



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 10:53 AM EDT

PDB ID : 9BMZ / pdb_00009bmz
EMDB ID : EMD-44716
Title : State-2 of motor domain from full-length human dynein-1 in apo condition
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.97 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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

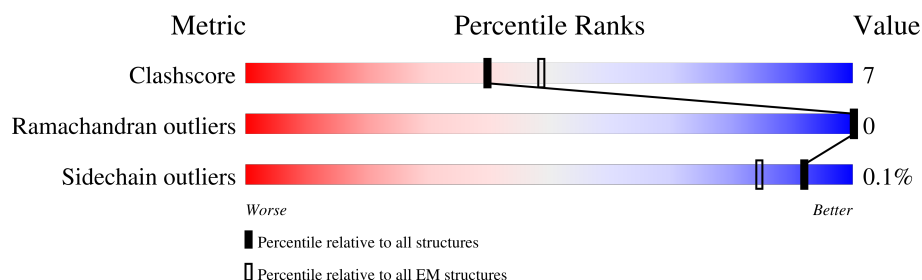
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.97 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	4646	<div> <div>9%</div> <div>52%</div> <div>11%</div> <div>37%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	4705	-	-	X	-
4	MG	A	4706	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 23707 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
			Total	C	N	O	S		
1	A	2937	23593	15028	4070	4378	117	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



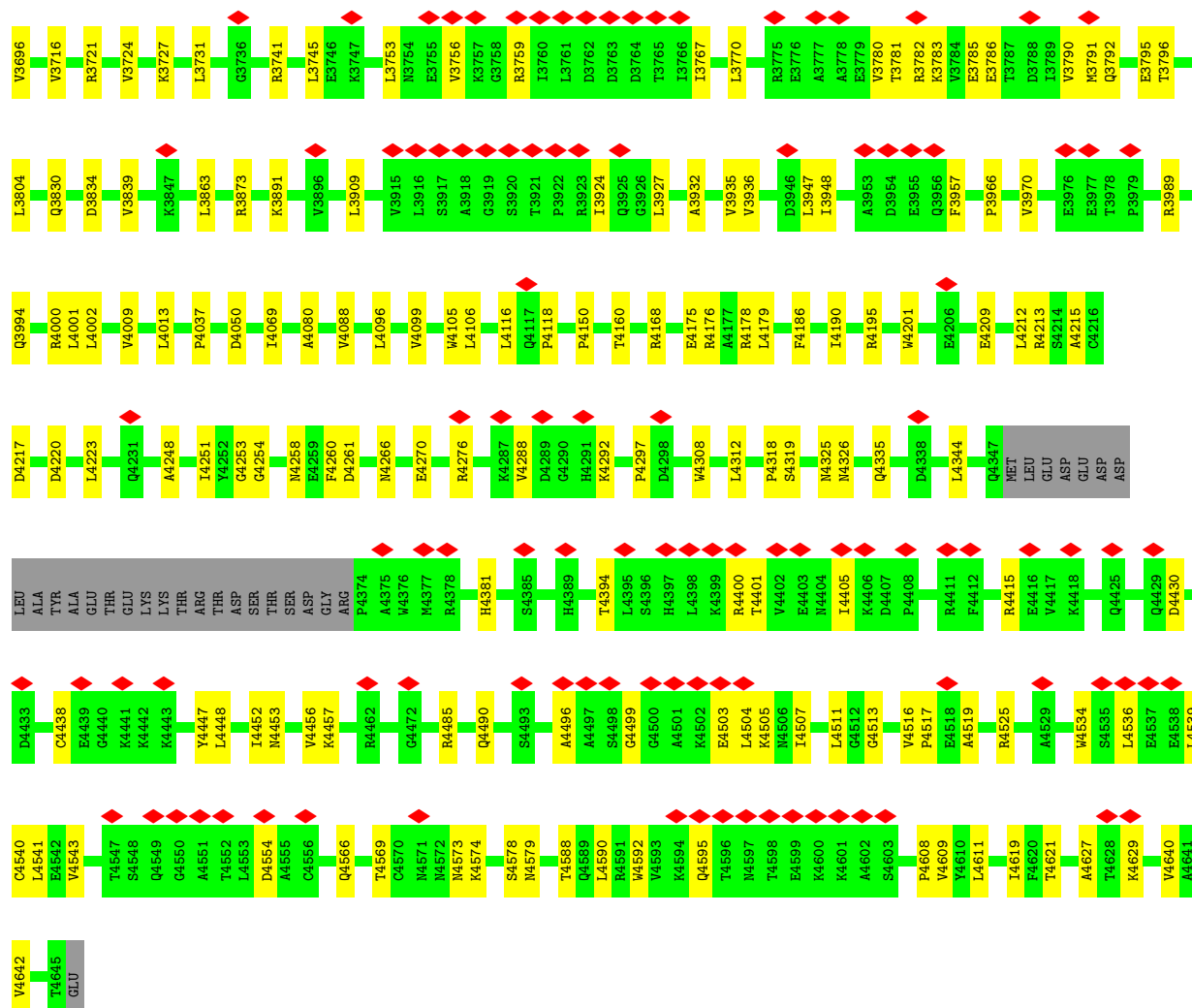
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Mg 2 2	0



L3547	A3458	ALA	L3218	D3124	L2976	W2825	E2629	E2629	E2126	S2290	E2126	
L3553	Q3459	GLN	R3219	Y3125	R2977	A2829	K2633	K2633	N2130	L2296	N2130	
E3558	A3460	ASN	R3220	M3126	V2979	D2840	E2665	E2665	L2131	Q2296	L2131	
R3569	T3461	TYR	D3221	V3128	L2980	R2844	E2665	E2665	F2132	R2297	F2132	
L3560	A3462	ASP	L3222	V3129	K2989	W2845	E2665	E2665	E2133	R2298	E2133	
W3562	K3463	MET	R3223	K3132	W2998	T2846	E2665	E2665	Q2134	V2307	Q2134	
Q3563	D3464	LEU	L3224	L3133	F3004	H2857	E2665	E2665	E2135	D2308	E2135	
P3568	L3465	LYS	K3225	P3134	L3005	D2862	E2665	E2665	T2136	W2311	T2136	
A3466	A3466	ARG	S3226	Q3135	E3006	E2864	E2665	E2665	L2137	V2312	L2137	
A3467	A3467	PRO	Q3227	P3136	E3006	E2864	E2665	E2665	L2138	N2314	L2138	
V3468	V3468	GLU	E3228	P3137	T3010	E2864	E2665	E2665	K2148	N2316	K2148	
F3469	F3469	ASN	L3229	R3140	A3013	E2864	E2665	E2665	L2149	D2320	L2149	
A3470	A3470	ASN	E3230	E3141	N3014	E2864	E2665	E2665	L2157	D2321	L2157	
F3471	F3471	GLN	V3231	A3142	V3017	E2864	E2665	E2665	L2161	T2326	L2161	
Y3472	Y3472	VAL	K3232	I3143	P3018	E2864	E2665	E2665	V2164	E2331	V2164	
R3473	R3473	LYS	N3233	N3145	G3019	E2864	E2665	E2665	F2165	N2338	F2165	
R3474	R3474	LEU	A3234	N3154	L3020	E2864	E2665	E2665	R2172	F2343	R2172	
S3475	S3475	GLU	A3235	V3148	D3024	E2864	E2665	E2665	E2173	F2344	E2173	
T3476	T3476	ASP	A3236	F3150	E3035	E2864	E2665	E2665	E2174	F2345	E2174	
A3477	A3477	ALA	N3237	H3151	E3035	E2864	E2665	E2665	T2175	Q2346	T2175	
L3478	L3478	LYS	D3238	Q3152	Q3038	E2864	E2665	E2665	E2181	A2354	E2181	
L3479	L3479	ASP	K3239	L3154	K3039	E2864	E2665	E2665	E2205	R2358	E2205	
R3480	R3480	ASN	L3240	L3161	M3043	E2864	E2665	E2665	V2211	E2366	V2211	
S3481	S3481	GLN	K3241	A3162	L3044	E2864	E2665	E2665	T2214	L2369	T2214	
L3482	L3482	GLN	K3242	K3163	D3045	E2864	E2665	E2665	M2221	L2374	M2221	
S3483	S3483	LYS	K3242	T3168	F3054	E2864	E2665	E2665	Q2224	D2388	Q2224	
R3486	R3486	ALA	VAL	T3172	S3072	E2864	E2665	E2665	Q2229	E2389	Q2229	
E3487	E3487	VAL	LYS	Y3176	E3073	E2864	E2665	E2665	K2230	GLY	K2230	
E3490	E3490	GLN	GLN	L3177	R3077	E2864	E2665	E2665	S2231	ASP	S2231	
K3491	K3491	ILE	ALA	D3178	R3078	E2864	E2665	E2665	W2234	GLU	W2234	
E3494	E3494	ASP	LYS	F3179	L3085	E2864	E2665	E2665	L2244	ALA	L2244	
T3495	T3495	ASP	LYS	N3180	R3088	E2864	E2665	E2665	E2245	GLN	E2245	
F3496	F3496	LEU	LYS	H3182	D3096	E2864	E2665	E2665	K2257	ARG	K2257	
K3497	K3497	LEU	LYS	N3181	K3097	E2864	E2665	E2665	W2271	LYS	W2271	
I3498	I3498	SER	VAL	K3207	R3206	E2864	E2665	E2665	W2275	GLY	W2275	
Q3499	Q3499	ILE	MET	E3210	K3207	E2864	E2665	E2665	D2277	GLY	D2277	
I3503	I3503	ALA	GLN	T3211	E3210	E2864	E2665	E2665	R2285	GLY	R2285	
S3510	S3510	TYR	ILE	V3212	E3210	E2864	E2665	E2665				
G3665	G3665	ALA	GLN	D3213	E3210	E2864	E2665	E2665				
G3666	G3666	ALA	GLN	Q3214	E3210	E2864	E2665	E2665				
Q3667	Q3667	GLY	GLN	V3215	E3210	E2864	E2665	E2665				
K3615	K3615	PRO	LEU	E3216	E3210	E2864	E2665	E2665				
F3516	F3516	PRO	THR	E3217	E3210	E2864	E2665	E2665				
A3517	A3517	VAL	THR	E3217	E3210	E2864	E2665	E2665				
F3520	F3520	LYS	ASP	E3217	E3210	E2864	E2665	E2665				
K3524	K3524	TRP	TRP	E3217	E3210	E2864	E2665	E2665				
R3525	R3525	ALA	LYS	E3217	E3210	E2864	E2665	E2665				
W3532	W3532	ALA	GLN	E3217	E3210	E2864	E2665	E2665				
Q3538	Q3538	LYS	GLN	E3217	E3210	E2864	E2665	E2665				
A3539	A3539	MET	GLN	E3217	E3210	E2864	E2665	E2665				
D3546	D3546	SER	SER	E3217	E3210	E2864	E2665	E2665				



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65852	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)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.158	Depositor
Minimum map value	-1.216	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.33	Depositor
Map size (Å)	444.4032, 444.4032, 444.4032	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1573, 1.1573, 1.1573	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, MG

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	0.26	0/24093	0.48	0/32651

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	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2091	ARG	Sidechain
1	A	2358	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23593	0	23659	326	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	81	0	36	1	0
3	A	31	0	12	4	0
4	A	2	0	0	4	0
All	All	23707	0	23707	326	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 7.

The worst 5 of 326 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:1913:THR:HG1	4:A:4705:MG:MG	0.77	0.87
1:A:3127:PRO:HG3	1:A:3538:GLN:HG2	1.64	0.77
1:A:1959:GLU:HB3	1:A:1962:ARG:HD3	1.71	0.72
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.22	0.72
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	1.72	0.71

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	2929/4646 (63%)	2879 (98%)	50 (2%)	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	2605/4125 (63%)	2602 (100%)	3 (0%)	92 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2047	GLN
1	A	3480	LYS
1	A	4573	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1855	GLN
1	A	1867	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ATP	A	4702	4	28,33,33	0.85	1 (3%)	34,52,52	0.87	1 (2%)
2	ADP	A	4704	-	24,29,29	0.79	0	29,45,45	0.91	2 (6%)
2	ADP	A	4703	-	24,29,29	0.93	1 (4%)	29,45,45	0.79	1 (3%)
2	ADP	A	4701	4	24,29,29	0.80	0	29,45,45	0.74	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	A	4702	4	-	4/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4703	-	-	2/12/32/32	0/3/3/3
2	ADP	A	4701	4	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4702	ATP	C1'-N9	-2.12	1.44	1.49
2	A	4703	ADP	C8-N7	-2.05	1.31	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4703	ADP	C5-C6-N6	2.46	124.05	120.31
2	A	4704	ADP	C5-C6-N6	2.28	123.78	120.31
3	A	4702	ATP	C5-C6-N6	2.26	123.75	120.31
2	A	4701	ADP	C5-C6-N6	2.25	123.74	120.31
2	A	4704	ADP	C4'-O4'-C1'	-2.24	107.88	109.92

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4702	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	O4'-C4'-C5'-O5'
2	A	4704	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	C3'-C4'-C5'-O5'

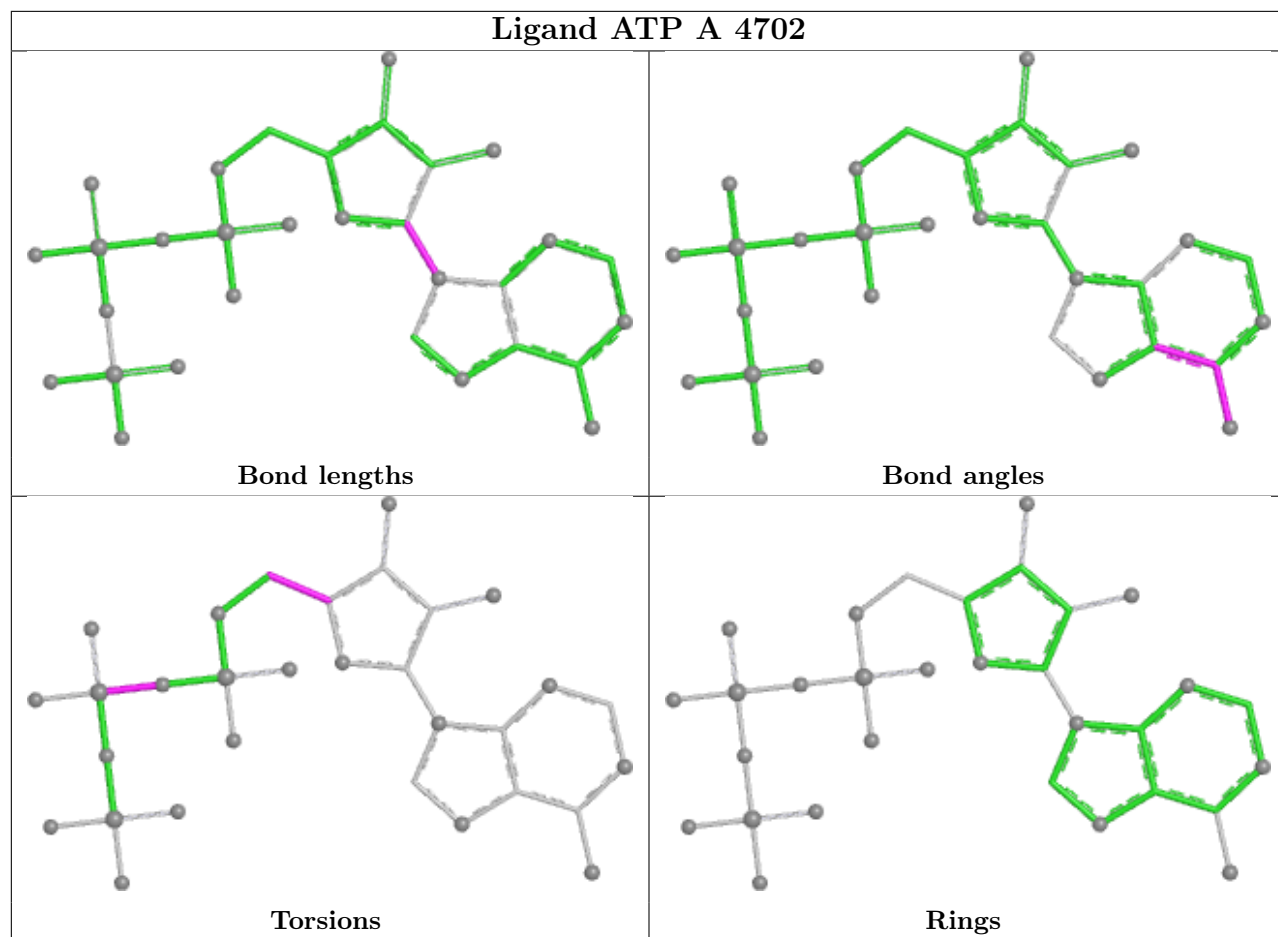
There are no ring outliers.

2 monomers are involved in 5 short contacts:

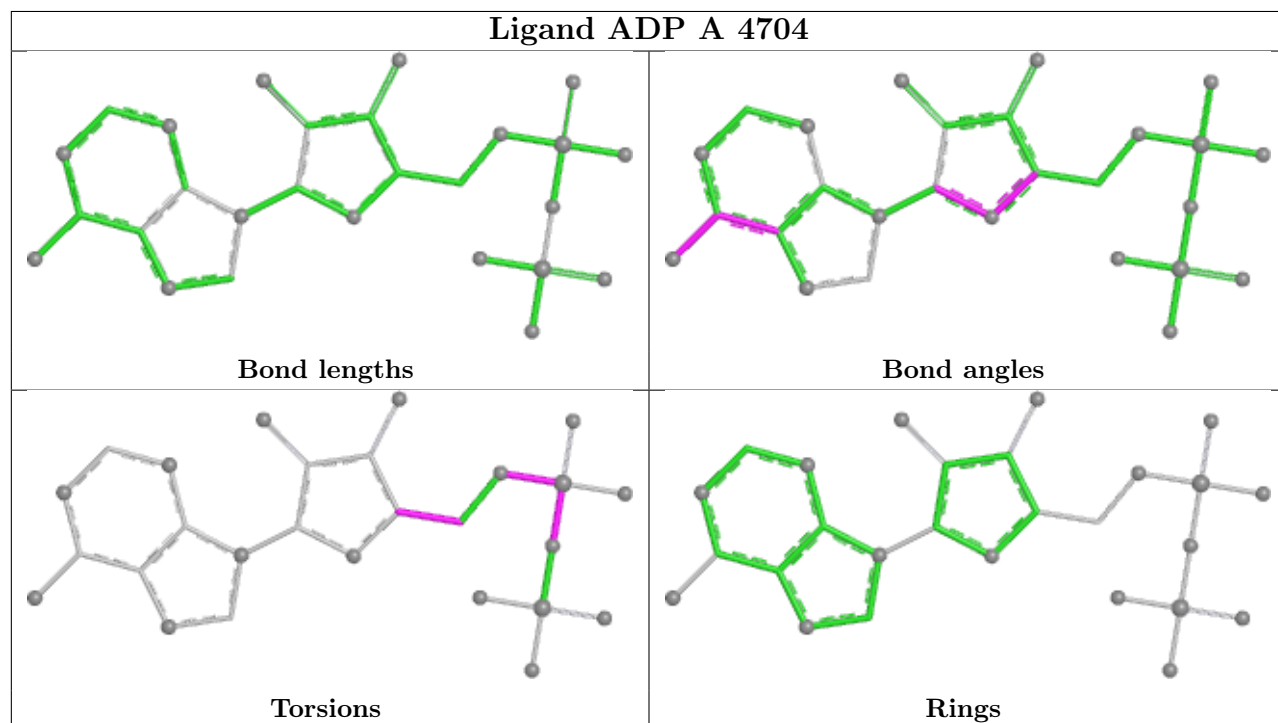
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	4	0
2	A	4704	ADP	1	0

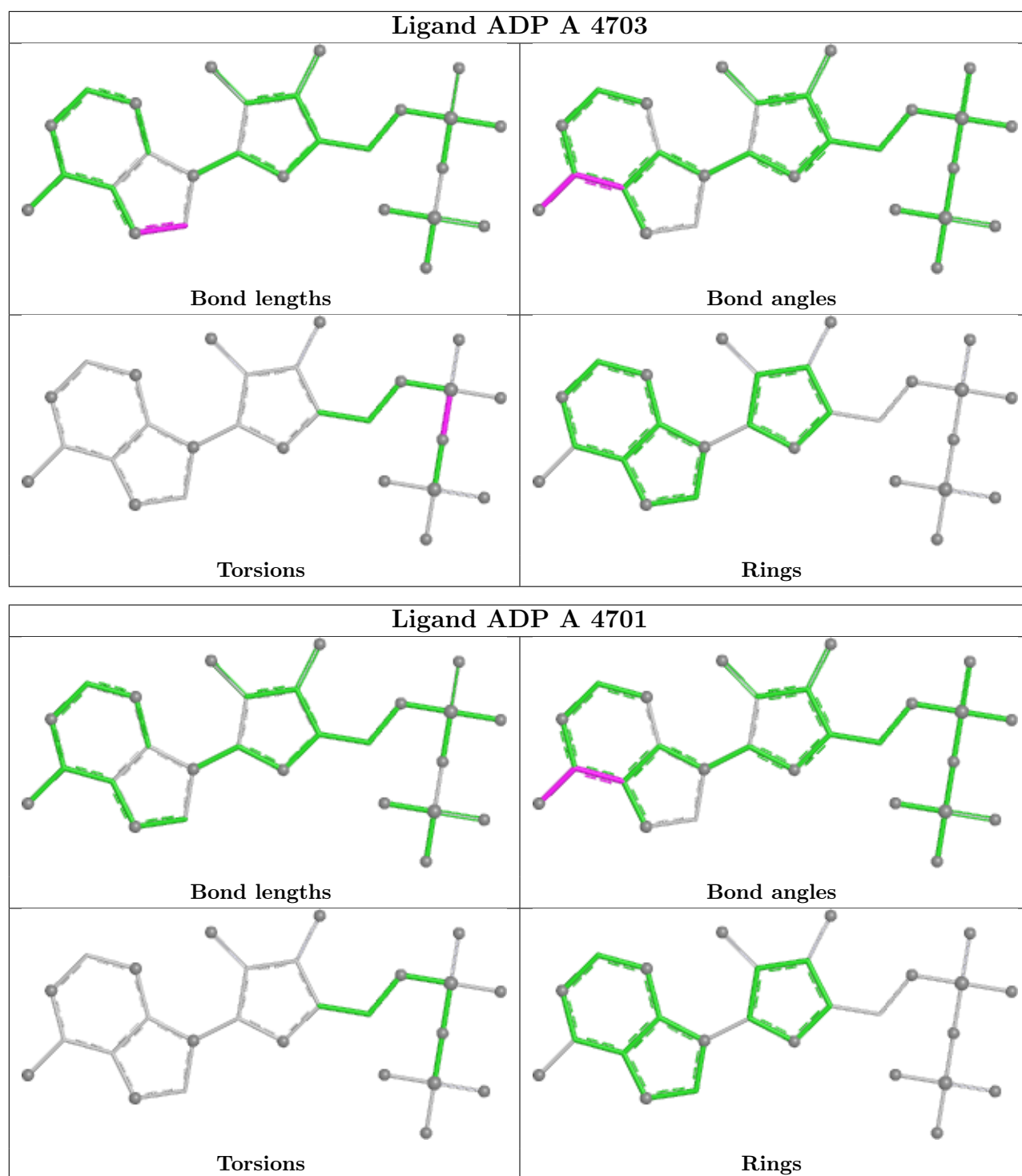
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP A 4702



Ligand ADP A 4704





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

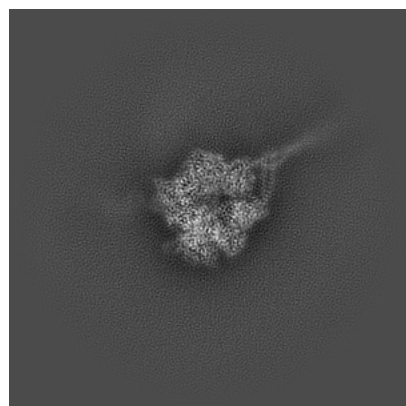
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44716. These allow visual inspection of the internal detail of the map and identification of artifacts.

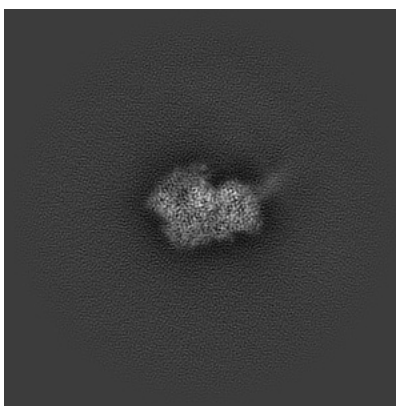
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

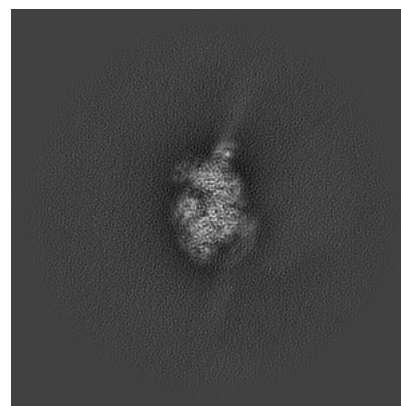
6.1.1 Primary map



X

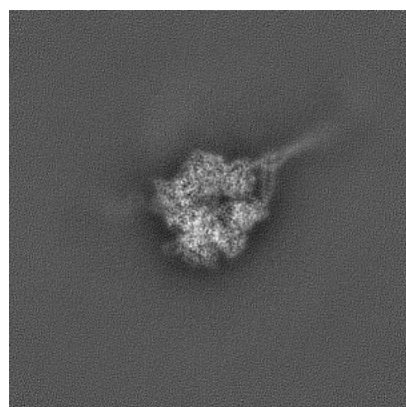


Y

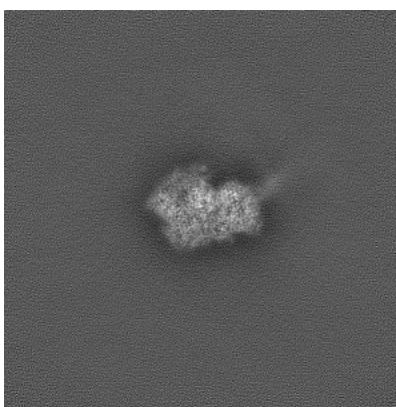


Z

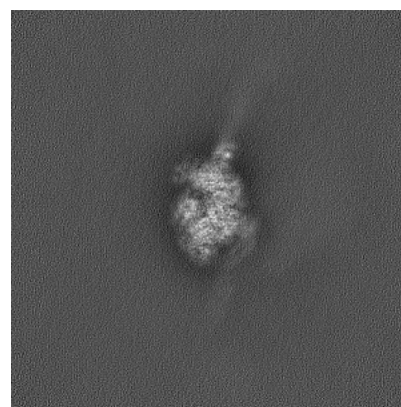
6.1.2 Raw map



X



Y

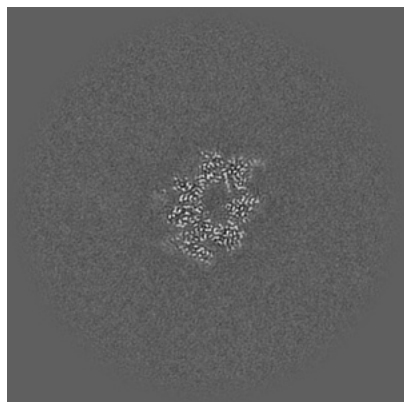


Z

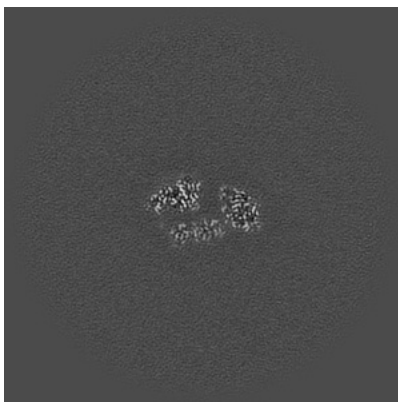
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

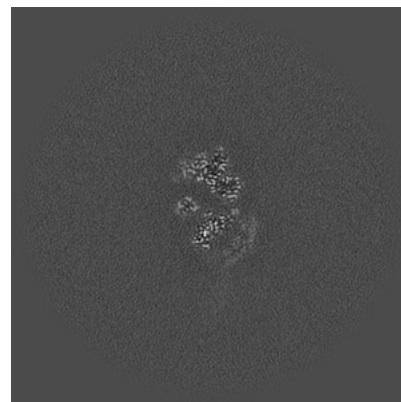
6.2.1 Primary map



X Index: 192

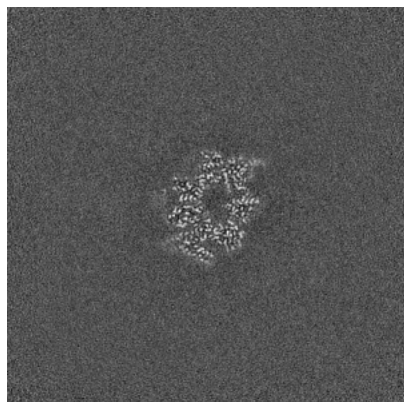


Y Index: 192

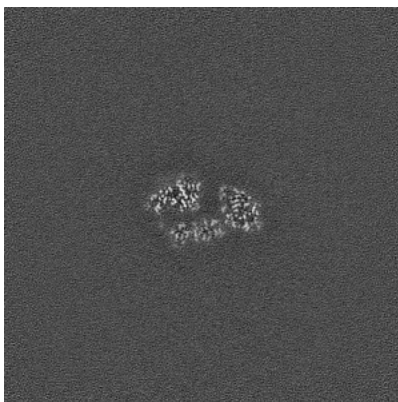


Z Index: 192

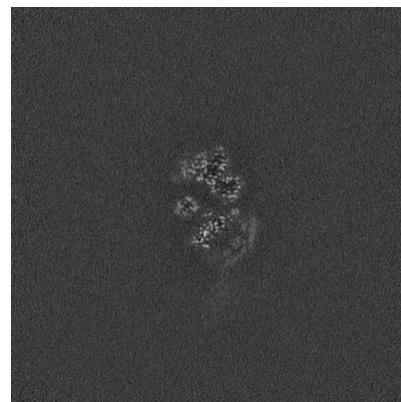
6.2.2 Raw map



X Index: 192



Y Index: 192

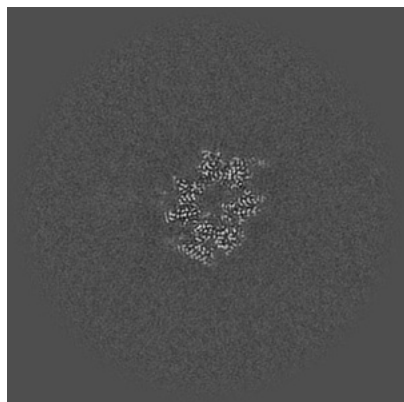


Z Index: 192

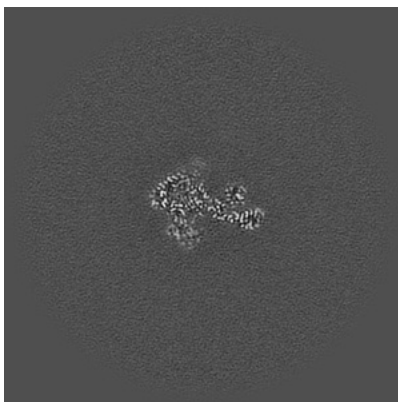
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

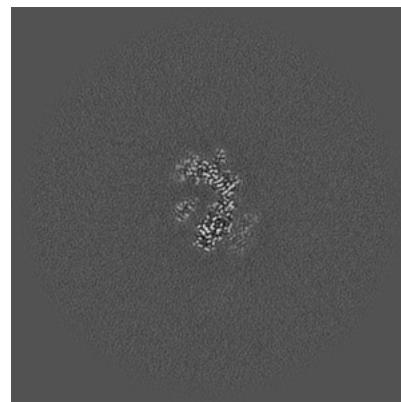
6.3.1 Primary map



X Index: 194

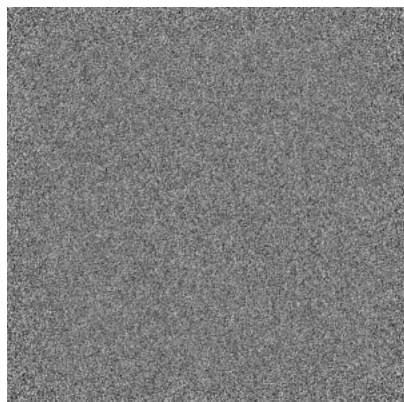


Y Index: 181

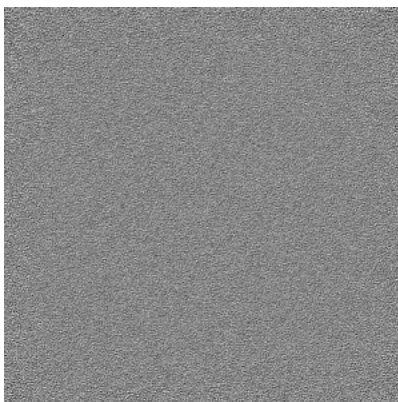


Z Index: 185

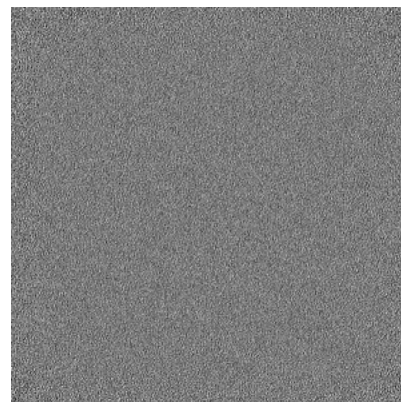
6.3.2 Raw map



X Index: 0



Y Index: 0

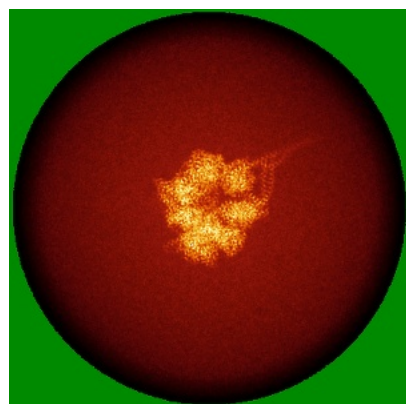


Z Index: 0

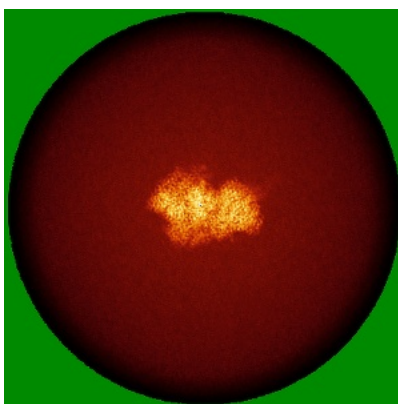
The images above show the largest variance slices of the map in three orthogonal directions.

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

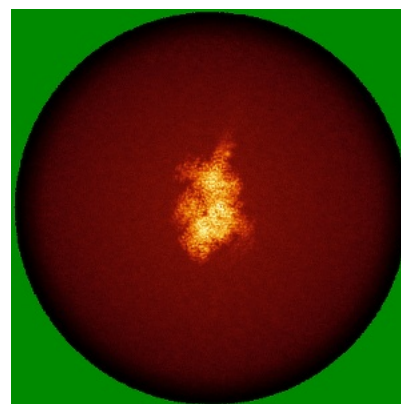
6.4.1 Primary map



X

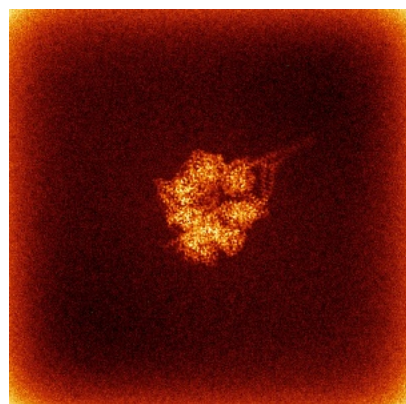


Y

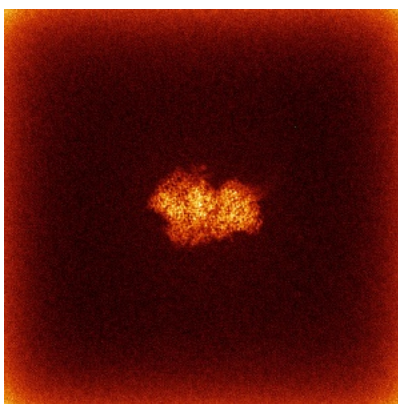


Z

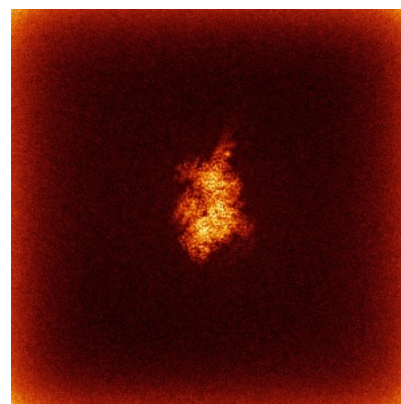
6.4.2 Raw map



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 0.33. 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.

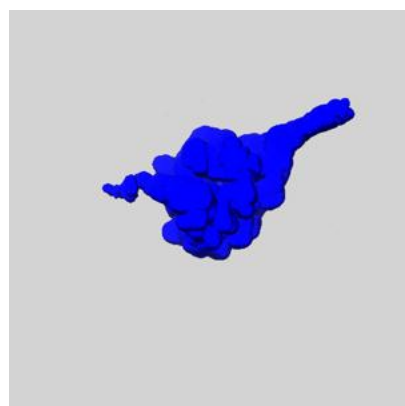
6.6 Mask visualisation [i](#)

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

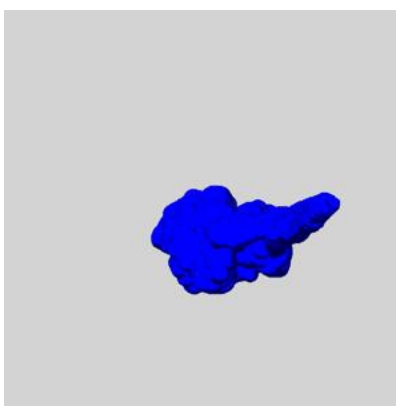
A mask typically either:

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

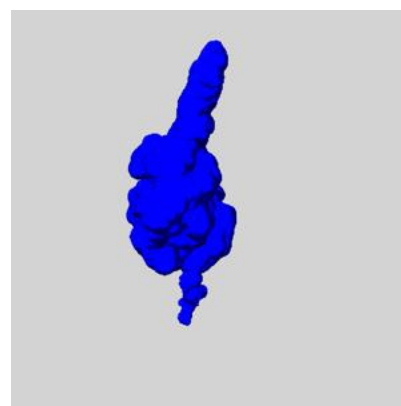
6.6.1 emd_44716_msk_1.map [i](#)



X



Y

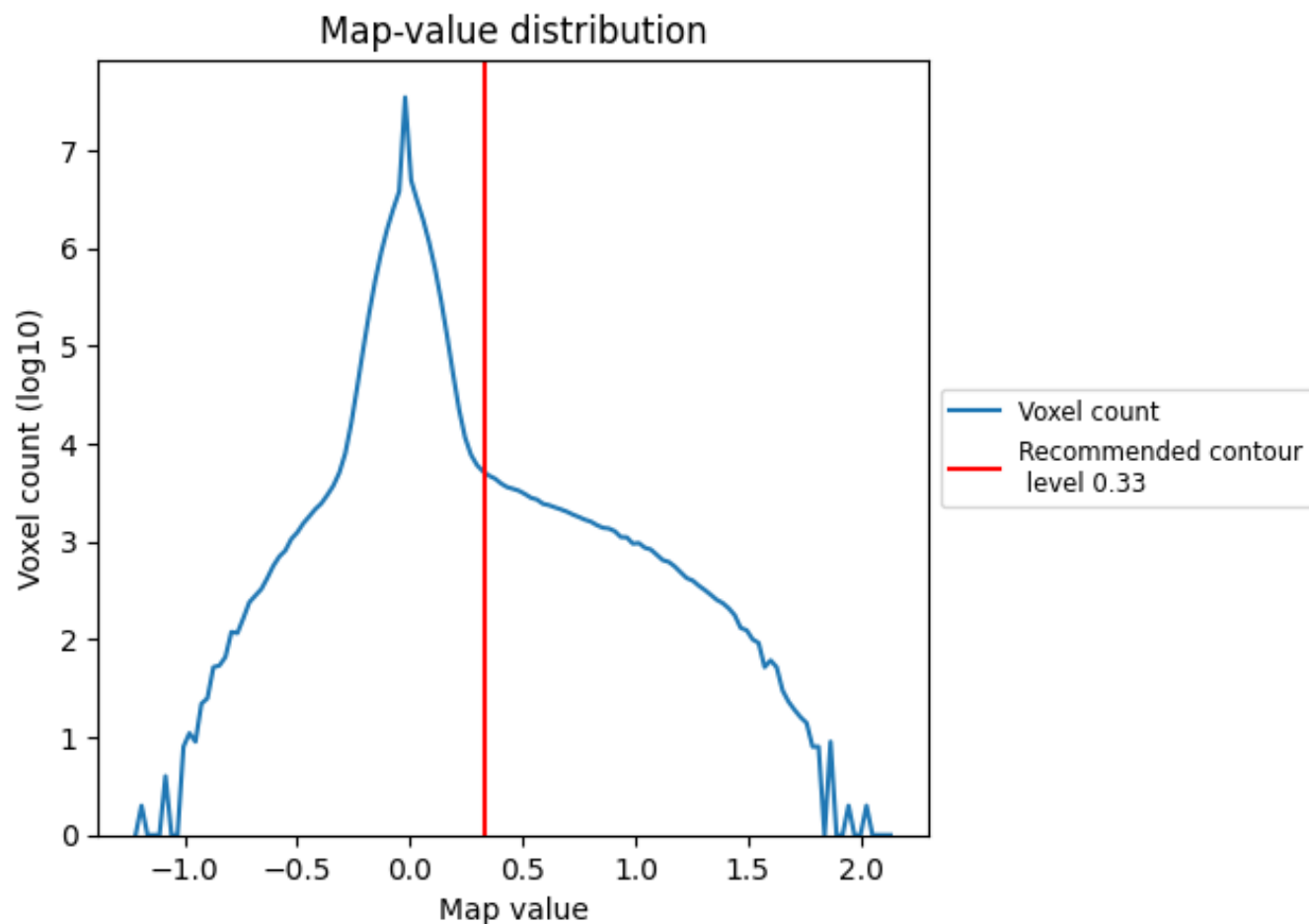


Z

7 Map analysis [i](#)

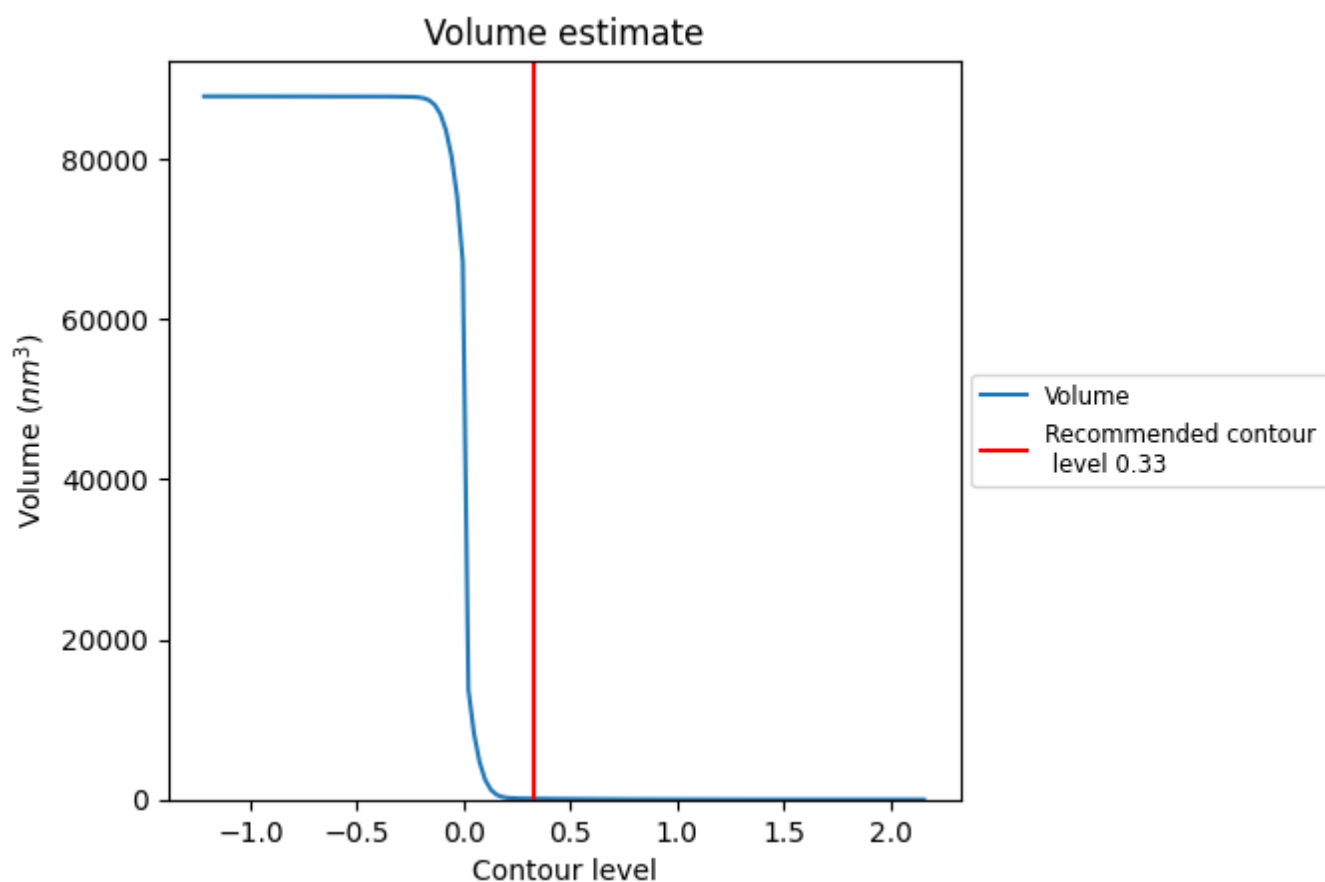
This section contains the results of statistical analysis of the map.

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.

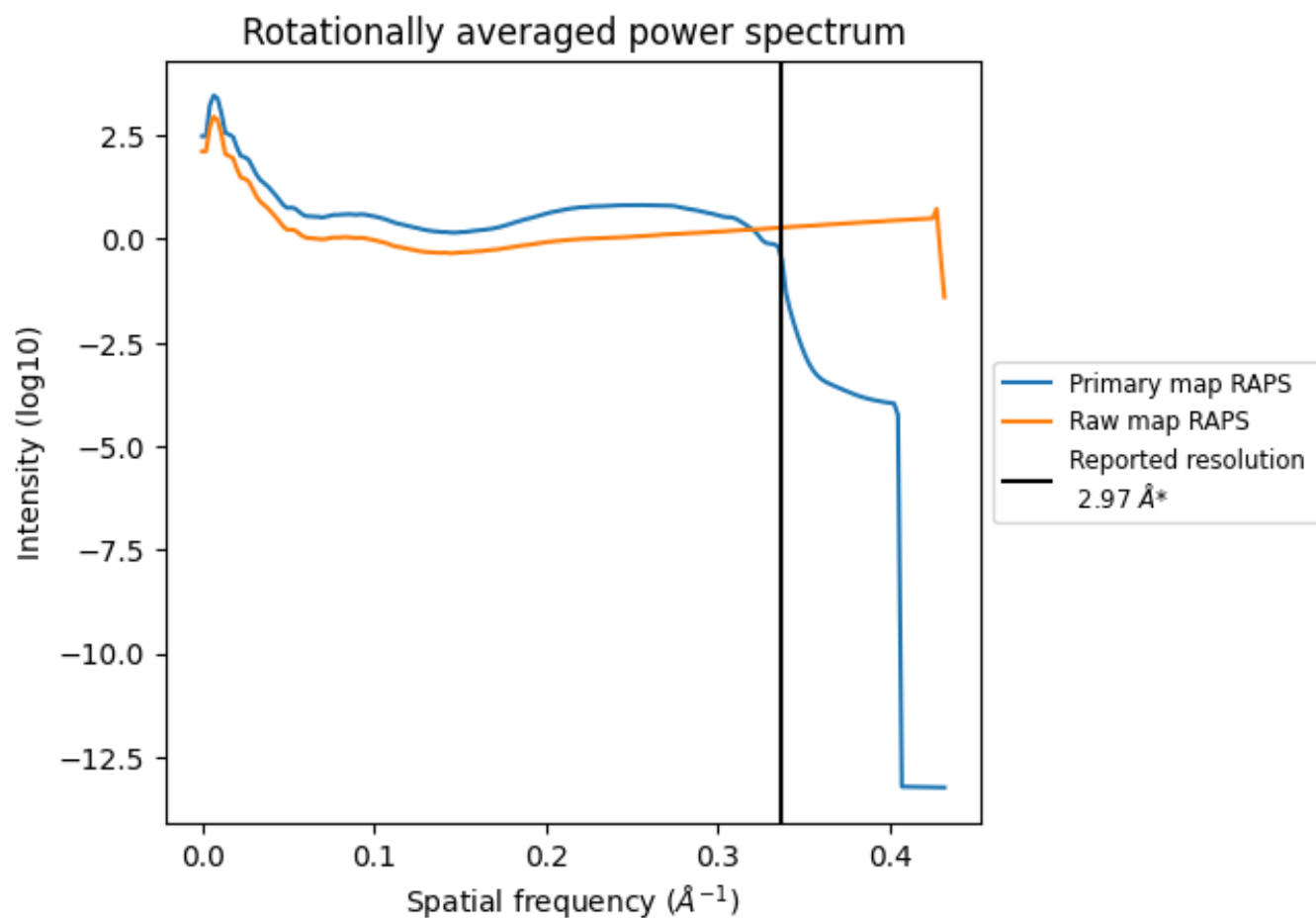
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112 nm³; this corresponds to an approximate mass of 101 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 ⓘ

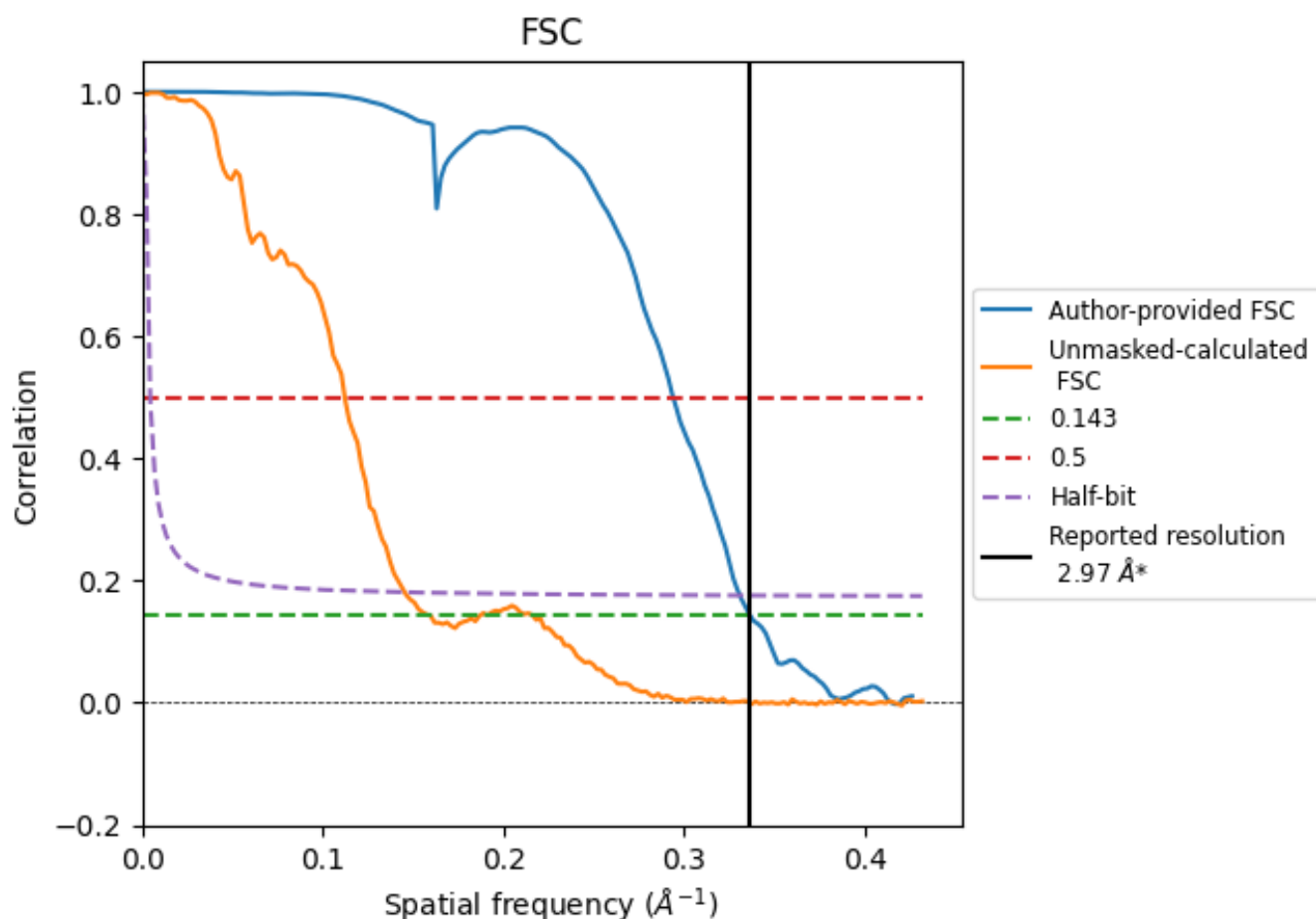


*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

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 0.337 Å⁻¹

8.2 Resolution estimates [i](#)

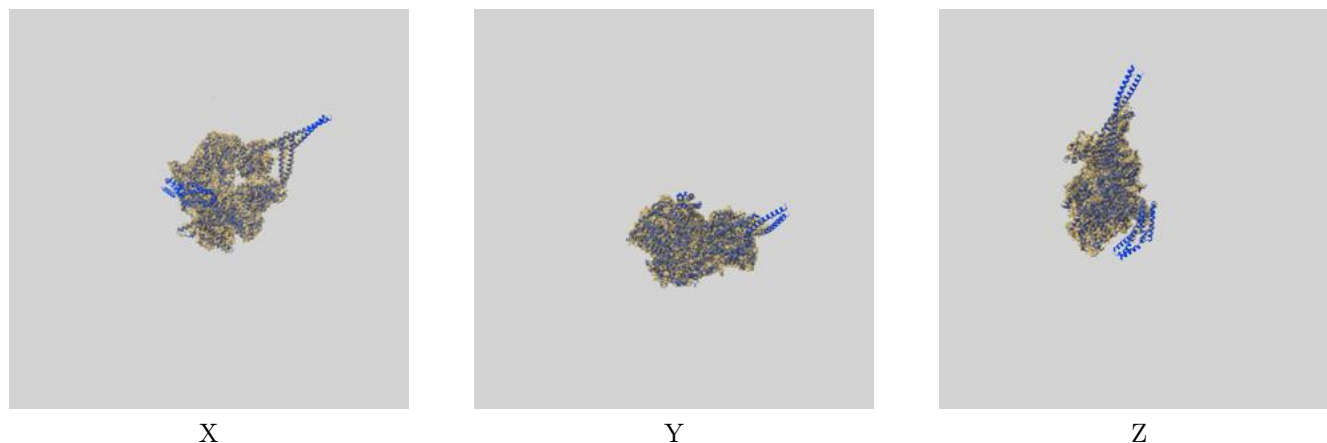
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.97	3.40	3.02
Unmasked-calculated*	6.29	8.91	6.88

*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 6.29 differs from the reported value 2.97 by more than 10 %

9 Map-model fit [i](#)

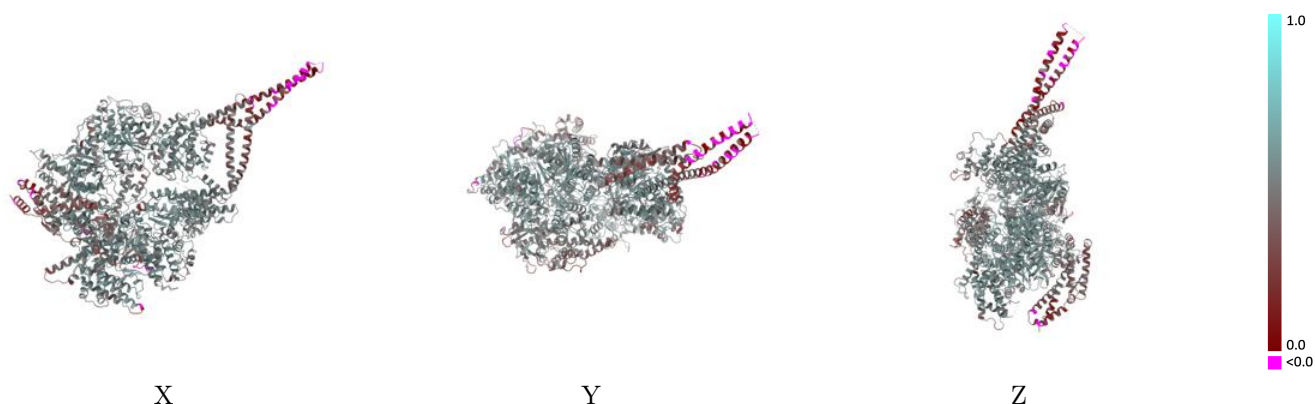
This section contains information regarding the fit between EMDB map EMD-44716 and PDB model 9BMZ. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



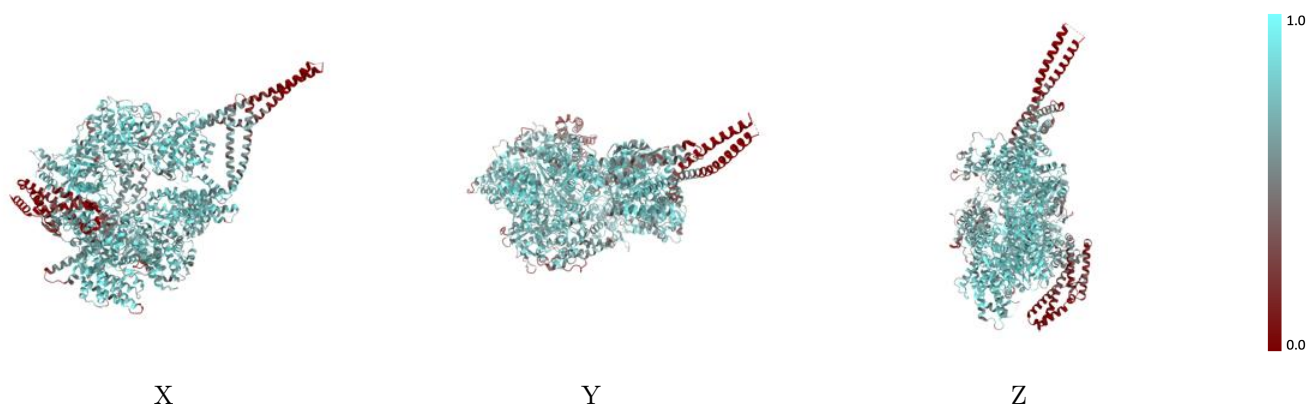
The images above show the 3D surface view of the map at the recommended contour level 0.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



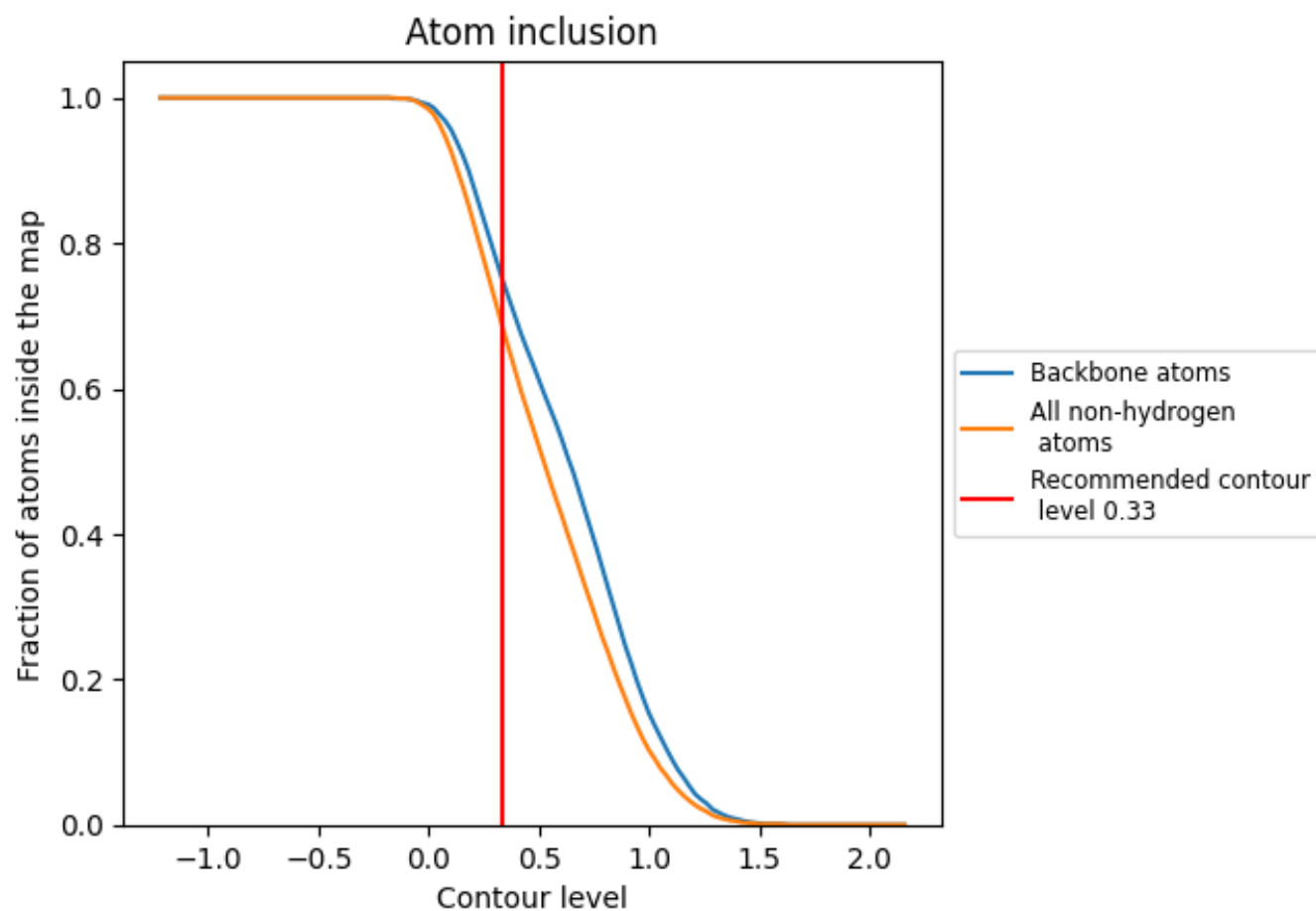
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.33).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 69% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6890	<div></div> 0.4900
A	<div></div> 0.6890	<div></div> 0.4900

