



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 01:10 AM UTC

PDB ID : 9BN3 / pdb_00009bn3
EMDB ID : EMD-44720
Title : The alpha registry-locked dynein motor domain mutant in 5mM ATP condition, class1
Authors : Chai, P.; Zhang, K.
Deposited on : 2024-05-02
Resolution : 2.80 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

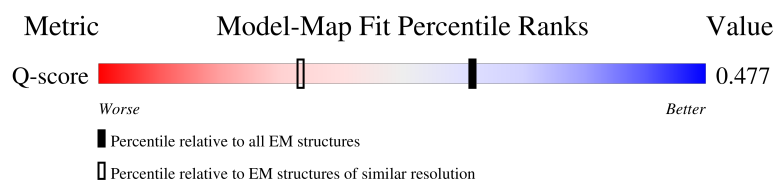
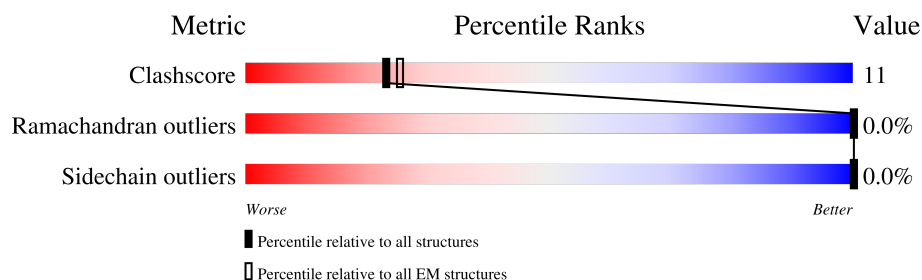
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23152 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.

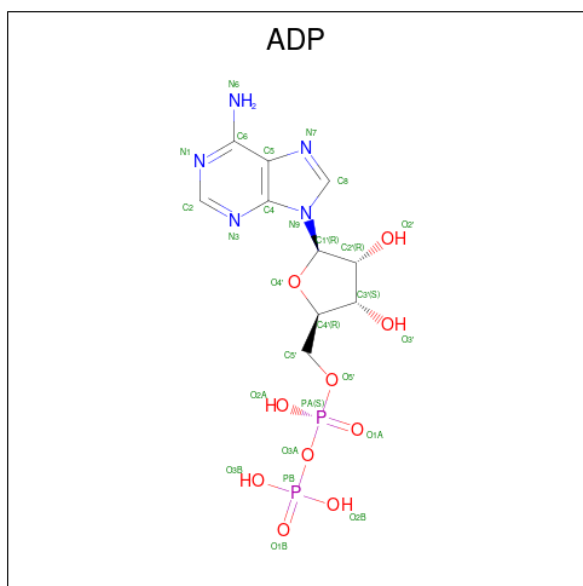
- Molecule 1 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	2866	23040	14688	3978	4259	115	0	0

There is a discrepancy between the modelled and reference sequences:

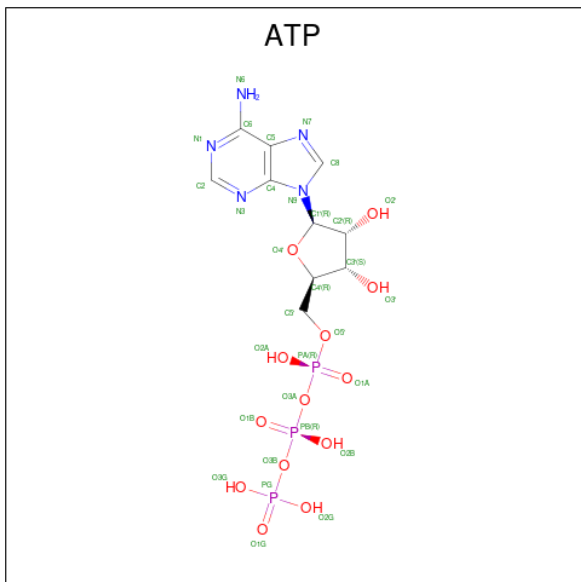
Chain	Residue	Modelled	Actual	Comment	Reference
A	2389	ASP	GLU	conflict	UNP Q14204

- 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
			Total	C	N	O	P	
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0
2	A	1	27	10	5	10	2	0

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

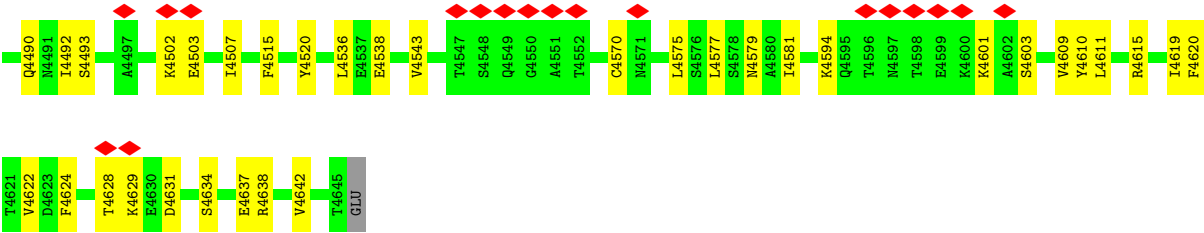


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	31	10	5	13	3	0



ARG	P3137	K3050	K2966	D2862	L2759	Q2654	Q2554	Q2424	V2345	E2242	GLU	K2007
ILE	S3138	Y3051	E2970	R2863	L2762	L2655	D2566	F2427	Q2346	R2243	GLU	K2018
LYS	R3139	K3052	E2971	E2864	A2766	V2660	V2569	T2428	Y2350	E2245	ARG	M2019
GLN	R3140	K3053	D2971	K2865	A2766	L2661	R2576	S2429	A2351	E2246	GLY	PRO
GLY	E3141	F3054	L2976	A2866	T2770	F2662	H2577	N2430	L2353	V2247	ALA	GLY
LEU	V3144	T3055	L2976	M2867	T2770	C2663	R2576	N2430	A2354	E2248	VAL	TYR
GLU	V3145	I3059	V2979	S2868	M2773	D2664	R2576	L2437	L2355	K2261	ASP	ALA
VAL	S3146	F3066	L2980	R2869	V2774	E2665	H2577	F2438	V2356	Y2265	GLY	ALA
ASN	C3147	T3067	R2981	P2870	V2774	E2665	L2581	H2439	R2357	D2265	SER	ARG
ALA	V3148	M3068	R2981	L2871	R2783	L2668	L2581	A2440	R2358	D2266	ASN	ASN
ALA	H3151	N3069	K2986	S2878	R2783	P2669	V2584	F2441	M2361	D2269	L2028	L2034
ASP	Q3152	P3070	N2987	K2879	T2785	D2670	V2584	Q2442	N2130	P2270	L2131	L2035
LYS	L3153	S3071	E2988	D2880	Q2786	M2671	L2592	Q2442	P2132	R2273	P2132	F2036
LYS	L3154	S3072	K2988	D2880	Q2786	K2673	L2592	H2445	E2133	D2277	R2133	R2037
LEU	H3155	S3073	D2995	D2885	L2802	F2682	L2593	L2449	V2368	F2280	Q2134	S2038
LYS	Q3156	G3074	E2996	Q2886	V2802	F2682	L2593	R2451	L2369	K2286	E2135	L2039
LYS	A3157	G3074	E2997	E2887	L2806	M2686	P2596	C2454	S2370	V2291	L2138	P2044
LYS	N3158	L3075	S2997	E2887	L2806	M2686	P2596	C2454	T2371	R2292	E2152	R2046
MET	N3158	L3075	S2997	E2887	L2806	M2686	P2596	C2454	T2371	R2292	D2153	F2059
VAL	K3163	K3076	N2998	R2890	A2809	D2697	L2605	S2457	L2374	V2291	L2160	L2065
LYS	R3164	R3077	L3000	K2894	L2810	D2697	L2605	L2458	N2377	R2292	L2161	A2066
GLN	M3169	R3078	D3001	K2898	L2816	K2702	R2610	L2462	L2382	G2293	L2161	L2067
GLN	A3079	A3080	F3004	E2903	P2817	L2703	P2613	R2467	R2383	L2295	V2164	K2068
ALA	T3172	T3081	K3005	E2904	V2818	E2704	D2614	R2468	L2389	Q2296	F2165	L2069
GLY	Y3176	A3084	E3006	L2905	G2820	R2705	D2615	V2469	L2389	W2300	R2179	V2070
LYS	L3085	F3086	M3008	D2906	L2821	Q2707	E2616	A2470	D2389	D2306	ASP	F2071
LYS	F3086	N3087	G3015	V2910	T2822	F2708	V2617	Q2471	GLY	V2307	L2188	L2075
VAL	L3193	N3092	F3021	N2913	R2720	S2623	P2622	Y2472	GLU	D2307	D2195	Q2079
MET	E3195	K3093	E3022	N2913	K2721	S2624	S2623	D2478	ALA	D2308	D2195	Q2079
GLN	Q3197	F3094	G3023	T2922	R2726	A2625	T2626	M2481	GLN	P2309	E2205	Y2086
ILE	Q3198	G3095	G3023	D2923	R2726	T2627	T2627	Q2485	ARG	F2310	L2208	L2090
GLN	M3199	G3095	G3023	R2924	V2731	E2628	E2628	R2488	LYS	W2311	Q2209	L2093
GLN	L3200	D3096	E3025	L2925	P2732	E2629	L2630	L2498	LYS	V2312	L2210	L2097
LEU	N3202	A3101	Y3026	Q2928	V2733	E2629	L2630	L2498	GLY	E2313	L2213	G2101
HIS	G3203	V3105	L3029	Q2928	V2733	E2629	L2630	L2498	ASP	E2314	L2213	L2093
LYS	G3204	M3113	M3030	P2929	V2734	E2629	L2630	L2498	GLY	D2320	L2220	L2097
GLN	L3205	M3113	M3030	P2929	V2734	E2629	L2630	L2498	GLY	M2221	G2227	K2104
GLY	K3207	M3113	M3030	P2929	V2734	E2629	L2630	L2498	GLY	S2226	K2227	K2105
VAL	K3207	M3113	M3030	P2929	V2734	E2629	L2630	L2498	GLY	S2226	K2227	K2105
ILE	K3209	M3119	K3032	L2933	R2844	T2845	E2640	P2527	ALA	G2330	K2230	E2106
ASP	E3210	P3123	C3032	L2933	R2844	T2845	E2640	P2527	ALA	E2331	K2230	E2106
LYS	T3211	D3124	C3033	L2935	R2844	T2845	E2640	P2527	ALA	E2331	K2230	E2106
GLN	V3212	Y3125	C3033	L2935	R2844	T2845	E2640	P2527	ALA	E2331	K2230	E2106
MET	Q3213	K3126	C3033	L2935	R2844	T2845	E2640	P2527	ALA	E2331	K2230	E2106
SER	D3213	P3127	C3033	L2935	R2844	T2845	E2640	P2527	ALA	E2331	K2230	E2106
VAL	Q3214	V3128	C3033	L2935	R2844	T2845	E2640	P2527	ALA	E2331	K2230	E2106
LYS	V3215	V3129	C3033	L2935	R2844	T2845	E2640	P2527	ALA	E2331	K2230	E2106
GLY	V3215	V3129	C3033	L2935	R2844	T2845	E2640	P2527	ALA	E2331	K2230	E2106
ASP	E3216	Y3130	E3040	L2961	R2763	L2756	E2646	Q2416	ALA	G2330	K2230	E2106
ASP	E3217	L3131	G3041	L2961	R2763	L2756	E2646	Q2416	ALA	E2331	K2230	E2106
LYS	R3218	K3132	L3042	K2962	R2757	L2756	E2646	Q2416	ALA	E2331	K2230	E2106
VAL	R3219	L3133	L3044	H2964	R2757	L2756	E2646	Q2416	ALA	E2331	K2230	E2106
LYS	R3220	P3134	D3045	R2965	R2757	L2756	E2646	Q2416	ALA	E2331	K2230	E2106
ASP	Q3135	Q3135	S3046	R2965	R2757	L2756	E2646	Q2416	ALA	E2331	K2230	E2106
LEU	LEU	P3136	E3048	R2965	R2757	L2756	E2646	Q2416	ALA	E2331	K2230	E2106
LEU	LEU	P3136	E3048	R2965	R2757	L2756	E2646	Q2416	ALA	E2331	K2230	E2106





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	433112	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	2.677	Depositor
Minimum map value	-1.892	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	412.488, 412.488, 412.488	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: ADP, ATP

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	0.15	1/23533 (0.0%)	0.36	4/31898 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3587	PRO	CG-CD	-5.96	1.30	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3587	PRO	N-CD-CG	-10.98	86.73	103.20
1	A	3587	PRO	CA-CB-CG	-8.66	88.05	104.50
1	A	3587	PRO	N-CA-CB	-6.07	98.07	103.35
1	A	3587	PRO	CA-N-CD	-5.47	104.34	112.00

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	23040	0	23108	513	0
2	A	81	0	36	0	0
3	A	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23152	0	23156	513	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 513 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	1.26	0.79
1:A:4043:MET:HB2	1:A:4127:THR:HA	1.63	0.79
1:A:1511:PRO:HG3	1:A:3628:ARG:HE	1.47	0.78
1:A:3209:LYS:HG3	1:A:3486:ARG:HH21	1.48	0.78
1:A:3137:PRO:HB3	1:A:3141:GLU:HB2	1.66	0.77

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	2854/4646 (61%)	2750 (96%)	103 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4172	SER

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	2548/4125 (62%)	2547 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
1	A	4029	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2689	HIS
1	A	4326	ASN
1	A	3200	HIS
1	A	3880	HIS
1	A	3182	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	$\# Z > 2$
2	ADP	A	4703	-	28,29,29	1.41	4 (14%)	43,45,45	1.81	9 (20%)
3	ATP	A	4702	-	32,33,33	0.34	0	48,52,52	0.31	0
2	ADP	A	4704	-	28,29,29	1.39	4 (14%)	43,45,45	1.82	10 (23%)
2	ADP	A	4701	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)

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	4703	-	-	3/16/32/32	0/3/3/3
3	ATP	A	4702	-	-	5/22/38/38	0/3/3/3
2	ADP	A	4704	-	-	3/16/32/32	0/3/3/3
2	ADP	A	4701	-	-	3/16/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4703	ADP	C5-C4	4.67	1.47	1.39
2	A	4701	ADP	C5-C4	4.61	1.47	1.39
2	A	4704	ADP	C5-C4	4.60	1.47	1.39
2	A	4701	ADP	C5-C6	2.71	1.48	1.41
2	A	4703	ADP	C5-C6	2.62	1.48	1.41

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4701	ADP	C5-C4-N3	-5.69	118.89	126.72
2	A	4704	ADP	C5-C4-N3	-5.65	118.94	126.72
2	A	4703	ADP	C5-C4-N3	-5.64	118.95	126.72
2	A	4703	ADP	N3-C4-N9	4.51	134.84	127.17
2	A	4704	ADP	N3-C4-N9	4.48	134.79	127.17

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

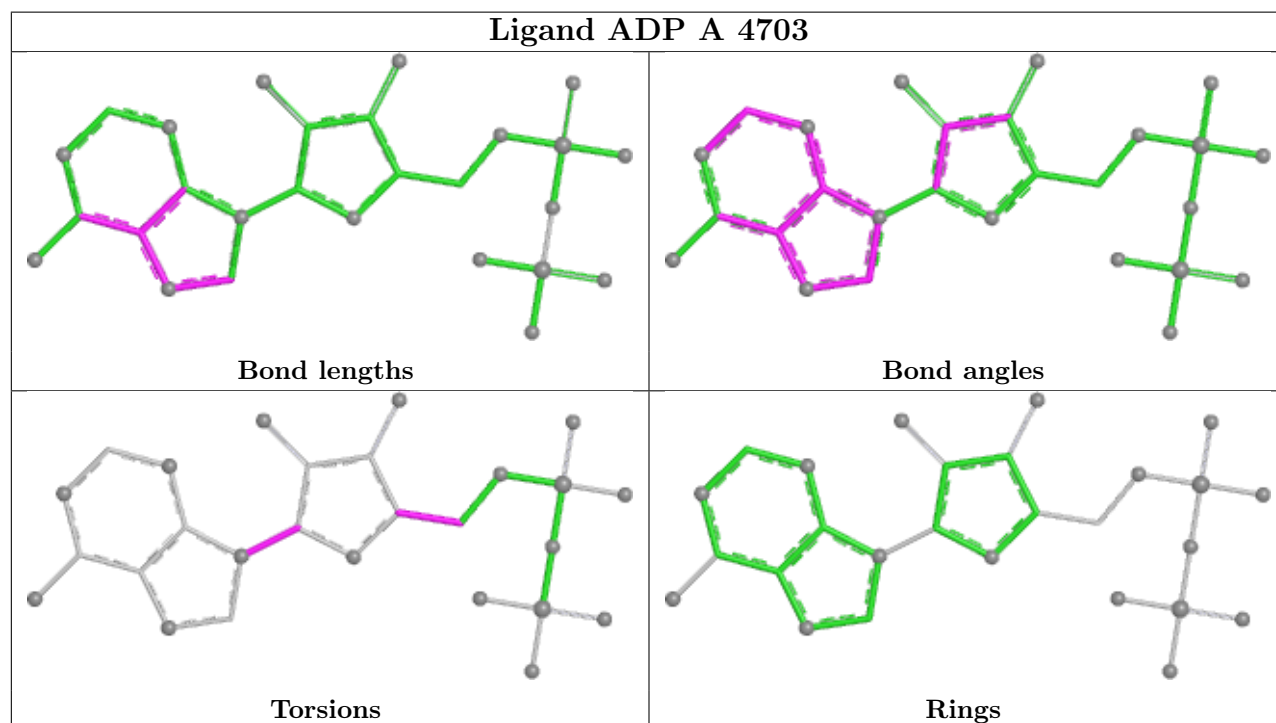
Mol	Chain	Res	Type	Atoms
2	A	4701	ADP	C5'-O5'-PA-O1A
2	A	4701	ADP	C5'-O5'-PA-O2A
2	A	4701	ADP	C5'-O5'-PA-O3A
2	A	4704	ADP	C5'-O5'-PA-O1A
2	A	4704	ADP	O4'-C4'-C5'-O5'

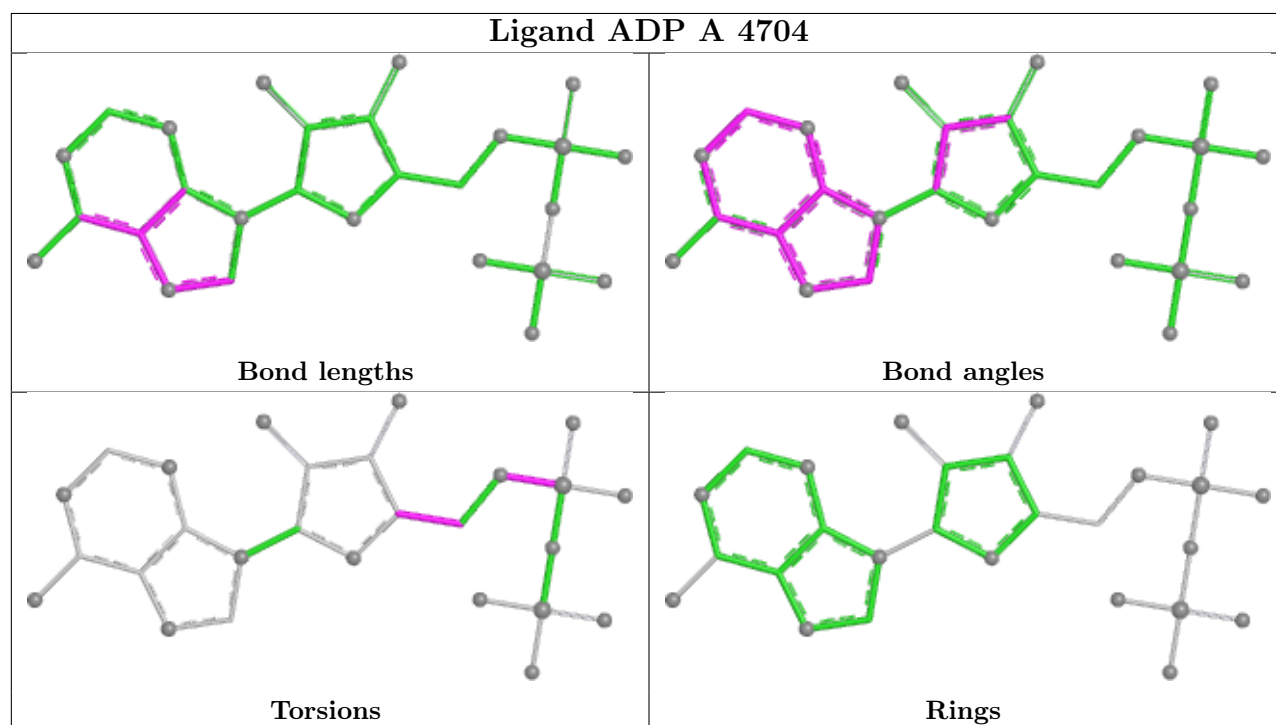
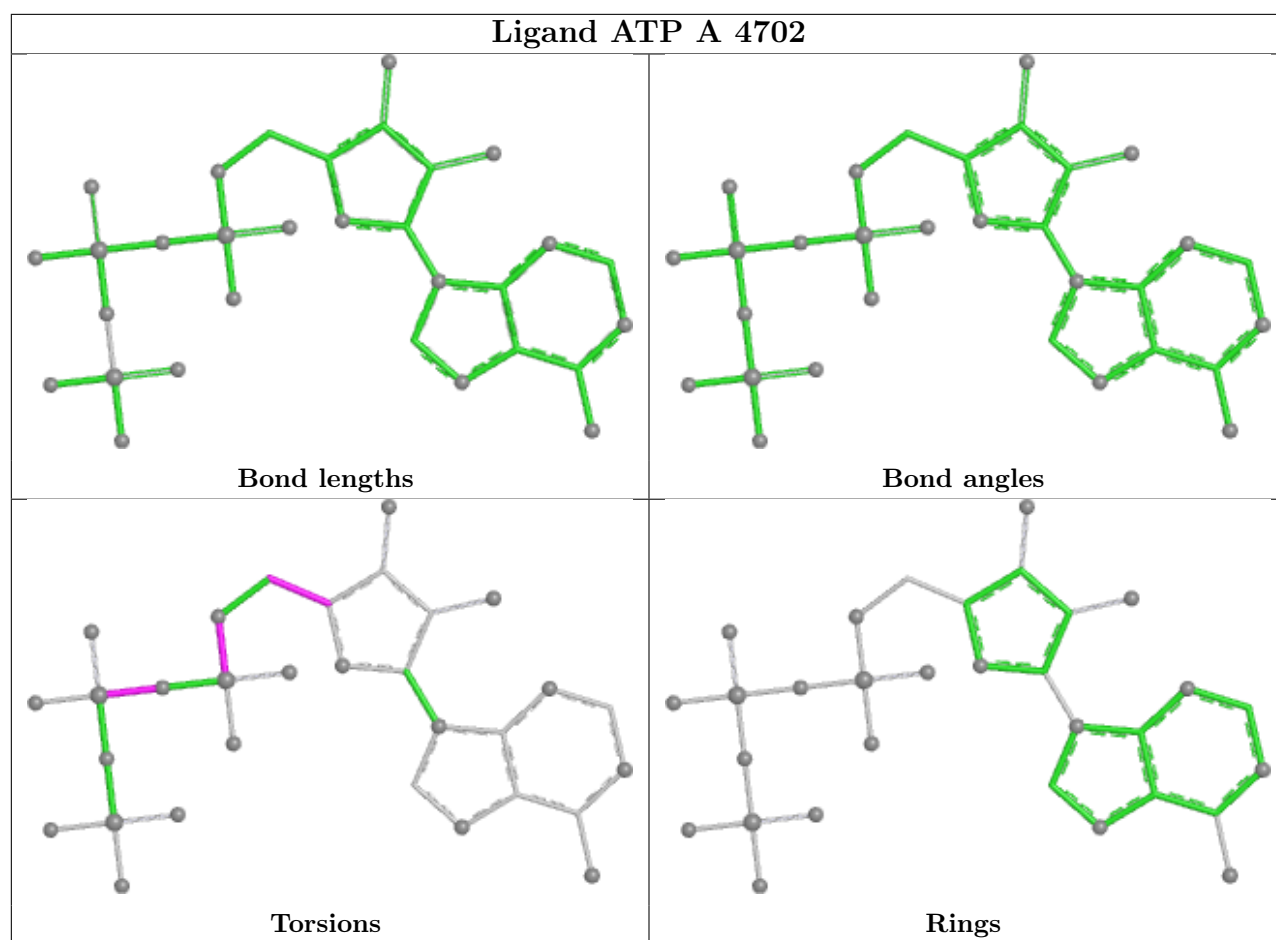
There are no ring outliers.

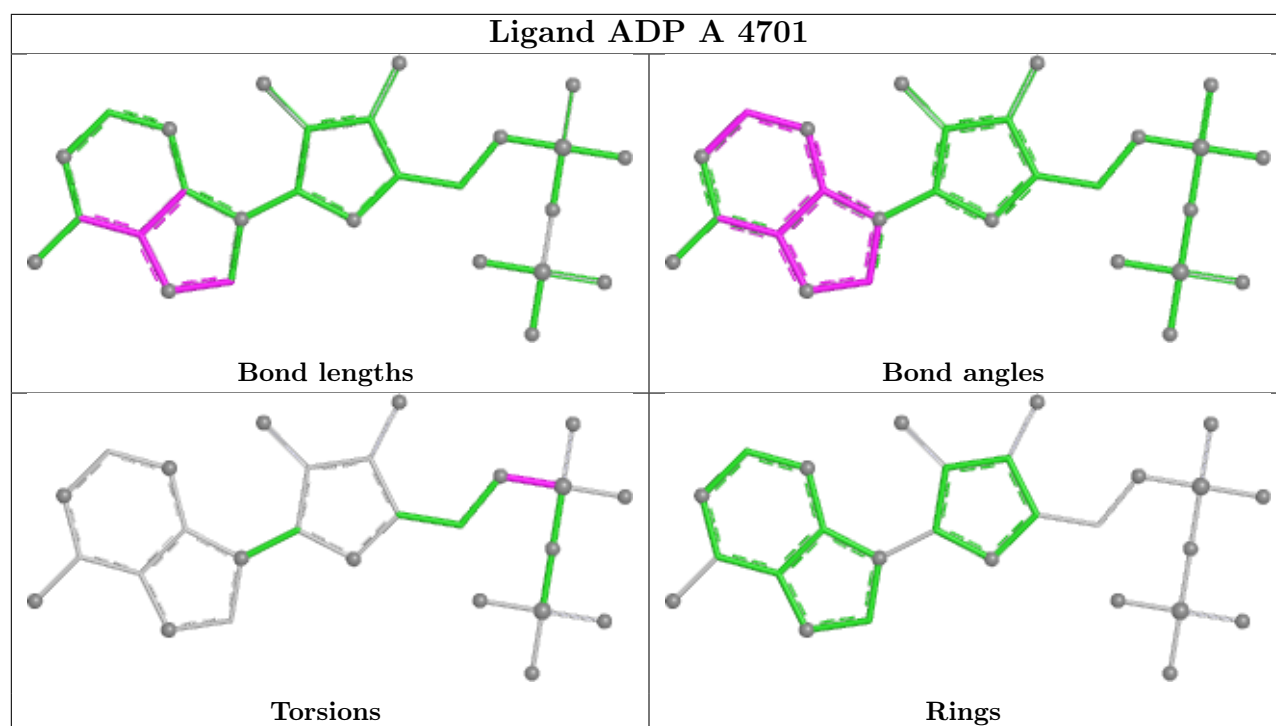
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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.

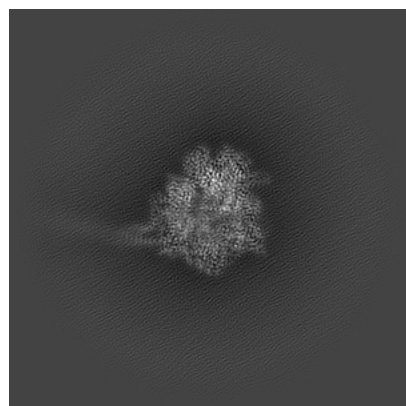
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44720. These allow visual inspection of the internal detail of the map and identification of artifacts.

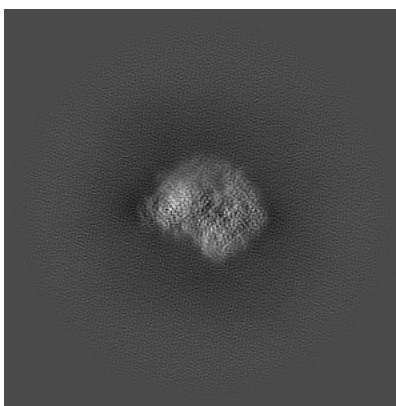
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

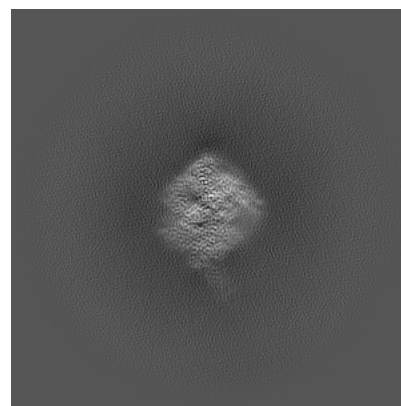
6.1.1 Primary map



X

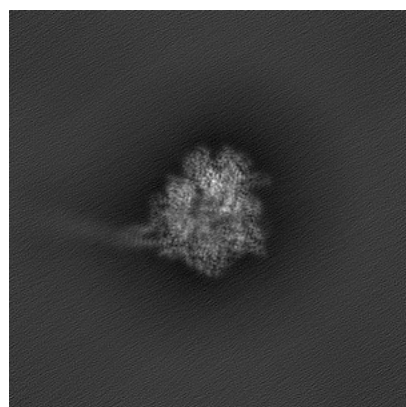


Y

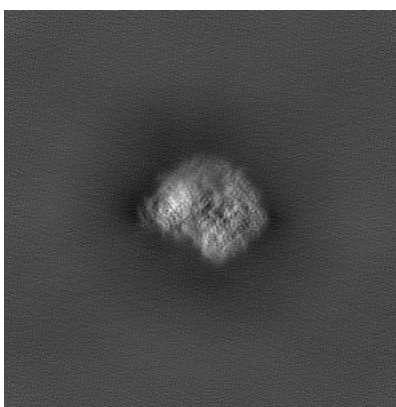


Z

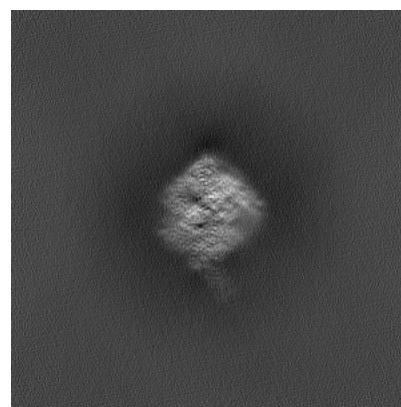
6.1.2 Raw map



X



Y

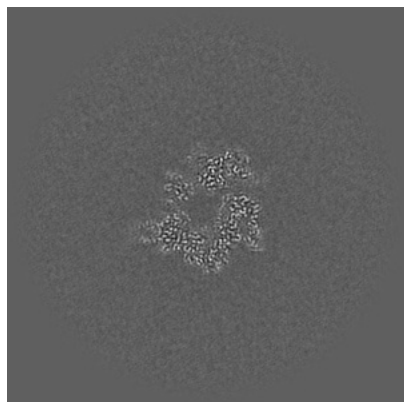


Z

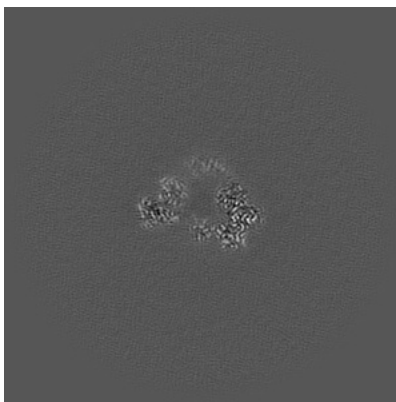
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

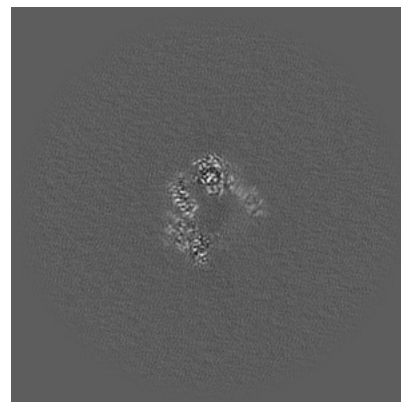
6.2.1 Primary map



X Index: 180

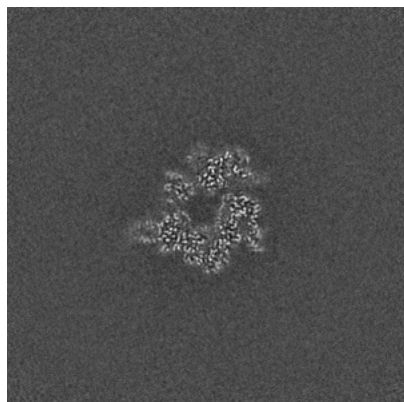


Y Index: 180

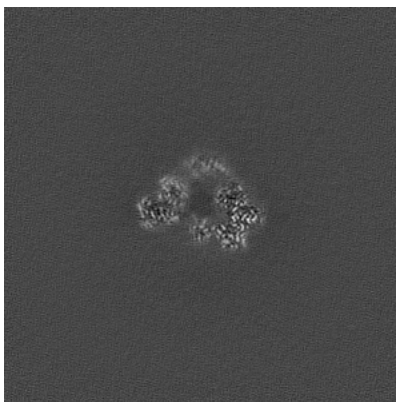


Z Index: 180

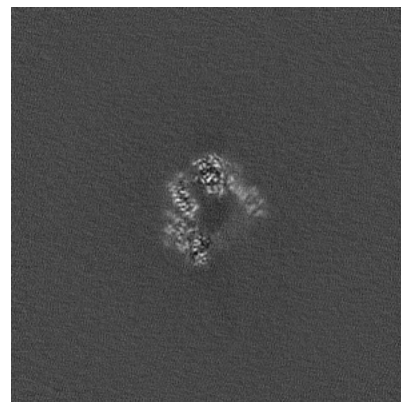
6.2.2 Raw map



X Index: 180



Y Index: 180

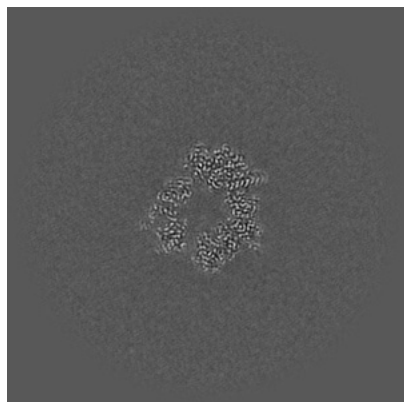


Z Index: 180

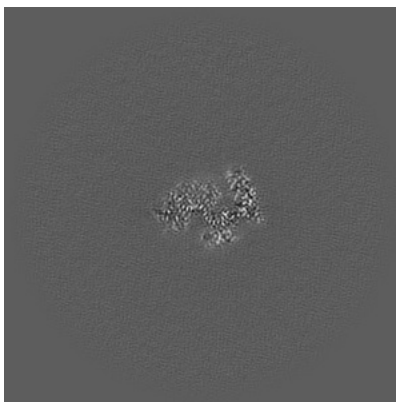
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

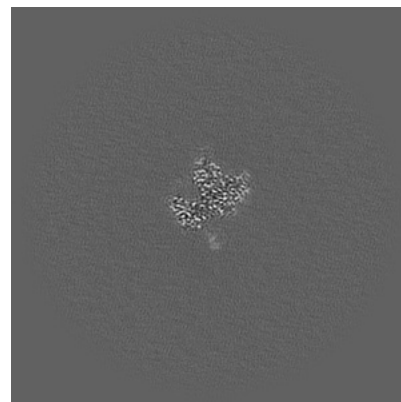
6.3.1 Primary map



X Index: 174

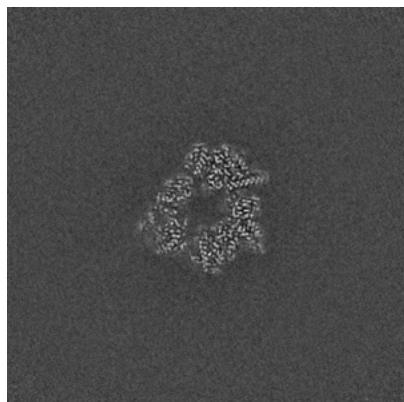


Y Index: 202

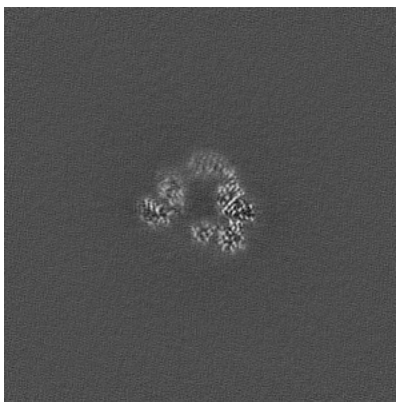


Z Index: 209

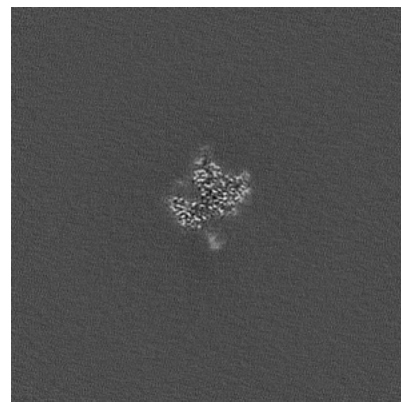
6.3.2 Raw map



X Index: 175



Y Index: 183

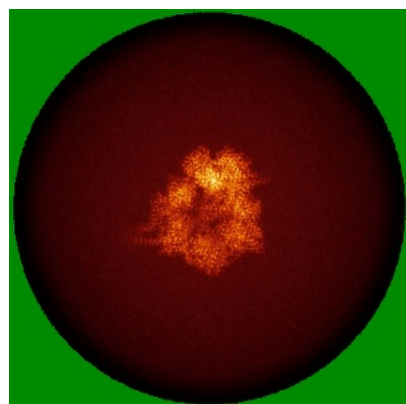


Z Index: 209

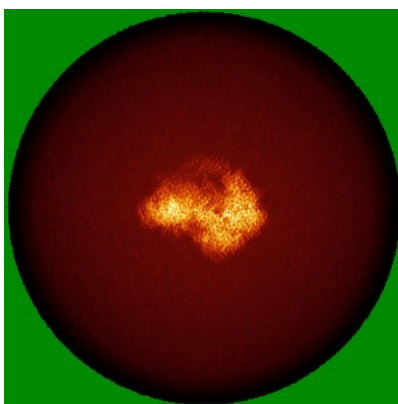
The images above show the largest variance slices of the map in three orthogonal directions.

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

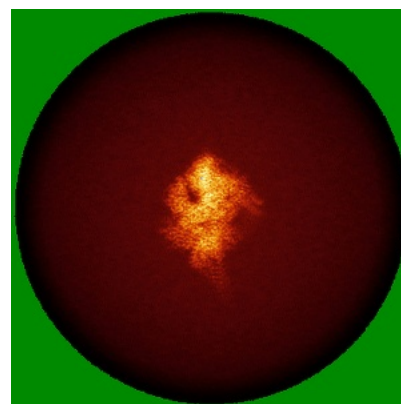
6.4.1 Primary map



X

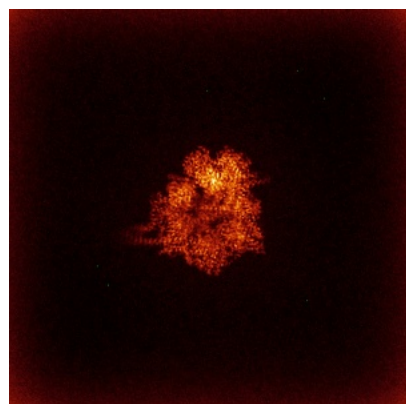


Y

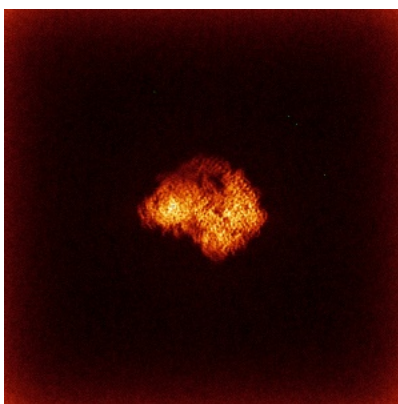


Z

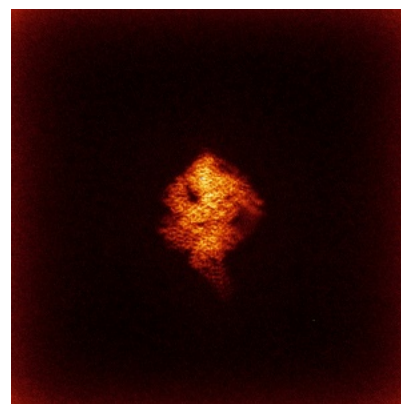
6.4.2 Raw map



X



Y

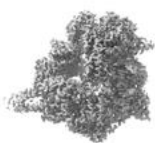


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

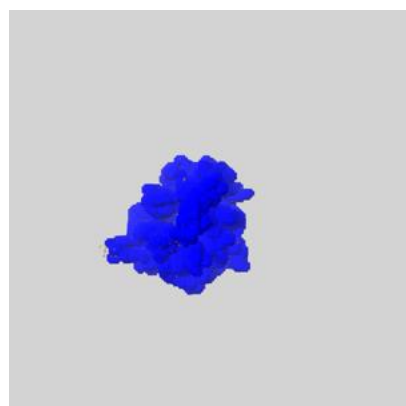
6.6 Mask visualisation [i](#)

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

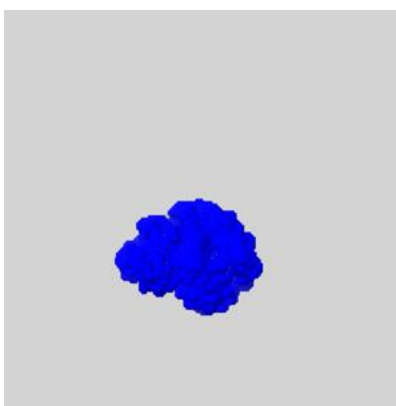
A mask typically either:

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

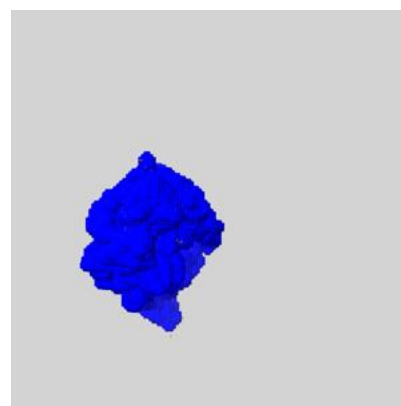
6.6.1 emd_44720_msk_1.map [i](#)



X



Y

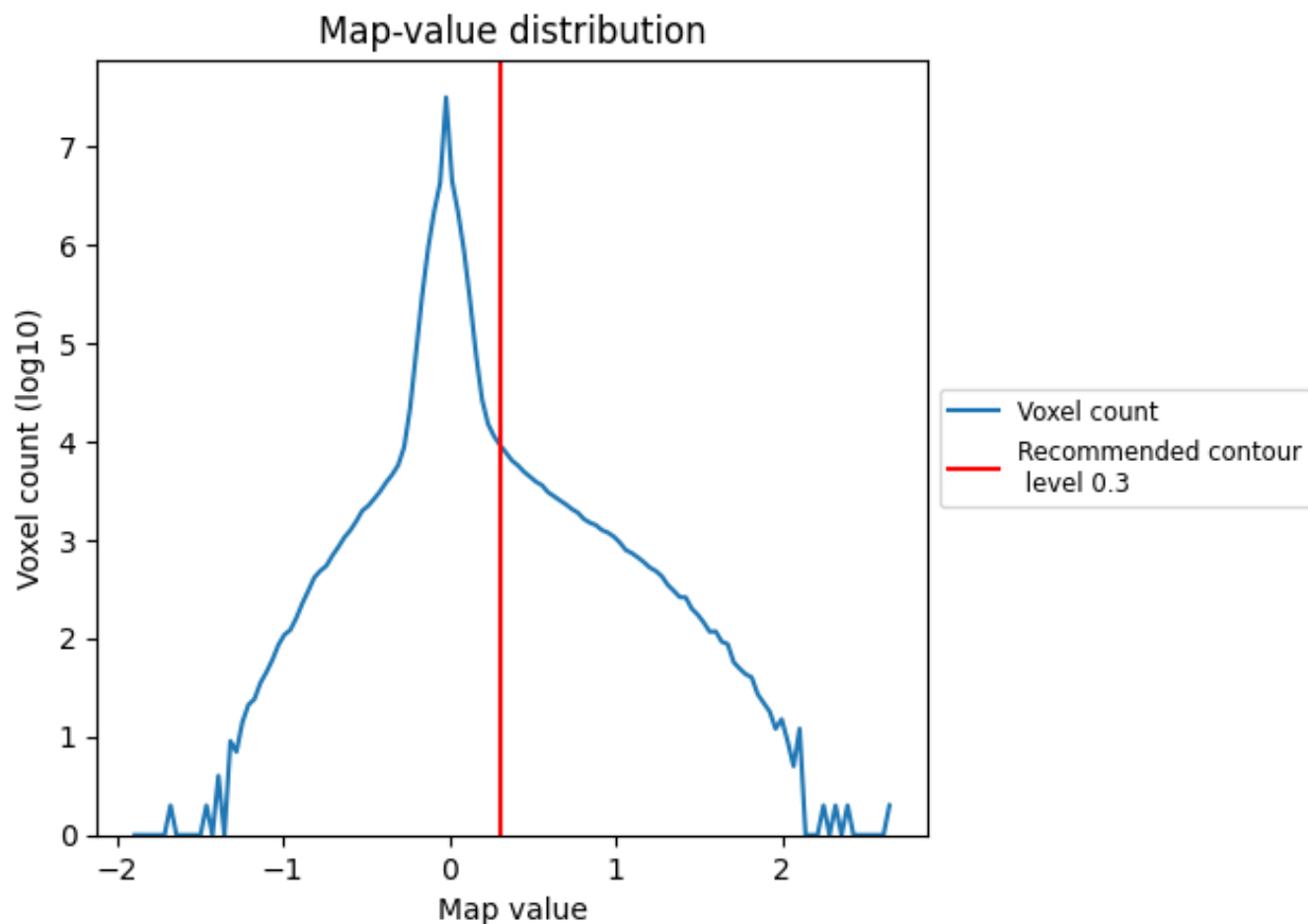


Z

7 Map analysis [i](#)

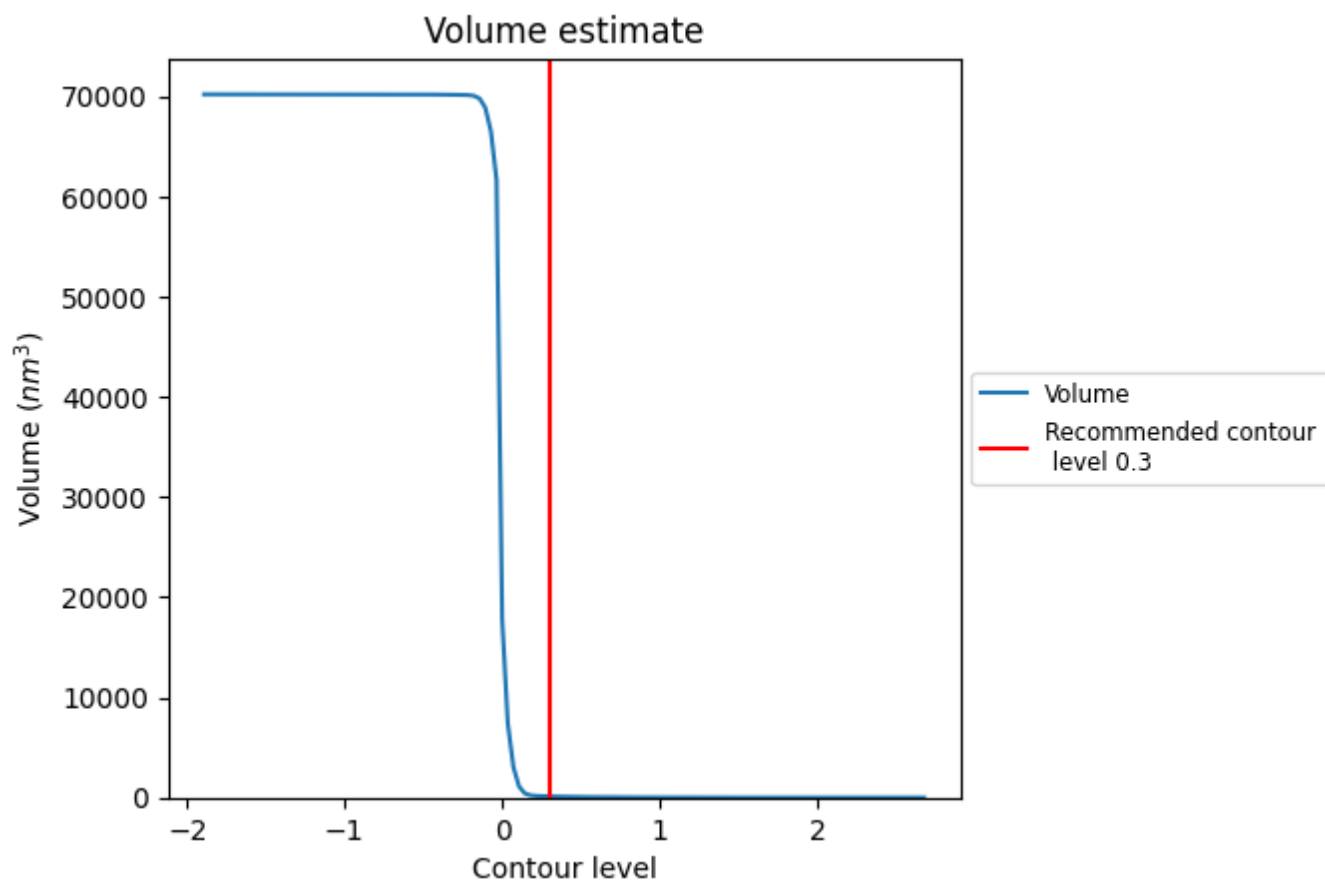
This section contains the results of statistical analysis of the map.

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.

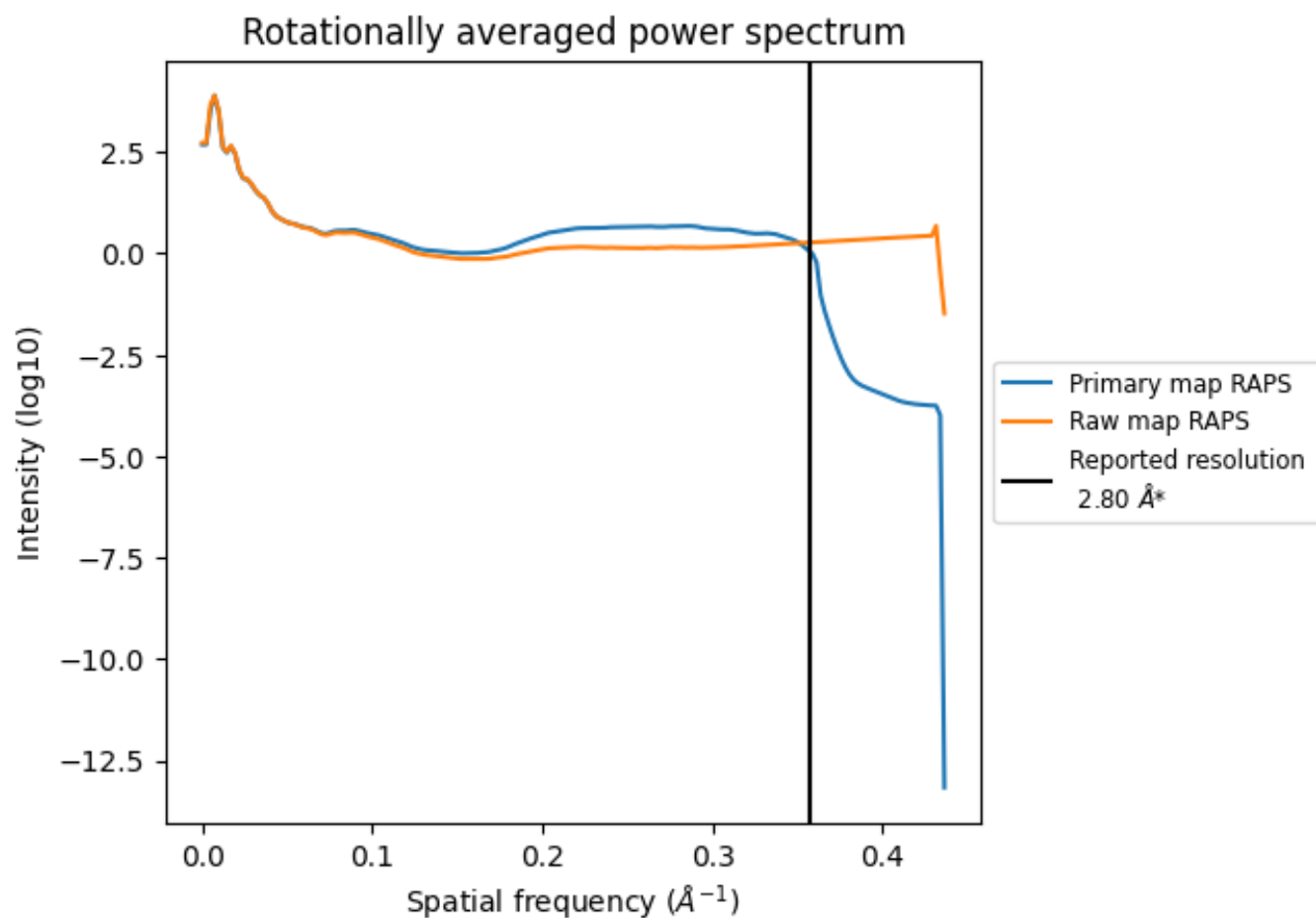
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 ⓘ

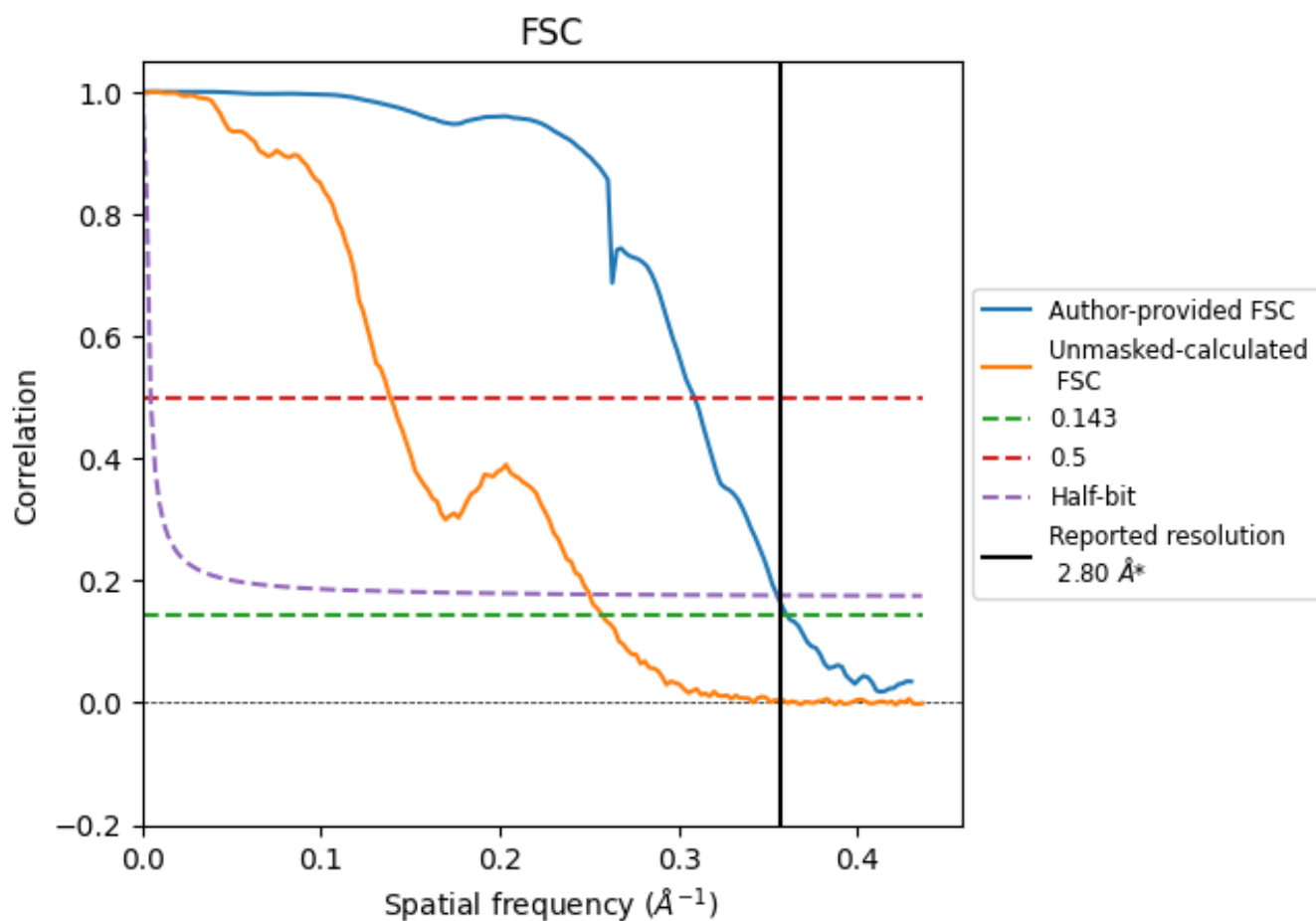


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

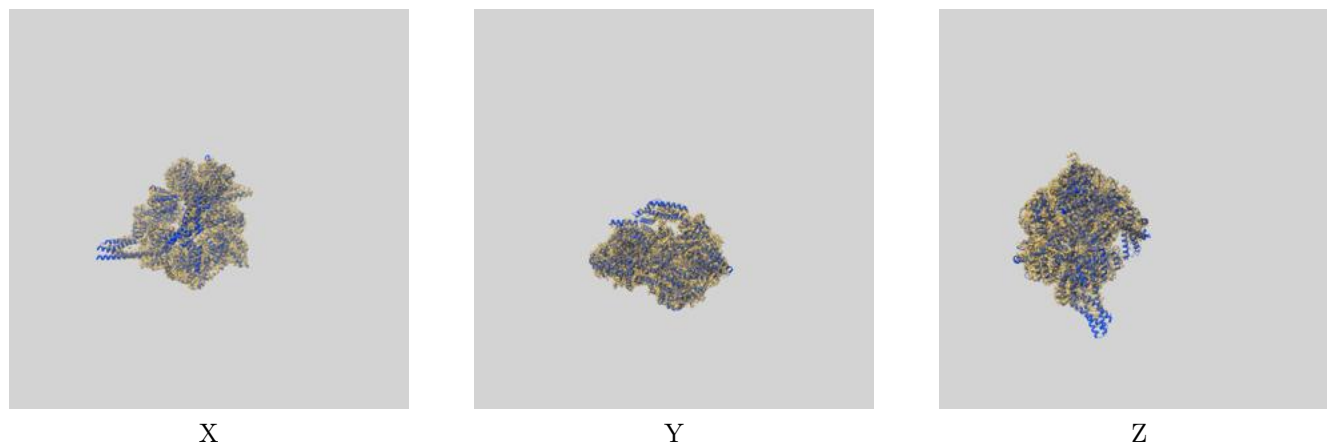
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.77	3.24	2.81
Unmasked-calculated*	3.89	7.21	4.00

*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 3.89 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

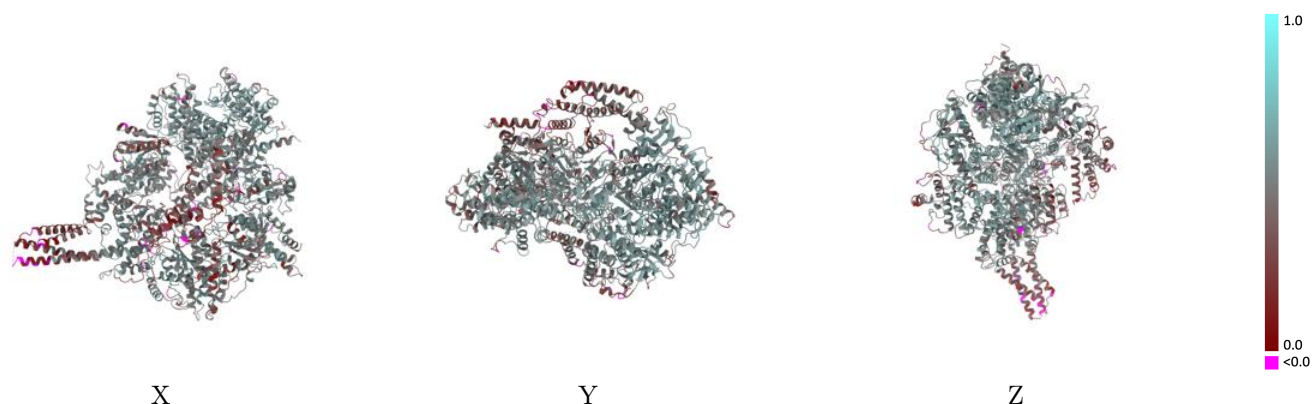
This section contains information regarding the fit between EMDB map EMD-44720 and PDB model 9BN3. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



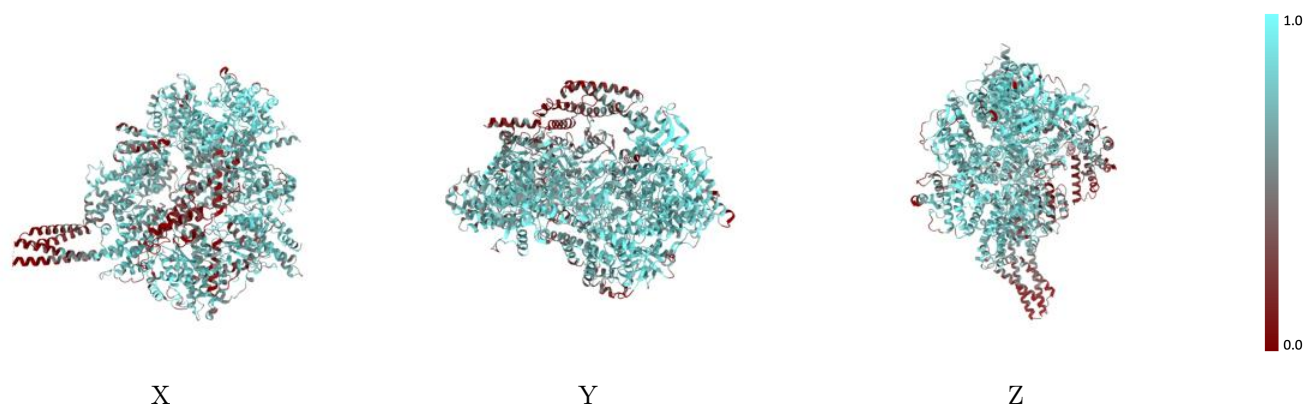
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



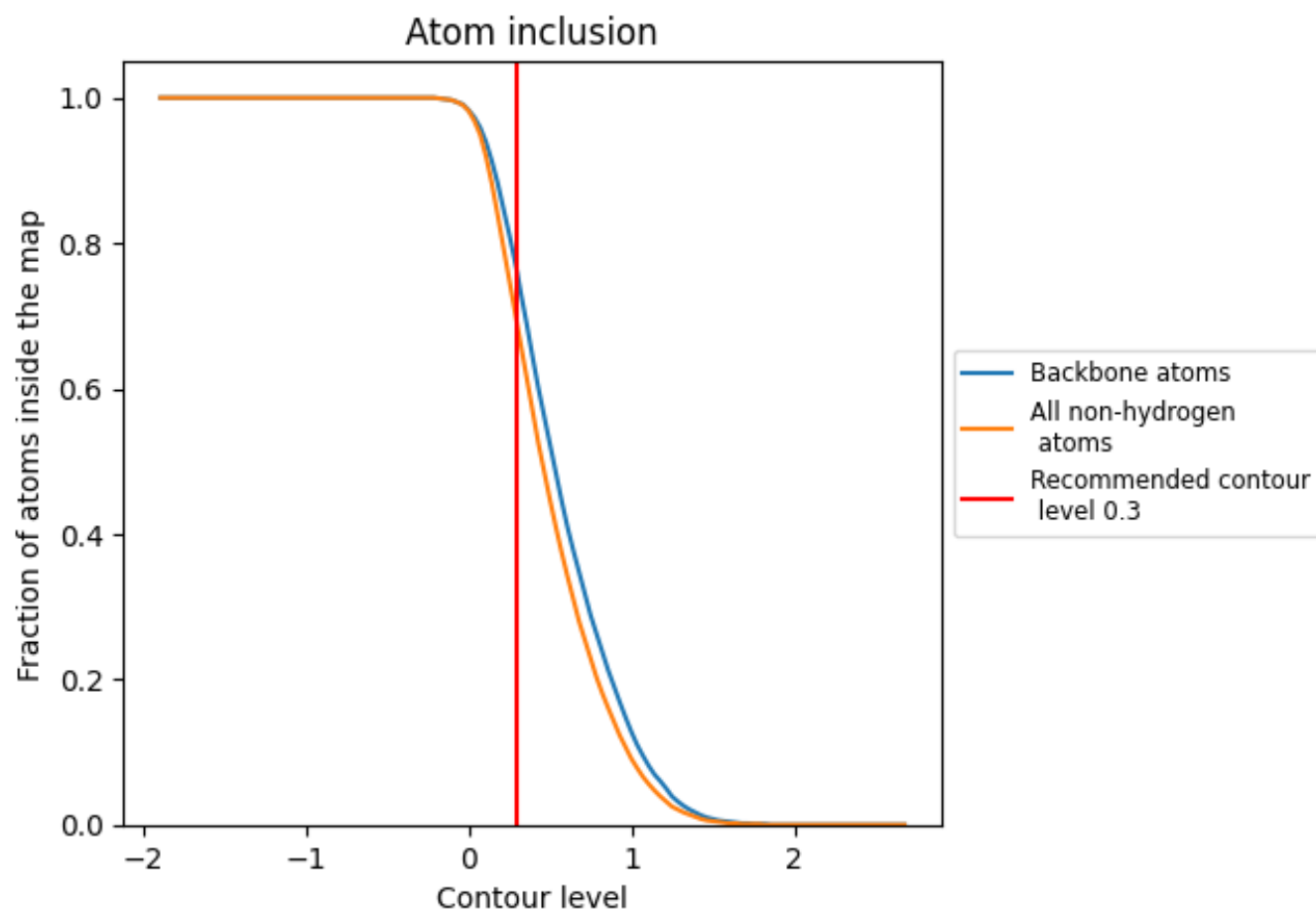
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.4770
A	0.6880	0.4770

