



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 06:05 am GMT

PDB ID : 6YVD
EMDB ID : EMD-10944
Title : Head segment of the *S.cerevisiae* condensin holocomplex in presence of ATP
Authors : Merkel, F.; Haering, C.H.; Hassler, M.; Lee, B.G.; Loewe, J.
Deposited on : 2020-04-28
Resolution : 7.60 Å(reported)

This is a Full wwPDB EM Validation 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

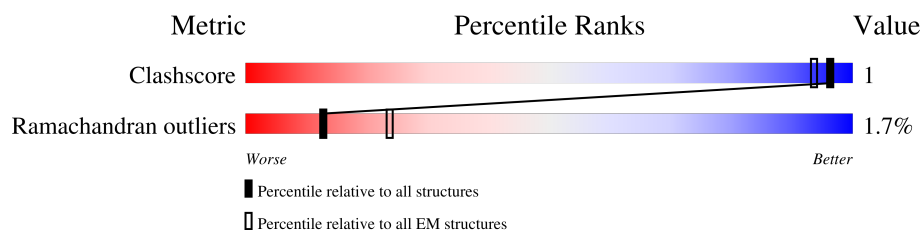
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.60 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	158937	4297
Ramachandran outliers	154571	4023

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	B	811	
2	A	1035	
3	C	1170	
4	D	1478	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8732 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Condensin complex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	B	101	Total	C	N	O	0	0
			502	300	101	101		

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	755	LEU	-	expression tag	UNP P38170
B	756	VAL	-	expression tag	UNP P38170
B	757	GLY	-	expression tag	UNP P38170
B	758	GLY	-	expression tag	UNP P38170
B	759	GLY	-	expression tag	UNP P38170
B	760	HIS	-	expression tag	UNP P38170
B	761	HIS	-	expression tag	UNP P38170
B	762	HIS	-	expression tag	UNP P38170
B	763	HIS	-	expression tag	UNP P38170
B	764	HIS	-	expression tag	UNP P38170
B	765	HIS	-	expression tag	UNP P38170
B	766	GLY	-	expression tag	UNP P38170
B	767	GLY	-	expression tag	UNP P38170
B	768	HIS	-	expression tag	UNP P38170
B	769	HIS	-	expression tag	UNP P38170
B	770	HIS	-	expression tag	UNP P38170
B	771	HIS	-	expression tag	UNP P38170
B	772	HIS	-	expression tag	UNP P38170
B	773	HIS	-	expression tag	UNP P38170
B	774	GLY	-	expression tag	UNP P38170
B	775	GLY	-	expression tag	UNP P38170
B	776	ARG	-	expression tag	UNP P38170
B	777	ILE	-	expression tag	UNP P38170
B	778	PHE	-	expression tag	UNP P38170
B	779	TYR	-	expression tag	UNP P38170
B	780	PRO	-	expression tag	UNP P38170
B	781	TYR	-	expression tag	UNP P38170
B	782	ASP	-	expression tag	UNP P38170

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

- Molecule 2 is a protein called Condensin complex subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	A	799	Total	C	N	O	0	0
			3974	2376	799	799		

- Molecule 3 is a protein called Structural maintenance of chromosomes protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	446	Total	C	N	O	0	0
			2207	1315	446	446		

- Molecule 4 is a protein called Structural maintenance of chromosomes protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	414	Total 2049	C 1221	N 414	O 414	0	0

There are 71 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	14	ALA	SER	conflict	UNP Q12267
D	30	GLU	ASP	conflict	UNP Q12267
D	143	SER	ARG	conflict	UNP Q12267
D	425	ARG	LYS	conflict	UNP Q12267
D	546	ASP	ASN	conflict	UNP Q12267
D	697	ALA	VAL	conflict	UNP Q12267
D	704	ILE	VAL	conflict	UNP Q12267
D	1028	ASN	ASP	conflict	UNP Q12267
D	1052	THR	ASN	conflict	UNP Q12267
D	1165	ASP	ALA	conflict	UNP Q12267
D	1177	VAL	ILE	conflict	UNP Q12267
D	1419	ARG	-	expression tag	UNP Q12267
D	1420	ILE	-	expression tag	UNP Q12267
D	1421	PRO	-	expression tag	UNP Q12267
D	1422	GLY	-	expression tag	UNP Q12267
D	1423	LEU	-	expression tag	UNP Q12267
D	1424	ILE	-	expression tag	UNP Q12267
D	1425	ASN	-	expression tag	UNP Q12267
D	1426	GLY	-	expression tag	UNP Q12267
D	1427	ALA	-	expression tag	UNP Q12267
D	1428	THR	-	expression tag	UNP Q12267
D	1429	GLY	-	expression tag	UNP Q12267
D	1430	TRP	-	expression tag	UNP Q12267
D	1431	SER	-	expression tag	UNP Q12267
D	1432	HIS	-	expression tag	UNP Q12267
D	1433	PRO	-	expression tag	UNP Q12267
D	1434	GLN	-	expression tag	UNP Q12267
D	1435	PHE	-	expression tag	UNP Q12267
D	1436	GLU	-	expression tag	UNP Q12267
D	1437	LYS	-	expression tag	UNP Q12267
D	1438	ALA	-	expression tag	UNP Q12267
D	1439	GLY	-	expression tag	UNP Q12267
D	1440	GLY	-	expression tag	UNP Q12267
D	1441	GLY	-	expression tag	UNP Q12267
D	1442	SER	-	expression tag	UNP Q12267
D	1443	GLY	-	expression tag	UNP Q12267

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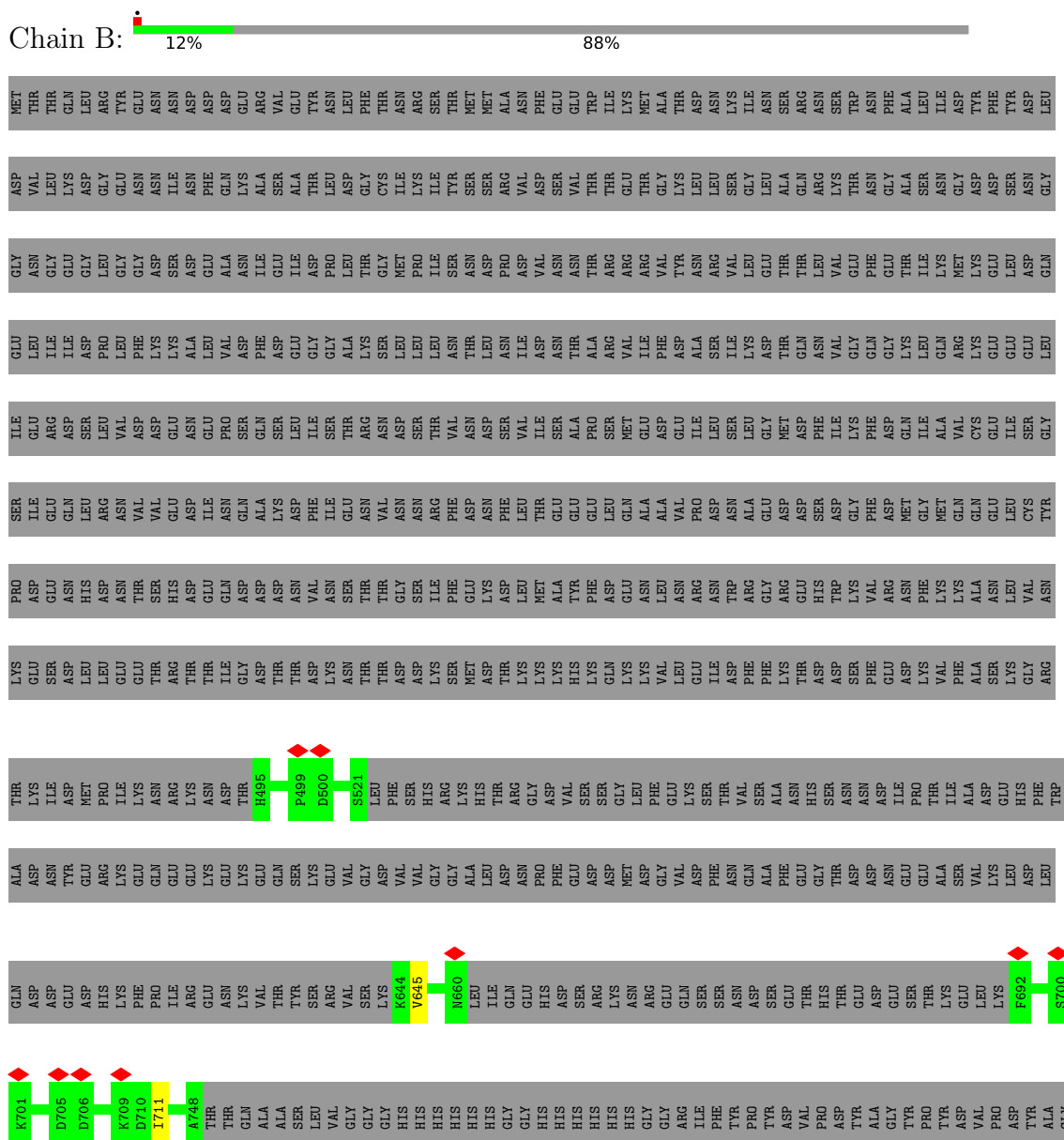
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1444	GLY	-	expression tag	UNP Q12267
D	1445	GLY	-	expression tag	UNP Q12267
D	1446	SER	-	expression tag	UNP Q12267
D	1447	GLY	-	expression tag	UNP Q12267
D	1448	GLY	-	expression tag	UNP Q12267
D	1449	GLY	-	expression tag	UNP Q12267
D	1450	SER	-	expression tag	UNP Q12267
D	1451	TRP	-	expression tag	UNP Q12267
D	1452	SER	-	expression tag	UNP Q12267
D	1453	HIS	-	expression tag	UNP Q12267
D	1454	PRO	-	expression tag	UNP Q12267
D	1455	GLN	-	expression tag	UNP Q12267
D	1456	PHE	-	expression tag	UNP Q12267
D	1457	GLU	-	expression tag	UNP Q12267
D	1458	LYS	-	expression tag	UNP Q12267
D	1459	GLY	-	expression tag	UNP Q12267
D	1460	GLY	-	expression tag	UNP Q12267
D	1461	GLY	-	expression tag	UNP Q12267
D	1462	SER	-	expression tag	UNP Q12267
D	1463	GLY	-	expression tag	UNP Q12267
D	1464	GLY	-	expression tag	UNP Q12267
D	1465	GLY	-	expression tag	UNP Q12267
D	1466	SER	-	expression tag	UNP Q12267
D	1467	GLY	-	expression tag	UNP Q12267
D	1468	GLY	-	expression tag	UNP Q12267
D	1469	GLY	-	expression tag	UNP Q12267
D	1470	SER	-	expression tag	UNP Q12267
D	1471	TRP	-	expression tag	UNP Q12267
D	1472	SER	-	expression tag	UNP Q12267
D	1473	HIS	-	expression tag	UNP Q12267
D	1474	PRO	-	expression tag	UNP Q12267
D	1475	GLN	-	expression tag	UNP Q12267
D	1476	PHE	-	expression tag	UNP Q12267
D	1477	GLU	-	expression tag	UNP Q12267
D	1478	LYS	-	expression tag	UNP Q12267

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: Condensin complex subunit 2







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	87744	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 ($e^-/\text{\AA}^2$)	45	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	0.209	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	244.79999, 244.79999, 244.79999	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.448, 2.448, 2.448	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	B	0.30	0/499	0.48	0/692
2	A	0.29	0/3966	0.47	0/5527
3	C	0.30	0/2205	0.50	0/3070
4	D	0.31	0/2047	0.52	0/2850
All	All	0.29	0/8717	0.49	0/12139

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
2	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	614	THR	Peptide

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	B	502	0	206	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3974	0	1747	0	0
3	C	2207	0	970	3	0
4	D	2049	0	899	7	0
All	All	8732	0	3822	10	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.

All (10) 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:C:146:MET:CB	3:C:1114:VAL:CB	2.73	0.66
3:C:1036:VAL:O	3:C:1040:PHE:N	2.33	0.61
4:D:1291:ALA:O	4:D:1292:GLU:CB	2.53	0.56
3:C:1049:PRO:O	3:C:1050:ASN:CB	2.57	0.53
4:D:211:GLN:O	4:D:212:ASP:CB	2.62	0.47
4:D:1323:LEU:O	4:D:1325:GLY:N	2.48	0.47
4:D:1374:LYS:O	4:D:1375:ASN:CB	2.65	0.44
4:D:1289:GLY:O	4:D:1290:ASN:CB	2.65	0.43
4:D:1299:LEU:O	4:D:1300:ASP:CB	2.68	0.41
4:D:1355:ALA:O	4:D:1356:ALA:HB3	2.21	0.41

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	B	95/811 (12%)	89 (94%)	4 (4%)	2 (2%)	7	36
2	A	783/1035 (76%)	753 (96%)	29 (4%)	1 (0%)	51	86
3	C	442/1170 (38%)	377 (85%)	54 (12%)	11 (2%)	5	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	410/1478 (28%)	337 (82%)	58 (14%)	15 (4%)	3	24
All	All	1730/4494 (38%)	1556 (90%)	145 (8%)	29 (2%)	13	42

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	981	LYS
3	C	982	VAL
3	C	983	ASN
3	C	1115	ASP
4	D	175	PRO
4	D	253	LYS
4	D	289	GLU
4	D	294	ASP
4	D	1291	ALA
4	D	1292	GLU
4	D	1300	ASP
4	D	1324	SER
1	B	711	ILE
2	A	787	VAL
3	C	117	ILE
3	C	1050	ASN
4	D	212	ASP
4	D	1290	ASN
3	C	10	GLY
3	C	12	LYS
3	C	26	GLN
4	D	272	ILE
4	D	336	TYR
4	D	1375	ASN
1	B	645	VAL
3	C	1017	THR
4	D	244	SER
4	D	160	VAL
3	C	74	VAL

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 monosaccharides 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.

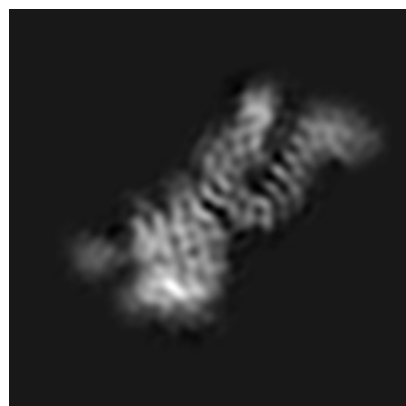
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10944. These allow visual inspection of the internal detail of the map and identification of artifacts.

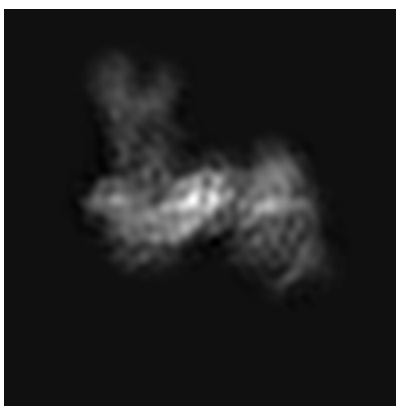
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

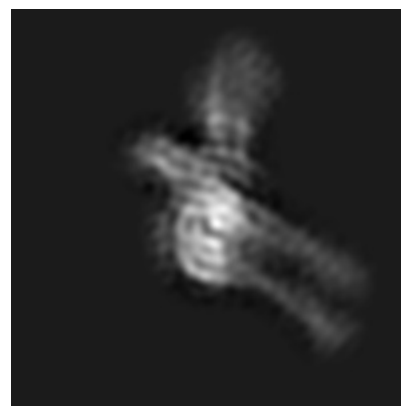
6.1.1 Primary map



X

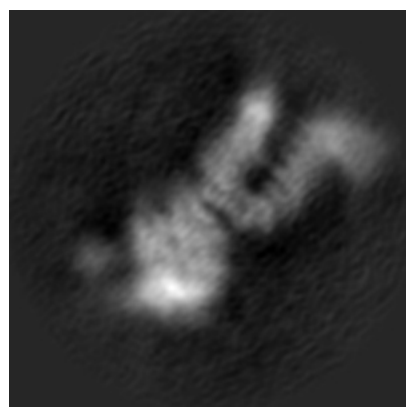


Y

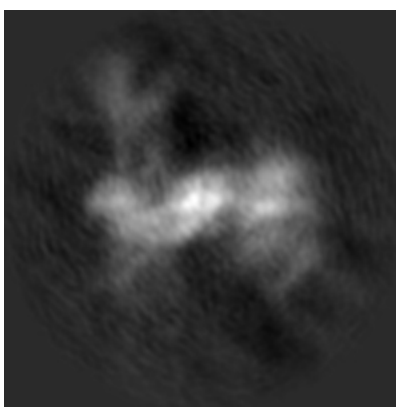


Z

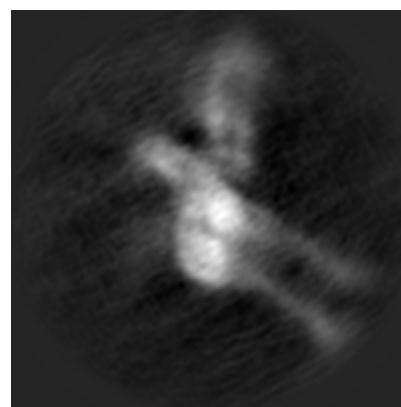
6.1.2 Raw map



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: 50

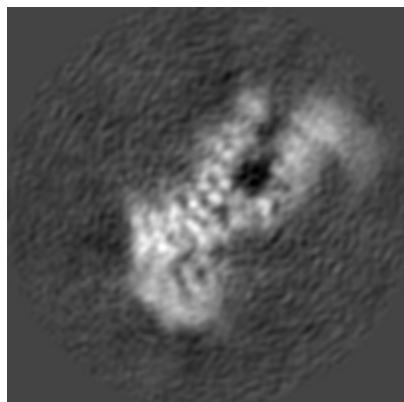


Y Index: 50

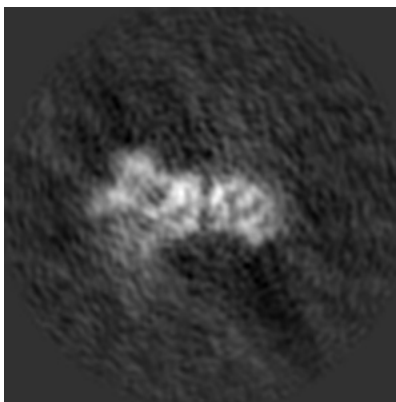


Z Index: 50

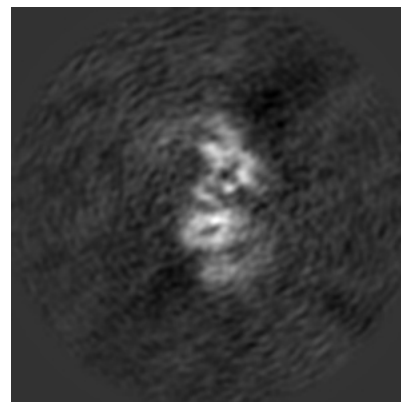
6.2.2 Raw map



X Index: 50



Y Index: 50



Z Index: 50

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: 51

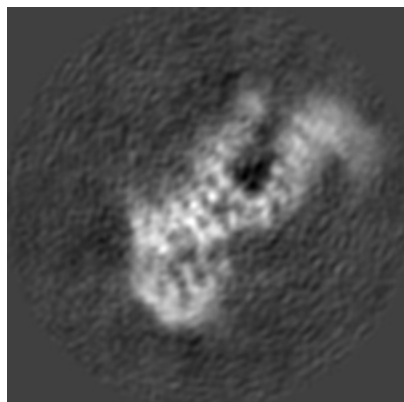


Y Index: 41

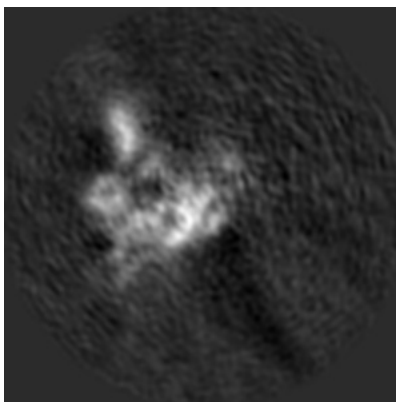


Z Index: 44

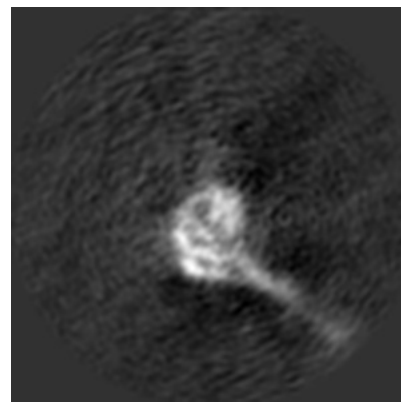
6.3.2 Raw map



X Index: 51



Y Index: 42

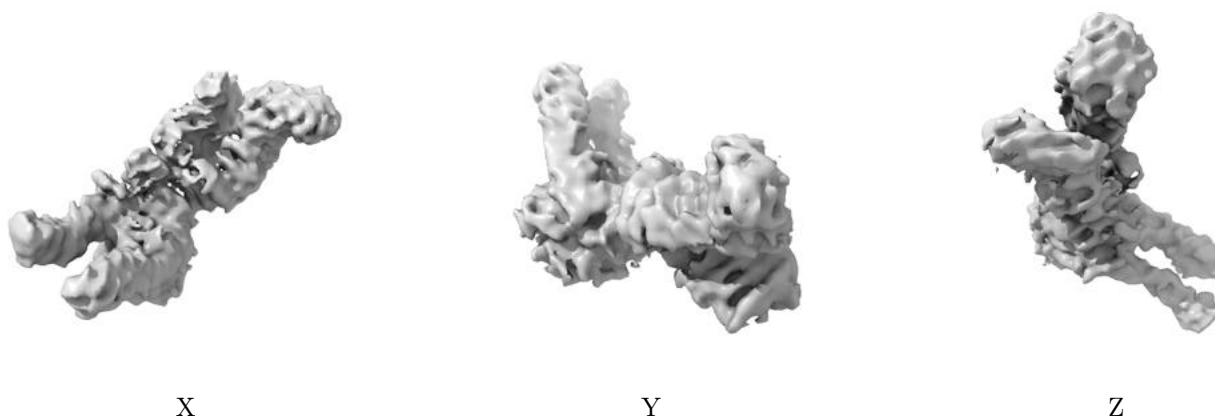


Z Index: 43

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

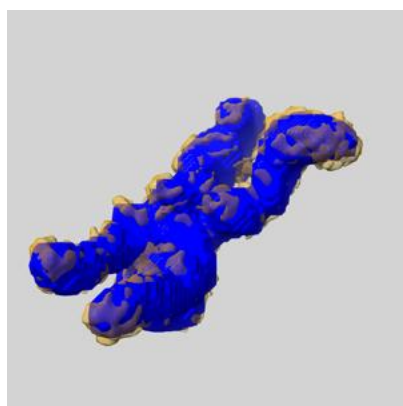
6.5 Mask visualisation [i](#)

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

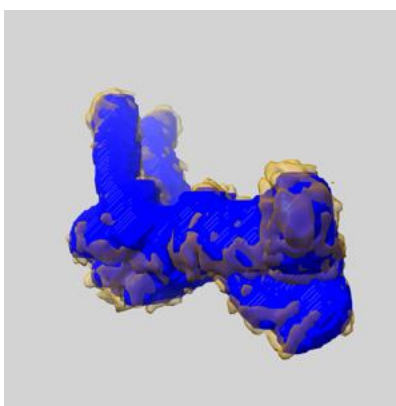
A mask typically either:

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

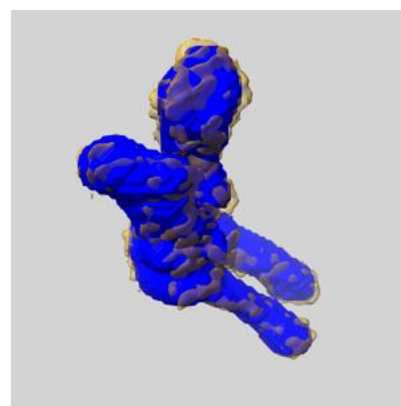
6.5.1 emd_10944_msk_1.map [i](#)



X



Y

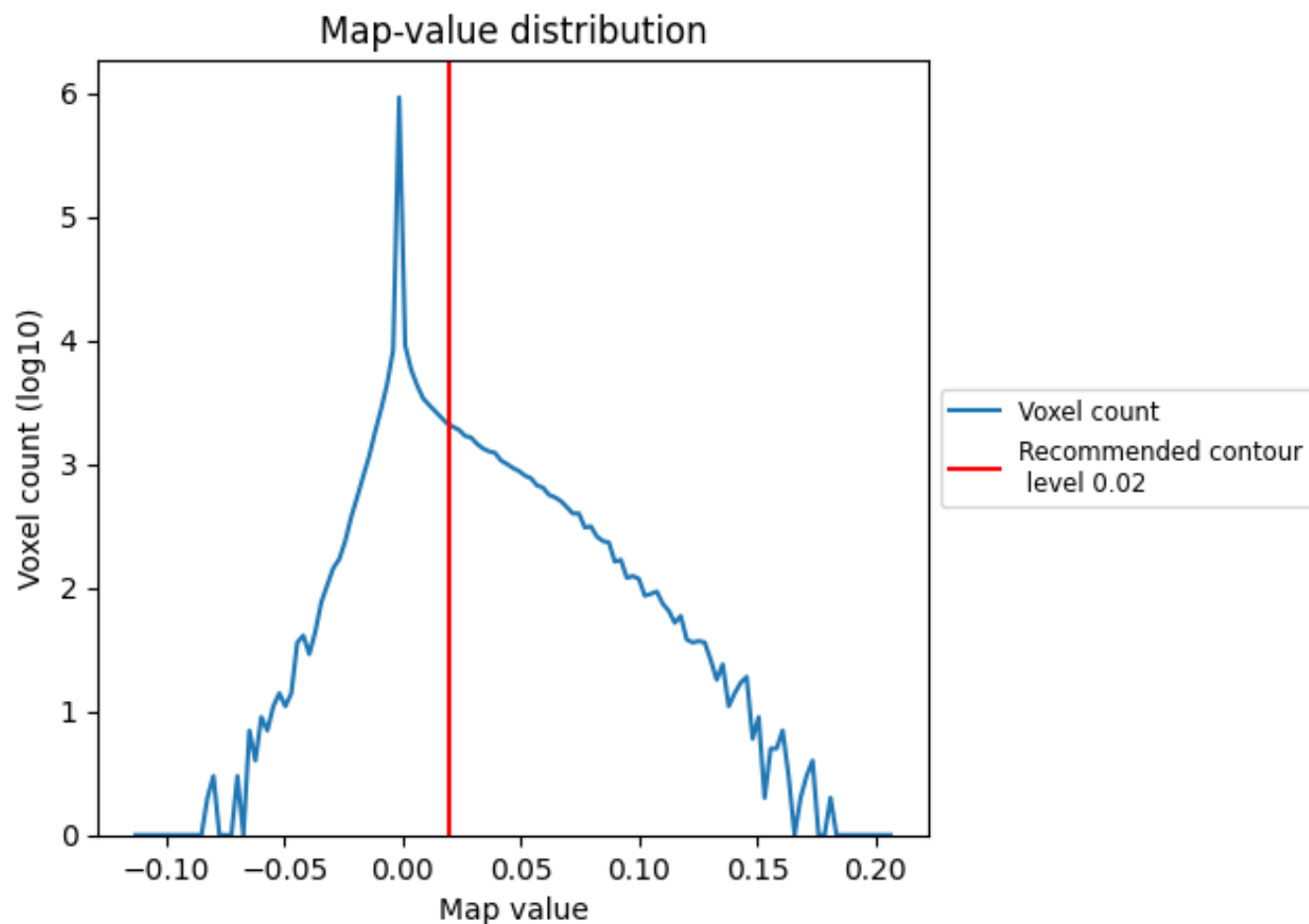


Z

7 Map analysis [i](#)

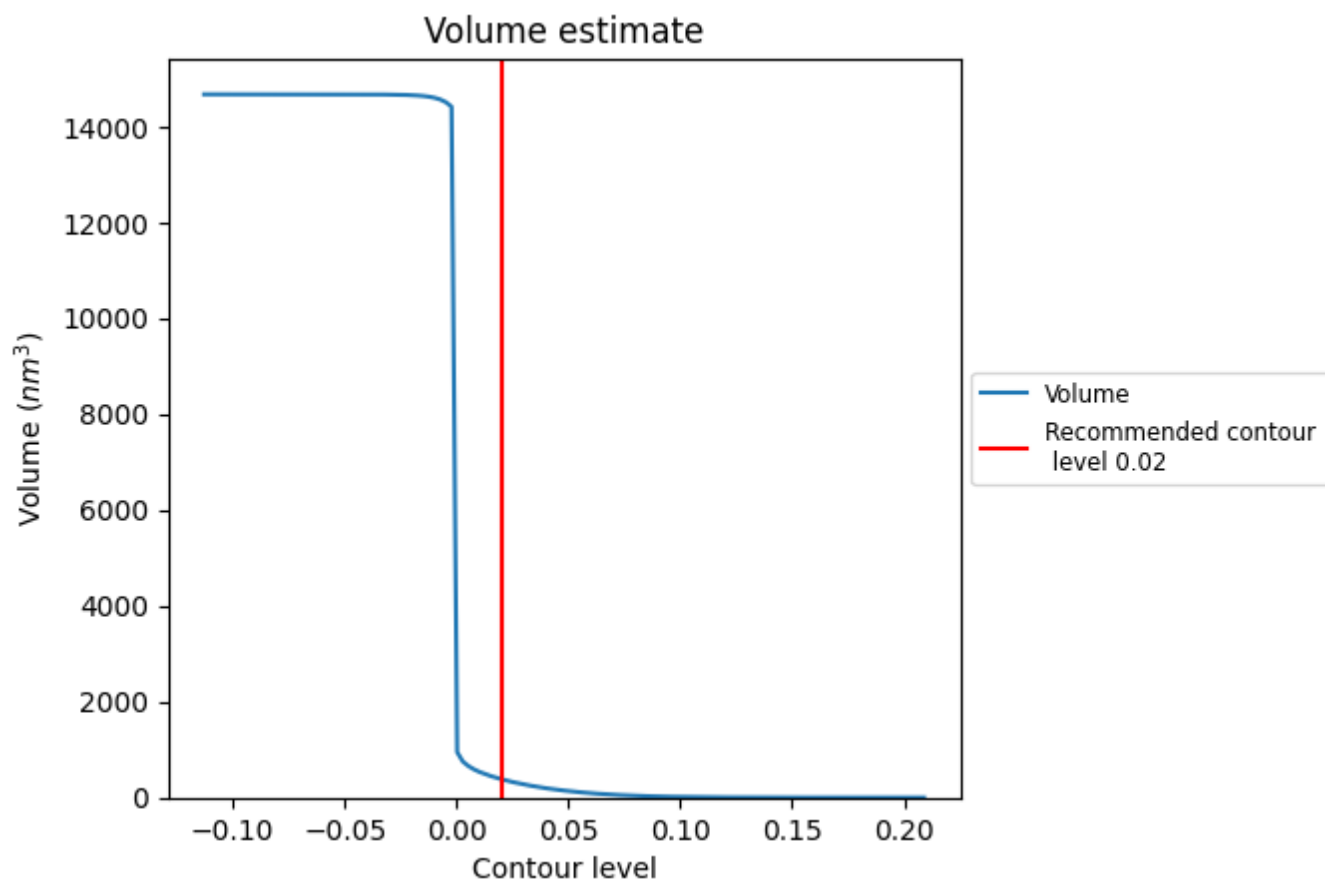
This section contains the results of statistical analysis of the map.

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.

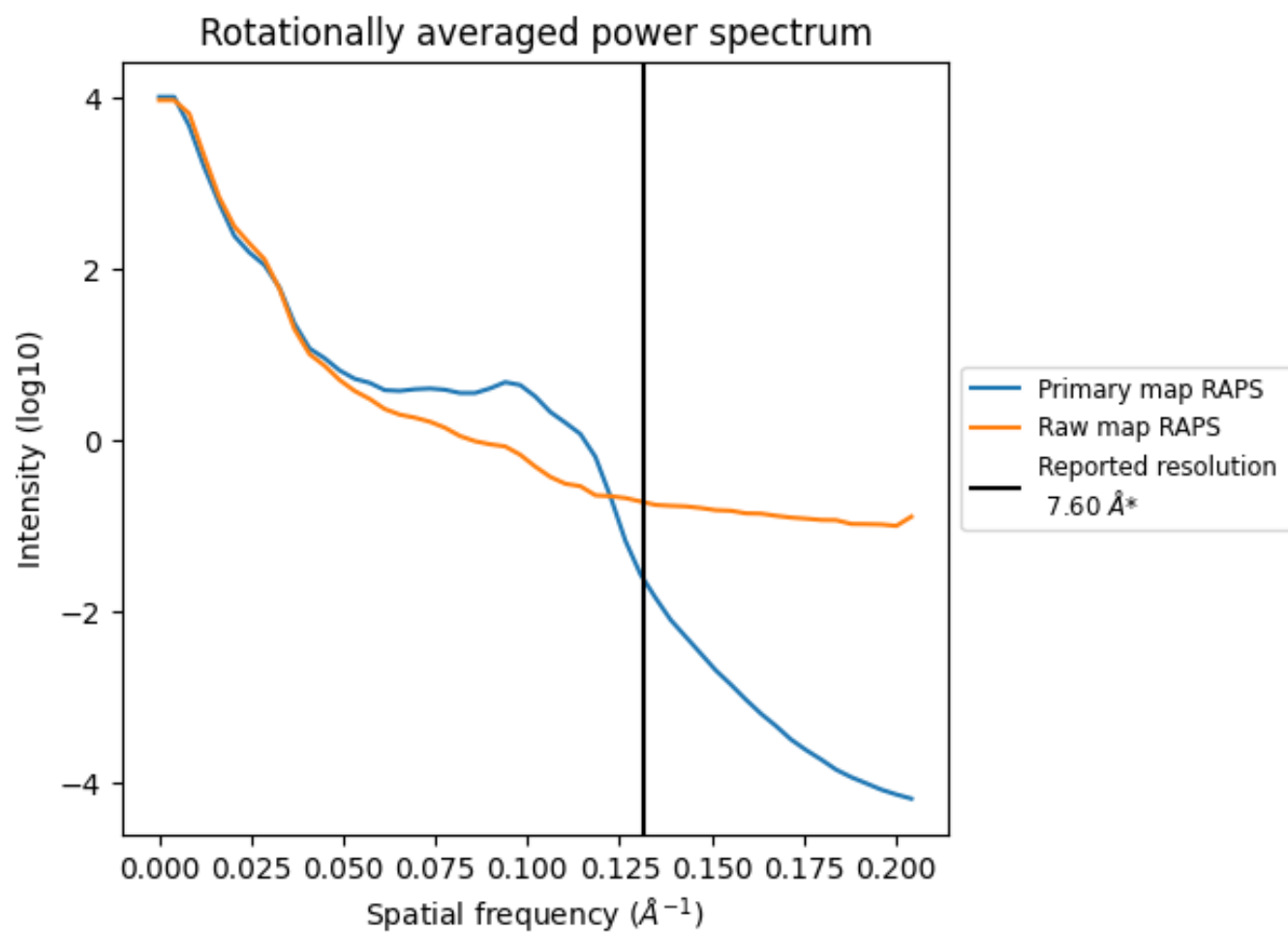
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 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 ⓘ

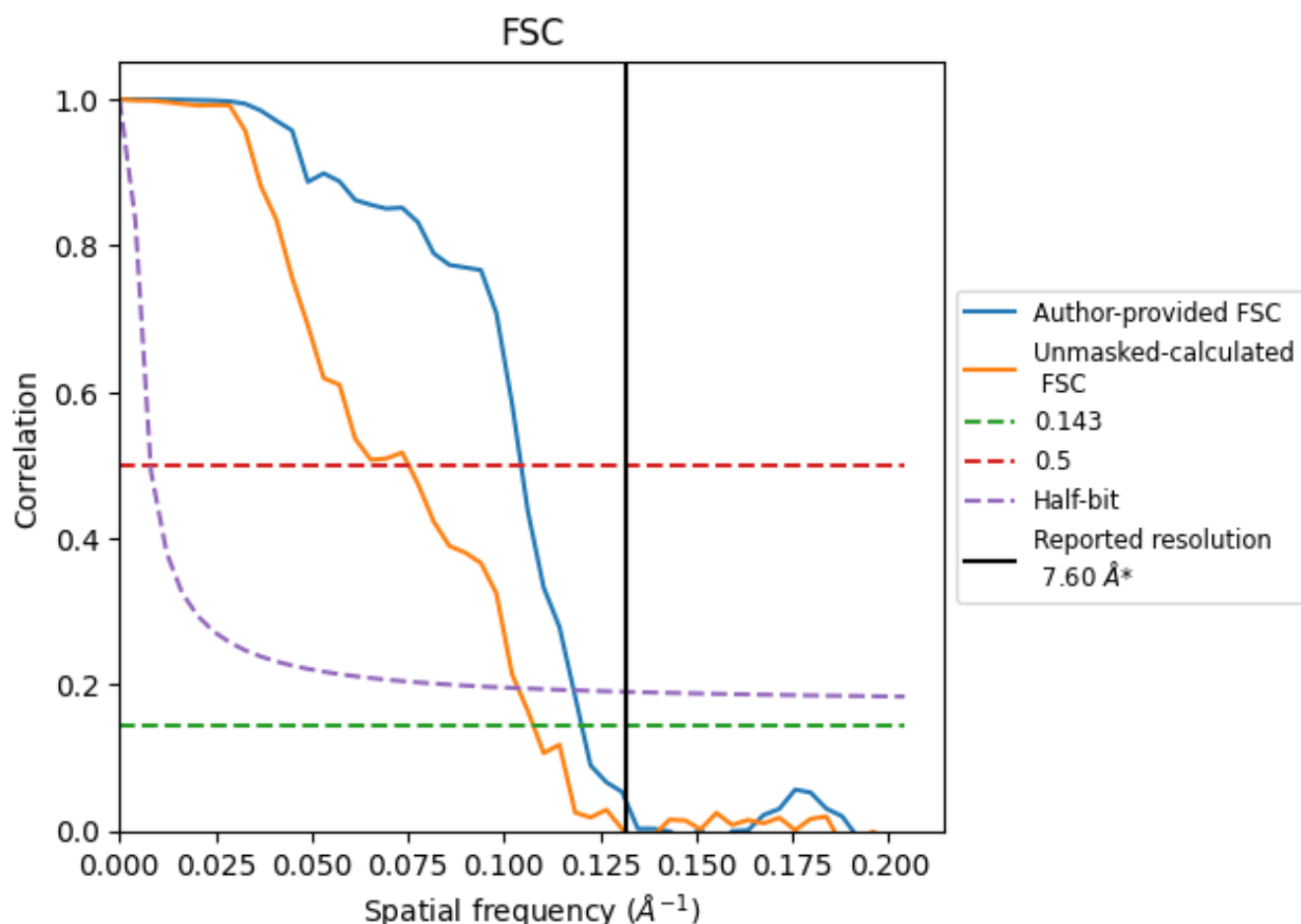


*Reported resolution corresponds to spatial frequency of 0.132 Å⁻¹

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 0.132 Å⁻¹

8.2 Resolution estimates [i](#)

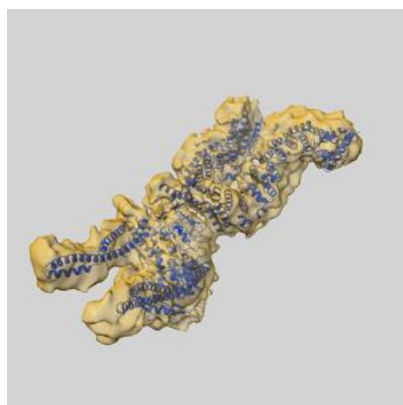
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.60	-	-
Author-provided FSC curve	8.32	9.58	8.47
Unmasked-calculated*	9.29	13.30	9.65

*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 9.29 differs from the reported value 7.6 by more than 10 %

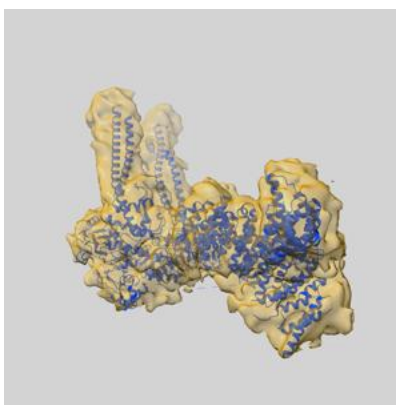
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10944 and PDB model 6YVD. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

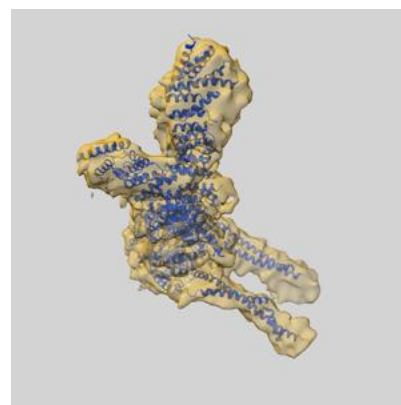
9.1 Map-model overlay [i](#)



X



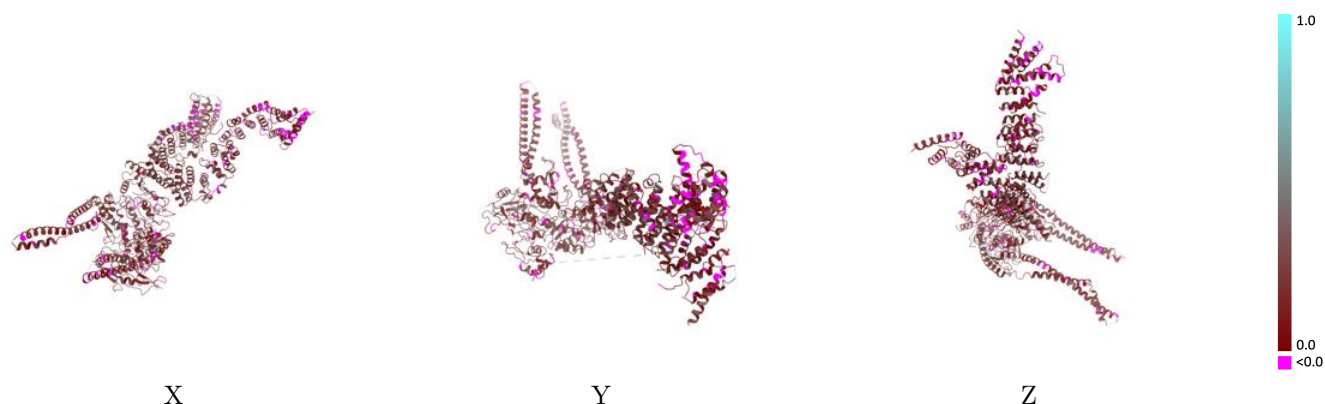
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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](#)



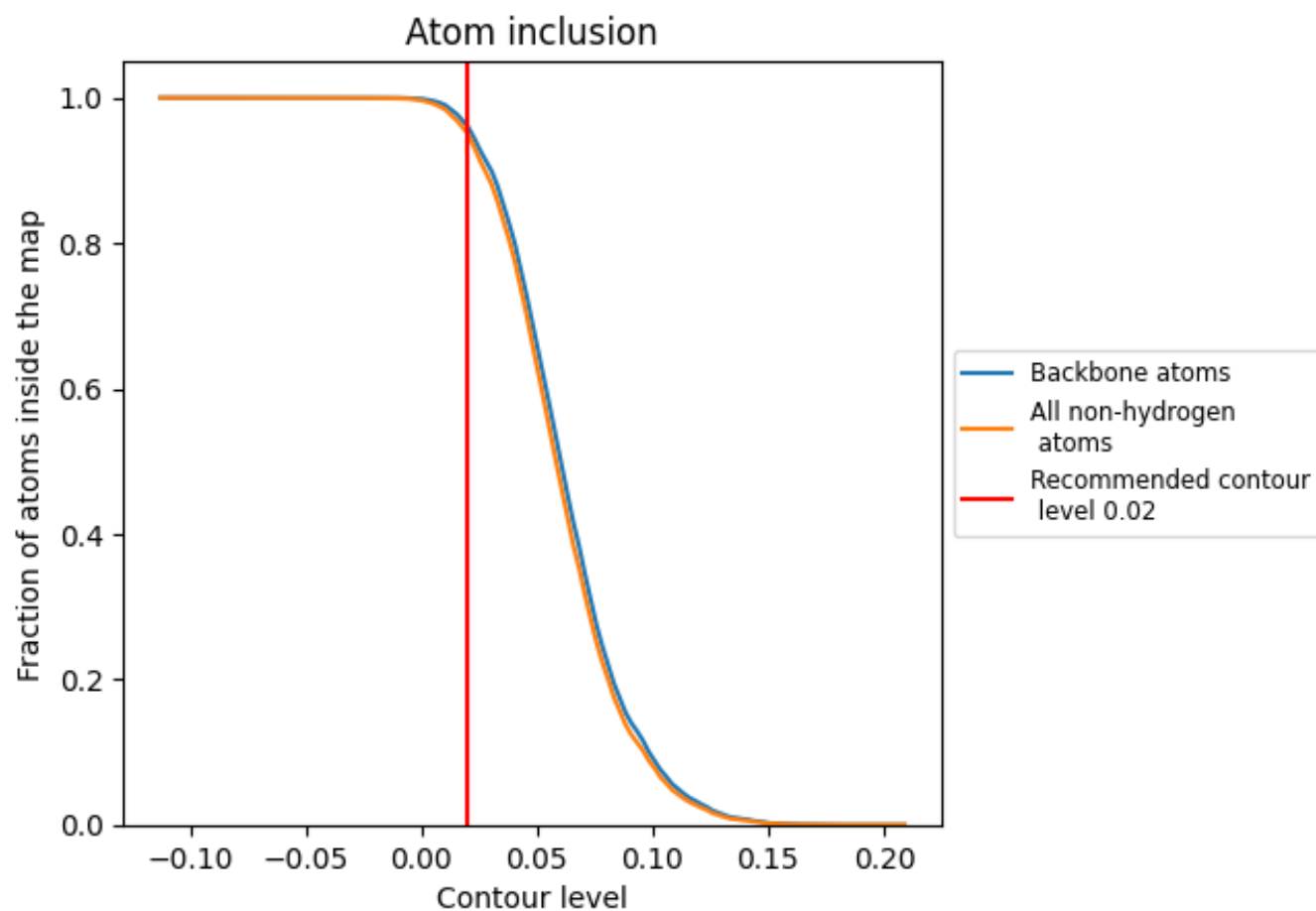
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9508	<div></div> 0.1600
A	<div></div> 0.9333	<div></div> 0.1480
B	<div></div> 0.8765	<div></div> 0.1560
C	<div></div> 0.9805	<div></div> 0.1740
D	<div></div> 0.9707	<div></div> 0.1670

