



wwPDB EM Validation Summary Report ⓘ

Apr 2, 2024 – 11:00 pm BST

PDB ID : 8PR1
EMDB ID : EMD-17831
Title : Cytoplasmic dynein-B heavy chain bound to IC-LC tower
Authors : Singh, K.; Lau, C.K.; Manigrasso, G.; Gassmann, R.; Carter, A.P.
Deposited on : 2023-07-12
Resolution : 8.20 Å (reported)
Based on initial model : 7Z8G

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:

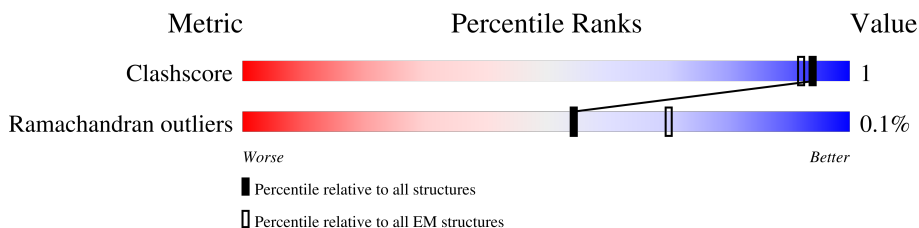
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 8.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




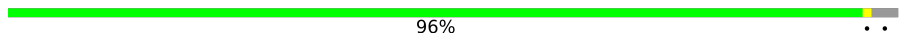
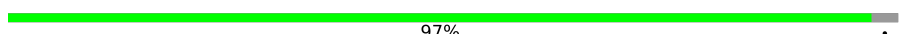
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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

Mol	Chain	Length	Quality of chain
1	D	89	
1	E	89	
2	I	612	
2	J	612	
3	K	113	
3	L	113	
4	A	4646	
4	G	4646	
5	F	492	

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Mol	Chain	Length	Quality of chain
5	H	492	 69% 30%
6	s	96	 96%
6	t	96	 97%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17871 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 Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	D	89	Total	C	N	O	0	0
			441	263	89	89		
1	E	89	Total	C	N	O	0	0
			441	263	89	89		

- Molecule 2 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	425	Total	C	N	O	0	0
			2100	1250	425	425		
2	J	432	Total	C	N	O	0	0
			2134	1270	432	432		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	484	SER	THR	conflict	UNP Q13409
I	499	GLY	ASP	conflict	UNP Q13409
J	484	SER	THR	conflict	UNP Q13409
J	499	GLY	ASP	conflict	UNP Q13409

- Molecule 3 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	113	Total	C	N	O	0	0
			558	332	113	113		
3	L	113	Total	C	N	O	0	0
			558	332	113	113		

- Molecule 4 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	A	857	Total	C	N	O	0	0
			4248	2534	857	857		
4	G	619	Total	C	N	O	0	0
			3067	1829	619	619		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1567	GLU	ARG	engineered mutation	UNP Q14204
A	1610	GLU	LYS	engineered mutation	UNP Q14204
G	1567	GLU	ARG	engineered mutation	UNP Q14204
G	1610	GLU	LYS	engineered mutation	UNP Q14204

- Molecule 5 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	F	344	Total	C	N	O	0	0
			1700	1012	344	344		
5	H	344	Total	C	N	O	0	0
			1700	1012	344	344		

- Molecule 6 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	t	93	Total	C	N	O	0	0
			462	276	93	93		
6	s	93	Total	C	N	O	0	0
			462	276	93	93		

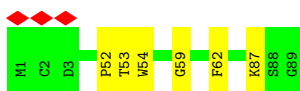
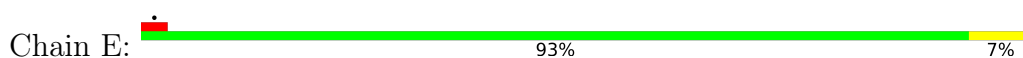
3 Residue-property plots i

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.

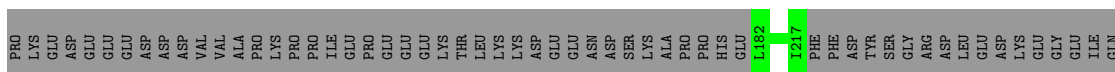
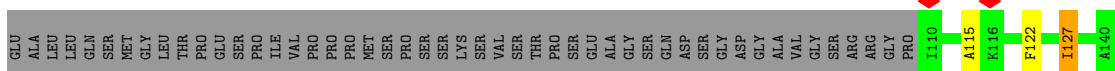
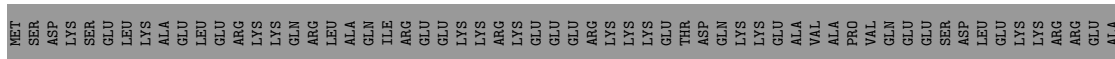
- Molecule 1: Dynein light chain 1, cytoplasmic



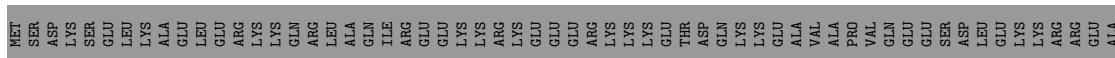
- Molecule 1: Dynein light chain 1, cytoplasmic



- Molecule 2: Cytoplasmic dynein 1 intermediate chain 2



- Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

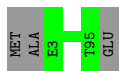


E1324	E1325	L1326	G1331	V1332	W1333	S1334	E1335	L1336	S1337	K1338	V1339	W1340	E1341	Q1342	I1343	I1344	D1344	Q1345	M1346	K1347	GLN	ARG	LEU	LEU	GLY	LYS	TYR	MET	GLY	PHE	GLN	ASP	GLY	THR	GLY	ASP	GLY	LEU	GLU	ASP	GLY										
I1224	M1225	Q1235	V1236	A1237	N1238	L1239	Q1240	M1241	K1242	I1243	V1244	A1249	R1253	T1254	T1255	D1256	L1257	T1259	D1260	W1261	E1262	K1263	K1264	K1265	P1266	G1269	N1270	L1271	R1272	E1295	K1299	E1302	A1303	L1304	E1306	L1307	D1308	T1309	G1310	L1311	L1312	S1313	G1314	R1318	V1319	Q1320	V1321	A1322	L1323		
GLY	ILE	ASP	SER	VAL	VAL	ARG	GLY	GLU	TRP	GLN	ASP	GLY	VAL	VAL	GLN	ASP	GLY	ASP	GLY	TRP	GLN	VAL	GLY	LEU	TRP	GLY	THR	PRO	ASP	ASN	THR	ASP	GLY	ARG	GLU	VAL	VAL	ASP	GLY	TRP	THR	ASP	GLY	THR	ASP	GLY	LEU	GLU	VAL	ASP	GLY
GLY	ILE	ASP	SER	VAL	VAL	ARG	GLY	GLU	TRP	GLN	ASP	GLY	VAL	VAL	GLN	ASP	GLY	ASP	GLY	TRP	GLN	VAL	GLY	LEU	TRP	GLY	THR	PRO	ASP	ASN	THR	ASP	GLY	ARG	GLU	VAL	VAL	ASP	GLY	TRP	THR	ASP	GLY	THR	ASP	GLY	LEU	GLU	VAL	ASP	GLY
GLY	ILE	ASP	SER	VAL	VAL	ARG	GLY	GLU	TRP	GLN	ASP	GLY	VAL	VAL	GLN	ASP	GLY	ASP	GLY	TRP	GLN	VAL	GLY	LEU	TRP	GLY	THR	PRO	ASP	ASN	THR	ASP	GLY	ARG	GLU	VAL	VAL	ASP	GLY	TRP	THR	ASP	GLY	THR	ASP	GLY	LEU	GLU	VAL	ASP	GLY
GLY	ILE	ASP	SER	VAL	VAL	ARG	GLY	GLU	TRP	GLN	ASP	GLY	VAL	VAL	GLN	ASP	GLY	ASP	GLY	TRP	GLN	VAL	GLY	LEU	TRP	GLY	THR	PRO	ASP	ASN	THR	ASP	GLY	ARG	GLU	VAL	VAL	ASP	GLY	TRP	THR	ASP	GLY	THR	ASP	GLY	LEU	GLU	VAL	ASP	GLY
GLY	ILE	ASP	SER	VAL	VAL	ARG	GLY	GLU	TRP	GLN	ASP	GLY	VAL	VAL	GLN	ASP	GLY	ASP	GLY	TRP	GLN	VAL	GLY	LEU	TRP	GLY	THR	PRO	ASP	ASN	THR	ASP	GLY	ARG	GLU	VAL	VAL	ASP	GLY	TRP	THR	ASP	GLY	THR	ASP	GLY	LEU	GLU	VAL	ASP	GLY
GLY	ILE	ASP	SER	VAL	VAL	ARG	GLY	GLU	TRP	GLN	ASP	GLY	VAL	VAL	GLN	ASP	GLY	ASP	GLY	TRP	GLN	VAL	GLY	LEU	TRP	GLY	THR	PRO	ASP	ASN	THR	ASP	GLY	ARG	GLU	VAL	VAL	ASP	GLY	TRP	THR	ASP	GLY	THR	ASP	GLY	LEU	GLU	VAL	ASP	GLY
GLY	ILE	ASP	SER	VAL	VAL	ARG	GLY	GLU	TRP	GLN	ASP	GLY	VAL	VAL	GLN	ASP	GLY	ASP	GLY	TRP	GLN	VAL	GLY	LEU	TRP	GLY	THR	PRO	ASP	ASN	THR	ASP	GLY	ARG	GLU	VAL	VAL	ASP	GLY	TRP	THR	ASP	GLY	THR	ASP	GLY	LEU	GLU	VAL	ASP	GLY
GLY	ILE	ASP	SER	VAL	VAL	ARG	GLY	GLU	TRP	GLN	ASP	GLY	VAL	VAL	GLN	ASP	GLY	ASP	GLY	TRP	GLN	VAL	GLY	LEU	TRP	GLY	THR	PRO	ASP	ASN	THR	ASP	GLY	ARG	GLU	VAL	VAL	ASP	GLY	TRP	THR	ASP	GLY	THR	ASP	GLY	LEU	GLU	VAL	ASP	GLY

ILE	ALA	ASP	THR	THR	THR	TYR	LEU	SER	LEU	ASN	ASP	ALA
ARG	LYS	ILE	THR	ASP	THR	ARG	LEU	ASP	THR	PRO	PHE	ASP
GLN	ASP	ILE	THR	ASP	THR	ARG	LEU	ASP	THR	PRO	PHE	ASP
LYS	ARG	SER	THR	VAL	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
THR	ASP	ILE	THR	VAL	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
LYS	GLY	VAL	THR	ASP	THR	ARG	LEU	ASP	THR	PRO	PHE	ASP
HIS	PHE	LEU	ARG	THR	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
GLU	GLN	THR	VAL	THR	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
LEU	THR	HIS	VAL	THR	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
ALA	VAL	LYS	SER	GLY	THR	ASP	THR	LEU	ASP	THR	PRO	PHE
PHE	GLU	PRO	PRO	ASP	THR	ASP	THR	LEU	ASP	THR	PRO	PHE
PHE	GLY	GLU	THR	ASP	THR	ASP	THR	LEU	ASP	THR	PRO	PHE
THR	PHE	LEU	THR	THR	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
ALA	GLU	ARG	VAL	THR	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
TRP	LEU	HIS	VAL	THR	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
TYR	LEU	ARG	THR	THR	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
ILE	HIS	VAL	THR	THR	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
GLY	ALA	THR	THR	THR	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP
ALA	THR	LYS	THR	THR	ASP	THR	LEU	ASP	THR	PRO	PHE	ASP

● Molecule 4: Cytoplasmic dynein 1 heavy chain 1





- Molecule 6: Dynein light chain roadblock-type 1

Chain s:  96% ..



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42405	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.118, 2.118, 2.118	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	D	0.32	0/440	0.72	0/612
1	E	0.31	0/440	0.65	0/612
2	I	0.34	0/2097	0.69	1/2916 (0.0%)
2	J	0.33	0/2131	0.62	0/2963
3	K	0.29	0/557	0.57	0/774
3	L	0.29	0/557	0.60	0/774
4	A	0.33	0/4245	0.57	0/5916
4	G	0.33	0/3064	0.63	1/4268 (0.0%)
5	F	0.31	0/1699	0.62	0/2365
5	H	0.31	0/1699	0.62	0/2365
6	s	0.37	0/461	0.62	0/642
6	t	0.30	0/461	0.68	0/642
All	All	0.33	0/17851	0.62	2/24849 (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	I	0	2
2	J	0	1
4	A	0	4
4	G	0	1
5	H	0	2
6	s	0	1
All	All	0	11

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	876	GLU	N-CA-CB	5.78	121.01	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	364	VAL	C-N-CA	5.72	134.30	122.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	985	GLU	Peptide
4	A	991	MET	Peptide
2	I	127	ILE	Peptide
2	I	339	ASN	Peptide
2	J	128	VAL	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	D	441	0	204	3	0
1	E	441	0	204	4	0
2	I	2100	0	939	7	0
2	J	2134	0	954	6	0
3	K	558	0	261	2	0
3	L	558	0	261	0	0
4	A	4248	0	1890	5	0
4	G	3067	0	1346	4	0
5	F	1700	0	746	2	0
5	H	1700	0	746	2	0
6	s	462	0	192	0	0
6	t	462	0	192	0	0
All	All	17871	0	7935	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 31 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:E:54:TRP:HA	1:E:87:LYS:HA	1.89	0.55
2:J:411:MET:HA	2:J:423:VAL:HA	1.89	0.54
4:A:530:VAL:HA	4:A:549:ALA:HB1	1.91	0.52
2:I:286:VAL:HA	2:I:304:HIS:HA	1.93	0.50
2:J:365:GLY:HA3	2:J:370:HIS:HA	1.94	0.50

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	D	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
1	E	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
2	I	419/612 (68%)	398 (95%)	20 (5%)	1 (0%)	47	81
2	J	426/612 (70%)	400 (94%)	25 (6%)	1 (0%)	47	81
3	K	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
3	L	111/113 (98%)	109 (98%)	2 (2%)	0	100	100
4	A	851/4646 (18%)	826 (97%)	25 (3%)	0	100	100
4	G	613/4646 (13%)	598 (98%)	15 (2%)	0	100	100
5	F	342/492 (70%)	327 (96%)	15 (4%)	0	100	100
5	H	342/492 (70%)	323 (94%)	19 (6%)	0	100	100
6	s	91/96 (95%)	81 (89%)	10 (11%)	0	100	100
6	t	91/96 (95%)	82 (90%)	9 (10%)	0	100	100
All	All	3571/12096 (30%)	3413 (96%)	156 (4%)	2 (0%)	54	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	127	ILE
2	J	138	VAL

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

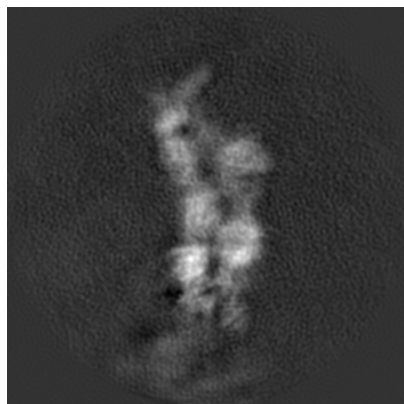
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17831. These allow visual inspection of the internal detail of the map and identification of artifacts.

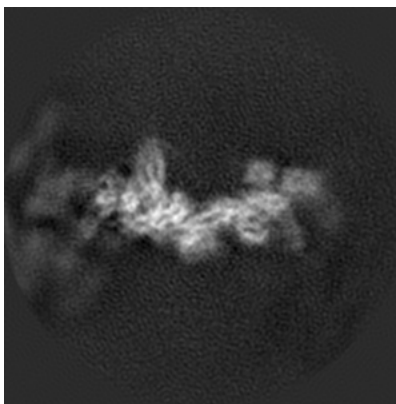
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

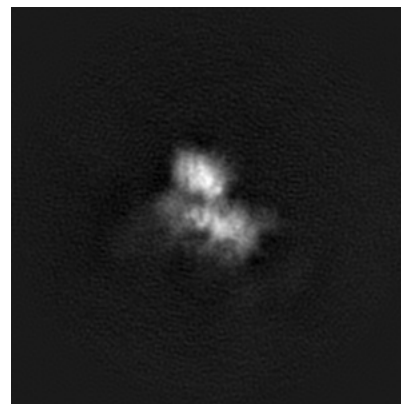
6.1.1 Primary map



X

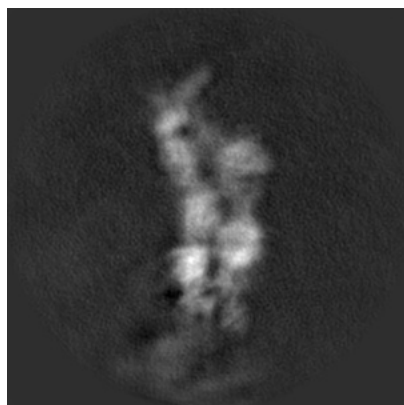


Y

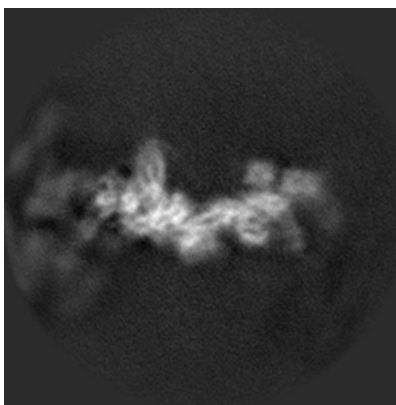


Z

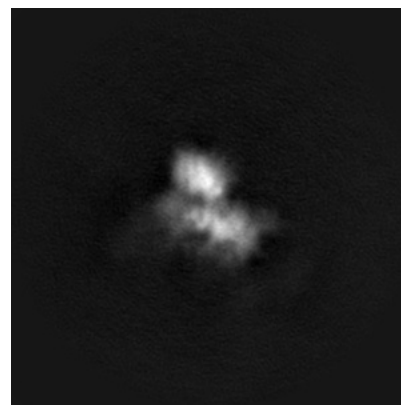
6.1.2 Raw map



X



Y

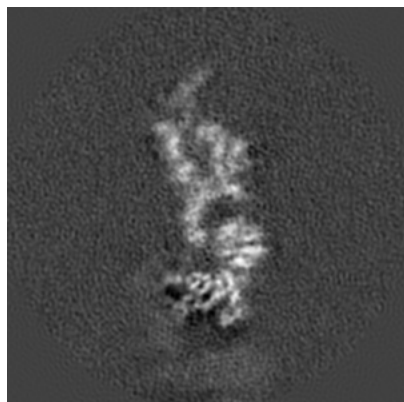


Z

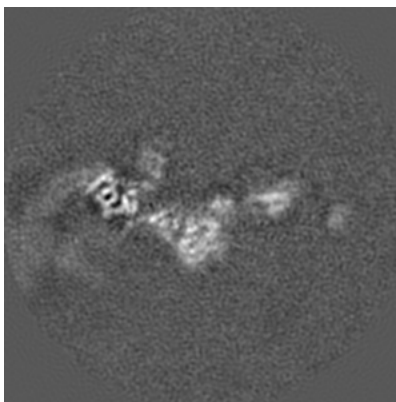
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

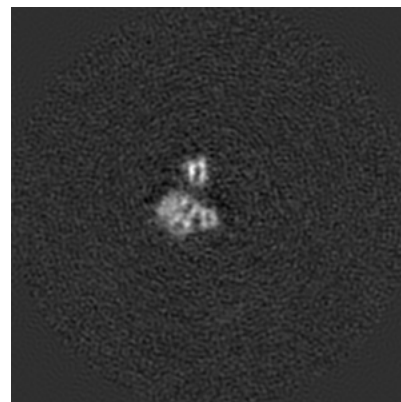
6.2.1 Primary map



X Index: 100

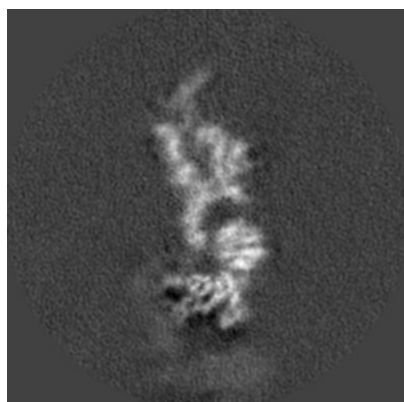


Y Index: 100

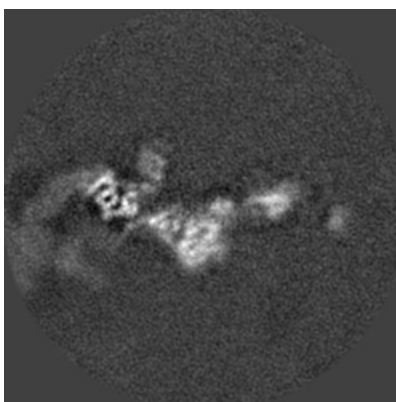


Z Index: 100

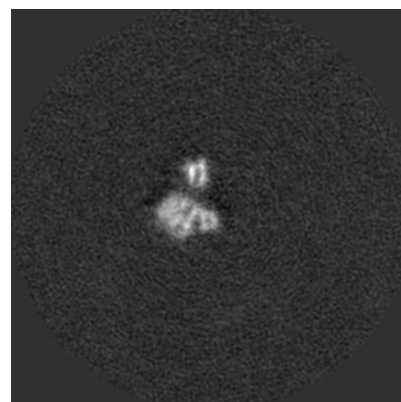
6.2.2 Raw map



X Index: 100



Y Index: 100



Z Index: 100

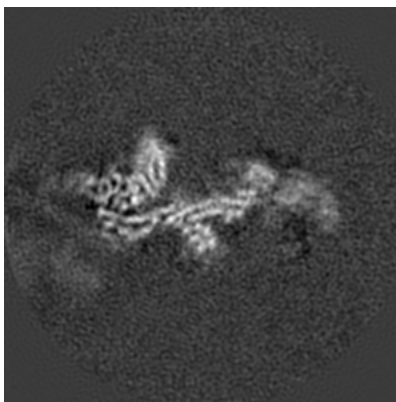
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

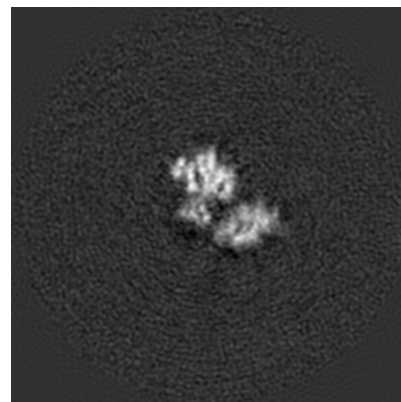
6.3.1 Primary map



X Index: 97

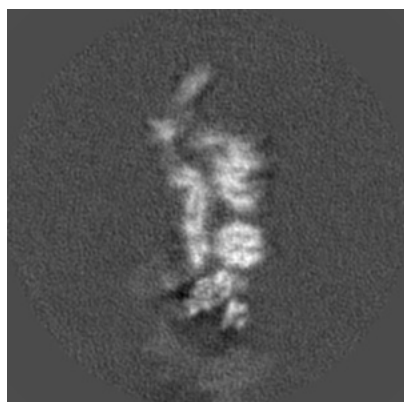


Y Index: 92

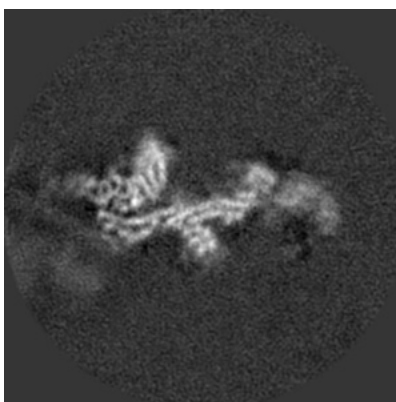


Z Index: 77

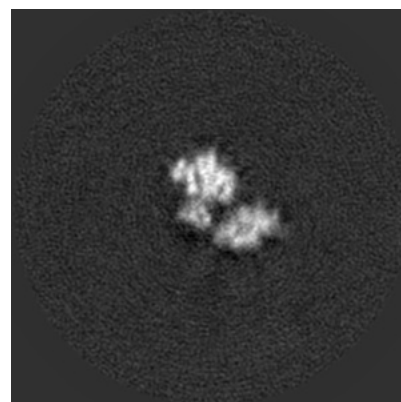
6.3.2 Raw map



X Index: 97



Y Index: 92

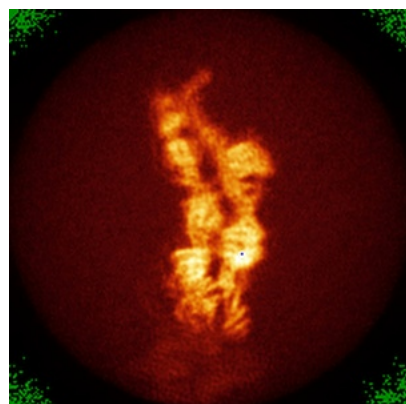


Z Index: 77

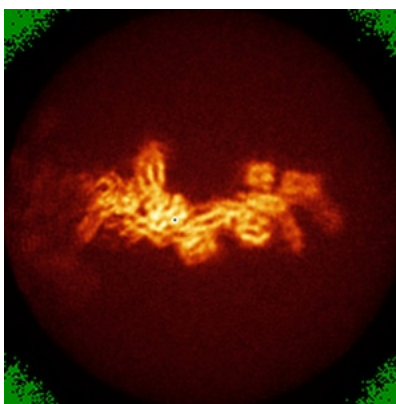
The images above show the largest variance slices of the map in three orthogonal directions.

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

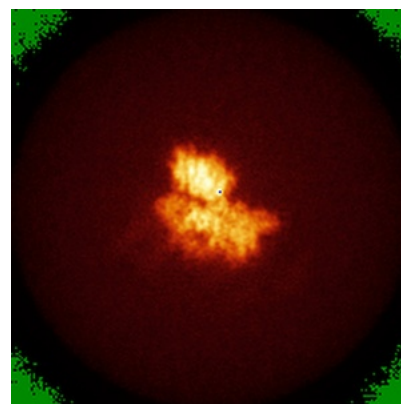
6.4.1 Primary map



X

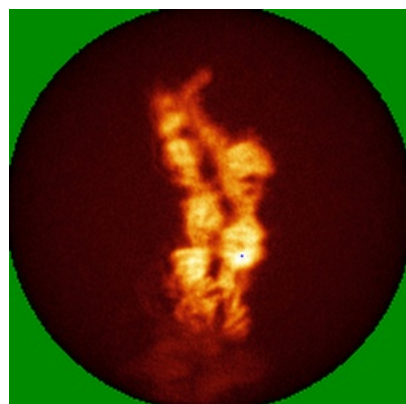


Y

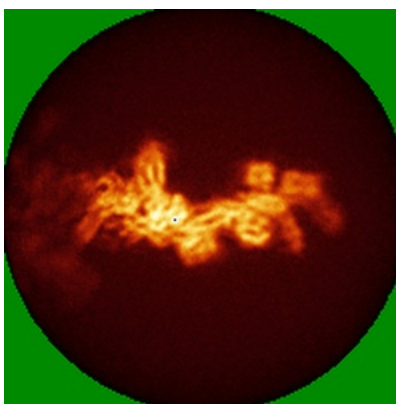


Z

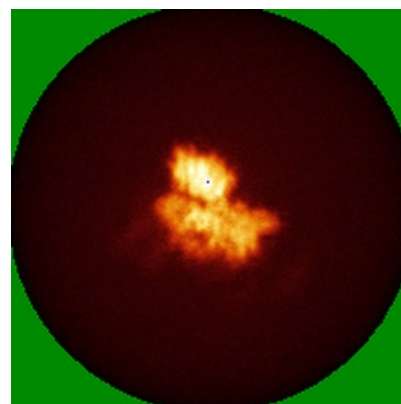
6.4.2 Raw map



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



X



Y



Z

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



X



Y



Z

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.

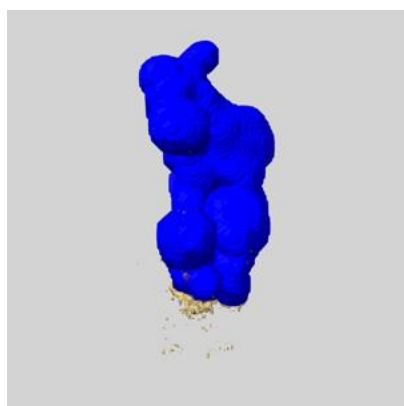
6.6 Mask visualisation [i](#)

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

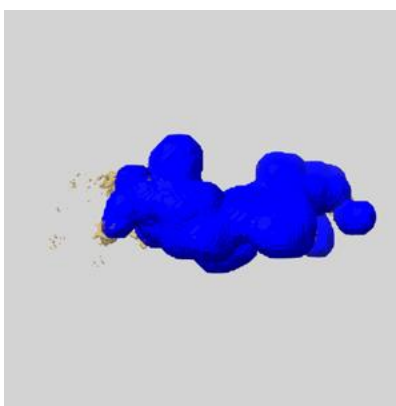
A mask typically either:

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

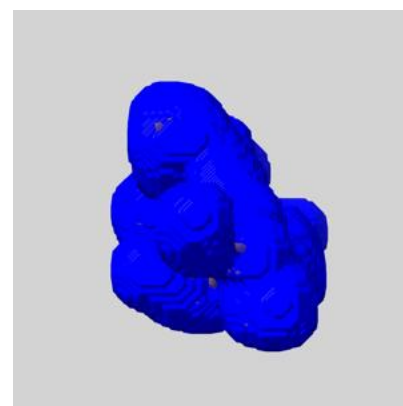
6.6.1 emd_17831_msk_1.map [i](#)



X



Y

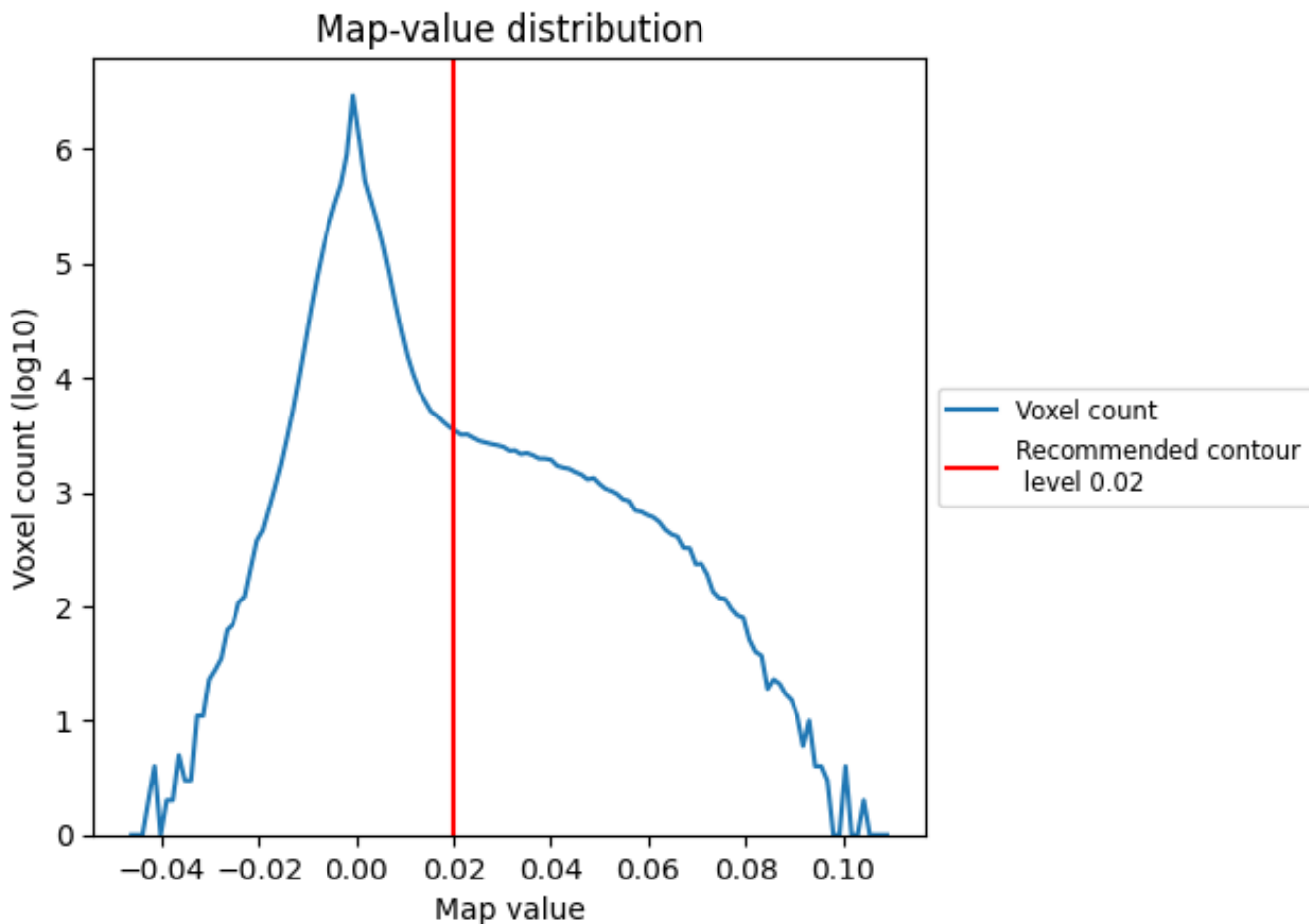


Z

7 Map analysis [i](#)

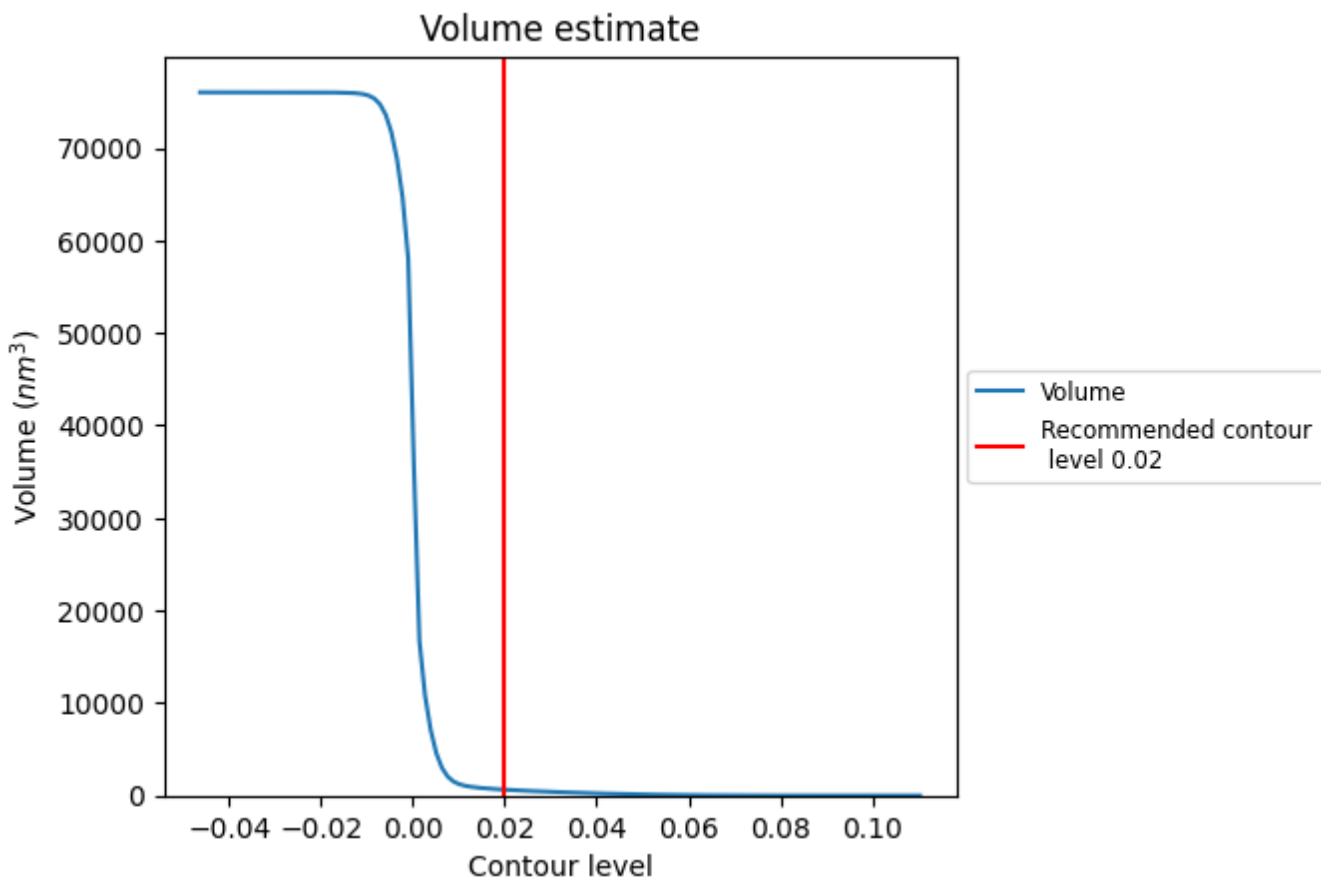
This section contains the results of statistical analysis of the map.

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.

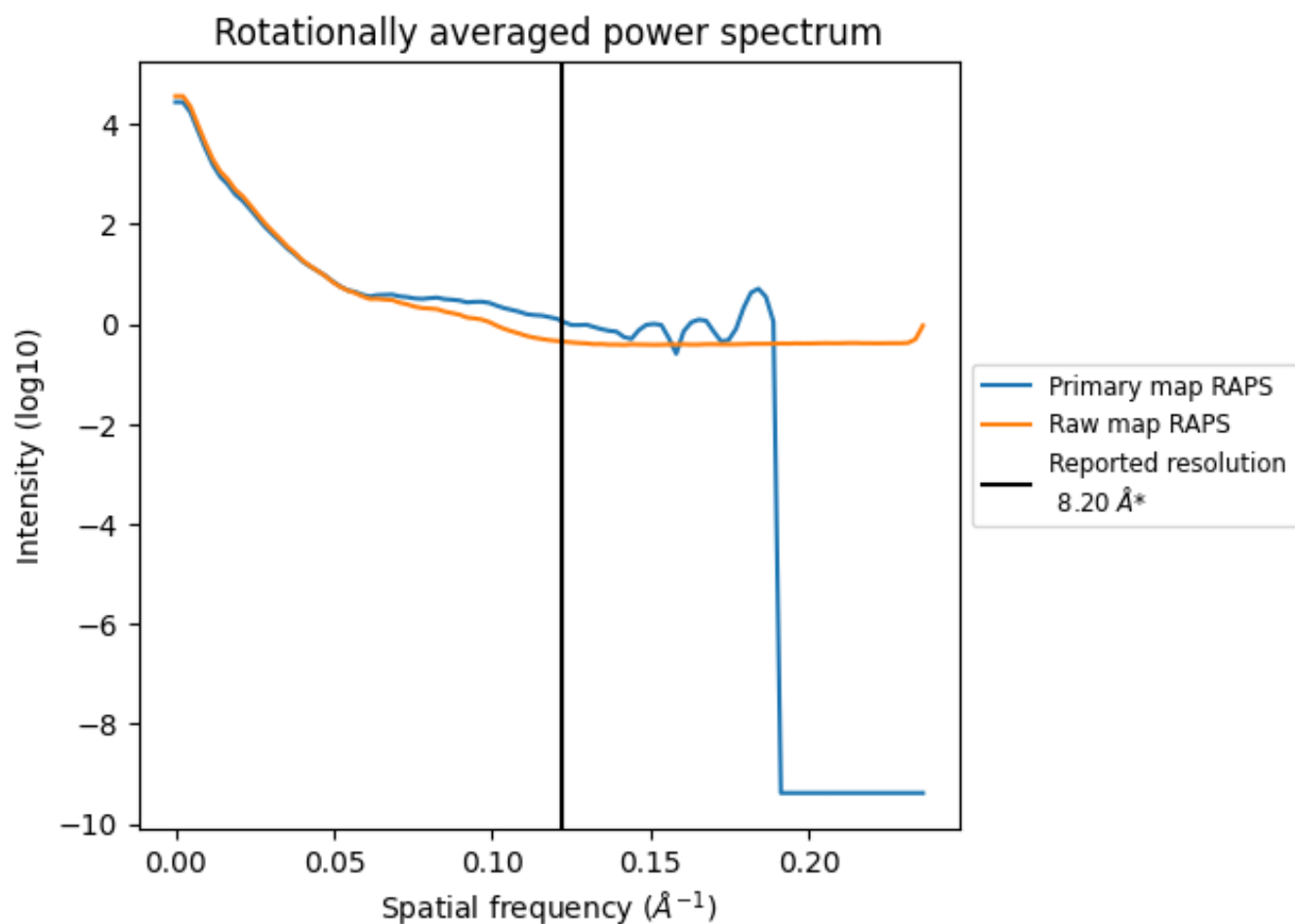
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 635 nm^3 ; this corresponds to an approximate mass of 573 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](#)

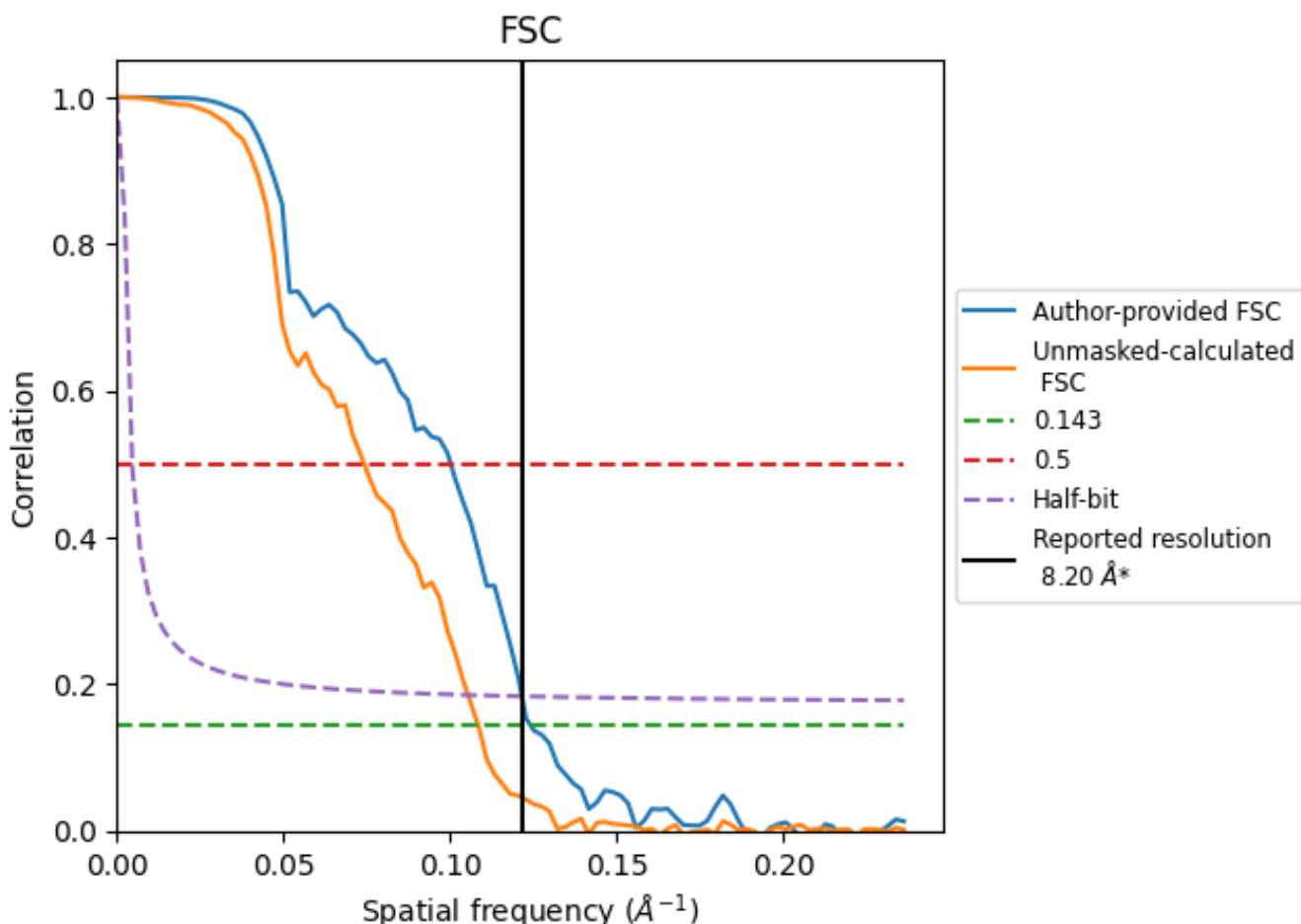


*Reported resolution corresponds to spatial frequency of 0.122 Å⁻¹

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 0.122 Å⁻¹

8.2 Resolution estimates [i](#)

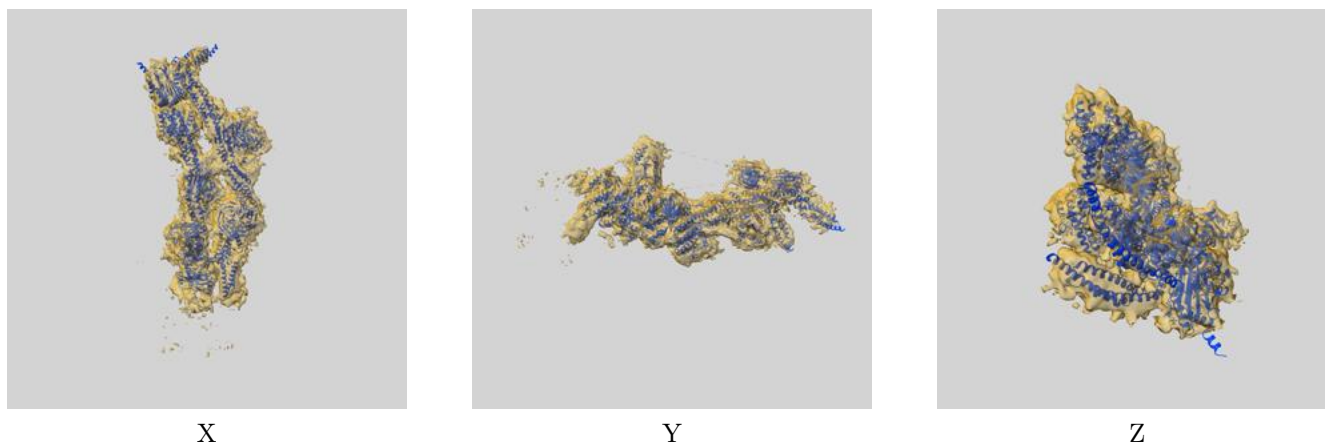
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.20	-	-
Author-provided FSC curve	8.06	9.99	8.23
Unmasked-calculated*	9.23	13.48	9.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.23 differs from the reported value 8.2 by more than 10 %

9 Map-model fit [i](#)

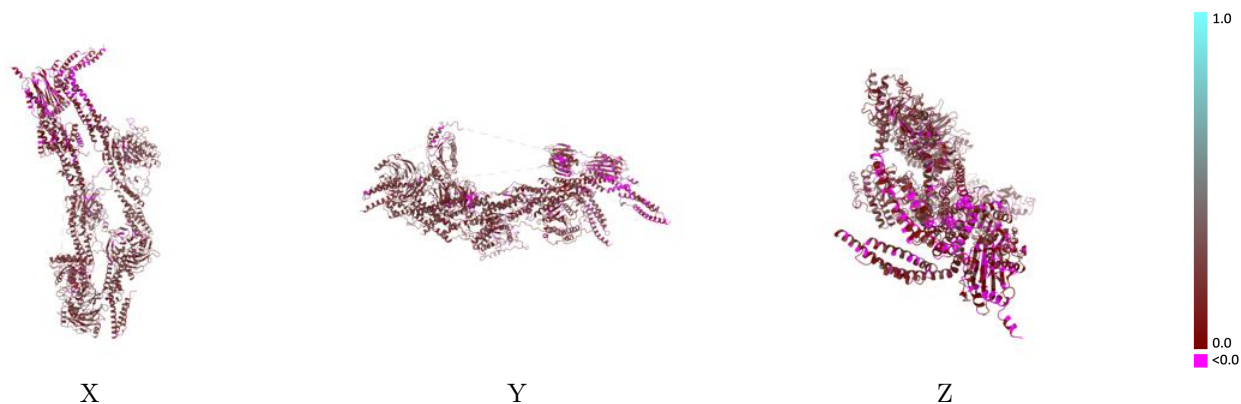
This section contains information regarding the fit between EMDB map EMD-17831 and PDB model 8PR1. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



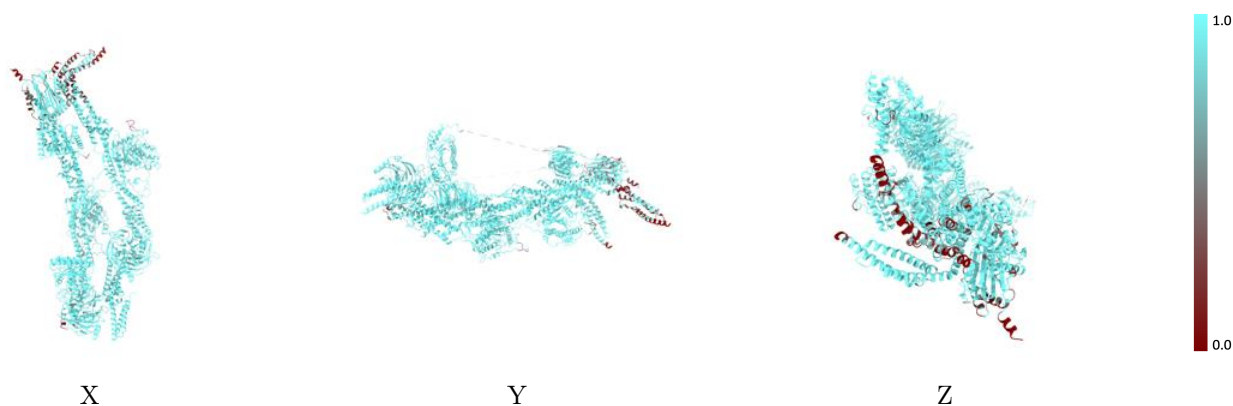
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



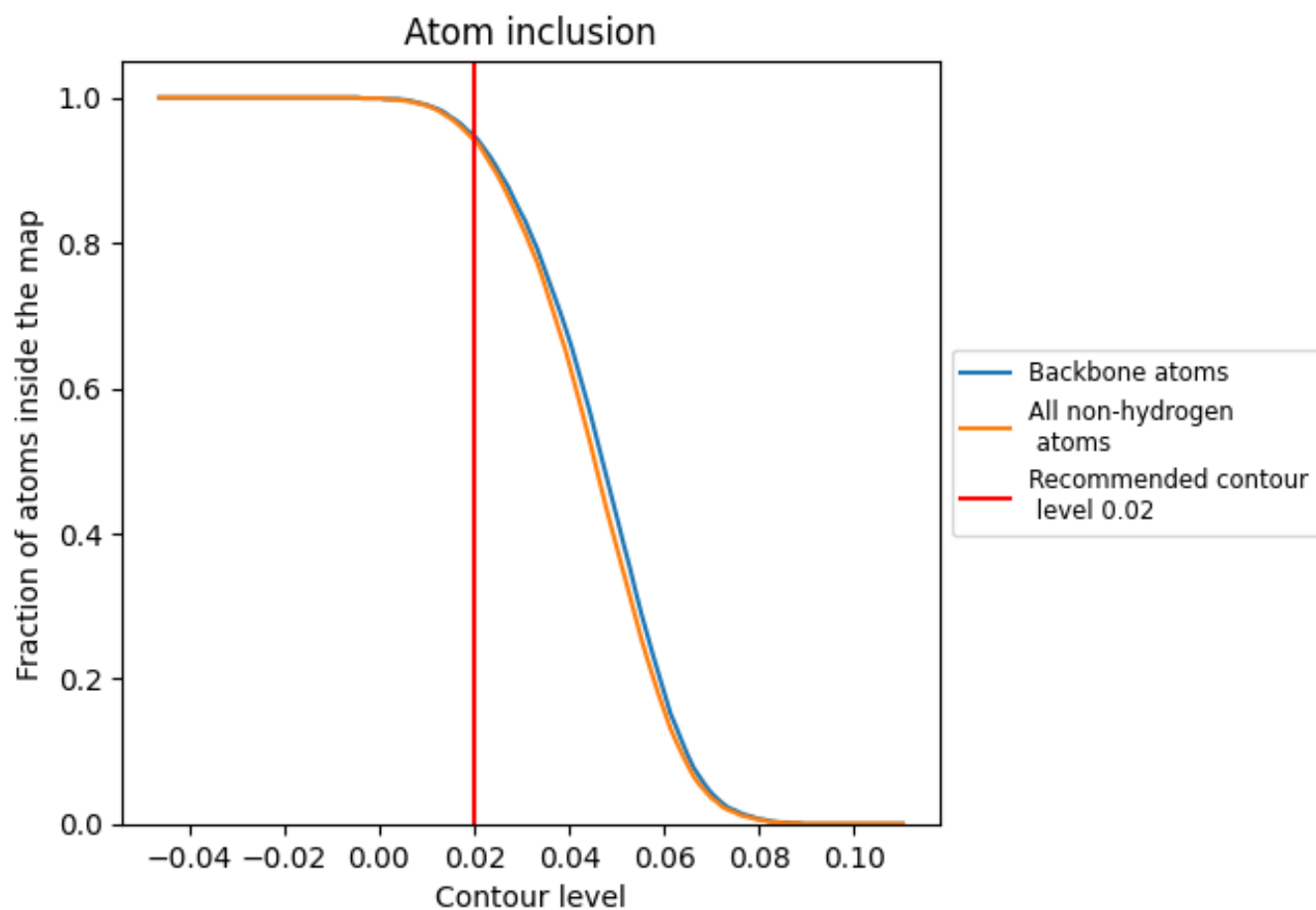
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

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	 0.9420	 0.1930
A	 0.9020	 0.1880
D	 0.9800	 0.1290
E	 0.9710	 0.1140
F	 0.9720	 0.1940
G	 0.9660	 0.2150
H	 0.9790	 0.2010
I	 0.9520	 0.2460
J	 0.9770	 0.1980
K	 0.8410	 0.0900
L	 0.7060	 0.0590
s	 0.9890	 0.1800
t	 1.0000	 0.2230

