



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 04:40 AM UTC

PDB ID : 8U95 / pdb_00008u95
EMDB ID : EMD-42024
Title : The structure of myosin heavy chain from *Drosophila melanogaster* flight muscle thick filaments
Authors : Abbasi Yeganeh, F.; Rastegarpouyani, H.; Li, J.; Taylor, K.A.
Deposited on : 2023-09-18
Resolution : 4.70 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:

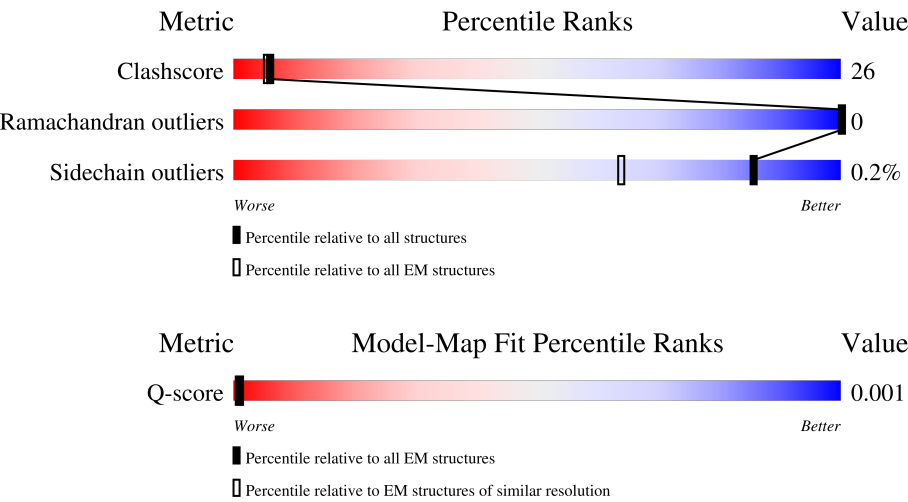
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	1989 (4.20 - 5.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1949	52% 26%25%48%
1	B	1949	52% 24%27%48%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16352 atoms, of which 0 are hydrogens and 0 are deuteriums.

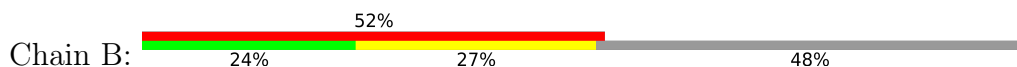
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Myosin heavy chain, isoform U.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1009	Total	C	N	O	S	0	0
			8176	4946	1527	1695	8		
1	B	1009	Total	C	N	O	S	0	0
			8176	4946	1527	1695	8		



- Molecule 1: Myosin heavy chain, isoform U

[illegible]

R1381	E1321	K1261	E1201	E1141	R1081	K1021	Q961	VAL	GLY	MET	THR	THR	LEU	ASN	LYS
S1382	S1322	L1262	M1202	L1142	K1082	V1022	K961	SER	LYS	ARG	THR	THR	THR	ASP	ALA
E1383	R1323	D1263	A1203	E1143	D1083	K1023	A963	ILE	ILE	GLN	ARG	LEU	THR	THR	THR
E1384	E1324	E1264	E1204	E1144	K1084	A1024	E964	GLU	LYS	ILE	SER	VAL	VAL	VAL	GLN
L1385	R1325	T1265	Q1205	L1145	E1085	K1025	Q965	ASP	TRP	TRP	THR	THR	THR	PHE	THR
E1386	A1326	N1266	V1206	G1146	L1086	L1026	D966	GLU	MET	MET	GLN	GLN	ASP	ASP	PHE
E1387	T1327	R1267	D1207	E1147	S1087	E1027	K967	ILE	GLN	GLN	PRO	PRO	GLN	SER	SER
A1388	L1328	T1268	Q1208	R1148	S1088	Q1028	A968	ARG	TRP	GLY	HIS	HIS	PHE	ALA	GLU
K1389	L1329	L1269	Q1209	L1149	T1089	Q1029	T969	LEU	ALA	ILE	VAL	VAL	LYS	LYS	LEU
R1390	G1330	N1270	N1210	E1150	T1090	L1030	K970	GLU	ARG	LYS	CYS	CYS	SER	THR	THR
K1391	K1331	D1271	K1211	E1151	A1091	D1031	D971	LYS	LYS	ILE	ILE	ILE	ASN	ASN	THR
L1392	F1332	F1272	L1212	A1152	K1092	E1032	H972	ALA	LEU	GLU	ILE	ILE	LYS	HIS	HIS
Q1393	R1333	D1273	K1213	G1153	L1093	L1033	Q973	LYS	ARG	PRO	PRO	PRO	LEU	LEU	LEU
A1394	A1334	A1274	A1214	Q1154	E1094	E1034	I974	ALA	LYS	LYS	GLU	GLU	ILE	ILE	LYS
R1395	L1335	S1275	K1215	A1155	D1095	D1035	R975	GLU	GLY	CYS	LYS	LYS	GLU	SER	SER
E1396	E1336	K1276	A1216	T1156	E1096	S1036	N976	GLU	PHE	THR	GLN	GLN	ILE	ALA	ALA
A1397	H1337	K1277	E1217	S1157	Q1097	L1037	L977	LEU	LYS	LYS	LYS	LYS	THR	ALA	PRO
K1398	D1338	K1278	K1218	A1158	V1098	E1038	N978	ALA	ALA	VAL	VAL	VAL	ASP	GLY	LYS
A1399	L1339	L1279	E1219	Q1159	V1099	R1039	D979	VAL	GLU	ILE	ASP	ASP	GLY	GLN	LYS
E1400	D1340	S1280	K1220	I1160	V1100	E1040	E980	VAL	GLN	GLU	GLU	GLU	GLN	GLN	PRO
E1401	M1341	I1281	N1221	E1161	L1101	K1041	I981	VAL	ARG	THR	THR	THR	ALA	ALA	PRO
T1402	L1342	E1282	E1222	L1162	K1102	K1042	A982	VAL	VAL	THR	HIS	HIS	SER	SER	PRO
T1403	R1343	N1283	Y1223	N1163	H1103	V1043	H983	ARG	ALA	GLU	GLU	GLU	ALA	LYS	LYS
E1404	E1344	S1284	Y1224	K1164	Q1104	R1044	Q984	LYS	LYS	LEU	VAL	VAL	GLY	GLY	PRO
S1405	Q1345	D1285	G1225	K1165	R1105	G1045	D985	GLU	VAL	ASN	MET	MET	GLY	GLY	GLY
L1406	V1346	L1286	Q1226	R1166	Q1106	D1046	E928	GLU	VAL	ASP	HIS	HIS	GLN	GLN	GLN
N1407	E1347	L1287	L1227	E1167	I1107	V1047	L987	ALA	ALA	ASP	THR	THR	ALA	ALA	ALA
K1408	E1348	R1288	N1228	A1168	K1108	E1048	I988	ASN	ASN	ARG	CYS	CYS	GLY	GLY	HIS
Q1409	E1349	D1289	L1229	E1169	E1109	R1049	N989	ALA	LYS	GLY	ASN	ASN	GLY	ALA	ALA
C1410	A1350	L1290	D1230	L1170	L1110	S1050	K990	LYS	LEU	ASN	VAL	VAL	GLY	GLY	ILE
T1411	E1351	E1291	R1231	S1171	Q1111	K1051	L991	LEU	LEU	ASN	THR	THR	LYS	LYS	HIS
G1412	G1352	E1292	A1232	K1172	A1112	R1052	N992	ALA	ALA	LYS	GLY	GLY	GLY	GLY	GLY
L1413	R1353	A1293	G1233	L1173	R1113	K1053	K993	LYS	LYS	VAL	ILE	ILE	ALA	ALA	ALA
E1414	A1354	E1294	V1234	R1174	I1114	V1054	E994	THR	THR	ARG	ARG	ARG	GLY	GLY	GLY
K1415	D1355	S1295	D1235	R1175	E1115	E1055	K995	ALA	THR	ARG	ILE	ILE	PHE	CYS	CYS
T1416	L1356	Q1296	H1236	D1176	E1116	G1056	K996	LEU	TRP	ALA	CYS	CYS	VAL	VAL	VAL
K1417	Q1357	V1297	I1237	L1177	L1117	D1057	M997	LEU	TRP	GLY	ARG	ARG	THR	SER	SER
Q1418	R1358	S1298	T1238	E1178	E1118	L1058	Q998	ASP	TRP	VAL	LYS	LYS	VAL	VAL	TYR
R1419	Q1359	Q1299	N1239	E1179	E1119	K1059	G999	SER	TYR	SER	GLY	GLY	PHE	SER	ASN
L1420	L1360	L1300	E1240	N1181	E1120	L1060	E1000	LEU	LEU	GLY	GLN	GLN	ALA	ALA	THR
S1421	S1361	S1301	K1241	E1182	V1121	T1061	T1001	SER	TRP	MET	MET	MET	TYR	TYR	TYR
T1422	K1362	K1302	A1242	I1183	E1122	Q1062	N1002	LYS	LYS	GLY	GLY	GLY	GLY	GLY	LYS
E1423	A1363	I1303	A1243	Q1183	A1123	E1063	Q1003	ALA	LYS	LEU	VAL	VAL	ARG	GLN	GLN
V1424	K1364	K1304	Q1244	H1184	E1124	A1064	K1004	LEU	THR	TRP	TRP	TRP	VAL	GLN	GLN
E1425	A1365	I1305	Q1245	E1185	R1125	V1065	T1005	ALA	ALA	ALA	ALA	ALA	ARG	GLY	GLY
D1426	E1366	S1306	K1246	S1186	Q1126	A1066	G1006	THR	THR	THR	THR	THR	VAL	VAL	VAL
L1427	A1367	L1307	T1247	T1187	A1127	D1067	E1007	ASP	ASP	ASP	GLY	GLY	GLY	GLY	GLY
Q1428	Q1368	T1308	A1248	E1188	R1128	L1068	E1008	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
L1429	V1369	T1309	K1249	A1189	A1129	E1069	L1009	SER	SER	SER	LEU	LEU	LEU	LEU	LEU
E1430	W1370	Q1310	Q1250	N1190	K1130	E1070	Q1010	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
V1431	R1371	L1311	L1251	L1191	A1131	N1071	A1011	ALA	LYS	LYS	LYS	LYS	PRO	ASN	ASN
D1432	S1372	E1312	Q1252	R1192	E1132	K1072	A1012	GLY	TRP	TRP	TRP	TRP	GLY	GLY	GLY
R1433	K1373	D1313	H1253	K1193	K1133	R1073	E1013	LYS	GLN	GLN	GLN	GLN	GLU	GLU	GLU
A1434	Y1374	T1314	L1254	K1194	Q1134	E1074	D1014	GLY	GLY	VAL	VAL	VAL	PHE	GLN	GLN
N1435	E1375	K1315	L1255	H1195	R1135	L1075	K1015	ALA	ARG	ARG	ARG	ARG	ARG	GLY	GLY
E1436	S1376	R1316	N1256	N1196	A1136	E1076	I1016	LEU	LYS	LYS	LYS	LYS	PRO	ASN	ASN
T1437	D1377	L1317	E1257	D1197	D1137	Q1077	N1017	LEU	PRO	ASP	ASP	ASP	ASP	GLU	GLU
A1438	G1378	A1318	V1258	L1197	L1138	T1078	H1018	GLN	LEU	LEU	LEU	LEU	PHE	LEU	LEU
N1439	V1379	D1319	Q1259	V1199	A1139	T1079	L1019	TYR	ASN	ASP	ASP	ASP	ASP	ASP	PRO
A1440	A1380	E1320	S1260	A1200	R1140	Q1080	N1020								



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	19.048	Depositor
Minimum map value	-4.384	Depositor
Average map value	0.028	Depositor
Map value standard deviation	0.633	Depositor
Recommended contour level	2.79	Depositor
Map size (Å)	1021.44006, 1021.44006, 1021.44006	wwPDB
Map dimensions	768, 768, 768	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/8212	0.62	0/10958
1	B	0.22	0/8212	0.70	3/10958 (0.0%)
All	All	0.21	0/16424	0.66	3/21916 (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
1	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1786	GLU	N-CA-CB	5.33	118.54	110.28
1	B	1007	GLU	CA-C-N	-5.09	112.58	120.31
1	B	1007	GLU	C-N-CA	-5.09	112.58	120.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1331	LYS	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	A	8176	0	8192	467	0
1	B	8176	0	8192	496	0
All	All	16352	0	16384	861	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 26.

The worst 5 of 861 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1224:TYR:HA	1:B:1227:LEU:HD12	1.50	0.93
1:A:1015:LYS:HZ1	1:B:1016:ILE:HG12	1.33	0.90
1:A:1755:LYS:HA	1:A:1758:MET:HE2	1.56	0.87
1:A:1223:TYR:OH	1:B:1226:GLN:NE2	2.09	0.85
1:A:1582:PHE:HB3	1:A:1586:ARG:HH12	1.45	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1007/1949 (52%)	999 (99%)	8 (1%)	0	100	100
1	B	1007/1949 (52%)	989 (98%)	18 (2%)	0	100	100
All	All	2014/3898 (52%)	1988 (99%)	26 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	A	866/1669 (52%)	865 (100%)	1 (0%)	88	88
1	B	866/1669 (52%)	863 (100%)	3 (0%)	86	84
All	All	1732/3338 (52%)	1728 (100%)	4 (0%)	85	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1089	ILE
1	B	1514	GLN
1	B	1635	ASN
1	B	1653	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1226	GLN
1	B	1734	GLN
1	B	1250	GLN
1	B	1635	ASN
1	B	1836	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.

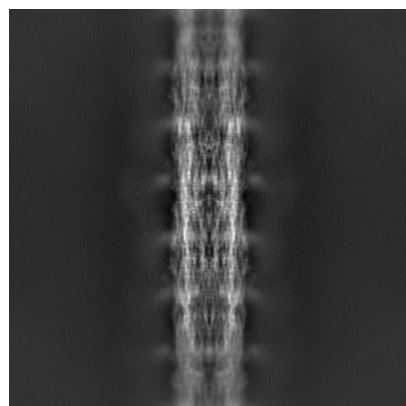
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42024. These allow visual inspection of the internal detail of the map and identification of artifacts.

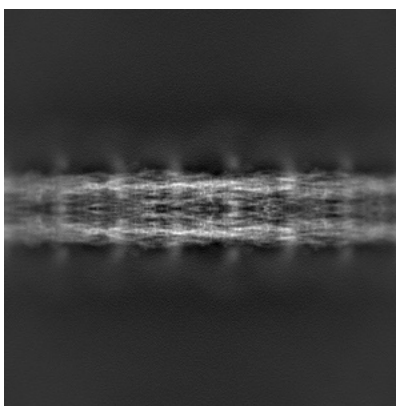
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

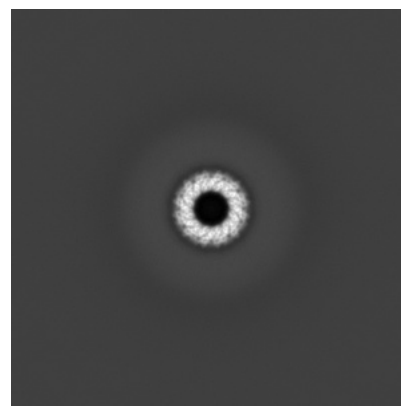
6.1.1 Primary map



X

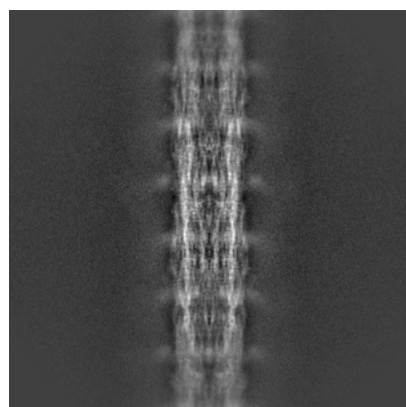


Y

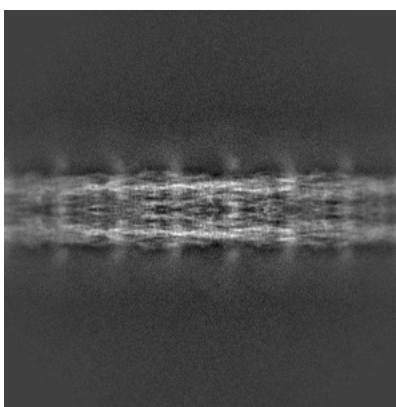


Z

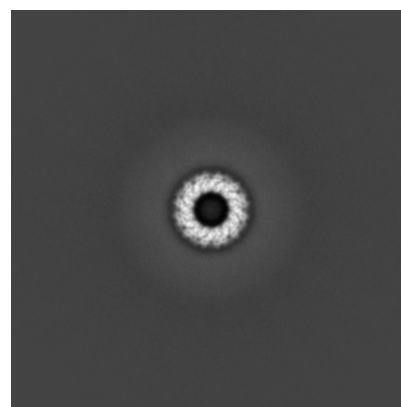
6.1.2 Raw map



X



Y

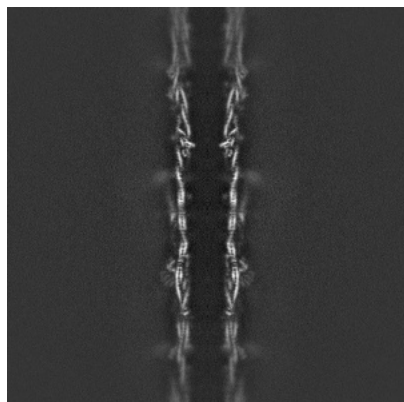


Z

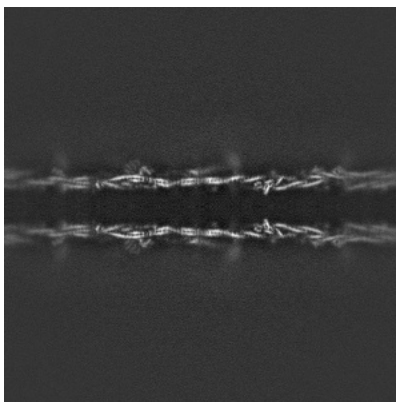
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

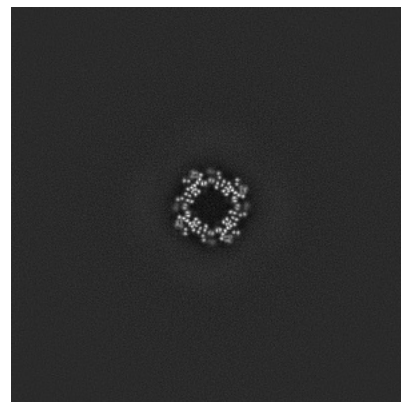
6.2.1 Primary map



X Index: 384

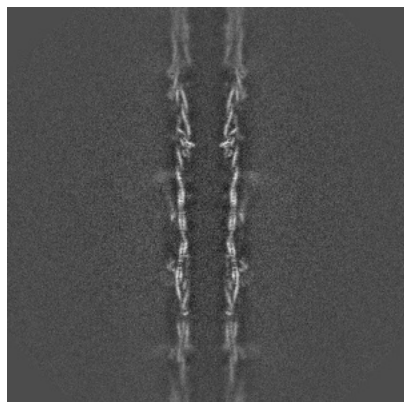


Y Index: 384

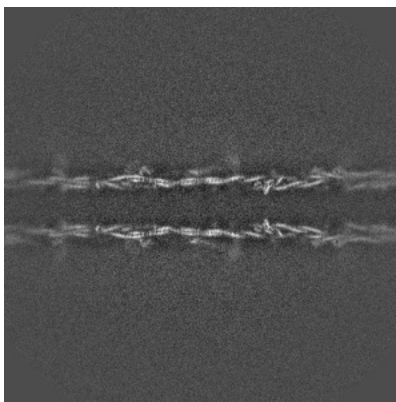


Z Index: 384

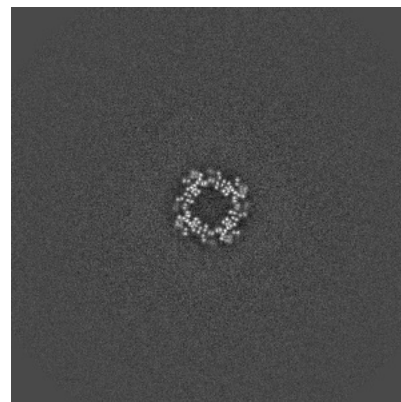
6.2.2 Raw map



X Index: 384



Y Index: 384

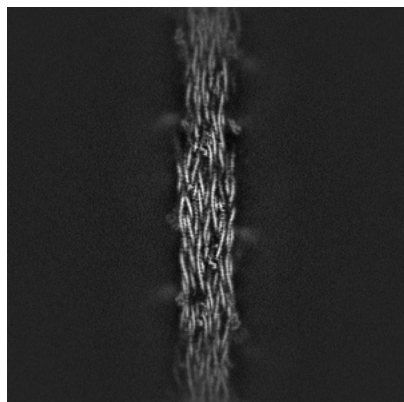


Z Index: 384

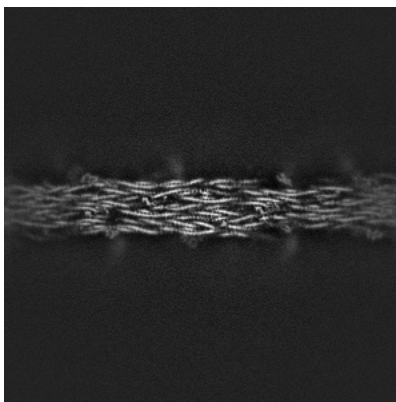
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

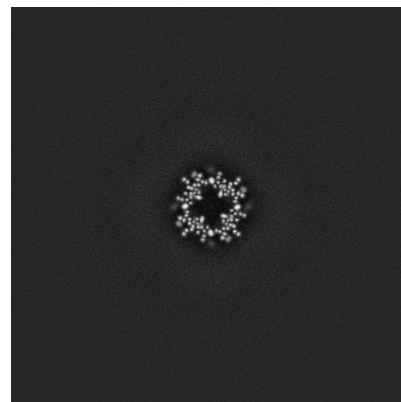
6.3.1 Primary map



X Index: 429

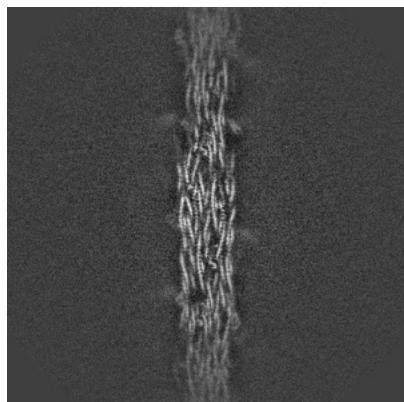


Y Index: 339

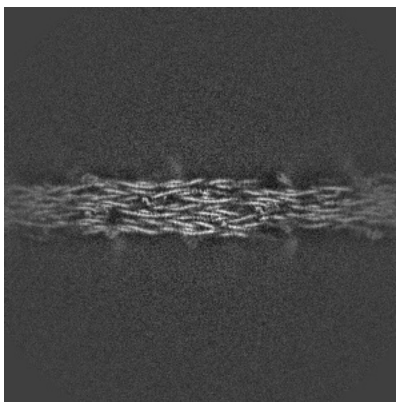


Z Index: 395

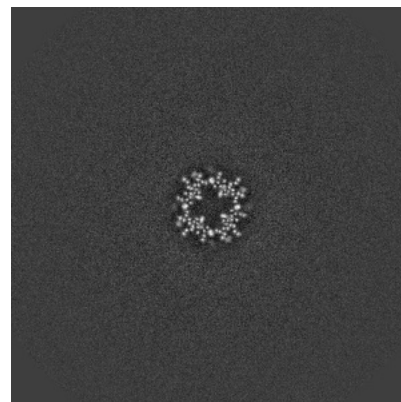
6.3.2 Raw map



X Index: 429



Y Index: 339

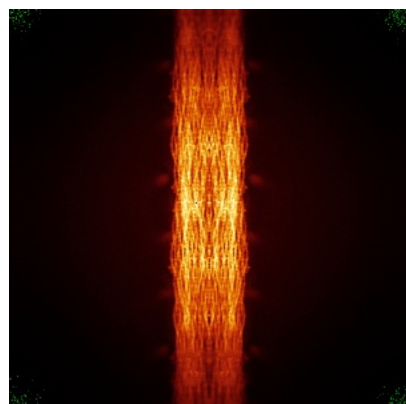


Z Index: 395

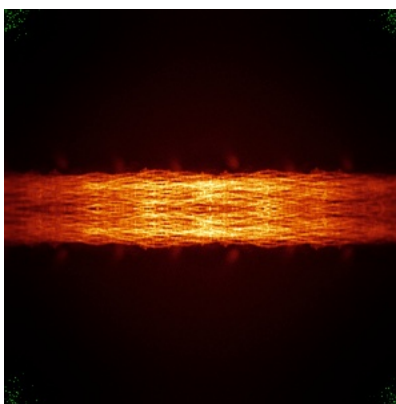
The images above show the largest variance slices of the map in three orthogonal directions.

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

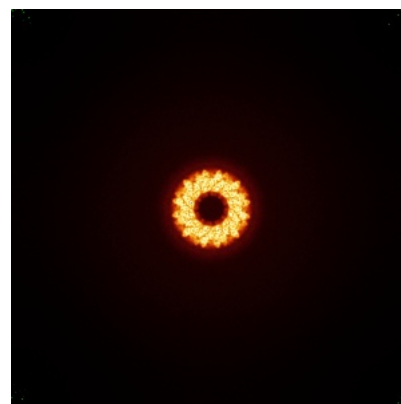
6.4.1 Primary map



X

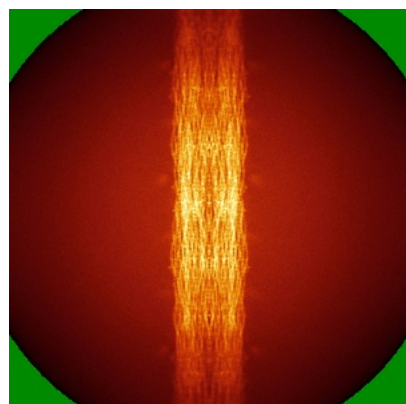


Y

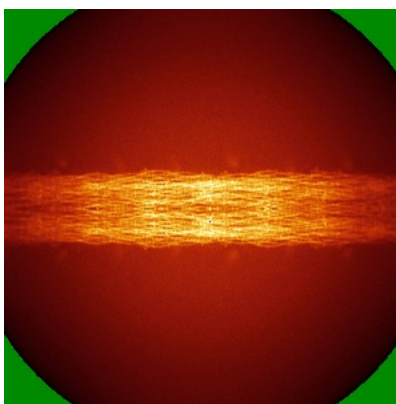


Z

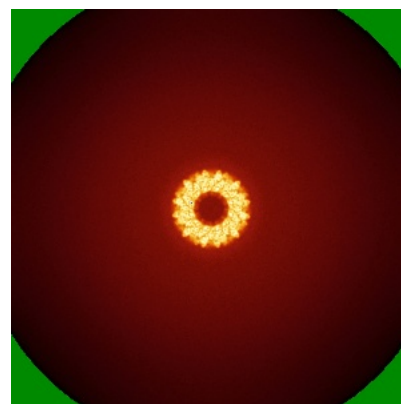
6.4.2 Raw map



X



Y

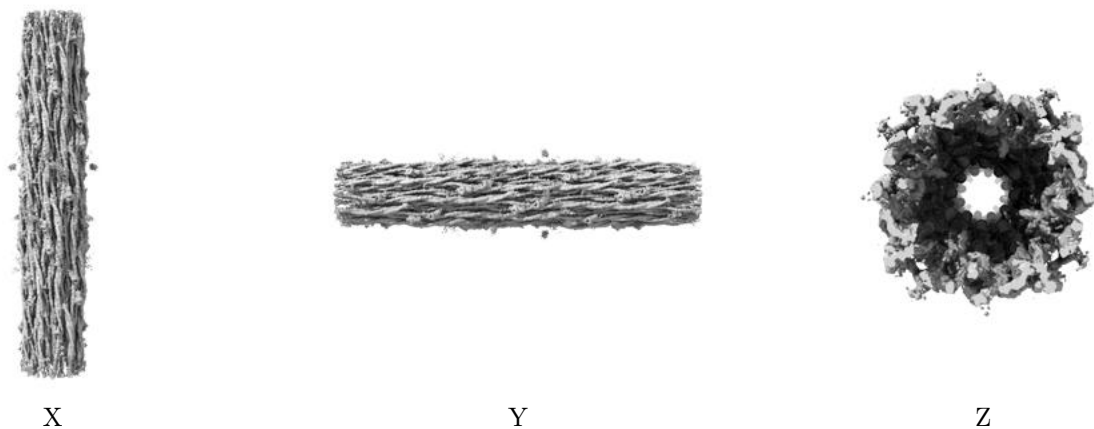


Z

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.

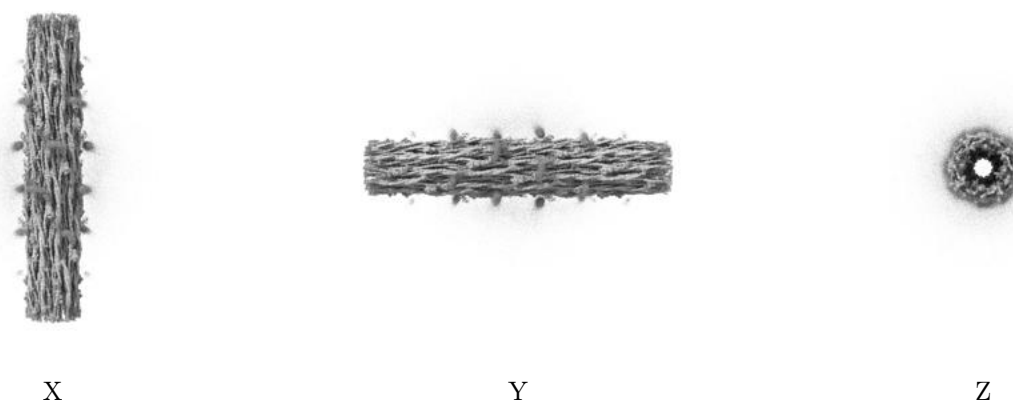
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.79. 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.

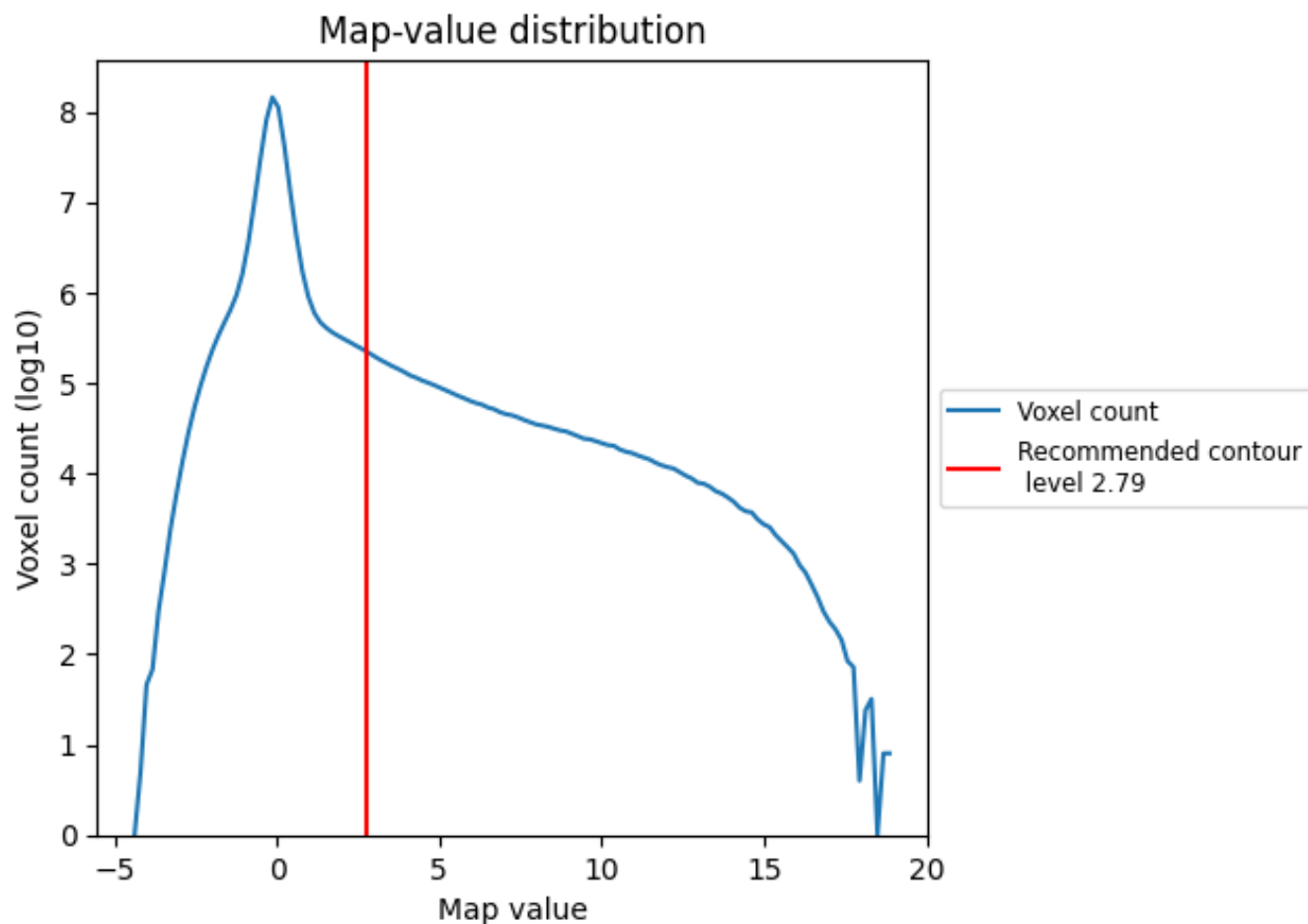
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

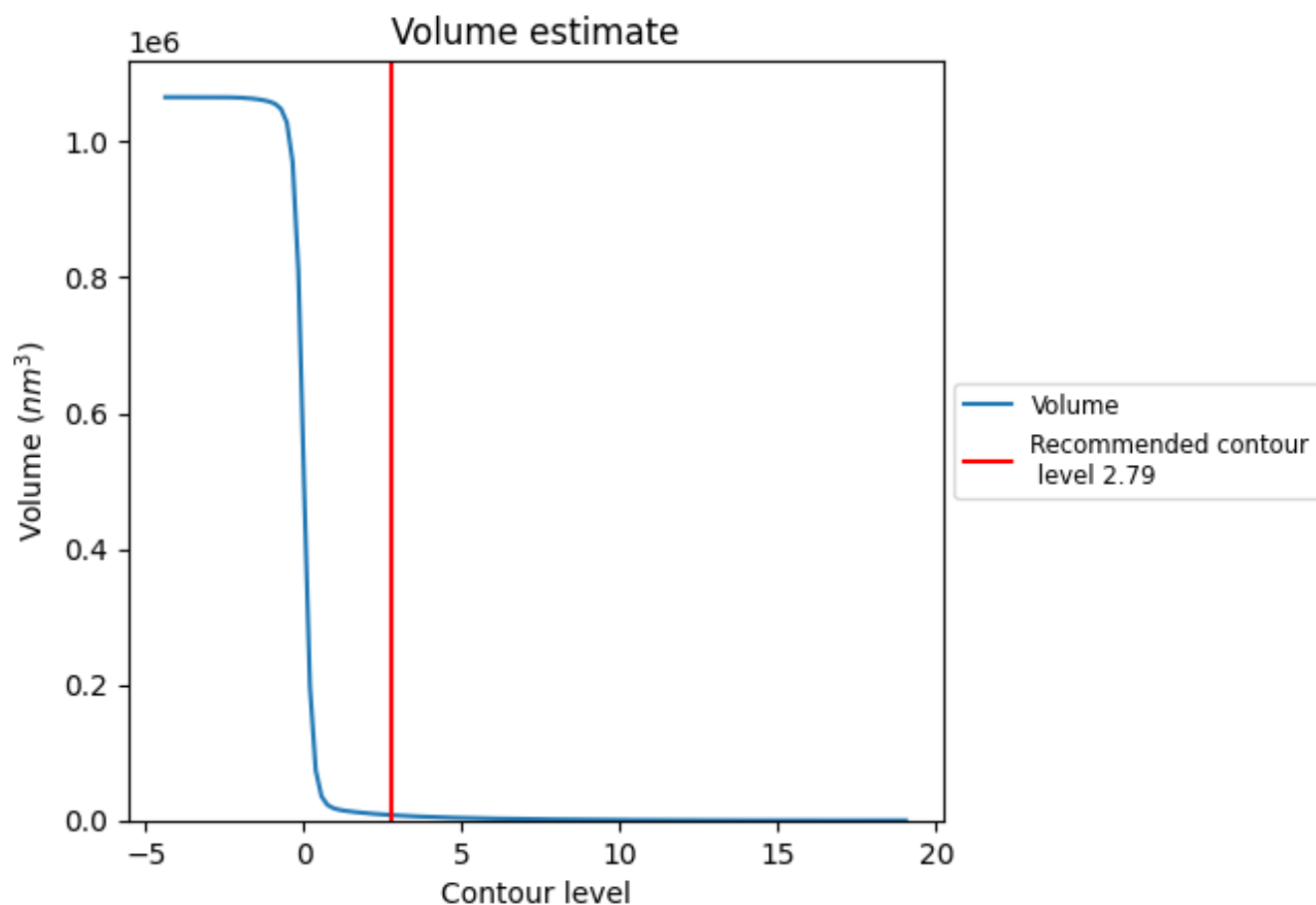
This section contains the results of statistical analysis of the map.

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.

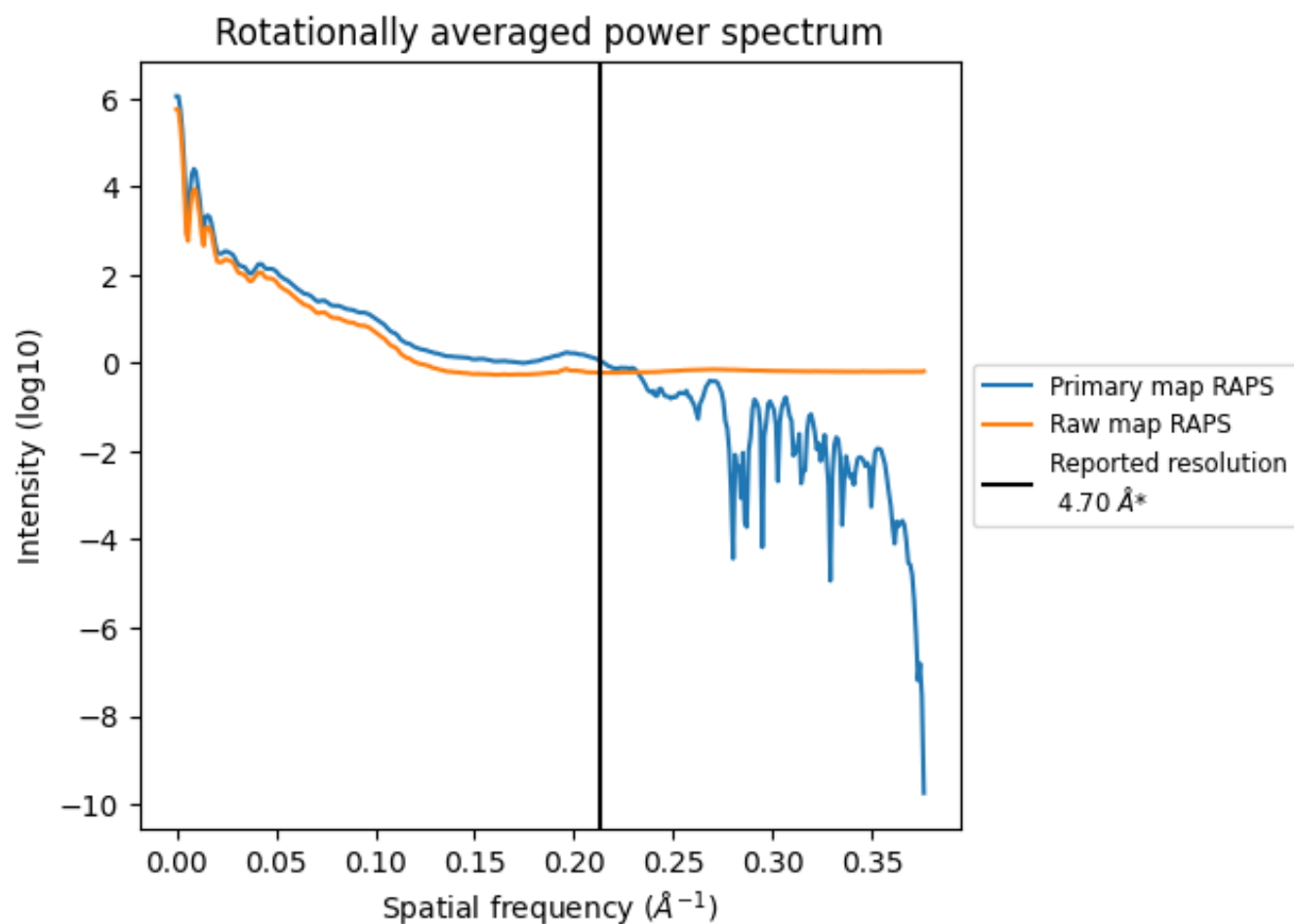
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7791 nm³; this corresponds to an approximate mass of 7038 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 ⓘ

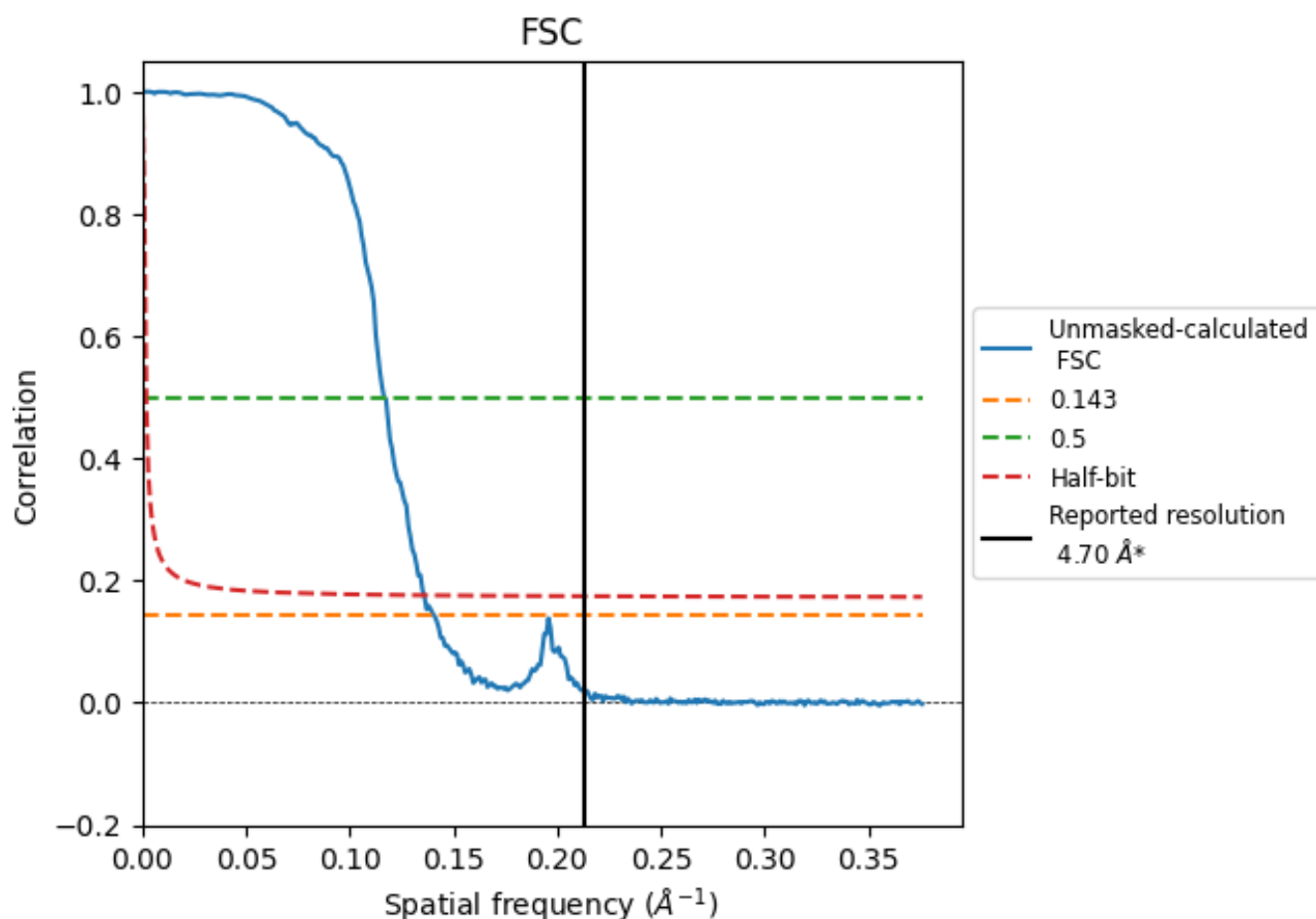


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 $\text{\AA}^{-1}$

8.2 Resolution estimates ⓘ

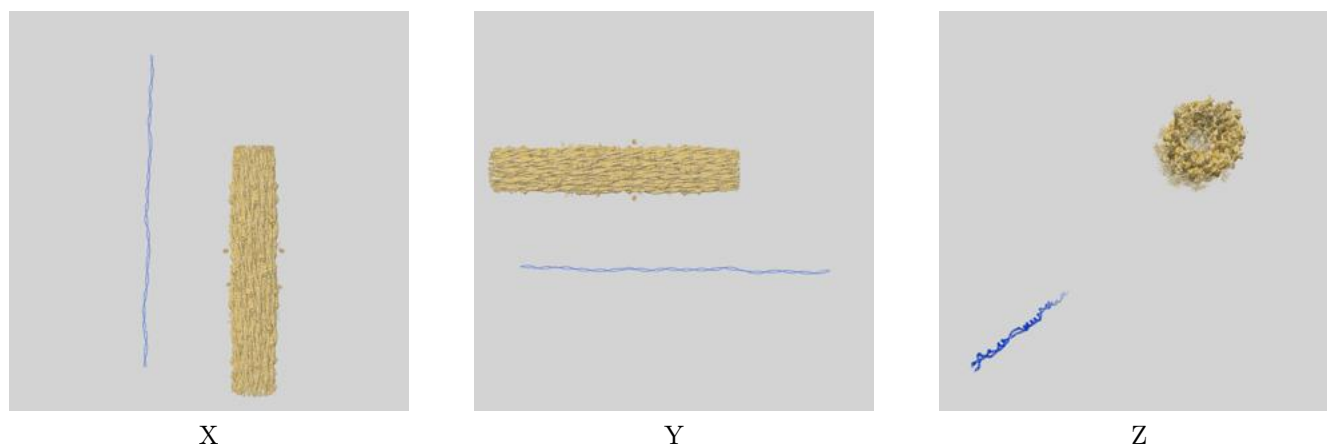
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	4.70
Author-provided FSC curve	-	-	-	-
Unmasked-calculated*	7.11	8.57	7.36	-

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

9 Map-model fit [i](#)

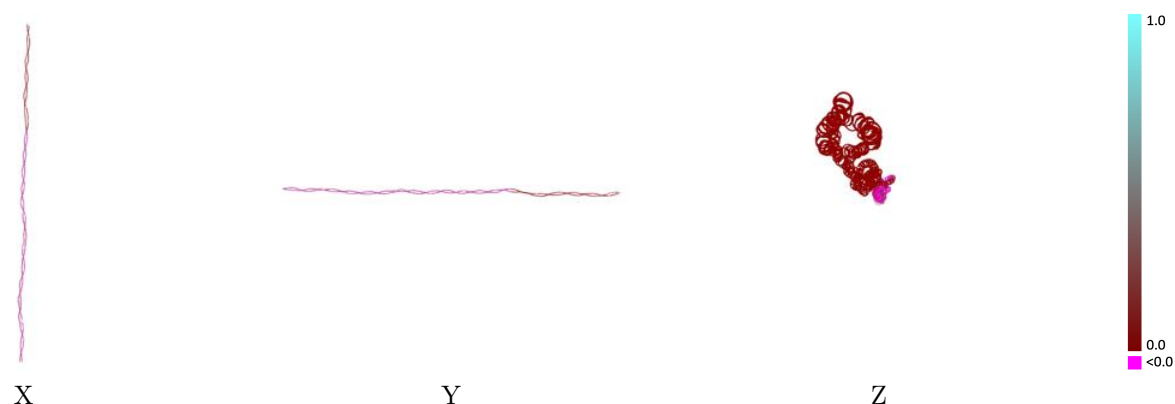
This section contains information regarding the fit between EMDB map EMD-42024 and PDB model 8U95. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



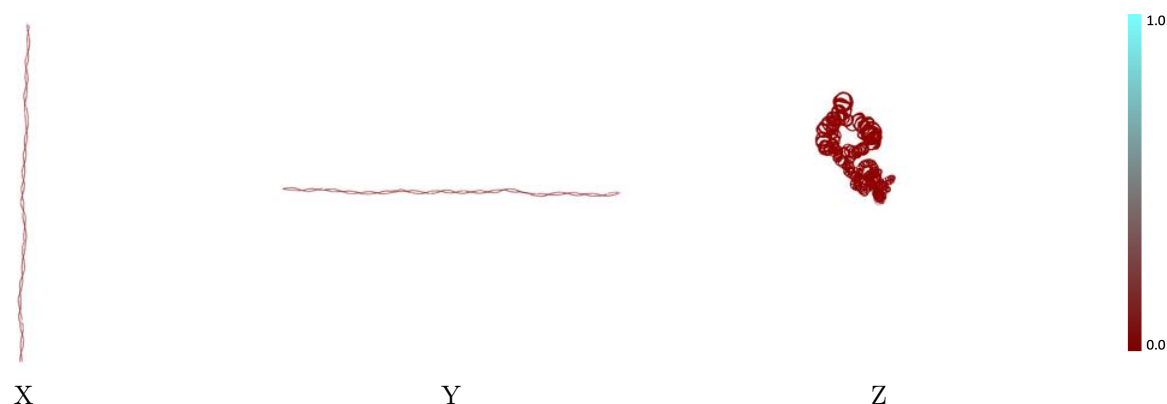
The images above show the 3D surface view of the map at the recommended contour level 2.79 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



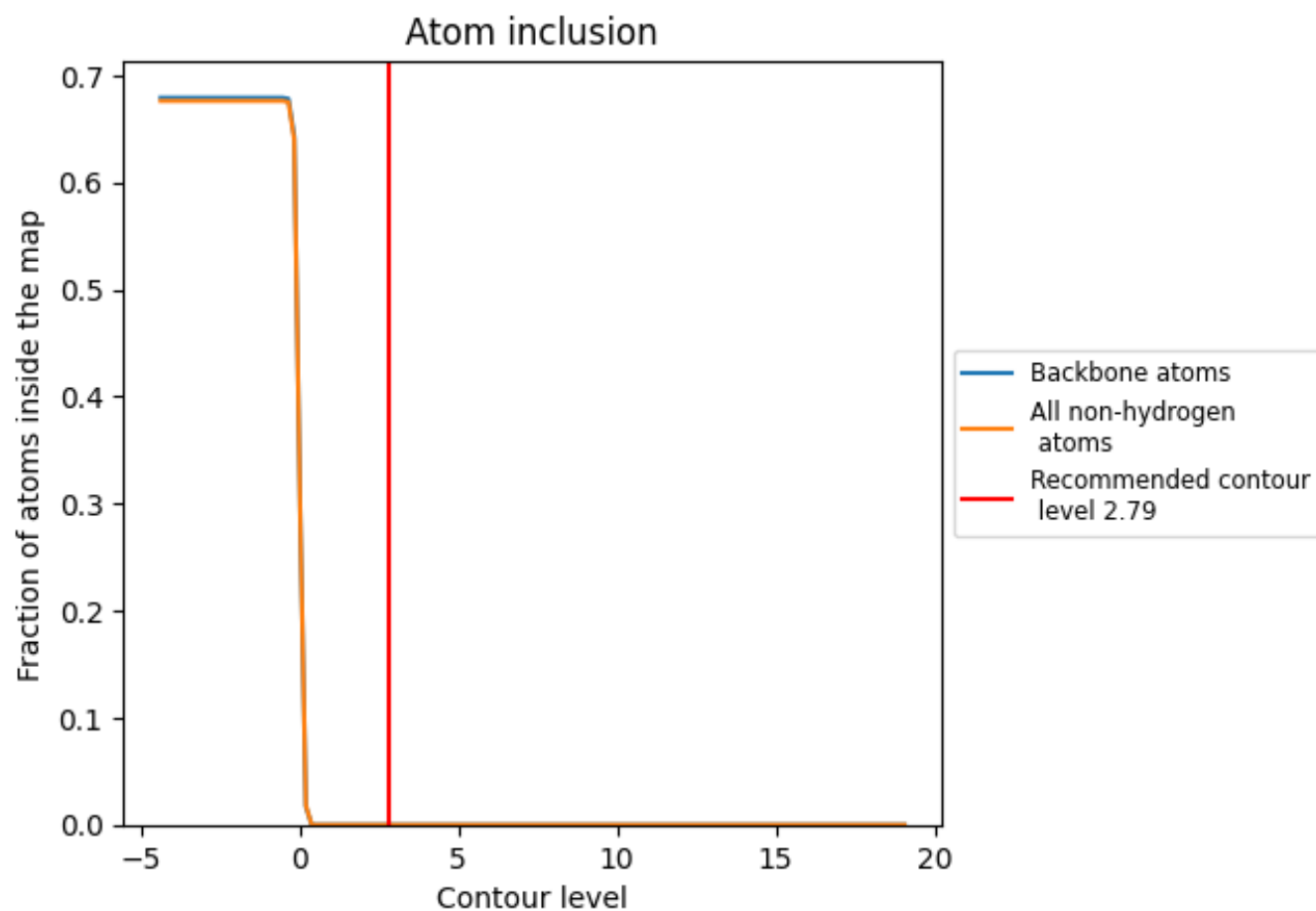
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.79).

9.4 Atom inclusion ⓘ



At the recommended contour level, 0% of all backbone atoms, 0% 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 (2.79) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0010
A	0.0000	0.0030
B	0.0000	-0.0010

