



wwPDB EM Validation Summary Report ⓘ

Dec 9, 2024 – 10:24 AM EST

PDB ID : 9CYX
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.dev113
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) : 2.40

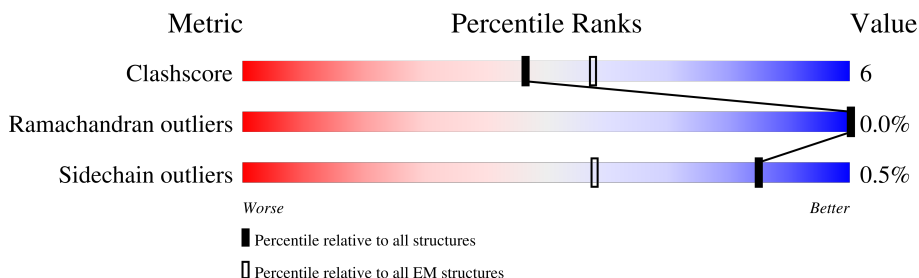
1 Overall quality at a glance

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)
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	B	1275	
1	H	1275	
1	I	1275	
2	A	1288	
3	Q	417	
3	R	417	

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		

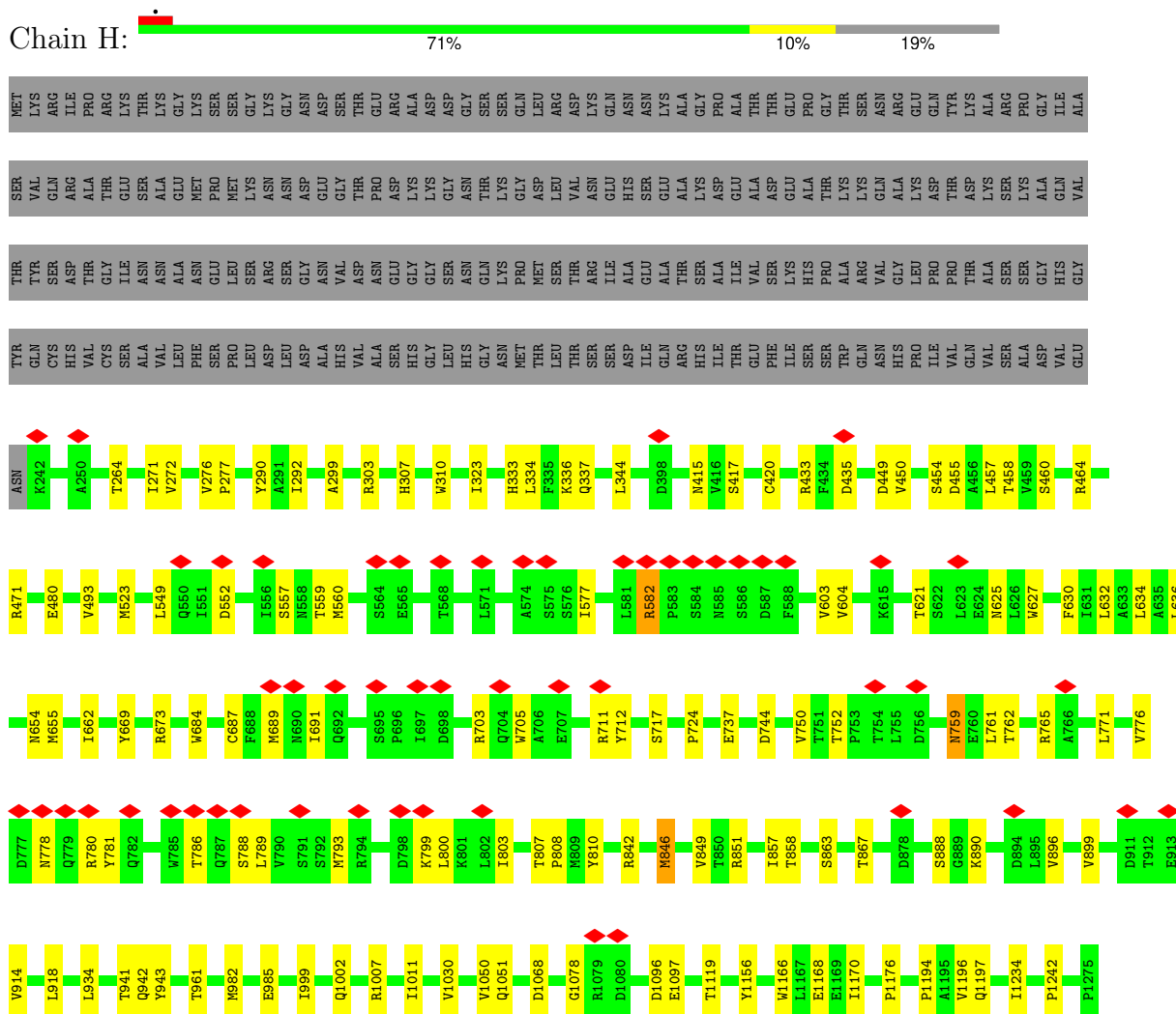
- Molecule 3 is a protein called Inner capsid protein sigma-2.

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		

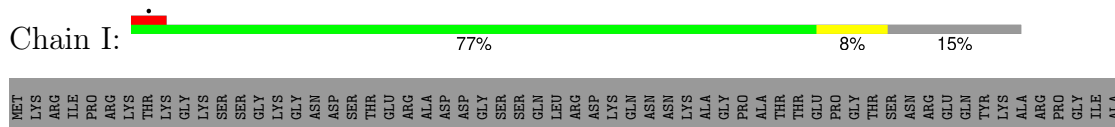
3 Residue-property plots

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.

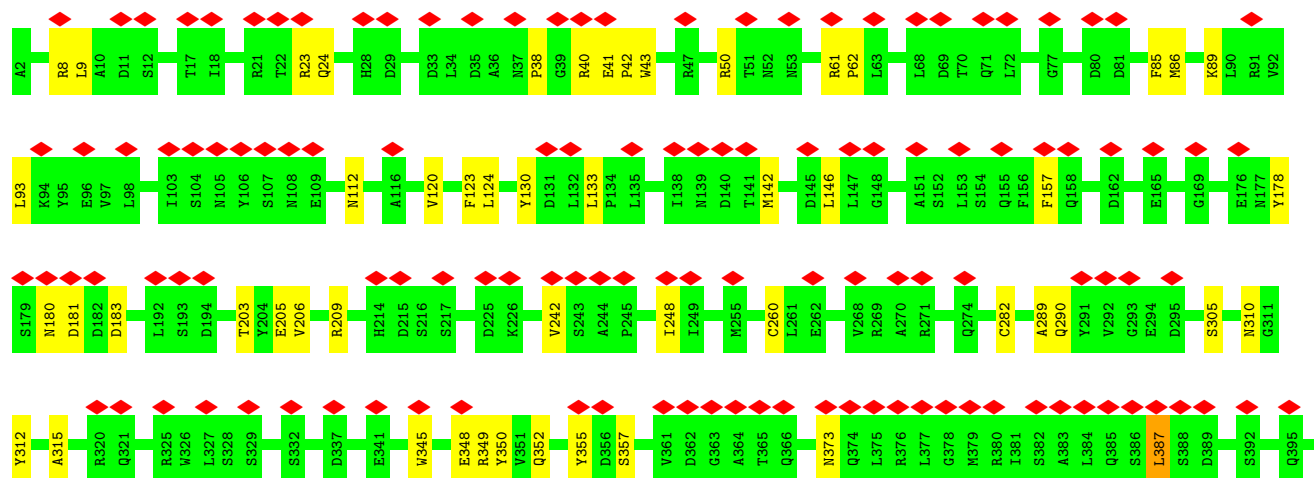
• Molecule 1: Lambda 1



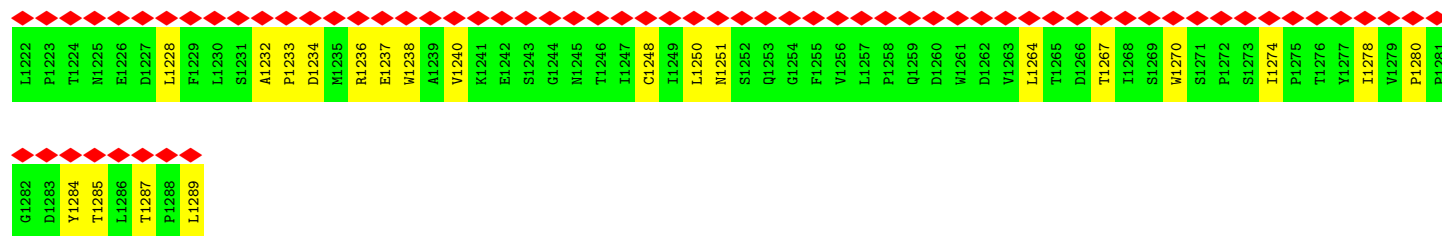
• Molecule 1: Lambda 1



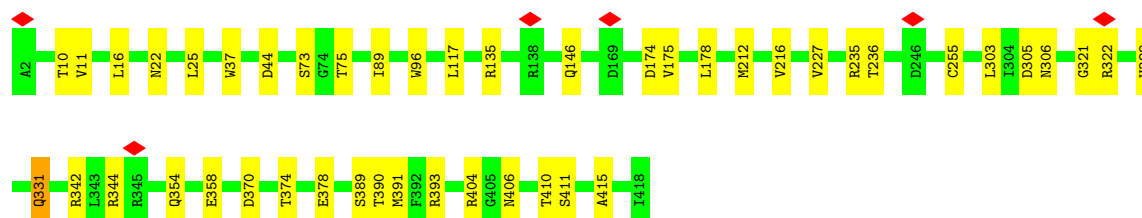
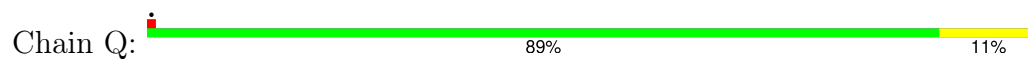




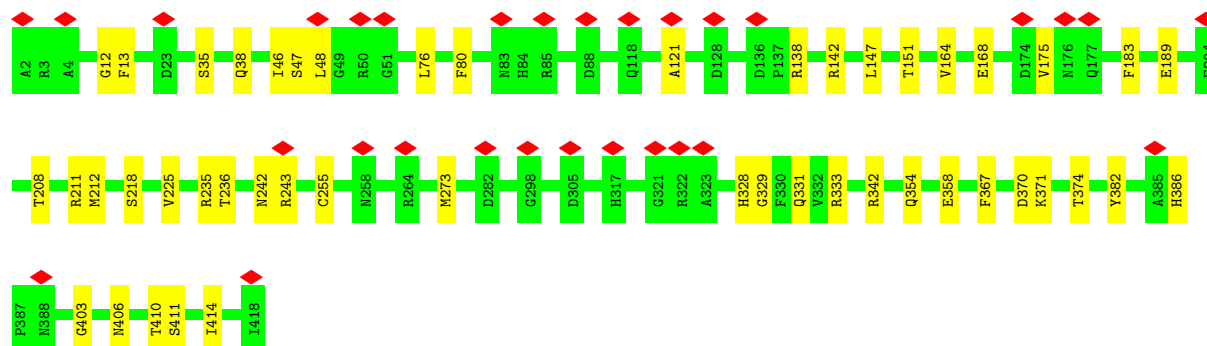
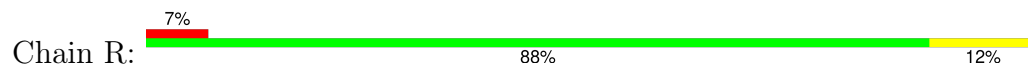
Q1162	W1163	Q1164	I1165	A1166	P1167	P1168	K1169	K1170	F1171	Q1172	F1173	F1174	S1175	SER	ALA	SER	GLY	T1180	L1181	V1182	M1183	M1184	V1185	K1186	L1187	D1188	I1189	A1190	D1191	K1192	Y1193	L1194	L1195	Y1196	Y1197	I1198	D1199	D1200	V1201	Q1202	S1203	R1204	D1205	V1206	F1207	F1208	Y1209	I1210	Q1211	H1212	P1213	L1214	Q1215	L1216	L1217	N1218	T1219	I1220	T1221			
Q1102	A1103	L1104	V1105	G1106	S1107	N1108	A1109	M1108	P1110	P1111	V1112	S1113	L1114	G1115	S1116	F1117	V1118	D1119	T1120	S1121	P1122	D1123	V1124	D1125	I1126	T1127	D1128	A1129	V1130	P1131	A1132	Q1133	L1134	D1135	Y1136	I1137	I1138	A1139	G1140	T1141	D1142	V1143	D1144	I1145	T1146	V1147	N1148	P1149	I1150	Y1151	R1152	L1153	M1154	T1155	F1156	V1157	R1158	Y1159	D1160	G1161		
L1042	V1043	I1044	P1045	G1046	F1047	M1048	A1049	P1048	Q1050	D1051	V1052	F1053	M1054	C1055	Y1056	F1057	V1058	S1059	A1060	L1061	A1062	F1063	S1064	T1065	E1066	D1067	V1068	N1069	A1070	A1071	M1072	I1073	P1074	Q1075	V1076	S1077	A1078	Q1079	F1080	D1081	A1082	T1083	K1084	G1085	E1086	W1087	L1088	L1089	D1090	W1091	V1092	F1093	S1094	D1095	A1096	G1097	Y1098	T1100	T1101			
W981	V982	P983	L984	S985	Y986	D987	L988	P989	W990	T991	R992	L993	A994	L995	L996	E997	S998	T999	T1000	L1001	S1002	S1003	I1006	R1007	A1008	A1009	E1010	L1011	M1012	Y1013	P952	K953	F954	G955	R956	D957	E958	P959	S960	P961	D962	H1024	G1025	L1026	P1027	M1028	E1029	K1030	R1031	G1032	N1033	F1034	T1035	V1036	G1037	Q1038	N1039	C1040	S1041			
V921	V922	L923	V924	Q925	V926	N927	C928	P929	T930	D931	V932	V933	R934	S935	I936	K937	Q938	Y939	L940	E941	I942	D943	S944	T945	N946	K947	R948	Y949	R950	P951	L992	K953	F954	G955	R956	D957	E958	P959	S960	P961	D962	H1024	G1025	L1026	P1027	M1028	E1029	K966	Q968	Q909	R910	I911	R912	V913	L914	S915	W974	P975	N976	C977	I978	T980
C860	W861	R862	W863	R864	F867	L868	E869	L870	D871	Y872	L873	S874	D875	C876	W877	T878	T879	C880	V881	R882	G883	D884	I885	V886	T887	C888	R889	L890	S891	L892	G893	A894	A895	A896	A897	C898	R899	P900	T902	P903	A904	A905	A906	F907	Q908	Q909	R910	I911	R912	V913	L914	S915	K916	S917	T918	A919	N920					
Y799	G800	S801	R802	S803	H804	V805	C806	L807	T808	M810	F813	E814	V815	S816	S817	A818	V819	W820	D821	G822	D823	W824	V825	L826	D827	O828	G829	T830	G831	L832	K833	T834	W835	R836	I837	E838	L839	T840	P841	R842	T843	S844	P845	V846	T847	C848	Q849	R850	I851	R852	T854	A855	C731	Q856	P857	S858	G859					
G735	W736	A737	R738	K739	S740	I743	Y744	E745	T746	H747	G748	A749	W750	V751	L752	T753	W754	T755	S756	R757	A761	S762	A763	R764	L826	R765	K766	L769	R770	Y771	T772	P773	L774	I775	T776	L837	P777	R778	S779	W780	E781	W782	A783	W785	T786	I787	R789	A790	D791	P792	W793	L794	W795	E796	W797	W798						
W666	T667	S668	G669	F672	F673	L674	V675	D676	H677	F678	G679	R680	Y681	E682	T683	I687	S688	R689	S693	D698	D699	G700	S701	S702	W703	I706	E707	T708	I709	S710	T711	E712	N713	G715	F716	S717	N718	W719	T720	Q721	A722	F723	R724	I725	G726	I727	S728	G729	L730	C731	A732	W733	Y734									
S600	S601	C602	M603	H604	A605	T606	P608	G609	G610	S611	F612	V613	W614	K615	I616	N617	F618	P619	T620	R621	P622	W624	H625	Y626	K630	I631	L632	P633	N634	I635	T636	S637	G638	L640	F644	V645	T646	N647	E650	L651	F652	V653	A655	F656	H659	Q660	H661	S662	S663	L664	T665											
P532	W533	I534	Q535	G536	K537	L538	S539	G540	V541	P542	P543	P544	V547	R548	G551	Y552	D553	V554	A555	R556	A557	D561	L562	A563	R564	P567	S568	G569	D570	Y571	Q572	Y575	D579	Q580	V581	W582	S444	A513	G516	A519	G520	H521	S522	G523	A524	D525	Q526	L593	V595	E596	L598	L599										
D464	E465	G468	R469	S470	R476	R477	R478	G479	D480	R481	S482	L483	W484	K485	D486	V489	L490	K491	H492	A493	Y494	Q495	A496	I497	D498	P499	N500	T501	K503	E504	Y505	Y438	Y439	S508	R509	Q510	S511	V512	G516	A519	G520	H521	S522	G523	A524	D525	Q526	L593	V595	E596	L598	L599										
Y400	T401	D402	D403	Q404	A405	A406	M407	D408	E409	G410	D411	L412	M413	W414	S415	R416	T418	Q419	L420	P421	L422	R423	P424	D425	I429	W430	D433	A434	L435	S436	Y437	Y438	Y439	D440	Y441	R442	R443	S444	A445	R446	Y447	V448	L449	S450	S451	E452	L453	P454	Q455	P457	D458	T459	Y460	G463								



• 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 (\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 (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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	0/1060	0.53	0/1420
1	H	0.35	0/8385	0.54	0/11486
1	I	0.34	0/8795	0.52	0/12048
2	A	0.31	0/10385	0.52	1/14172 (0.0%)
3	Q	0.33	0/3403	0.53	0/4634
3	R	0.31	0/3403	0.53	0/4634
All	All	0.33	0/35431	0.53	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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	987	ASP	CB-CG-OD2	5.26	123.03	118.30

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	85	0
1	I	8562	0	8451	61	0
2	A	10127	0	9910	198	0
3	Q	3317	0	3216	30	0
3	R	3317	0	3216	28	0
All	All	34537	0	33910	403	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 403 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	76
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%)	79	87
1	I	959/1114 (86%)	959 (100%)	0	100	100
2	A	1118/1120 (100%)	1110 (99%)	8 (1%)	81	88
3	Q	353/353 (100%)	351 (99%)	2 (1%)	84	90
3	R	353/353 (100%)	352 (100%)	1 (0%)	91	94
All	All	3812/5168 (74%)	3794 (100%)	18 (0%)	85	91

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

Mol	Chain	Res	Type
2	A	1248	CYS
3	R	333	ARG
3	Q	331	GLN
2	A	716	PHE
2	A	984	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	214	HIS
2	A	240	GLN
3	R	386	HIS
2	A	1251	ASN
1	I	249	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.

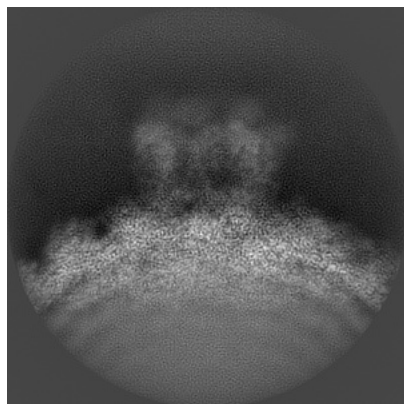
6 Map visualisation [i](#)

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.

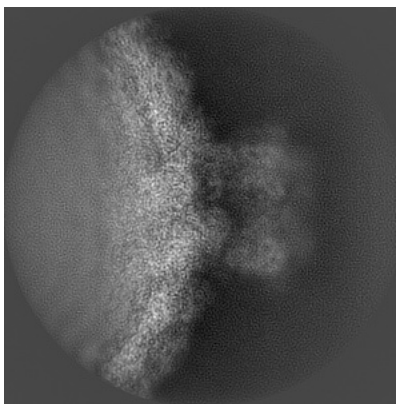
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

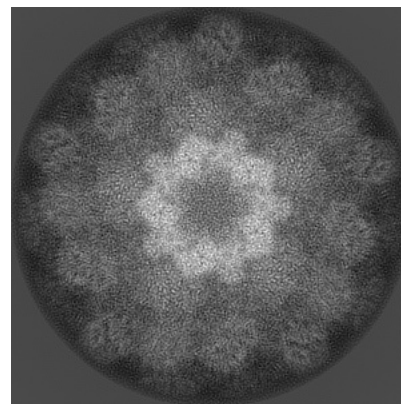
6.1.1 Primary map



X

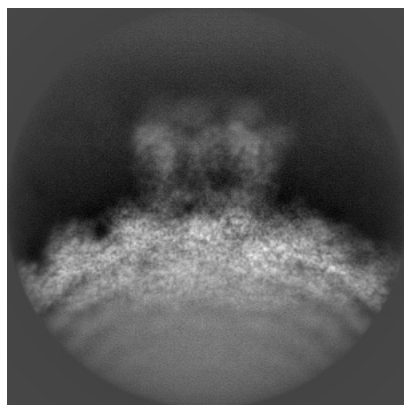


Y

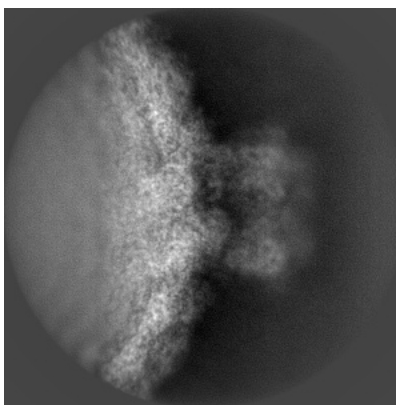


Z

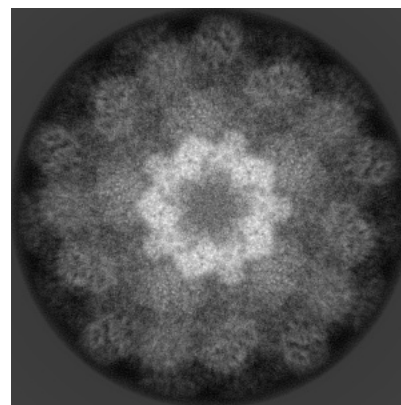
6.1.2 Raw map



X



Y

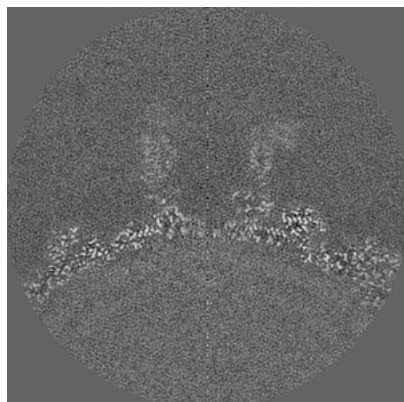


Z

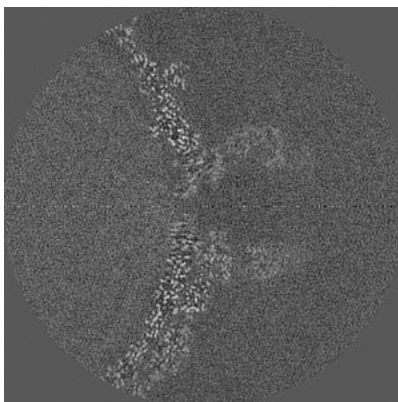
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

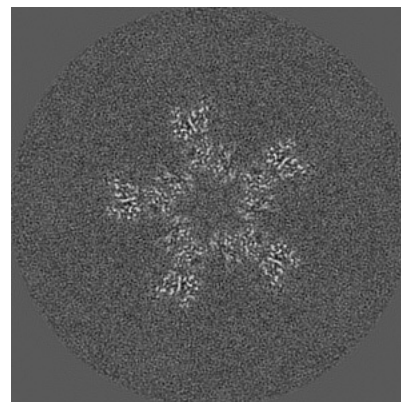
6.2.1 Primary map



X Index: 192

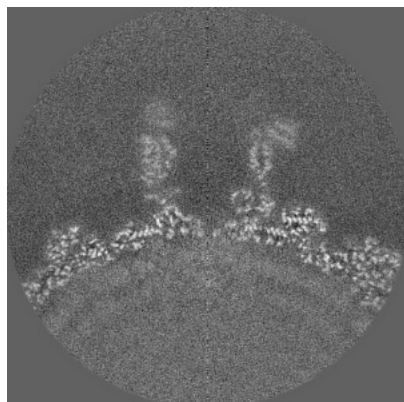


Y Index: 192

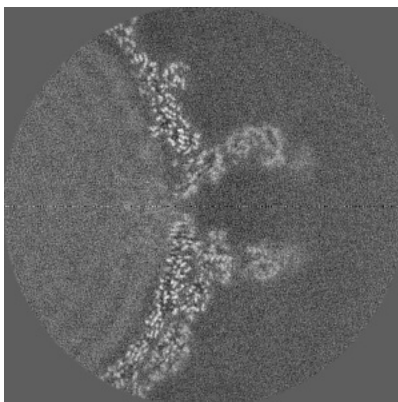


Z Index: 192

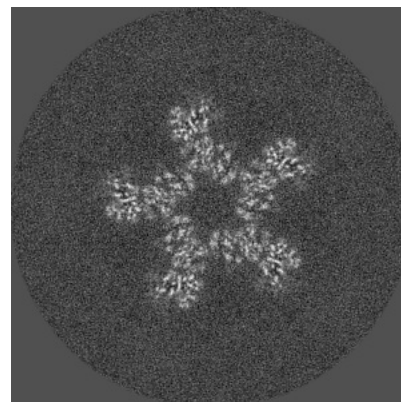
6.2.2 Raw map



X Index: 192



Y Index: 192

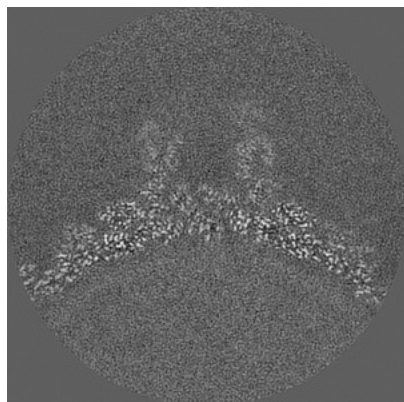


Z Index: 192

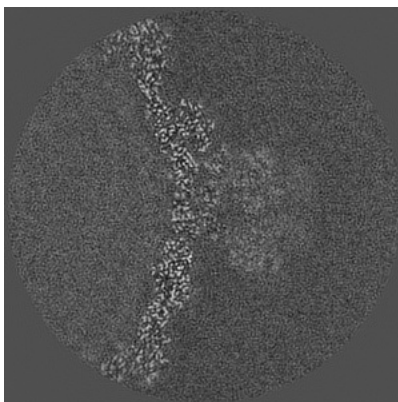
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

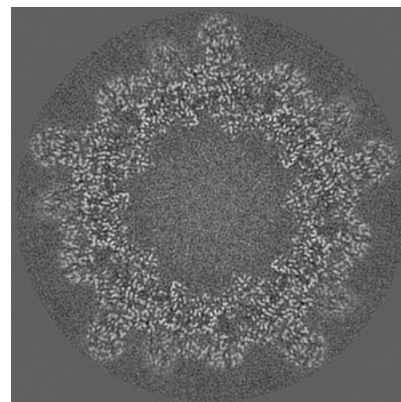
6.3.1 Primary map



X Index: 165

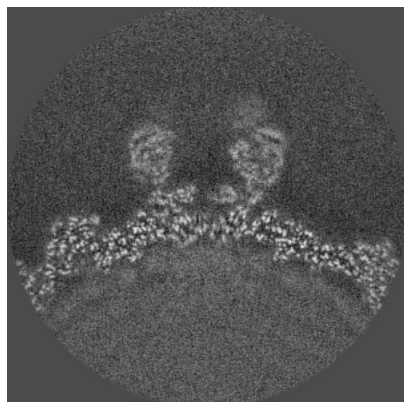


Y Index: 235

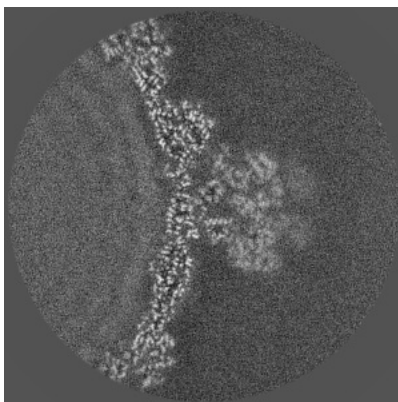


Z Index: 146

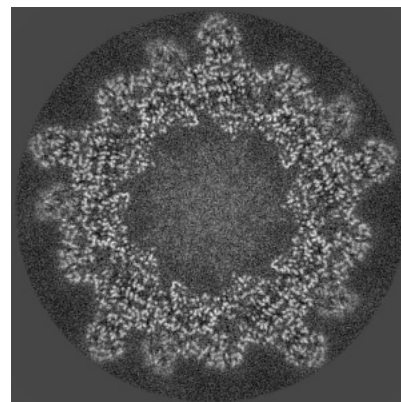
6.3.2 Raw map



X Index: 214



Y Index: 238

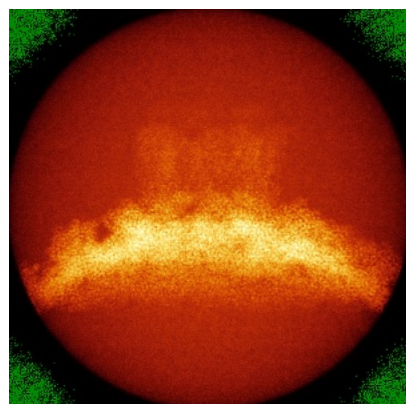


Z Index: 146

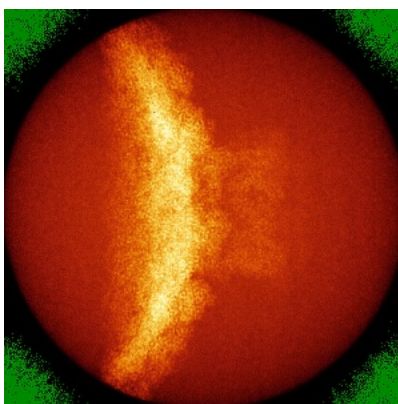
The images above show the largest variance slices of the map in three orthogonal directions.

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

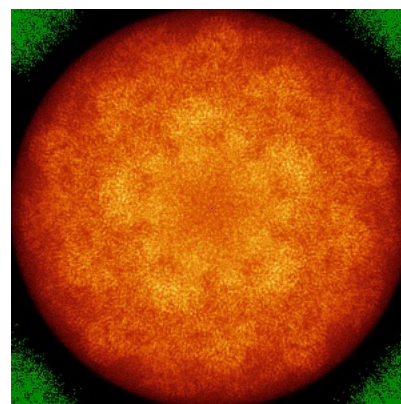
6.4.1 Primary map



X

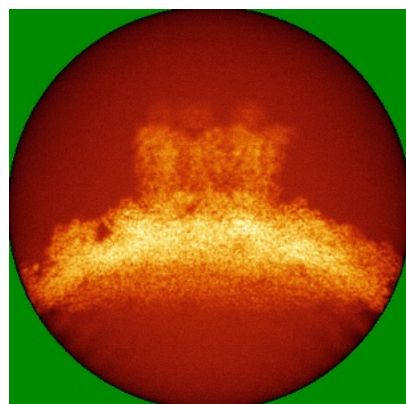


Y

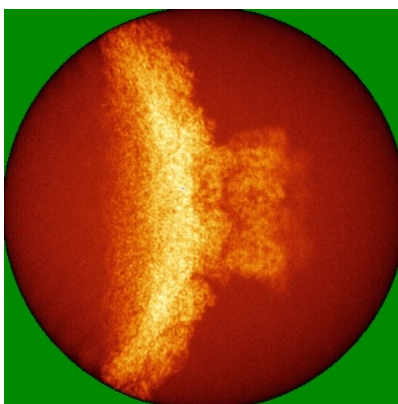


Z

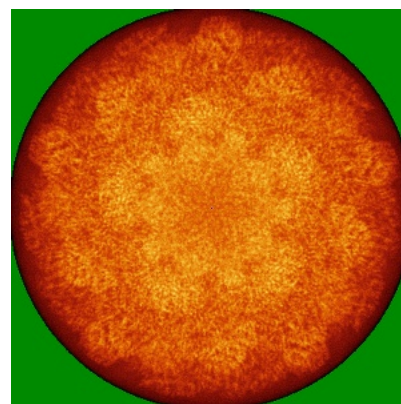
6.4.2 Raw map



X



Y

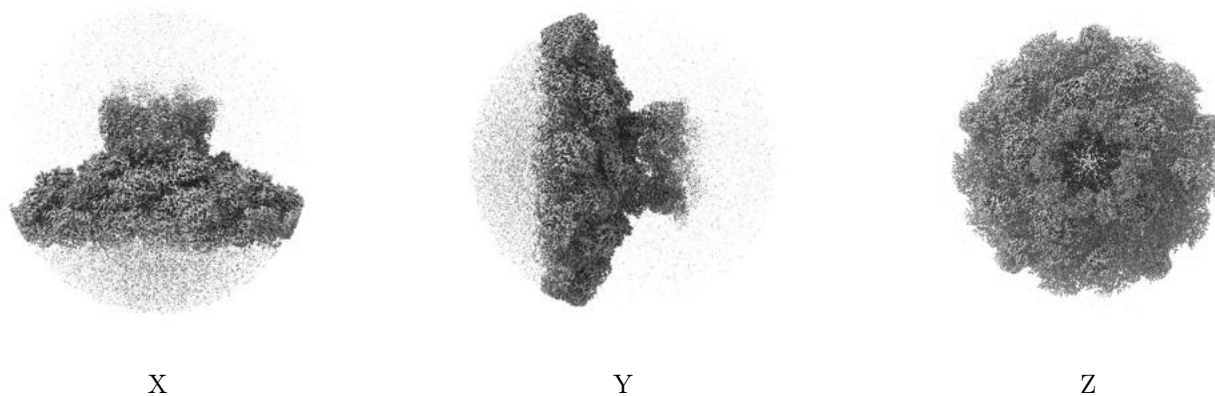


Z

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.

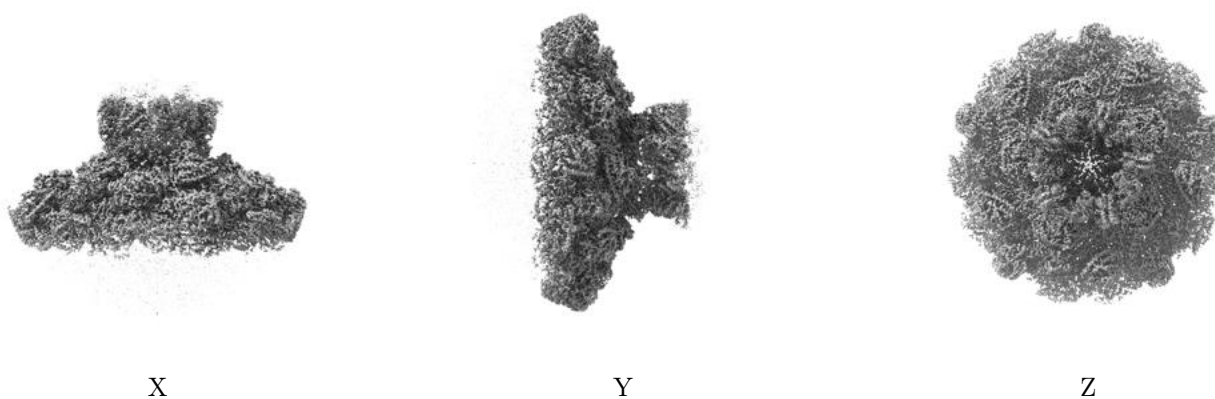
6.5 Orthogonal surface views [i](#)

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.

6.5.2 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.

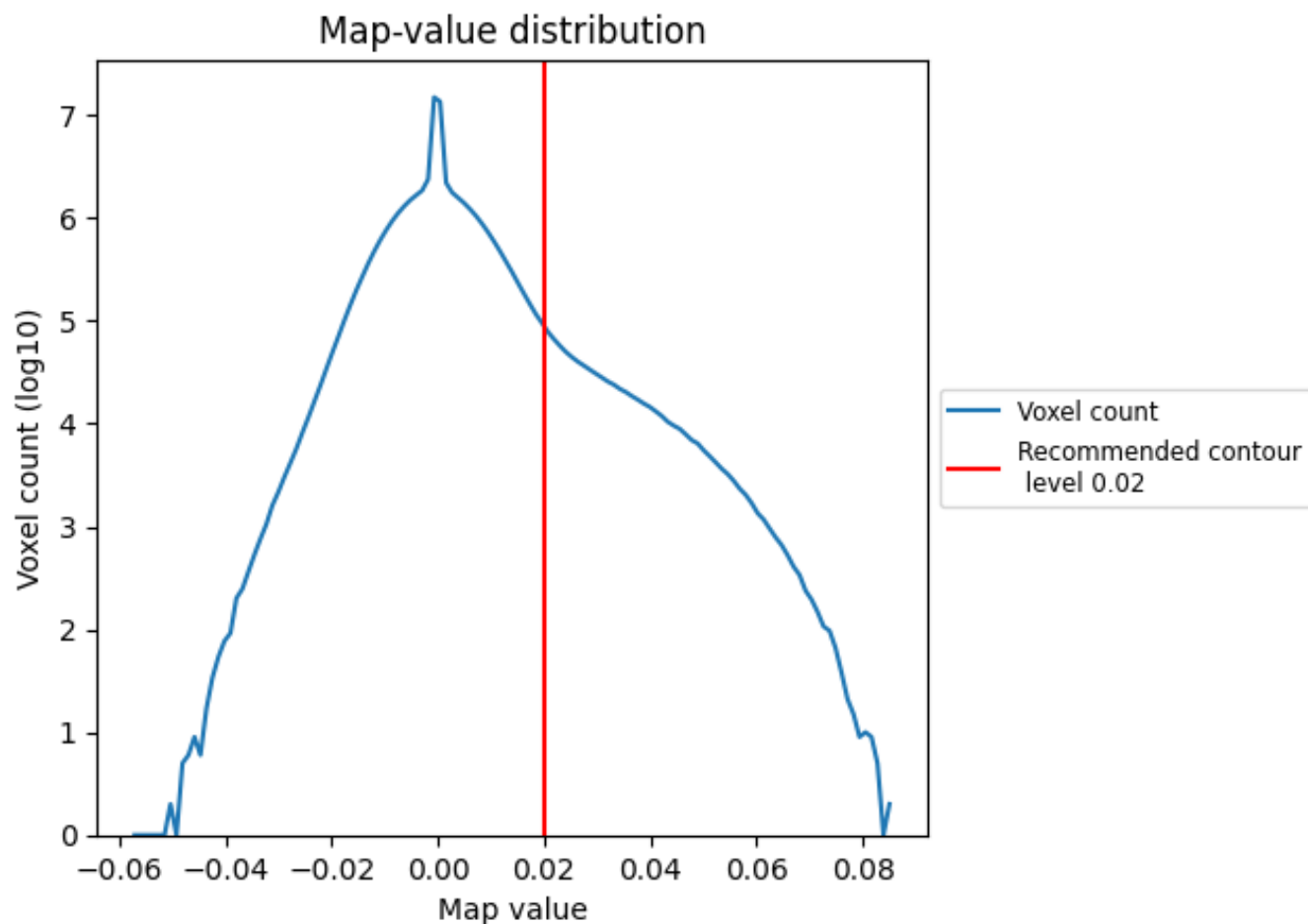
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

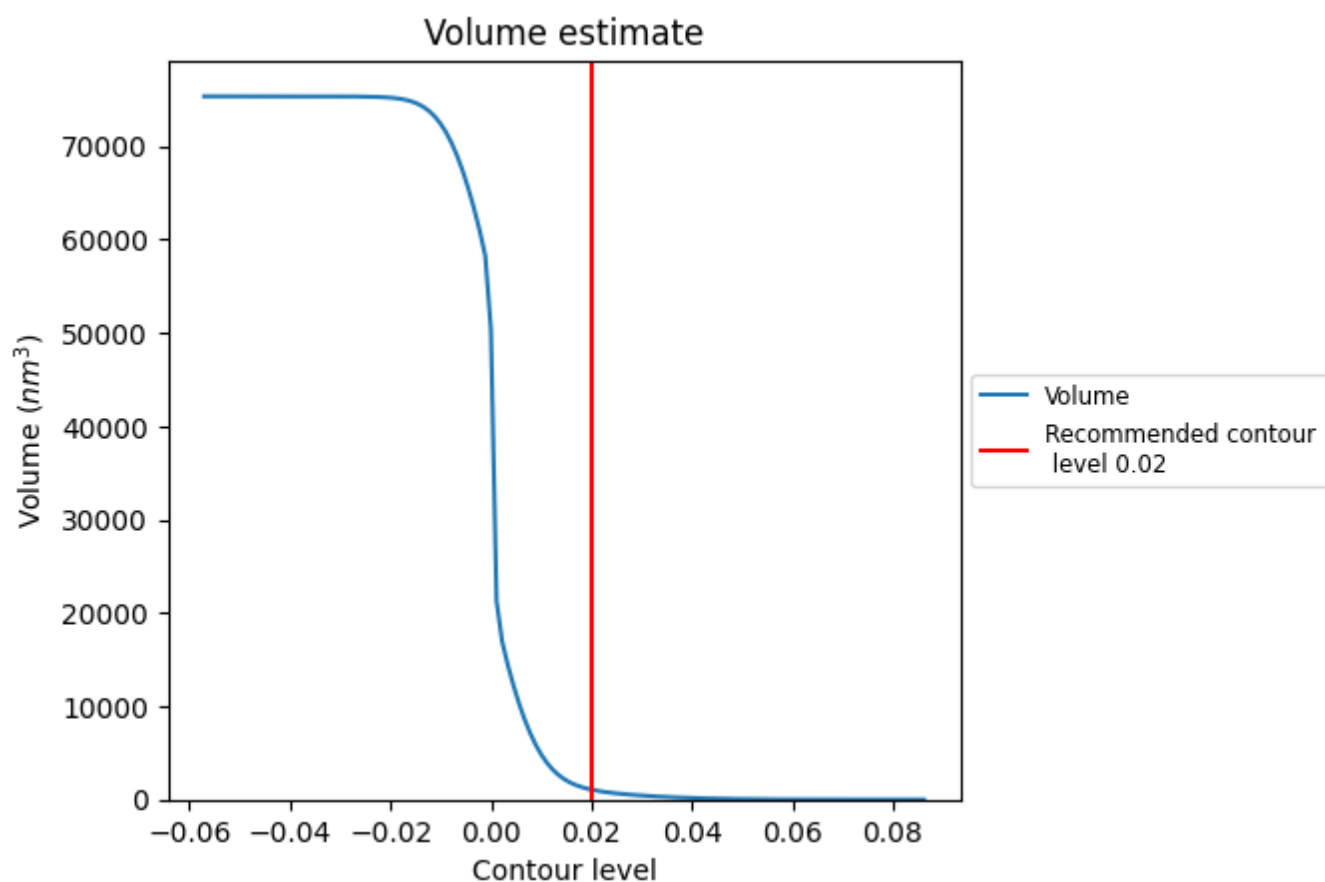
This section contains the results of statistical analysis of the map.

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.

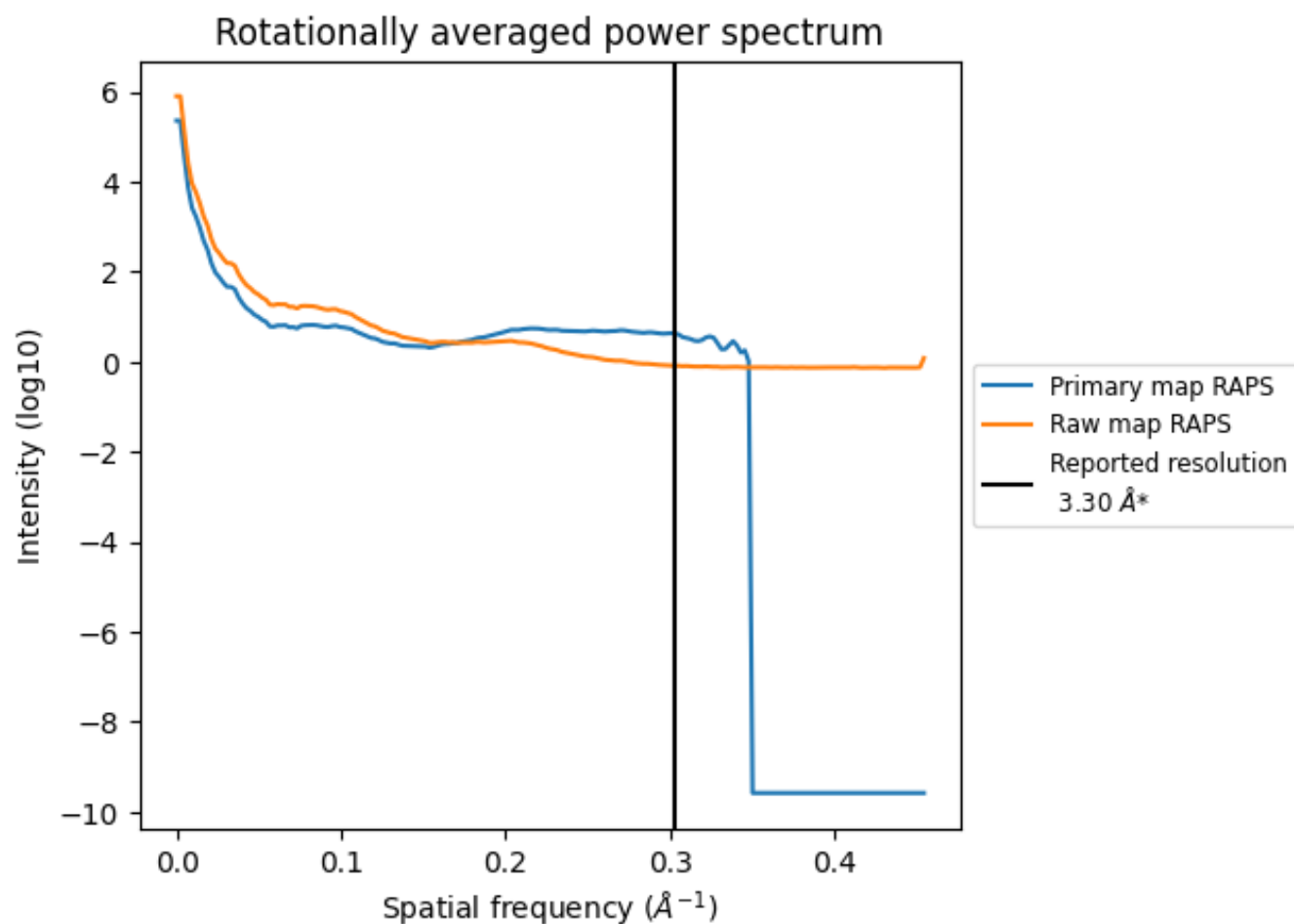
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1064 nm³; 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 ⓘ

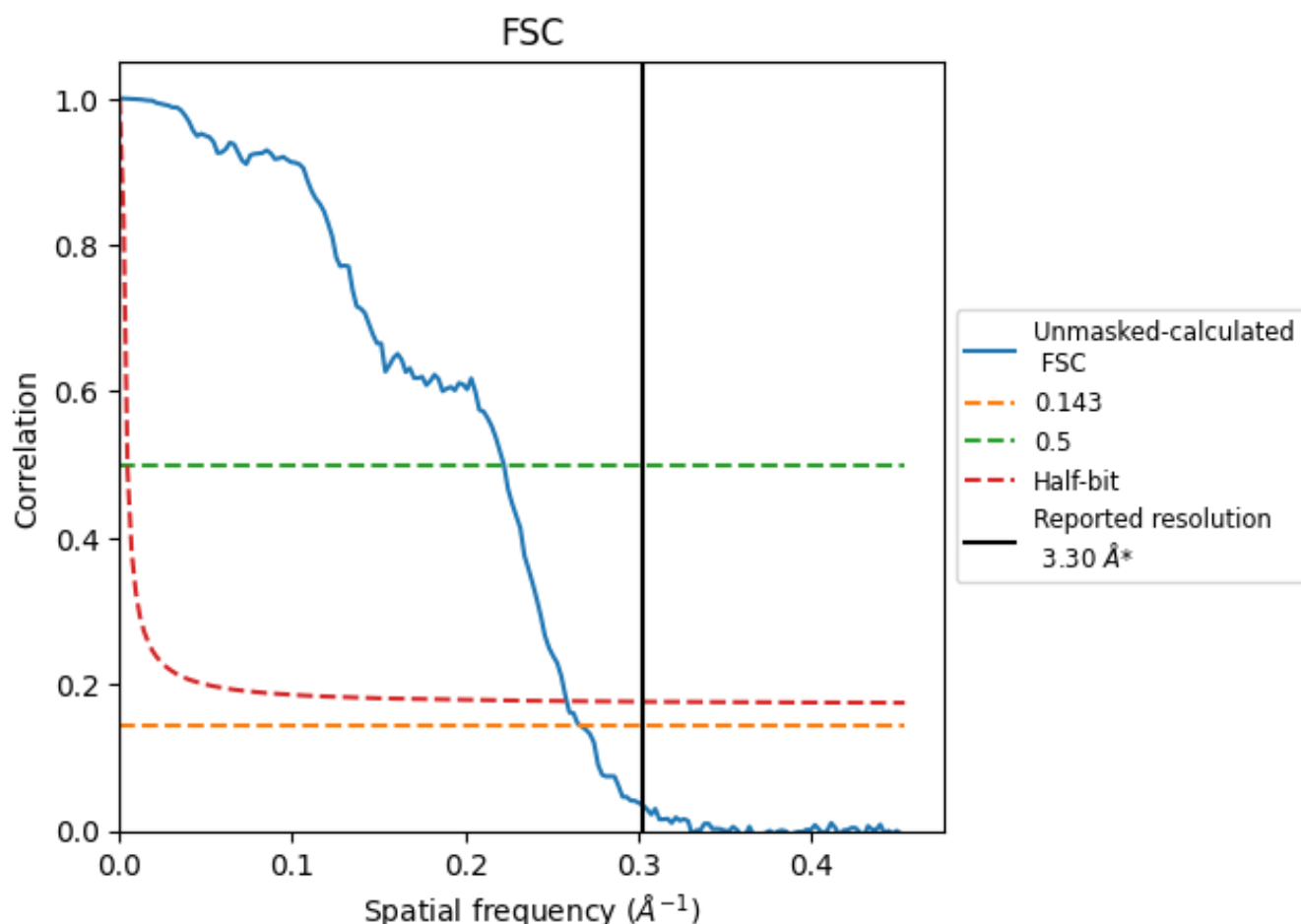


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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](#)

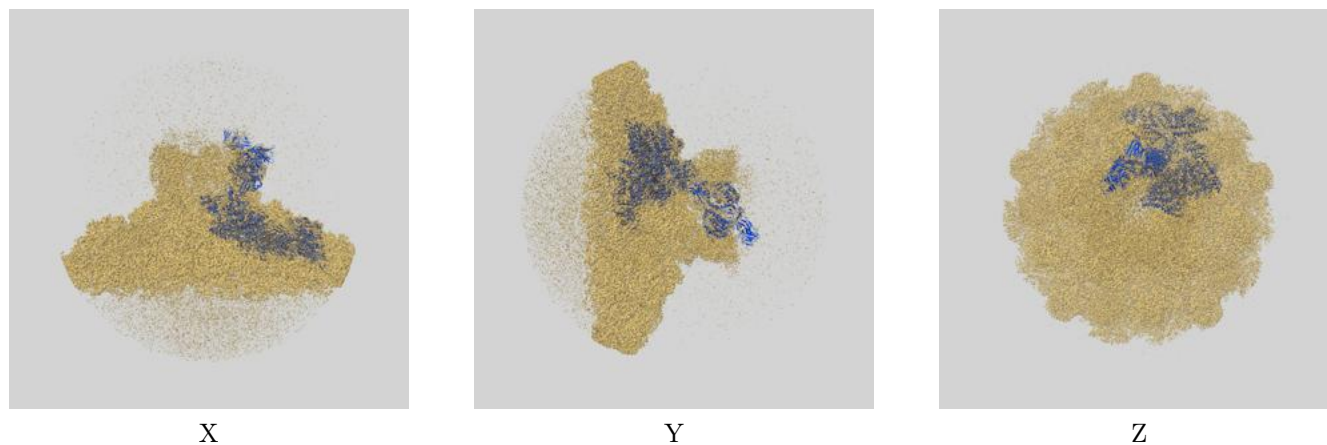
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.74	4.49	3.86

*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](#)

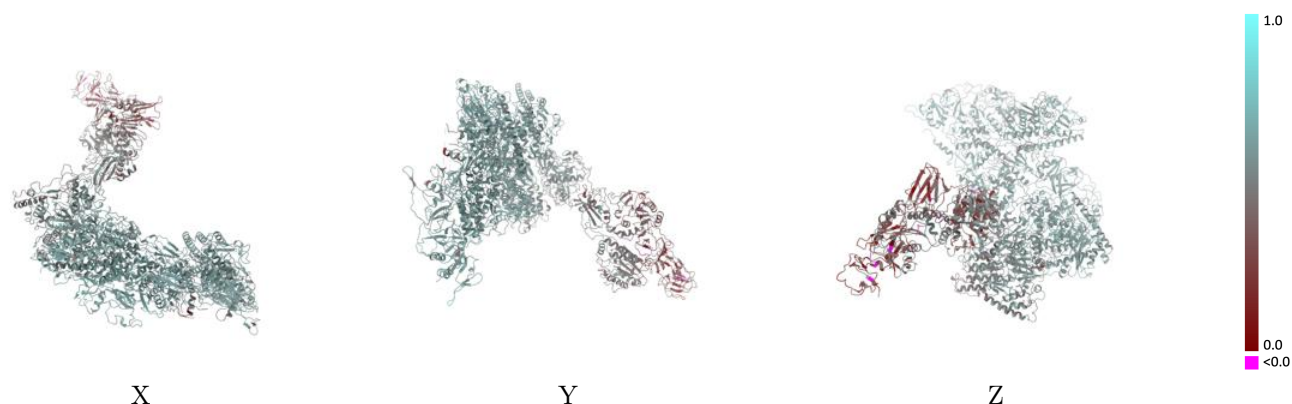
This section contains information regarding the fit between EMDB map EMD-46053 and PDB model 9CYX. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



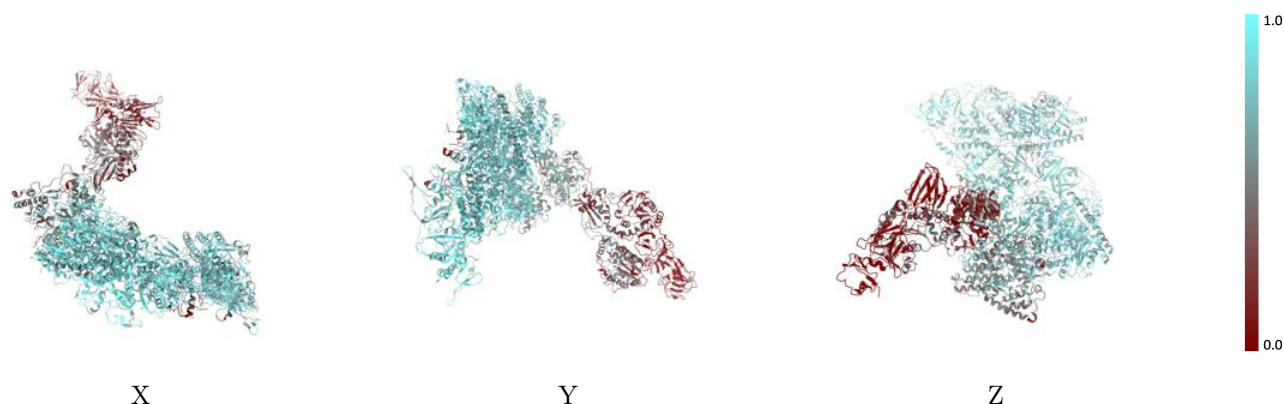
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



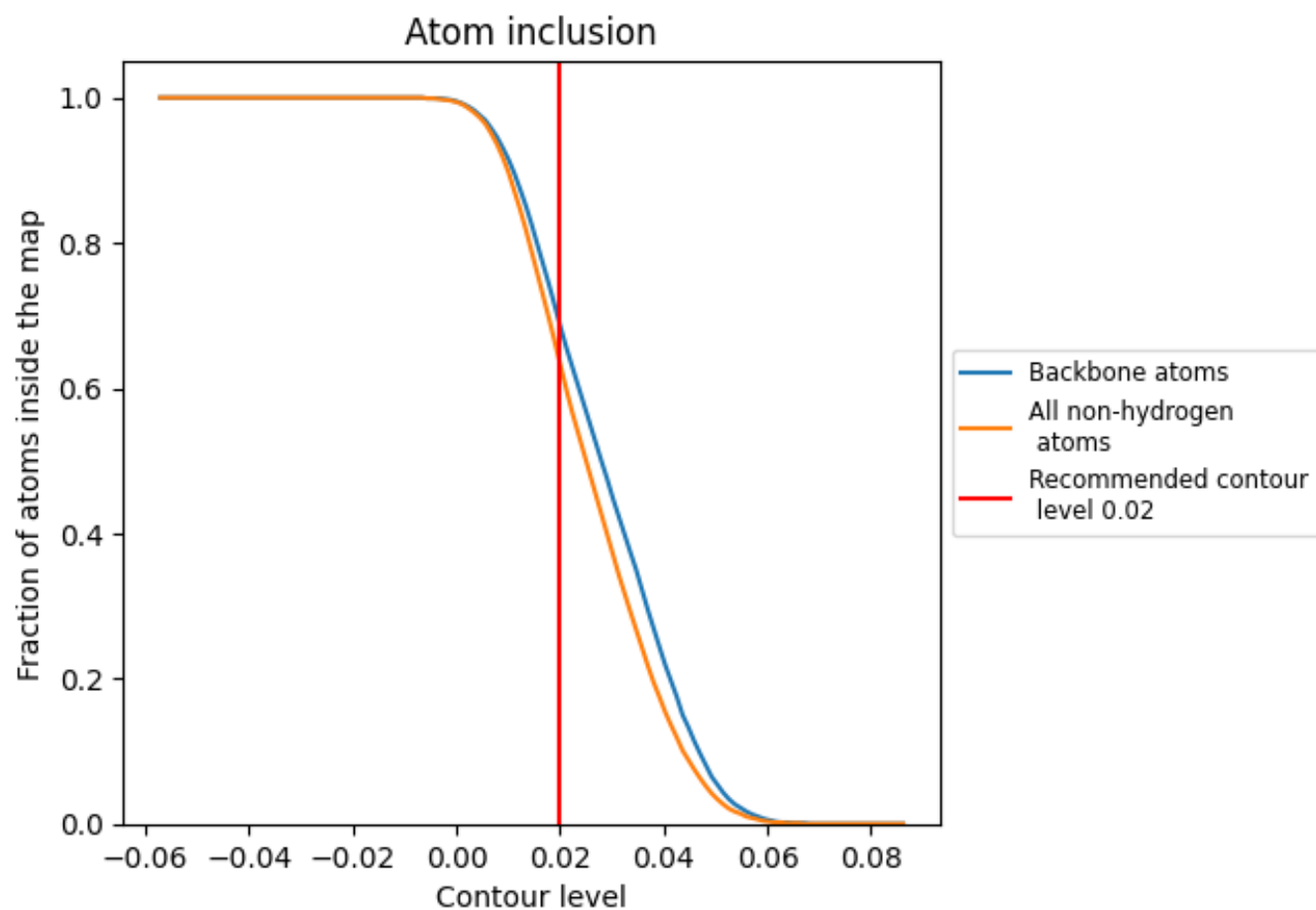
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0

0.0

<0.0