



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:59 PM UTC

PDB ID : 9CYX / pdb_00009cyx
EMDB ID : EMD-46053
Title : Cryo-EM structure of MRV full core
Authors : Liu, X.Y.; Xia, X.; Martynowycz, M.W.; Gonen, T.; Zhou, Z.H.
Deposited on : 2024-08-02
Resolution : 3.30 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:

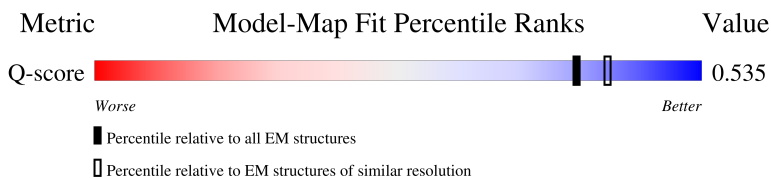
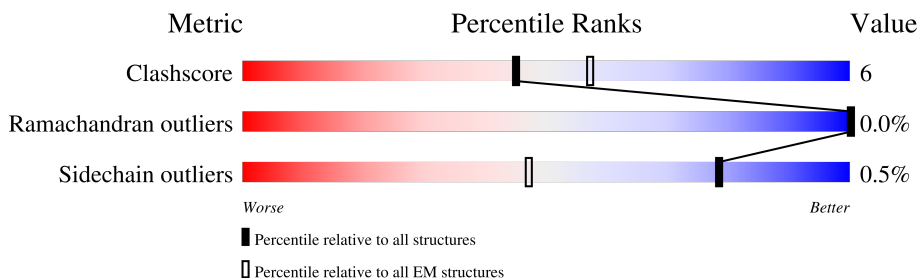
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.30 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	15087 (2.80 - 3.80)

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	1275	 10% 89%
1	H	1275	 70% 11% 19%
1	I	1275	 76% 9% 15%
2	A	1288	 66% 77% 22%

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Mol	Chain	Length	Quality of chain
3	Q	417	 88% 11%
3	R	417	 7% 88% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34537 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 Lambda 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	1034	Total	C	N	O	S	0	0
			8164	5220	1378	1517	49		
1	I	1085	Total	C	N	O	S	0	0
			8562	5471	1450	1590	51		
1	B	140	Total	C	N	O	S	0	0
			1050	622	198	226	4		

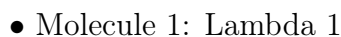
- Molecule 2 is a protein called Outer capsid protein lambda-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1284	Total	C	N	O	S	0	0
			10127	6468	1700	1917	42		

- Molecule 3 is a protein called Inner capsid protein sigma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	417	Total	C	N	O	S	0	0
			3317	2096	599	605	17		
3	R	417	Total	C	N	O	S	0	0
			3317	2096	599	605	17		

Frequency	Percentage
Daily	76%
Weekly	9%
Monthly	15%



A horizontal bar chart with a grey background. The x-axis represents percentages from 0% to 100%. A green bar extends to the 89% mark. Above the bar, there are two small red squares and one small yellow square. Below the bar, the text '10%' is positioned at the start of the green bar, and '89%' is positioned at the end of the green bar.

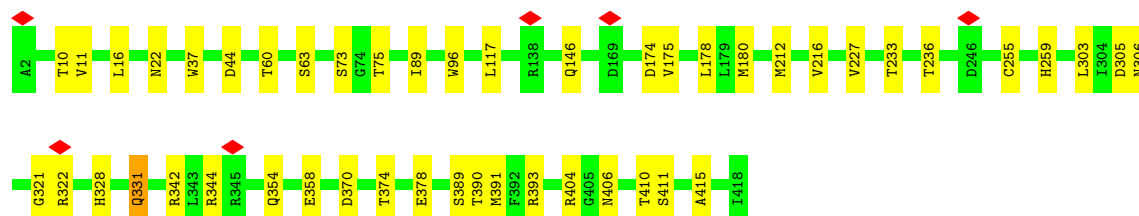
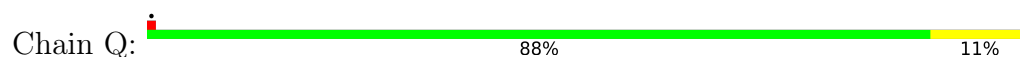
Response	Percentage
Yes	89%
No	10%



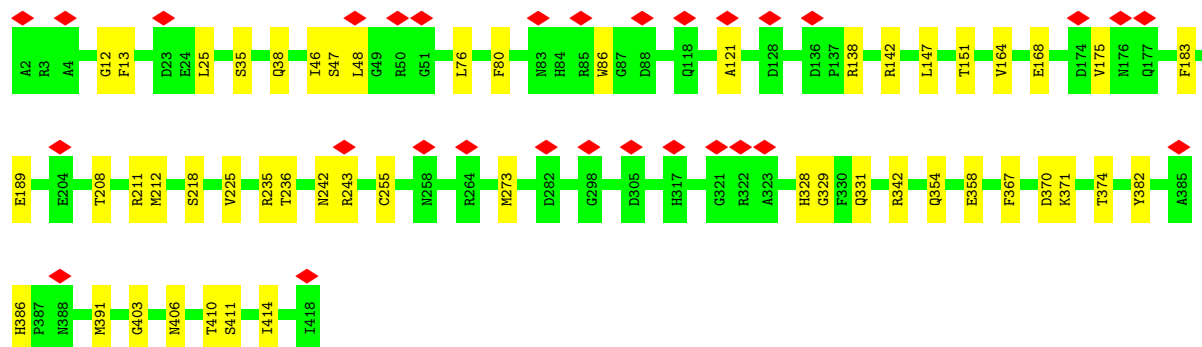
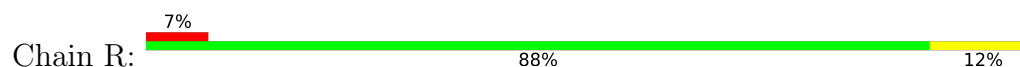
A1096	V1036	P975	T854	V793	G729	Q660	L594	Q526	P457	D389	T298
G1097	G1037	N976	A855	L794	L730	H661	V595	P527	D458	D389	S305
I1098	Q1038	C977	Q856	F795	C731	S662	E596	L528	T459	S392	N310
Y1099	M1039	S978	P857	E796	A732	S663	S997	V529	Y460	Q395	G311
T1100	C1040	S979	S858	W797	W733	L664	L599	E531	G463	Y400	Y312
Q1102	S1041	T980	C859	W798	W734	T665	S900	P532	D464	T401	A315
A1103	L1042	W981	C980	S799	G735	W666	S601	W333	E465	I402	R320
L1104	V1043	W982	C800	G800	W736	T667	C602	Q535	G468	D403	Q321
L1105	I1044	W861	A801	S802	W737	S668	M603	G536	R469	Q404	R320
V1106	P1045	W863	S802	R803	R738	G669	H604	K537	S470	A405	Q321
G1106	G1046	R864	H804	W805	S740	F672	T606	I538	R476	A406	R325
S1107	F1047	F867	W805	C806	I743	F673	A607	S539	K477	M407	W326
M1108	M1048	L868	C806	L807	Y744	L674	P608	G540	V478	D408	L327
A1109	A1049	E869	L807	T808	E745	V675	G609	V541	I478	E409	S329
M1110	Q1050	L870	T808	W746	W746	D676	G610	P542	G479	G410	S329
P1111	D1051	D871	W809	S746	W747	H677	G610	F543	D480	D411	S332
W1112	V1052	W872	W810	H810	H747	F678	S611	P544	S482	L412	S332
S1113	F1053	R873	F813	F813	G748	Y679	F612	V547	L483	M413	D337
L1114	M1054	L873	E814	E814	A749	R680	V613	R548	V484	V414	E341
G1115	N1055	S874	W815	W815	R750	Y681	V614	K485	V484	S415	E341
S1116	C1055	D875	S816	S816	W751	T683	K615	D486	R486	R416	W345
F1117	Y1056	G876	S817	S817	L752	Y682	I616	G551	V489	L417	W345
M1118	F1057	W877	S818	S818	T753	T687	N617	Y552	V489	L417	W345
W1119	M1058	L878	A818	A818	T754	S688	F618	D553	L490	T418	E348
V1120	S1059	T879	W819	W819	T755	R689	F619	V554	K911	Q419	R349
D1120	A1060	C880	W820	W820	S756	R689	T620	A555	H492	L420	Y350
S1121	L1061	W881	D821	D821	R757	S693	R621	R556	A493	P421	Q352
P1122	A1062	R882	C822	C822	R757	S693	P622	G557	L422	L422	Y355
D1123	F1063	C833	D823	D823	A761	D698	V623	D561	R423	R423	Y355
W1124	S1064	D884	W824	W824	S762	W624	W624	L562	P424	P424	D356
D1125	T1065	T885	W825	W825	A763	D699	H625	A563	A496	R425	D356
I1126	E1066	W886	L826	L826	R764	G700	Y626	R564	I497	D425	S357
T1127	D1067	T887	L827	L827	R765	S701	Y626	R564	D498	I429	Y361
M1128	N1068	C888	D828	D828	W766	S702	K630	P567	P499	W430	V361
A1129	Q1069	W889	C829	C829	L769	V703	I631	S568	N500	W430	D362
M1130	A1070	L890	T830	T830	R770	I706	L632	G569	T501	D433	G363
P1131	L1011	S891	W831	W831	Y771	E707	P633	D570	G502	A434	A364
A1132	M1012	L892	P832	P832	L772	T708	N634	Y571	K503	L435	T365
Q1133	K1014	C893	E833	E833	P773	I709	I635	Q572	E504	S436	Q366
L1134	I1015	A895	K835	K835	L774	S710	T636	Y575	Y506	Y437	N373
D1135	M1016	A896	W836	W836	I775	S711	Y638	Y575	L506	Y438	Q374
F1136	P1017	A897	L837	L837	L776	I711	M639	D579	R507	Y439	L375
L1137	I1018	A898	E838	E838	D776	E712	L640	Q580	S508	D440	R376
T1138	M1019	A899	E839	E839	P777	W713	F644	V581	R509	Y441	L377
A1139	Q1078	E897	E839	E839	R778	P714	V645	V582	S511	M442	G378
G1140	F1079	K899	L839	L839	R779	G715	T646	D583	Q510	R443	M379
L1141	D1080	S900	W840	W840	S799	F716	N647	H584	V512	S444	R380
D1142	I1021	H901	T840	T840	L780	S717	N647	H584	A513	H445	I381
W1143	H1024	T902	A841	A841	E781	W719	E650	H585	G516	R446	A382
G1144	G1025	F903	T843	T843	Q783	W720	L651	H585	A519	V447	A383
T1145	L1026	D904	S844	S844	A784	T721	F652	D586	G520	V448	L384
F1146	P1027	A905	W846	W846	W785	Q721	F653	L588	H521	L449	Q385
E1147	M1028	A906	T847	T847	I787	A722	V654	L588	G520	L449	Q385
W1148	E1029	F907	C848	C848	I787	A723	A655	S889	H521	S450	S386
M1149	Q1030	Q908	W849	W849	L788	R724	A655	I590	S522	S450	S386
P1150	L1089	Q909	D850	D850	P789	I725	F656	S591	G523	E452	L387
G1151	D1090	C970	L910	L910	A790	G726	H659	S592	A524	L453	S388
W1151	M1091	R971	T851	T851	D791	I727	H659	G593	D525	P454	S388
F1152	V1092	T972	R852	R852	F792	S728	H659	G593	D525	P454	S388
L1153	F1093	A973	P853	P853	S728	S728	H659	G593	D525	P454	S388
M1154	S1094	W974	P853	P853	S728	S728	H659	G593	D525	P454	S388
T1155	D1095	W974	P853	P853	S728	S728	H659	G593	D525	P454	S388



• Molecule 3: Inner capsid protein sigma-2



• Molecule 3: Inner capsid protein sigma-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	10857	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	0.23	0/1060	0.41	0/1420
1	H	0.32	1/8385 (0.0%)	0.53	1/11486 (0.0%)
1	I	0.28	0/8795	0.47	0/12048
2	A	0.29	0/10385	0.49	0/14172
3	Q	0.25	0/3403	0.41	0/4634
3	R	0.24	0/3403	0.44	0/4634
All	All	0.29	1/35431 (0.0%)	0.48	1/48394 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	854	ARG	N-CA	5.08	1.49	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	854	ARG	CB-CA-C	-5.11	109.72	117.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	992	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1050	0	1035	10	0
1	H	8164	0	8082	93	0
1	I	8562	0	8451	71	0
2	A	10127	0	9910	211	0
3	Q	3317	0	3216	30	0
3	R	3317	0	3216	30	0
All	All	34537	0	33910	434	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 6.

The worst 5 of 434 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)
2:A:1237:GLU:HB2	2:A:1289:LEU:HB2	1.48	0.93
2:A:8:ARG:HB2	2:A:716:PHE:CD2	2.05	0.90
2:A:413:MET:SD	2:A:722:ALA:HB1	2.14	0.88
1:I:186:CYS:SG	1:I:199:HIS:NE2	2.48	0.86
1:H:1234:ILE:HD11	1:H:1242:PRO:HA	1.58	0.85

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	136/1275 (11%)	131 (96%)	5 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	1032/1275 (81%)	999 (97%)	33 (3%)	0	100	100
1	I	1081/1275 (85%)	1031 (95%)	50 (5%)	0	100	100
2	A	1280/1288 (99%)	1203 (94%)	76 (6%)	1 (0%)	48	75
3	Q	415/417 (100%)	403 (97%)	12 (3%)	0	100	100
3	R	415/417 (100%)	405 (98%)	10 (2%)	0	100	100
All	All	4359/5947 (73%)	4172 (96%)	186 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	850	ASP

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	B	115/1114 (10%)	115 (100%)	0	100	100
1	H	914/1114 (82%)	907 (99%)	7 (1%)	73	79
1	I	959/1114 (86%)	959 (100%)	0	100	100
2	A	1118/1120 (100%)	1108 (99%)	10 (1%)	70	78
3	Q	353/353 (100%)	352 (100%)	1 (0%)	86	86
3	R	353/353 (100%)	353 (100%)	0	100	100
All	All	3812/5168 (74%)	3794 (100%)	18 (0%)	78	83

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	984	LEU
3	Q	331	GLN
2	A	1248	CYS
2	A	387	LEU
2	A	847	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
3	Q	214	GLN
3	R	300	GLN
3	Q	300	GLN
3	R	114	GLN
3	R	328	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](#)

There are no chain breaks in this entry.

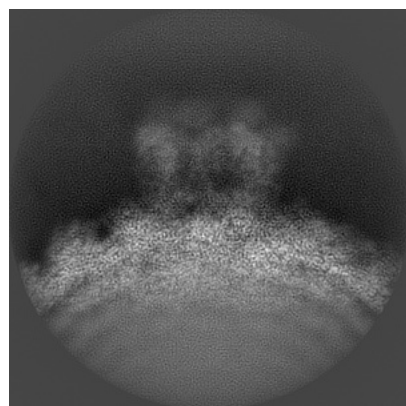
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46053. These allow visual inspection of the internal detail of the map and identification of artifacts.

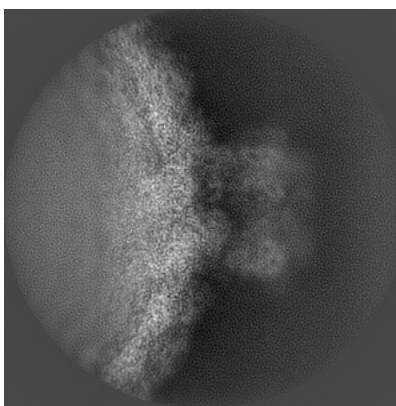
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

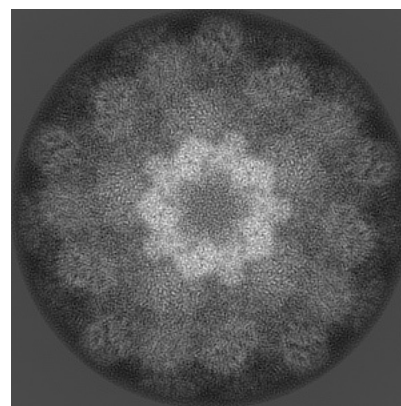
6.1.1 Primary map



X

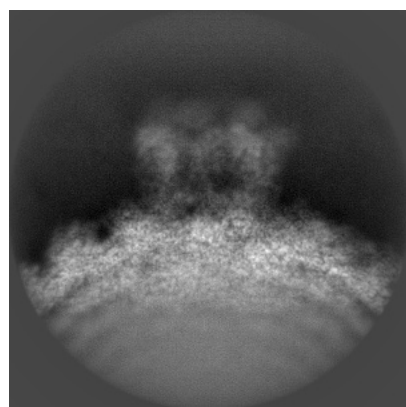


Y

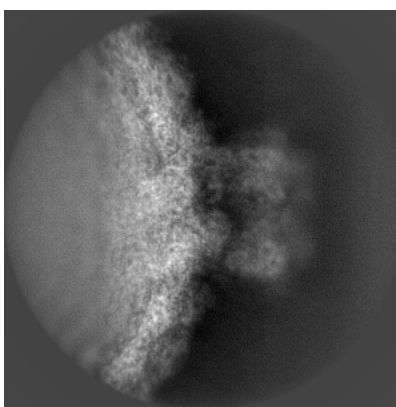


Z

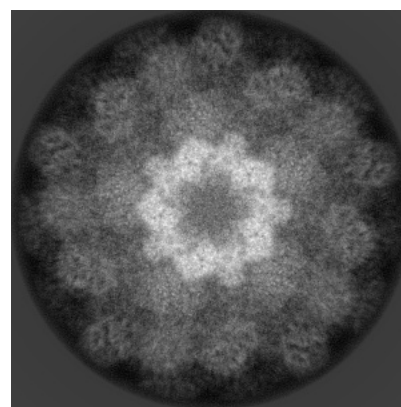
6.1.2 Raw map



X



Y

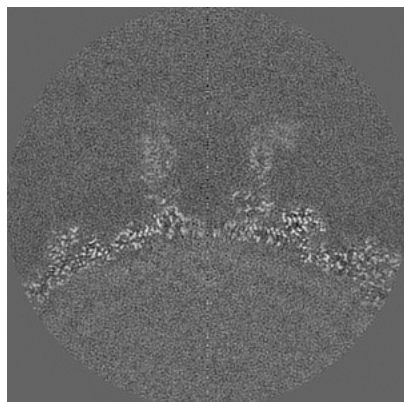


Z

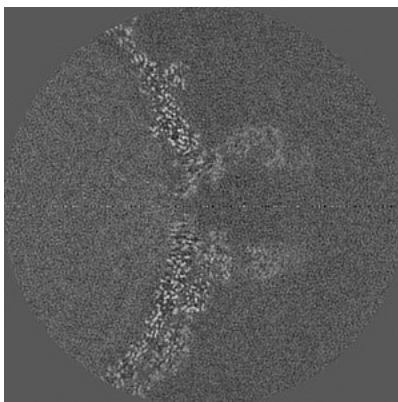
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

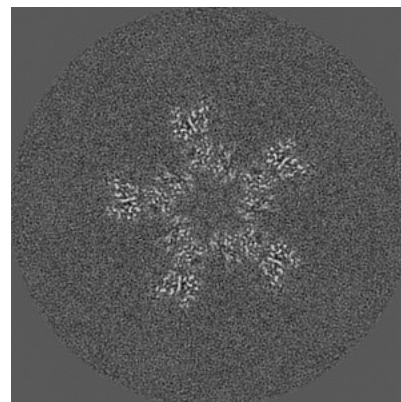
6.2.1 Primary map



X Index: 192

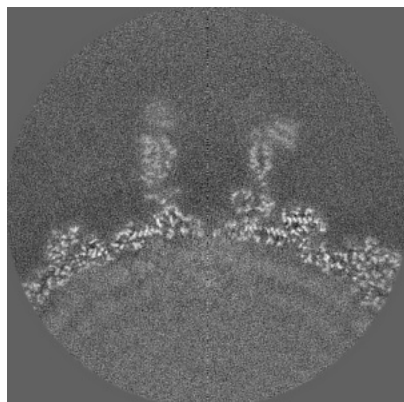


Y Index: 192

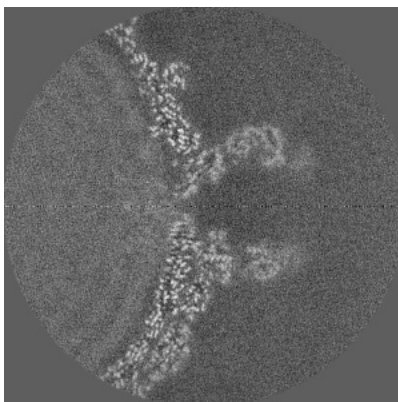


Z Index: 192

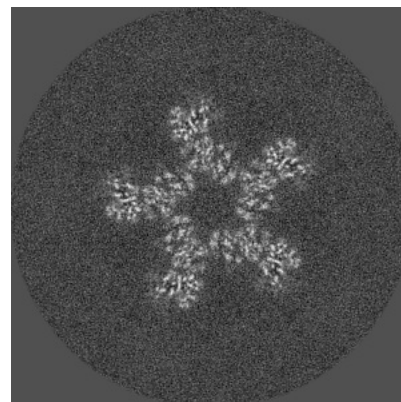
6.2.2 Raw map



X Index: 192



Y Index: 192

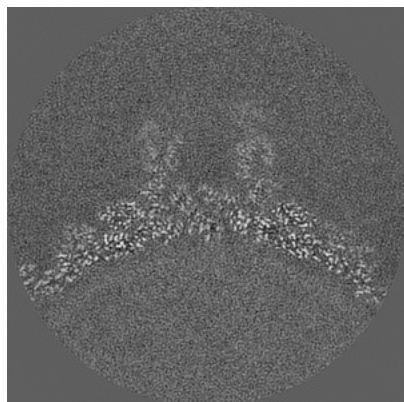


Z Index: 192

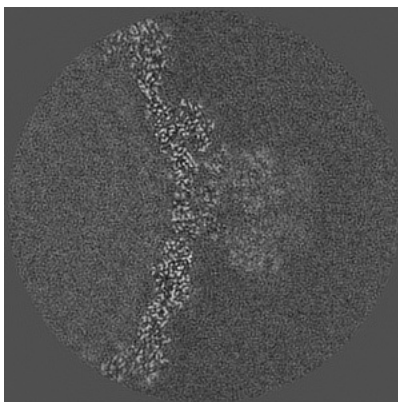
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

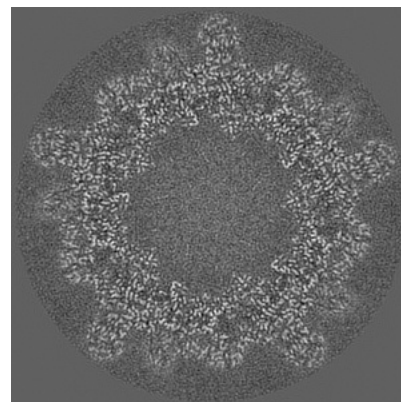
6.3.1 Primary map



X Index: 165

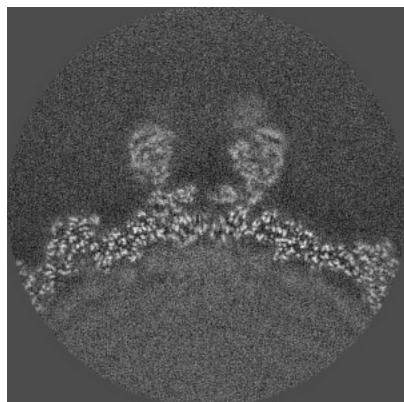


Y Index: 235

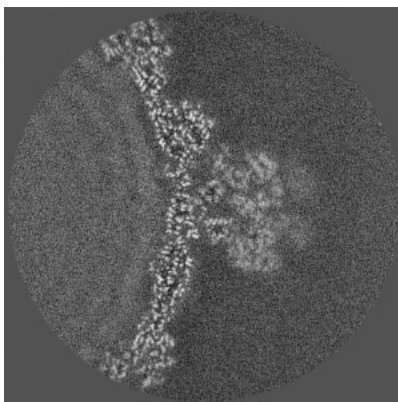


Z Index: 146

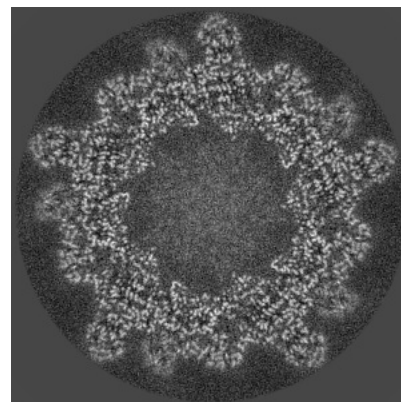
6.3.2 Raw map



X Index: 214



Y Index: 238

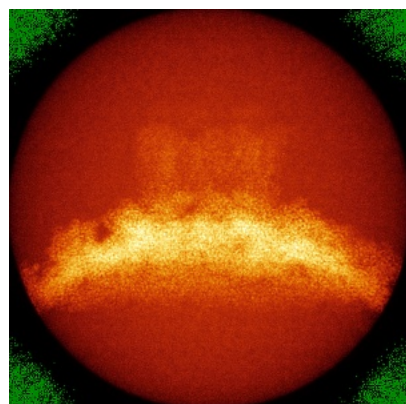


Z Index: 146

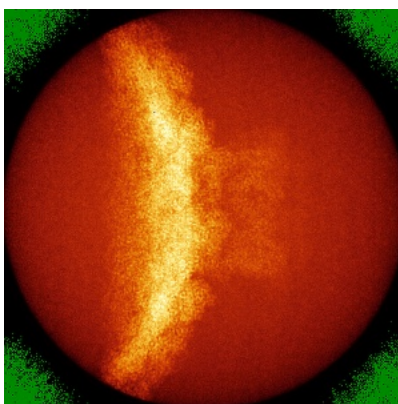
The images above show the largest variance slices of the map in three orthogonal directions.

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

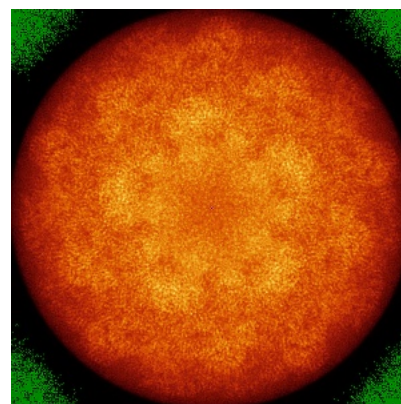
6.4.1 Primary map



X

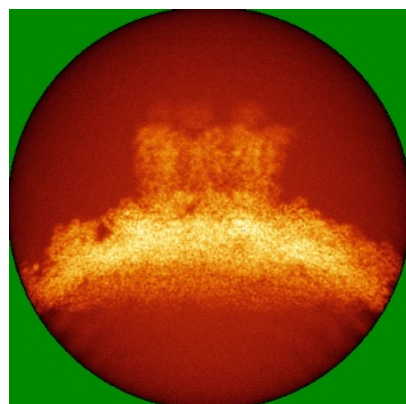


Y

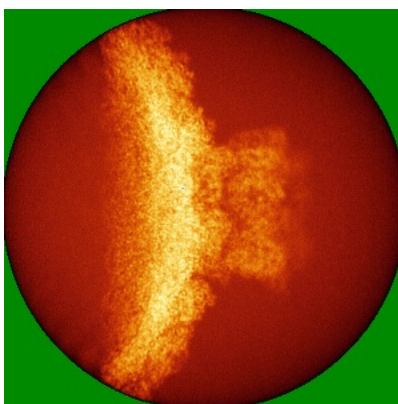


Z

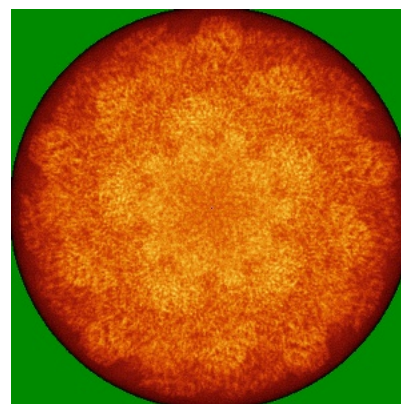
6.4.2 Raw map



X



Y

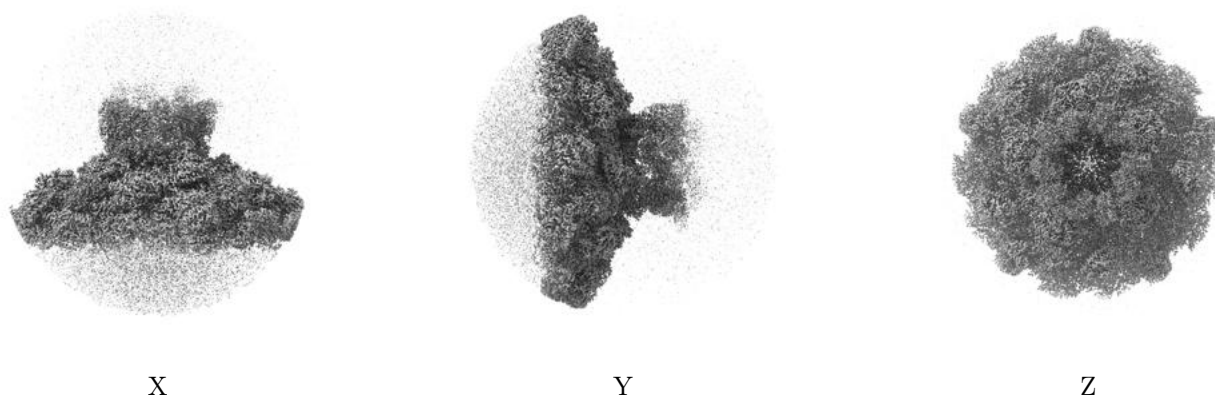


Z

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

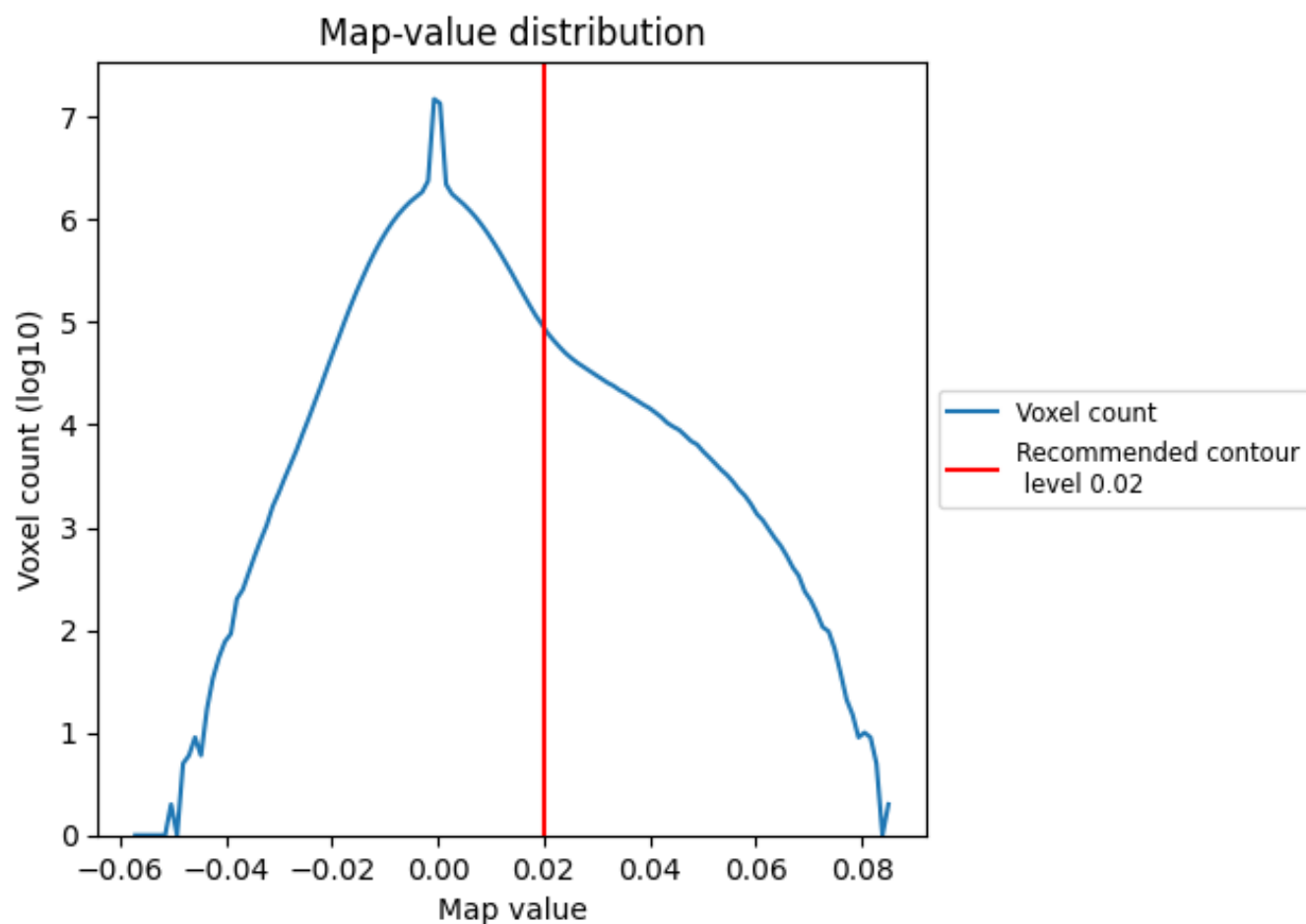
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

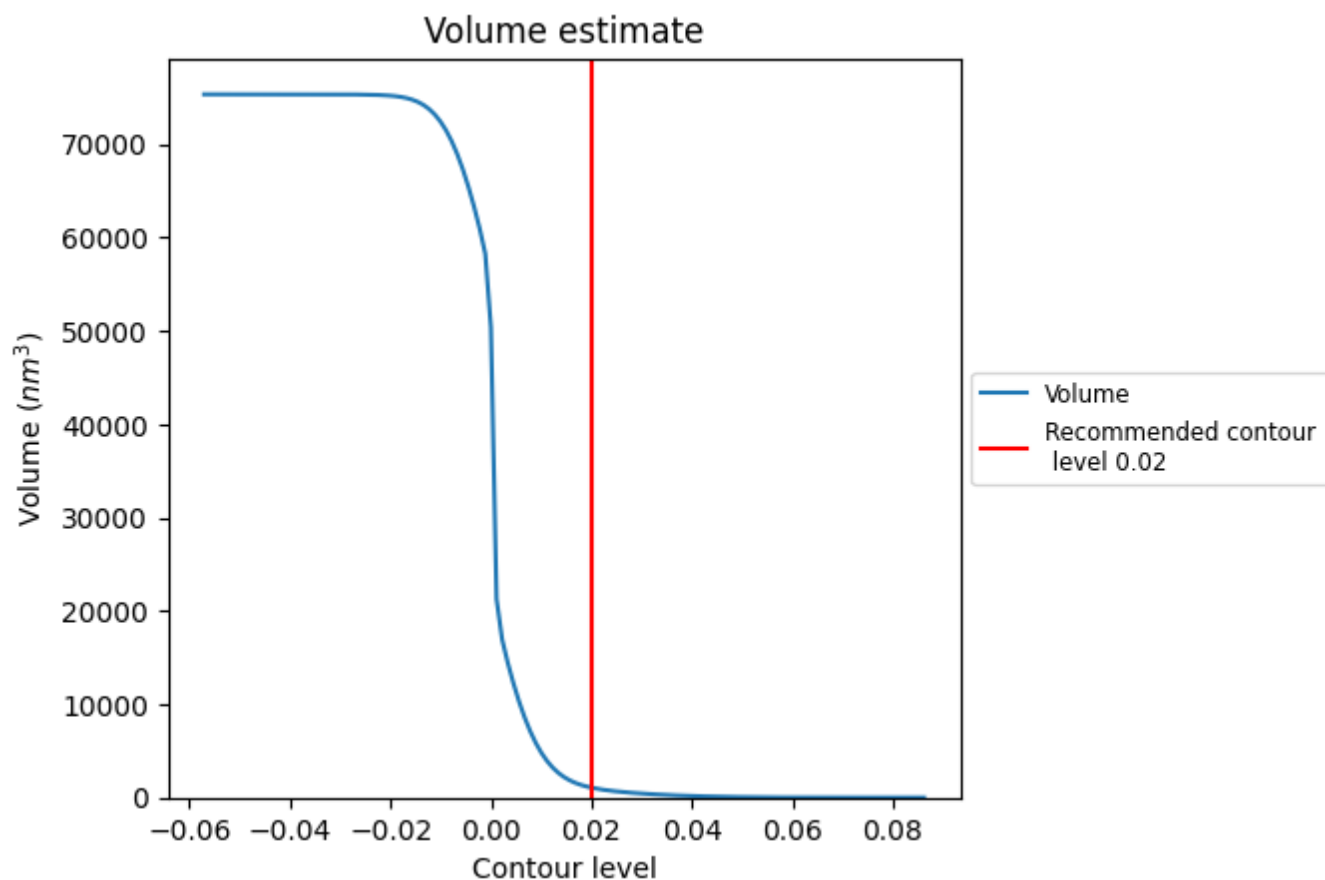
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

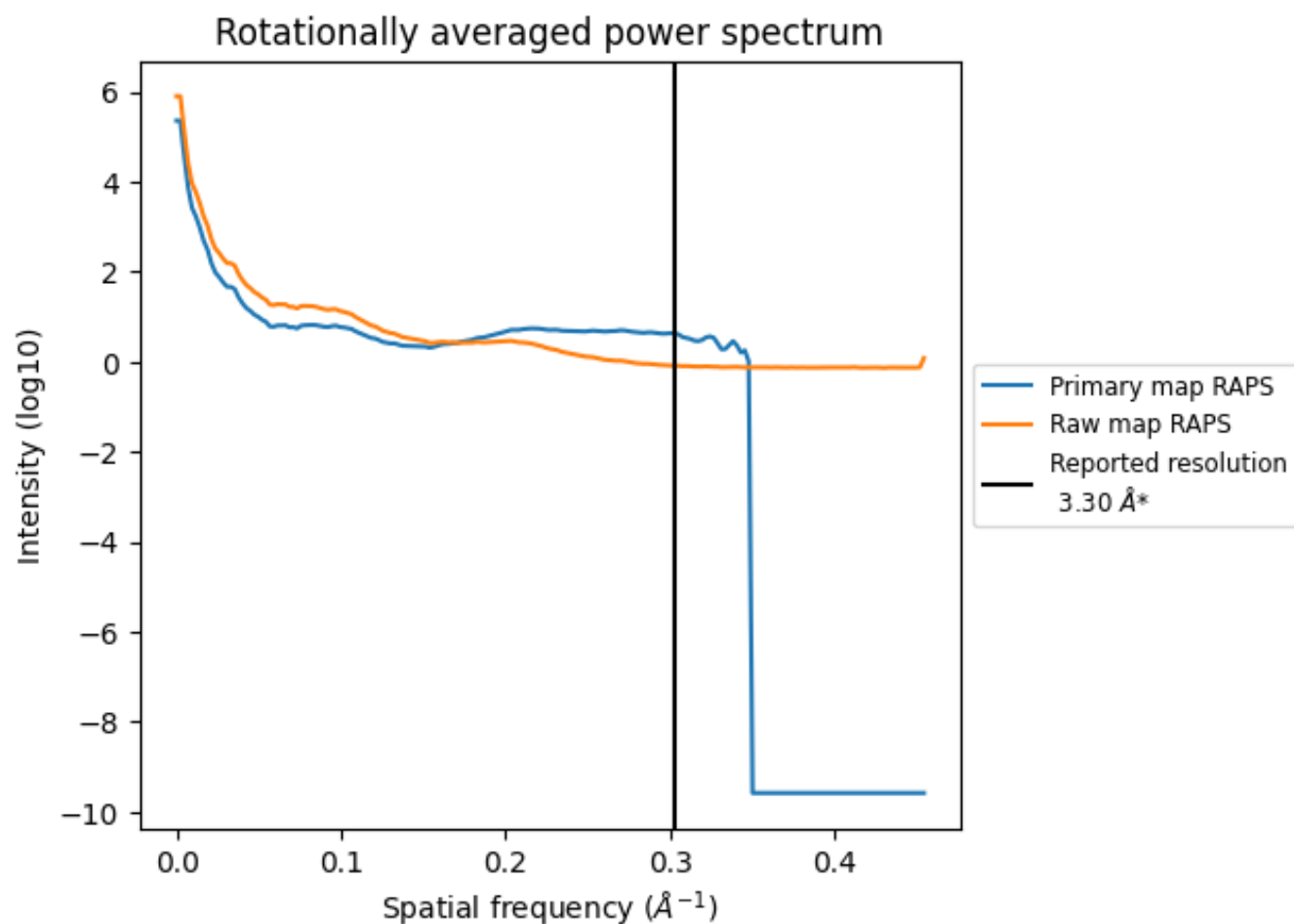
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1064 nm^3 ; this corresponds to an approximate mass of 961 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 ⓘ

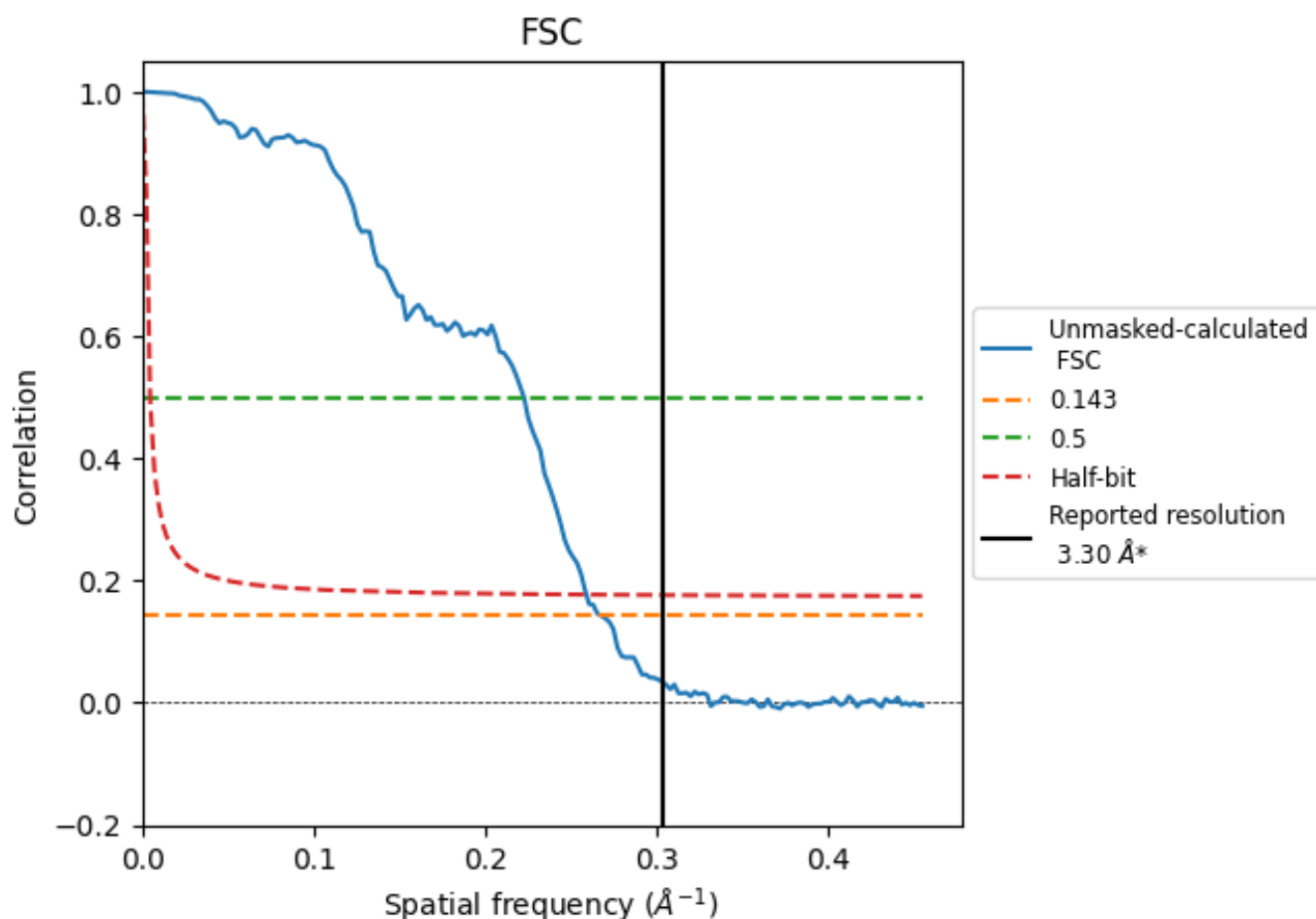


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

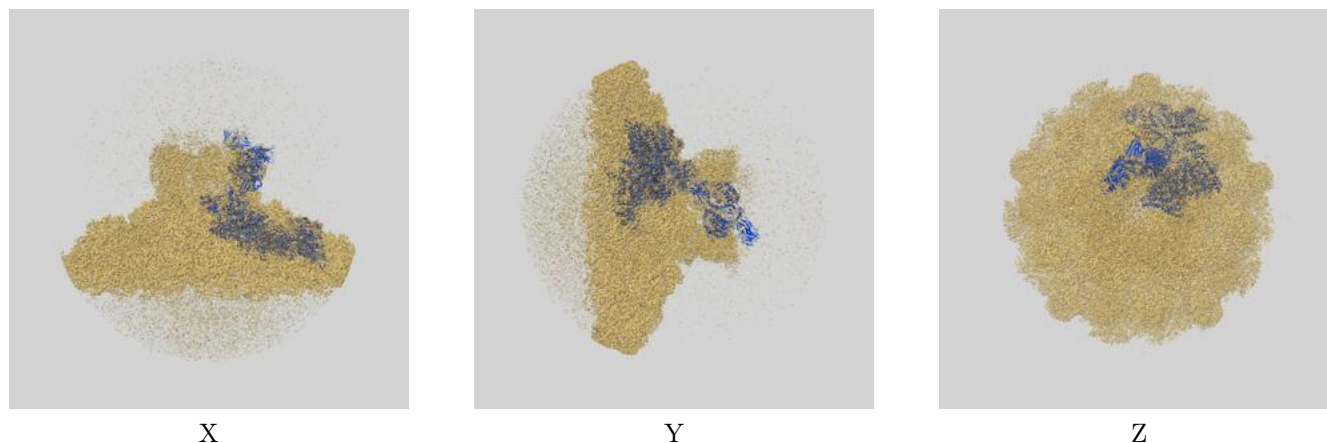
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	4.49	3.86

*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 3.74 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

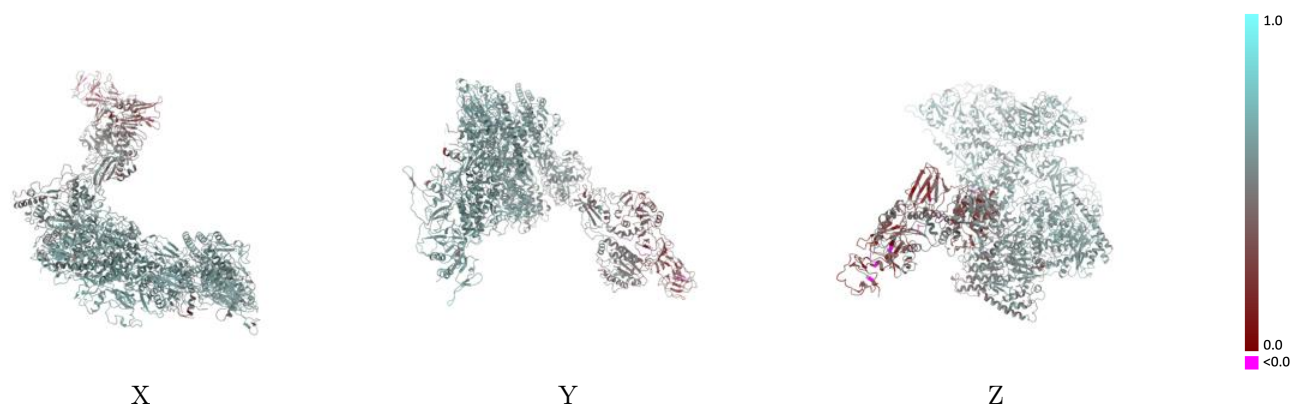
This section contains information regarding the fit between EMDB map EMD-46053 and PDB model 9CYX. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



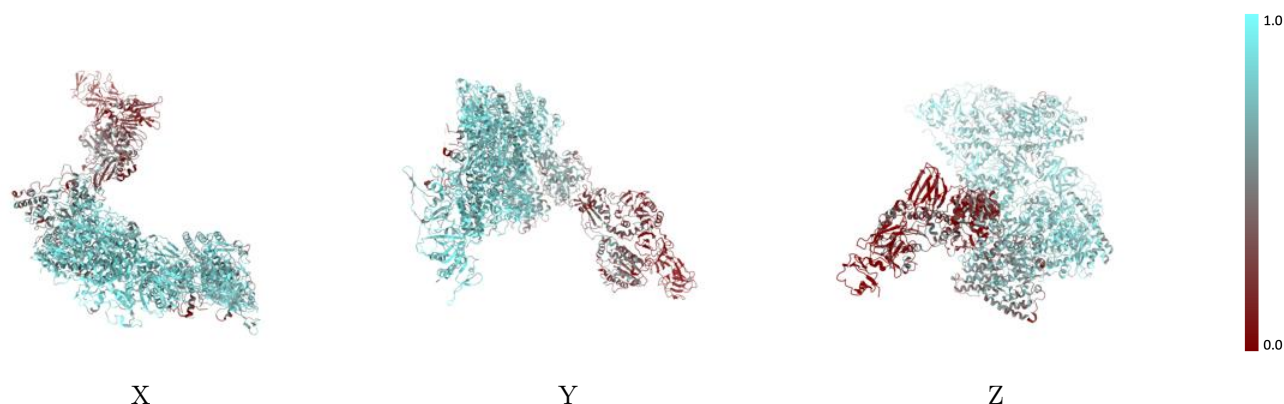
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



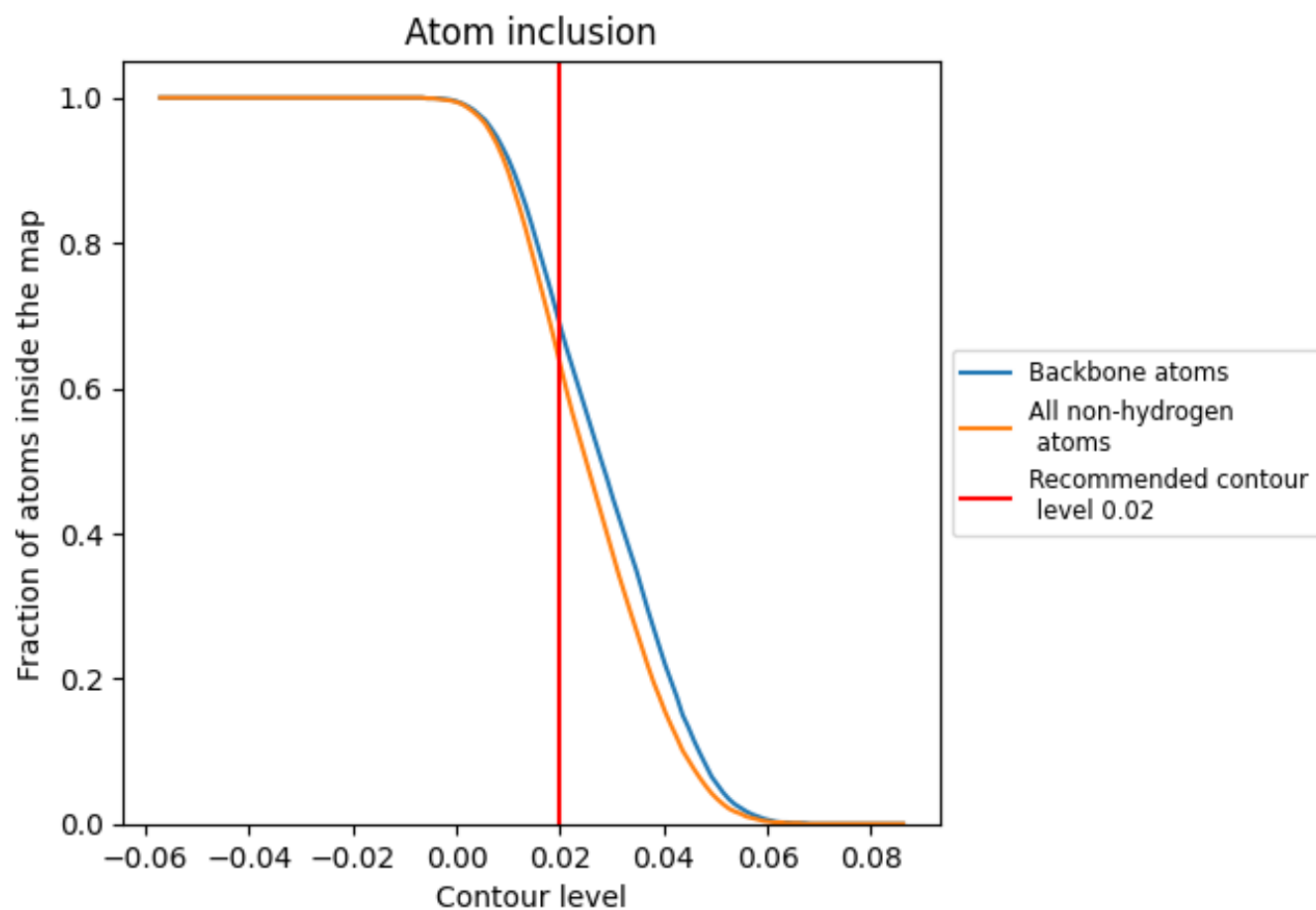
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 69% of all backbone atoms, 63% 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	0.6340	0.5350
A	0.3150	0.4260
B	0.6570	0.5750
H	0.7700	0.5740
I	0.7710	0.5810
Q	0.8140	0.5950
R	0.7310	0.5740

1.0

0.0

<0.0