



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 10:23 AM EDT

PDB ID : 9BMW / pdb_00009bmw
EMDB ID : EMD-44713
Title : State-7b-post2 of motor domain from full-length human dynein-1 in 5 mM ADP
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 3.30 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

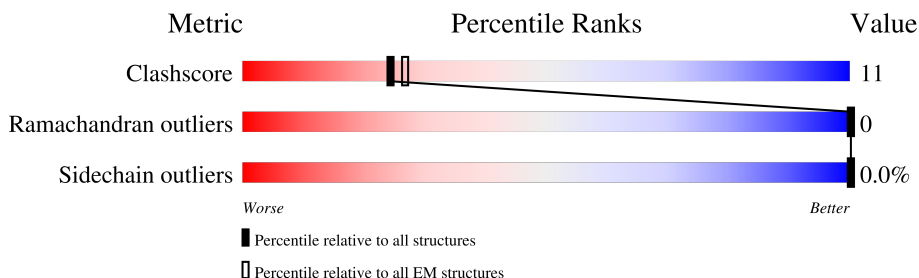
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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>10%</div> <div>49%</div> <div>17%</div> <div>35%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24617 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	3043	24503	15606	4234	4541	122	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	C	N	O	P	0
			31	10	5	13	3	

- 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



ARG	ILE	ALA	GLU	V3129	K3062	E2970	D2851	R2753	W2858	E2487	R2396	S2260	T2127
VAL	PRO	VAL	LEU	Y3130	T3065	D2971	H2857	A2754	L2859	R2397	R2397	H2263	L2131
GLU	THR	ILE	GLU	D3131	T3065	D2971	H2857	N2755	V2660	R2398	R2398	L2264	P2132
PRO	ILE	GLU	VAL	K3132	S3066	D2972	N2860	E2767	F2662	R2399	G2400	G2265	E2133
LEU	VAL	ALA	ASN	L3133	Q3057	D2973	R2869	P2768	C2863	G2401	E2402	G2266	Q2134
ARG	ASN	ASN	ALA	Q3134	V3058	D2976	Y2873	M2773	D2864	E2403	E2403	Y2267	E2135
ASN	PHE	ALA	ALA	Q3135	I3059	L2976	L2877	E2775	L2666	E2404	E2404	L2268	
GLU	SER	VAL	ALA	P3136	V3064	V2979	Y2873	V2774	N2667	E2405	E2405		T2138
GLN	GLU	LYS	ASN	R3140	V3065	L2980	Y2873	E2775	L2666	E2406	E2406	R2273	Q2139
GLY	GLU	ASP	ASP	E3141	R2981	R2981	L2877	E2775	E2666	E2406	E2406	V2291	S2140
LEU	ILE	ILE	LYS	S3146	T3067	S2983	L2877	T2778	N2667	E2406	E2406	R2292	V2141
SER	ASP	LYS	LYS		K3068	N2987	D2880	E2782	K2873	E2406	E2406		V2146
ASP	ALA	GLN	LYS		N3069	E2987	D2880	E2782	T2876	E2407	E2407		L2149
GLU	ASP	ALA	MET	V3150	P3070	K2988	L2882	E2783	Q2877	E2408	E2408		L2156
GLY	GLU	VAL	VAL	H3151	S3071	E2989	P2883	E2784	R2878	E2409	E2409		L2166
ASN	LYS	VAL	ASP		S3072	L2990	E2887	T2785	F2882	E2409	E2409		L2157
GLY	GLU	VAL	GLU	L3154	E3073	D2992	E2887	Q2786	F2882	E2409	E2409		D2304
MET	MET	VAL	GLN	H3155	F2992	F2992	E2888	D2787	L2883	E2409	E2409		G2305
GLN	LYS	VAL	GLN	L3155	L2993	L2993	E2888	T2788	R2884	E2409	E2409		D2306
GLN	LYS	VAL	GLU	T3172	K3074	K2994	L2889	Q2789	V2887	E2409	E2409		W2311
ALA	ASN	MET	ALA		L3075	D2995	K2898	H2790	T2895	E2409	E2409		L2161
ASN	GLU	ASN	ALA	L3186	K3076	E2996	K2898	E2791	F2895	E2409	E2409		L2315
GLU	MET	ASN	GLU		R3077	S2997	Y2901	Y2792	T2895	E2409	E2409		L2191
GLY	MET	ASN	GLU	L3186	R3078	N2997	Y2901	Y2792	T2895	E2409	E2409		T2192
VAL	SER	PRO	LYS	S3192	A3079	N2998	L2905	R2797	R2705	E2409	E2409		G2200
ASN	ASN	PRO	LYS	E3193	A3080	V2999	L2905	R2797	L2706	E2409	E2409		L2324
GLU	GLN	PRO	VAL	L3194	T3081	L3000	L2909	W2802	Q2707	E2409	E2409		L2325
MET	SER	ALA	ALA	E3195	F3086	F3004	V2910	W2803	C2712	E2409	E2409		T2326
ILE	TYR	VAL	VAL	E3196	R3087	L3005	L2916	L2806	H2713	E2409	E2409		L2327
ASN	TYR	VAL	GLN	Q3197	R3088	E3006	L2916	F2807	P2714	E2409	E2409		W2204
GLY	GLU	LEU	GLU	Q3198	C3089	L3007	V2919	L2816	R2720	E2409	E2409		E2205
VAL	GLU	LEU	GLN	H3199	V3090	R3007	L2920	P2817	L2723	E2409	E2409		K2206
ALA	VAL	GLU	GLN	L3200	L3091	K3008	L2921	L2816	L2723	E2409	E2409		Y2211
SER	ASN	ASN	ASN	H3200	N3092	L3020	L2922	P2817	L2723	E2409	E2409		H2218
ASN	ASN	ASN	ASN	N3092	N3092	L3020	L2923	P2817	L2723	E2409	E2409		W2221
ILE	ARG	ILE	ARG	W3093	N3092	L3020	L2924	L2816	L2723	E2409	E2409		V2222
ALA	ALA	CYS	ALA	F3094	N3092	L3020	L2925	P2817	L2723	E2409	E2409		G2224
SER	ALA	LEU	LEU	E3100	N3092	L3020	L2926	L2816	L2723	E2409	E2409		F2343
GLY	GLY	GLY	GLN	Y3103	N3092	L3020	L2927	P2817	L2723	E2409	E2409		E2344
VAL	VAL	GLU	VAL	K3107	N3092	L3020	L2928	P2817	L2723	E2409	E2409		V2345
SER	PRO	SER	ILE	E3108	N3092	L3020	L2929	P2817	L2723	E2409	E2409		Q2346
ALA	MET	THR	ALA	F3109	N3092	L3020	L2930	P2817	L2723	E2409	E2409		R2358
VAL	VAL	THR	ALA	T3208	N3092	L3020	L2935	P2817	L2723	E2409	E2409		M2373
LYS	LYS	ASP	ASP	K3209	N3092	L3020	L2936	P2817	L2723	E2409	E2409		W2234
TRP	TRP	TRP	TRP	E3210	N3092	L3020	L2944	P2817	L2723	E2409	E2409		K2236
ALA	ILE	GLN	GLN	T3211	N3092	L3020	R2948	P2817	L2723	E2409	E2409		V2237
ALA	ALA	ILE	VAL	V3212	N3092	L3020	P2949	P2817	L2723	E2409	E2409		L2382
GLN	LYS	ARG	LYS	D3213	N3092	L3020	V2950	P2817	L2723	E2409	E2409		P2386
ALA	ASN	ASN	GLU	Q3214	N3092	L3020	N2954	P2817	L2723	E2409	E2409		E2242
ASN	ASN	ASN	ASN	V3215	N3092	L3020	G2955	P2817	L2723	E2409	E2409		E2248
TYR	TYR	ILE	ASP	E3216	N3092	L3020	L2956	P2817	L2723	E2409	E2409		G2390
ALA	ALA	MET	ASP	E3217	N3092	L3020	K2962	P2817	L2723	E2409	E2409		E2391
ASP	ASP	ARG	ARG	L3218	N3092	L3020	R2965	P2817	L2723	E2409	E2409		D2392
MET	MET	GLU	GLU	R3219	N3092	L3020	K2966	P2817	L2723	E2409	E2409		A2258
LEU	LEU	ASN	ASN	R3220	N3092	L3020	K2966	P2817	L2723	E2409	E2409		E2393
ALA	ALA	PHE	PHE	D3221	N3092	L3020	K2966	P2817	L2723	E2409	E2409		L2259
				LEU	N3092	L3020	K2966	P2817	L2723	E2409	E2409		A2394
				ARG	N3092	L3020	K2966	P2817	L2723	E2409	E2409		Q2395
				ILE	N3092	L3020	K2966	P2817	L2723	E2409	E2409		
				LYS	N3092	L3020	K2966	P2817	L2723	E2409	E2409		
				LYS	N3092	L3020	K2966	P2817	L2723	E2409	E2409		
				SER	N3092	L3020	K2966	P2817	L2723	E2409	E2409		
				GLN	N3092	L3020	K2966	P2817	L2723	E2409	E2409		

WORLDWIDE
PDB
PROTEIN DATA BANK

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41042	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.144	Depositor
Minimum map value	-0.610	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	329.984, 329.984, 329.984	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0312, 1.0312, 1.0312	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.27	0/25022	0.50	0/33900

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	24503	0	24573	518	0
2	A	81	0	36	2	0
3	A	31	0	12	2	0
4	A	2	0	0	0	0
All	All	24617	0	24621	518	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 11.

The worst 5 of 518 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:1698:ILE:HD13	1:A:1701:TRP:HE1	1.44	0.82
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.65	0.77
1:A:2221:MET:HG2	1:A:2343:PHE:HB2	1.66	0.77
1:A:3601:MET:HE2	1:A:3634:LEU:HD23	1.66	0.76
1:A:4326:ASN:HD22	1:A:4581:ILE:HD13	1.49	0.74

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	3035/4646 (65%)	2967 (98%)	68 (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	2706/4125 (66%)	2705 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3078	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2416	GLN
1	A	2577	HIS
1	A	2588	HIS

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	$\# Z > 2$
2	ADP	A	4701	-	24,29,29	0.85	0	29,45,45	1.24	2 (6%)
3	ATP	A	4702	4	28,33,33	0.70	0	34,52,52	0.59	1 (2%)
2	ADP	A	4703	-	24,29,29	0.87	0	29,45,45	1.25	2 (6%)
2	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.25	2 (6%)

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
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4702	4	-	3/18/38/38	0/3/3/3
2	ADP	A	4703	-	-	5/12/32/32	0/3/3/3
2	ADP	A	4704	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	N3-C2-N1	-3.85	123.45	128.67
2	A	4704	ADP	N3-C2-N1	-3.73	123.61	128.67
2	A	4703	ADP	N3-C2-N1	-3.69	123.67	128.67
2	A	4704	ADP	C4-C5-N7	-2.43	106.77	109.34
2	A	4703	ADP	C4-C5-N7	-2.42	106.78	109.34

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4703	ADP	C5'-O5'-PA-O1A
2	A	4703	ADP	C5'-O5'-PA-O2A
2	A	4703	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A

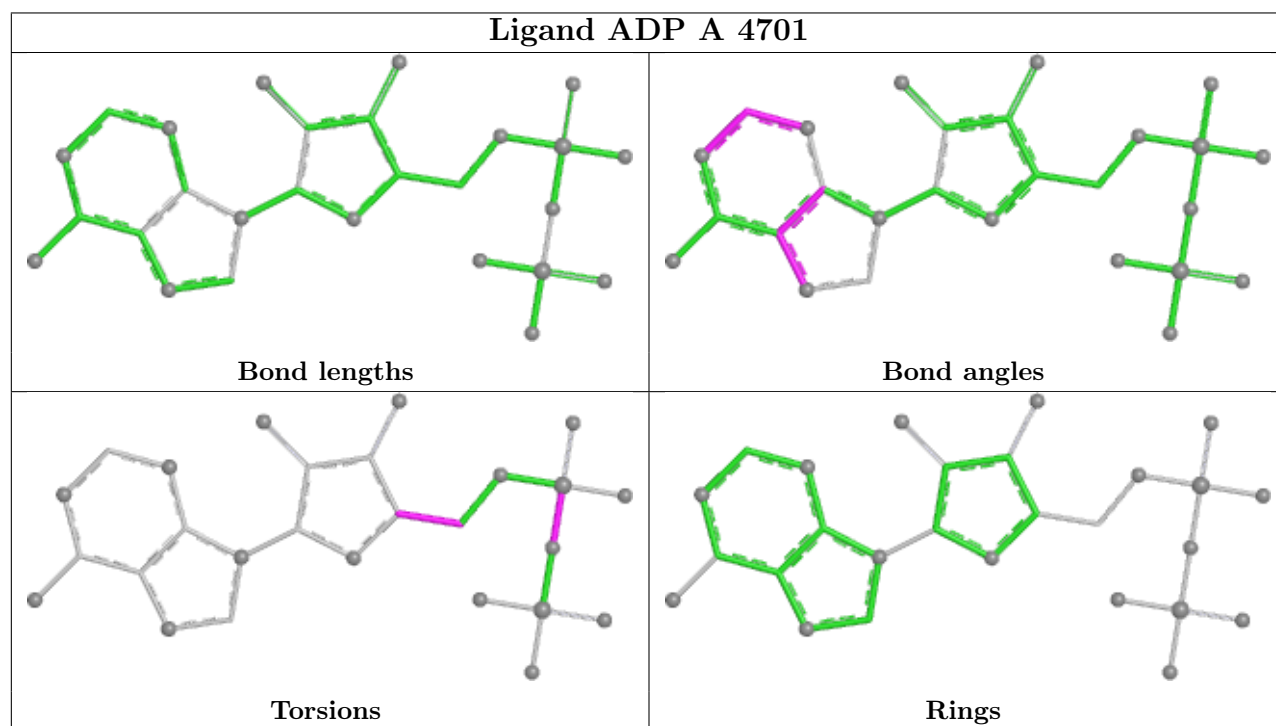
There are no ring outliers.

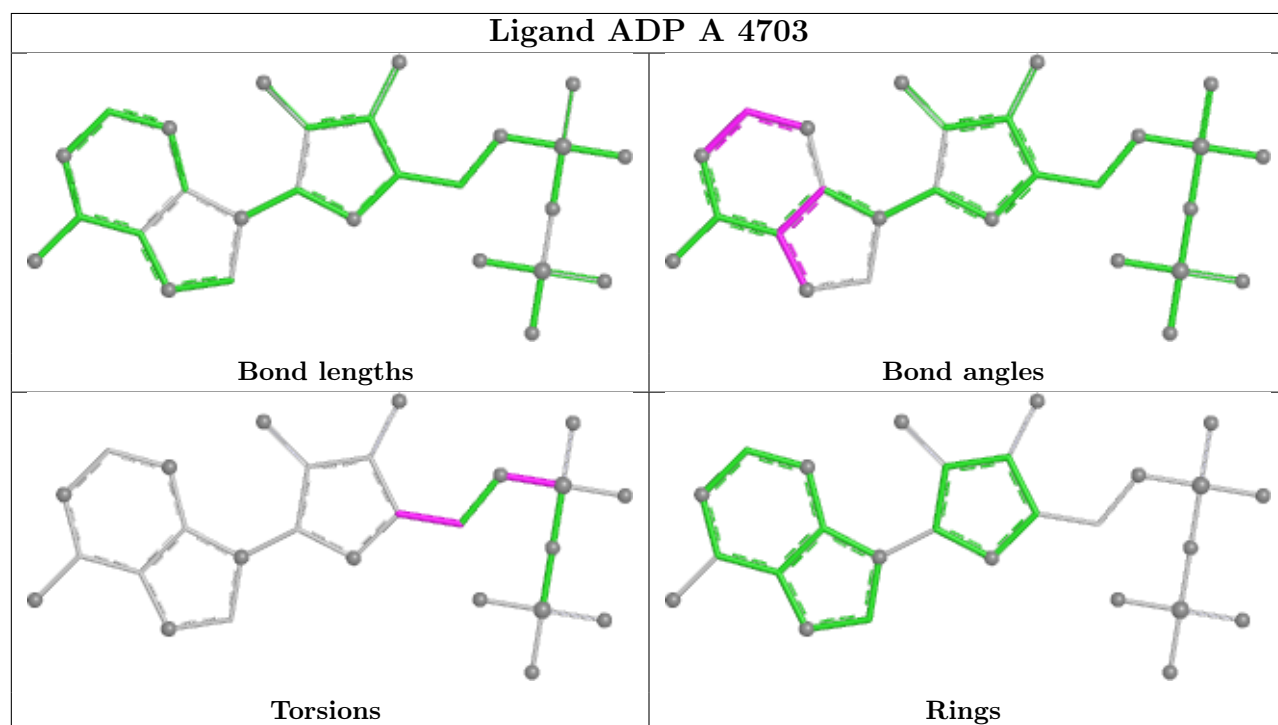
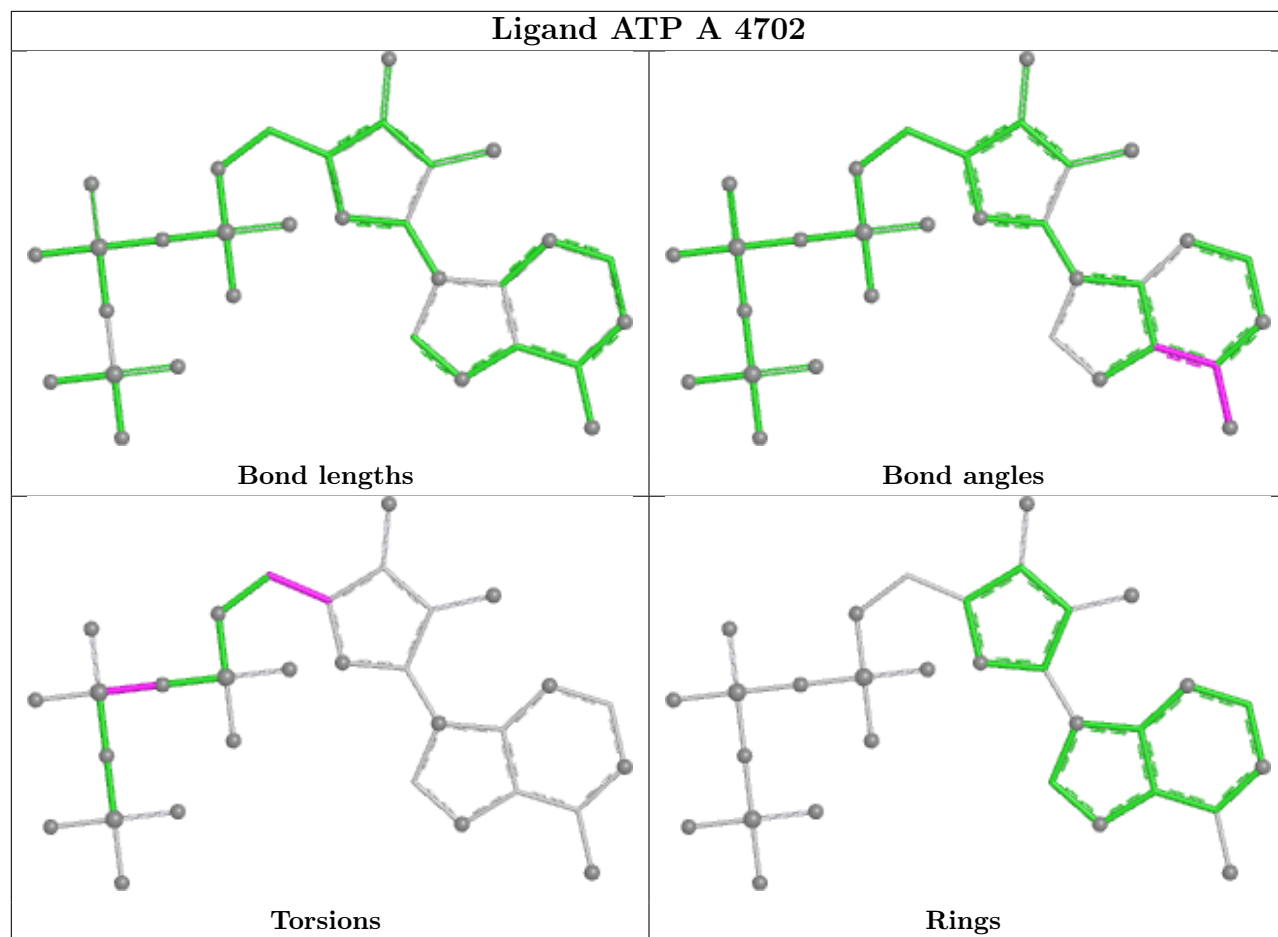
3 monomers are involved in 4 short contacts:

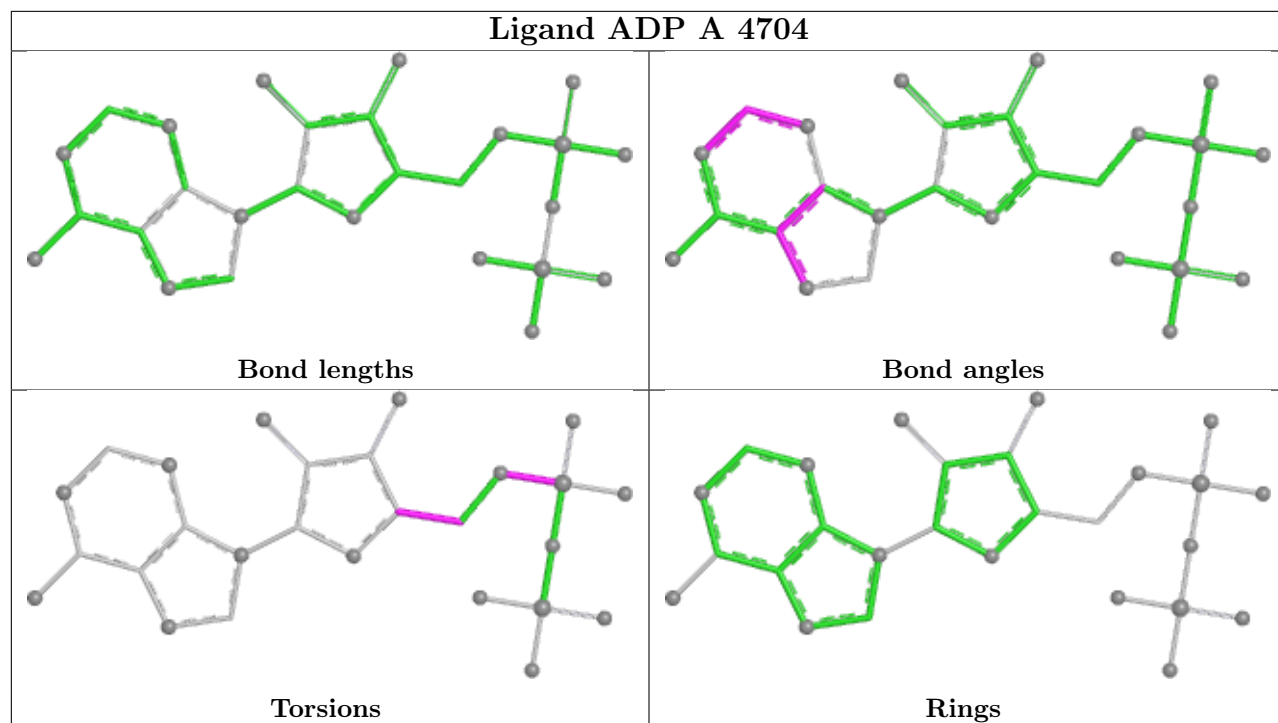
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	1	0
3	A	4702	ATP	2	0
2	A	4704	ADP	1	0

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.







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.

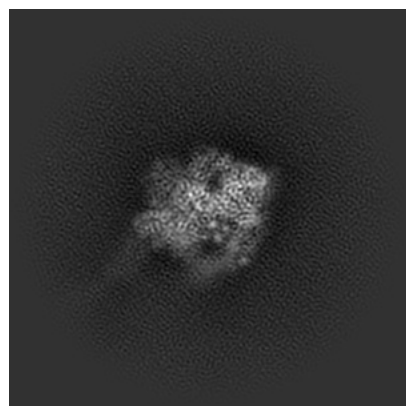
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44713. These allow visual inspection of the internal detail of the map and identification of artifacts.

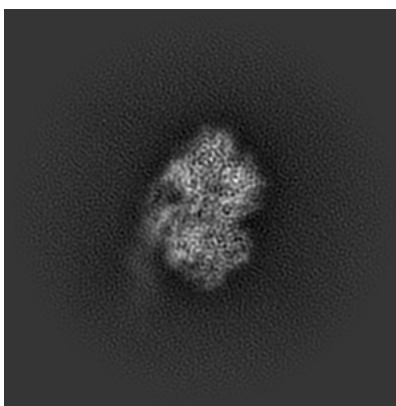
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

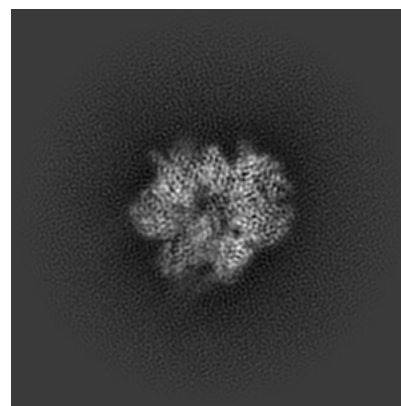
6.1.1 Primary map



X

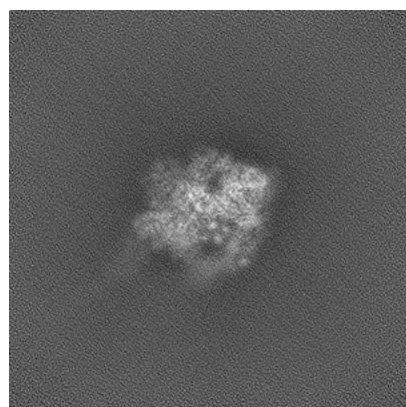


Y

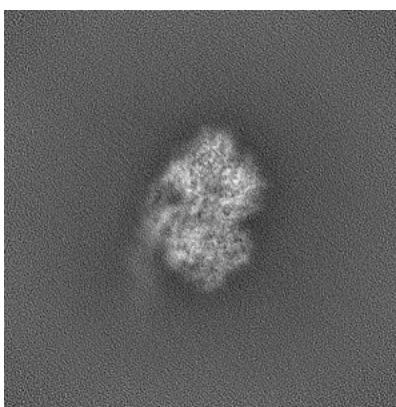


Z

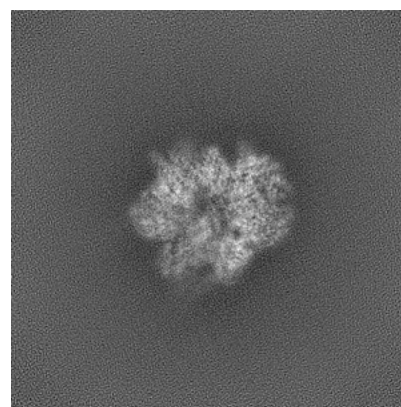
6.1.2 Raw map



X



Y

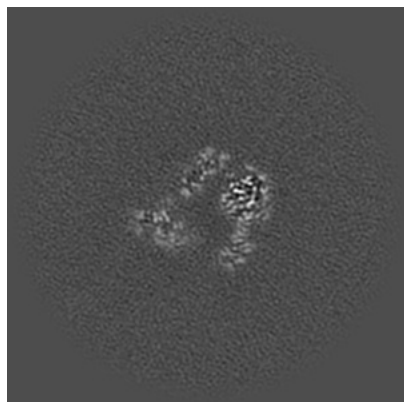


Z

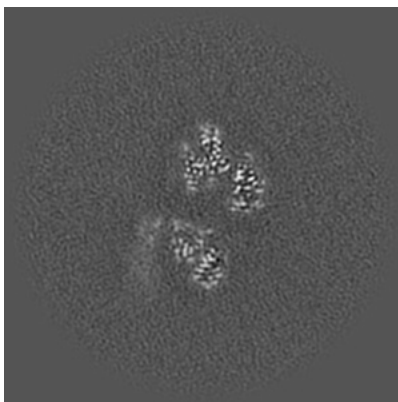
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

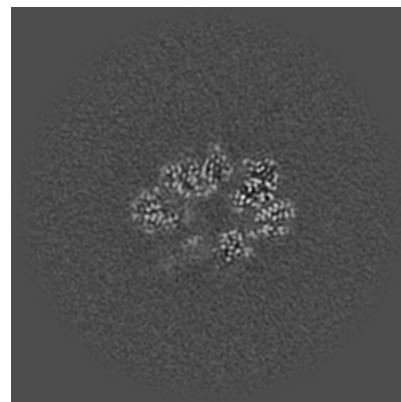
6.2.1 Primary map



X Index: 160

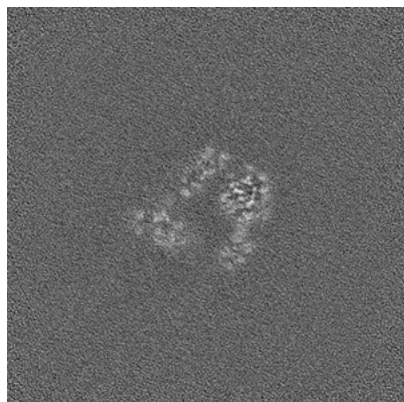


Y Index: 160

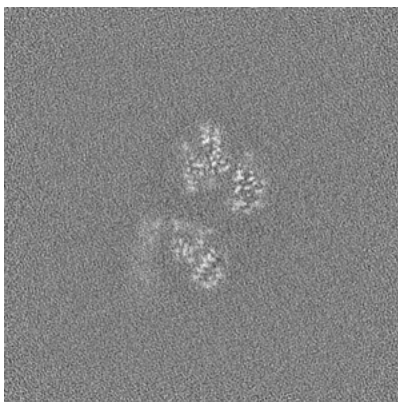


Z Index: 160

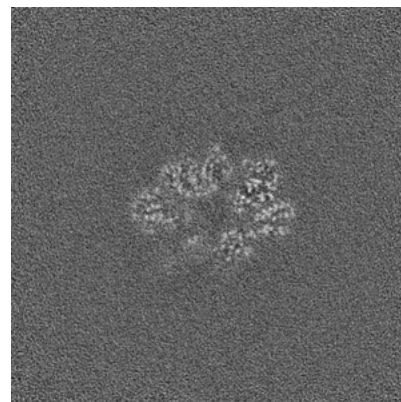
6.2.2 Raw map



X Index: 160



Y Index: 160

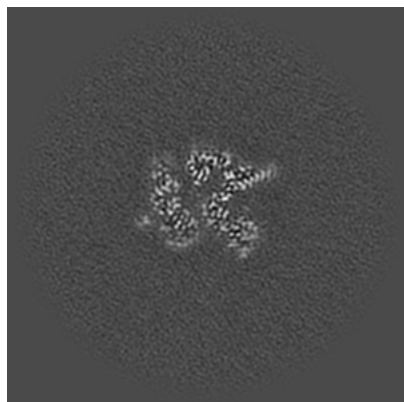


Z Index: 160

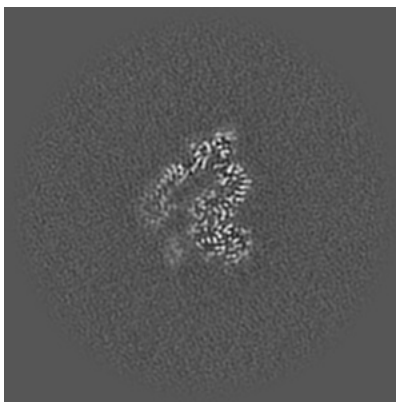
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

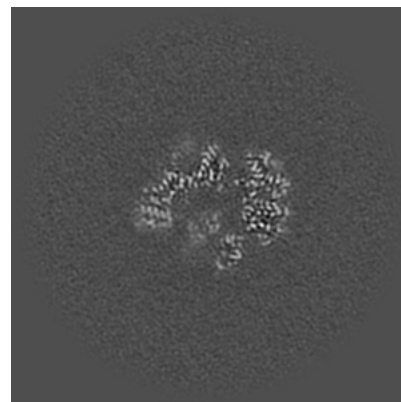
6.3.1 Primary map



X Index: 183

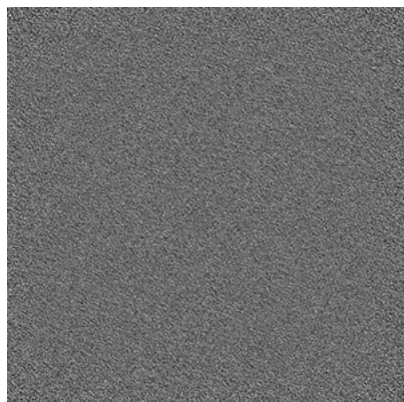


Y Index: 181

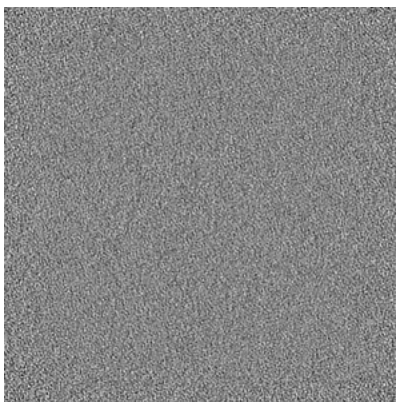


Z Index: 172

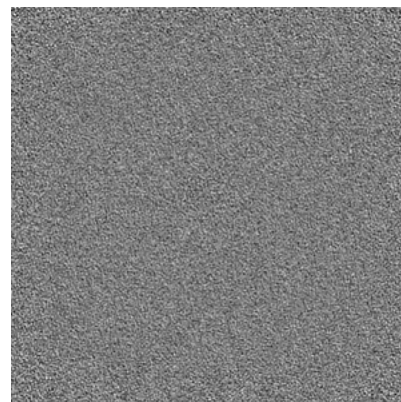
6.3.2 Raw map



X Index: 0



Y Index: 0

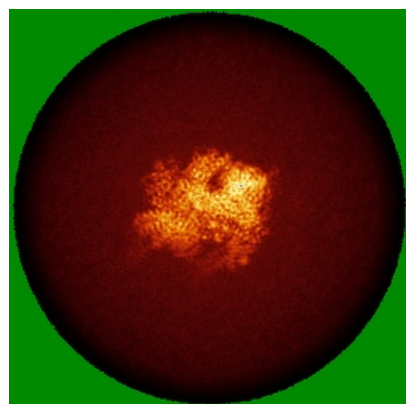


Z Index: 0

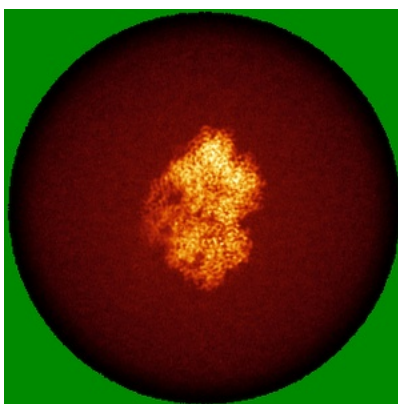
The images above show the largest variance slices of the map in three orthogonal directions.

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

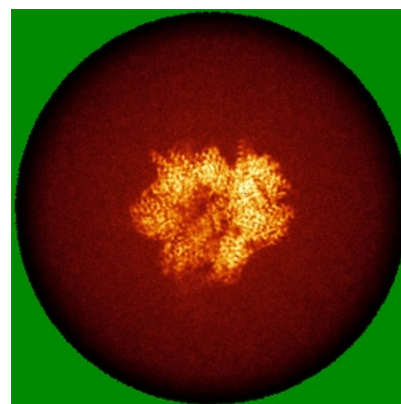
6.4.1 Primary map



X

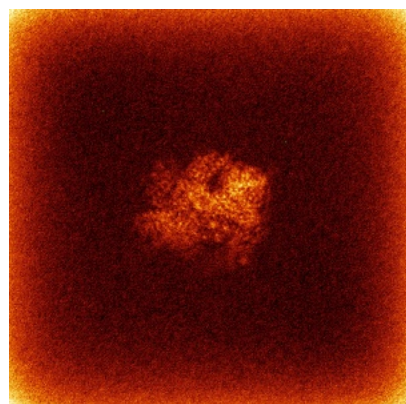


Y

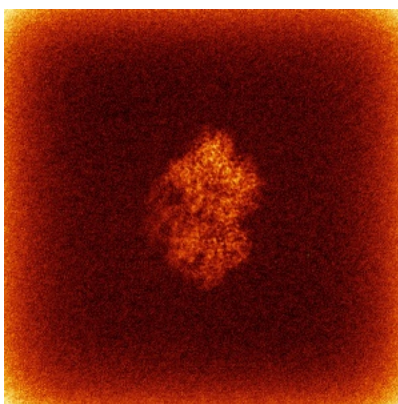


Z

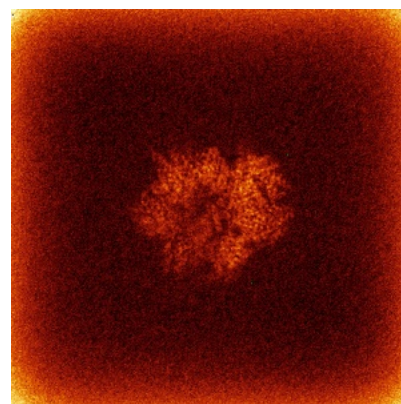
6.4.2 Raw map



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](#)

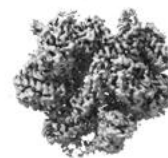
6.5.1 Primary map



X



Y



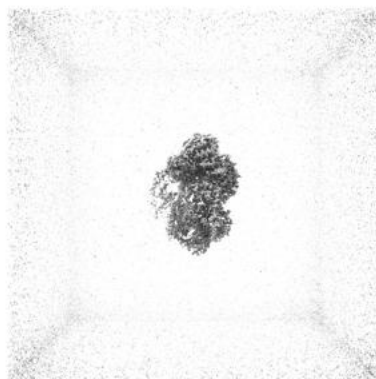
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

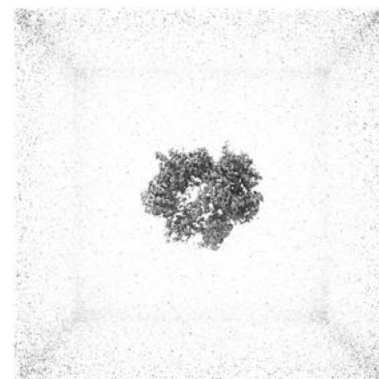
6.5.2 Raw map



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.

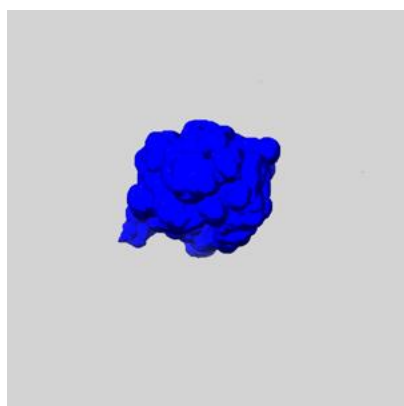
6.6 Mask visualisation [i](#)

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

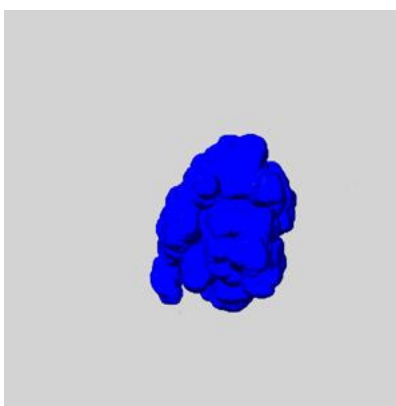
A mask typically either:

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

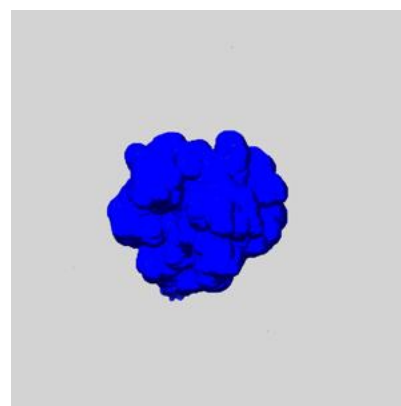
6.6.1 emd_44713_msk_1.map [i](#)



X



Y

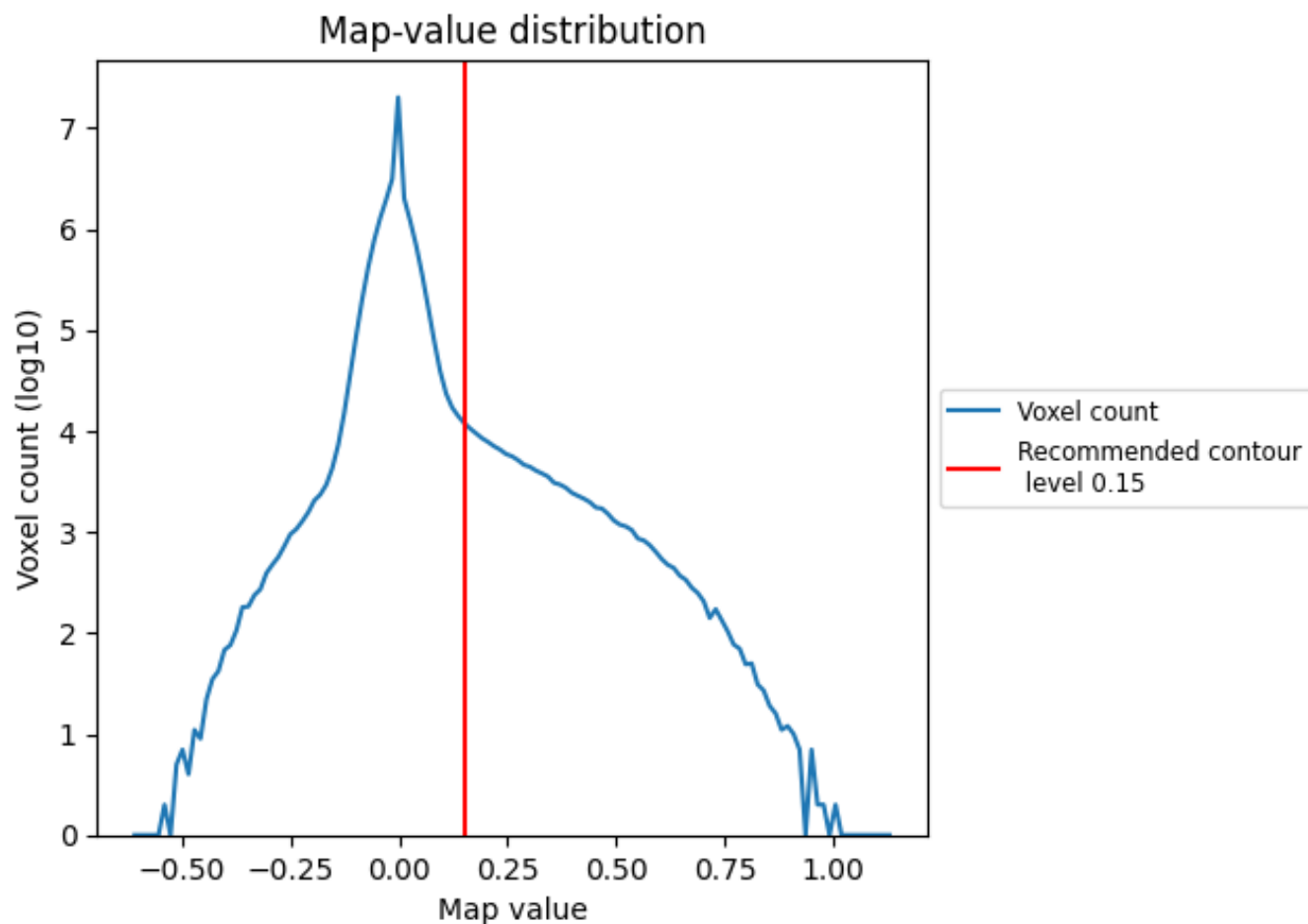


Z

7 Map analysis [i](#)

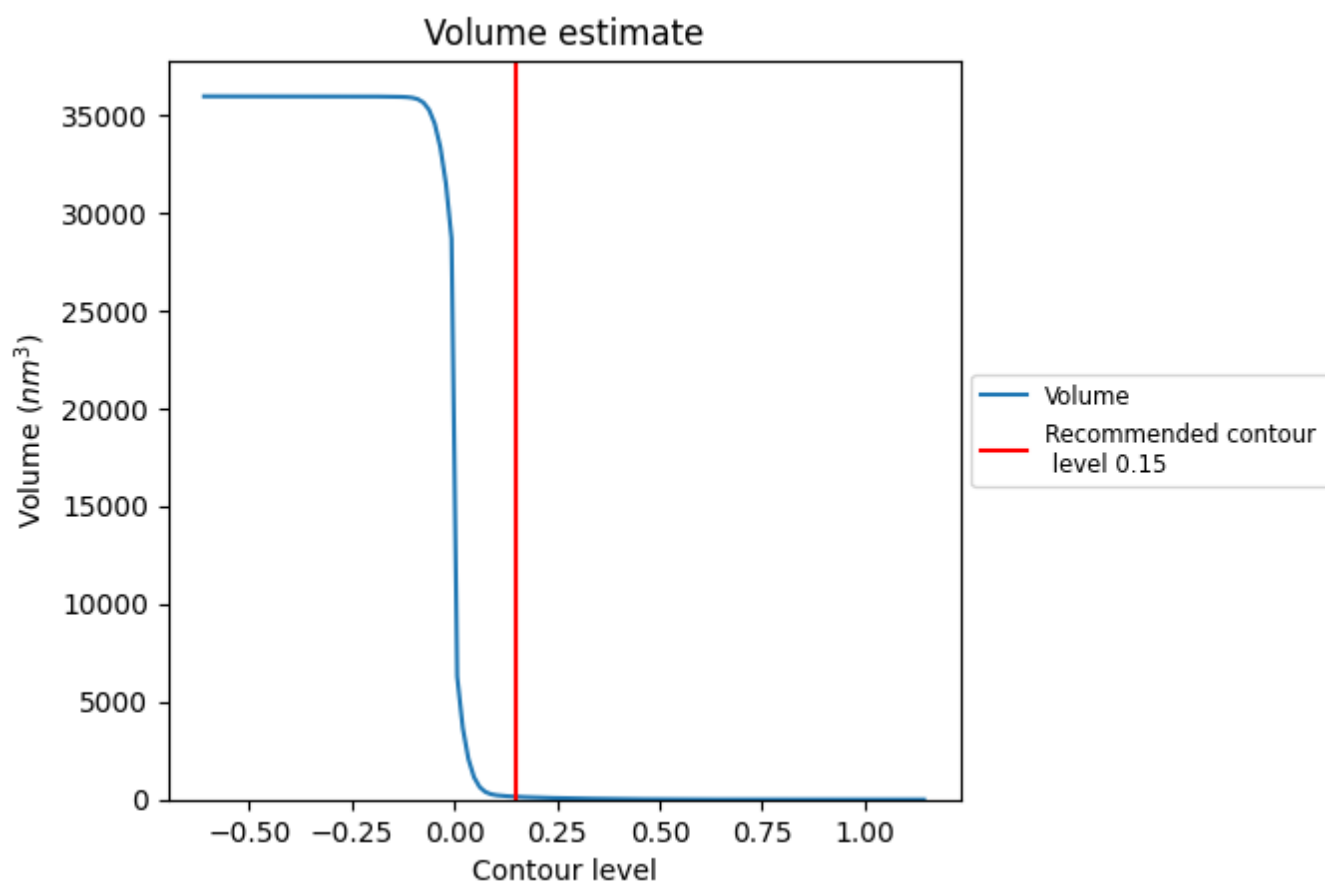
This section contains the results of statistical analysis of the map.

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.

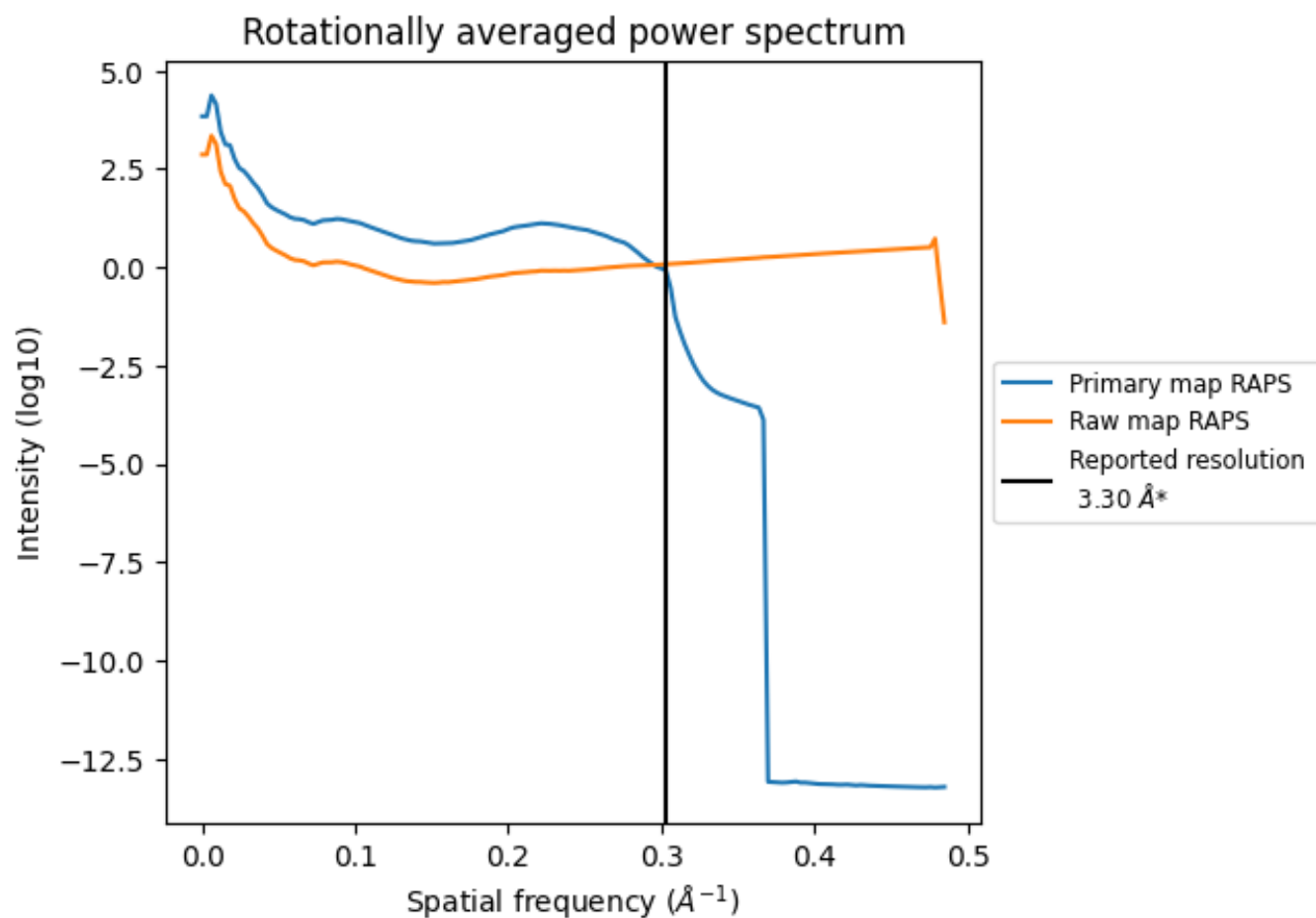
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 146 nm³; this corresponds to an approximate mass of 132 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 ⓘ

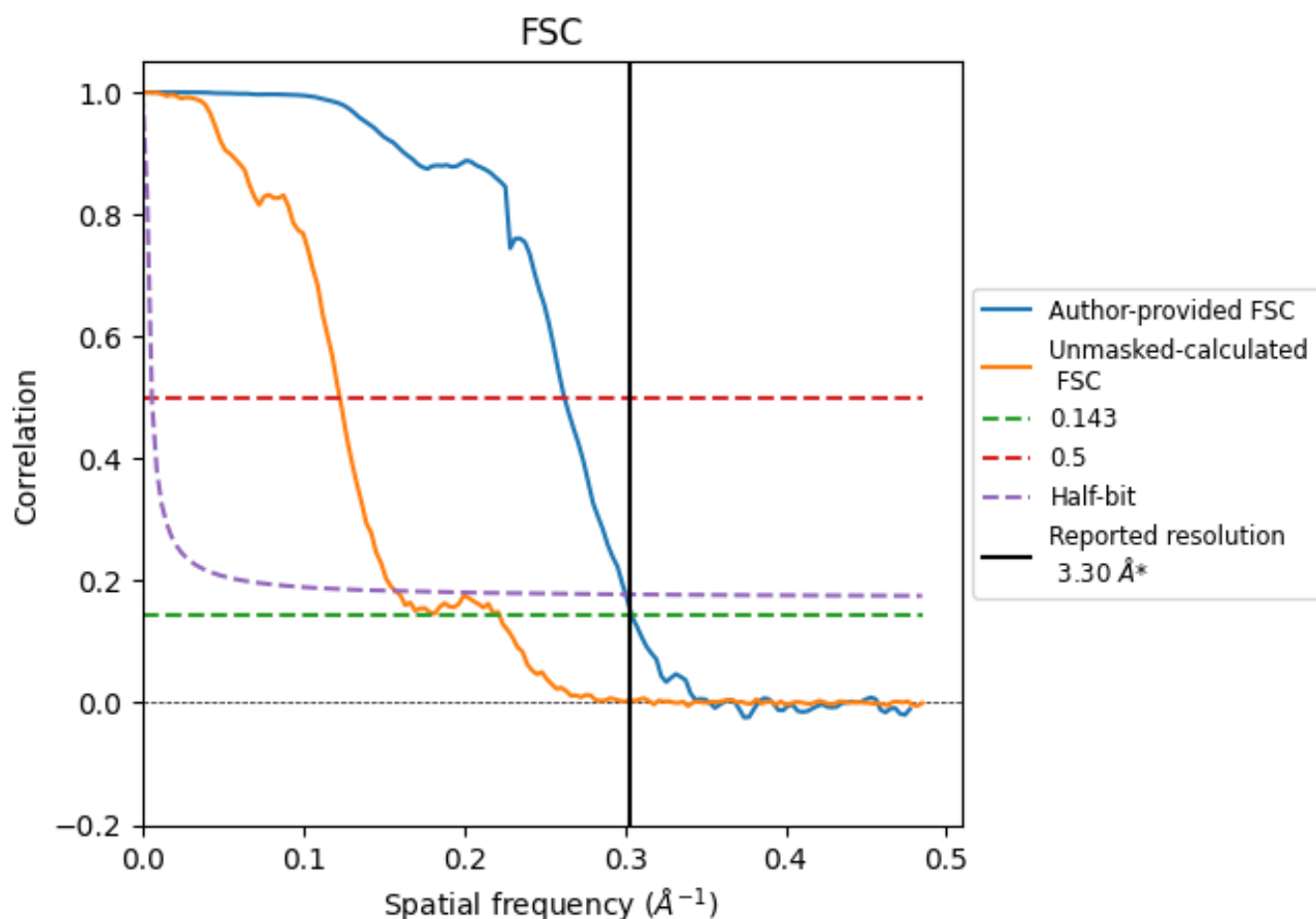


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

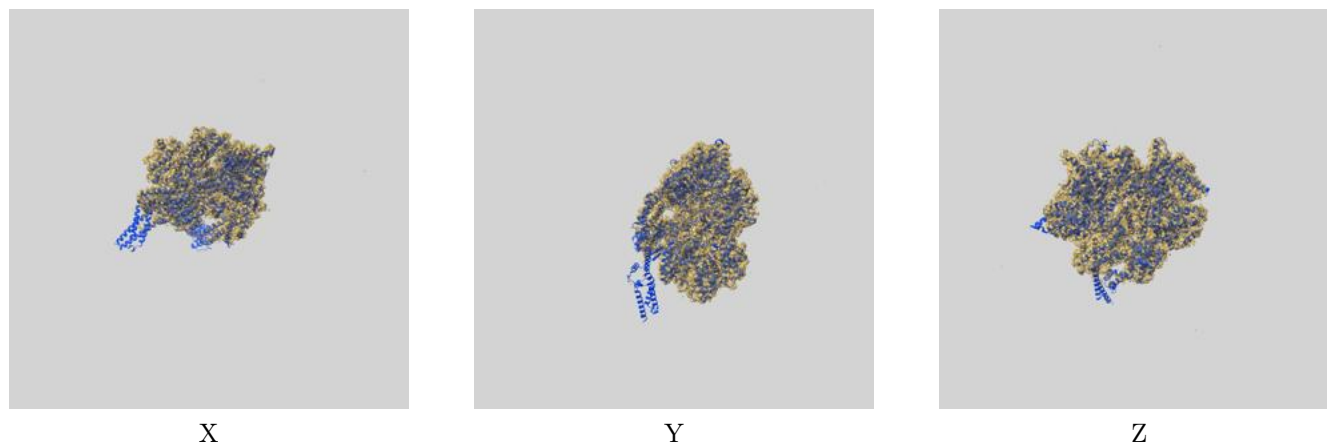
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.81	3.33
Unmasked-calculated*	4.50	8.14	6.34

*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 4.50 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

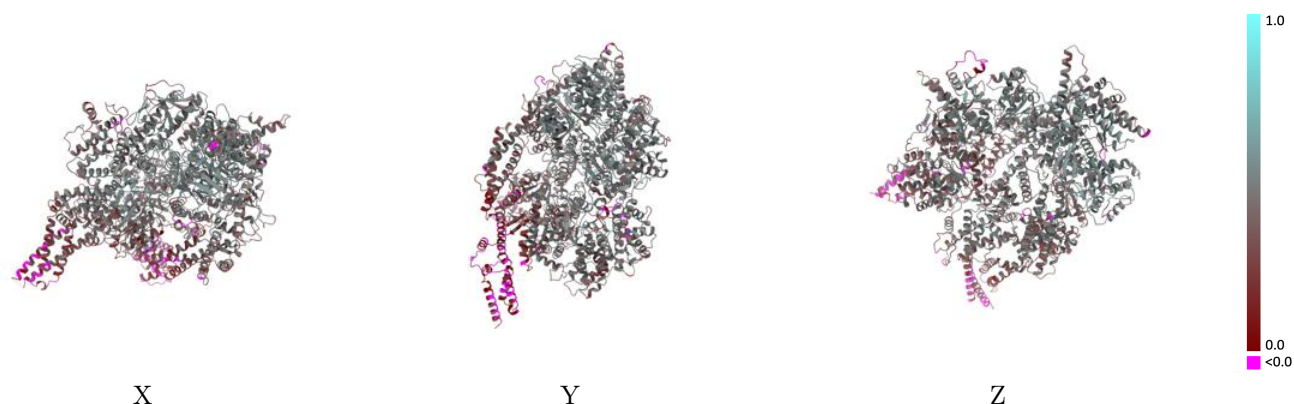
This section contains information regarding the fit between EMDB map EMD-44713 and PDB model 9BMW. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



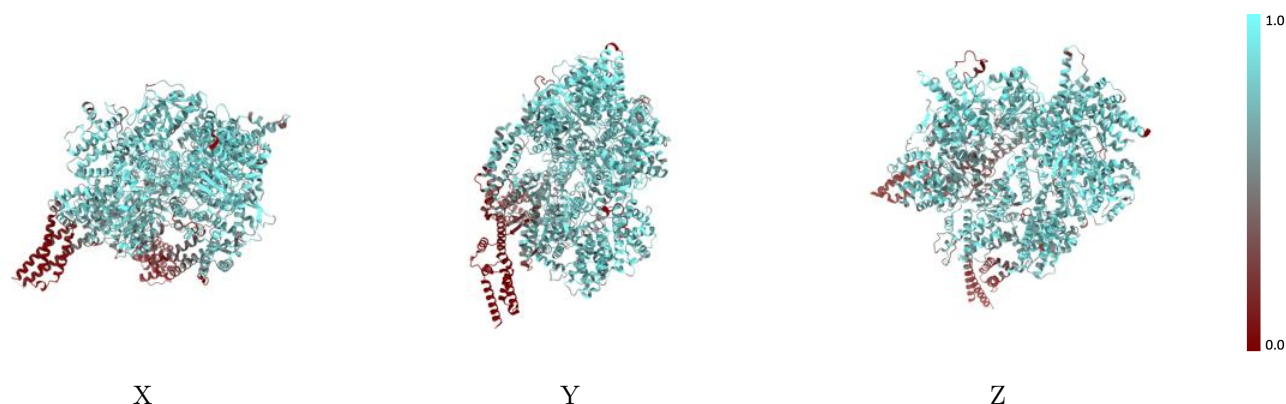
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



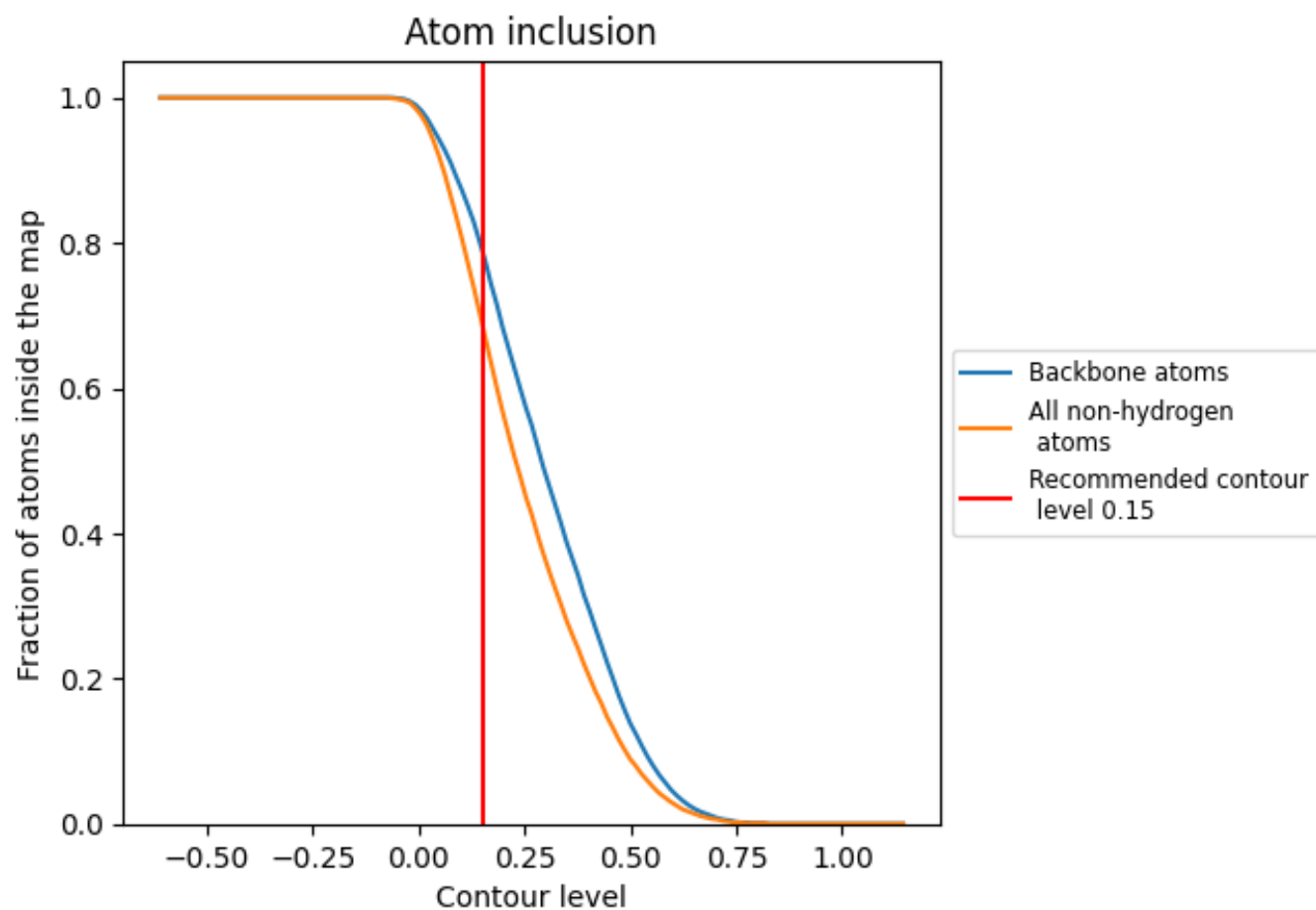
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6880	<div></div> 0.4110
A	<div></div> 0.6880	<div></div> 0.4110

