



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 10:37 PM EST

PDB ID : 7JPU
EMDB ID : EMD-22423
Title : Structure of an endocytic receptor
Authors : Gully, B.S.; Rossjohn, J.; Berry, R.
Deposited on : 2020-08-09
Resolution : 5.00 Å(reported)
Based on initial models : 1DQO, 1QDD, 2V5P

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.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) : 2.31.2

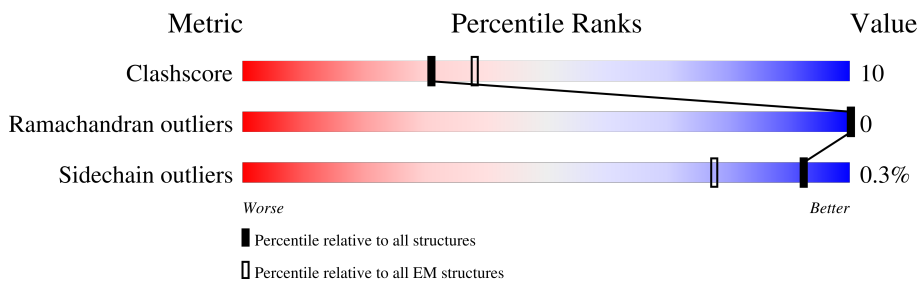
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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
Sidechain outliers	154315	3826

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	1722	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 51% 16% 33%</p>
1	B	1722	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8% 52% 15% 33%</p>
1	C	1722	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8% 51% 16% 33%</p>
1	D	1722	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">8% 53% 14% 33%</p>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 35936 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 Lymphocyte antigen 75.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1156	Total 8986	C 5794	N 1522	O 1611	S 59	0	0
1	B	1156	Total 8986	C 5794	N 1522	O 1611	S 59	0	0
1	C	1156	Total 8986	C 5794	N 1522	O 1611	S 59	0	0
1	D	1155	Total 8978	C 5788	N 1521	O 1610	S 59	0	0

VAL	N585	E873	Y776	S842	L926	I1012	GLU	E1300	GLY	E1300	LYS	ASP	LYS	ASP	HIS
GLU	W586	A674	L777	N643	P927	G1013	THR	Q1301	ASN	Q1301	ARG	TYR	ASP	ASP	ASP
THR	N587	A680	R778	H644	E931	L1014	V1108	L1302	THR	L1302	GLU	THR	GLY	GLY	GLY
VAL	E590	A683	P779	S845	LYS	W1025	I1117	L1306	LYS	L1306	PHE	GLU	PHE	ALA	ALA
ASP	P591	H684	C782	A664	TYR	E1030	P1119	A1309	ASN	A1309	LEU	THR	ASN	TYR	TYR
THR	V598	V691	D783	N665	VAL	T1031	K1120	A1311	VAL	A1311	THR	THR	THR	THR	THR
TYR	A599	V695	E787	I666	SER	T1032	T1121	V1312	PRO	V1312	GLY	PRO	GLY	GLY	GLY
SER	M600	K695	TRP	S667	LEU	Y1033	L1123	G1315	VAL	G1315	SER	PRO	PRO	PRO	PRO
D359	V607	E896	VAL	G668	GLU	L1039	W1124	I1316	ASP	I1316	PHE	ASP	ASP	ASP	ASP
T359	G607	E896	THR	D669	LYS	L1040	K1128	T1317	VAL	T1317	VAL	VAL	VAL	VAL	VAL
A363	K608	L701	CYS	K672	TYR	G1043	L1132	I1318	LYS	I1318	LYS	TYR	TYR	TYR	TYR
C364	V611	F705	GLN	R676	PRO	I1047	L1138	Y1318	PRO	Y1318	GLY	GLY	GLY	GLY	GLY
W365	I622	W710	ILE	S678	ASP	PRO	V1139	R1319	SER	R1319	GLU	GLU	GLU	GLU	GLU
G370	K625	L711	LYS	S679	SER	GLU	L1155	N1320	PRO	N1320	GLY	GLY	GLY	GLY	GLY
F371	MET	W712	ARG	E679	ALA	ASN	L1161	T1329	VAL	T1329	THR	THR	THR	THR	THR
G372	SER	I713	THR	H680	ALA	PHE	L1162	P1330	LEU	P1330	THR	THR	THR	THR	THR
Y373	ASN	G714	PRO	P681	VAL	PHE	W1162	L1331	ASN	L1331	VAL	VAL	VAL	VAL	VAL
L374	ASP	L715	LYS	S681	GLN	GLU	I1163	H1335	THR	H1335	THR	THR	THR	THR	THR
L375	ALA	P720	THR	I682	CYS	GLU	G1164	W1336	TRP	W1336	GLN	GLN	GLN	GLN	GLN
V376	SER	ASP	PRO	D683	SER	GLU	L1165	R1337	PRO	R1337	ASP	ASP	ASP	ASP	ASP
N377	GLY	TRP	ASP	H684	GLU	SER	F1166	A1338	THR	A1338	THR	THR	THR	THR	THR
E378	LEU	G724	TRP	H685	TRP	ILE	E1171	L1349	THR	L1349	THR	THR	THR	THR	THR
S379	LYS	W728	ASN	PHE	ILE	C1060	F1178	S1353	THR	S1353	THR	THR	THR	THR	THR
N380	GLU	I729	PRO	THR	THR	A1061	D1178	T1354	VAL	T1354	THR	THR	THR	THR	THR
K384	ALA	D730	ASP	SER	THR	L1062	F1184	H1356	GLU	H1356	GLU	GLU	GLU	GLU	GLU
K388	PRO	S731	PRO	ARG	ARG	I1063	S1185	G1357	LEU	G1357	LEU	LEU	LEU	LEU	LEU
C389	PRO	R731	LYS	ARG	ARG	L1064	R1186	F1357	LEU	R1186	LEU	LEU	LEU	LEU	LEU
C390	ASP	T732	GLY	ARG	THR	M1065	W1187	I1360	LEU	W1187	LEU	LEU	LEU	LEU	LEU
A392	TRP	I732	ILE	HIS	HIS	Q1067	W1187	Q1361	ALA	W1187	ALA	ALA	ALA	ALA	ALA
ALA	K508	G737	GLY	ARG	ARG	K1068	W1187	D1270	VAL	D1270	VAL	VAL	VAL	VAL	VAL
S393	C514	I737	PRO	THR	THR	T1078	N1191	E1272	GLY	E1272	GLY	GLY	GLY	GLY	GLY
S394	Y515	M738	PRO	PHE	PHE	S1079	L1194	H1273	LEU	L1194	LEU	LEU	LEU	LEU	LEU
D395	T526	I739	PRO	THR	THR	C1080	E1195	V1274	LEU	E1195	LEU	LEU	LEU	LEU	LEU
L396	R535	F740	PRO	THR	THR	H1084	D1196	H1275	ALA	D1196	ALA	ALA	ALA	ALA	ALA
I397	N542	M741	PRO	PHE	PHE	H1088	C1197	T1275	VAL	C1197	VAL	VAL	VAL	VAL	VAL
K411	M545	E742	PRO	GLY	GLY	L1088	V1198	K1276	ASP	V1198	ASP	ASP	ASP	ASP	ASP
L412	F556	F743	PRO	GLU	GLU	Y1092	T1202	K1277	HIS	T1202	HIS	HIS	HIS	HIS	HIS
H413	F559	Q744	PRO	ASP	ASP	SER	T1208	Q1278	ASN	T1208	ASN	ASN	ASN	ASN	ASN
M414	G559	Q745	PRO	ASP	ASP	VAL	Y1209	K1279	ASN	Y1209	ASN	ASN	ASN	ASN	ASN
E415	E568	D746	PRO	ASP	ASP	VAL	D1210	H1279	ASN	D1210	ASN	ASN	ASN	ASN	ASN
E419	F566	Y747	PRO	ASP	ASP	VAL	P1216	L1286	THR	P1216	THR	THR	THR	THR	THR
E420	H661	D748	PRO	ASP	ASP	VAL	G1217	L1287	THR	G1217	THR	THR	THR	THR	THR
W421	G559	I749	PRO	ASP	ASP	LYS	A1218	S1288	THR	A1218	THR	THR	THR	THR	THR
W422	E568	R750	PRO	ASP	ASP	ARG	I1219	L1378	THR	I1219	THR	THR	THR	THR	THR
S437	A572	D751	PRO	ASP	ASP	THR	P1216	S1376	THR	P1216	THR	THR	THR	THR	THR
D438	A572	C752	PRO	ASP	ASP	LEU	G1217	L1377	THR	G1217	THR	THR	THR	THR	THR
G439	G576	A753	PRO	ASP	ASP	GLN	A1218	L1378	THR	A1218	THR	THR	THR	THR	THR
T440	F563	M754	PRO	ASP	ASP	ASN	I1219	C1379	THR	I1219	THR	THR	THR	THR	THR
Y465	S584	V755	PRO	ASP	ASP	ALA	Y1221	K1293	THR	Y1221	THR	THR	THR	THR	THR
L466	E672	W757	PRO	ASP	ASP	SER	Y1222	F1297	THR	Y1222	THR	THR	THR	THR	THR
		F758	PRO	ASP	ASP	THR	S1223	V1298	THR	V1298	THR	THR	THR	THR	THR
		H759	PRO	ASP	ASP	THR		L1299	THR	L1299	THR	THR	THR	THR	THR
		R772	PRO	ASP	ASP	THR			THR		THR	THR	THR	THR	THR
		E773	PRO	ASP	ASP	THR			THR		THR	THR	THR	THR	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	102569	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 ($e^-/\text{\AA}^2$)	63	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	0.071	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	248.04, 248.04, 248.04	wwPDB
Map dimensions	234, 234, 234	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.24	0/9247	0.45	1/12580 (0.0%)
1	B	0.24	0/9247	0.44	1/12580 (0.0%)
1	C	0.24	0/9247	0.45	1/12580 (0.0%)
1	D	0.24	0/9239	0.44	2/12569 (0.0%)
All	All	0.24	0/36980	0.45	5/50309 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1370	VAL	C-N-CA	6.15	137.07	121.70
1	C	1370	VAL	C-N-CA	6.12	137.00	121.70
1	D	1370	VAL	C-N-CA	6.11	136.97	121.70
1	B	1370	VAL	C-N-CA	6.00	136.69	121.70
1	D	412	LEU	CA-CB-CG	5.61	128.20	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8986	0	8303	186	0
1	B	8986	0	8303	161	0
1	C	8986	0	8303	185	0
1	D	8978	0	8292	155	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	35936	0	33201	672	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 10.

The worst 5 of 672 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:A:423:ILE:HG23	1:A:463:VAL:HG13	1.54	0.89
1:C:423:ILE:HG23	1:C:463:VAL:HG13	1.60	0.84
1:B:421:VAL:HB	1:B:465:TYR:HB2	1.63	0.80
1:B:69:TRP:HE1	1:B:73:HIS:HA	1.45	0.79
1:B:713:ILE:HG13	1:B:755:VAL:H	1.48	0.78

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	1130/1722 (66%)	1046 (93%)	84 (7%)	0	100	100
1	B	1130/1722 (66%)	1052 (93%)	78 (7%)	0	100	100
1	C	1130/1722 (66%)	1051 (93%)	79 (7%)	0	100	100
1	D	1129/1722 (66%)	1050 (93%)	79 (7%)	0	100	100
All	All	4519/6888 (66%)	4199 (93%)	320 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	913/1536 (59%)	912 (100%)	1 (0%)	93	96
1	B	913/1536 (59%)	909 (100%)	4 (0%)	91	94
1	C	913/1536 (59%)	911 (100%)	2 (0%)	93	96
1	D	912/1536 (59%)	908 (100%)	4 (0%)	91	94
All	All	3651/6144 (59%)	3640 (100%)	11 (0%)	92	95

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	241	LYS
1	D	664	ARG
1	D	1133	LYS
1	D	910	LYS
1	B	1277	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1252	GLN
1	D	1157	HIS
1	C	249	ASN
1	D	1037	HIS
1	D	585	ASN

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.

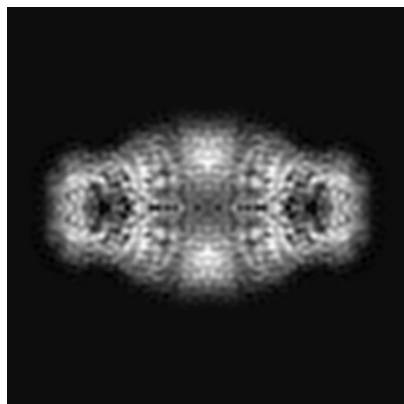
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22423. These allow visual inspection of the internal detail of the map and identification of artifacts.

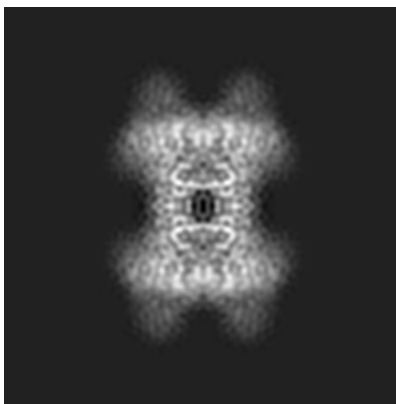
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

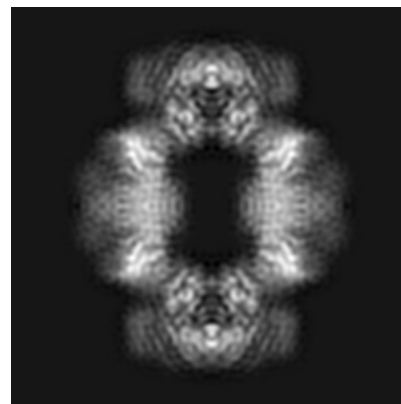
6.1.1 Primary map



X

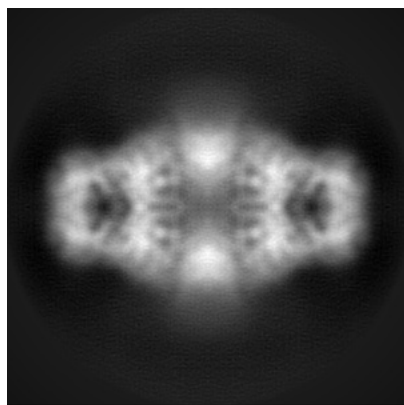


Y

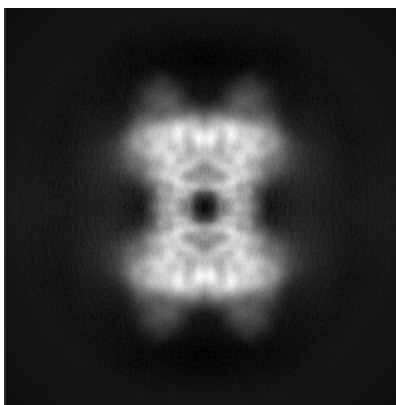


Z

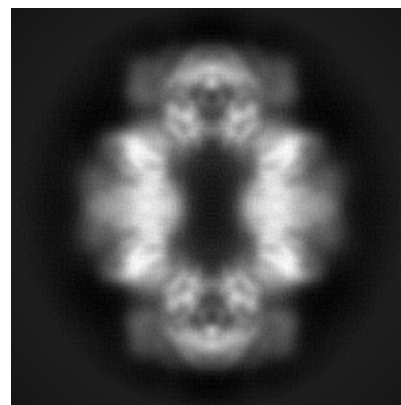
6.1.2 Raw map



X



Y



Z

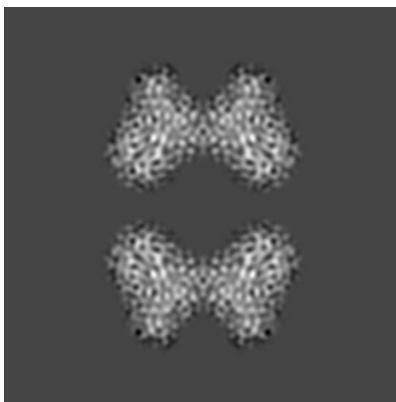
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 117

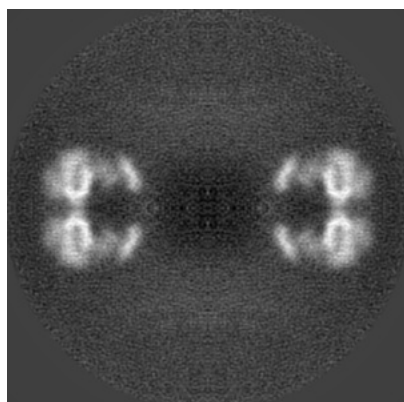


Y Index: 117

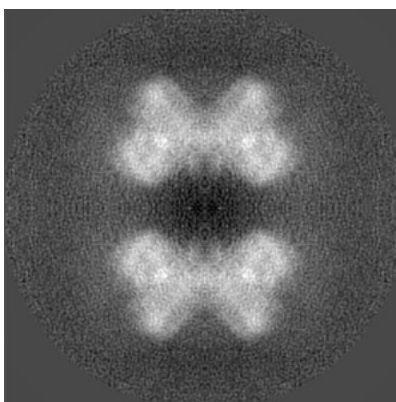


Z Index: 117

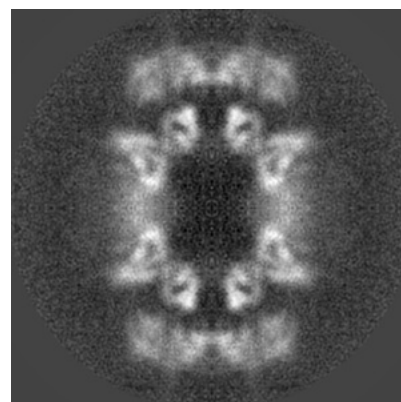
6.2.2 Raw map



X Index: 117



Y Index: 117

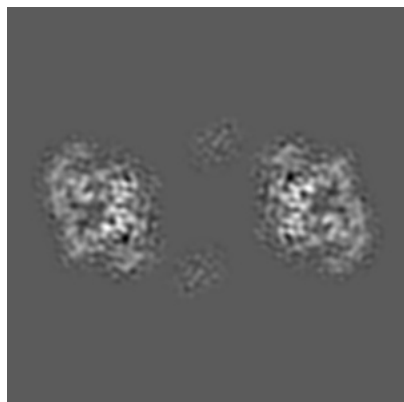


Z Index: 117

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: 130

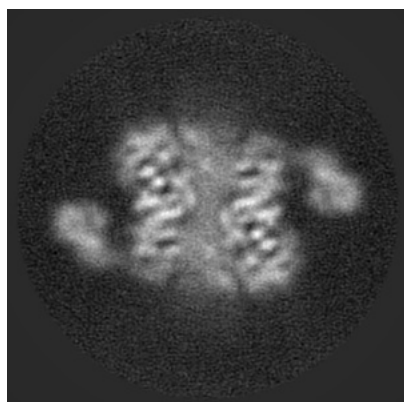


Y Index: 154

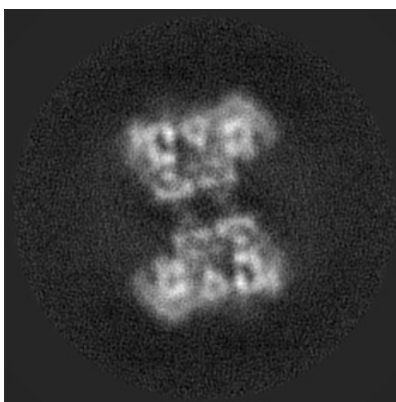


Z Index: 100

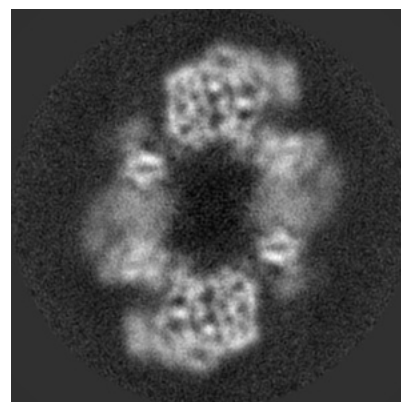
6.3.2 Raw map



X Index: 77



Y Index: 79

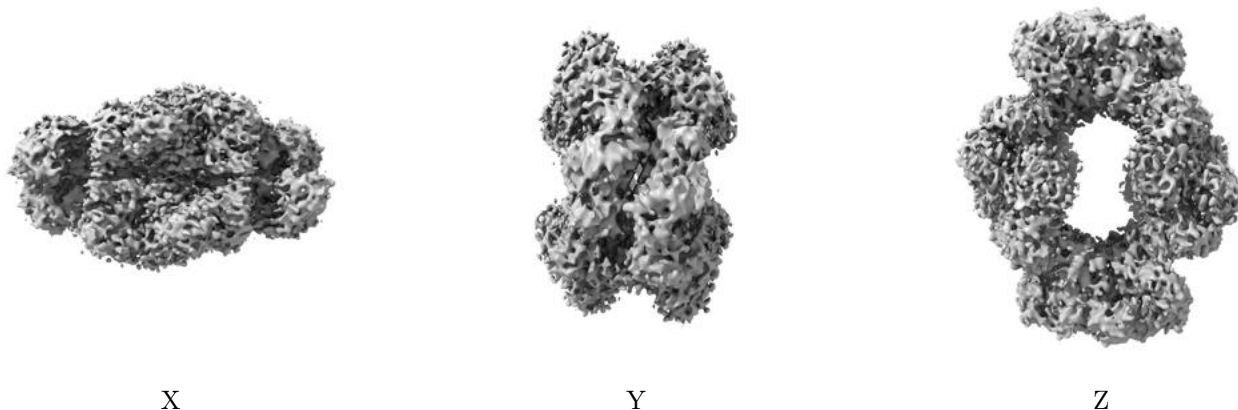


Z Index: 102

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

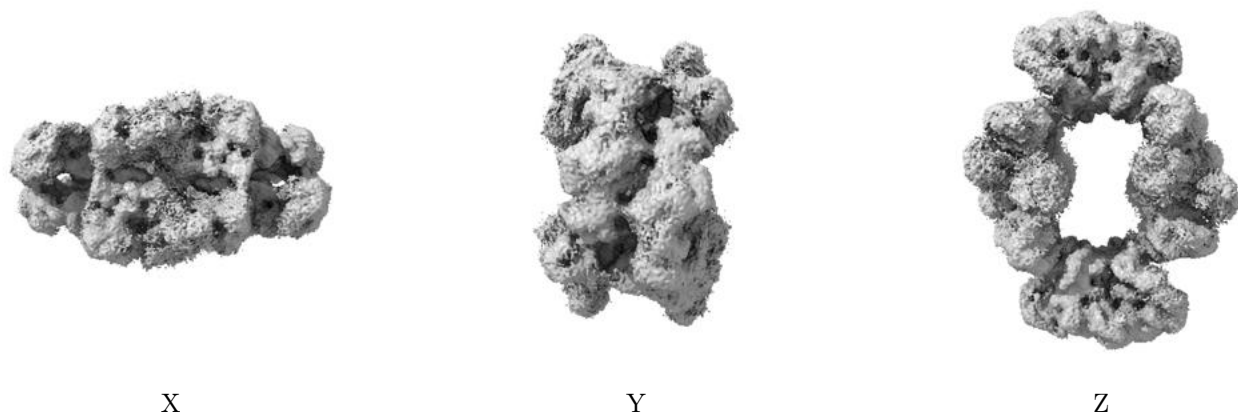
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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.

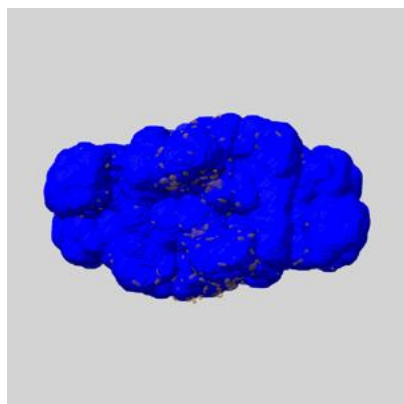
6.5 Mask visualisation [i](#)

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

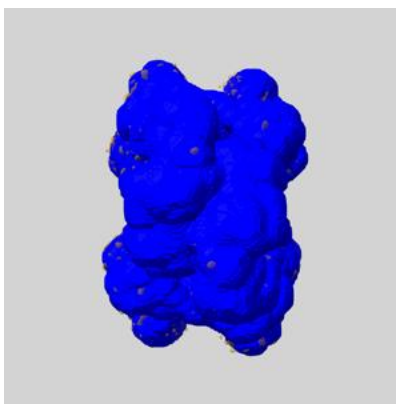
A mask typically either:

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

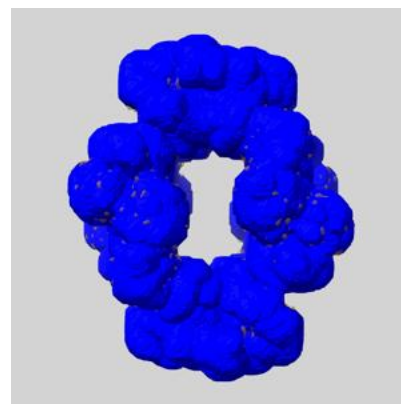
6.5.1 emd_22423_msk_1.map [i](#)



X



Y

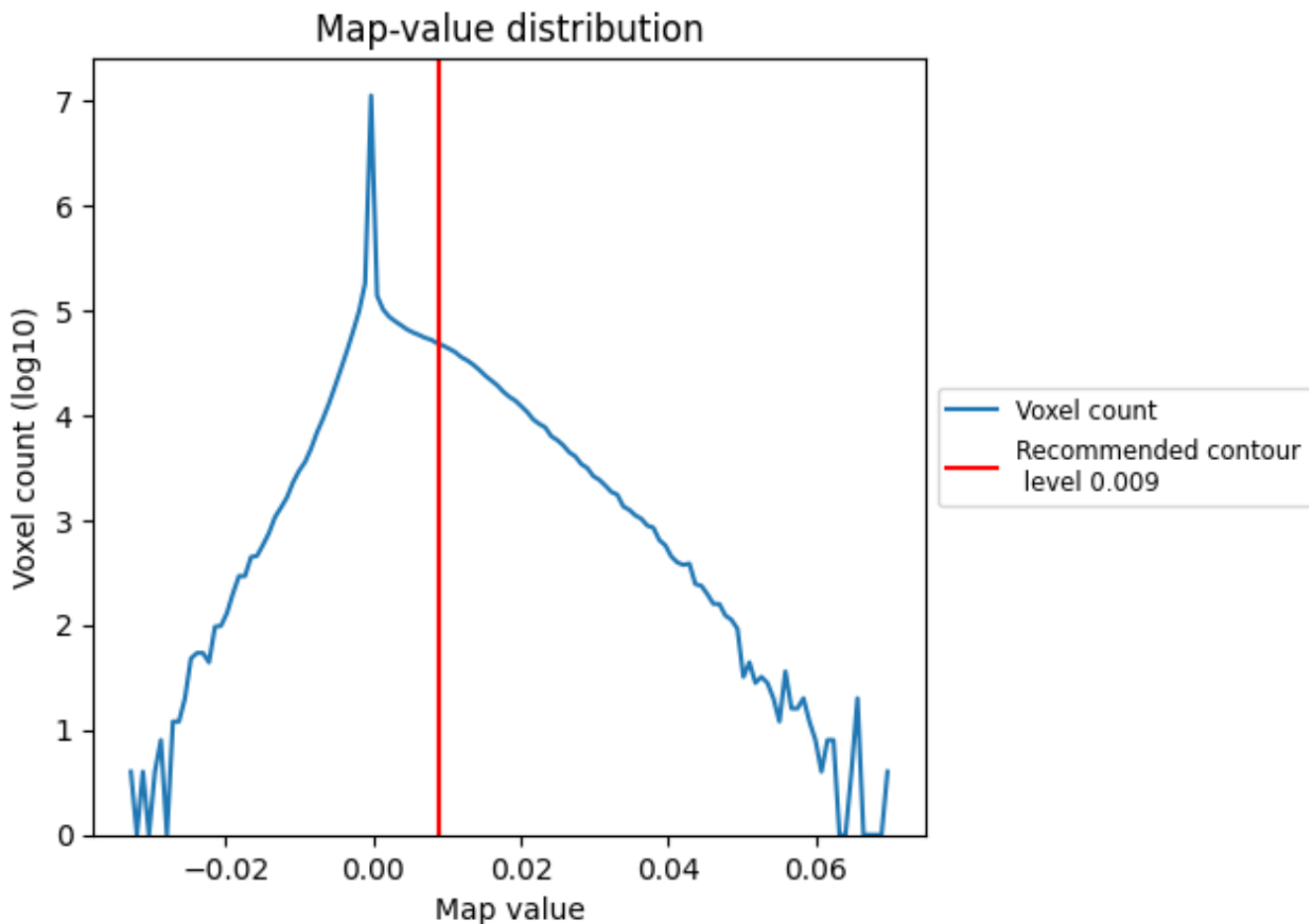


Z

7 Map analysis [i](#)

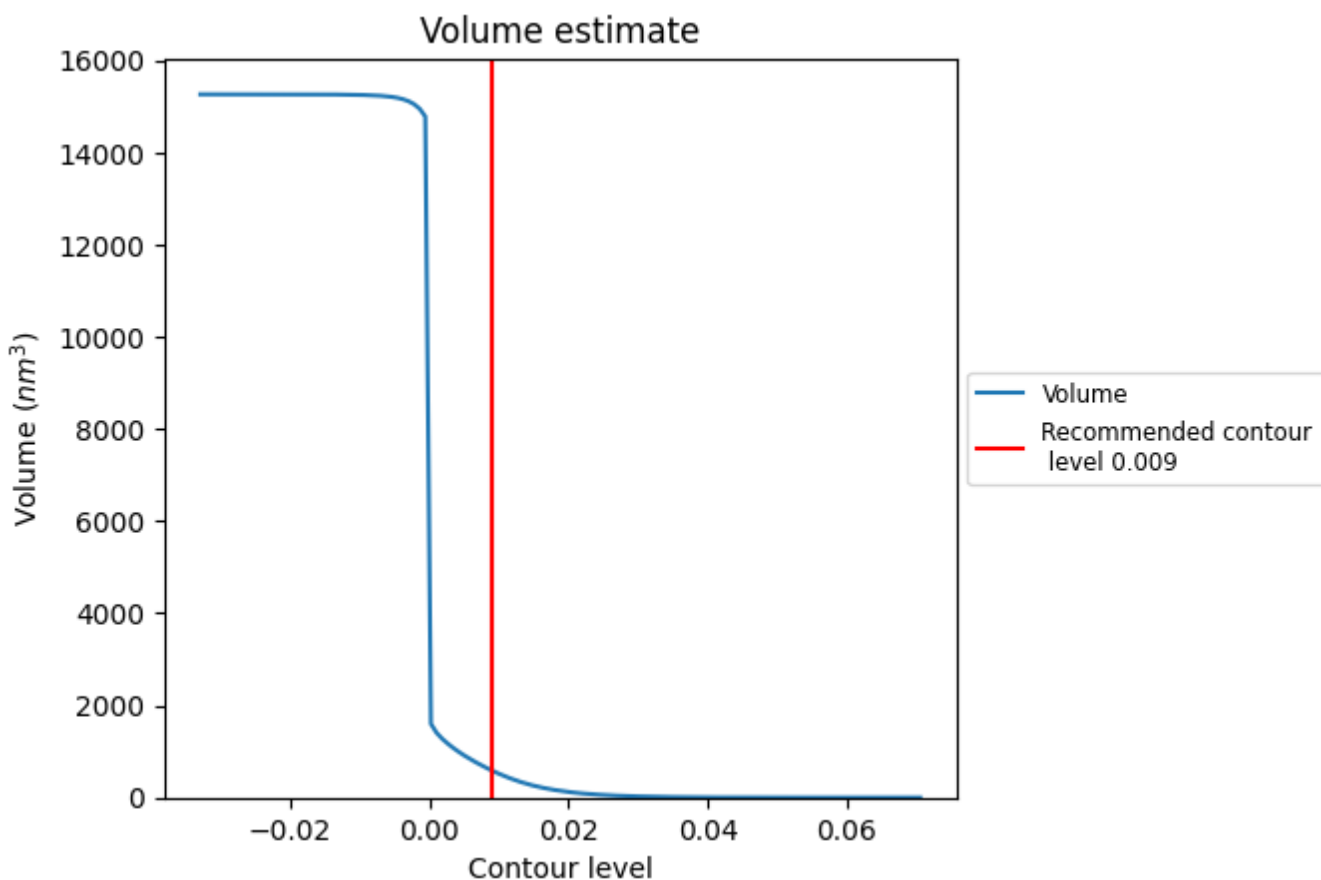
This section contains the results of statistical analysis of the map.

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.

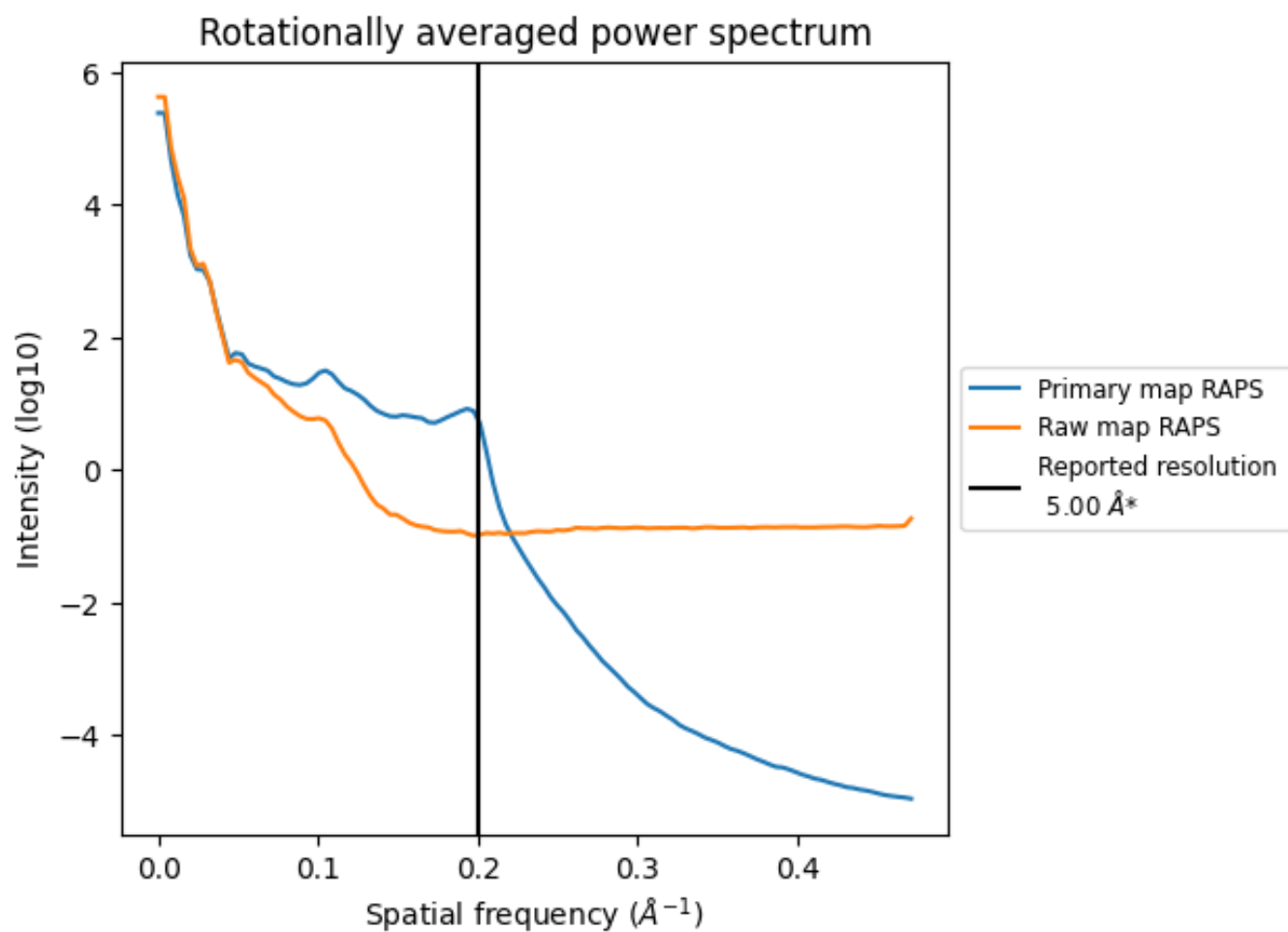
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 588 nm³; this corresponds to an approximate mass of 531 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 [i](#)

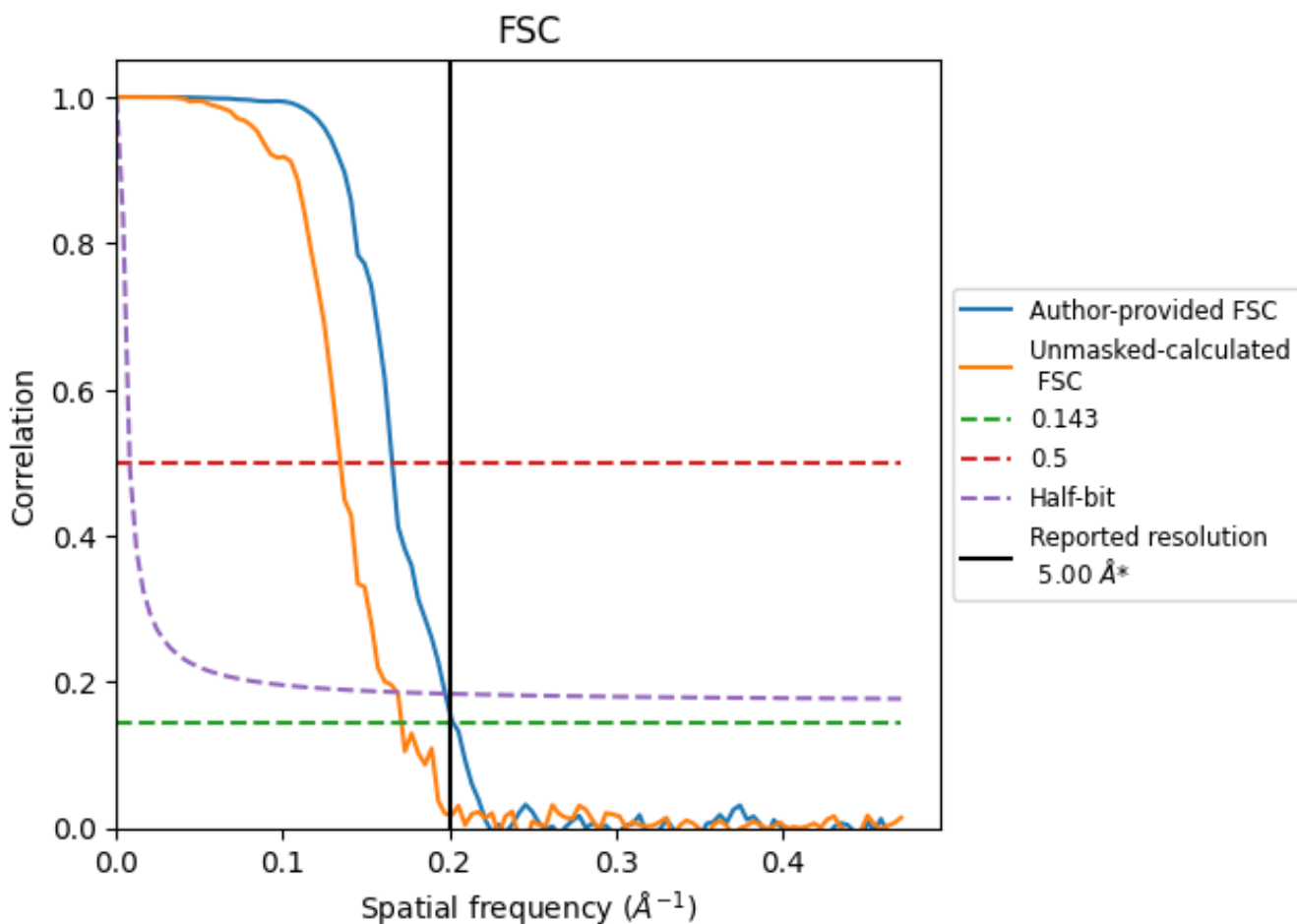


*Reported resolution corresponds to spatial frequency of 0.200 Å⁻¹

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 0.200 Å⁻¹

8.2 Resolution estimates [i](#)

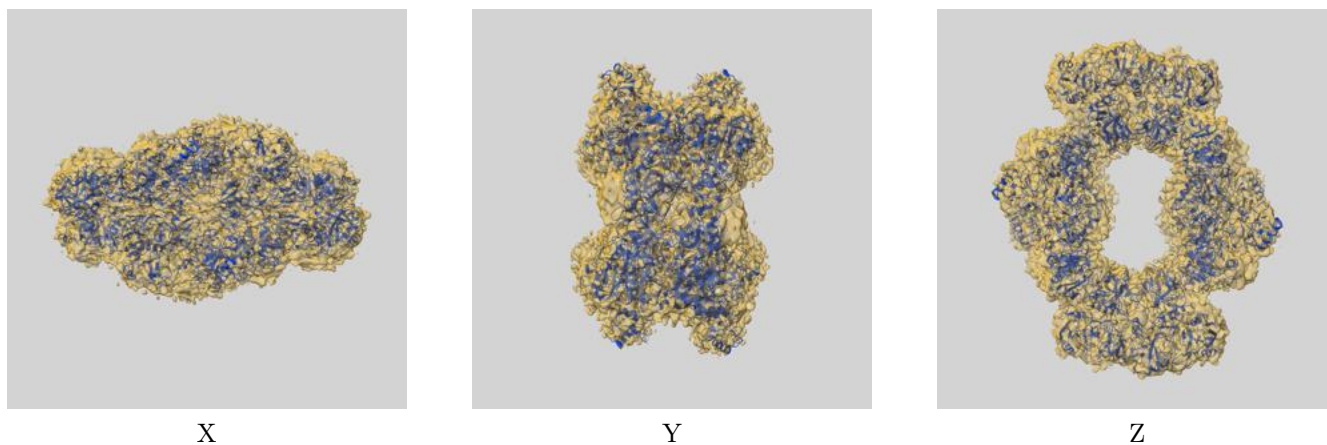
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	4.94	6.03	5.06
Unmasked-calculated*	5.83	7.43	5.93

*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 5.83 differs from the reported value 5.0 by more than 10 %

9 Map-model fit [i](#)

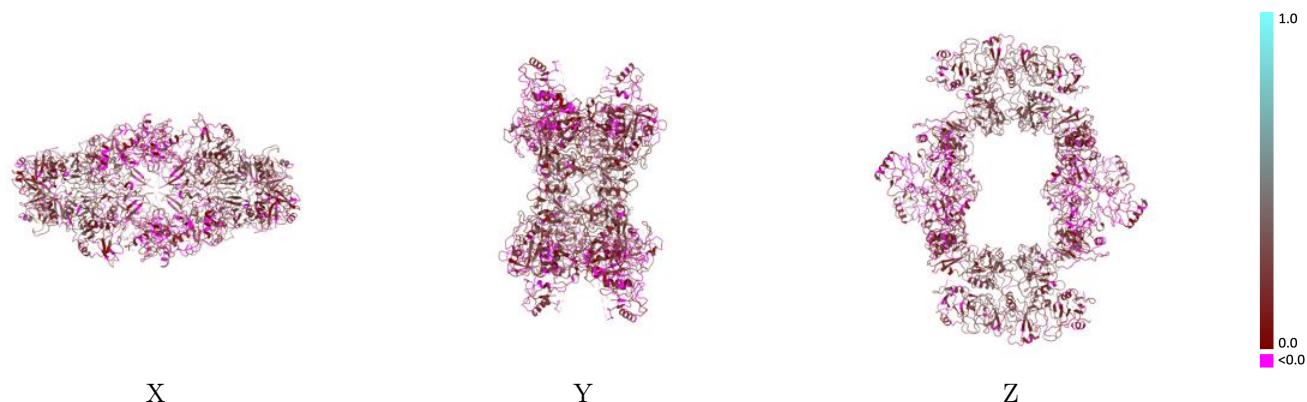
This section contains information regarding the fit between EMDB map EMD-22423 and PDB model 7JPU. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



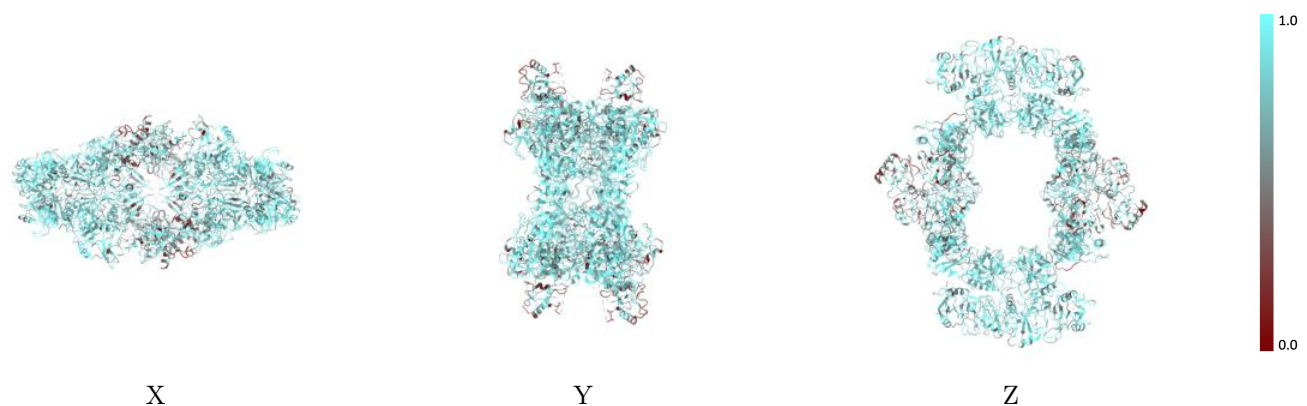
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



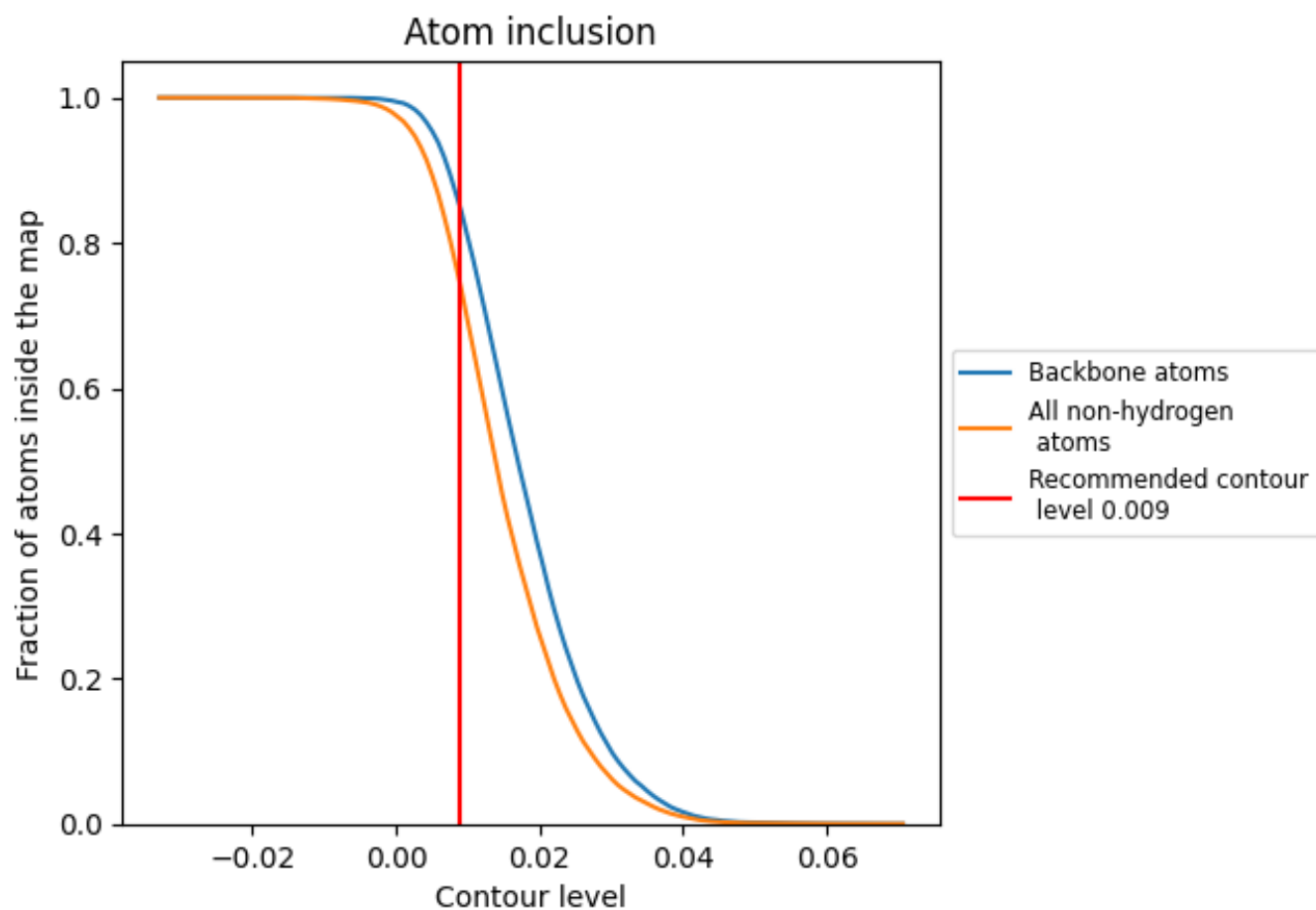
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).











9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7424	 0.1610
A	 0.7454	 0.1620
B	 0.7408	 0.1590
C	 0.7430	 0.1640
D	 0.7406	 0.1600

