



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 03:41 AM UTC

PDB ID : 8PQV / pdb_00008pqv
EMDB ID : EMD-17825
Title : Cytoplasmic dynein-1 motor domain in post-powerstroke state
Authors : Singh, K.; Lau, C.K.; Manigrasso, G.; Gassmann, R.; Carter, A.P.
Deposited on : 2023-07-12
Resolution : 4.00 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

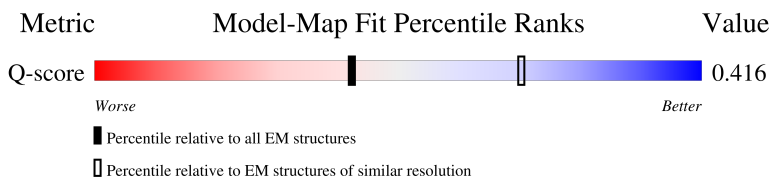
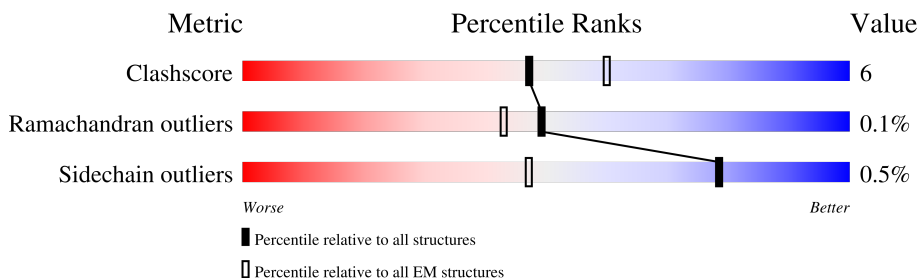
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	4646	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24122 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2996	Total	C	N	O	S	0	0
			24122	15366	4163	4472	121		

There are 2 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

S2506	R2358	V2207	T2017	E1871	I1571	K1447	VAL	Q1327	ASN	GLU	ALA	ASN	PHE
R2507	L2369	Y2211	P2020	Y1889	K1581	E1456	ALA	D1328	LYS	PHE	LEU	LEU	ASN
E2516	L2374	L2220	G2021	L1890	M1571	M1457	LEU	E1335	GLN	THR	GLN	GLN	GLN
R2519	R2383	S2231	T2017	T1891	Q1598	L1459	LEU	E1341	MET	ASN	GLN	GLN	LYS
R2520	E2389	W2234	ALA	F1905	L1601	E1461	Q1327	E1341	PRO	VAL	GLN	GLN	VAL
L2526	G2390	W2234	GLY	G1906	E1602	F1462	D1328	E1341	ASP	VAL	GLN	GLN	ASP
D2536	E2391	L2237	S2026	G1906	R1603	L1463	E1335	E1341	GLY	VAL	GLN	GLN	ASP
Y2537	D2392	L2238	L2035	K1912	L1604	K1464	E1335	E1341	ILE	VAL	GLN	GLN	LEU
E2538	E2393	K2239	L2039	T1913	L1607	R1467	E1335	E1341	ASN	PRO	VAL	VAL	ILE
G2543	A2394	E2242	L2039	R1925	I1611	E1468	E1335	E1341	LEU	PRO	VAL	VAL	ILE
K2551	Q2395	A2258	A2066	R1925	I1611	W1469	E1335	E1341	GLU	PRO	VAL	VAL	ILE
A2563	R2396	A2258	L2069	C1932	E1620	N1471	E1335	E1341	GLY	PRO	VAL	VAL	ILE
V2569	ARG	D2269	Q2079	F1936	P1627	Q1481	E1335	E1341	ASP	GLU	PRO	VAL	ILE
G2570	LYS	T2272	L2080	M1941	R1628	C1484	E1335	E1341	THR	GLU	PRO	VAL	ILE
L2571	GLY	R2273	Q2083	I1944	K1649	R1485	E1335	E1341	ALA	GLU	PRO	VAL	ILE
L2572	LYS	E2274	Q2084	I1944	K1652	K1496	E1335	E1341	PHE	GLU	PRO	VAL	ILE
L2572	ASP	W2275	S2084	F1945	K1652	V1497	E1335	E1341	THR	GLU	PRO	VAL	ILE
L2572	GLU	T2276	H2085	W1946	I1684	K1498	E1335	E1341	VAL	GLU	PRO	VAL	ILE
R2576	GLY	D2277	K2104	G1947	I1684	E1499	E1335	E1341	ASP	GLU	PRO	VAL	ILE
L2581	E2406	G2278	K2112	L1948	I1686	V1504	E1335	E1341	THR	GLU	PRO	VAL	ILE
V2592	E2407	T2281	K2112	W1951	I1676	M1507	E1335	E1341	LYS	GLU	PRO	VAL	ILE
G2619	A2408	R2285	E2116	G1952	S1677	K1514	E1335	E1341	ASP	GLU	PRO	VAL	ILE
F2622	L2412	T2288	E2117	A1953	S1678	K1514	E1335	E1341	THR	GLU	PRO	VAL	ILE
S2623	T2415	D2289	R2118	W1954	E1680	L1521	E1335	E1341	GLN	GLU	PRO	VAL	ILE
T2644	A2420	S2290	G2119	D1958	E1683	E1524	E1335	E1341	VAL	GLU	PRO	VAL	ILE
G2647	Q2423	V2291	E2120	M1967	E1683	E1524	E1335	E1341	ASN	GLU	PRO	VAL	ILE
F2662	Q2431	R2292	A2121	L1968	I1698	A1532	E1335	E1341	LYS	GLU	PRO	VAL	ILE
L2666	L2432	L2295	D2123	S1972	W1701	L1702	E1335	E1341	THR	GLU	PRO	VAL	ILE
P2669	V2433	W2300	E2126	Q1979	V1721	V1724	E1335	E1341	ASP	GLU	PRO	VAL	ILE
R2678	T2434	D2304	I2136	M1987	V1721	V1724	E1335	E1341	GLN	GLU	PRO	VAL	ILE
R2694	K2435	G2305	L2137	P1988	V1721	V1724	E1335	E1341	ASP	GLU	PRO	VAL	ILE
Q2698	K2436	D2307	D2153	M1989	V1721	V1724	E1335	E1341	GLN	GLU	PRO	VAL	ILE
G2710	L2437	V2307	L2160	Y1990	V1721	V1724	E1335	E1341	THR	GLU	PRO	VAL	ILE
D2717	R2451	D2320	L2160	D1991	V1721	V1724	E1335	E1341	GLY	GLU	PRO	VAL	ILE
R2720	L2452	P2336	F2165	A1995	V1721	V1724	E1335	E1341	ASP	GLU	PRO	VAL	ILE
Y2735	R2453	P2337	Y2170	P1996	V1721	V1724	E1335	E1341	THR	GLU	PRO	VAL	ILE
	C2454	N2338	Y2170	L2002	V1721	V1724	E1335	E1341	GLY	GLU	PRO	VAL	ILE
	L2455	C2186	C2186	R2003	V1721	V1724	E1335	E1341	THR	GLU	PRO	VAL	ILE
	P2480	M2342	K2004	K2004	V1721	V1724	E1335	E1341	GLY	GLU	PRO	VAL	ILE
	R2488	F2343	M2189	Q2005	V1721	V1724	E1335	E1341	ASP	GLU	PRO	VAL	ILE
	T2498	E2344	Y2190	V2006	V1721	V1724	E1335	E1341	THR	GLU	PRO	VAL	ILE
	L2499	V2345	L2191	K2007	V1721	V1724	E1335	E1341	GLY	GLU	PRO	VAL	ILE
	D2505	A2354	W2202	D2011	V1721	V1724	E1335	E1341	THR	GLU	PRO	VAL	ILE



ARG
GLY
VAL
ALA
VAL
LEU
CYS
THR
GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67795	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	0.055	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	296.52002, 296.52002, 296.52002	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	0.21	0/24633	0.48	8/33378 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3690	PRO	CA-N-CD	-7.32	101.75	112.00
1	A	4418	LYS	CA-CB-CG	6.89	127.89	114.10
1	A	2480	PRO	CA-N-CD	-6.47	102.94	112.00
1	A	3503	ILE	CA-C-N	-6.42	112.46	122.42
1	A	3503	ILE	C-N-CA	-6.42	112.46	122.42

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	24122	0	24177	288	0
All	All	24122	0	24177	288	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 288 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:1416:LEU:O	1:A:1420:LEU:HB2	1.81	0.80
1:A:3502:THR:O	1:A:3504:ALA:N	2.22	0.73
1:A:1351:TRP:HB3	1:A:1429:LEU:HB3	1.74	0.70
1:A:3503:ILE:HG12	1:A:3503:ILE:O	1.93	0.67
1:A:2320:ASP:HB3	1:A:2358:ARG:HE	1.62	0.65

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	2984/4646 (64%)	2892 (97%)	89 (3%)	3 (0%)	48	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1996	PRO
1	A	3503	ILE
1	A	1421	HIS

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	2666/4125 (65%)	2652 (100%)	14 (0%)	81	82

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2810	LEU
1	A	3155	HIS
1	A	3703	VAL
1	A	3502	THR
1	A	3503	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4174	ASN
1	A	4231	GLN
1	A	4444	GLN
1	A	2005	GLN
1	A	1979	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

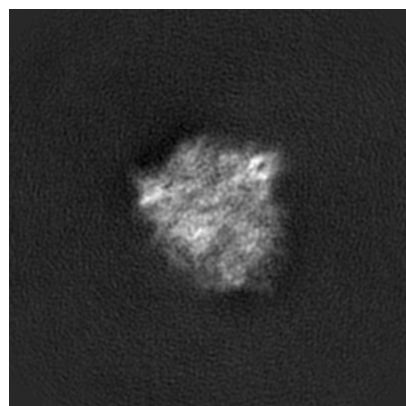
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17825. These allow visual inspection of the internal detail of the map and identification of artifacts.

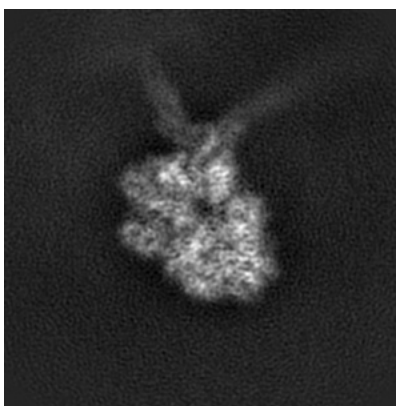
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

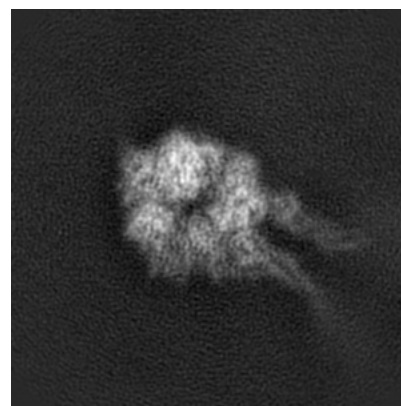
6.1.1 Primary map



X

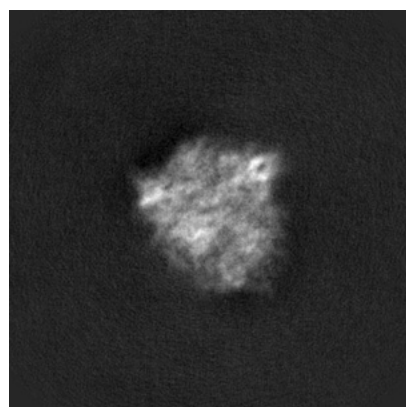


Y

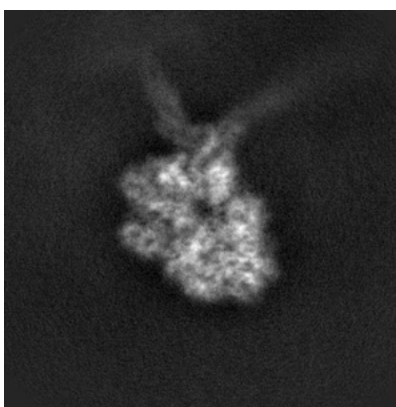


Z

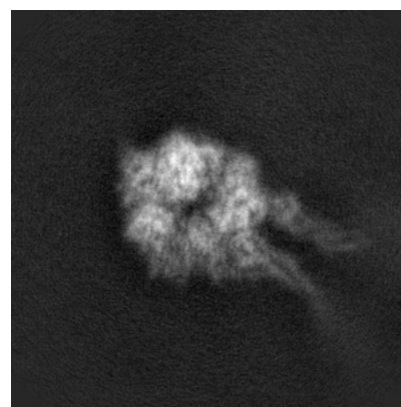
6.1.2 Raw map



X



Y



Z

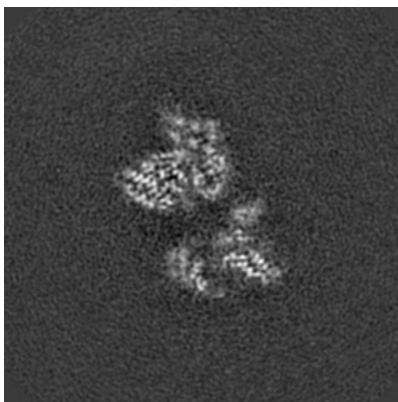
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

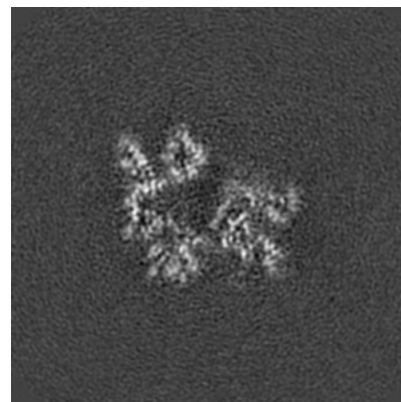
6.2.1 Primary map



X Index: 140



Y Index: 140

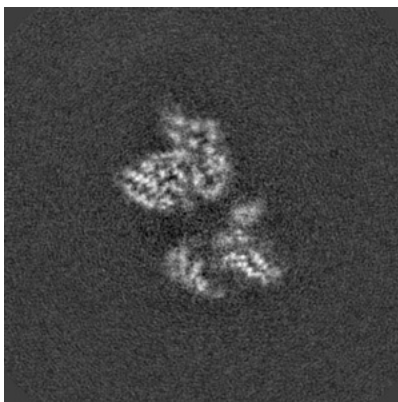


Z Index: 140

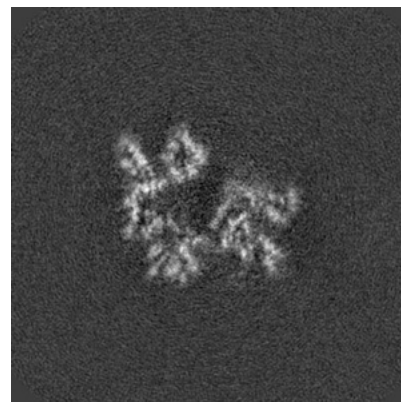
6.2.2 Raw map



X Index: 140



Y Index: 140

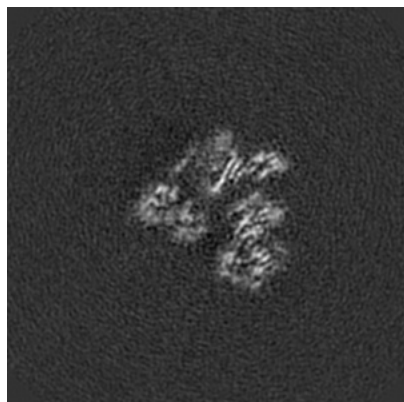


Z Index: 140

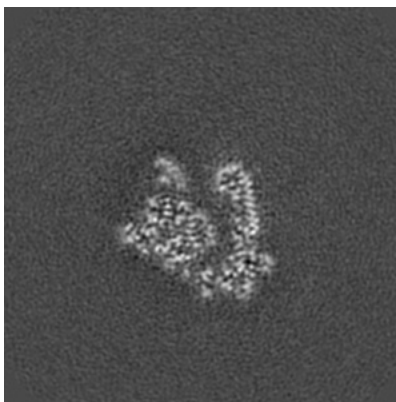
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

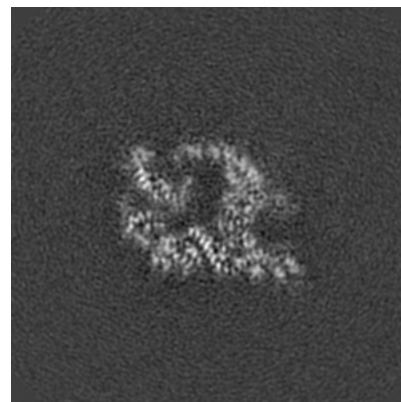
6.3.1 Primary map



X Index: 114

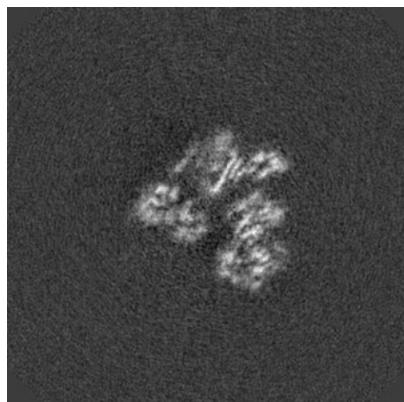


Y Index: 170

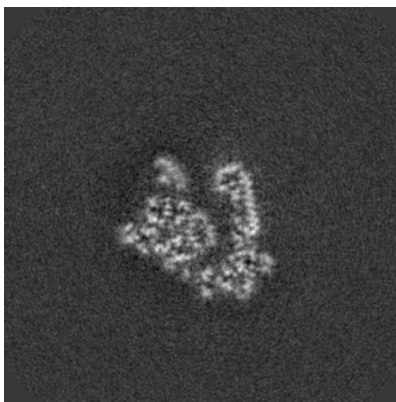


Z Index: 150

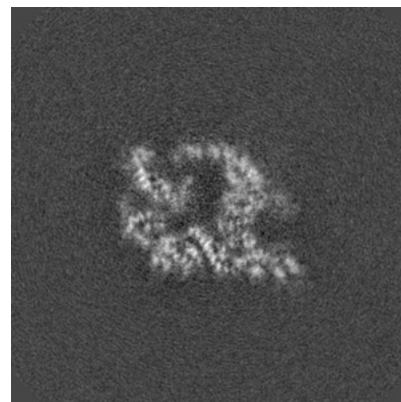
6.3.2 Raw map



X Index: 114



Y Index: 170

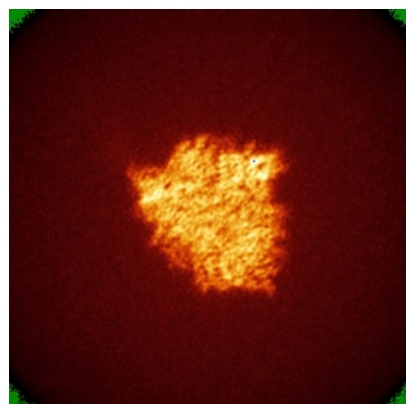


Z Index: 150

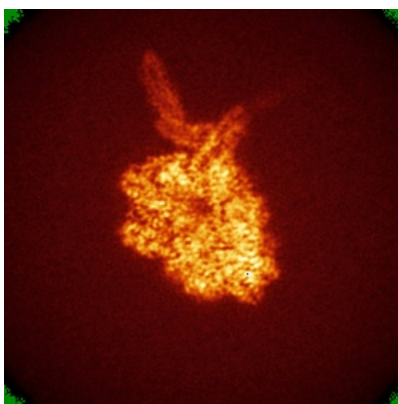
The images above show the largest variance slices of the map in three orthogonal directions.

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

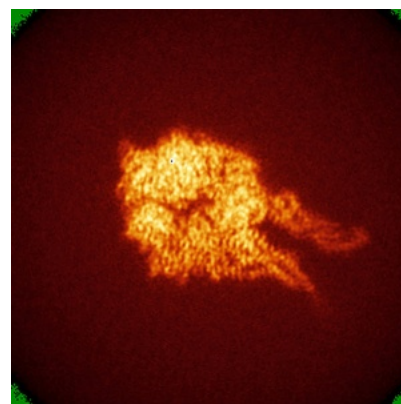
6.4.1 Primary map



X

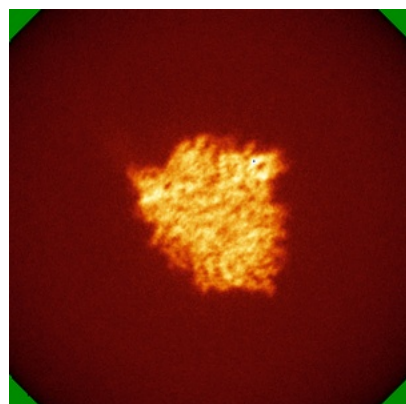


Y

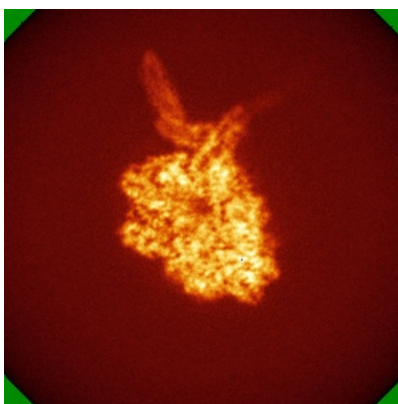


Z

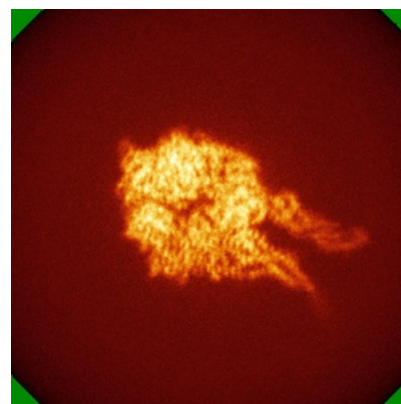
6.4.2 Raw map



X



Y

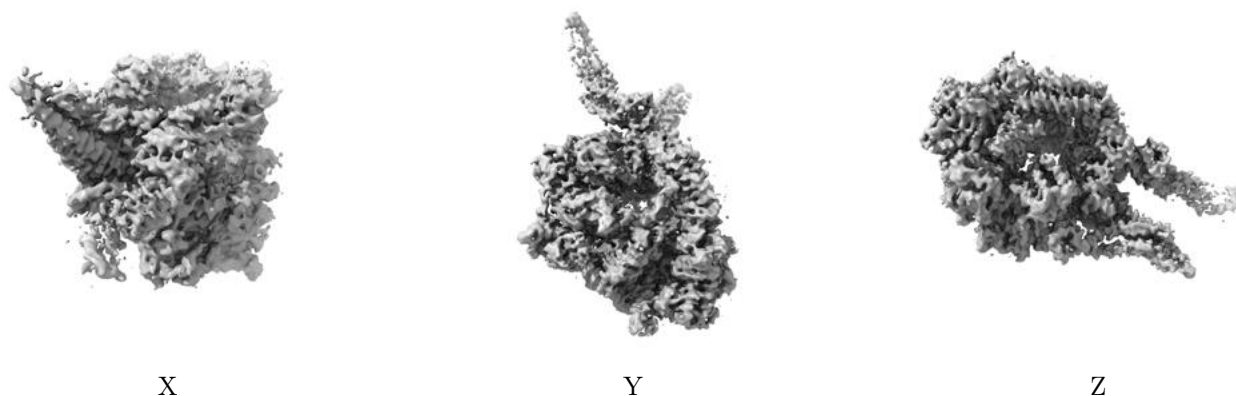


Z

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.

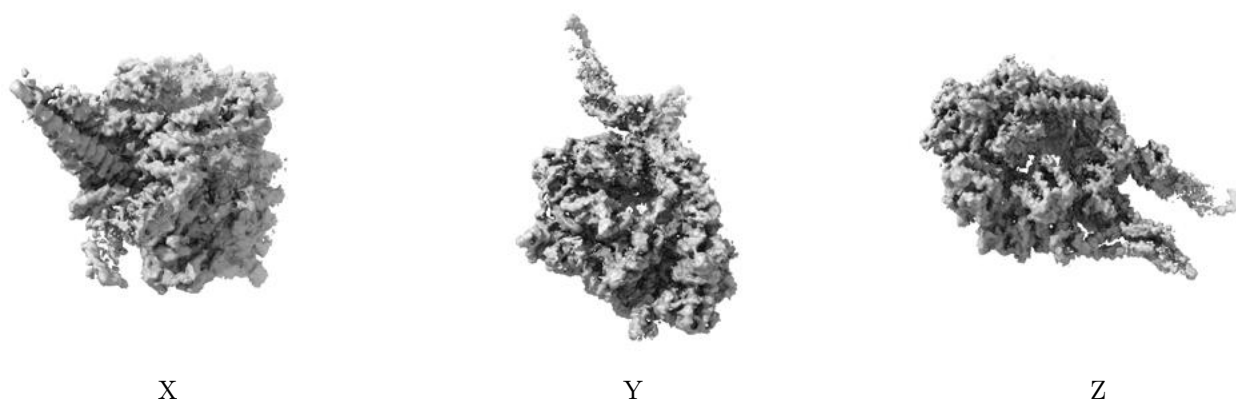
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. 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.

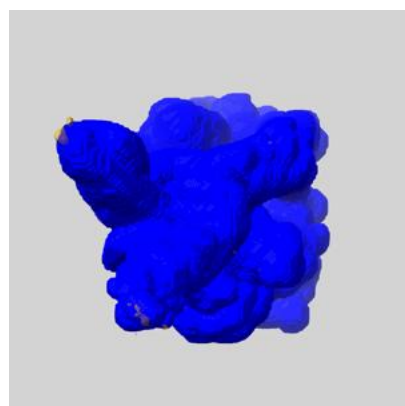
6.6 Mask visualisation [i](#)

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

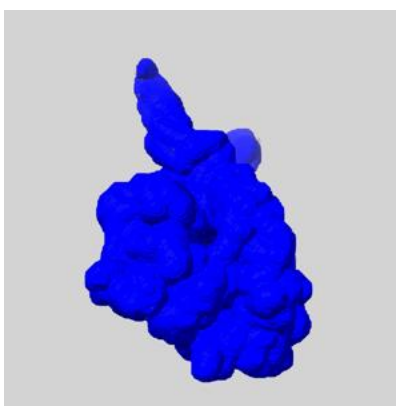
A mask typically either:

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

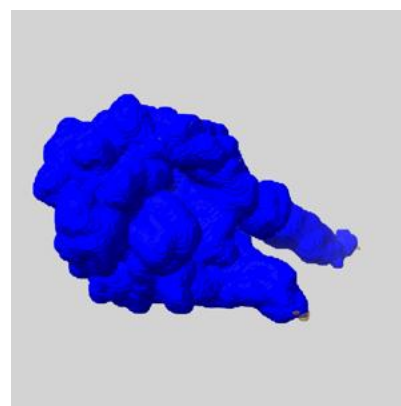
6.6.1 emd_17825_msk_1.map [i](#)



X



Y

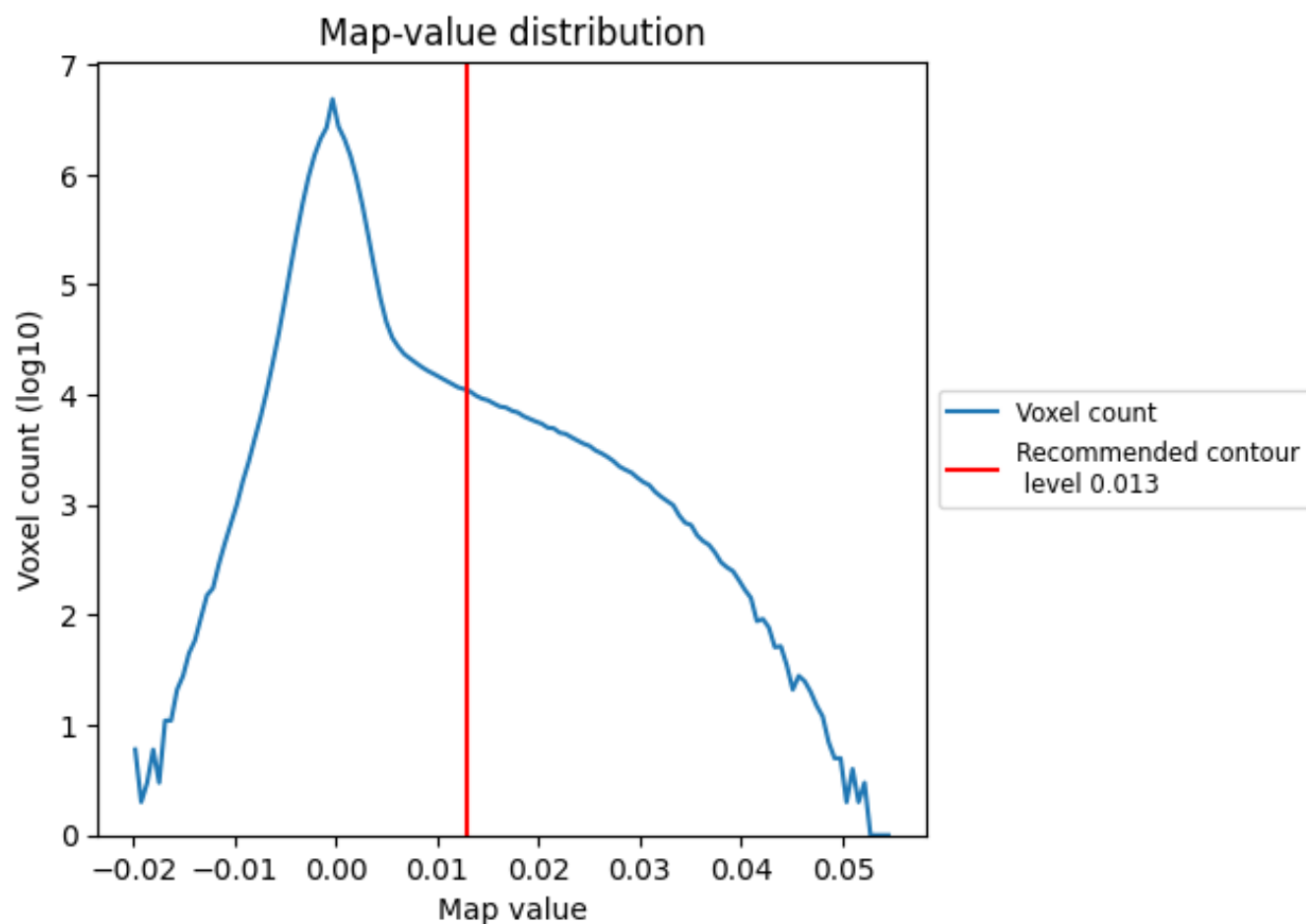


Z

7 Map analysis [i](#)

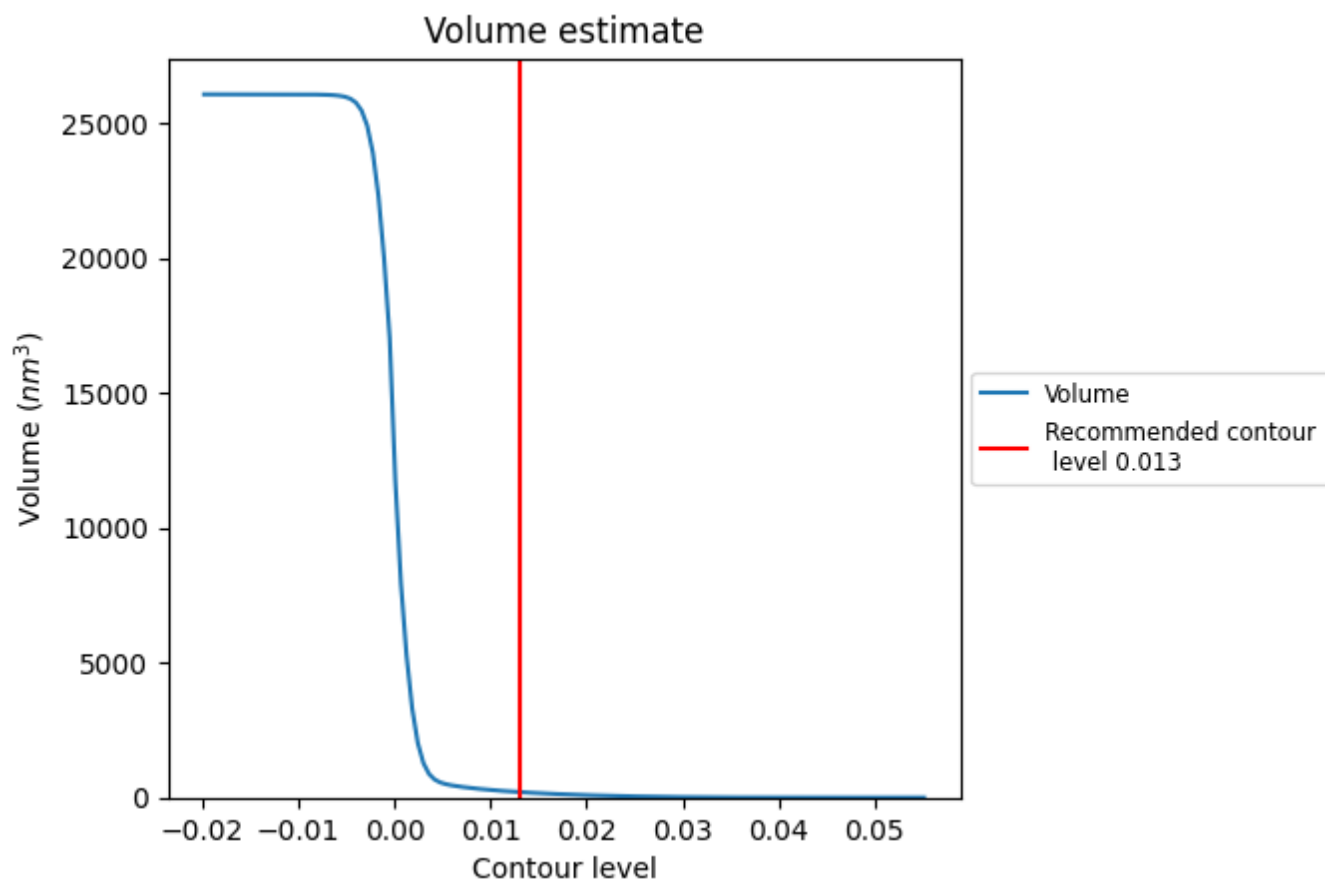
This section contains the results of statistical analysis of the map.

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.

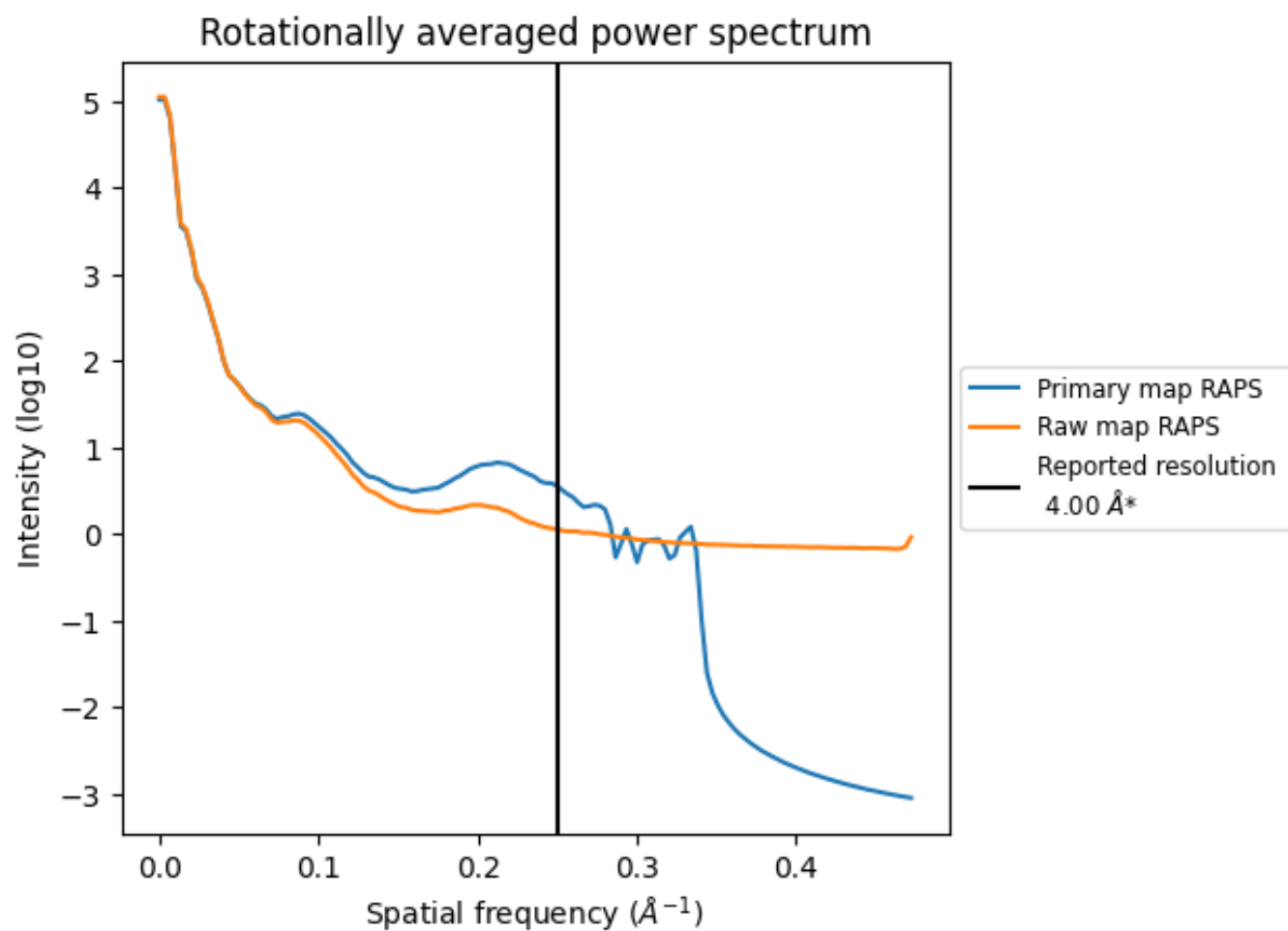
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 184 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 ⓘ

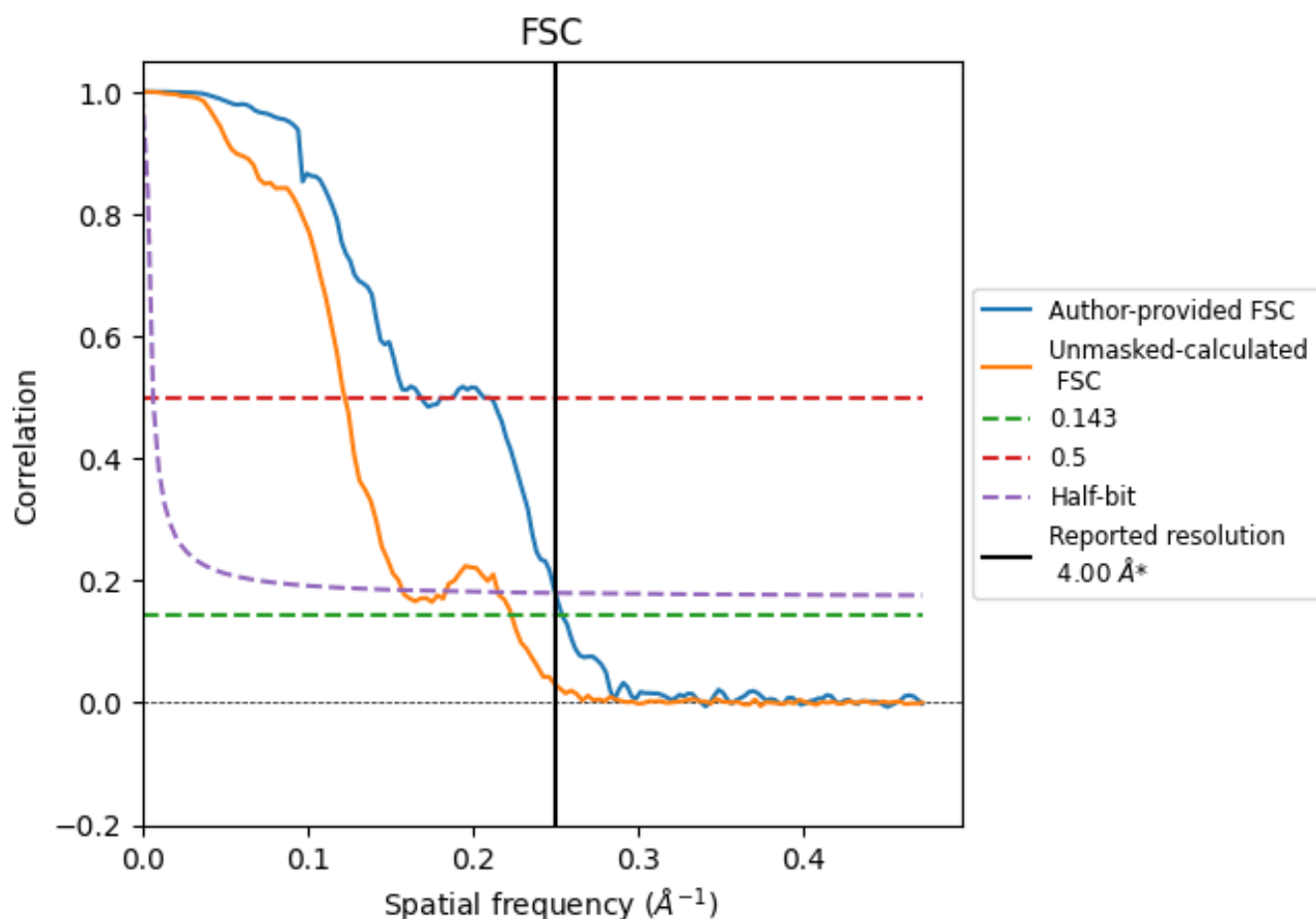


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

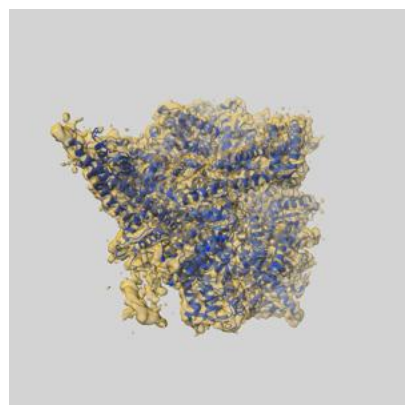
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.93	5.93	4.00
Unmasked-calculated*	4.47	8.16	6.35

*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 4.47 differs from the reported value 4.0 by more than 10 %

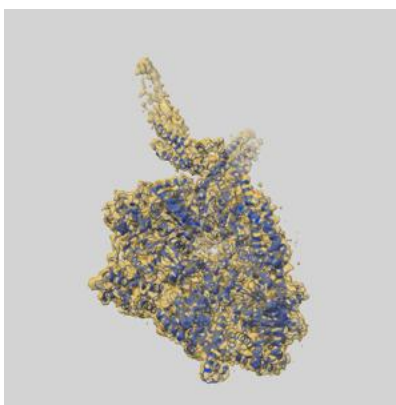
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17825 and PDB model 8PQV. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

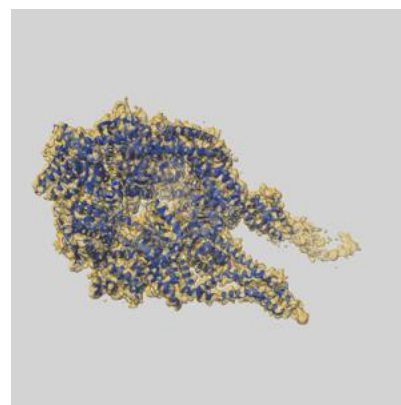
9.1 Map-model overlay [i](#)



X



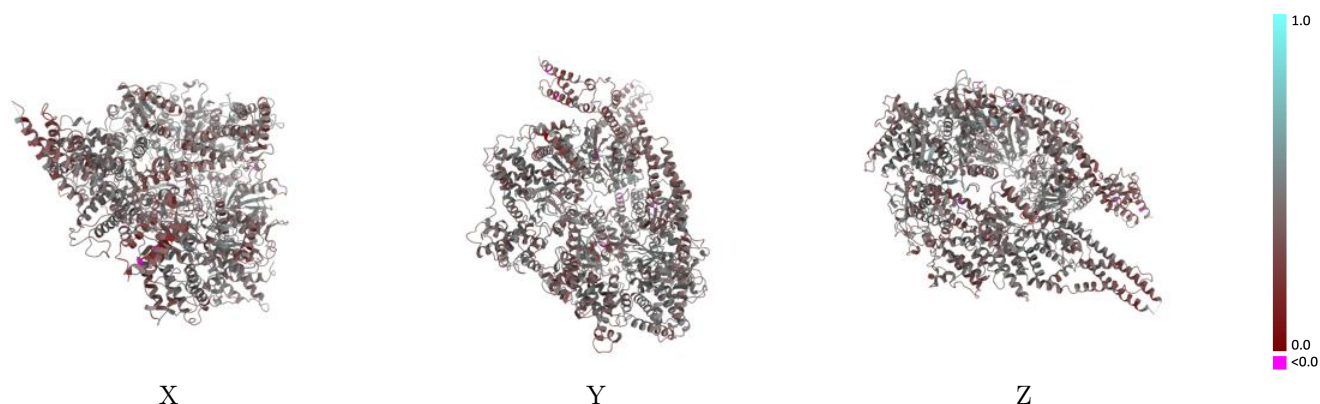
Y



Z

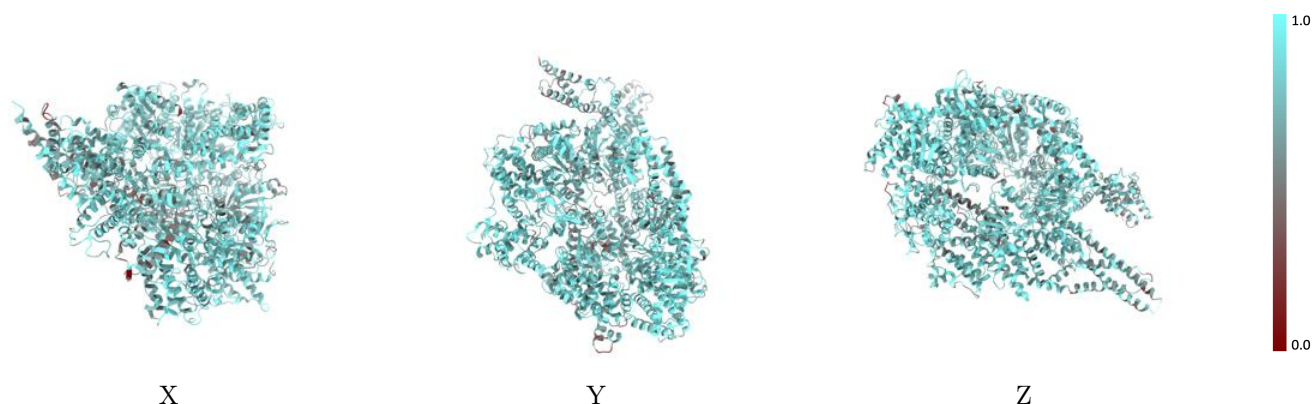
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



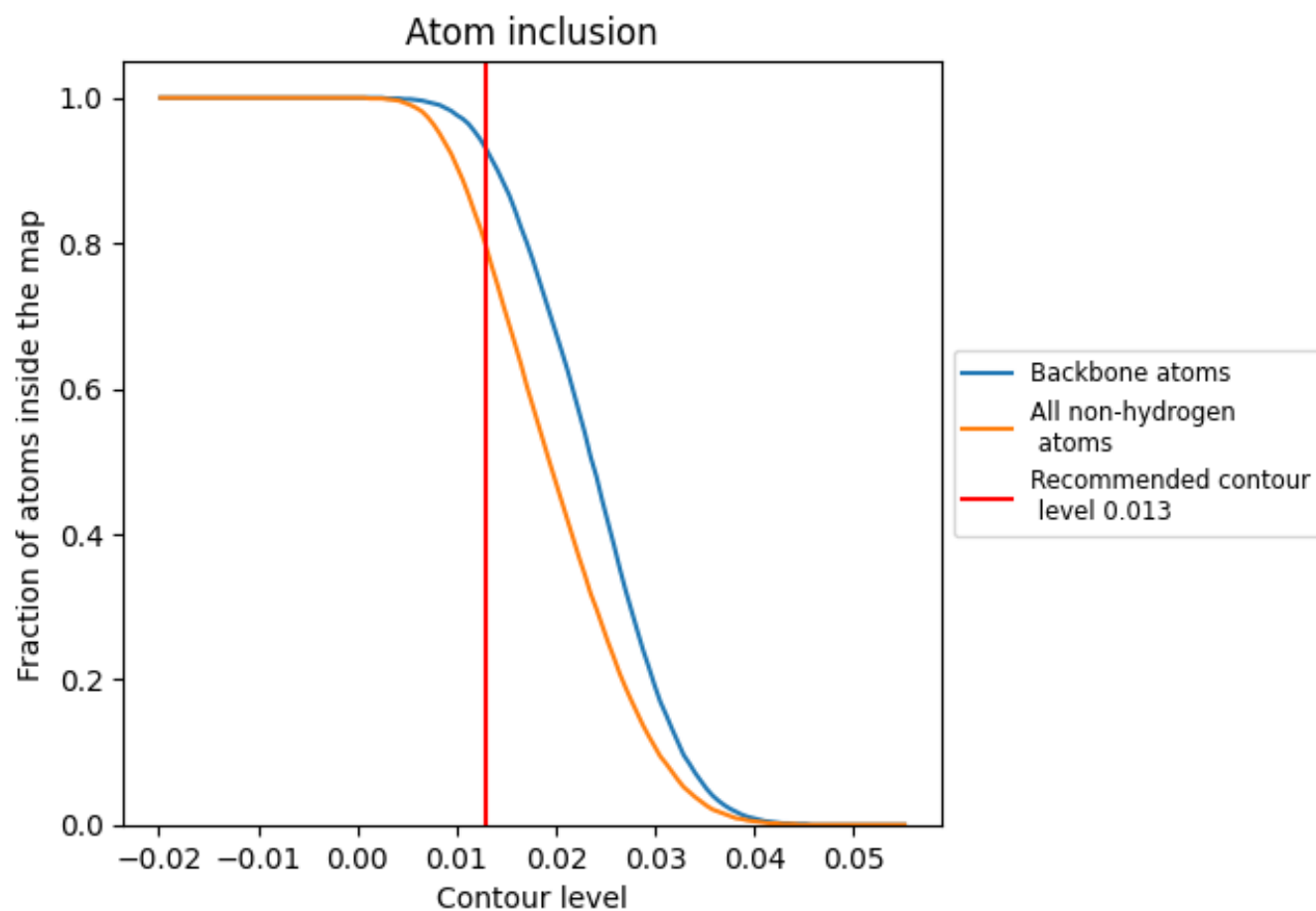
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 79% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7940	0.4160
A	0.7930	0.4160

