



## wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 12:27 PM EDT

PDB ID : 9BM4 / pdb\_00009bm4  
EMDB ID : EMD-44687  
Title : State-5b of motor domain from full-length human dynein-1 in 5 mM ATP  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-05-02  
Resolution : 3.48 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](mailto: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>.

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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

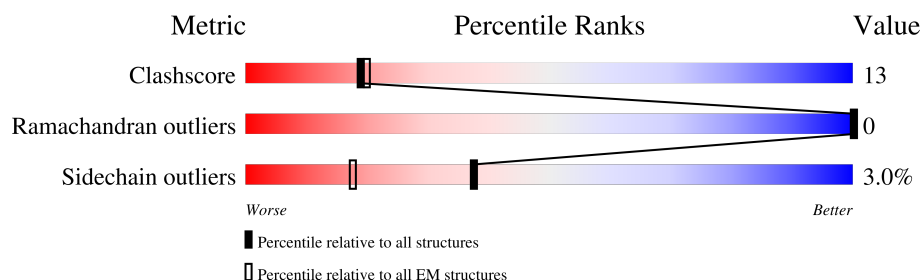
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.48 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  $\geq 3$ , 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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21801 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	2701	21684	13811	3743	4019	111	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

- 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
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	1	Total Mg 1 1	0

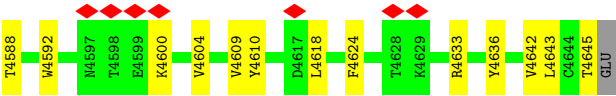




T3211	D3114	Q3032	L2920	E2839	12747	R6610	L2499	D2388	Q2299	L2191	E3078	K2007
V3212	L3115	E3035	D2923	D2840	Y2748	P2613	W2500	E2389	F2303	T2192	Q2079	P2010
D3213	E3116	D2841	F2926	E2842	G2749	D2614	S2501	GLU	D2308	K2206	H2085	D2011
Q3214	P3123	R2843	R2927	R2844	A2754	M2615	D2505	ASP	P2309	Q2212	Y2086	D2012
V3215	D3124	R2845	Q2928	W2846	R2757	S2623	S2506	GLU	E2310	T2216	D2087	A2013
V3216	G3041	T2846	Q2929	T2846	R2757	T2626	R2507	ALA	E2311	L2220	F2088	A2014
E3217	L3042	T2846	Q2930	T2846	R2757	T2626	R2507	GLN	W2312	L2220	G2089	F2015
L3218	M3043	L2850	G2931	T2846	R2757	T2626	R2507	ARG	E2313	L2220	L2090	T2016
R3219	L3044	L2850	H2932	T2846	R2757	T2626	R2507	ARG	E2314	L2222	V2096	T2017
R3220	H3047	H2857	L2933	H2857	R2763	Y2641	L2514	LYS	M2314	W2222	L2097	T2018
ASP	D3131	F2858	L2934	F2858	T2770	N2646	E2515	LYS	D2320	G2227	V2098	T2019
LEU	K3132	L2861	L2935	L2861	T2770	G2647	E2516	ASP	N2321	S2228	S2099	GLY
ARG	L3133	R2862	L2936	R2862	V2774	G2647	V2517	GLU	N2322	S2228	A2100	TVR
ILE	P3134	R2863	G2937	R2863	E2775	V2648	L2518	ASP	K2323	G2228	V2103	ALA
LYS	Q3135	E2864	V2938	E2864	E2775	V2648	T2521	GLY	L2324	M2232	R2107	GLY
SER	P3136	S2868	V2963	S2868	W2779	L2650	T2522	GLU	L2325	A2233	R2107	ARG
GLN	R3140	L2871	R2964	L2871	E2782	K2657	L2526	GLU	P2328	W2234	E2114	SER
GLU	S3146	L2872	K2966	L2872	R2783	W2658	P2527	ALA	N2329	L2244	K2115	L2028
VAL	G3147	Y2873	Y2967	Y2873	F2784	D2664	T2528	S2410	G2330	L2244	E2116	P2029
LYS	V3148	Y2873	T2968	Y2873	T2785	E2665	W2531	P2411	E2331	E2245	E2117	D2030
ASN	F3149	W2876	G2969	W2876	Q2786	L2666	W2531	L2413	R2332	P2256	R2118	N2031
ALA	V3150	K2879	E2974	K2879	T2788	P2689	T2534	Q2416	L2333	S2260	E2119	L2032
ALA	Q3151	D2880	D2975	D2880	T2788	P2689	T2534	R2417	P2337	K2261	E2120	F2036
ALA	Q3152	L2880	L2976	L2880	Q2789	D2670	T2535	R2418	N2338	R2261	E2121	R2037
ASN	T3153	Y2881	L2977	Y2881	R2790	Y2674	E2538	A2419	R2339	D2262	A2121	S2038
ASP	L3154	T2882	T2978	T2882	H2791	Y2674	E2538	L2419	R2340	R2263	D2123	L2039
LYS	N3158	P2883	R2981	P2883	Y2792	V2679	W2548	I2422	I2341	L2264	E2126	A2040
LEU	T3168	Q2886	D2995	Q2886	Y2794	V2679	V2557	M2423	M2342	Y2265	E2127	N2041
LYS	M3169	E2887	E2996	E2887	R2797	R2684	T2557	S2429	F2343	L2268	L2137	T2042
MET	A3170	E2888	S2997	E2888	Q2686	Q2686	T2559	V2429	E2345	D2269	L2137	R2046
LYS	I3171	L2889	M2998	L2889	V2687	V2687	T2559	V2433	V2345	P2270	I2138	I2049
ASP	R3175	R2890	S3002	R2890	W2802	E2688	A2563	L2437	Y2350	N2271	Q2139	L2052
GLN	A3184	D2891	G3003	D2891	R2803	E2688	A2563	L2437	A2351	T2272	S2140	V2062
ALA	K3190	Y2892	F3004	Y2892	R2804	H2689	D2566	E2444	L2352	R2273	V2141	M2063
LYS	R3191	K2894	L3005	K2894	G2805	H2689	D2566	E2444	A2354	E2274	C2142	L2054
LYS	E3195	R2896	E3006	R2896	L2806	F2692	V2569	R2451	L2355	W2275	E2143	Y2055
LYS	E3196	L2897	R3007	L2897	A2809	Q2698	L2581	L2452	V2356	G2278	K2148	S2056
VAL	Q3197	M2902	M3008	M2902	L2816	V2701	L2581	S2457	S2357	L2279	L2161	R2060
SER	Q3198	E2903	A3101	E2903	L2821	G2710	L2584	M2461	M2361	H2282	Q2169	L2065
GLN	M3199	D2906	N3014	D2906	L2822	K2721	L2585	Q2471	V2362	V2283	Y2170	A2066
ILE	H3200	V2907	L3020	V2907	R2823	R2729	H2588	D2478	W2363	L2284	T2176	V2067
GLN	L3201	W2908	F3021	W2908	L2824	H2730	K2589	F2479	F2364	A2177	A2177	K2068
GLU	V3105	L2909	G3024	L2909	A2826	V2731	P2590	D2478	S2365	L2288	T2176	I2069
GLN	K3106	V2910	D3024	V2910	Q2834	V2731	L2593	F2479	E2366	D2289	R2179	V2070
LEU	V3203	L2911	E3025	L2911	R2835	V2731	L2593	F2479	L2369	R2292	E2180	P2071
LYS	G3204	L2916	M3030	L2916	R2836	V2736	M2603	I2490	M2373	E2293	E2181	F2072
LYS	R3205	D2917	L3031	D2917	L2837	V2736	T2604	V2495	W2385	G2294	Q2187	K2074
GLN	K3206	H2918	T3031	H2918	Y2838	S2743	L2606	I2498	I2386	L2295	E2188	L2075
GLU	I3208	V2919		V2919			F2606		P2386	R2298	Y2190	D2077
K3209	E3210								L2387			







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	114327	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	0.703	Depositor
Minimum map value	-0.410	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.832, 0.832, 0.832	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0/22148	0.51	3/30024 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1766	LEU	CA-CB-CG	6.52	130.29	115.30
1	A	4451	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	4224	ASP	CB-CG-OD1	5.18	122.97	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21684	0	21717	549	0
2	A	54	0	24	4	0
3	A	62	0	24	5	0
4	A	1	0	0	0	0
All	All	21801	0	21765	549	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 13.

The worst 5 of 549 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:1659:ALA:HA	1:A:1926:PHE:HE1	1.24	1.00
1:A:1659:ALA:HA	1:A:1926:PHE:CE1	2.07	0.88
1:A:3759:ARG:HG3	1:A:3760:ILE:HG13	1.56	0.88
1:A:3030:MET:SD	1:A:3047:HIS:ND1	2.49	0.84
1:A:3845:ASN:HB3	1:A:3858:ILE:HD11	1.61	0.83

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	2687/4646 (58%)	2624 (98%)	63 (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	2400/4125 (58%)	2329 (97%)	71 (3%)	36	63

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3957	PHE
1	A	4095	MET
1	A	4314	ASP
1	A	2366	GLU
1	A	2332	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3198	GLN
1	A	3631	ASN
1	A	4526	GLN
1	A	3852	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 5 ligands modelled in this entry, 1 is 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	0.73	0	29,45,45	0.74	1 (3%)
3	ATP	A	4703	4	28,33,33	0.71	0	34,52,52	0.83	1 (2%)
2	ADP	A	4704	-	24,29,29	0.85	0	29,45,45	1.18	2 (6%)
3	ATP	A	4702	-	28,33,33	0.73	0	34,52,52	0.61	1 (2%)

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	-	-	2/12/32/32	0/3/3/3
3	ATP	A	4703	4	-	3/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	1/12/32/32	0/3/3/3
3	ATP	A	4702	-	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	N3-C2-N1	-3.56	123.84	128.67
2	A	4704	ADP	C4-C5-N7	-2.48	106.72	109.34
3	A	4702	ATP	C5-C6-N6	2.32	123.84	120.31
2	A	4701	ADP	C5-C6-N6	2.26	123.76	120.31
3	A	4703	ATP	C5-C6-N6	2.25	123.75	120.31

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

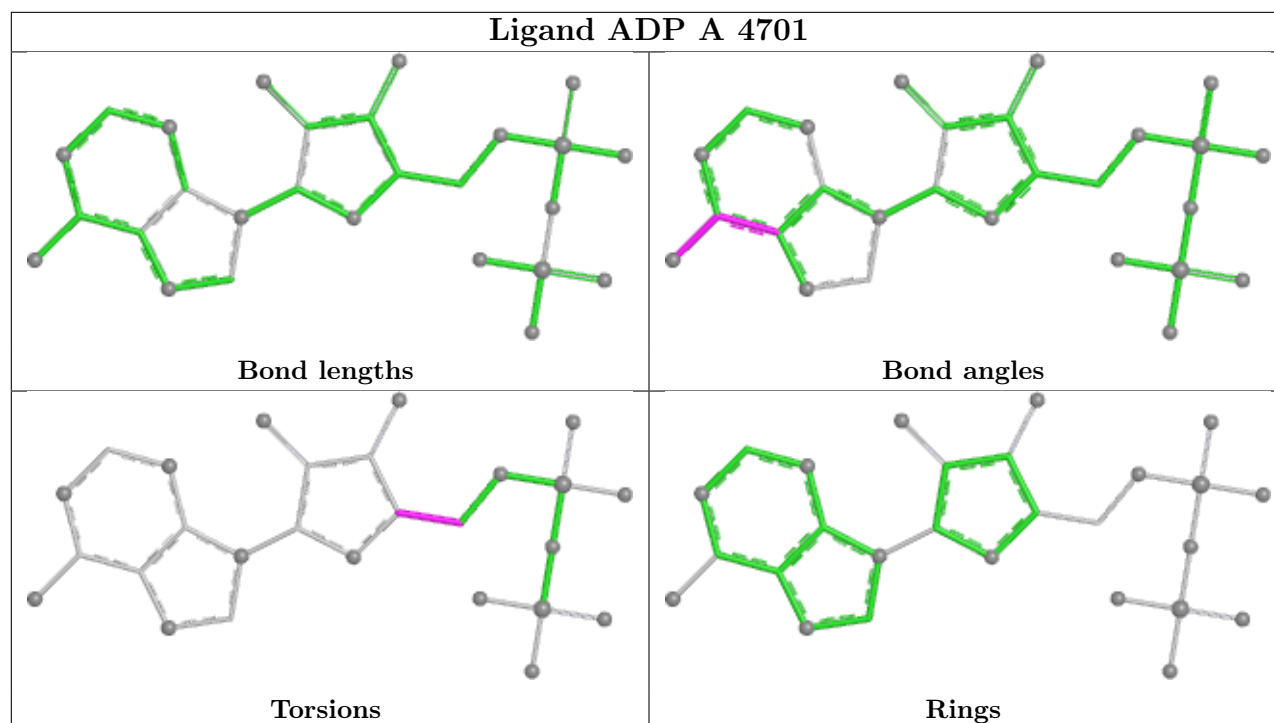
Mol	Chain	Res	Type	Atoms
2	A	4704	ADP	C5'-O5'-PA-O1A
3	A	4703	ATP	PB-O3B-PG-O3G
2	A	4701	ADP	O4'-C4'-C5'-O5'
2	A	4701	ADP	C3'-C4'-C5'-O5'
3	A	4702	ATP	O4'-C4'-C5'-O5'

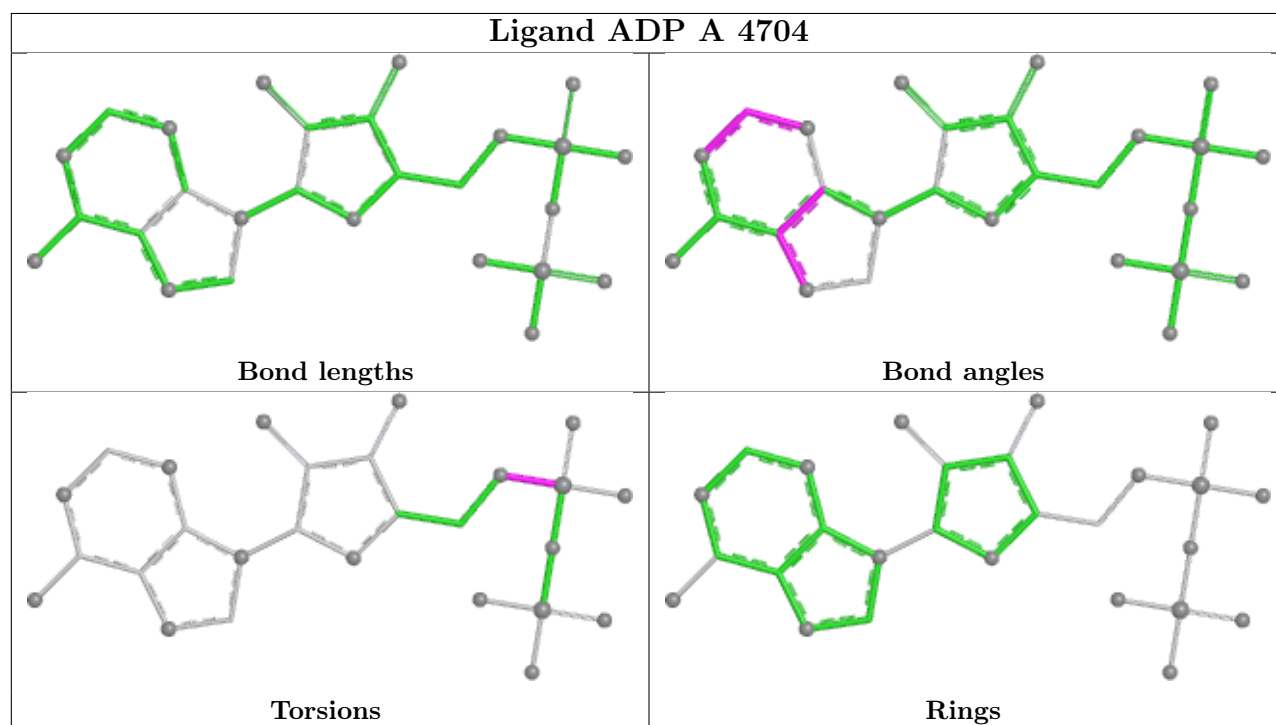
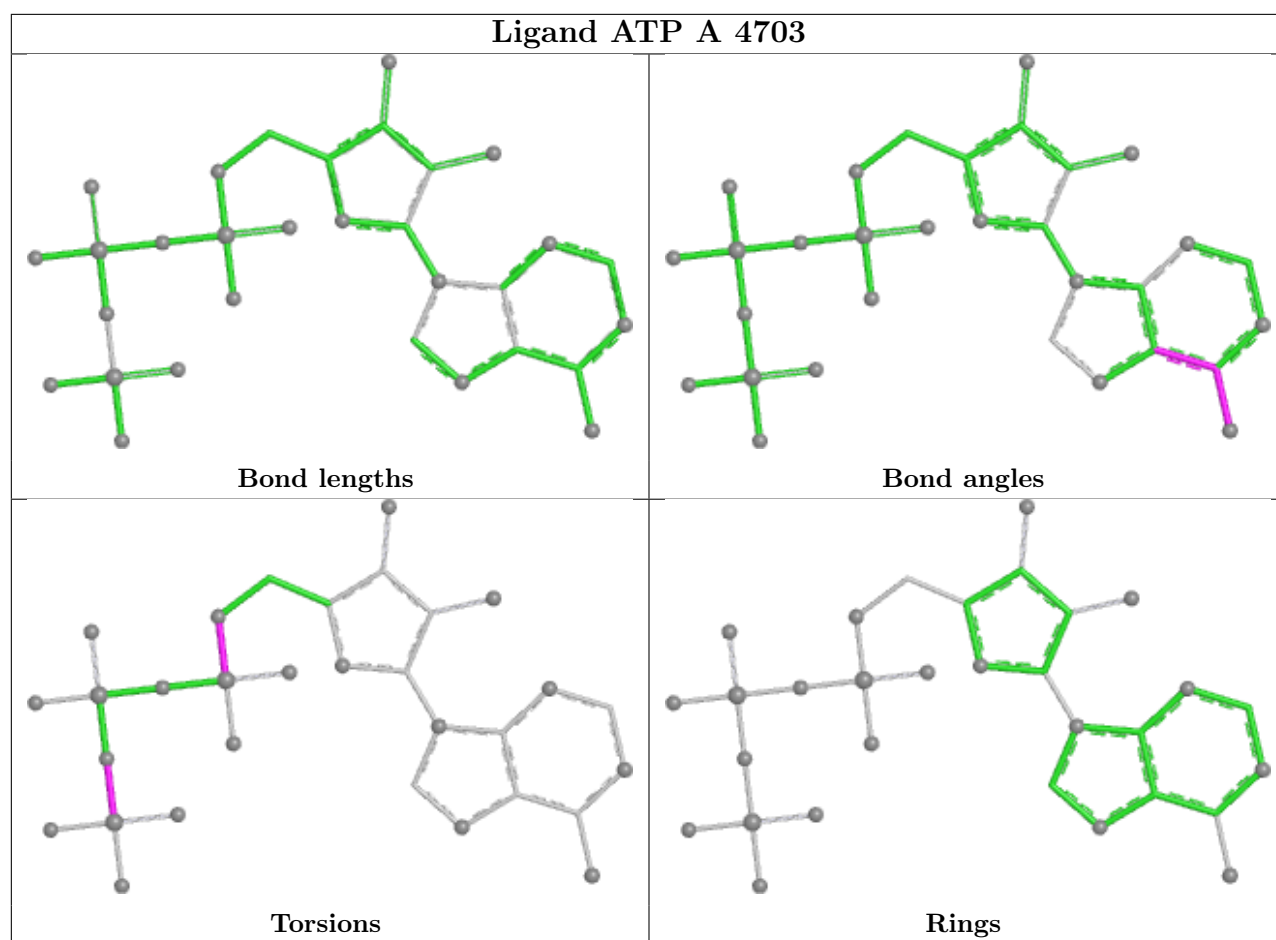
There are no ring outliers.

3 monomers are involved in 9 short contacts:

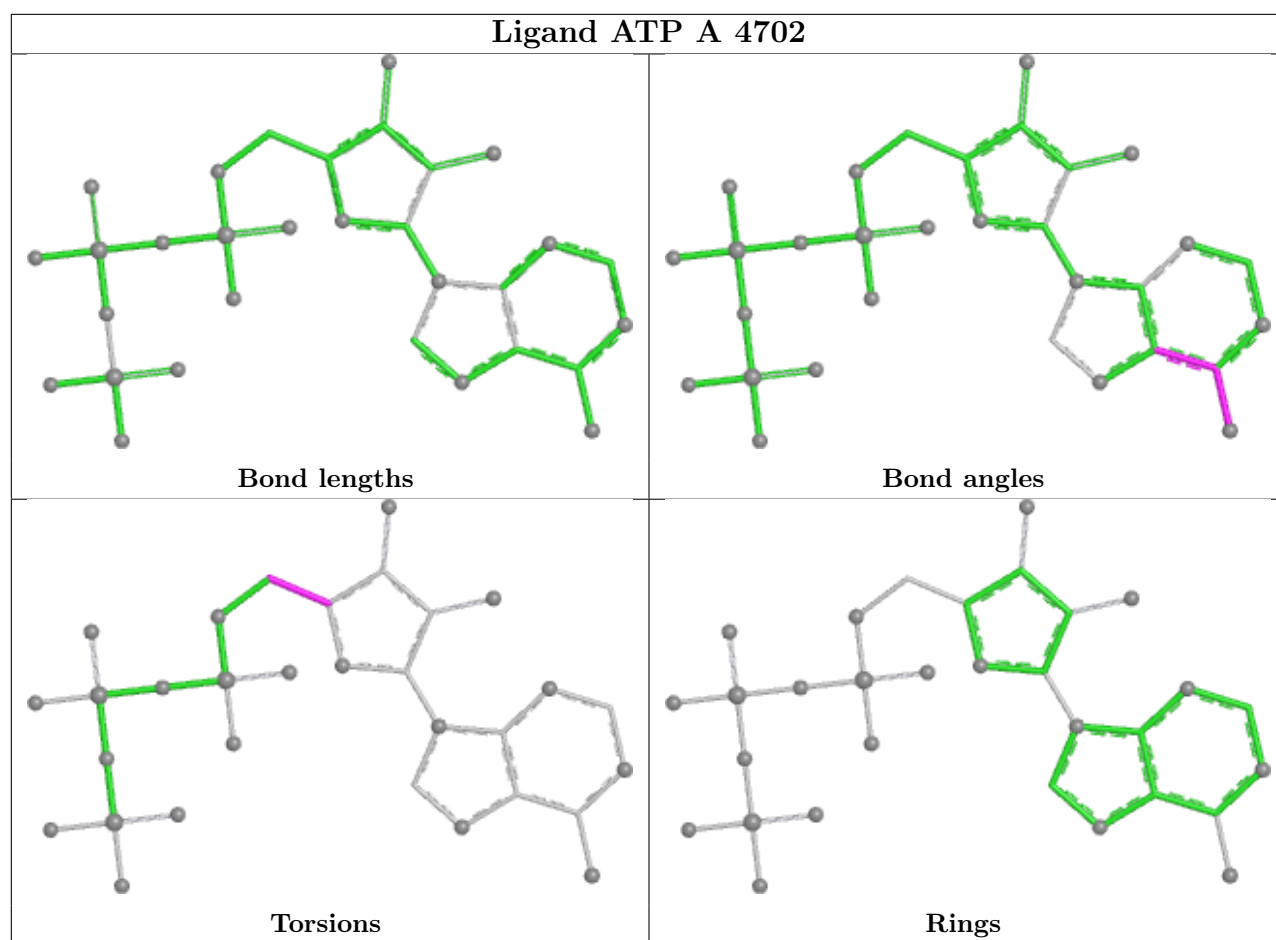
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	4	0
3	A	4703	ATP	3	0
3	A	4702	ATP	2	0

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.

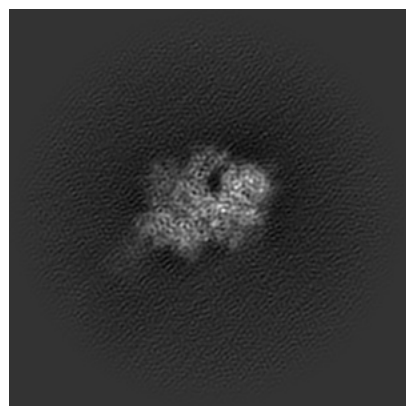
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44687. These allow visual inspection of the internal detail of the map and identification of artifacts.

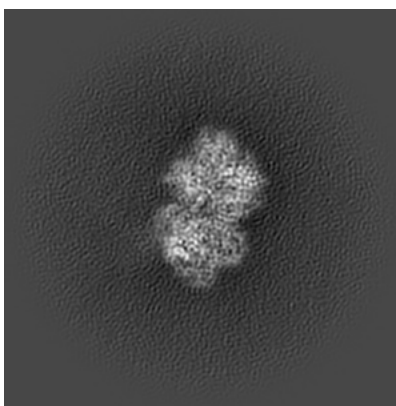
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

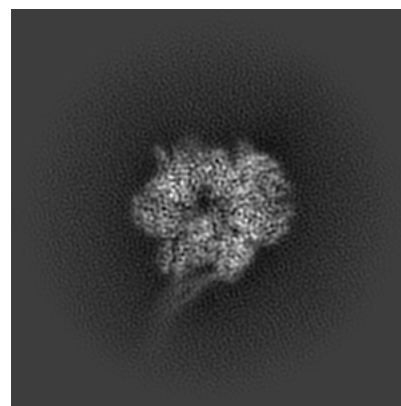
#### 6.1.1 Primary map



X

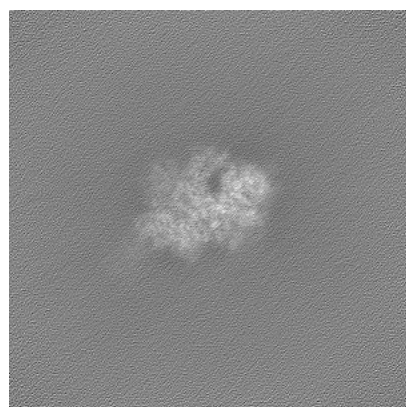


Y

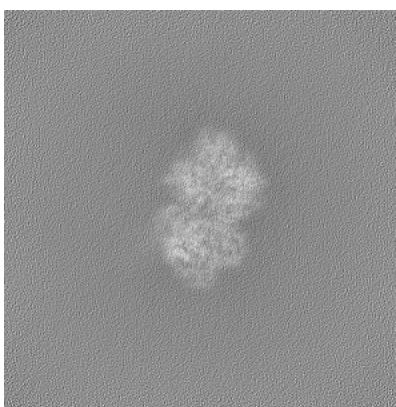


Z

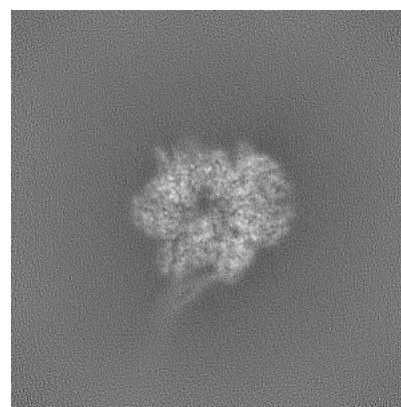
#### 6.1.2 Raw map



X



Y

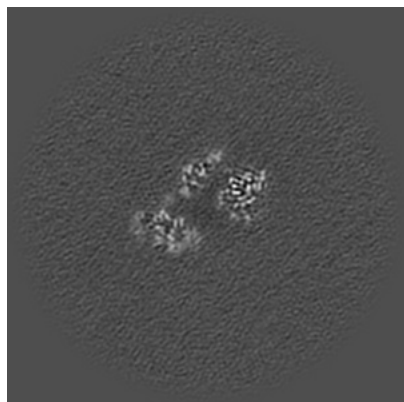


Z

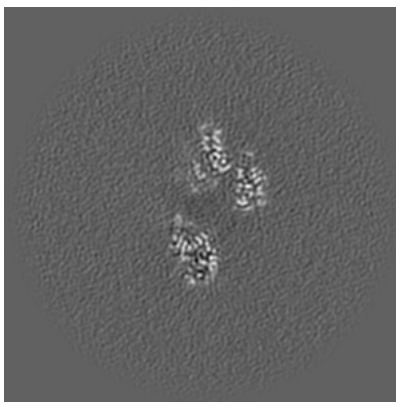
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

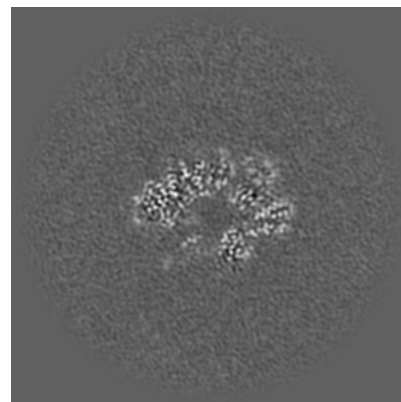
### 6.2.1 Primary map



X Index: 200

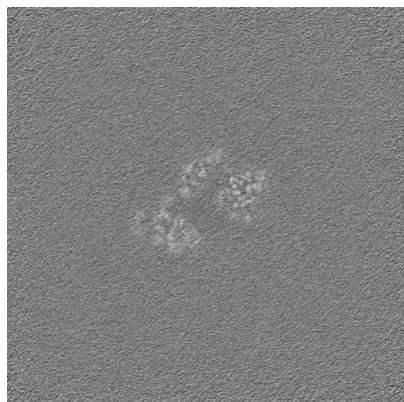


Y Index: 200

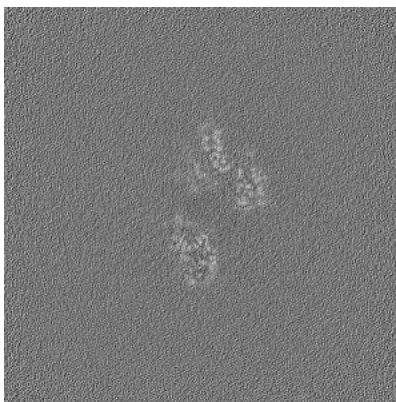


Z Index: 200

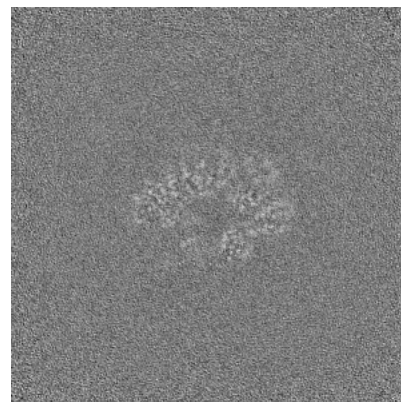
### 6.2.2 Raw map



X Index: 200



Y Index: 200

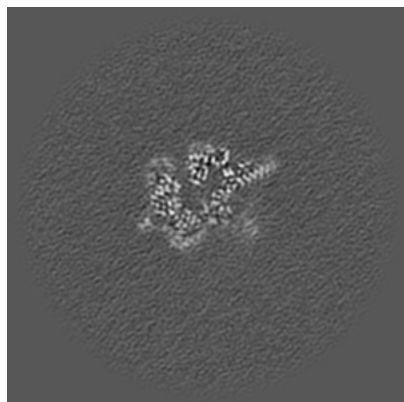


Z Index: 200

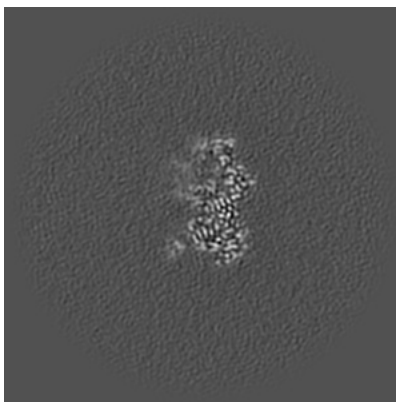
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

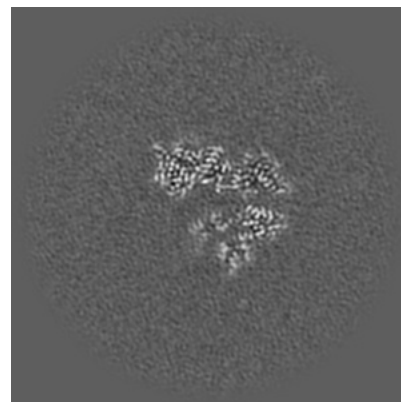
### 6.3.1 Primary map



X Index: 229

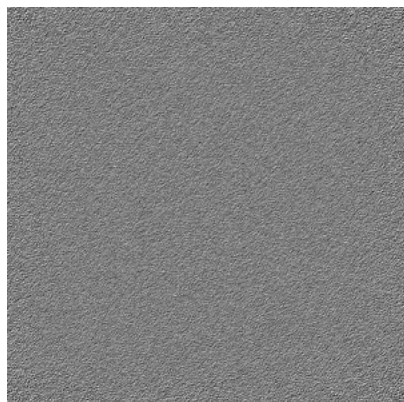


Y Index: 231

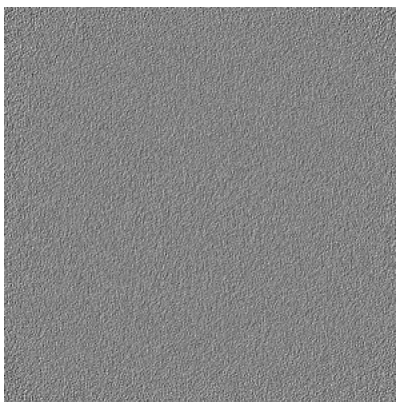


Z Index: 222

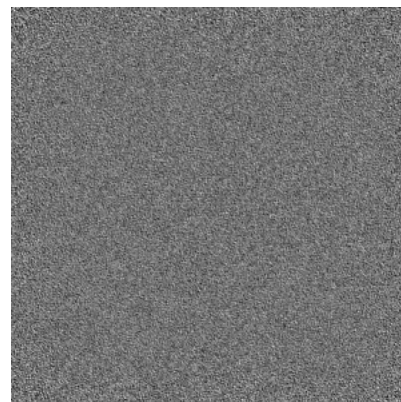
### 6.3.2 Raw map



X Index: 0



Y Index: 0



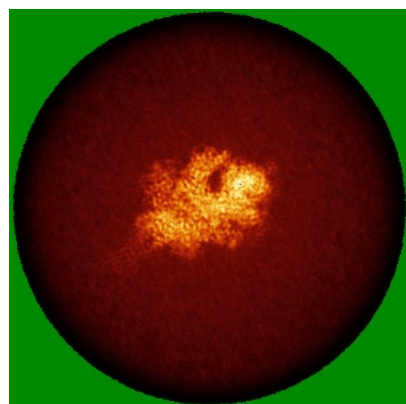
Z Index: 0

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

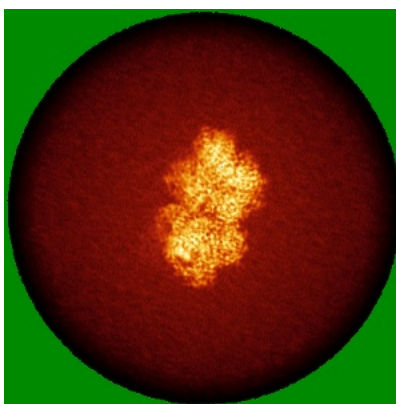


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

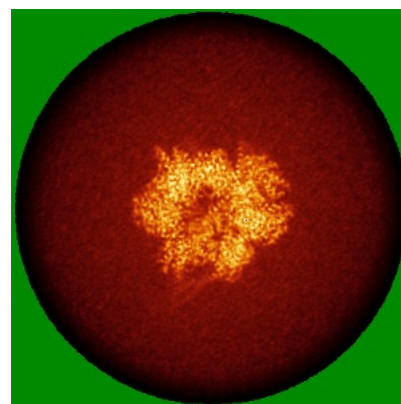
### 6.4.1 Primary map



X

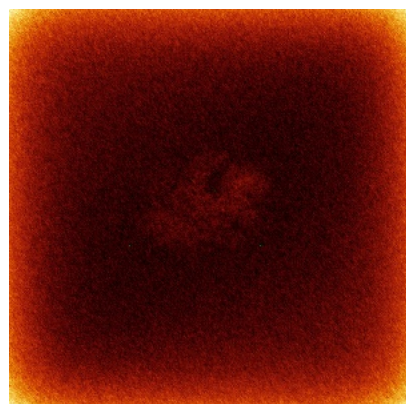


Y

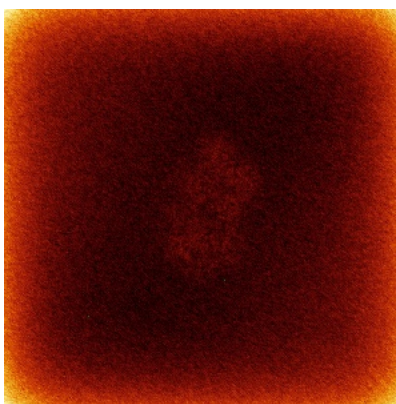


Z

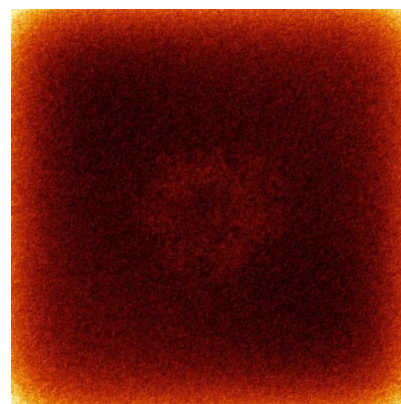
### 6.4.2 Raw map



X



Y

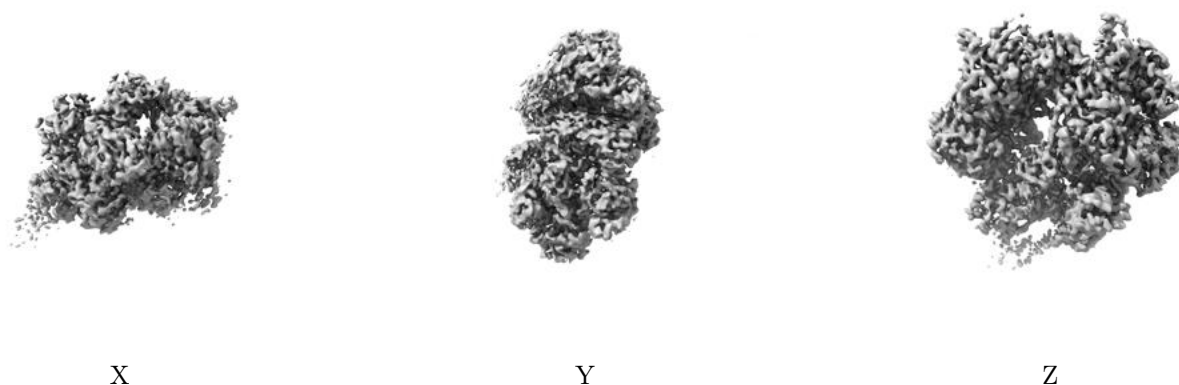


Z

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.

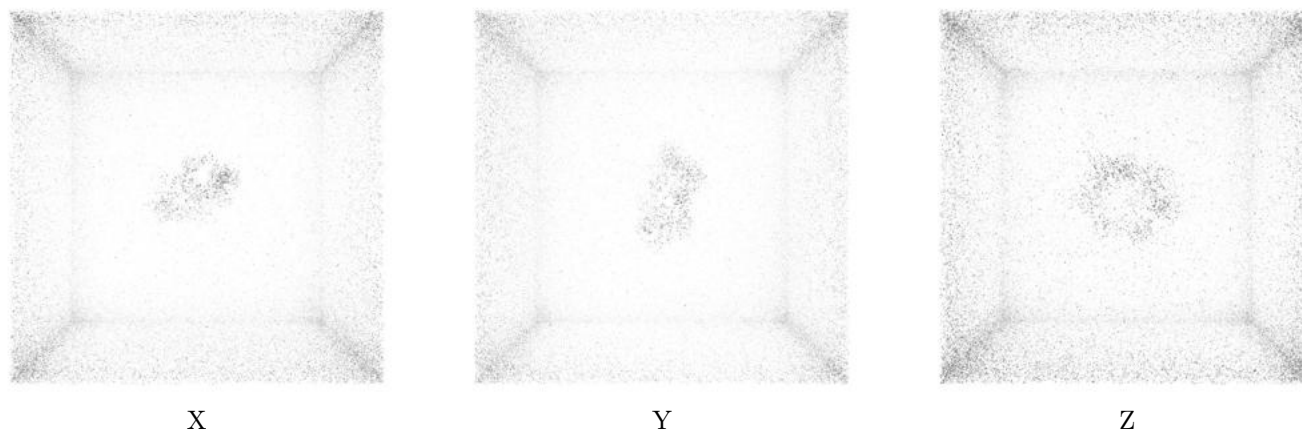
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

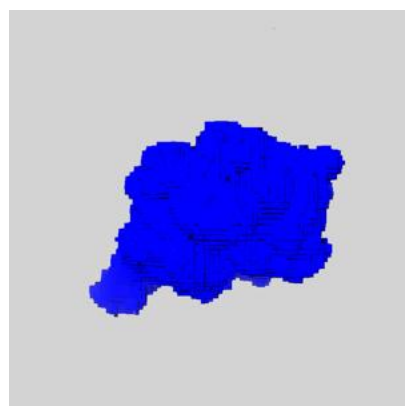
## 6.6 Mask visualisation [i](#)

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

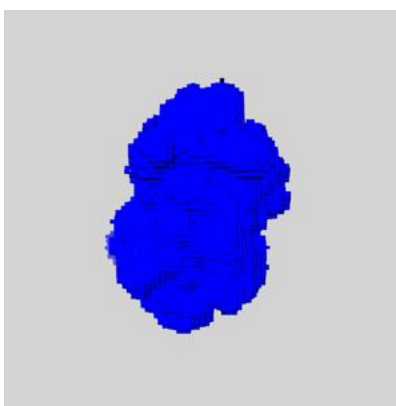
A mask typically either:

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

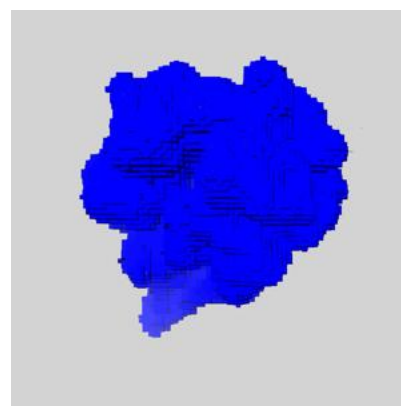
### 6.6.1 emd\_44687\_msk\_1.map [i](#)



X



Y

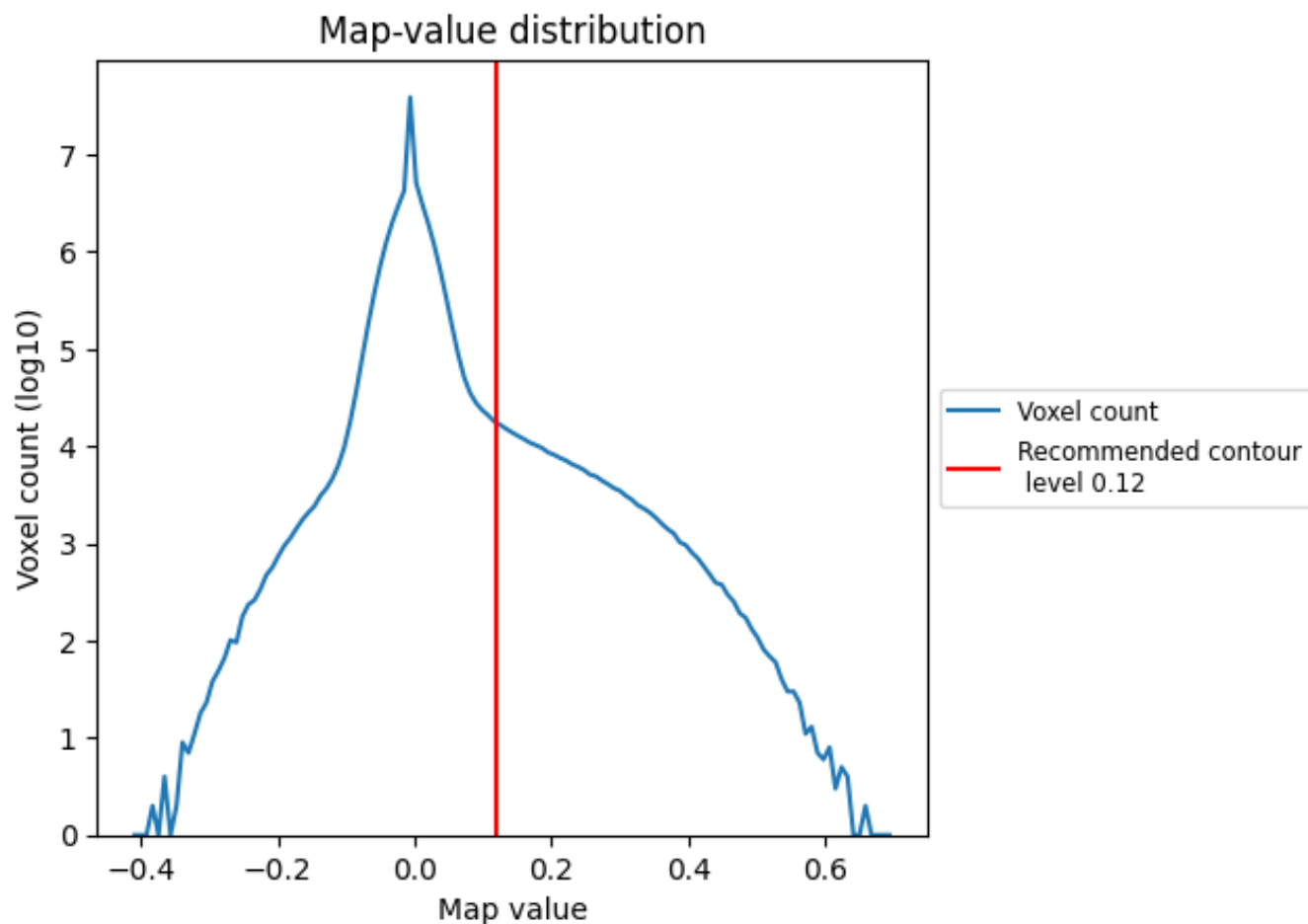


Z

## 7 Map analysis [i](#)

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

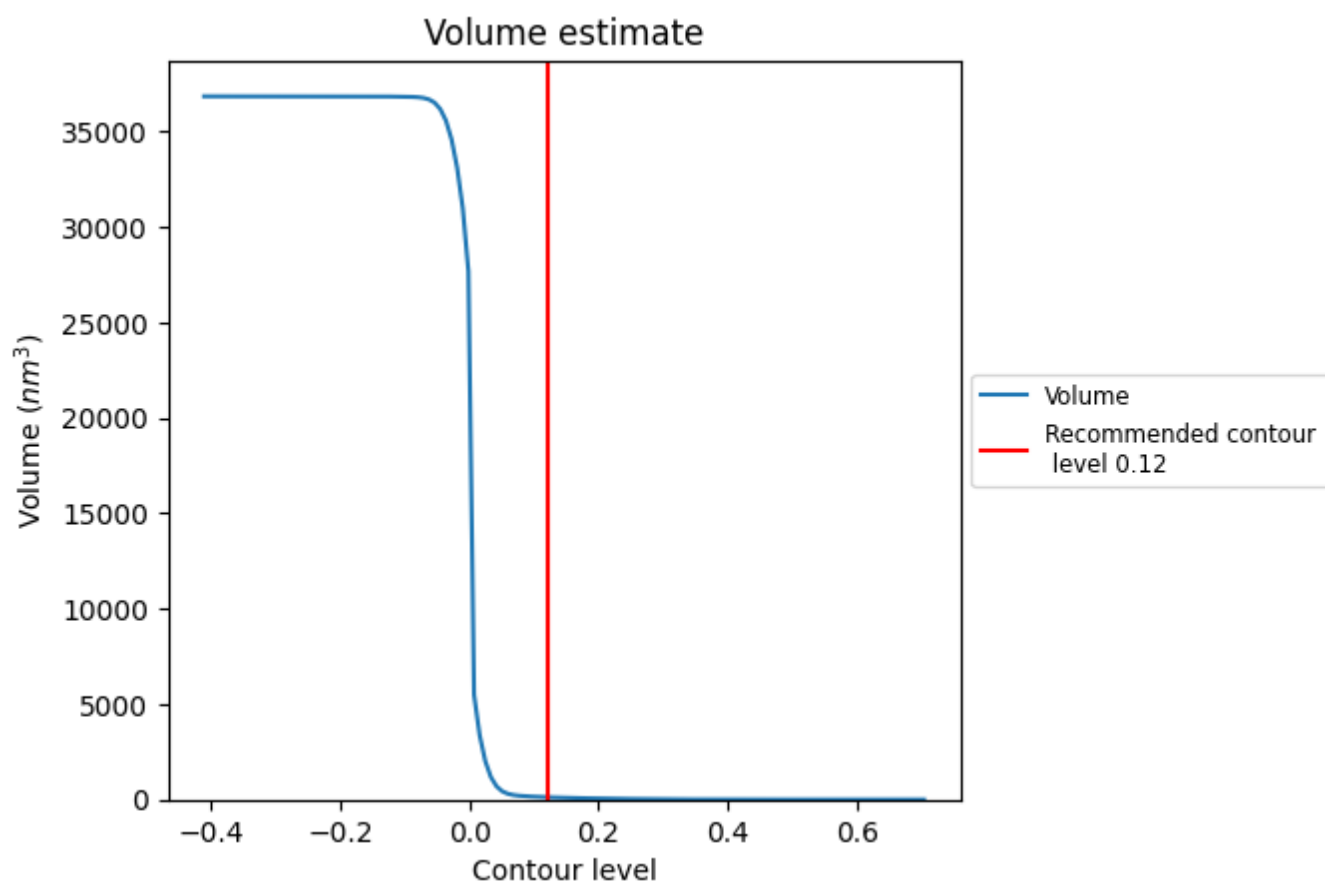
### 7.1 Map-value distribution [i](#)



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.



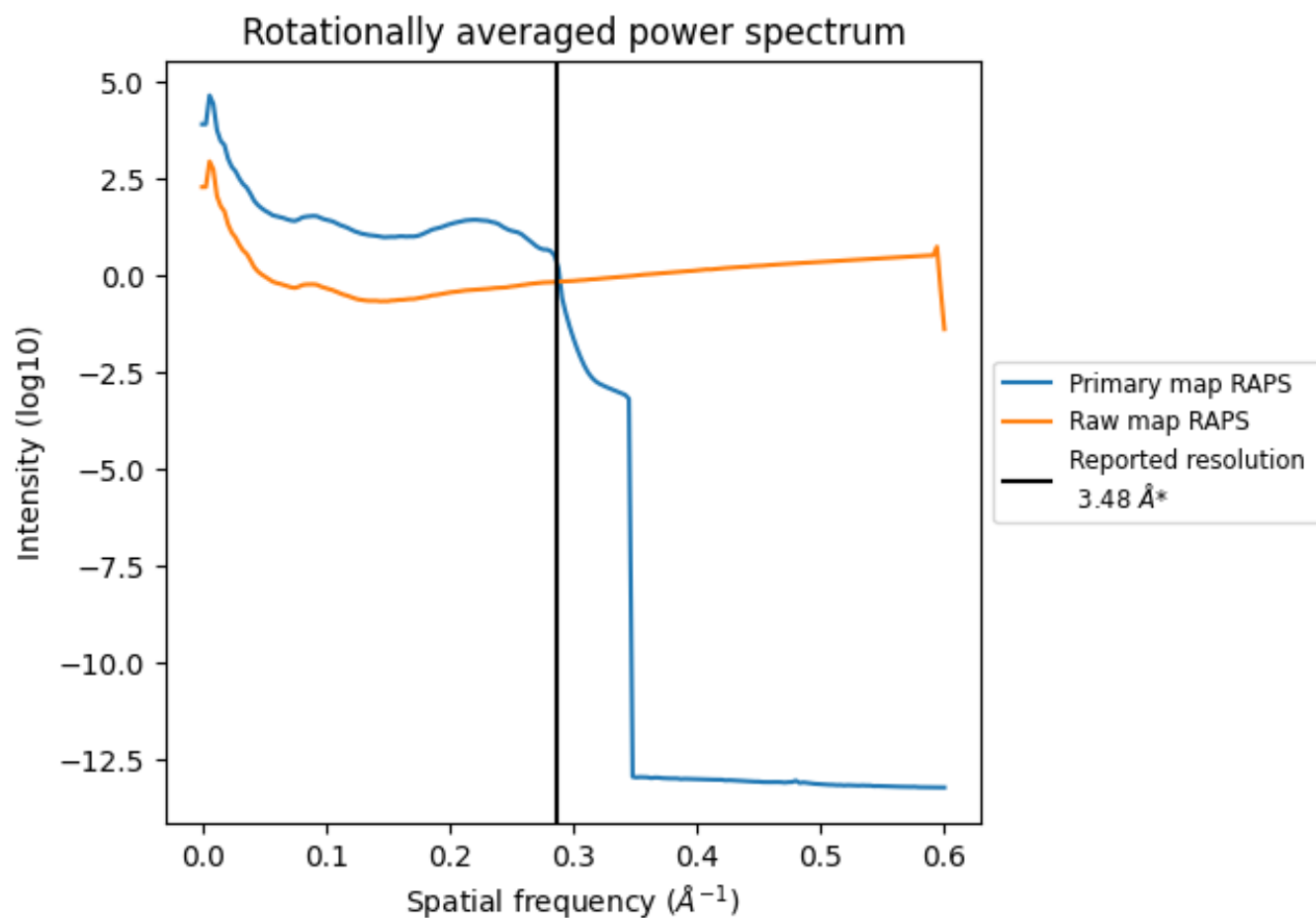
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 122 nm<sup>3</sup>; this corresponds to an approximate mass of 110 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 ⓘ

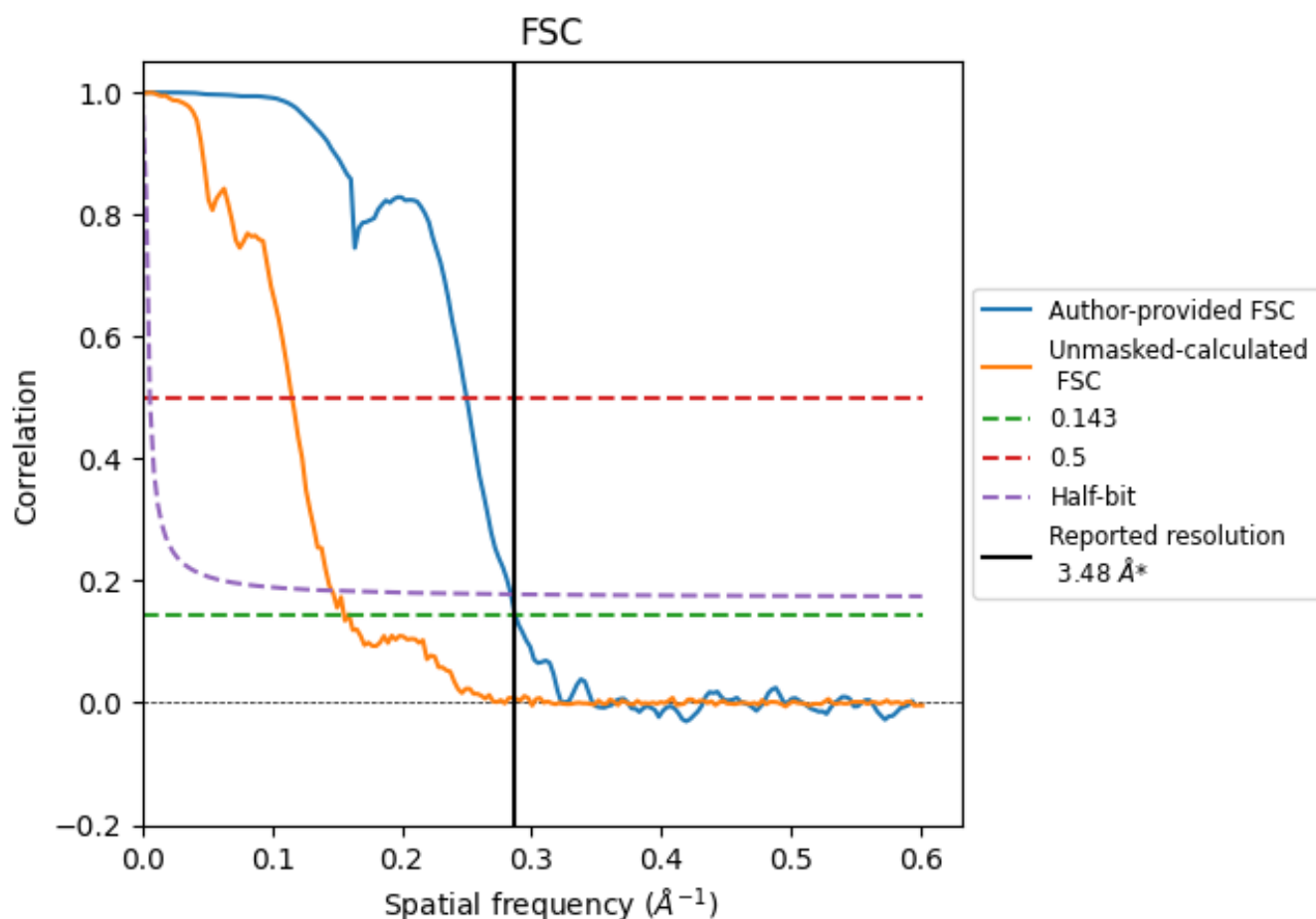


\*Reported resolution corresponds to spatial frequency of 0.287 Å<sup>-1</sup>

## 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 0.287 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

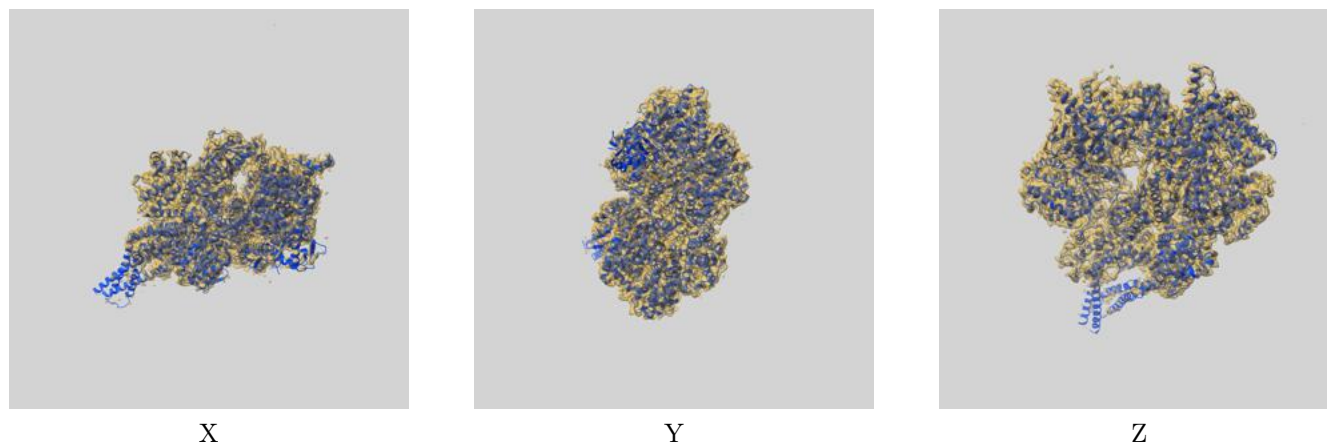
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.48	-	-
Author-provided FSC curve	3.48	4.00	3.52
Unmasked-calculated*	6.43	8.67	6.84

\*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 6.43 differs from the reported value 3.48 by more than 10 %

## 9 Map-model fit [i](#)

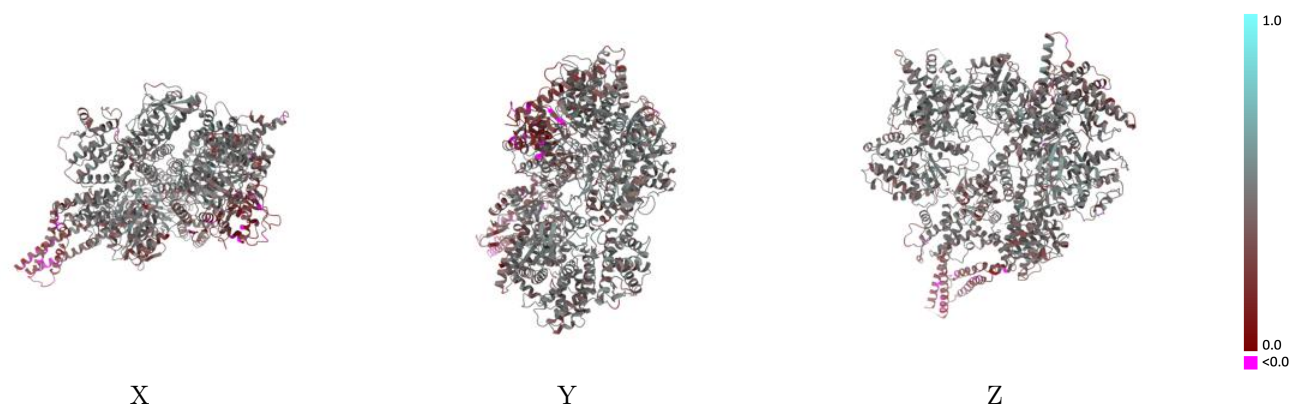
This section contains information regarding the fit between EMDB map EMD-44687 and PDB model 9BM4. Per-residue inclusion information can be found in section [3](#) on page [5](#).

### 9.1 Map-model overlay [i](#)



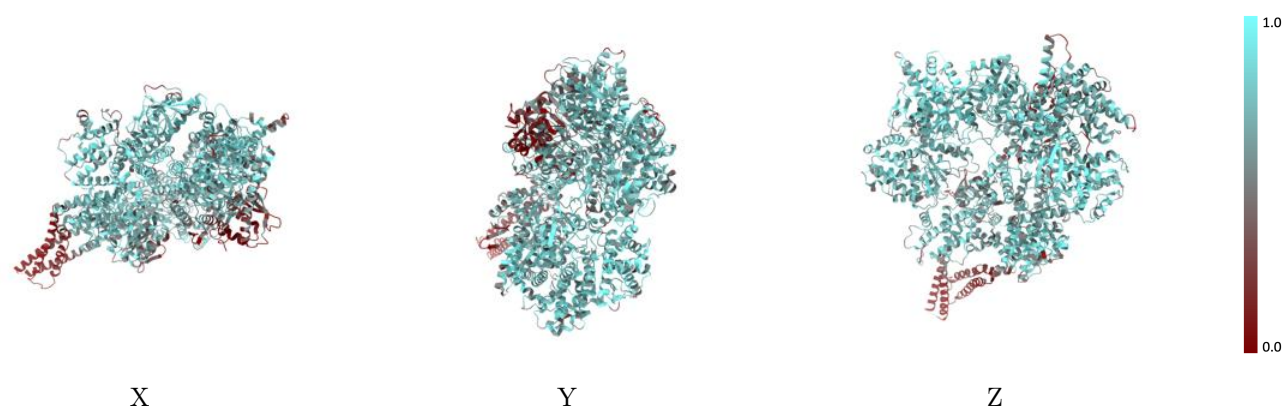
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



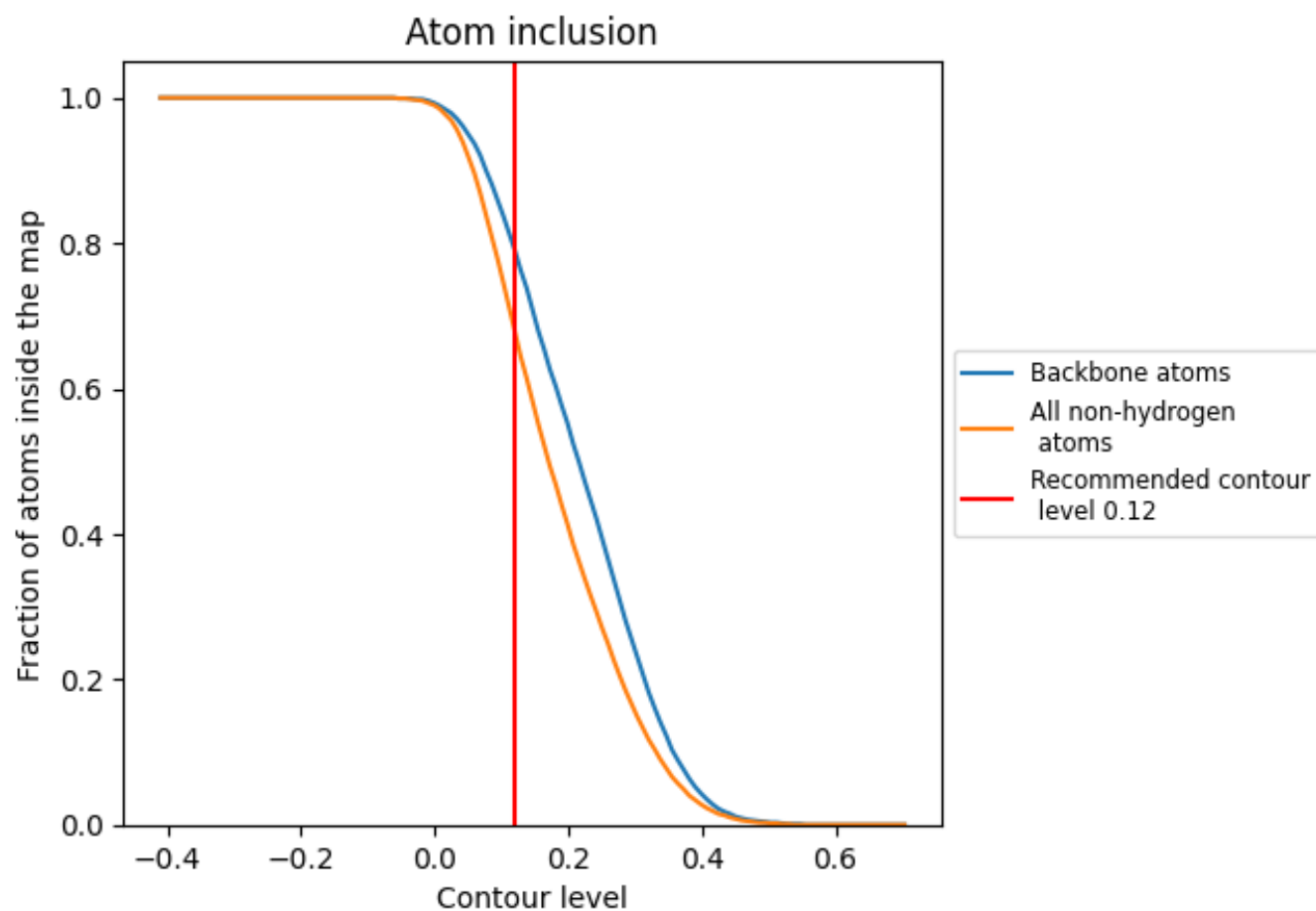
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 68% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6780	<div></div> 0.4220
A	<div></div> 0.6780	<div></div> 0.4220

