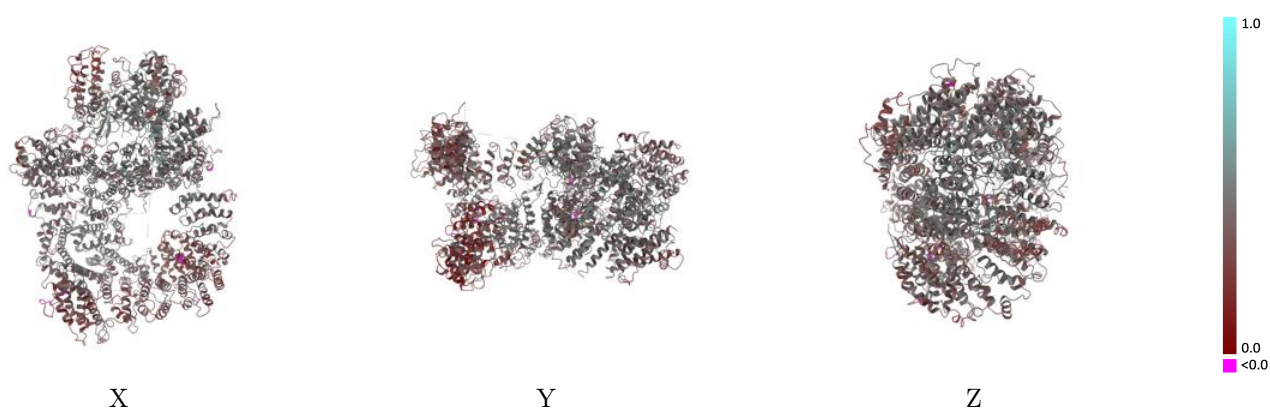
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11213 and PDB model 6ZH4. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

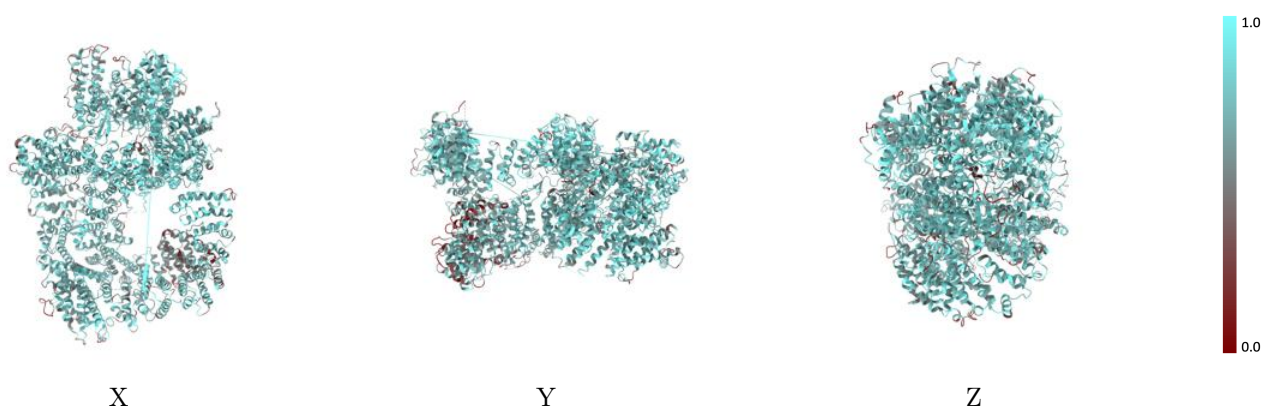
This section was not generated.

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



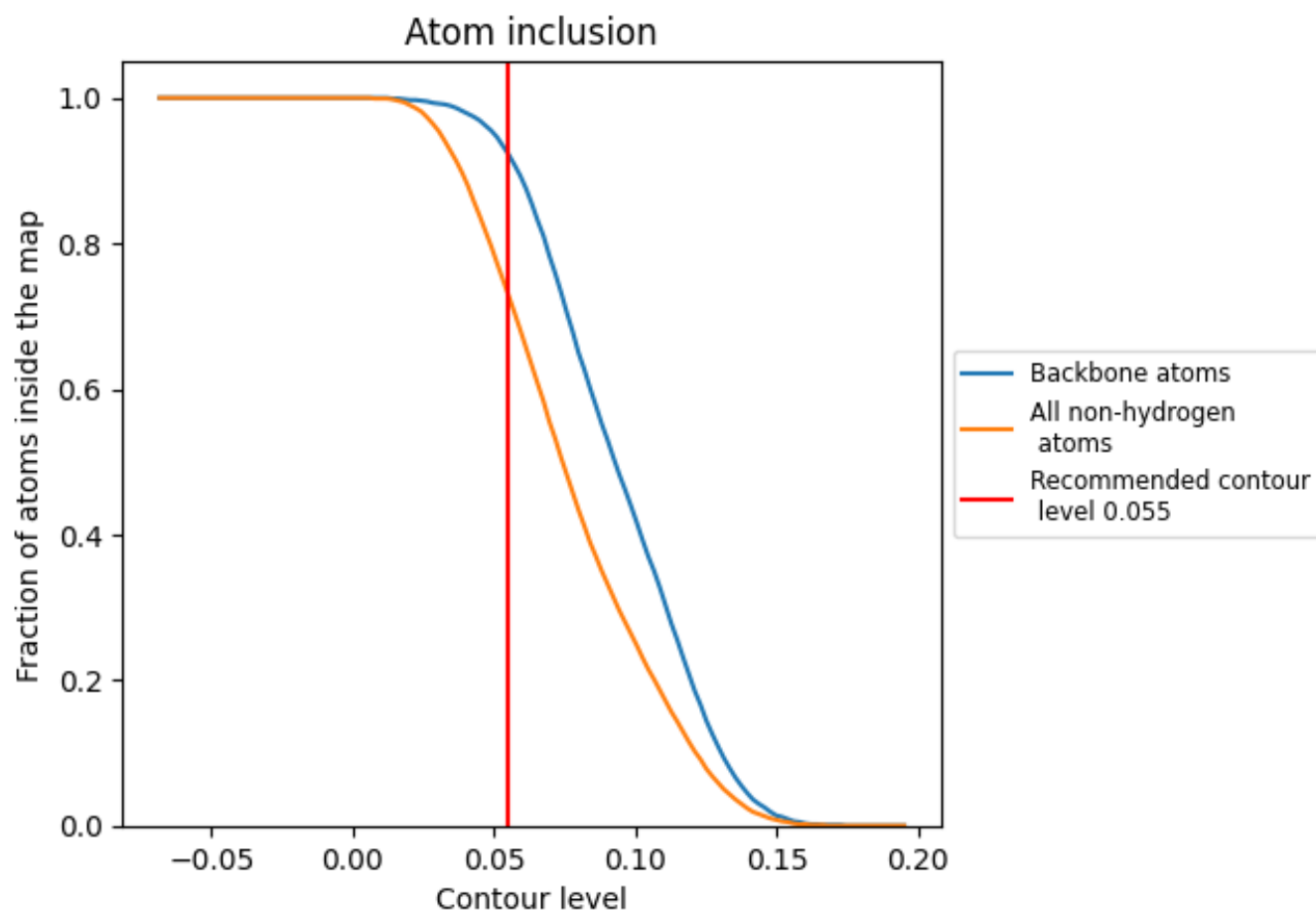
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 73% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7300	0.3980
A	0.7300	0.3980

