



wwPDB EM Validation Summary Report ⓘ

Apr 17, 2025 – 12:37 PM JST

PDB ID : 9IVD / pdb_00009ivd
EMDB ID : EMD-60925
Title : Cryo-EM structure of CyclinD1 bound AMBRA1-DDB1
Authors : Wang, Y.; Liu, M.; Su, M.-Y.; Stjepanovic, G.
Deposited on : 2024-07-23
Resolution : 3.55 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

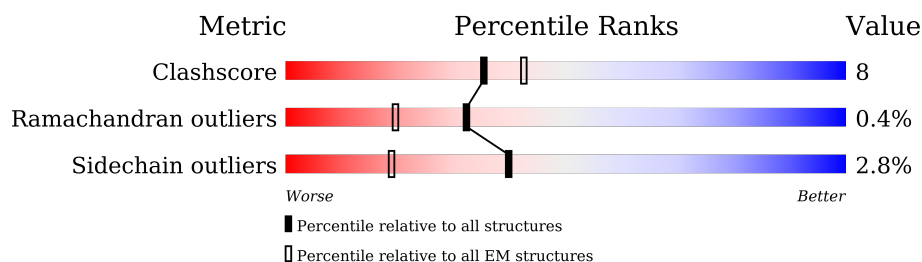
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.55 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	E	295	
2	B	396	
3	A	1140	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8628 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 G1/S-specific cyclin-D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	11	Total	C	N	O	P	S	
			89	50	14	23	1	1	

- Molecule 2 is a protein called Activating molecule in BECN1-regulated autophagy protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	364	Total	C	N	O	S		
			2824	1805	501	505	13	0	0

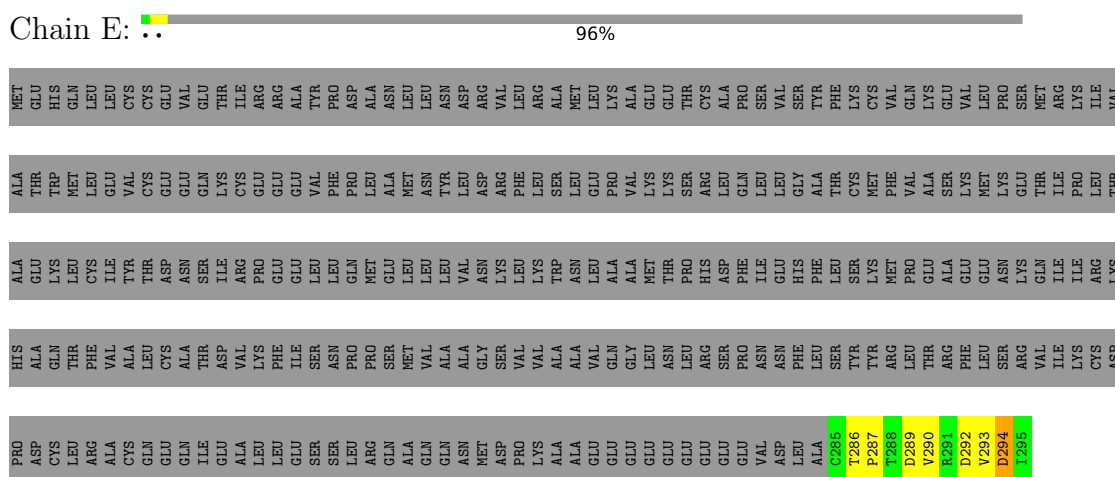
- Molecule 3 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	785	Total	C	N	O	S		
			5715	3689	981	1016	29	0	0

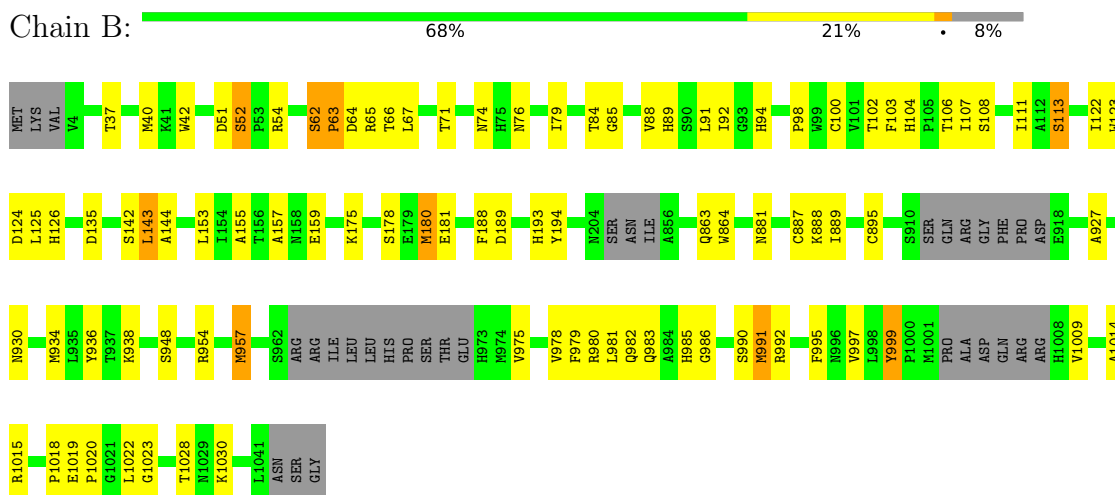
3 Residue-property plots

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: G1/S-specific cyclin-D1



• Molecule 2: Activating molecule in BECN1-regulated autophagy protein 1



• Molecule 3: DNA damage-binding protein 1



M1	L283	ASP	GLU	ASP	LEU	SER	L736	L880	GLU
N4	C313	THR	PRO	ILE	CYS	ASN	S737	I884	THR
Y5	D318	LEU	ALA	PRO	LEU	LYS	S738	N885	THR
V6	V321	VAL	LEU	LEU	GLY	VAL	D744	S886	P1023
P12	D330	SER	VAL	GLY	ASP	PHE	THR	T887	S1027
C18	D366	PHE	ASP	ASP	GLY	SER	SER	Y891	G1035
T24	LEU	THR	ASN	ASN	ALA	ASN	GLY	E892	V1040
N30	GLU	ARG	PRO	SER	TYR	LEU	T749	W893	T1041
K60	GLU	VAL	ALA	LEU	PHE	LYS	T750	L899	S1044
M64	ASN	VAL	LYS	CYS	GLY	GLU	S757	N904	E1045
R68	GLN	GLY	ILE	ILE	ASN	ASN	S762	H905	R1057
D75	G373	GLU	SER	GLY	THR	MET	F771	N907	E1069
T81	V376	GLU	ALA	THR	GLY	CYS	SER	M910	F1088
A82	G380	VAL	VAL	THR	LEU	PRO	SER	F920	F1097
K83	G385	THR	GLN	ARG	LYS	TYR	THR	L921	L922
K92	R388	LEU	VAL	ILE	LYS	PRO	F782	S929	V1108
Q93	I389	MET	VAL	LEU	VAL	ASP	L791	L933	V1109
S94	I390	GLY	VAL	THR	THR	LEU	L792	A934	M1111
I101	R391	PHE	ALA	LEU	GLY	ALA	H789	Y935	L1112
T118	N392	VAL	VAL	THR	THR	LEU	H790	F942	GLN
R129	GLY	ASP	GLY	ARG	GLN	ALA	L791	E943	TYR
M130	ILE	ASP	ALA	LEU	ASN	ASN	D795	E944	ASP
R134	HIS	GLU	THR	THR	THR	SER	E800	R947	GLY
D137	ALA	SER	PHE	LEU	LEU	THR	V801	D948	MET
P176	ILE	ASN	GLY	LYS	ARG	LEU	L802	F949	LYS
C179	ASP	VAL	PRO	MET	PHE	THR	Q806	N950	R1122
V195	LEU	ALA	GLN	ILE	GLY	THR	Q809	L960	E1123
F202	GLY	PRO	ILE	ARG	VAL	ILE	M810	N964	A1124
G205	LEU	THR	SER	ILE	PHE	ALA	Y812	V976	L1129
P206	PRO	THR	GLU	THR	CYS	CYS	K823	L992	I1139
W207	LEU	ALA	MET	MET	SER	ASP	F829	F998	H1140
I232	ARG	SER	GLU	THR	THR	THR	T833	H999	
I237	ASP	VAL	HIS	PHE	ARG	ARG	V849	L1000	
I253	PRO	LEU	GLU	THR	THR	THR	V850	G1010	
I258	ASN	ASN	VAL	GLU	VAL	THR	F851	V1013	
	ARG	VAL	ALA	VAL	ILE	TYR	E863	MET	
	GLU	SER	CYS	GLU	THR	SER	A869	GLN	
	THR	GLN	LEU	TYR	SER			ASN	
								LEU	
								GLY	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1015935	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.198	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.992	Depositor
Minimum map value	-0.437	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.192	Depositor
Map size (\AA)	217.6, 217.6, 217.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	E	0.31	0/77	1.00	1/101 (1.0%)
2	B	0.29	1/2896 (0.0%)	0.59	2/3946 (0.1%)
3	A	0.25	0/5821	0.51	0/7928
All	All	0.26	1/8794 (0.0%)	0.55	3/11975 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	63	PRO	CG-CD	-5.54	1.32	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	PRO	CA-N-CD	-11.80	94.97	111.50
2	B	63	PRO	N-CD-CG	-6.35	93.67	103.20
1	E	294	ASP	CB-CG-OD2	5.77	123.49	118.30

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	E	89	0	78	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2824	0	2751	59	0
3	A	5715	0	5486	69	0
All	All	8628	0	8315	131	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 8.

The worst 5 of 131 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)
3:A:886:SER:HB2	3:A:910:MET:H	1.35	0.90
2:B:63:PRO:HD2	2:B:64:ASP:H	1.45	0.81
2:B:63:PRO:HD2	2:B:64:ASP:N	2.02	0.73
3:A:18:CYS:N	3:A:313:CYS:SG	2.63	0.72
3:A:920:PHE:HB3	3:A:935:TYR:HB3	1.74	0.69

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	E	8/295 (3%)	8 (100%)	0	0	100	100
2	B	354/396 (89%)	315 (89%)	35 (10%)	4 (1%)	12	45
3	A	771/1140 (68%)	679 (88%)	91 (12%)	1 (0%)	48	79
All	All	1133/1831 (62%)	1002 (88%)	126 (11%)	5 (0%)	32	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	991	MET

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Mol	Chain	Res	Type
2	B	92	ILE
2	B	125	LEU
3	A	1124	ALA
2	B	122	ILE

5.3.2 Protein sidechains ⓘ

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	E	10/265 (4%)	9 (90%)	1 (10%)	6	28
2	B	296/338 (88%)	284 (96%)	12 (4%)	26	55
3	A	558/999 (56%)	547 (98%)	11 (2%)	50	72
All	All	864/1602 (54%)	840 (97%)	24 (3%)	40	64

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	179	CYS
3	A	744	ASP
3	A	330	ASP
3	A	789	HIS
2	B	180	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	904	ASN
3	A	950	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	TPO	E	286	1	8,10,11	1.07	0	10,14,16	1.92	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	E	286	1	-	1/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	E	286	TPO	P-OG1-CB	-5.43	106.82	123.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	286	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

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.

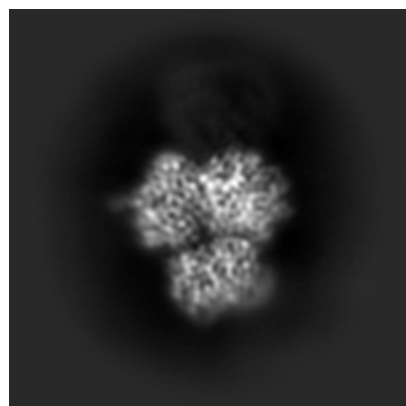
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60925. These allow visual inspection of the internal detail of the map and identification of artifacts.

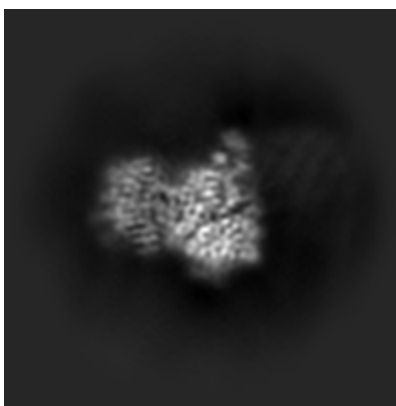
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

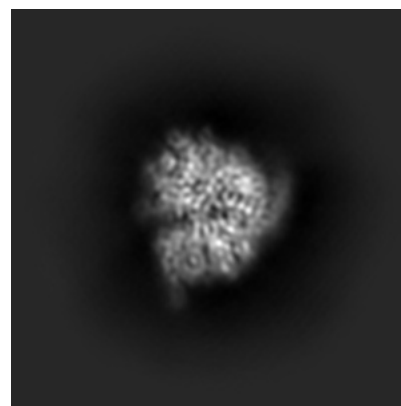
6.1.1 Primary map



X

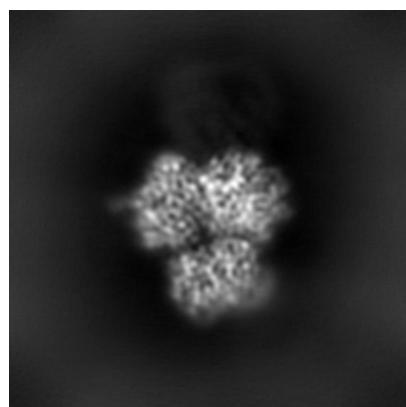


Y

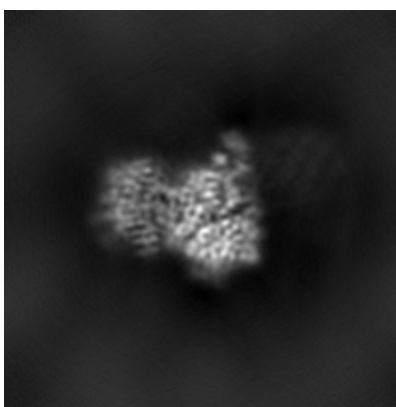


Z

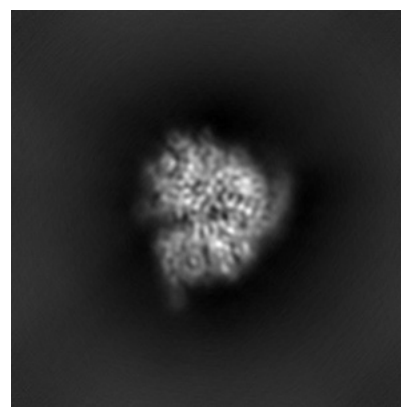
6.1.2 Raw map



X



Y

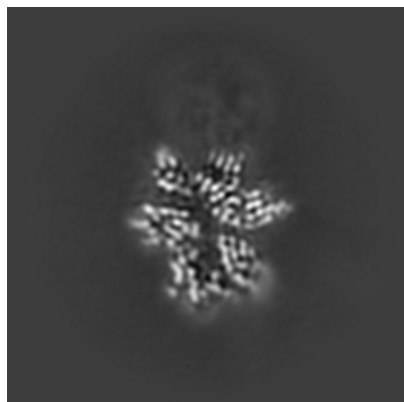


Z

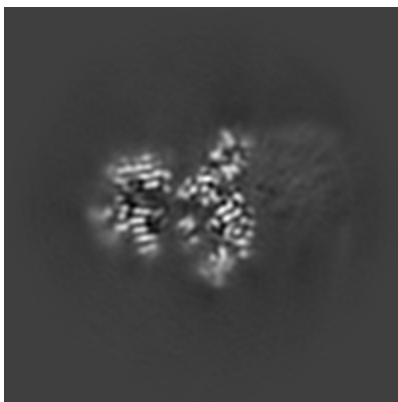
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

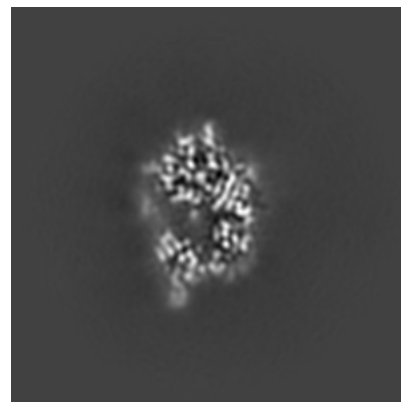
6.2.1 Primary map



X Index: 128

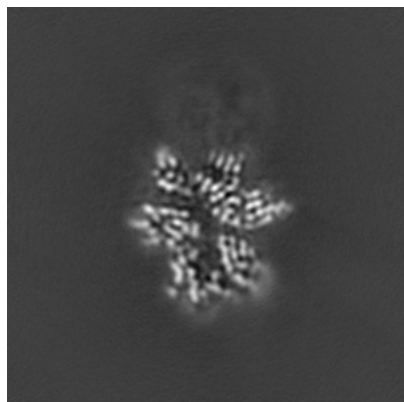


Y Index: 128

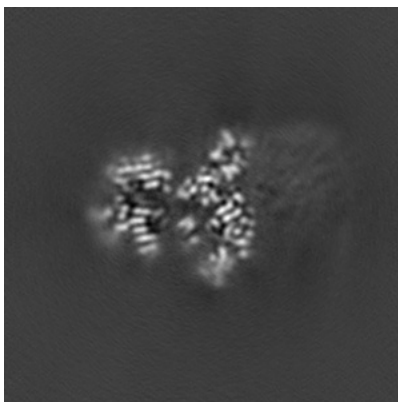


Z Index: 128

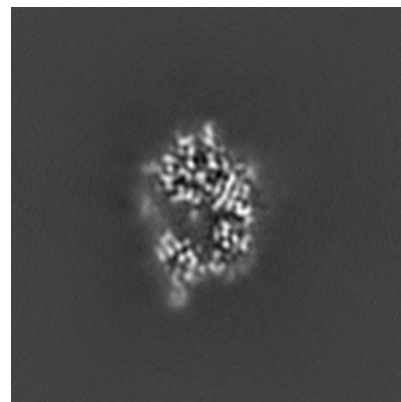
6.2.2 Raw map



X Index: 128



Y Index: 128

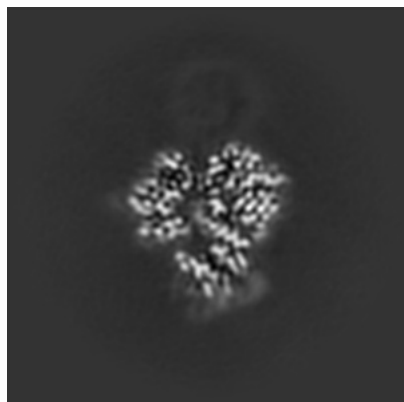


Z Index: 128

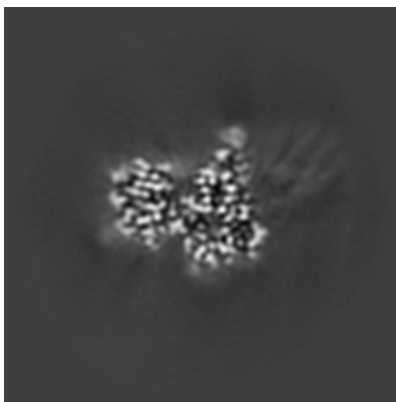
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

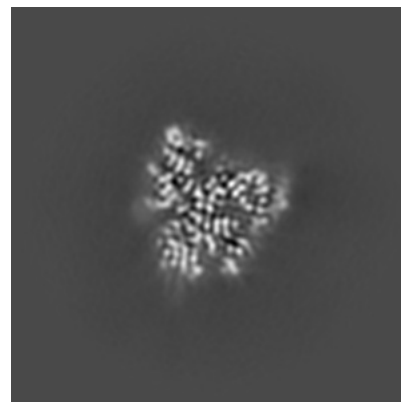
6.3.1 Primary map



X Index: 114

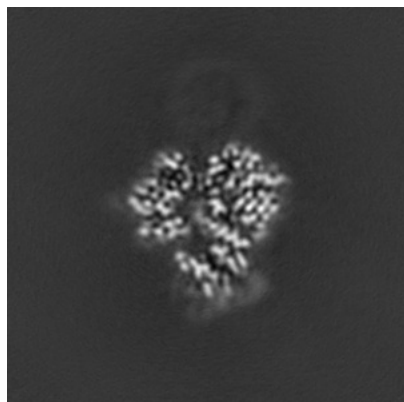


Y Index: 140

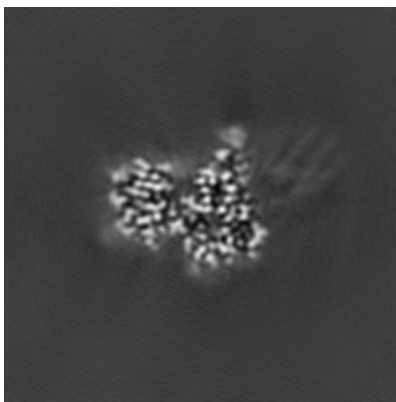


Z Index: 141

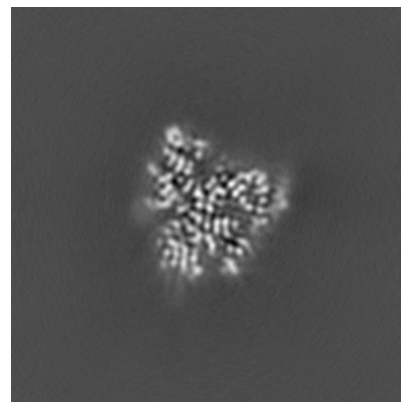
6.3.2 Raw map



X Index: 114



Y Index: 140

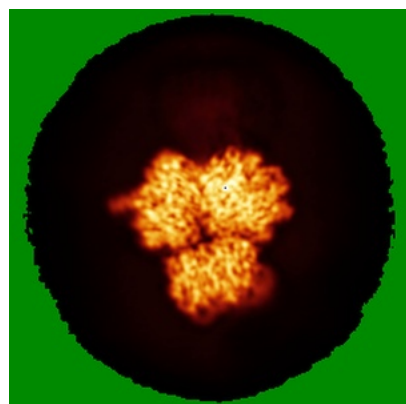


Z Index: 141

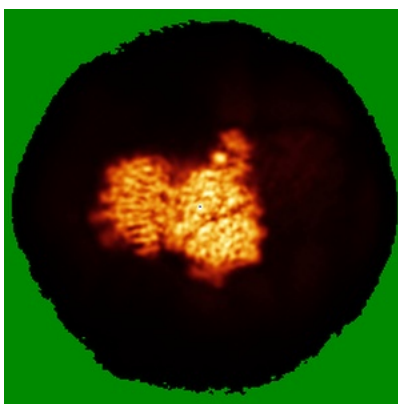
The images above show the largest variance slices of the map in three orthogonal directions.

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

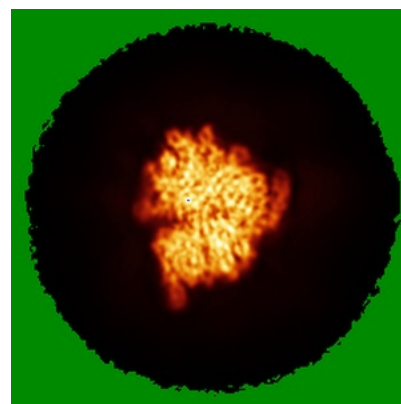
6.4.1 Primary map



X

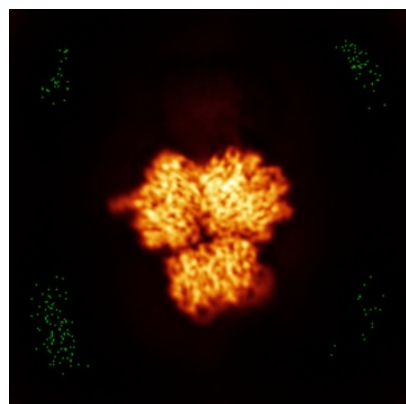


Y

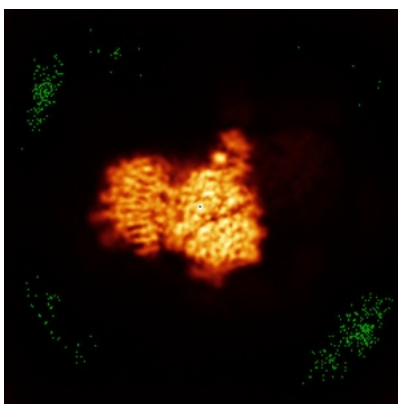


Z

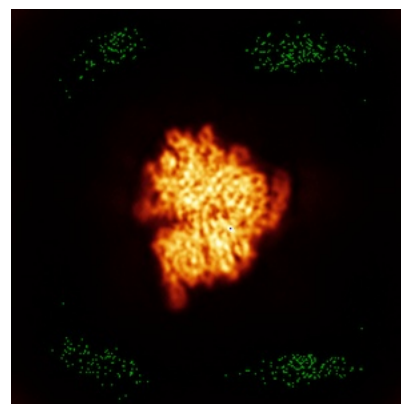
6.4.2 Raw map



X



Y

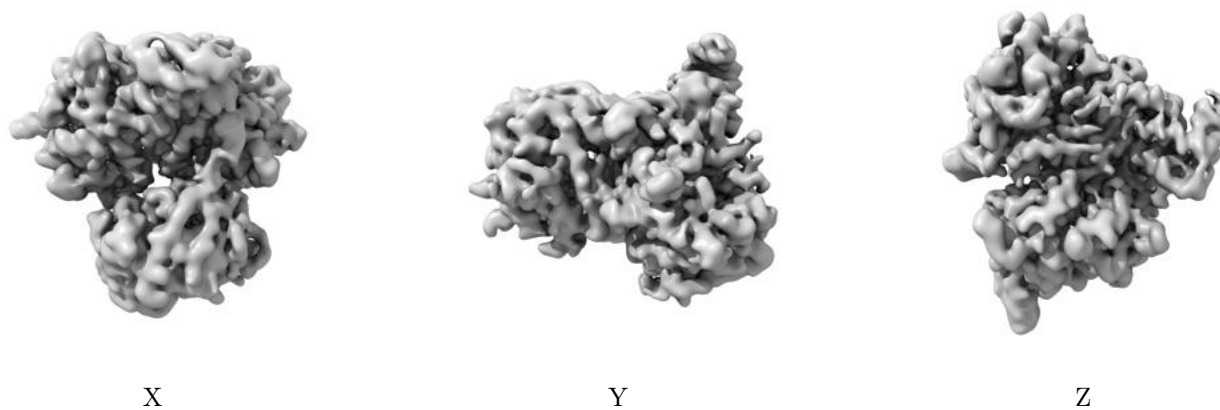


Z

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.

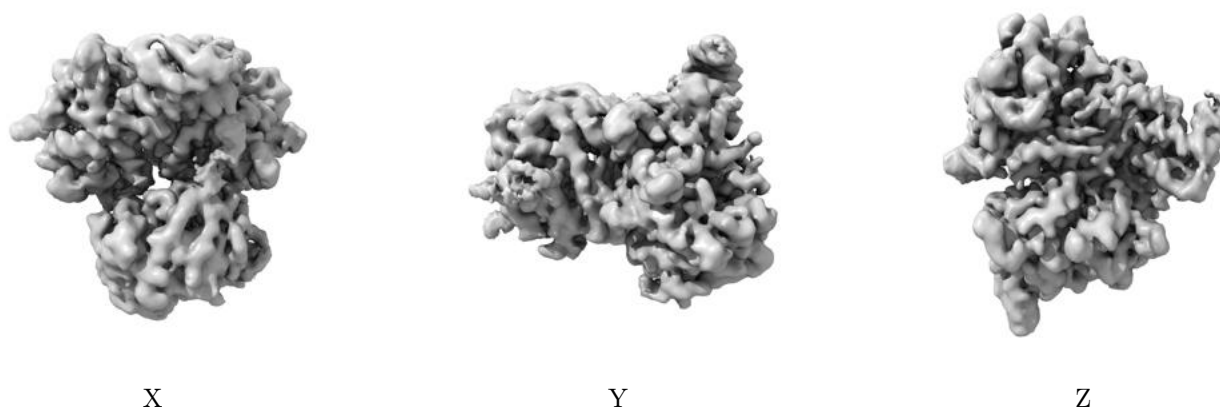
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.192. 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.

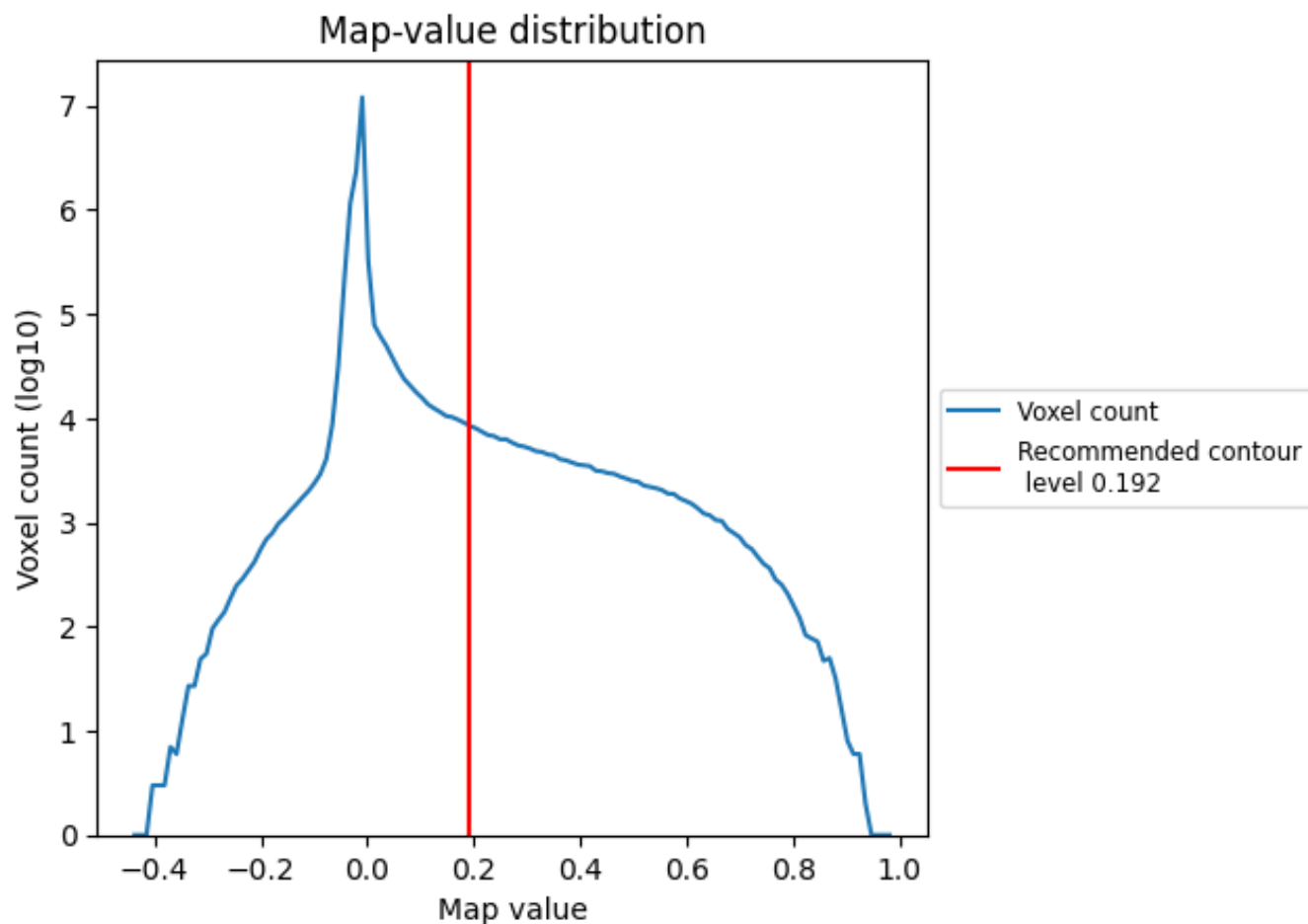
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

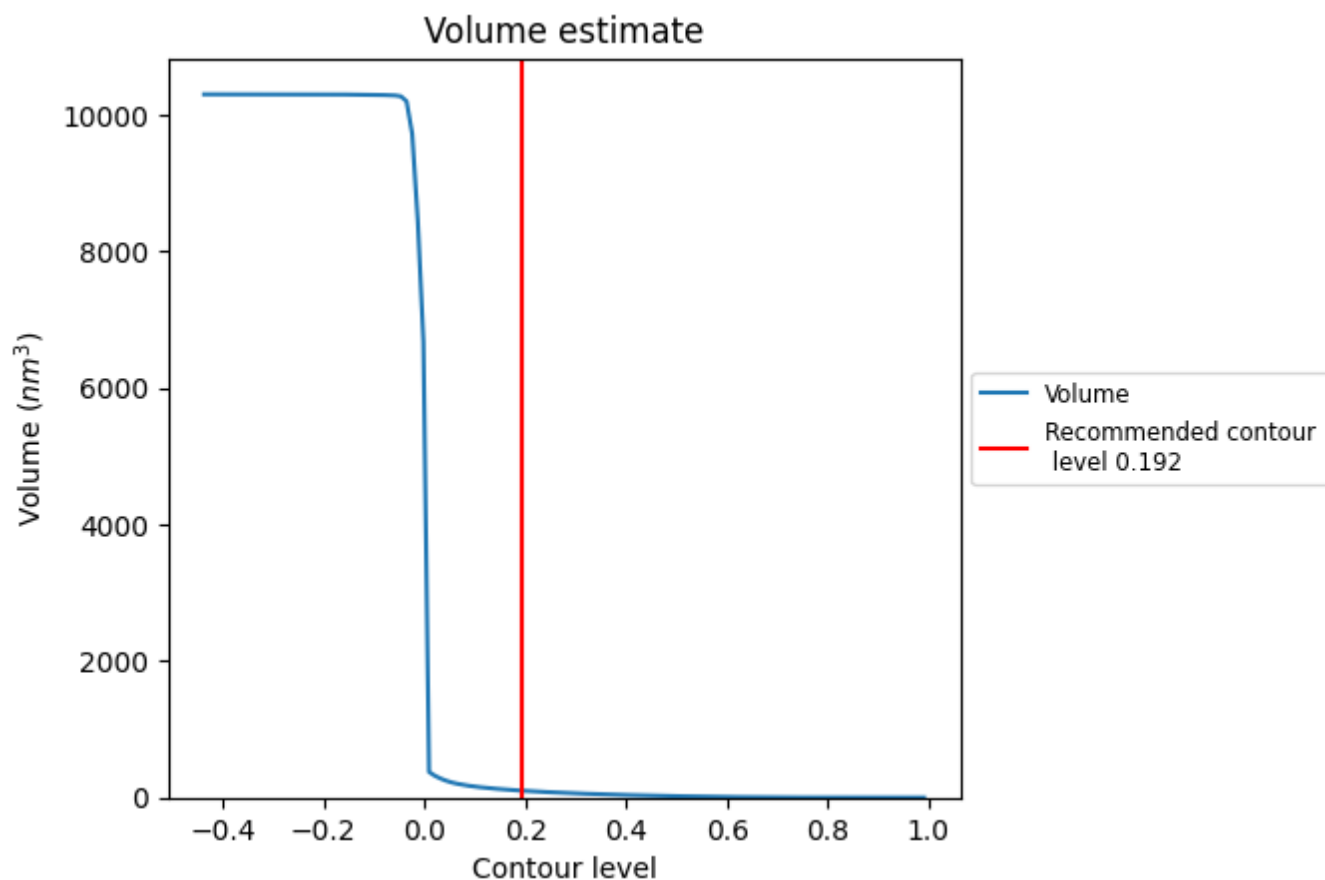
This section contains the results of statistical analysis of the map.

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.

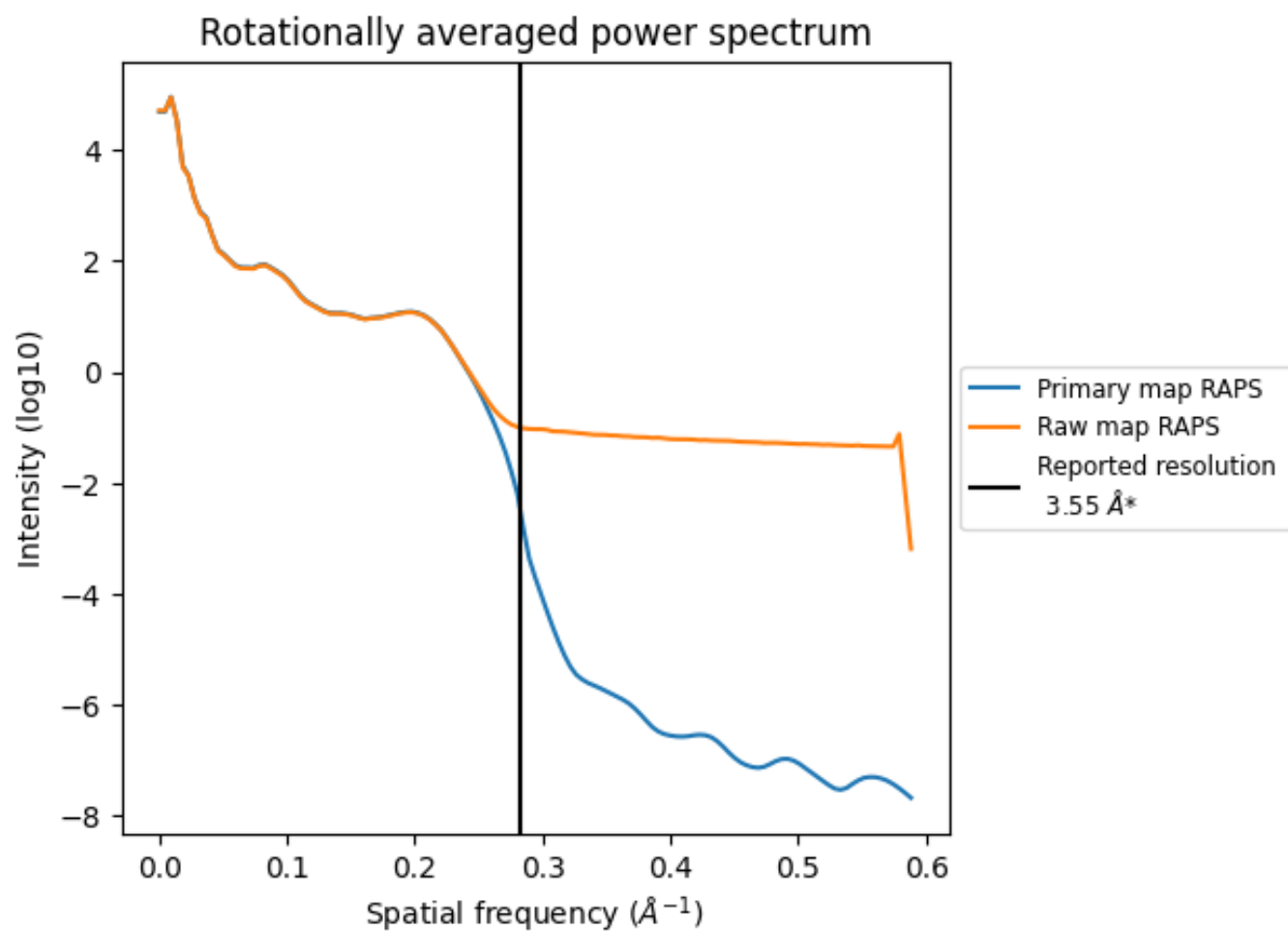
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 102 nm^3 ; this corresponds to an approximate mass of 92 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 ⓘ

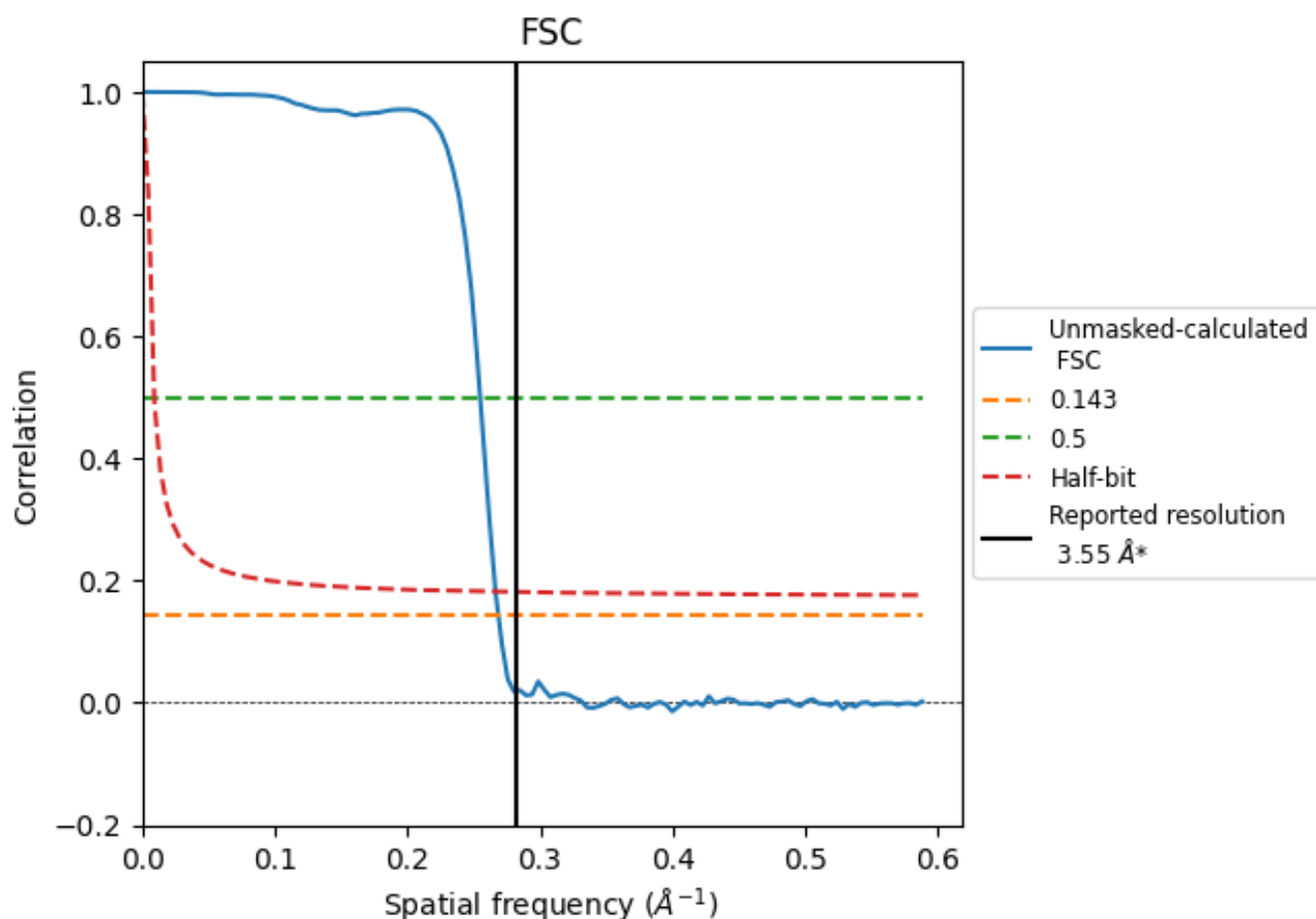


*Reported resolution corresponds to spatial frequency of 0.282 \AA^{-1}

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

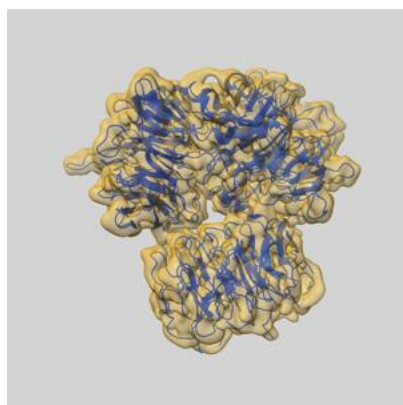
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	3.92	3.75

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

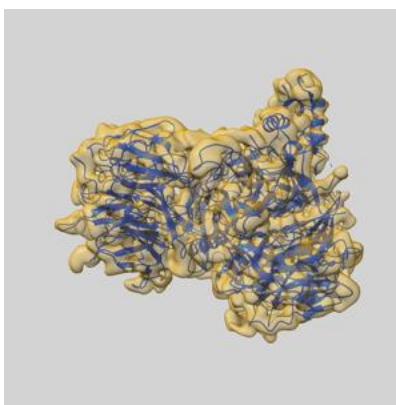
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60925 and PDB model 9IVD. Per-residue inclusion information can be found in section [3](#) on page [4](#).

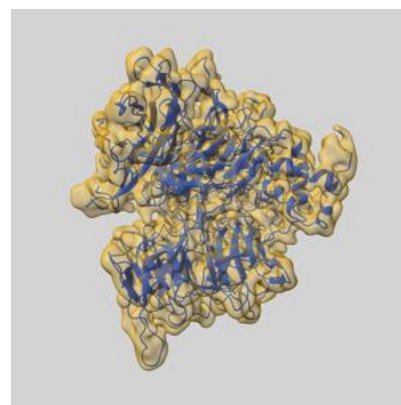
9.1 Map-model overlay [i](#)



X



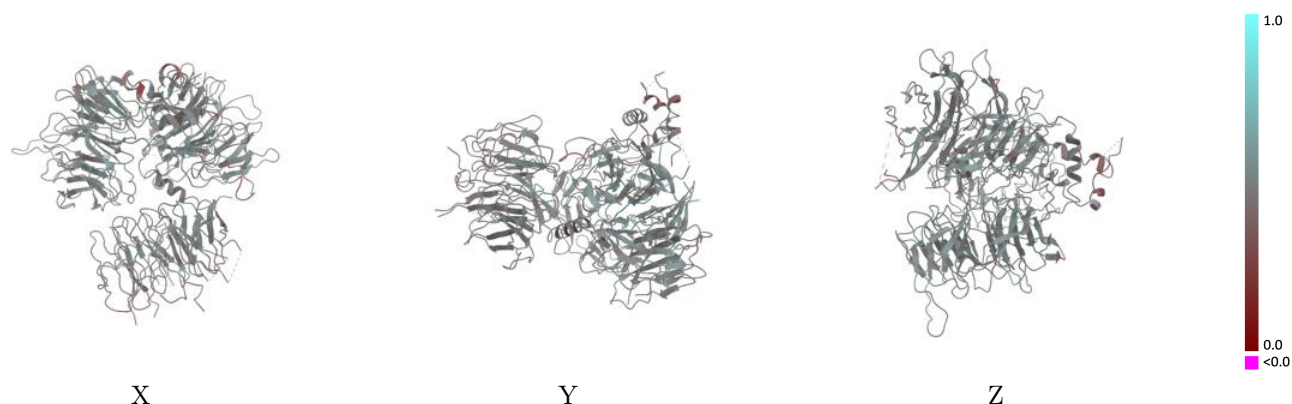
Y



Z

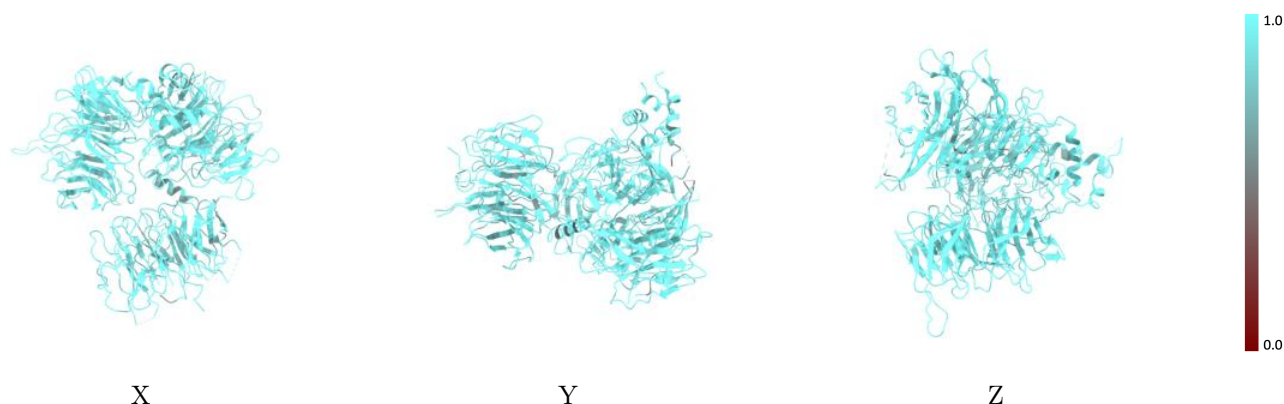
The images above show the 3D surface view of the map at the recommended contour level 0.192 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



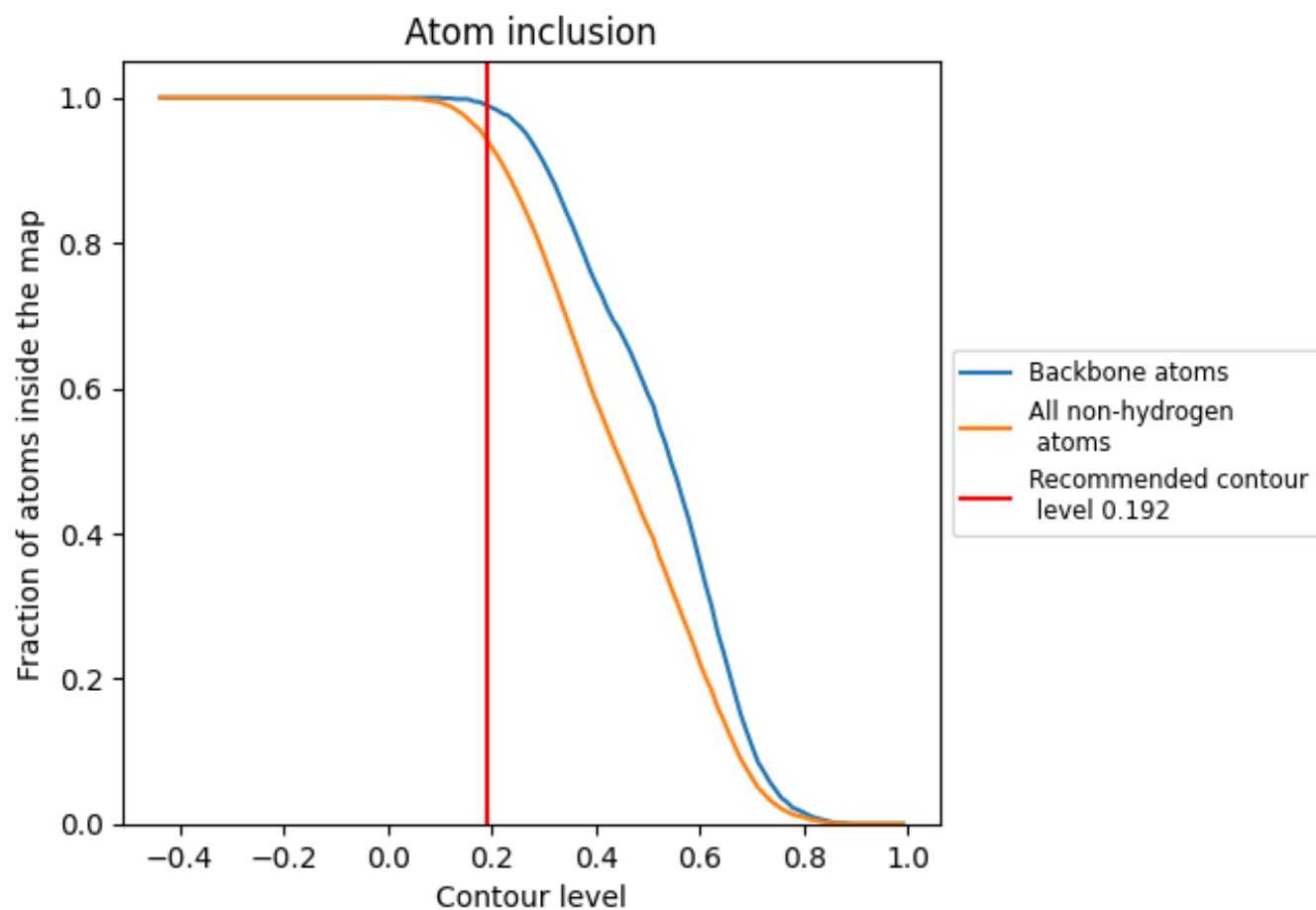
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.192).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.192) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9410	<div></div> 0.4820
A	<div></div> 0.9530	<div></div> 0.4890
B	<div></div> 0.9180	<div></div> 0.4680
E	<div></div> 0.8850	<div></div> 0.4250

