



## wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 01:02 PM EDT

PDB ID : 9BM7 / pdb\_00009bm7  
EMDB ID : EMD-44690  
Title : State-7b of motor domain from full-length human dynein-1 in 5 mM ATP  
Authors : Chai, P.; Zhang, K.  
Deposited on : 2024-05-02  
Resolution : 3.58 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

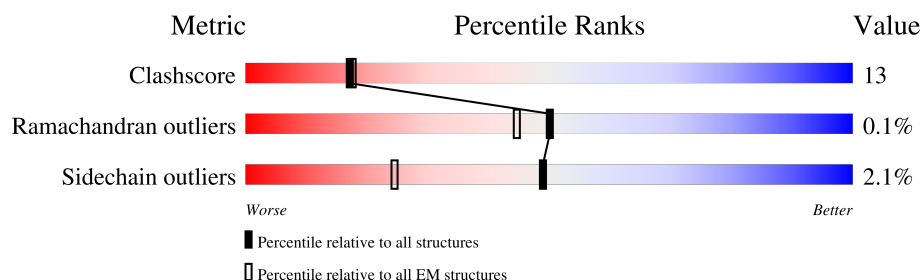
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.58 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 3 unique types of molecules in this entry. The entry contains 21818 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	2703	21702	13828	3748	4016	110	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

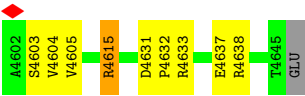




H3200	K3107	G3041	V2963	I2861	V2774	I2866	V2569	R2451	E2344	Y2265	E1233	D2030
L3201	T3110	L3042	R2964	D2862	E2775	N2867	V2569	L2452	V2345	L2268	I2136	K2033
N3202	R2965	M3043	R2966	R2863	N2779	P2869	L2572	R2453	Q2346	P2269	L2137	R2037
V3203	R2967	L3044	R2968	E2864	S2781	D2870	V2575	S2460	L2348	P2270	I2138	K2040
G3204	T2968	D3045	T2968	K2865	Q2781	D2870	V2575	M2461	L2348	P2270	I2139	M2041
L3205	R2968	H3047	R2968	A2866	E2782	Q2877	L2580	Q2464	R2358	T2271	E2143	T2042
R3206	R2969	E3048	F2972	H2867	F2784	I2880	T2583	A2465	M2361	T2272	M2145	D2045
K3207	D2973	E3048	D2973	T2785	T2785	S2881	T2583	C2466	V2362	R2273	M2146	L2048
I3208	E2974	L3050	E2974	Q2786	Q2786	F2882	T2583	C2466	V2362	R2273	M2146	L2049
K3209	D2975	Y3051	D2975	P2870	D2767	I2883	H2587	N2468	L2369	E2274	P2147	L2054
E3210	L2976	K3052	L2976	L2872	T2788	R2884	K2589	M2473	T2370	D2277	K2148	S2056
T3211	T2977	T3055	T2977	S2878	H2791	R2894	L2591	M2481	D2372	V2283	L2161	R2060
V3212	V2979	S3056	V2979	I2882	Y2792	D2697	V2592	Q2485	M2373	R2284	Y2170	L2065
Q3213	R2982	Q3057	R2982	I2882	R2797	Q2898	S2599	Q2491	I2374	R2285	L2178	L2066
Q3214	S2983	V3058	S2983	I2882	E2798	T2899	G2600	R2492	I2386	R2286	E2180	L2067
V3215	N2987	R3060	N2987	I2882	R2801	V2709	M2603	Y2493	D2387	S2290	L2182	K2068
E3216	V3064	N3061	V3064	I2882	V2802	A2711	T2604	L2494	D2388	V2291	L2191	L2069
L3218	V3065	V3065	V3065	I2882	V2802	A2711	T2604	L2494	D2388	R2292	T2192	H2085
R3219	F3066	F3066	F3066	I2882	R2804	C2712	F2606	V2495	GLY	R2293	D2195	L2090
E3220	T3067	T3067	T3067	I2882	G2805	P2714	S2607	A2497	GLY	E2294	W2203	R2091
ASP	S3138	M3068	M3068	I2882	R2811	D2717	A2608	I2498	ASP	Q2296	V2207	K2092
ARG	R3139	D2995	D2995	I2882	R2812	R2720	L2609	W2500	GLY	L2297	Y2211	K2094
LEU	R3140	P3070	P3070	I2882	L2813	R2721	L2612	L2502	GLY	K2298	Q2212	S2095
ILE	E3141	SER	SER	I2882	E2814	R2722	D2613	L2502	GLY	Q2299	I2213	L2097
LYS	N3145	SER	SER	I2882	T2815	L2723	D2614	L2514	GLY	W2302	L2220	V2098
SER	S3146	GLY	GLY	I2882	L2816	F2727	M2615	L2514	GLY	F2303	M2221	N2102
GLN	F3149	LEU	LEU	I2882	P2817	L2728	E2616	Y2517	GLY	V2307	V2223	R2105
GLU	V3150	ASP	ASP	I2882	V2818	R2729	L2620	I2518	GLY	D2308	S2226	R2107
VAL	H3151	ALA	ALA	I2882	E2819	H2730	L2620	P2530	ASP	W2311	K2230	E2114
ASN	Q3152	THR	THR	I2882	G2820	V2731	L2620	N2531	ASP	V2312	S2231	LYS
ALA	N3158	S3082	S3082	I2882	L2821	P2732	L2632	I2532	GLY	D2320	M2232	GLY
ALA	A3162	P3083	P3083	I2882	E2826	S2743	L2632	I2532	GLY	D2321	W2234	GLY
ASN	R3163	A3084	A3084	I2882	L2829	I2747	F2635	I2535	ALA	N2322	R2235	ARG
ASP	R3164	L3085	L3085	I2882	L2830	N2752	D2636	I2535	ALA	K2323	L2241	GLY
LYS	G3165	L3086	L3086	I2882	R2831	R2753	H2637	E2538	ALA	L2324	E2242	ALA
LEU	G3166	N3087	N3087	I2882	Q2834	A2754	Y2638	S2542	ALA	L2325	R2243	VAL
LYS	R3167	R3088	R3088	I2882	D2835	M2755	Y2638	G2543	ALA	T2327	L2244	ASP
LYS	T3168	G3089	G3089	I2882	E2839	L2756	Y2641	W2545	ALA	P2328	E2248	GLY
MET	M3169	V3090	V3090	I2882	E2841	R2757	T2644	W2548	ALA	N2329	K2257	L2127
VAL	L3170	L3091	L3091	I2882	E2842	R2763	L2650	I2556	ALA	G2330	L2241	GLY
LYS	R3174	N3092	N3092	I2882	R2843	Y2764	L2650	E2557	ALA	E2331	E2242	GLY
LYS	H3175	V3093	V3093	I2882	R2844	Y2765	L2650	A2563	ALA	R2332	L2244	GLY
GLN	Y3176	F3094	F3094	I2882	R2844	T2770	L2650	D2566	ALA	P2337	E2248	GLY
GLN	R3191	G3095	G3095	I2882	D2851	T2770	L2650	D2566	ALA	N2338	K2257	GLY
ALA	L3194	W3097	W3097	I2882	D2851	T2770	L2650	D2566	ALA	R2340	K2257	GLY
LYS	E3195	L3102	L3102	I2882	K2856	M2773	E2665	D2566	ALA	W2341	K2257	GLY
LYS	E3196	V3105	V3105	I2882	K2857	M2773	E2665	D2566	ALA	F2343	K2257	GLY
VAL	Q3197	G3106	G3106	I2882	K2857	M2773	E2665	D2566	ALA	F2343	K2257	GLY
MET	Q3198	G3106	G3106	I2882	K2857	M2773	E2665	D2566	ALA	F2343	K2257	GLY
SER	M3199	G3106	G3106	I2882	K2857	M2773	E2665	D2566	ALA	F2343	K2257	GLY
GLN		G3106	G3106	I2882	K2857	M2773	E2665	D2566	ALA	F2343	K2257	GLY







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66008	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	0.552	Depositor
Minimum map value	-0.340	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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, 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	0.29	0/22168	0.51	0/30054

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 [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	21702	0	21742	586	0
2	A	54	0	24	7	0
3	A	62	0	24	11	0
All	All	21818	0	21790	586	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 586 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:3151:HIS:HD1	1:A:3516:TYR:HH	0.95	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3660:VAL:HG22	1:A:3671:LEU:HD13	1.60	0.84
1:A:2437:LEU:HD22	1:A:2502:LEU:HD21	1.61	0.81
1:A:2221:MET:HE1	1:A:2343:PHE:HB2	1.63	0.79
1:A:1882:THR:HB	1:A:1883:PRO:HD2	1.64	0.79

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	2689/4646 (58%)	2606 (97%)	80 (3%)	3 (0%)	48 79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER
1	A	4251	ILE
1	A	2387	LEU

### 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	2401/4125 (58%)	2350 (98%)	51 (2%)	48 71

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3146	SER
1	A	3714	ASN
1	A	4491	ASN
1	A	3176	TYR
1	A	3619	PHE

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	3009	ASN
1	A	4065	GLN
1	A	4477	GLN
1	A	4326	ASN
1	A	2637	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](#)

4 ligands are modelled in this entry.

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	-	28,33,33	0.75	0	34,52,52	0.77	1 (2%)
2	ADP	A	4704	-	24,29,29	0.84	0	29,45,45	1.26	3 (10%)
3	ATP	A	4703	-	28,33,33	0.79	0	34,52,52	0.61	1 (2%)
2	ADP	A	4701	-	24,29,29	0.73	0	29,45,45	0.78	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	-	-	4/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	5/12/32/32	0/3/3/3
3	ATP	A	4703	-	-	4/18/38/38	0/3/3/3
2	ADP	A	4701	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4704	ADP	N3-C2-N1	-3.53	123.88	128.67
2	A	4704	ADP	C4-C5-N7	-2.68	106.51	109.34
3	A	4702	ATP	C5-C6-N6	2.37	123.92	120.31
2	A	4701	ADP	C5-C6-N6	2.30	123.82	120.31
3	A	4703	ATP	C5-C6-N6	2.27	123.77	120.31

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

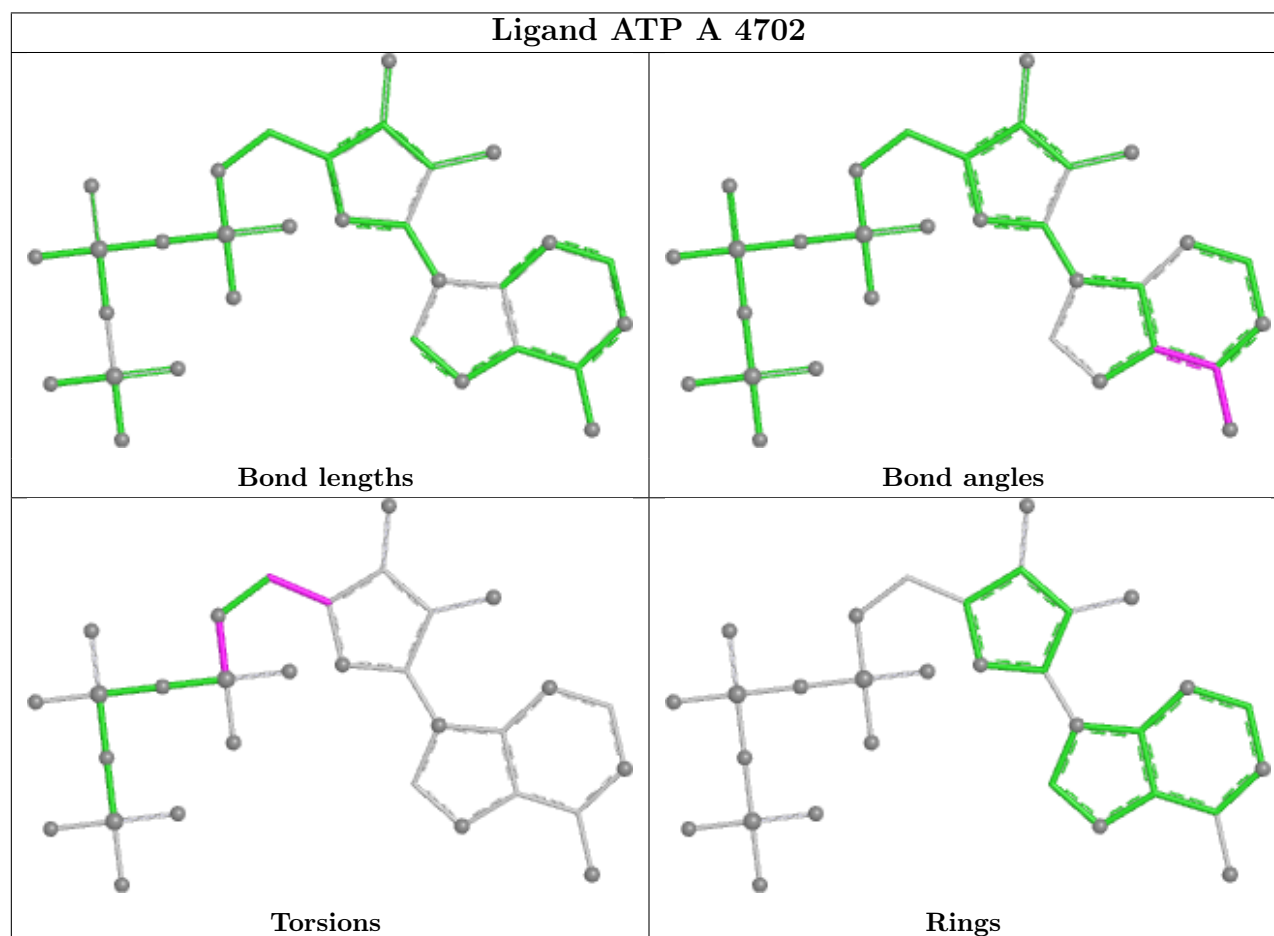
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	C5'-O5'-PA-O2A
2	A	4704	ADP	C5'-O5'-PA-O3A

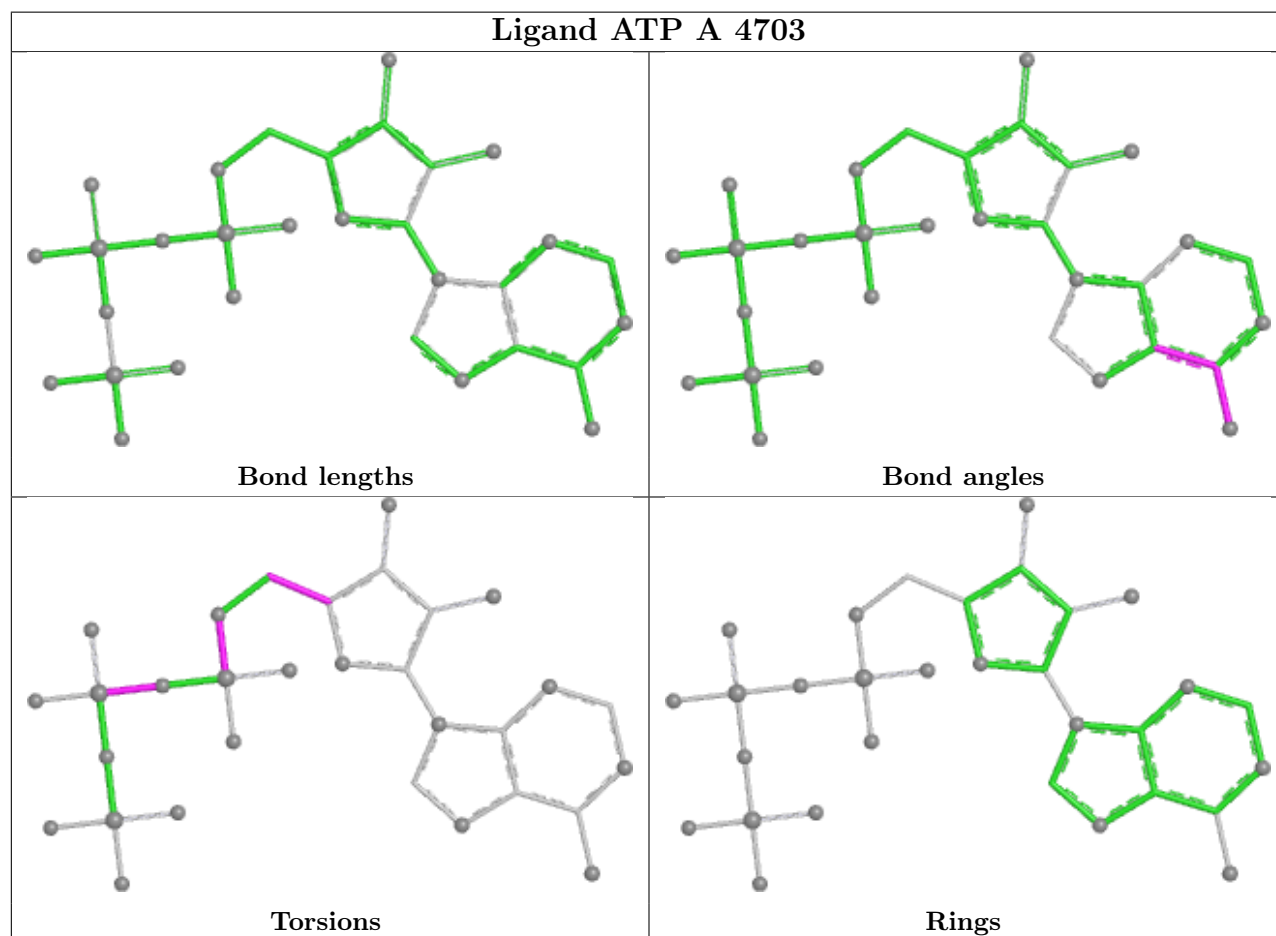
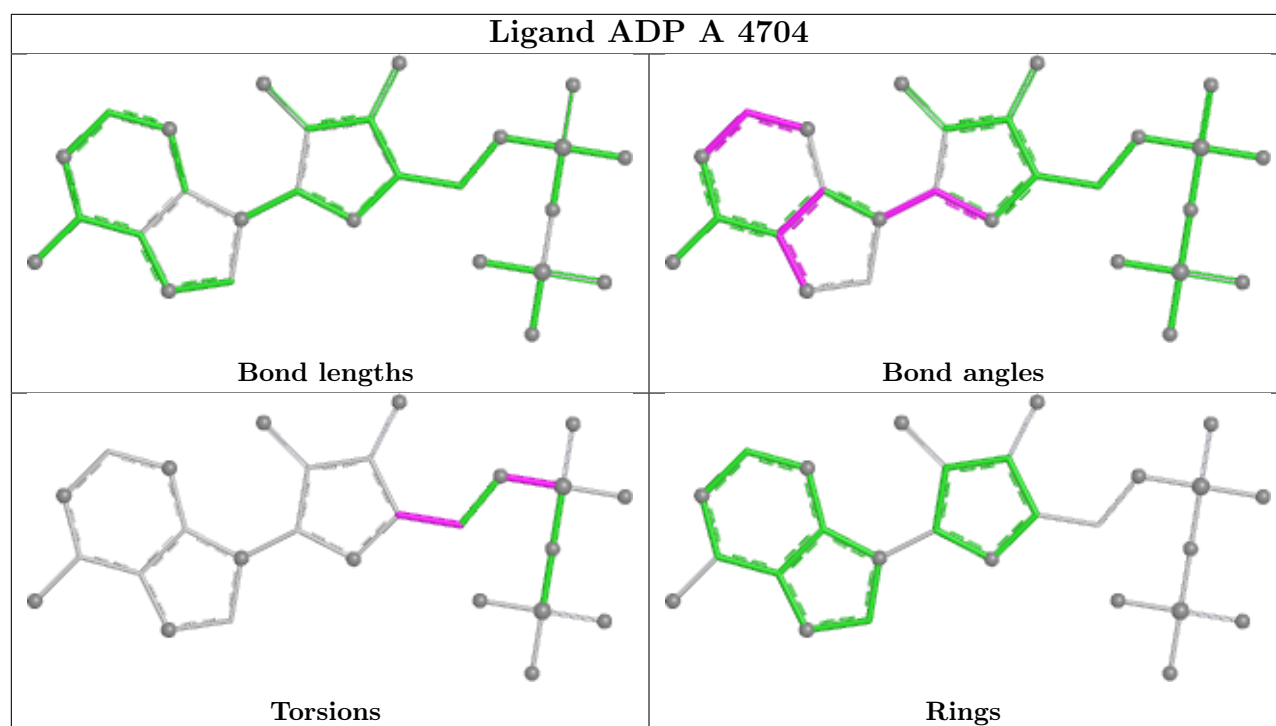
There are no ring outliers.

4 monomers are involved in 18 short contacts:

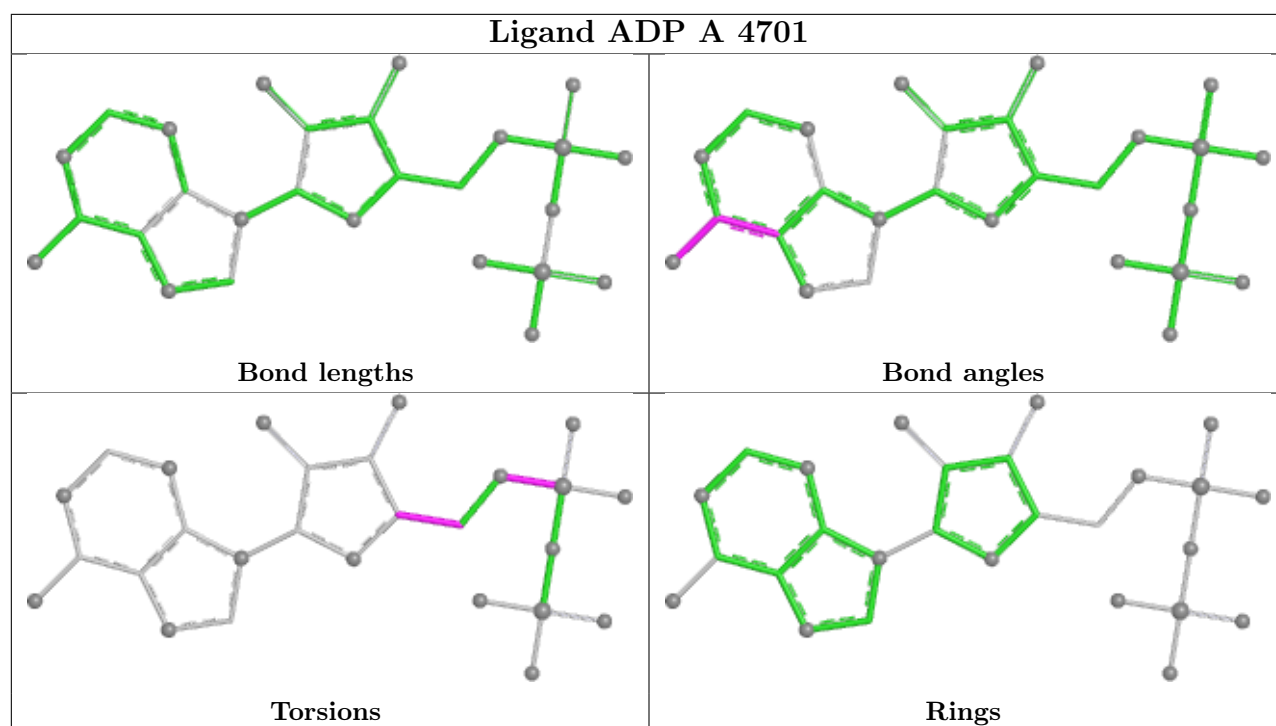
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4702	ATP	7	0
2	A	4704	ADP	2	0
3	A	4703	ATP	4	0
2	A	4701	ADP	5	0

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.

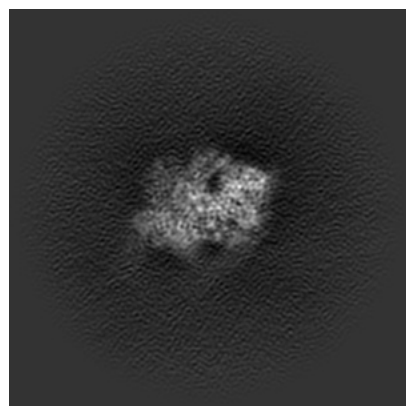
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44690. These allow visual inspection of the internal detail of the map and identification of artifacts.

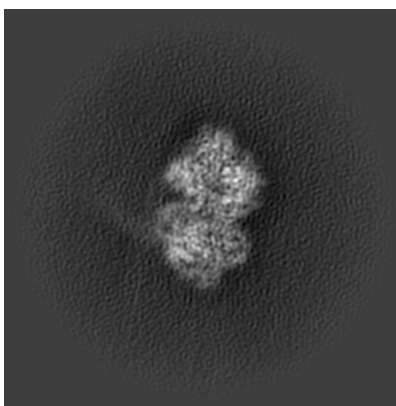
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

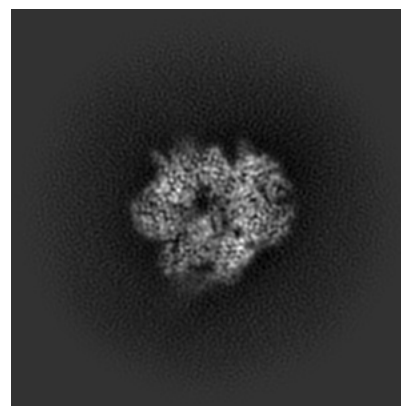
#### 6.1.1 Primary map



X

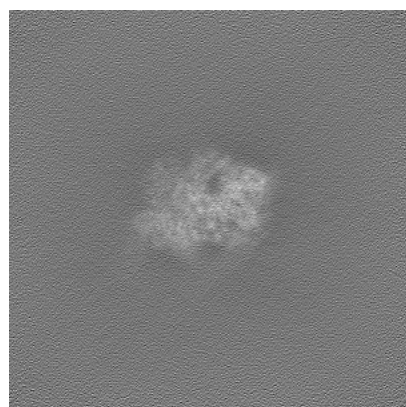


Y

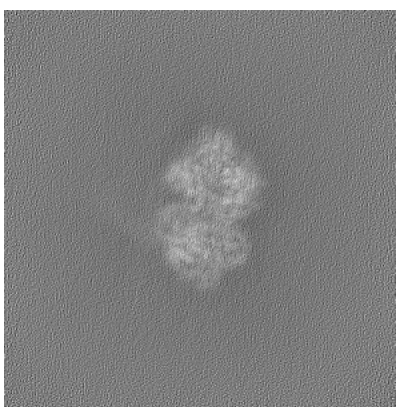


Z

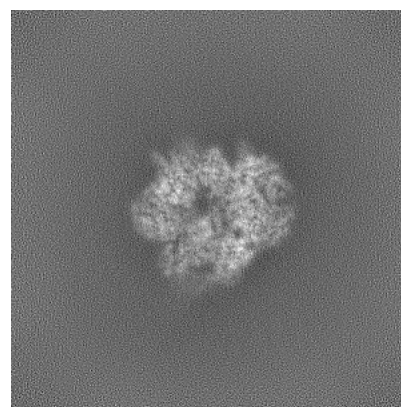
#### 6.1.2 Raw map



X



Y

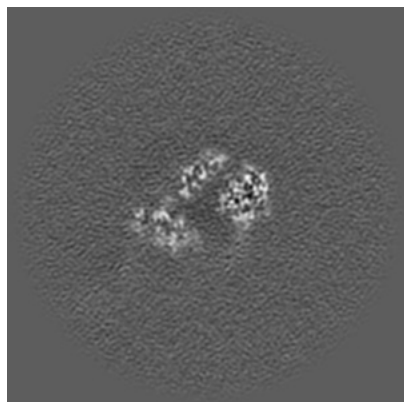


Z

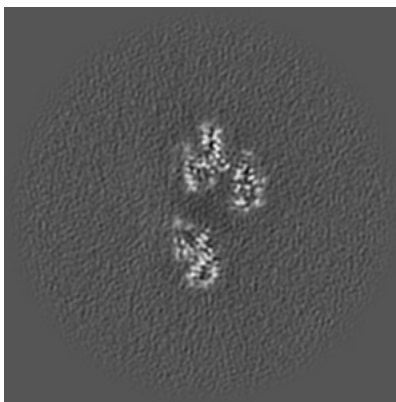
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

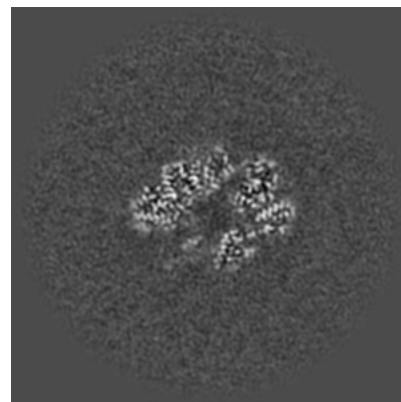
### 6.2.1 Primary map



X Index: 200

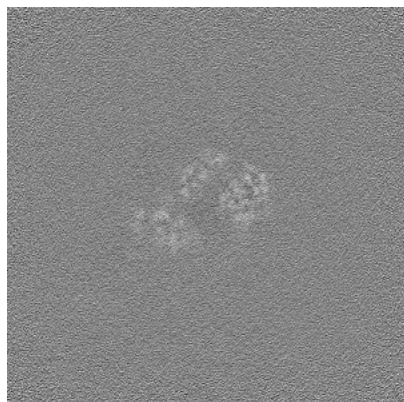


Y Index: 200

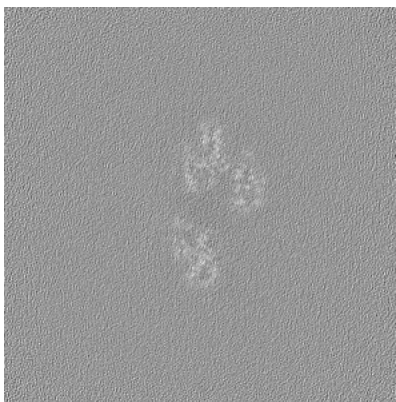


Z Index: 200

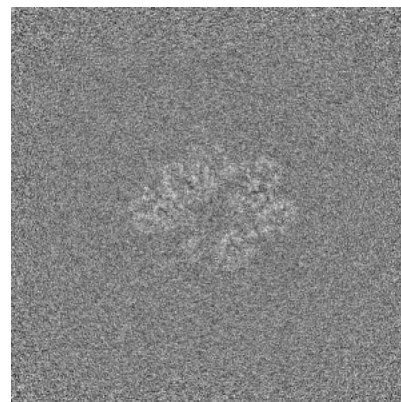
### 6.2.2 Raw map



X Index: 200



Y Index: 200

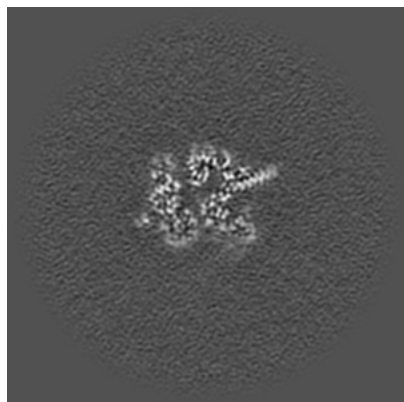


Z Index: 200

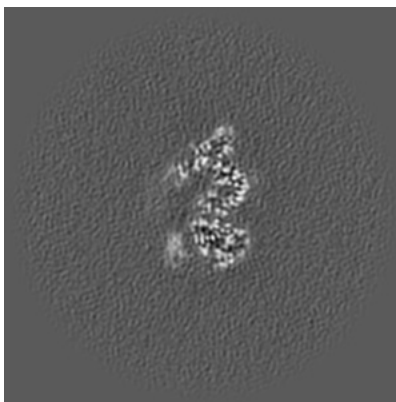
The images above show central slices of the map in three orthogonal directions.

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

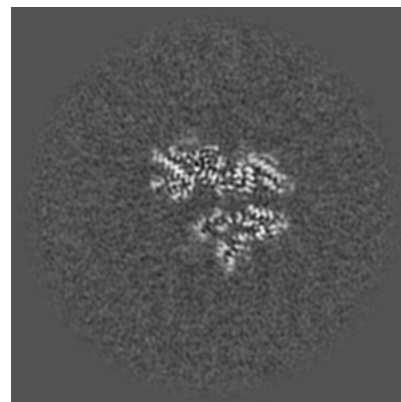
### 6.3.1 Primary map



X Index: 229

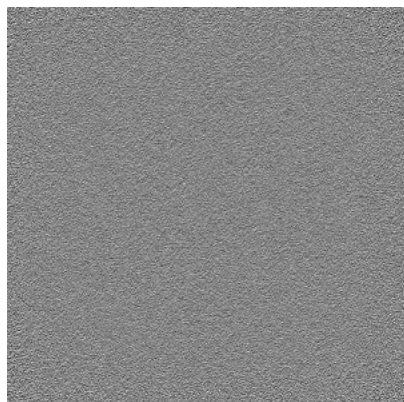


Y Index: 224

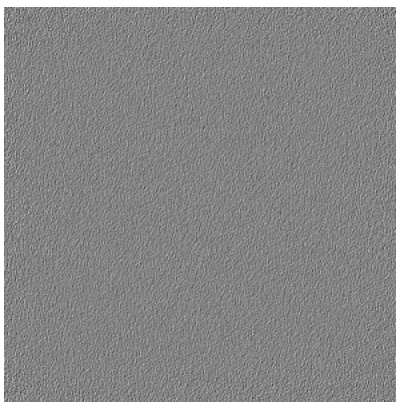


Z Index: 222

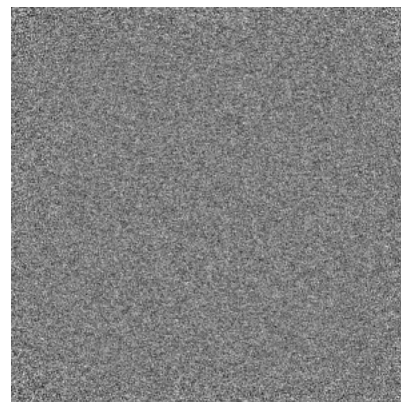
### 6.3.2 Raw map



X Index: 0



Y Index: 0



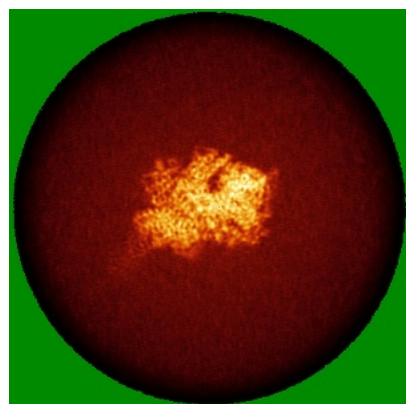
Z Index: 0

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

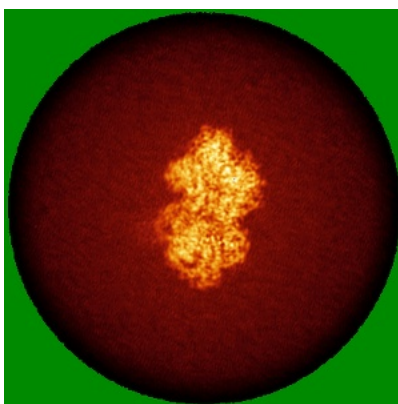


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

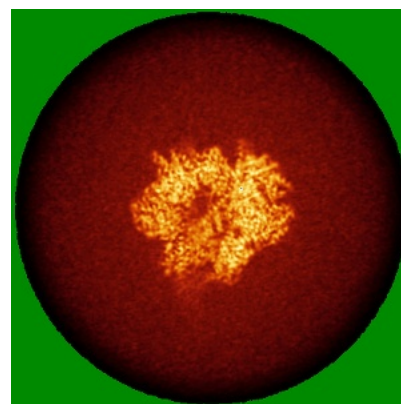
### 6.4.1 Primary map



X

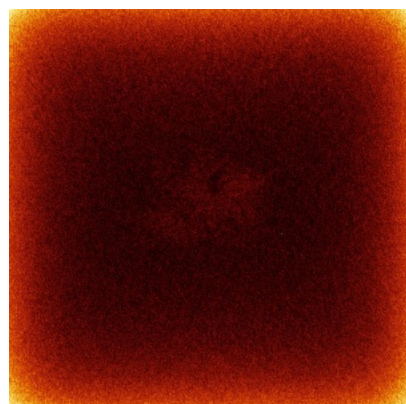


Y

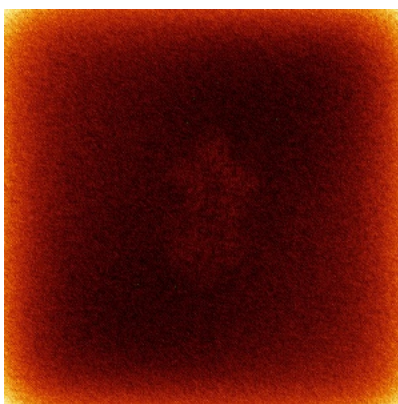


Z

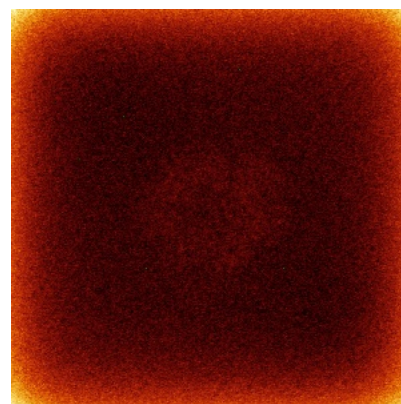
### 6.4.2 Raw map



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.

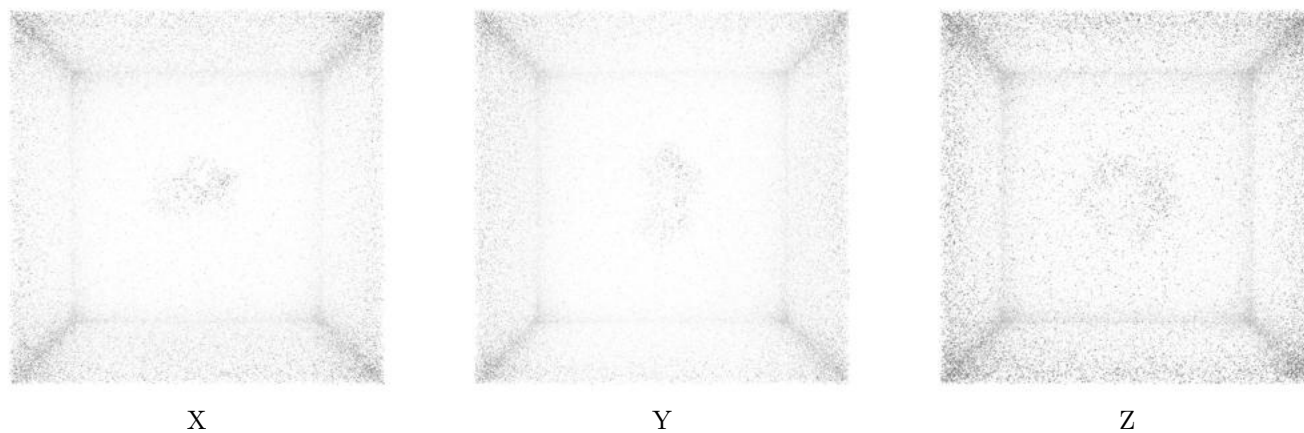
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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.

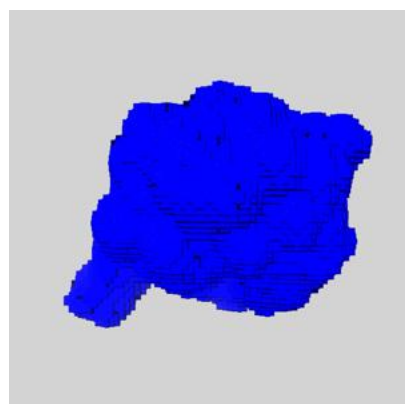
## 6.6 Mask visualisation [i](#)

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

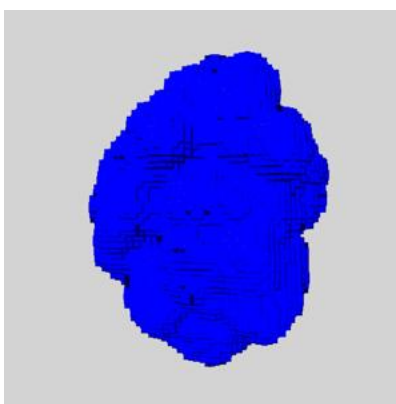
A mask typically either:

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

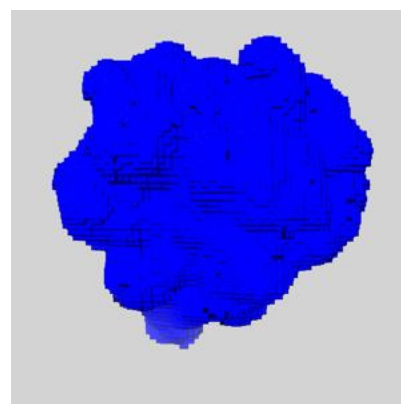
### 6.6.1 emd\_44690\_msk\_1.map [i](#)



X



Y

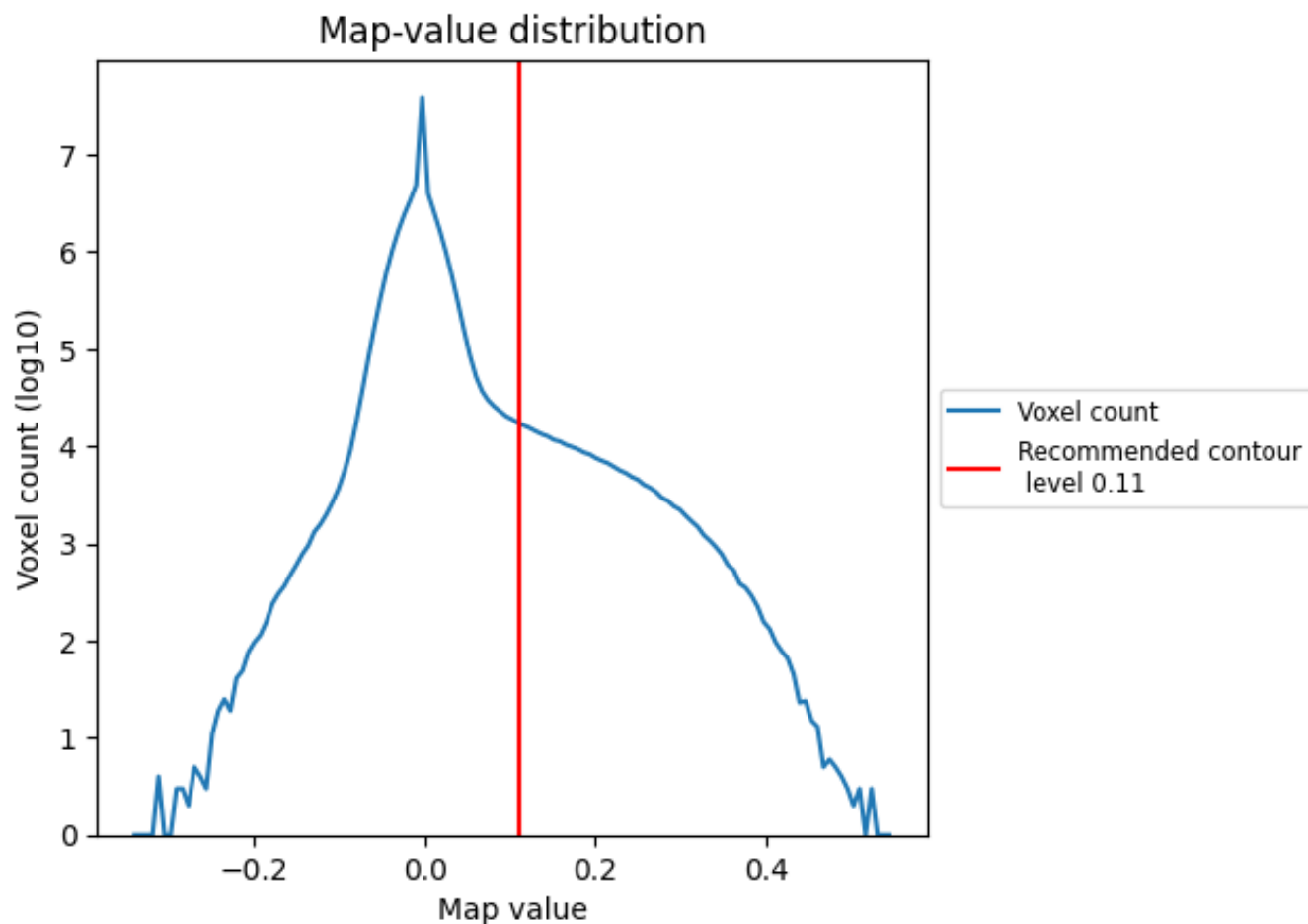


Z

## 7 Map analysis [i](#)

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

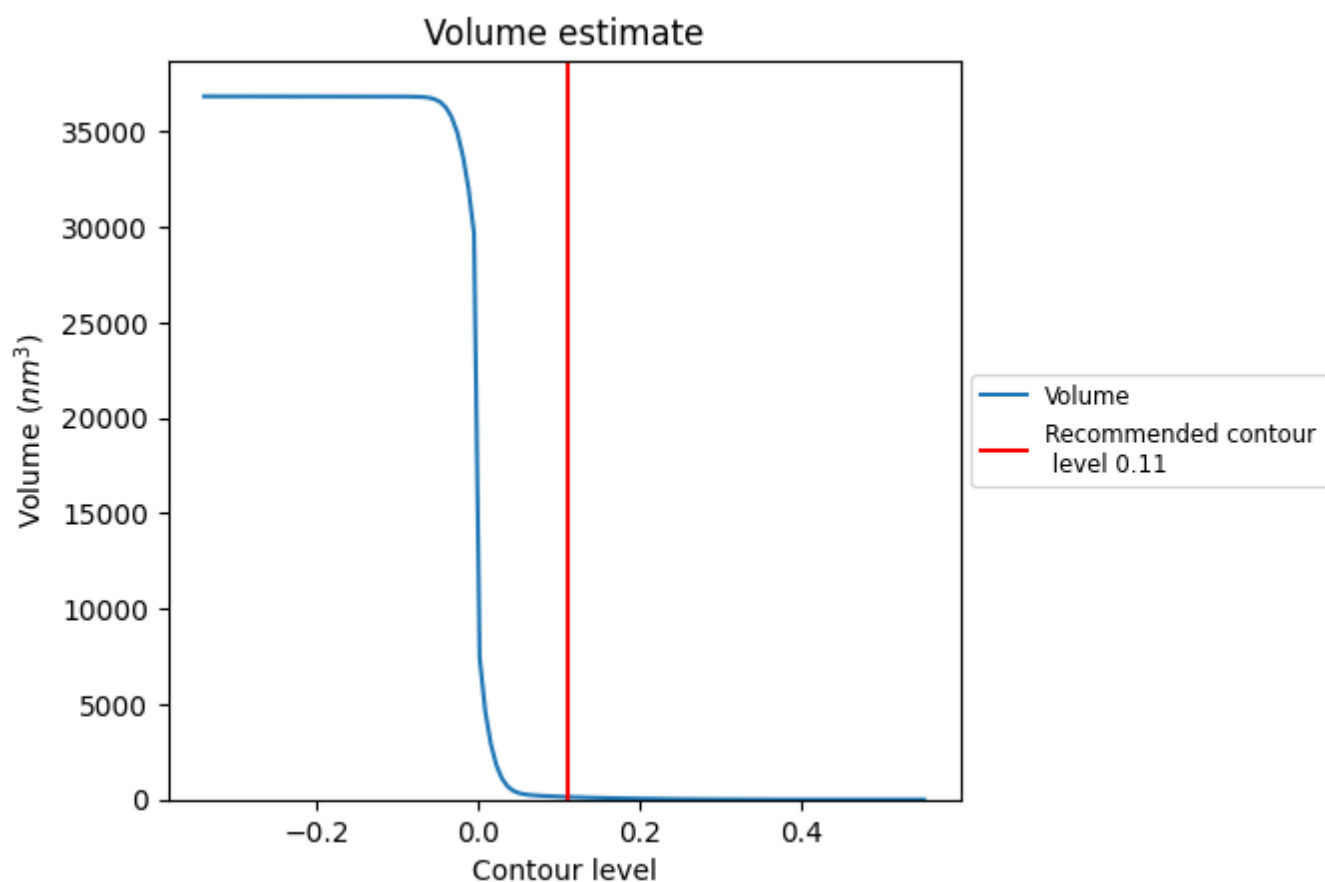
### 7.1 Map-value distribution [i](#)



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.



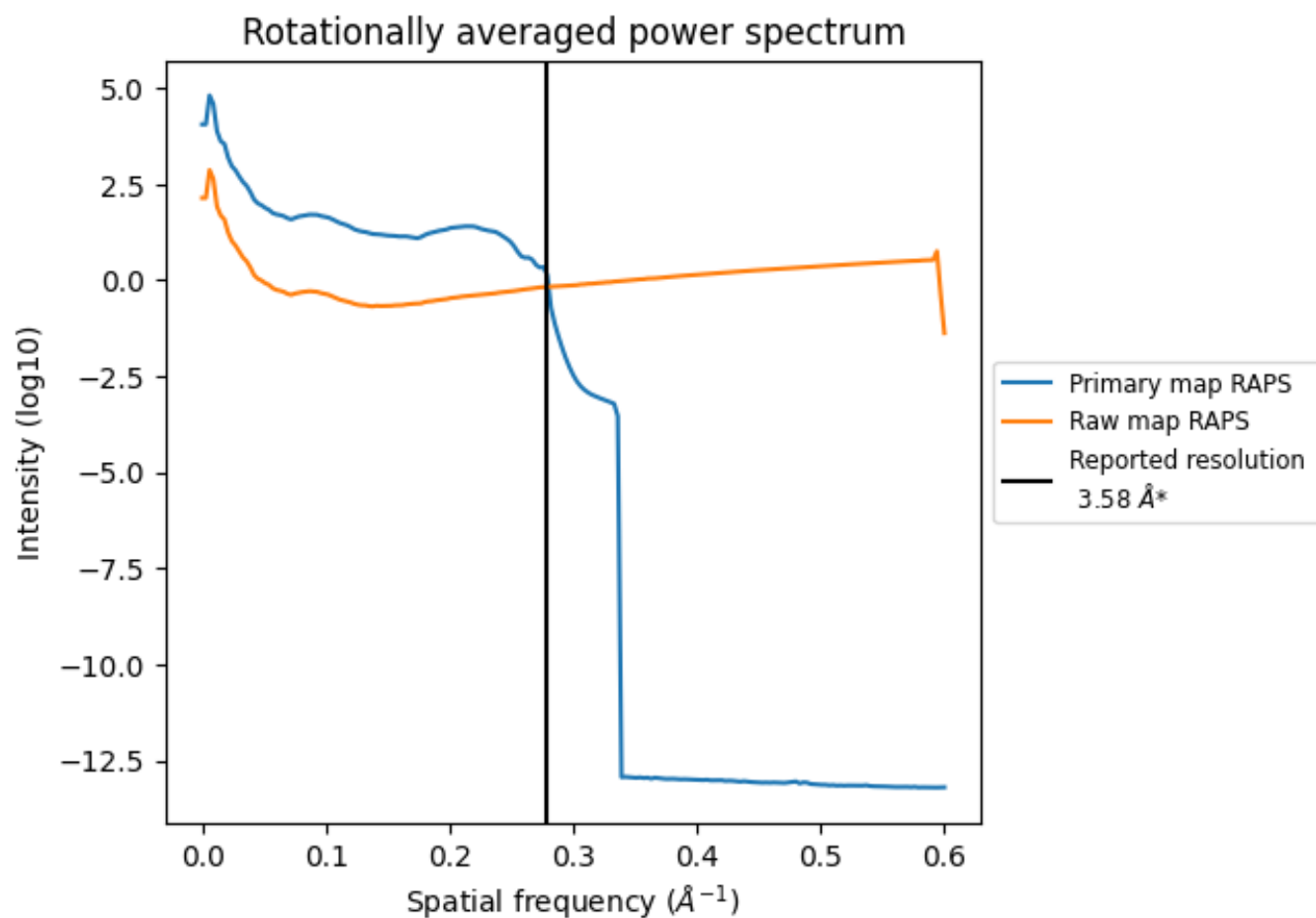
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm<sup>3</sup>; this corresponds to an approximate mass of 124 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 ⓘ

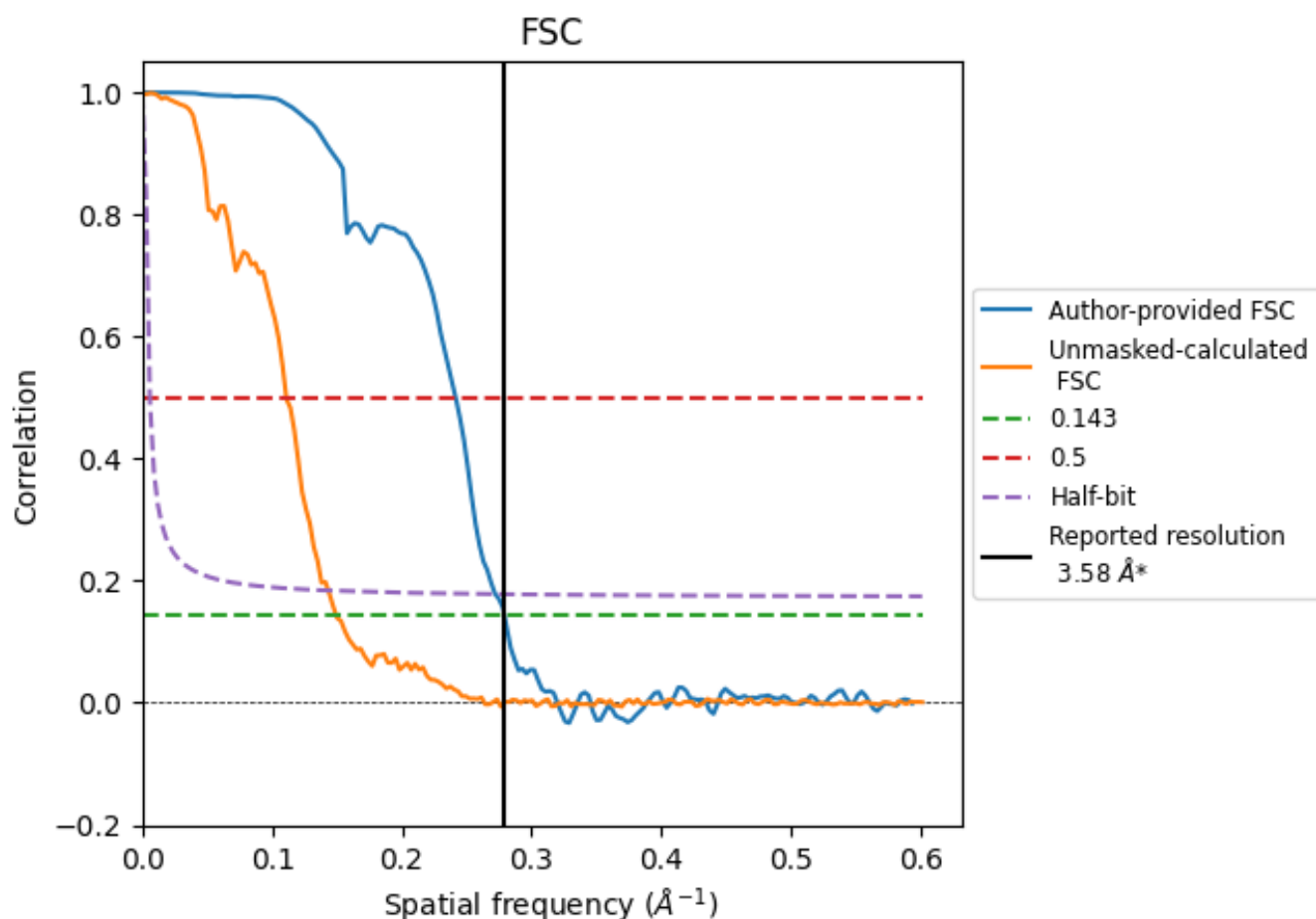


\*Reported resolution corresponds to spatial frequency of 0.279  $\text{\AA}^{-1}$

## 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 0.279  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

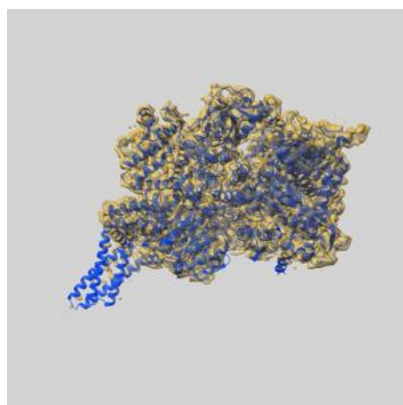
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	3.58	4.14	3.68
Unmasked-calculated*	6.68	9.01	6.97

\*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 6.68 differs from the reported value 3.58 by more than 10 %

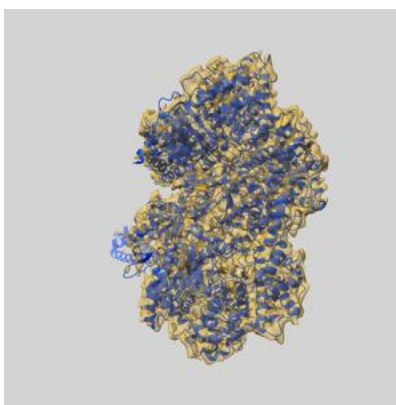
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44690 and PDB model 9BM7. Per-residue inclusion information can be found in section [3](#) on page [5](#).

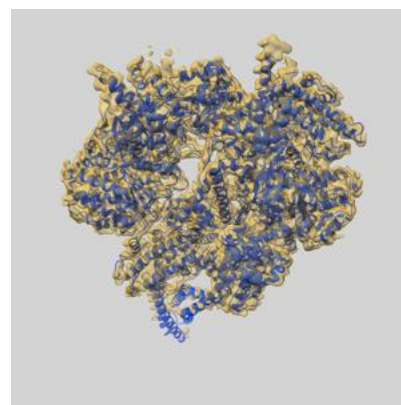
### 9.1 Map-model overlay [i](#)



X



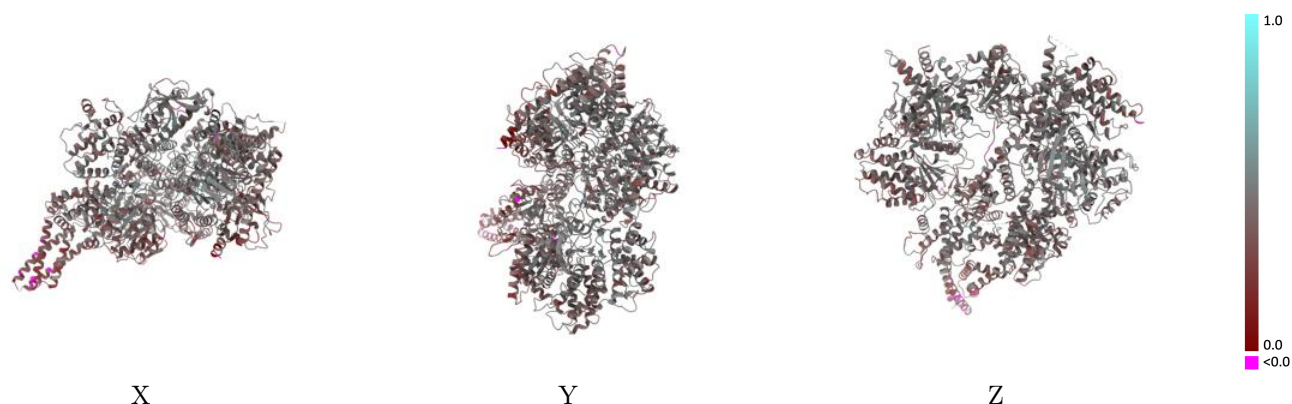
Y



Z

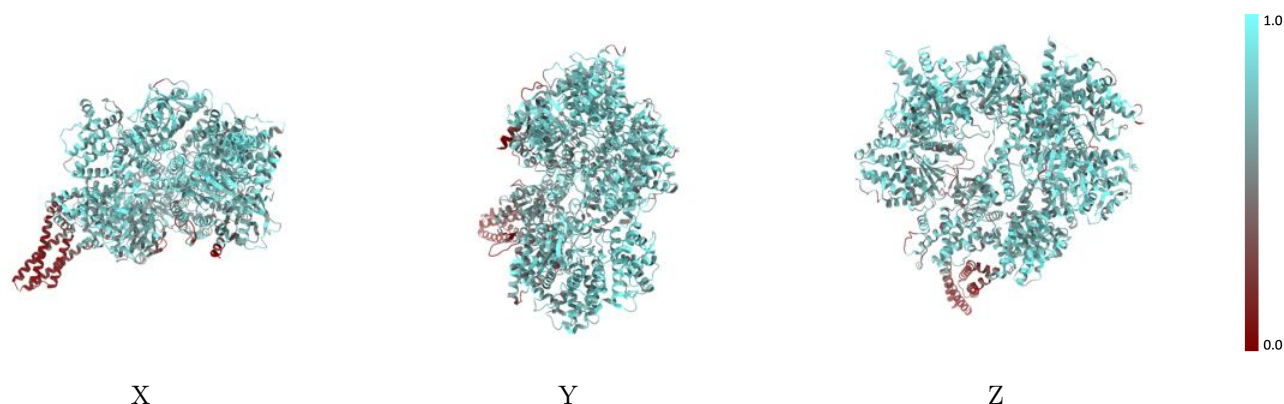
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



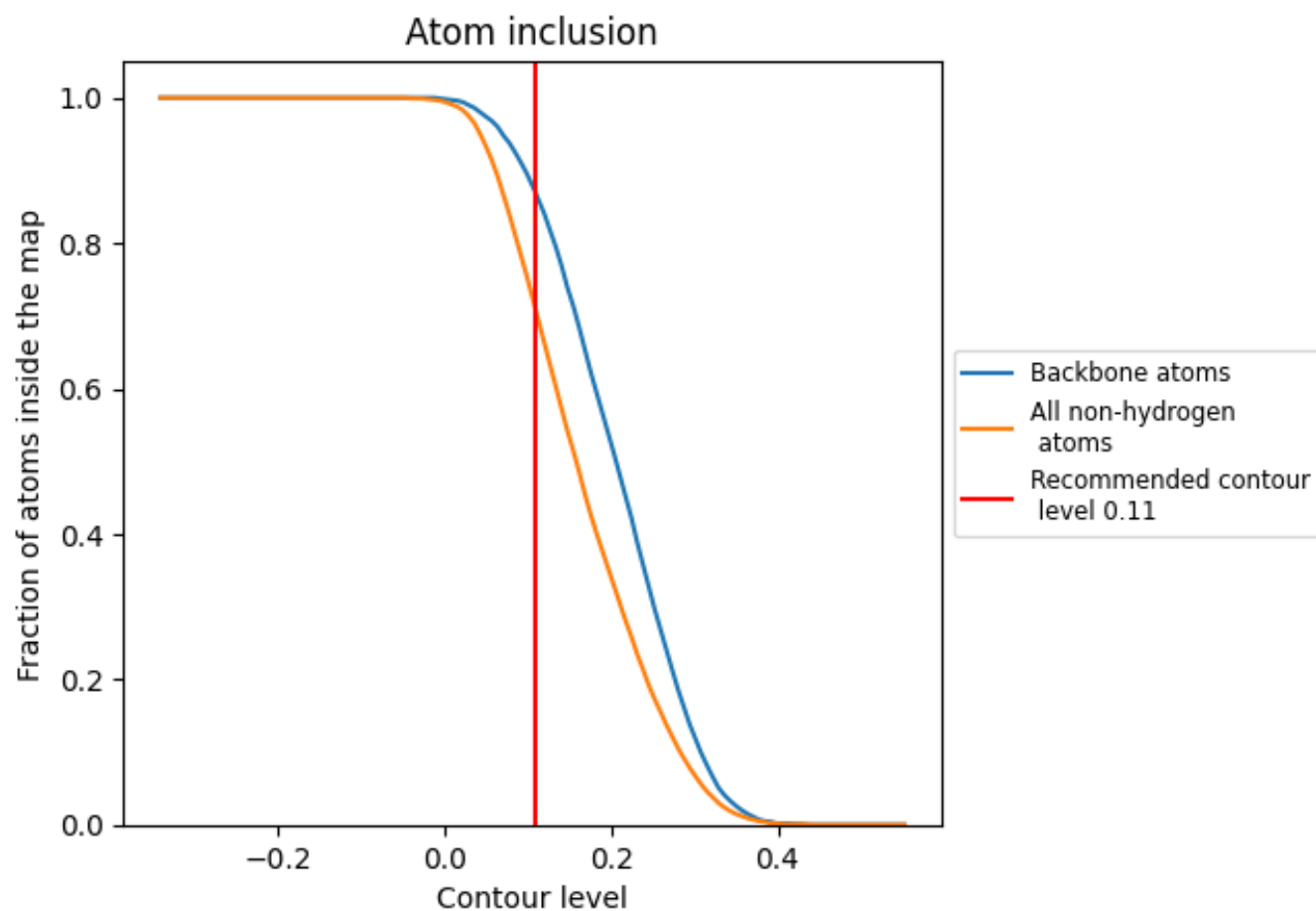
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 71% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7080	<div></div> 0.4100
A	<div></div> 0.7080	<div></div> 0.4100

