



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2025 – 01:09 PM EDT

PDB ID : 9BN4 / pdb_00009bn4
EMDB ID : EMD-44721
Title : The alpha registry-locked dynein motor domain mutant in 5mM ATP condition, class2
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at
<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

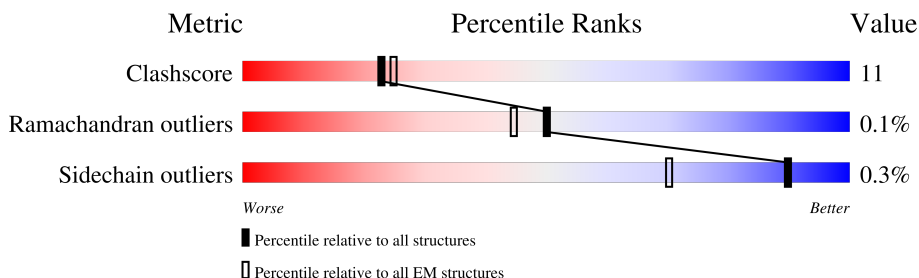
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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>13%</div> <div>45%</div> <div>16%</div> <div>39%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23078 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

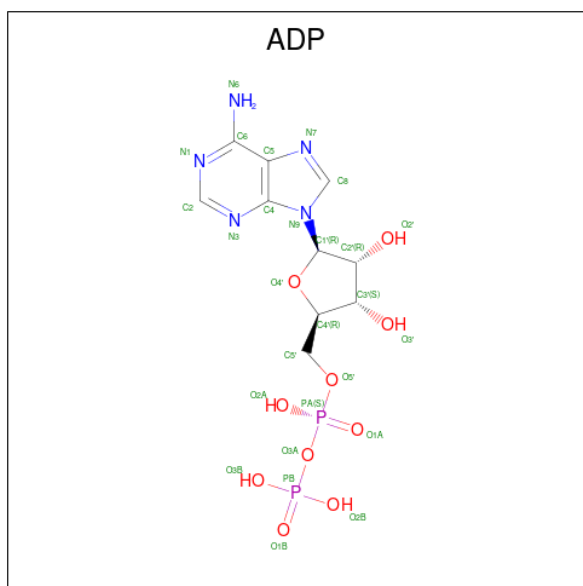
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2855	Total	C	N	O	S	0	0
			22962	14643	3963	4241	115		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2389	ASP	GLU	conflict	UNP Q14204

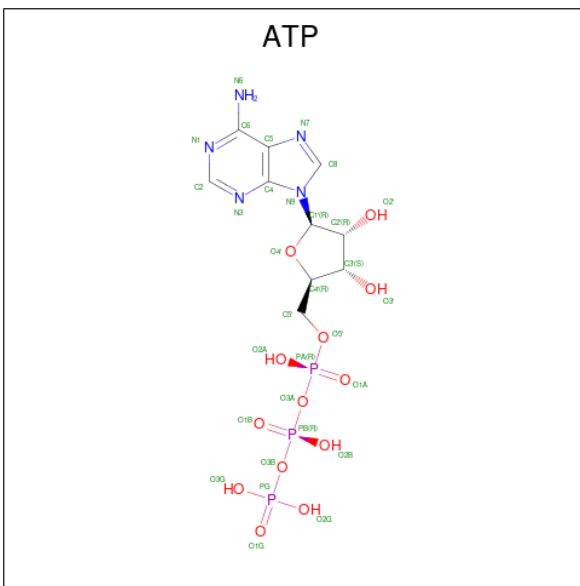
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- 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).

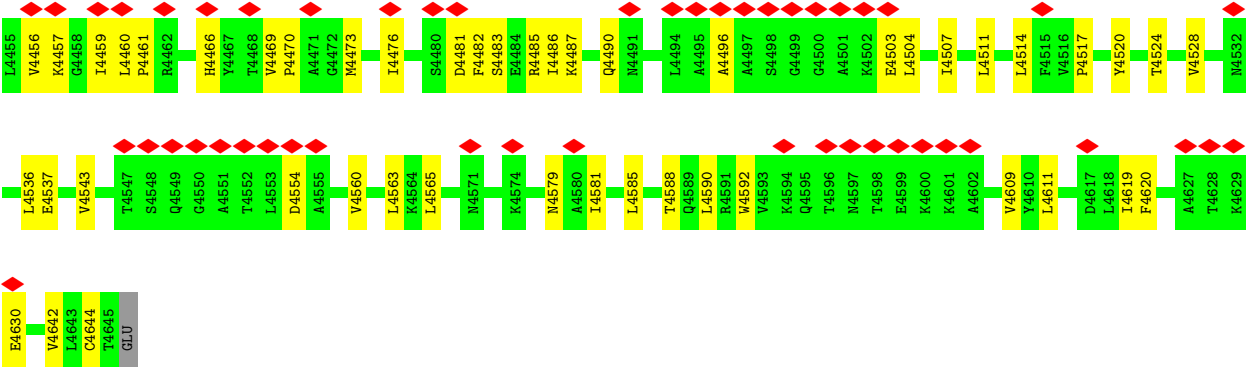


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0
3	A	1	Total 31	C 10	N 5	O 13	P 3	0



GLU	E3049	R2966	R2869	P2768	Q2654	K2529	Q2424	R2332	L2208	Q2079	A1995
LEU	T3055	G2969	P2870	L2769	K2657	P2530	P2425	P2336	Q2209	K2094	P1996
VAL	Q3156	E2970	I2871	A2772	W2658	W2531	T2426	P2337	L2210	S2099	C1999
ASN	I3059	L2976	Y2873	W2773	L2659	I2532	S2429	N2338	Q2212	S2099	E2000
ALA	N3061	L2977	S2874	V2774	P2662	E2544	N2430	N2339	I2213	G2101	L2001
ALA	Y3064	T2978	W2876	E2775	C2663	W2545	G2431	F2343	T2214	N2102	L2002
ALA	P3070	V2979	W2877	E2782	D2664	P2565	H2439	E2344	Q2215	R2105	W2003
ASN	P3070	L2980	R2878	R2783	E2665	P2566	H2439	E2345	M2221	E2106	K2004
ASP	K3163	R2981	K2879	T2785	L2668	D2566	Q2442	Q2346	R2107	R2106	W2006
LEU	SER	N2982	P2883	Q2786	P2669	D2573	Q2442	D2347	G2227	W2012	
LEU	GLU	N2987	V2884	D2787	D2670	R2576	H2445	L2348	K2230	R2113	
LYS	GLY	N2988	P2884	T2788	P2670	R2576	H2446	L2349	S2231	E2114	I2016
LYS	LEU	K2989	D2885	Q2789	F2682	L2581	M2447	Y2350	W2234	GLU	T2017
VAL	I2990	Q2886	Q2887	P2790	T2682	T2582	D2448	A2351	W2234	GLU	W2018
LYS	ASP	E2887	E2887	H2791	T2695	T2583	L2449	T2352	PRG	ARG	N2019
ASP	ARG	E2888	E2888	Y2792				R2358	GLY	GLY	PRO
ALA	ALA	D2891	D2891	I2793	Y2701	P2590	L2452	F2364	GLY	TYR	GLY
ALA	S2997	P2796	P2796	Y2794	R2705	C2594	R2453	ASP	ALA	ALA	ALA
ALA	N2998	E2797	E2797	P2798	V2709	P2596	C2454	S2370	VAL	GLY	GLY
LYS	S3002	L2897	L2897	E2798	C2712	L2593	L2452	T2372	K2257	ASP	ARG
LYS	F3004	V2898	V2898	R2801	N2713	G2595	R2454	D2371	S2260	ASP	ARG
VAL	L3091	E2902	E2902	W2802	P2714	T2602	D2478	L2382	L2261	GLY	ASN
MET	L3005	E2903	E2903	V2803	R2720	T2602	F2479	R2383	D2262	L2127	L2028
SER	K3007	D2906	D2906	R2804	K2721	L2605	E2484	P2386	D2263	D2030	F2029
GLN	M3008	L3011	L3011	E2814	R2729	F2606	E2484	GLY	Y2265	A2128	N2031
ILE	M3113	L3012	L3012	T2815	R2730	L2609	R2488	GLY	N2271	E2135	L2035
GLN	L3114	E3022	E3022	L2816	H2731	L2609	R2488	ASP	L2284	S2140	F2036
LEU	L3115	G3023	G3023	W2818	P2732	P2613	R2492	GLU	S2290	L2149	S2038
LYS	N3119	D3024	D3024	E2819	P2733	W2615	V2495	ALA	V2291	L2157	L2039
LYS	D3124	Y3025	Y3025	G2820	V2734	E2616	V2495	GLN	R2292	L2160	A2041
GLN	Y3125	Y3026	H2918	L2821	L2744	V2617	I2498	ARG	G2293	L2160	T2042
GLU	V3128	A3027	I2922	L2822	L2744	N2621	L2502	ARG	E2294	L2048	L2048
VAL	V3129	T3028	I2925	R2823	I2747	F2622	S2503	ARG	L2295	T2049	
ALA	V3130	M3030	F2926	D2840	F2751	S2623	G2504	LYS	Q2169	Q2169	
ASP	D3131	T3031	Q2927	R2844	N2752	T2626	D2505	GLY	Y2170	Y2170	
LYS	K3034	E3035	Q2928	L2855	R2753	T2627	S2506	LYS	H2171	H2171	
GLN	K3038	Q3038	Q2929	L2856	F2757	P2628	R2507	ASP	R2172	R2172	
MET	K3039	K3039	Q2930	K2856	R2757	E2629	L2508	GLU	G2173	G2173	
SER	G3041	G3041	H2932	H2857	I2758	H2637	L2509	GLY	E2174	E2174	
VAL	G3042	G3042	G2931	K2856	I2759	Y2638	L2614	GLU	V2307	V2307	
ASP	G3043	G3043	L2934	L2861	P2760	V2638	L2614	ALA	D2308	D2308	
LEU	L3044	L3044	L2934	N2860	S2761	T2644	L2618	ALA	P2309	P2309	
ASP	G3045	G3045	K2943	T2861	S2761	T2644	T2522	ALA	G2194	G2194	
ASP	L3046	L3046	T2944	D2862	L2762	P2645	T2522	ALA	D2195	D2195	
LEU	M3043	M3043	R2948	R2863	R2763	N2646	T2524	ALA	E2196	E2196	
LYS	L3044	L3044	R2948	R2864	R2765	G2647	P2525	ALA	E2197	E2197	
VAL	N3145	N3145	R2948	K2865	A2766	V2648	P2525	ALA	E2198	E2198	
PRO	F3149	F3149	S2957	K2866	E2767	P2652	T2527	ALA	W2203	W2203	
ASP	V3150	V3150	R2965	A2866	E2767	V2653	T2528	ALA	V2204	V2204	
LEU				M2867				ALA	E2205	E2205	
ARG				S2868				ALA	K2206	K2206	
ILE								ALA	V2207	V2207	
LYS								ALA			
SER								ALA			
GLN								ALA			

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	91718	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.072	Depositor
Minimum map value	-1.197	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.35	Depositor
Map size (\AA)	412.488, 412.488, 412.488	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1458, 1.1458, 1.1458	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	0.27	1/23454 (0.0%)	0.53	8/31791 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2328	PRO	CG-CD	-6.17	1.30	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2328	PRO	N-CD-CG	-11.60	85.79	103.20
1	A	2328	PRO	CA-N-CD	-9.86	97.70	111.50
1	A	2714	PRO	N-CD-CG	-8.44	90.54	103.20
1	A	2714	PRO	CA-CB-CG	-7.68	89.40	104.00
1	A	2714	PRO	CA-N-CD	-6.83	101.93	111.50

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	22962	0	23030	507	0
2	A	54	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	62	0	24	0	0
All	All	23078	0	23078	507	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 507 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:2925:ILE:HG13	1:A:2933:LEU:HD13	1.59	0.85
1:A:2929:PRO:HB3	1:A:3060:ARG:HA	1.56	0.85
1:A:2987:ASN:OD1	1:A:3061:ASN:ND2	2.10	0.85
1:A:2324:LEU:HD11	1:A:2332:ARG:HB3	1.61	0.82
1:A:2453:ARG:HB2	1:A:2729:ARG:HA	1.59	0.82

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	2841/4646 (61%)	2765 (97%)	72 (2%)	4 (0%)	48 77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER
1	A	4251	ILE
1	A	1730	ALA
1	A	2871	ILE

5.3.2 Protein sidechains ⓘ

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	2540/4125 (62%)	2533 (100%)	7 (0%)	91 97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2998	ASN
1	A	3608	LYS
1	A	3937	ARG
1	A	3741	ARG
1	A	2875	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3155	HIS
1	A	3631	ASN
1	A	3952	GLN
1	A	1867	ASN
1	A	1541	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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$
2	ADP	A	4701	-	24,29,29	0.88	0	29,45,45	1.24	2 (6%)
3	ATP	A	4702	-	28,33,33	0.65	0	34,52,52	0.59	1 (2%)
2	ADP	A	4704	-	24,29,29	0.87	0	29,45,45	1.24	2 (6%)
3	ATP	A	4703	-	28,33,33	0.67	0	34,52,52	0.60	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	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4702	-	-	7/18/38/38	0/3/3/3
2	ADP	A	4704	-	-	3/12/32/32	0/3/3/3
3	ATP	A	4703	-	-	5/18/38/38	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	4701	ADP	N3-C2-N1	-3.68	123.68	128.67
2	A	4704	ADP	N3-C2-N1	-3.58	123.81	128.67
2	A	4704	ADP	C4-C5-N7	-2.63	106.56	109.34
2	A	4701	ADP	C4-C5-N7	-2.55	106.64	109.34
3	A	4702	ATP	C5-C6-N6	2.31	123.83	120.31

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

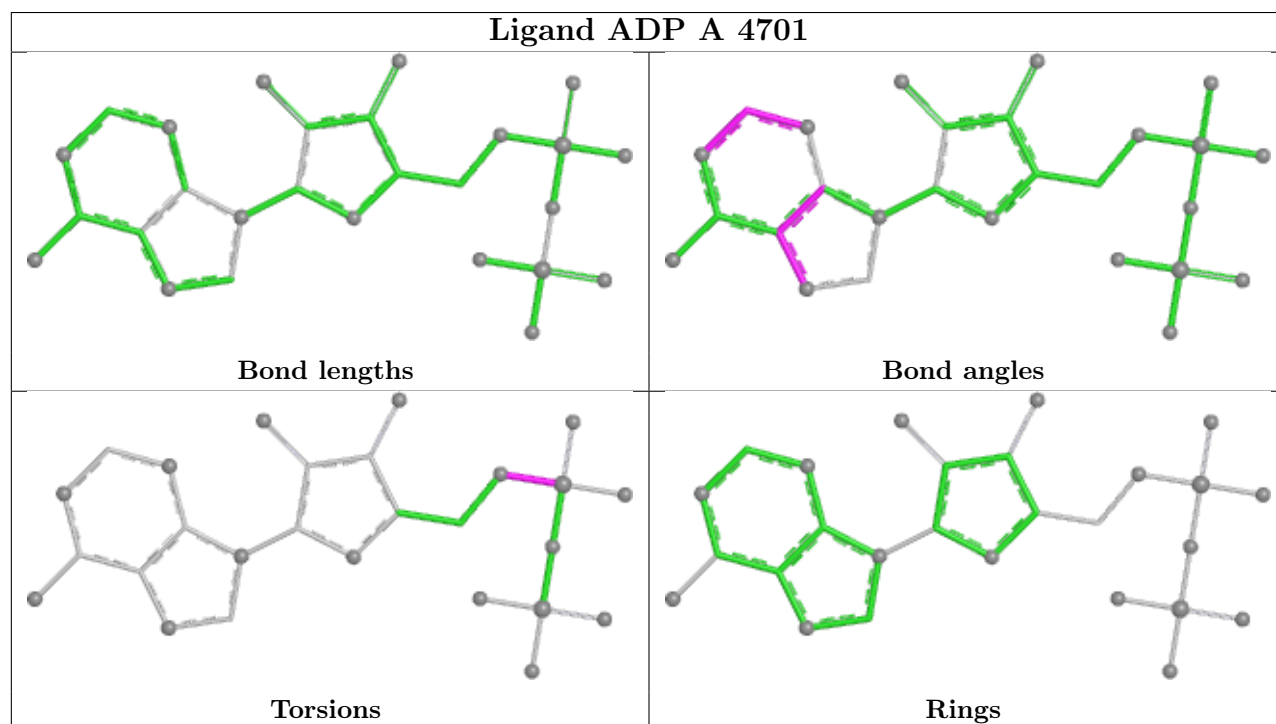
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	O4'-C4'-C5'-O5'

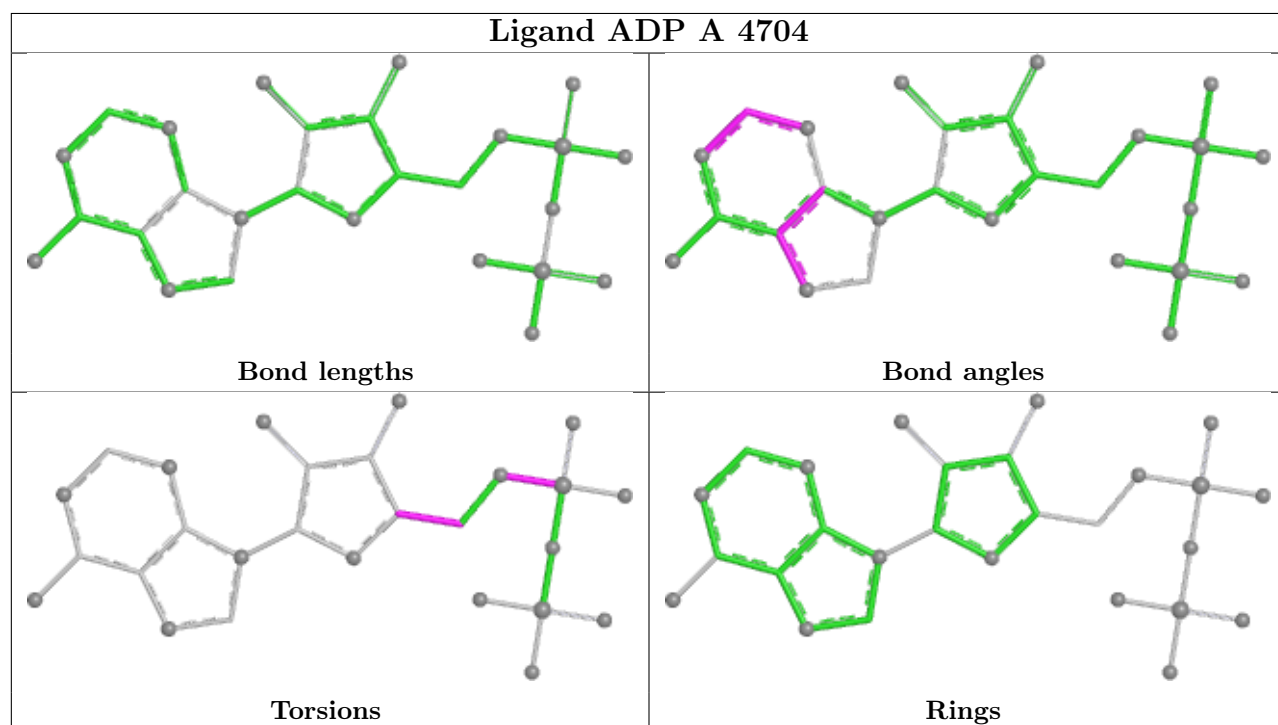
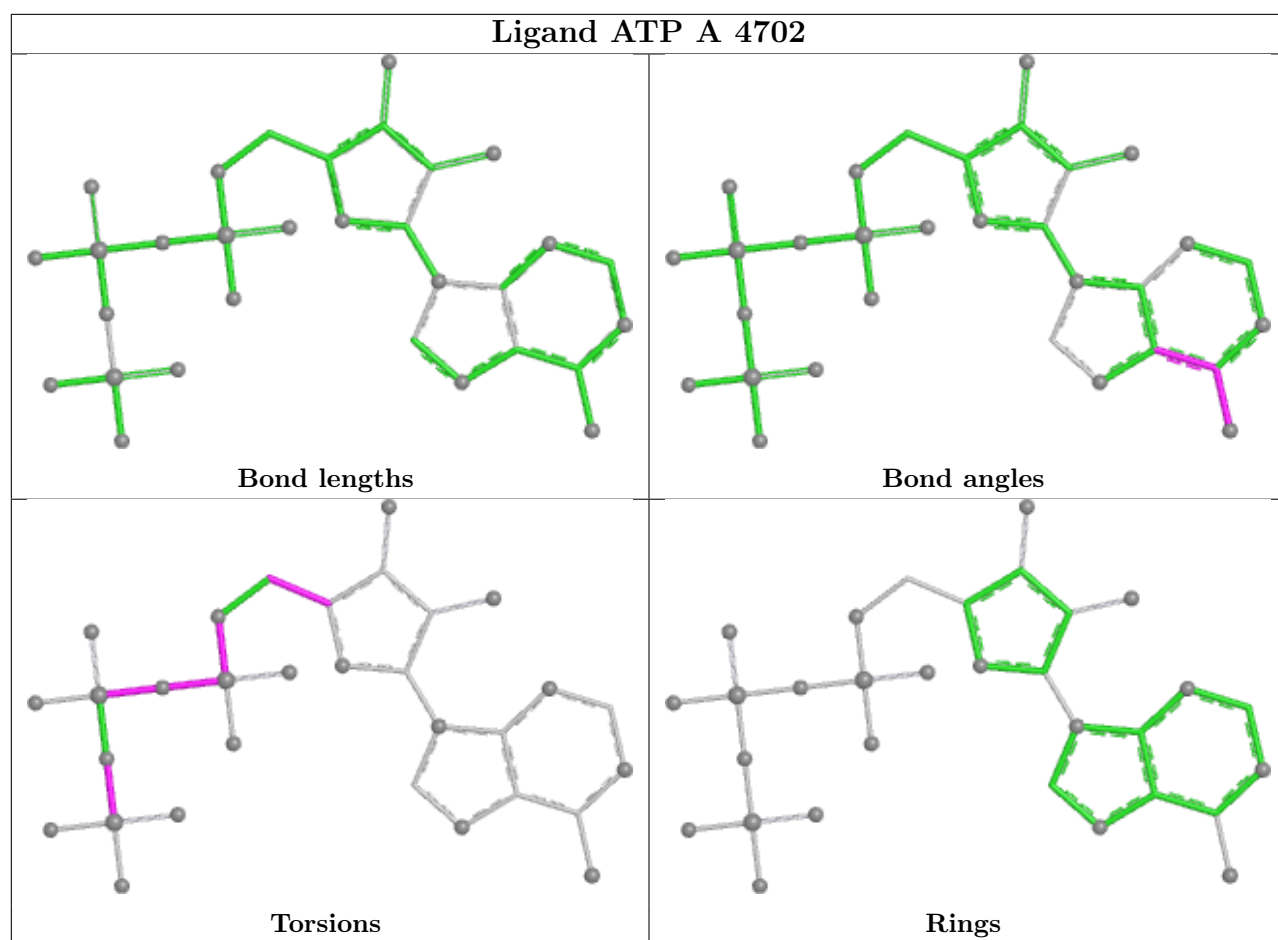
There are no ring outliers.

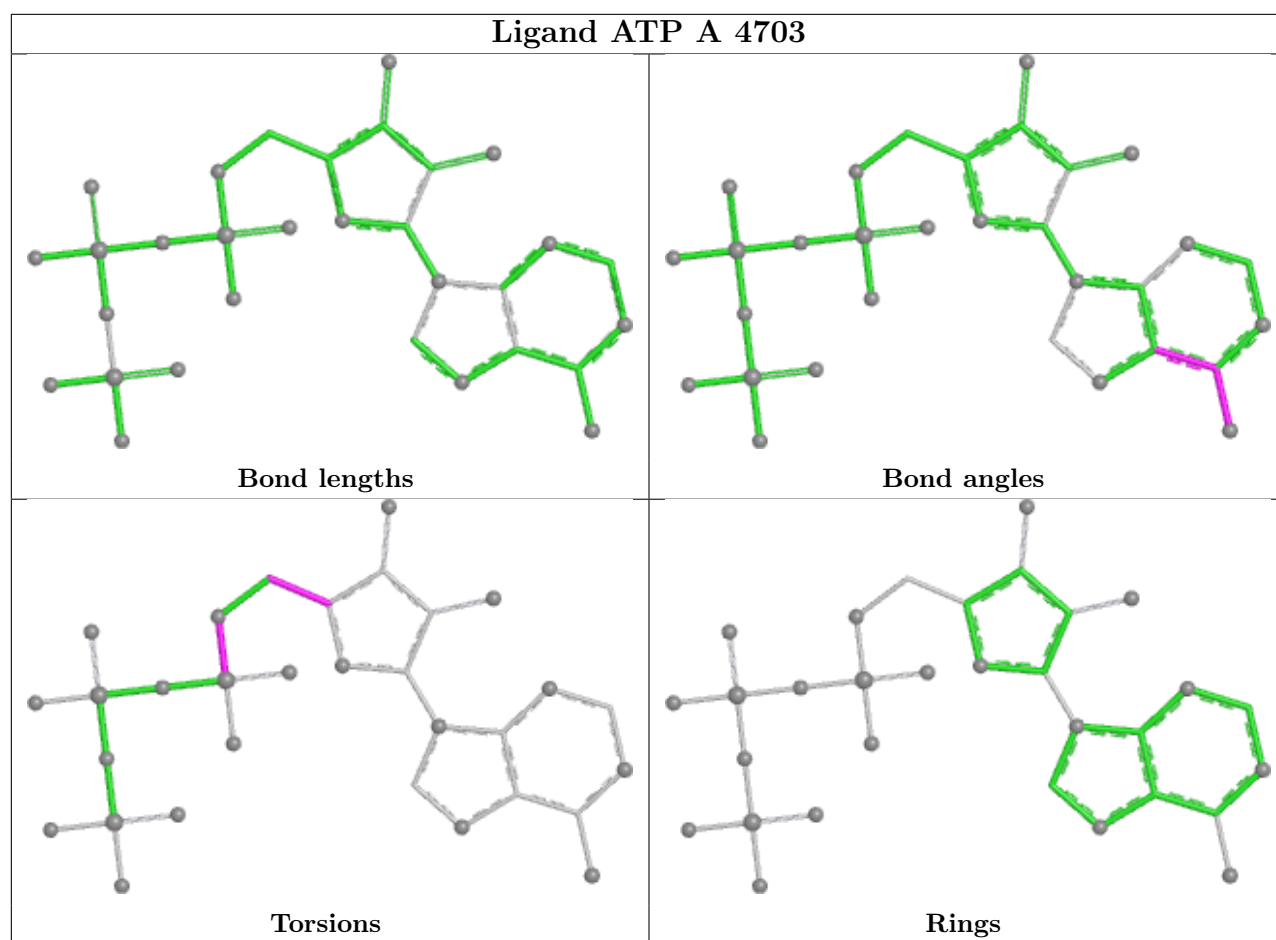
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4701	ADP	1	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.

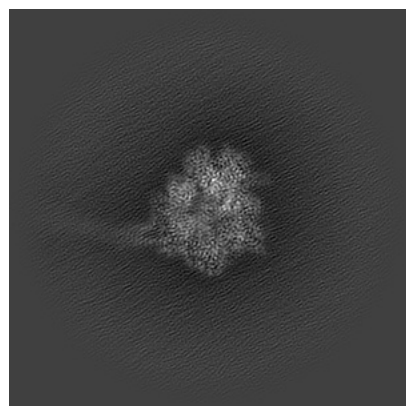
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44721. These allow visual inspection of the internal detail of the map and identification of artifacts.

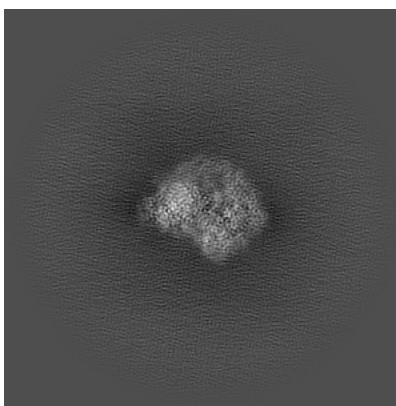
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

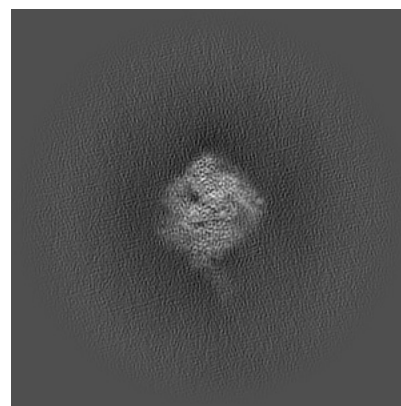
6.1.1 Primary map



X

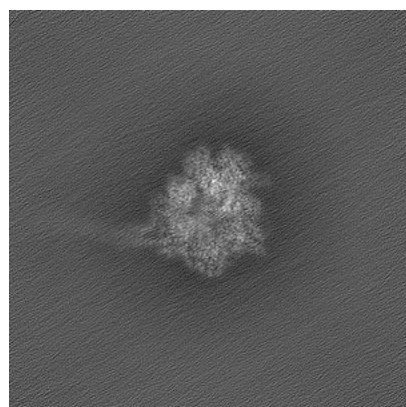


Y

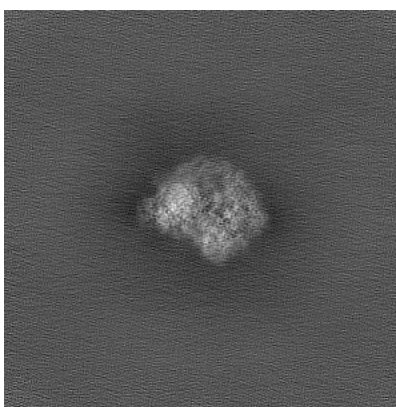


Z

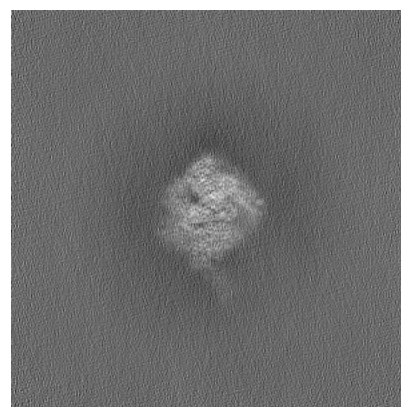
6.1.2 Raw map



X



Y

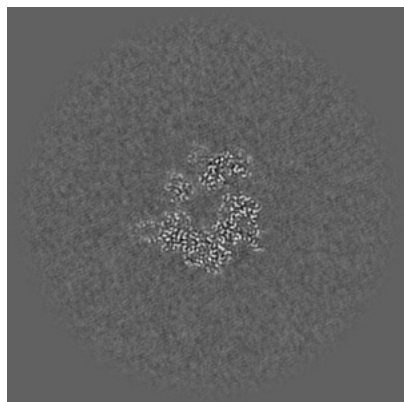


Z

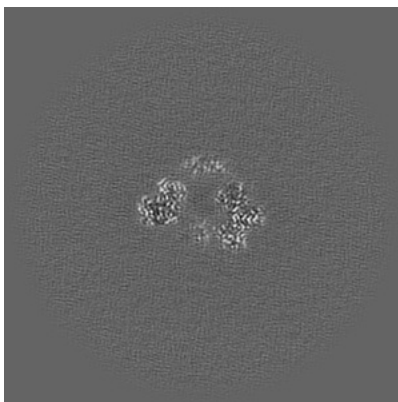
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

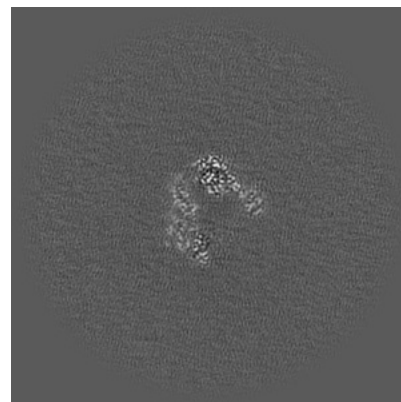
6.2.1 Primary map



X Index: 180

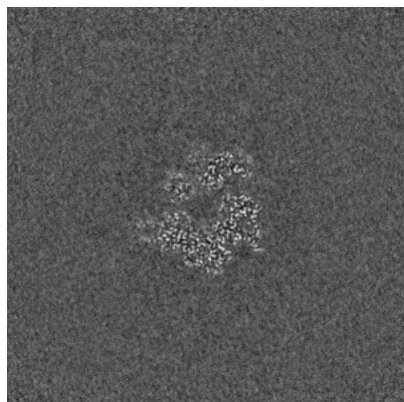


Y Index: 180

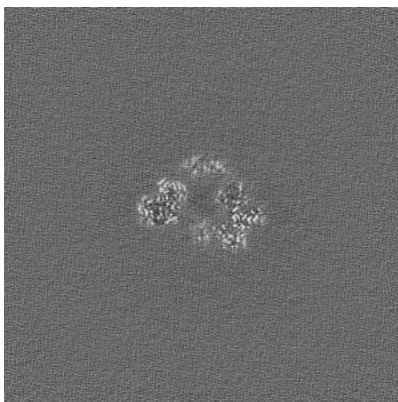


Z Index: 180

6.2.2 Raw map



X Index: 180



Y Index: 180

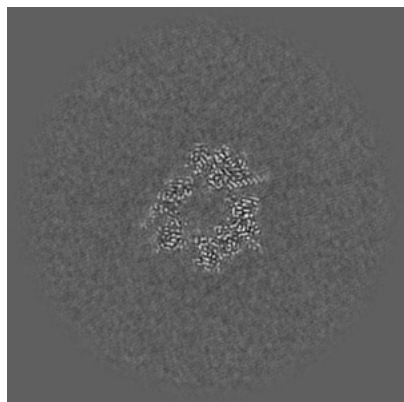


Z Index: 180

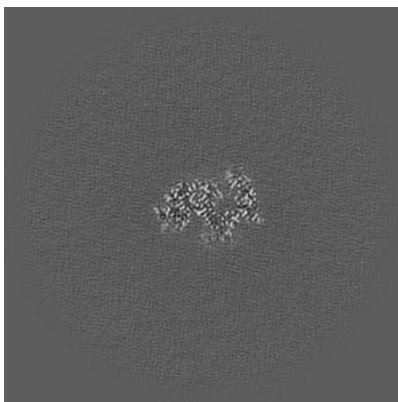
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

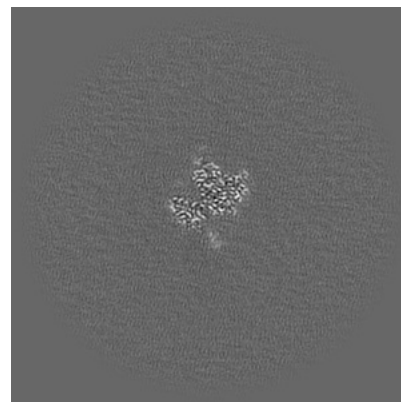
6.3.1 Primary map



X Index: 175

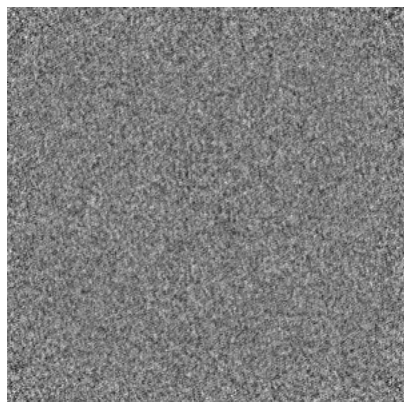


Y Index: 203

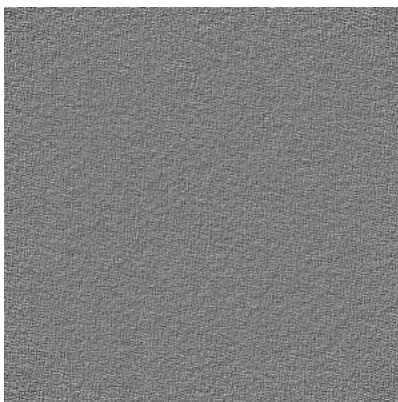


Z Index: 209

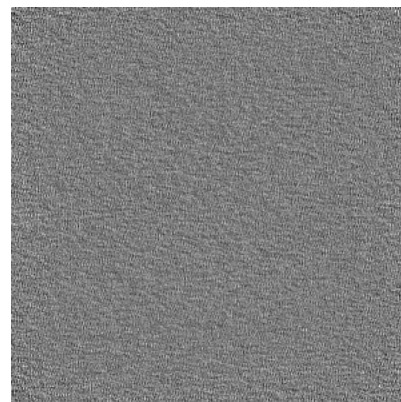
6.3.2 Raw map



X Index: 0



Y Index: 0

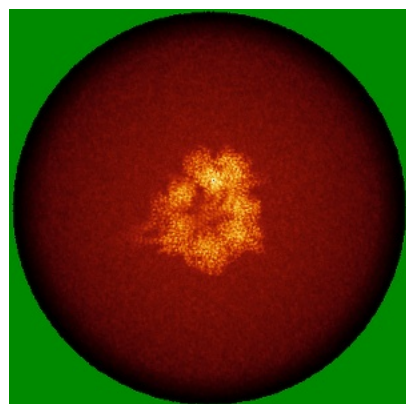


Z Index: 0

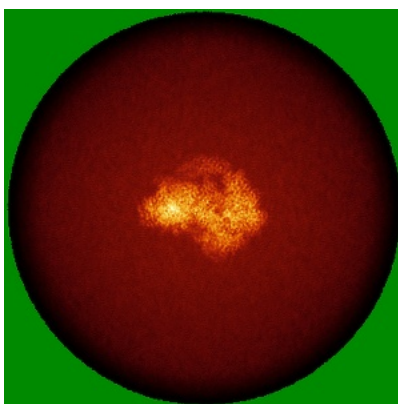
The images above show the largest variance slices of the map in three orthogonal directions.

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

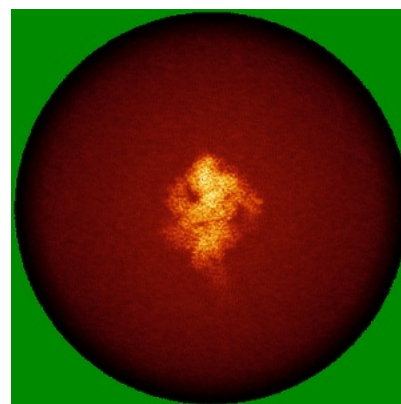
6.4.1 Primary map



X

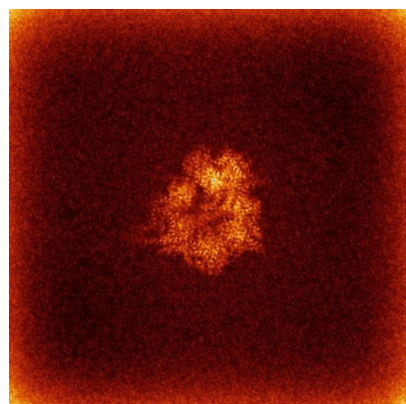


Y

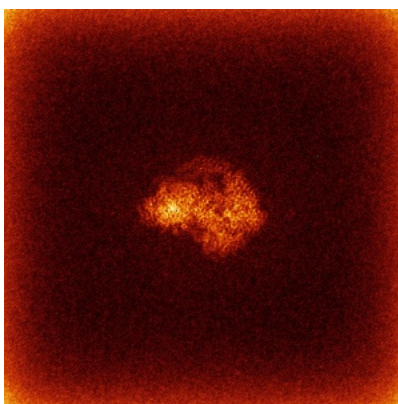


Z

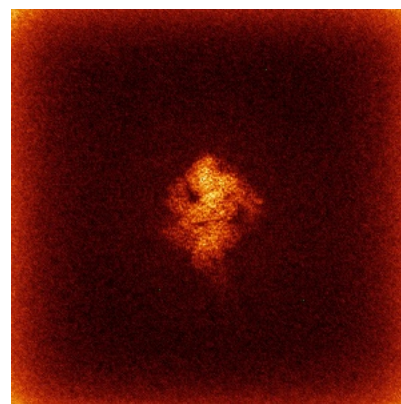
6.4.2 Raw map



X



Y

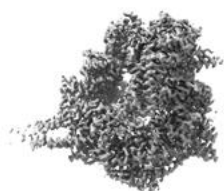


Z

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



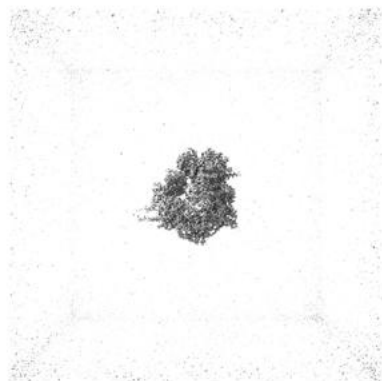
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

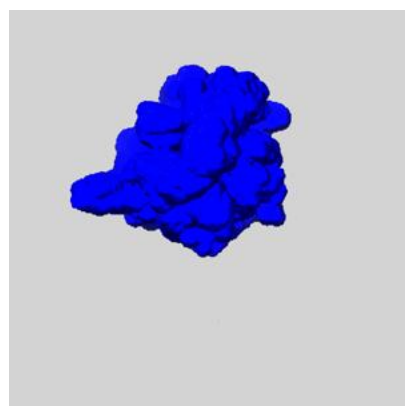
6.6 Mask visualisation [i](#)

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

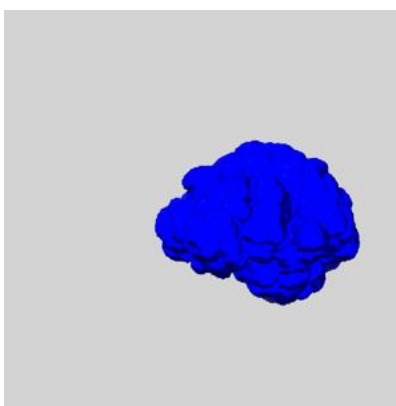
A mask typically either:

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

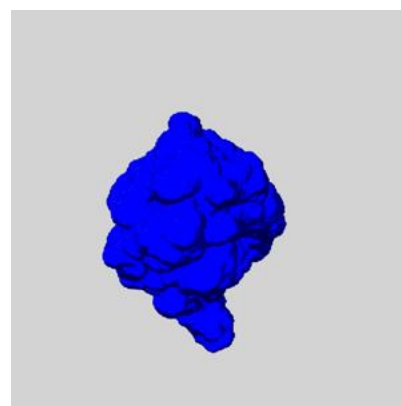
6.6.1 emd_44721_msk_1.map [i](#)



X



Y

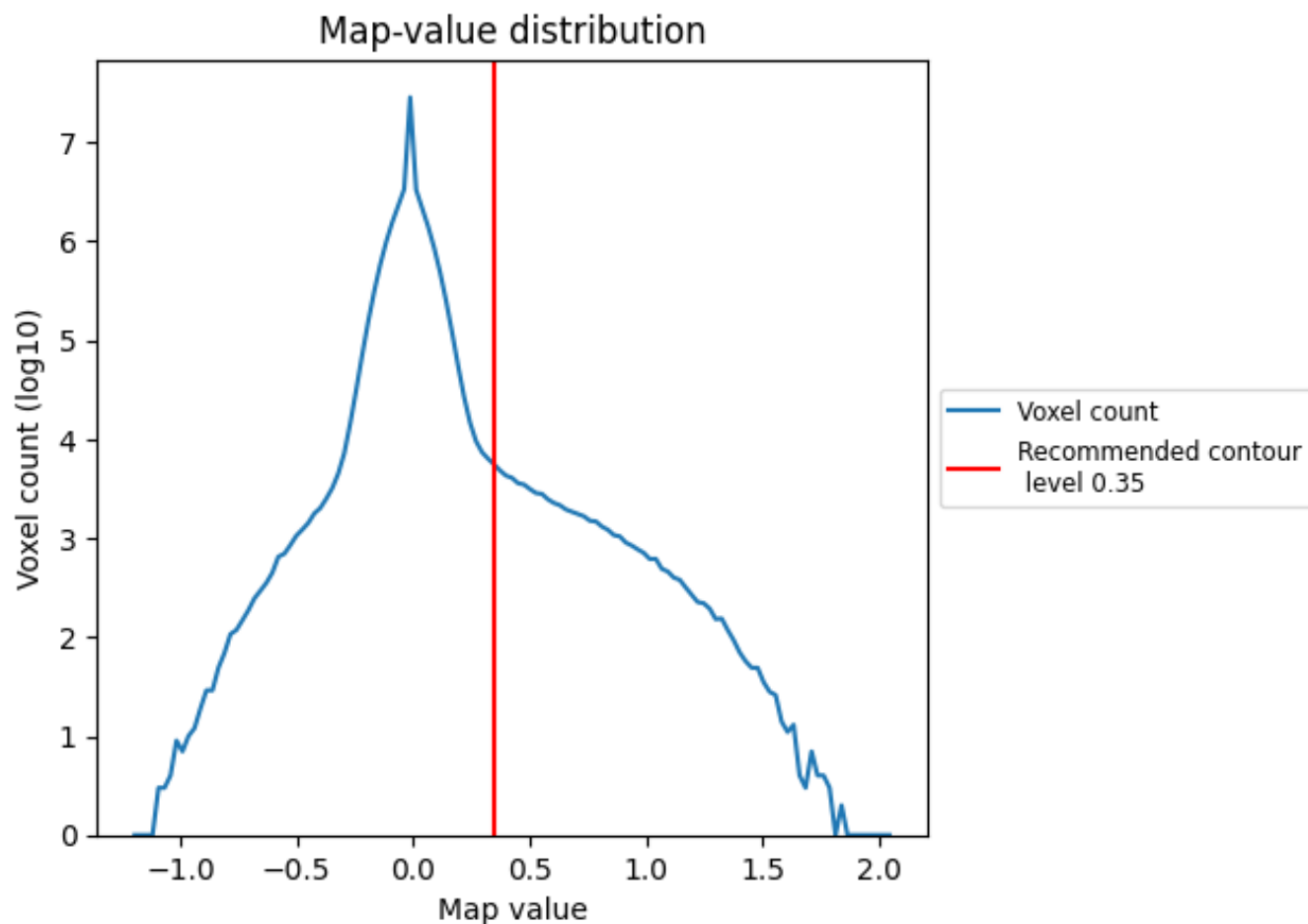


Z

7 Map analysis [i](#)

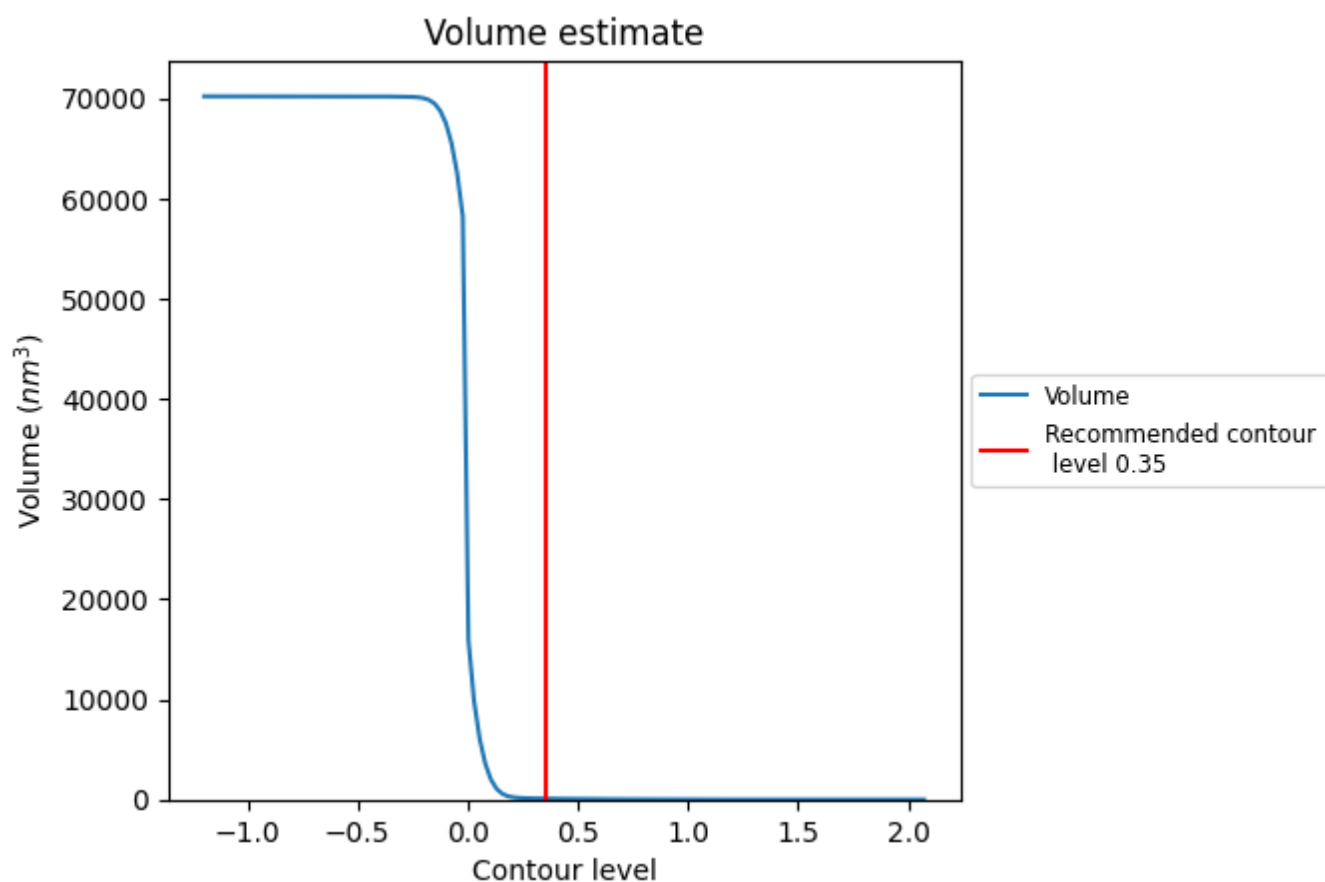
This section contains the results of statistical analysis of the map.

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.

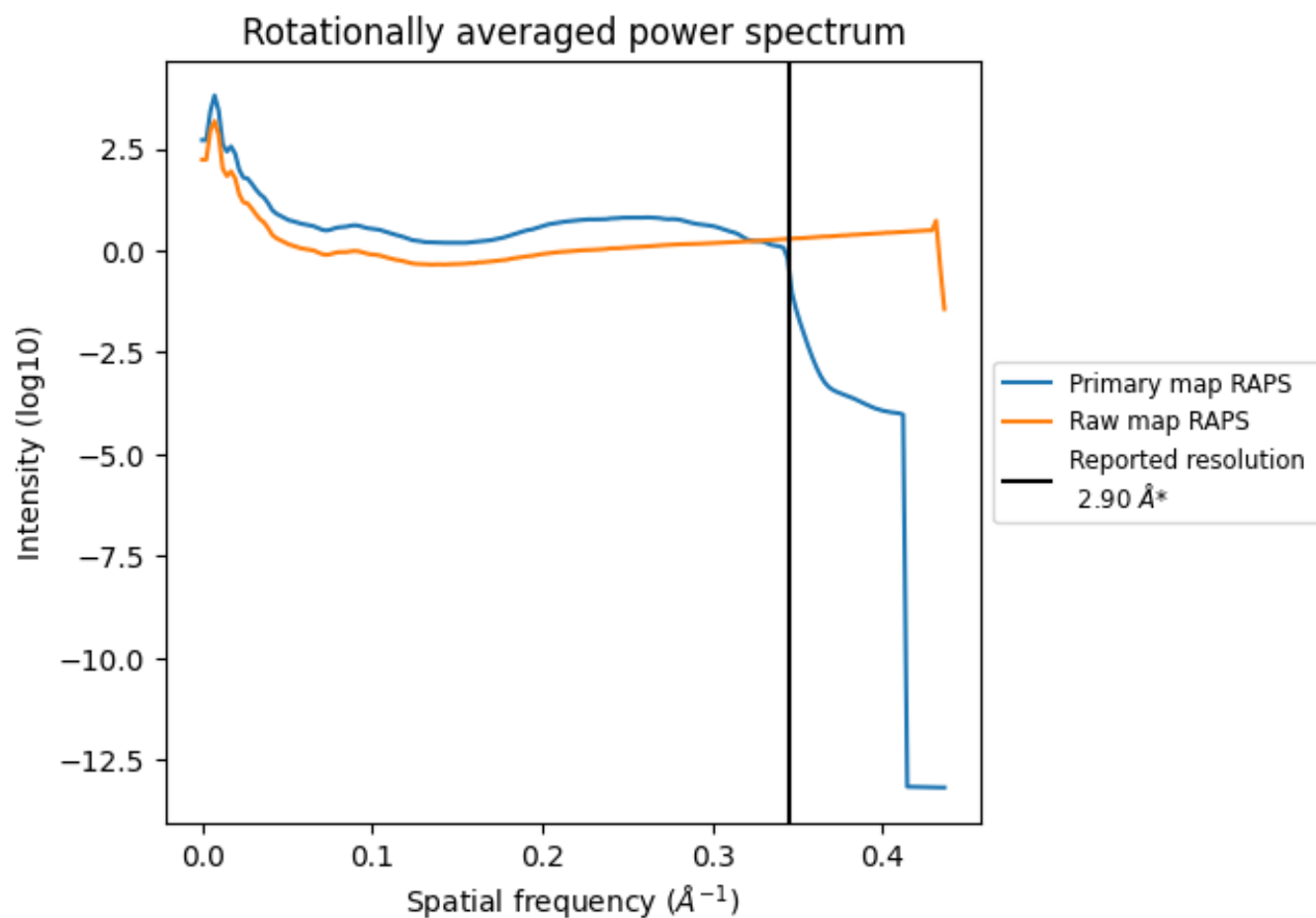
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm³; this corresponds to an approximate mass of 87 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 ⓘ

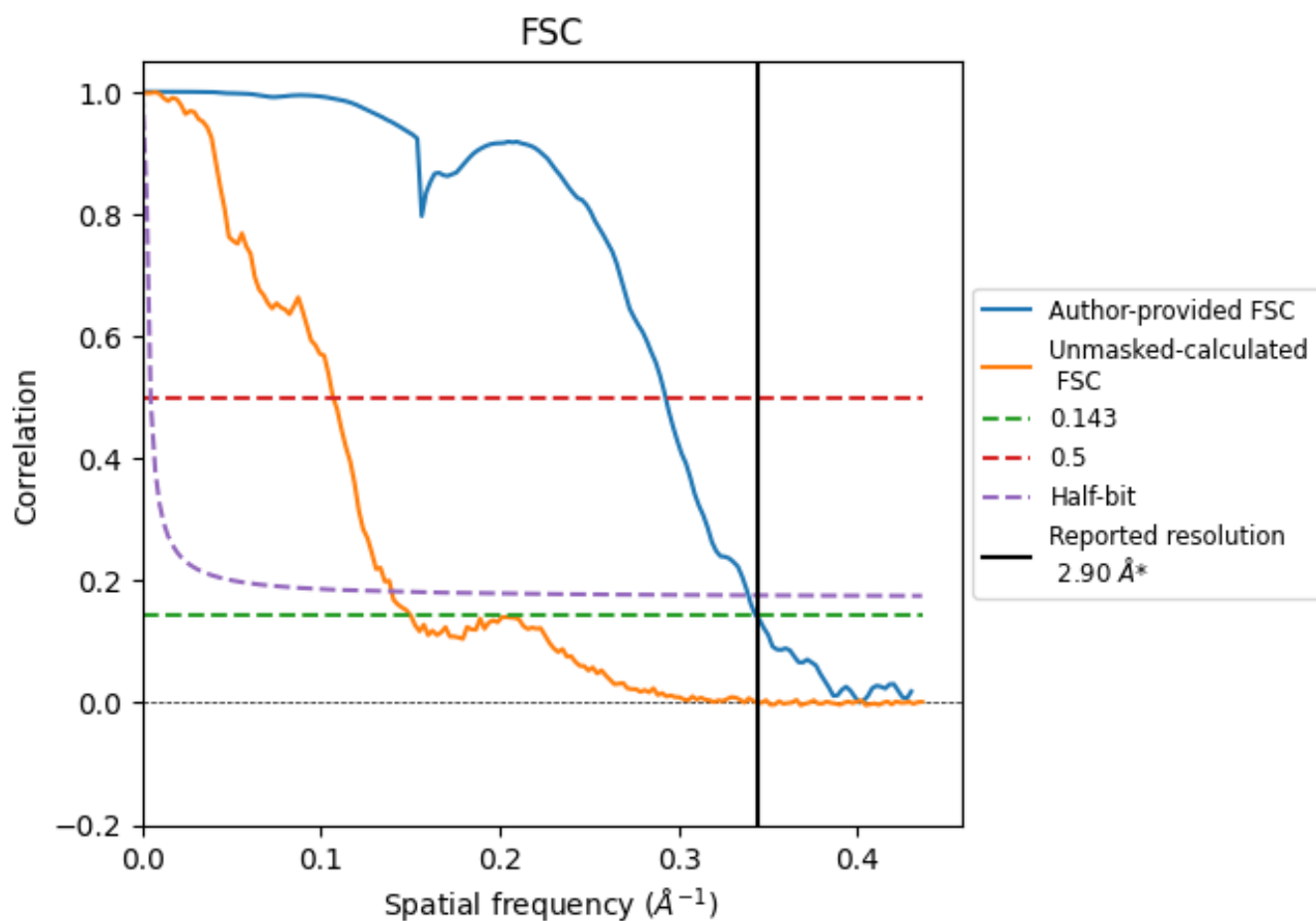


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

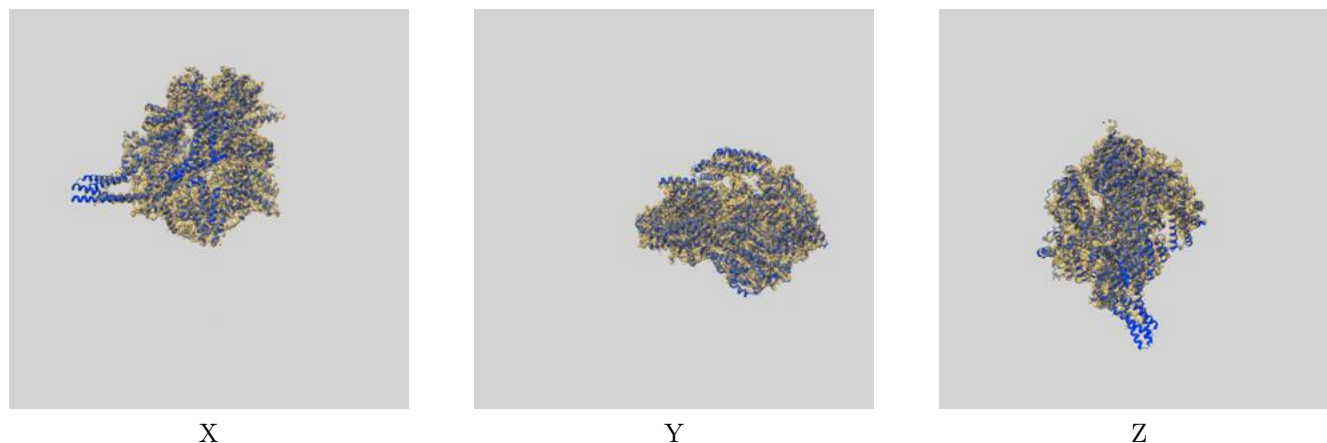
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.42	2.95
Unmasked-calculated*	6.66	9.37	7.16

*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 6.66 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

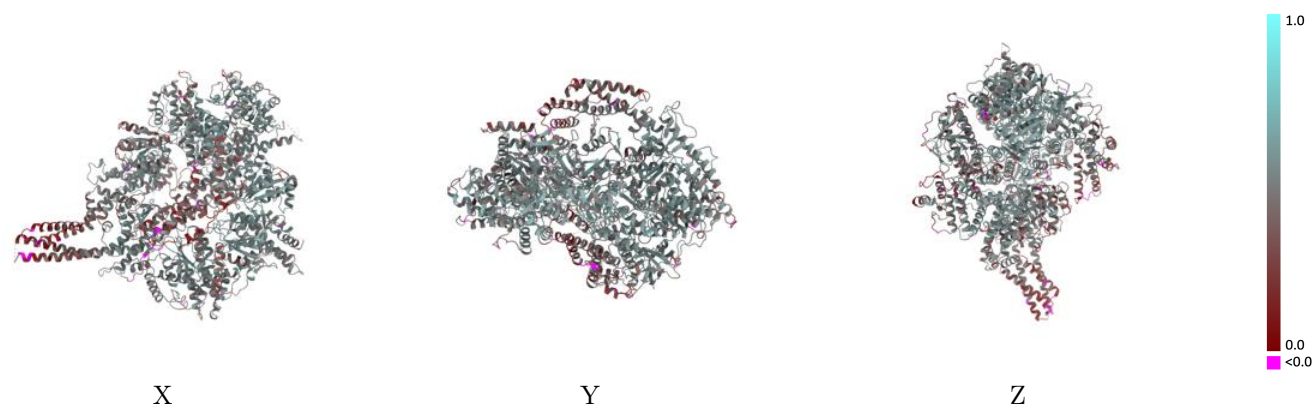
This section contains information regarding the fit between EMDB map EMD-44721 and PDB model 9BN4. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



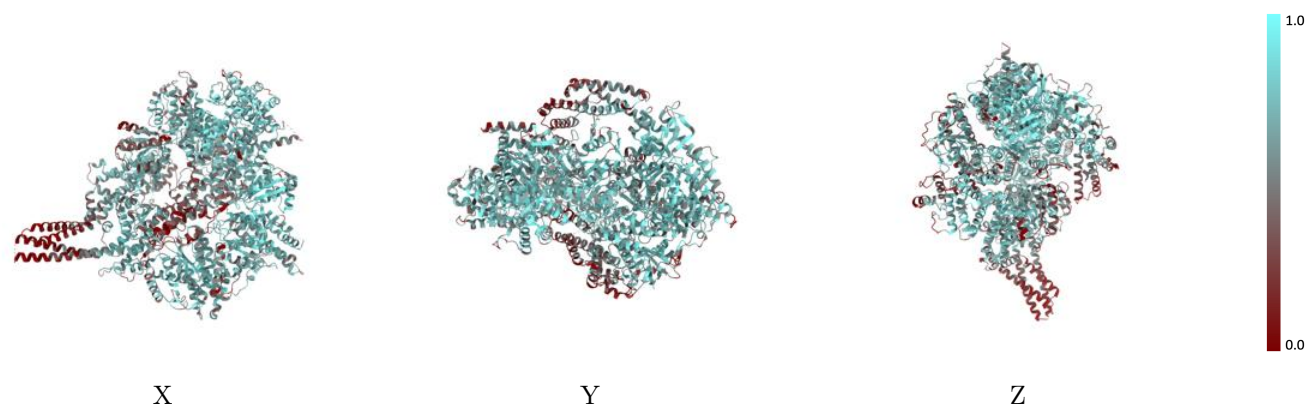
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



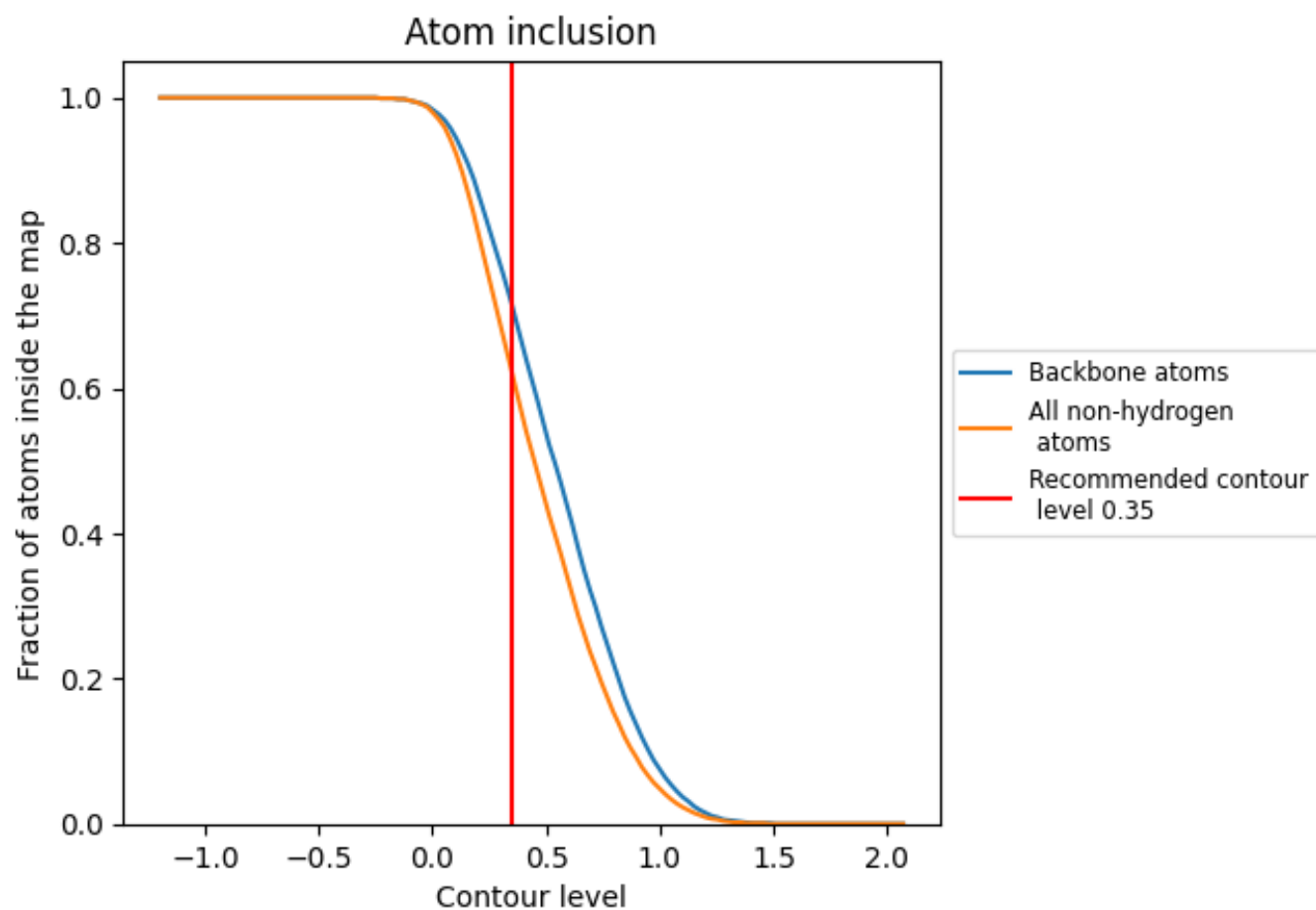
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 62% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6220	<div></div> 0.4680
A	<div></div> 0.6220	<div></div> 0.4680

