



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 02:55 PM UTC

PDB ID : 9DLE / pdb_00009dle
EMDB ID : EMD-46975
Title : CryoEM structures of yeast cytoplasmic dynein in the presence of ATP and Lis1.
Authors : Kendrick, A.A.; Leschziner, A.E.
Deposited on : 2024-09-10
Resolution : 3.40 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:

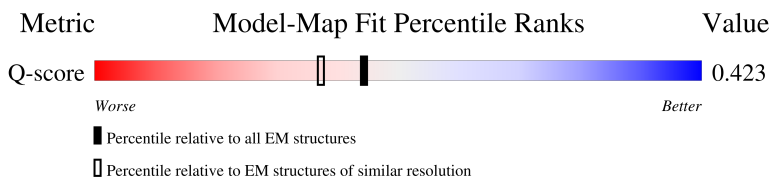
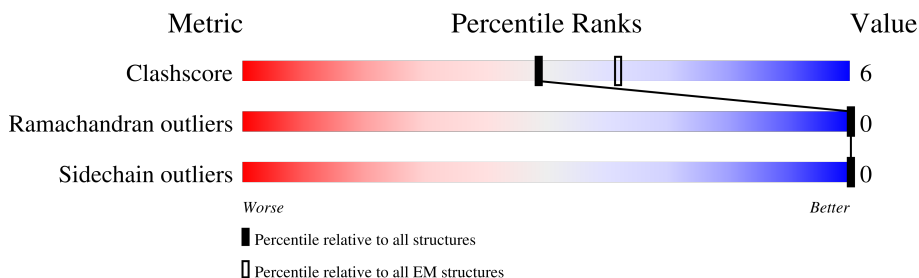
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.40 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	14717 (2.90 - 3.90)

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	2875	
2	B	495	
2	C	495	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22892 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 Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2300	Total	C	N	O	S	0	0
			17945	11552	2999	3314	80		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1220	GLY	-	expression tag	UNP P36022
A	1575	PHE	LEU	conflict	UNP P36022
A	1578	SER	PHE	conflict	UNP P36022
A	1668	GLU	GLN	conflict	UNP P36022
A	1777	VAL	ILE	conflict	UNP P36022
A	1984	VAL	ILE	conflict	UNP P36022
A	2936	VAL	ILE	conflict	UNP P36022
A	3266	GLN	ARG	conflict	UNP P36022
A	3343	GLY	ALA	conflict	UNP P36022
A	3444	VAL	ILE	conflict	UNP P36022
A	3556	ARG	LYS	conflict	UNP P36022
A	3742	ASP	ASN	conflict	UNP P36022
A	3895	VAL	PHE	conflict	UNP P36022
A	4072	ASP	ASN	conflict	UNP P36022

- Molecule 2 is a protein called Nuclear distribution protein PAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	352	Total	C	N	O	S	0	0
			2777	1788	485	489	15		
2	B	333	Total	C	N	O	S	0	0
			2057	1299	379	373	6		

There are 2 discrepancies between the modelled and reference sequences:

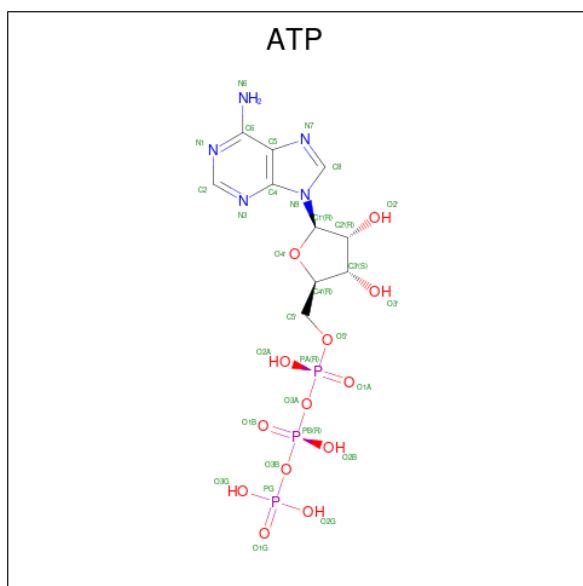
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP P39946

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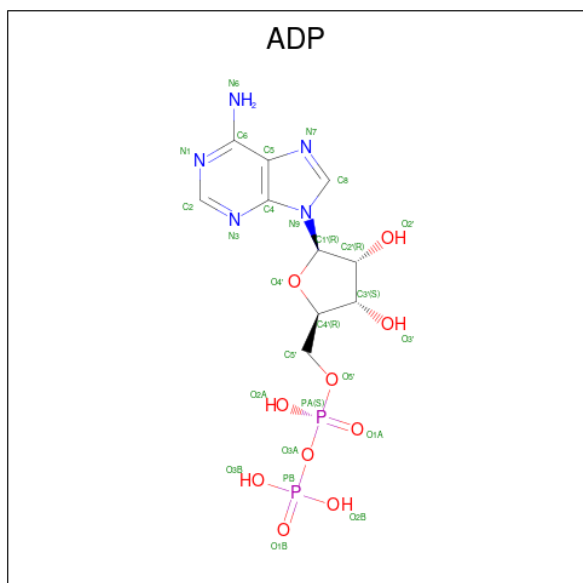
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P39946

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

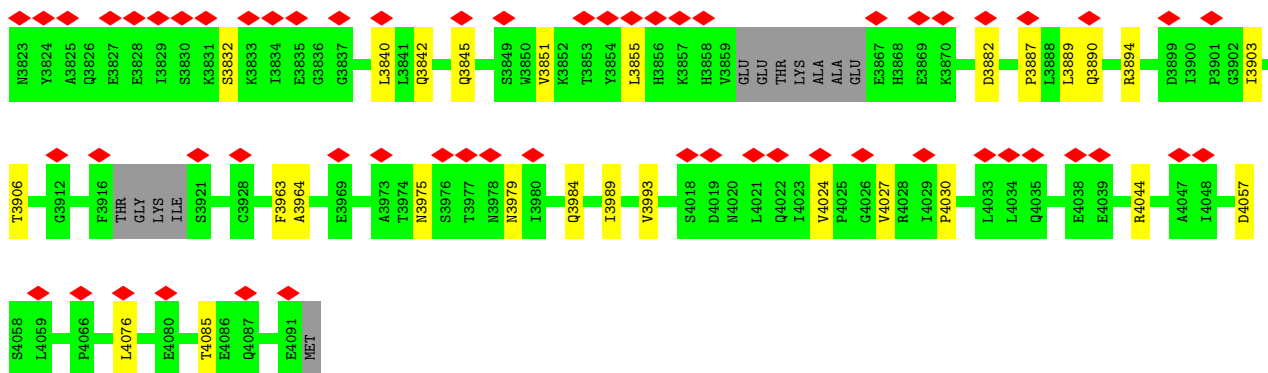


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

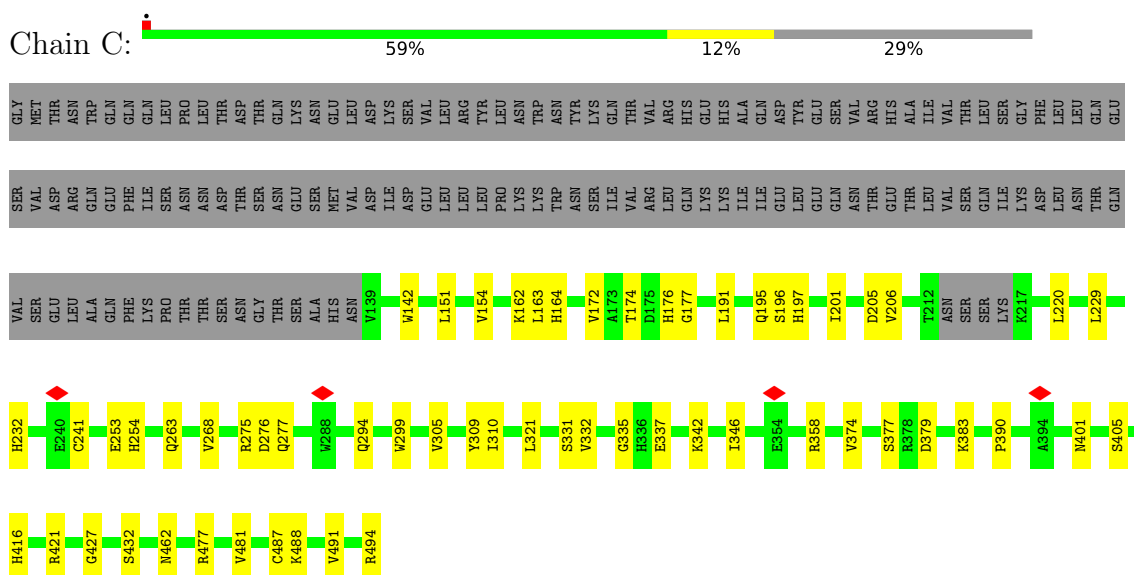
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	

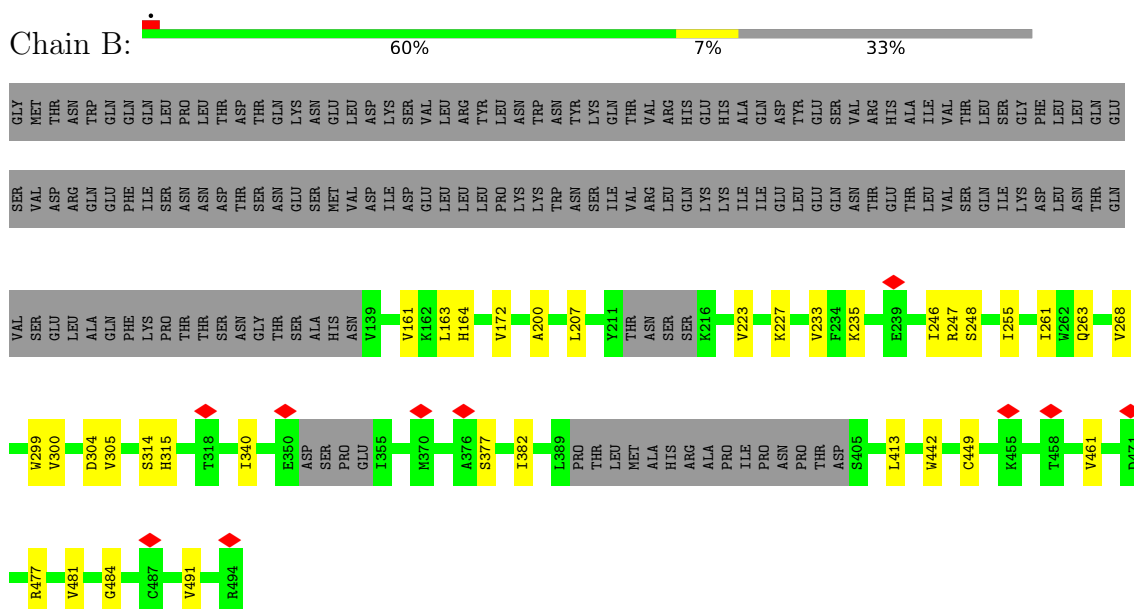
S3727	E3728	S3729	S3730	D3731	G3732	V3733	P3734	K3735	L3736	THR	VAL	ASP	THR	N3741	D3742	D3743	L3744	R3745	Y3746	K3747	K3748	D3749	K3754	I3757	W3762	N3765	Y3769	E3782	R3792	D3793	V3794	D3795	L3800	I3801	K3805	K3808	E3809	S3810	L3811	K3812	I3813	I3814	P3815	L3816	G3817	S3818	I3819	E3820			
LEU	GLU	ASN	ASP	E3582	L3583	M3584	V3585	E3603	F3608	P3609	Q3610	F3611	D3612	N3613	S3619	K3623	L3632	Q3637	Y3642	G3643	I3644	S3645	L3646	Q3647	Q3648	F3657	F3658	K3659	K3660	SER	ARG	GLU	THR	ARG	ALA	ALA	ARG	THR	I3674	V3682	F3686	D3691	M3700	L3726							
L3391	E3392	D3402	A3403	N3424	E3434	N3442	R3445	D3469	P3460	R3468	G3474	N3475	D3483	H3484	E3485	D3491	N3521	K3522	E3523	S3524	F3530	L3534	R3543	D3547	L3548	I3549	K3550	L3551	K3560	N3561	L3562	E3563	K3564	L3567	N3571	N3572	SER	GLN	GLY	ASN	MET										
ILE	ARG	ASP	VAL	GLU	ALA	ILE	THR	LYS	THR	MET	ASN	VAL	GLN	ALA	ASN	L3289	D3290	R3291	S3292	I3293	S3294	K3297	S3298	L3299	T3300	F3301	R3305	W3306	L3307	N3308	T3309	K3310	K3311	Q3312	F3313	T3316	L3320	I3325	Y3330	R3340	M3345	L3348	L3353	D3358	D3368	D3388					
TRP	VAL	ASP	ILE	ALA	GLN	ILE	PHE	SER	VAL	LEU	ASN	VAL	GLU	ASN	VAL	GLN	ALA	ASN	ILE	THR	ILE	GLU	PHE	GLU	SER	LEU	GLU	VAL	LEU	LEU	ALA	ALA	GLU	GLU	ILE	ASN	VAL	ILE	GLU	GLU	GLN	GLY	THR	PRO	LYS	GLN	TRP				
ARG	ASP	ILE	GLN	GLN	PHE	ILE	ARG	LYS	ASP	PHE	THR	ILE	HIS	GLN	VAL	HIS	TYR	ASP	THR	THR	LEU	HIS	ILE	LYS	PRO	GLN	GLN	ILE	LEU	THR	GLY	ILE	ARG	GLU	GLU	TYR	GLU	THR	GLU	GLU	GLY	THR	ARG	GLN							
GLU	VAL	VAL	MET	LYS	SER	ILE	GLN	ASP	ILE	GLN	PRO	THR	THR	GLU	ALA	GLU	GLY	VAL	VAL	VAL	ASN	ILE	LYS	GLN	GLN	LYS	GLN	LEU	THR	ILE	GLU	VAL	ASN	GLU	VAL	VAL	GLU	VAL	VAL	GLU	GLU	GLU	ASP	ILE	ARG	LYS					
N3032	E3033	L3034	ASN	LYS	THR	LEU	SER	LYS	LYS	SER	THR	THR	GLU	LEU	THR	GLU	GLY	VAL	VAL	VAL	ALA	ARG	LYS	THR	ASP	LYS	GLN	GLU	VAL	VAL	GLU	VAL	GLU	GLU	ILE	LYS	VAL	GLU	GLU	GLU	ASP	ILE	ARG	LYS	ARG	ASN	LYS				
V2626	Y2630	R2646	R2659	Q2684	L2695	D2703	E2706	L2712	V2713	E2717	V2733	L2734	V2739	D2740	H2741	L2742	R2743	R2744	L2745	M2757	L2769	T2770	R2771	V2773	Q2783	P2784	K2785	H2789	S2793	D2805	L2808	E2819	E2824	F2827	L2834																
A2838	D2839	T2840	F2841	D2842	D2850	L2856	L2867	L2873	F2877	V2878	F2889	S2899	W2932	M2938	E2939	F2940	E2947	V2948	N2949	L2950	E2951	L2952	T2961	D2962	R2963	A2964	V2965	N2967	L2968	V2982	G2983	V2984	N2985	L2993	K3006	E3022	E3026	S3027	V3028	L3029	V3031										
N3032	E3033	L3034	ASN	LYS	THR	LEU	SER	LYS	LYS	THR	GLU	LEU	THR	GLU	LYS	ALA	ARG	SER	THR	LEU	ASP	LYS	GLN	ARG	PRO	LYS	GLN	GLY	VAL	THR	ILE	GLU	GLU	ILE	LYS	VAL	GLN	GLU	GLU	ASP	ILE	ARG	LYS	ARG	ASN	LYS					
E2452	L2458	V2465	THR	THR	LYS	GLY	L2471	L2479	D2487	E2488	L2489	N2490	L2491	L2494	G2498	S2499	Q2500	V2503	R2507	E2511	K2512	V2523	N2536	P2537	P2538	R2543	M2546	S2547	E2548	R2549	R2552	Y2574	T2578	K2604	F2617	S2618	E2621														
E2285	L2290	Q2303	T2315	K2319	L2323	S2334	I2339	T2344	Y2345	T2346	G2347	H2348	D2349	E2352	I2361	ALA	ASN	ASN	ASP	LYS	L2366	S2367	F2368	E2374	V2391	I2392	P2393	I2403	F2404	N2408	L2409	L2416	G2421	M2426	T2427	M2428	R2433	N2434	Y2438	N2444											
N2173	K2174	P2179	N2180	G2181	E2182	R2183	I2186	P2187	L2188	R2191	E2195	L2199	R2209	F2215	K2225	A2236	LEU	ASP	ASN	LYS	LEU	SER	MET	PHE	E2245	K2248	S2254	D2255	S2256	F2257	D2258	N2259	A2260	S2261	L2262	N2264	L2265	L2272	I2276	V2278	F2281	L2284									
Y2061	Q2064	Q2068	V2073	G2074	W2084	H2097	K2098	H2099	V2103	I2104	T2110	S2113	S2117	M2118	L2119	K2120	A2121	T2122	L2123	E2124	W2125	K2126	D2127	R2136	T2141	T2142	G2143	T2144	F2145	K2146	R2149	V2152	V2153	D2159	F2160	E2161	V2162	V2163	E2164	A2165	L2170	D2171	D2172								



- Molecule 2: Nuclear distribution protein PAC1



- Molecule 2: Nuclear distribution protein PAC1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40384	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.902	Depositor
Minimum map value	-0.483	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.13	Depositor
Map size (\AA)	312.928, 312.928, 312.928	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.889, 0.889, 0.889	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, MG

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	0.14	0/18305	0.30	0/24808
2	B	0.12	0/2092	0.27	0/2882
2	C	0.18	0/2856	0.37	0/3892
All	All	0.14	0/23253	0.31	0/31582

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	17945	0	17534	206	0
2	B	2057	0	1448	20	0
2	C	2777	0	2696	38	0
3	A	31	0	12	2	0
4	A	81	0	36	1	0
5	A	1	0	0	0	0
All	All	22892	0	21726	260	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 6.

The worst 5 of 260 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)
2:C:401:ASN:O	2:C:405:SER:HB3	1.75	0.84
1:A:2488:GLU:HB3	1:A:2491:LEU:HD13	1.63	0.78
1:A:1645:PHE:HB2	1:A:1697:LYS:HG3	1.69	0.73
1:A:2444:ASN:HA	1:A:2487:ASP:HB2	1.73	0.70
1:A:1570:GLU:HB2	1:A:1585:VAL:HA	1.73	0.69

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	2272/2875 (79%)	2213 (97%)	59 (3%)	0	100	100
2	B	325/495 (66%)	314 (97%)	11 (3%)	0	100	100
2	C	348/495 (70%)	331 (95%)	17 (5%)	0	100	100
All	All	2945/3865 (76%)	2858 (97%)	87 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1914/2631 (73%)	1914 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	114/461 (25%)	114 (100%)	0	100	100
2	C	304/461 (66%)	304 (100%)	0	100	100
All	All	2332/3553 (66%)	2332 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	401	ASN
2	B	269	HIS
1	A	3761	ASN
1	A	3858	HIS
1	A	3914	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	A	4102	-	28,29,29	1.38	5 (17%)	43,45,45	1.82	8 (18%)
3	ATP	A	4101	-	32,33,33	0.57	1 (3%)	48,52,52	0.43	0
4	ADP	A	4103	-	28,29,29	1.41	4 (14%)	43,45,45	2.01	9 (20%)
4	ADP	A	4104	5	28,29,29	1.40	4 (14%)	43,45,45	1.91	8 (18%)

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
4	ADP	A	4102	-	-	7/16/32/32	0/3/3/3
3	ATP	A	4101	-	-	7/22/38/38	0/3/3/3
4	ADP	A	4103	-	-	4/16/32/32	0/3/3/3
4	ADP	A	4104	5	-	1/16/32/32	0/3/3/3

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4103	ADP	C5-C4	4.67	1.47	1.39
4	A	4104	ADP	C5-C4	4.60	1.47	1.39
4	A	4102	ADP	C5-C4	4.57	1.47	1.39
4	A	4104	ADP	C5-C6	2.58	1.48	1.41
4	A	4103	ADP	C5-C6	2.57	1.48	1.41

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4103	ADP	C5-C4-N3	-6.81	117.35	126.72
4	A	4104	ADP	C5-C4-N3	-6.36	117.97	126.72
4	A	4102	ADP	C5-C4-N3	-5.84	118.68	126.72
4	A	4103	ADP	N3-C4-N9	5.59	136.67	127.17
4	A	4104	ADP	N3-C4-N9	5.21	136.03	127.17

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4102	ADP	C5'-O5'-PA-O1A
4	A	4102	ADP	C5'-O5'-PA-O2A

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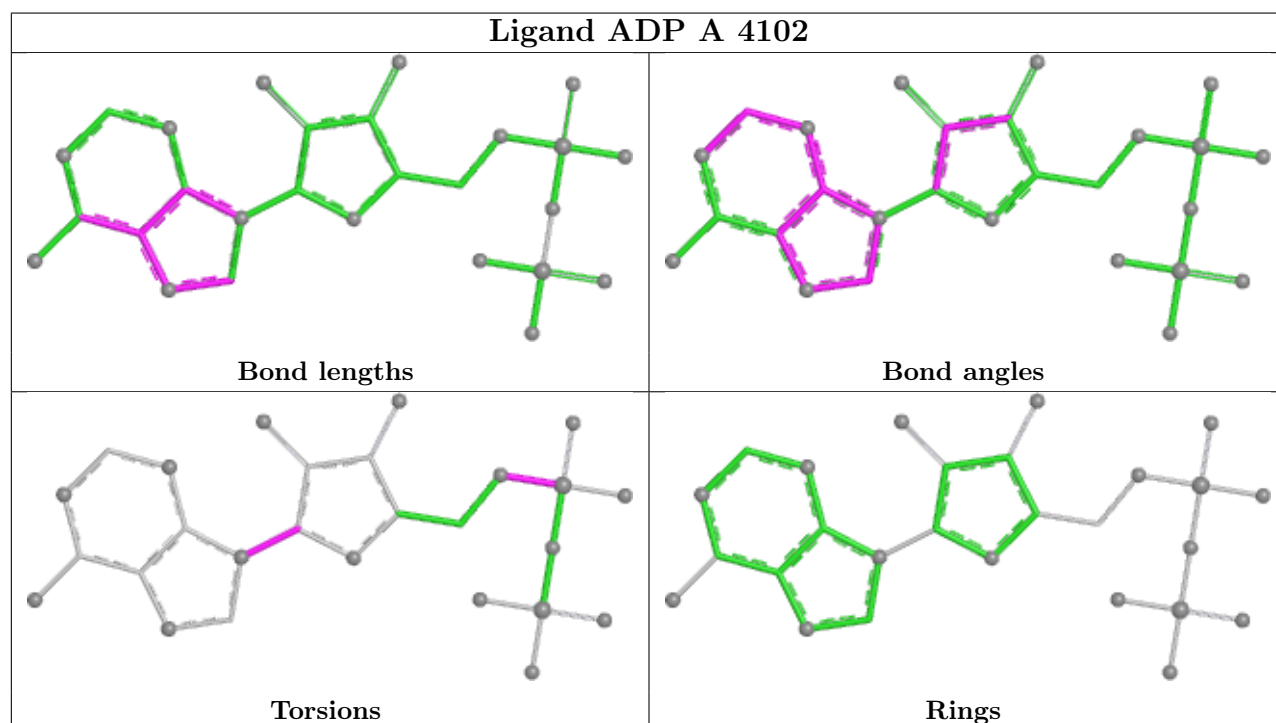
Mol	Chain	Res	Type	Atoms
4	A	4102	ADP	C5'-O5'-PA-O3A
3	A	4101	ATP	C3'-C4'-C5'-O5'
3	A	4101	ATP	O4'-C1'-N9-C8

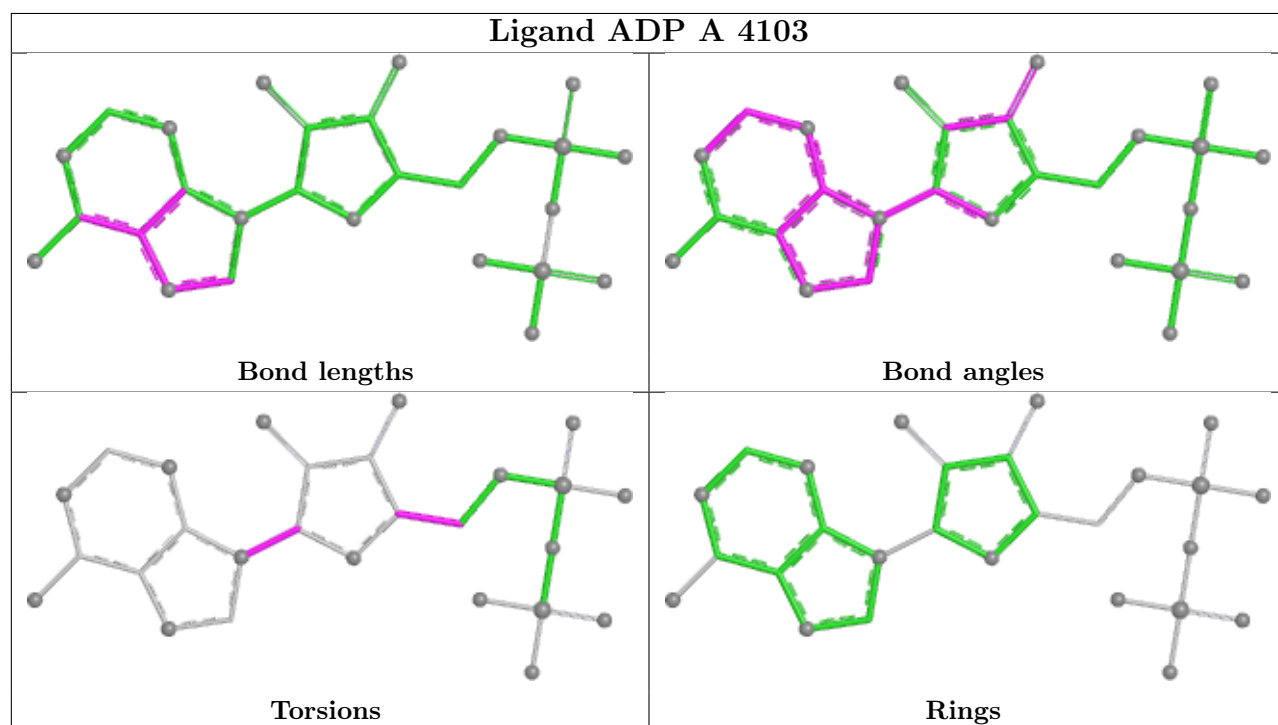
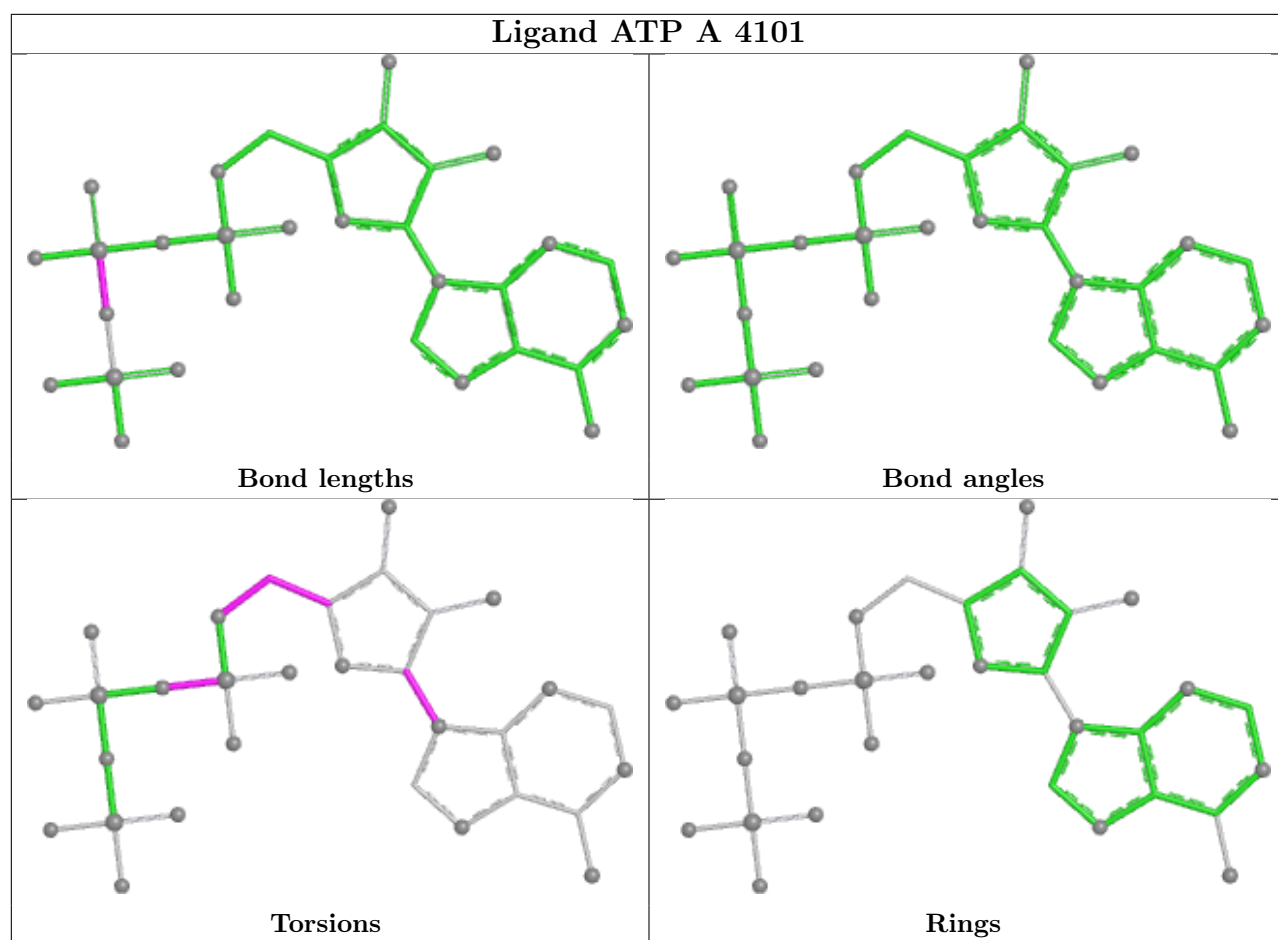
There are no ring outliers.

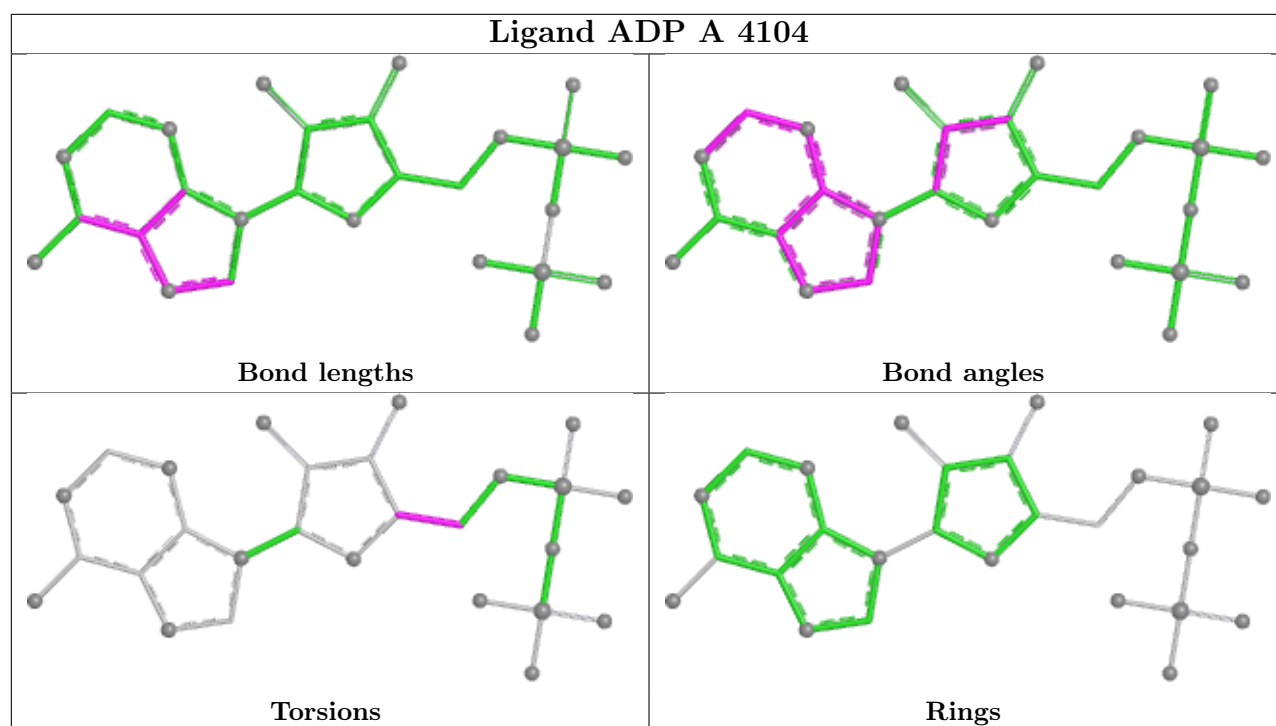
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4102	ADP	1	0
3	A	4101	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.

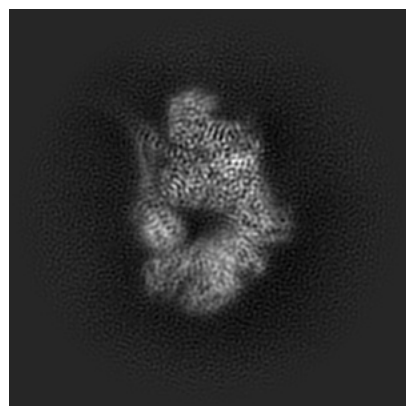
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46975. These allow visual inspection of the internal detail of the map and identification of artifacts.

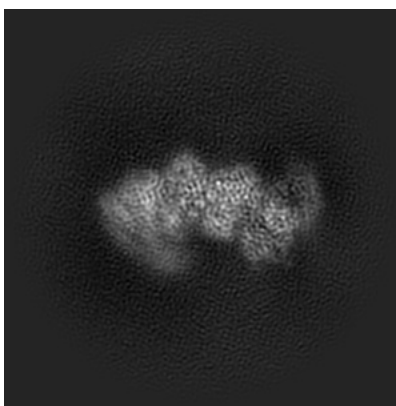
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

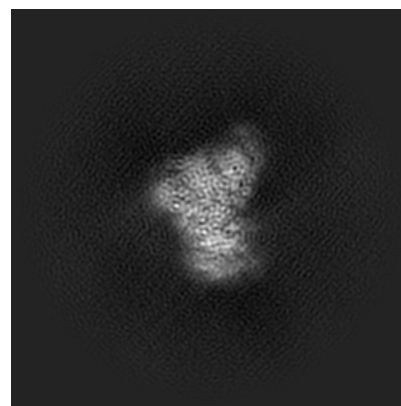
6.1.1 Primary map



X

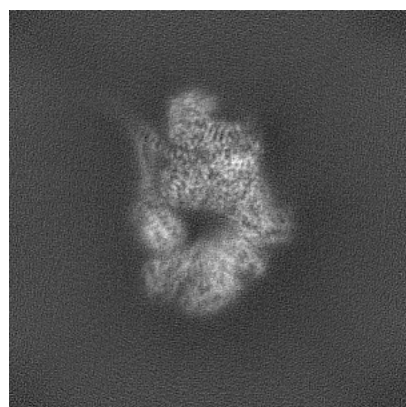


Y

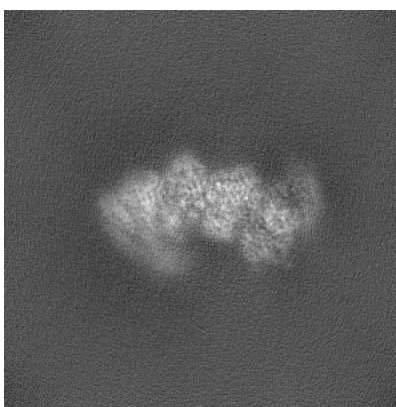


Z

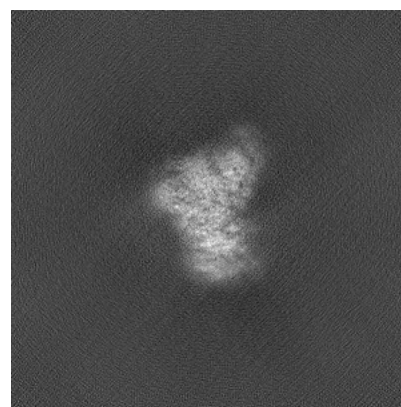
6.1.2 Raw map



X



Y

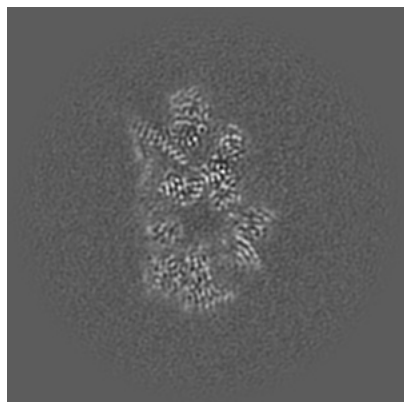


Z

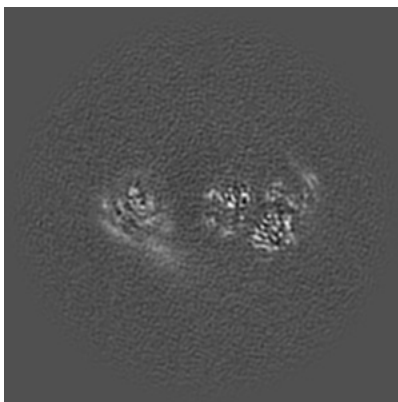
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

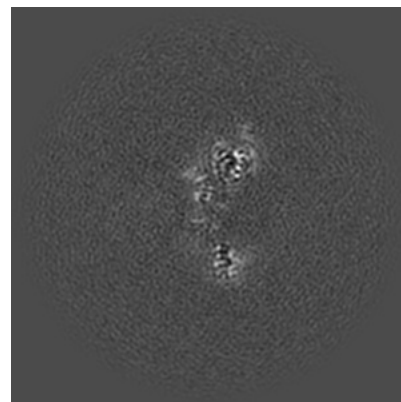
6.2.1 Primary map



X Index: 176

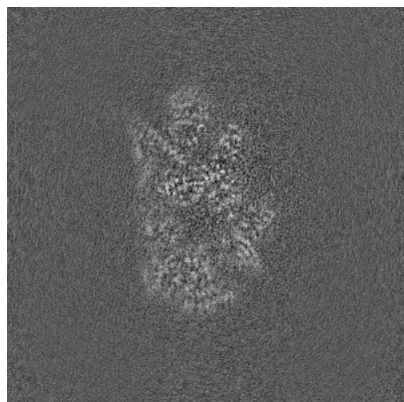


Y Index: 176

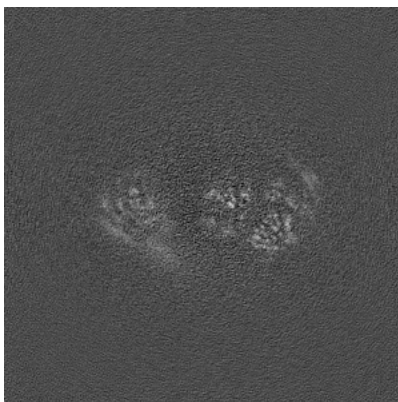


Z Index: 176

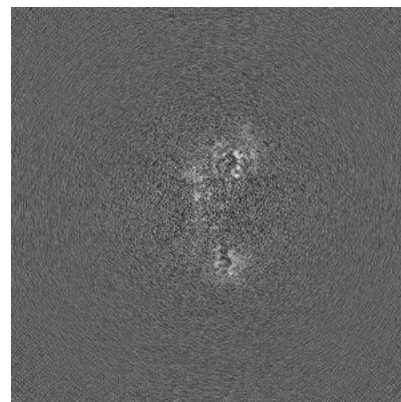
6.2.2 Raw map



X Index: 176



Y Index: 176

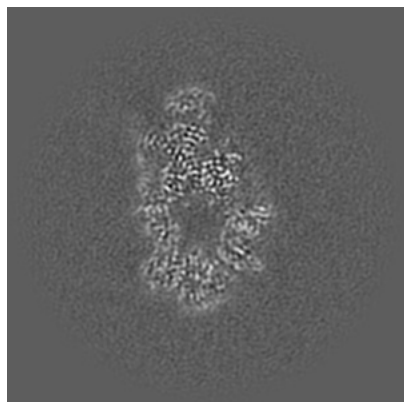


Z Index: 176

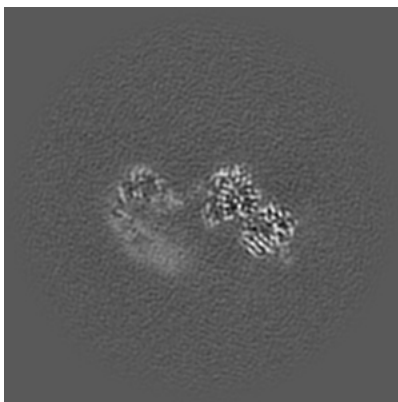
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

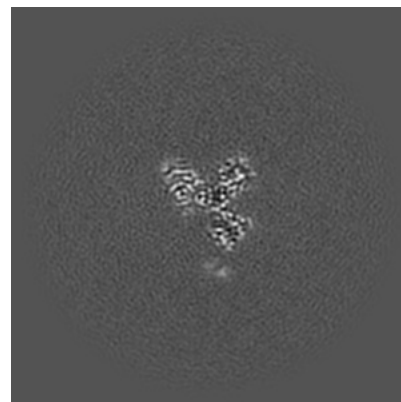
6.3.1 Primary map



X Index: 181

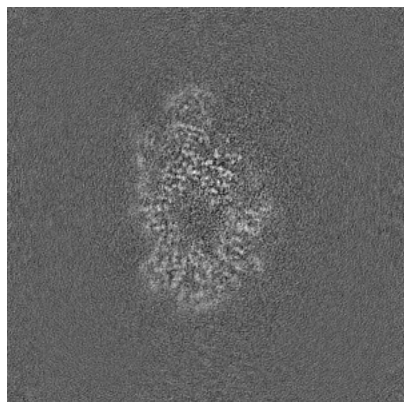


Y Index: 189

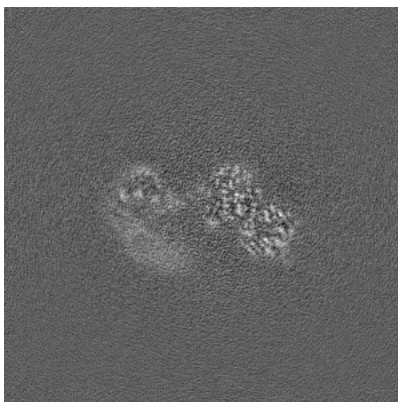


Z Index: 213

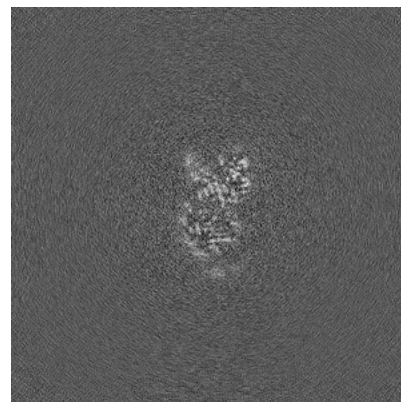
6.3.2 Raw map



X Index: 182



Y Index: 190

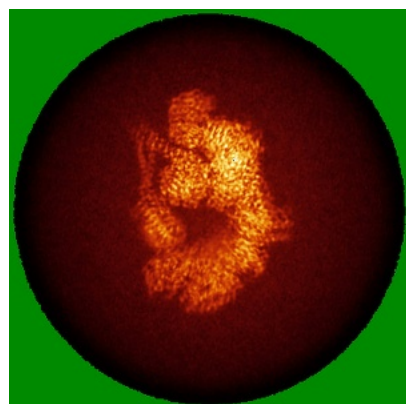


Z Index: 194

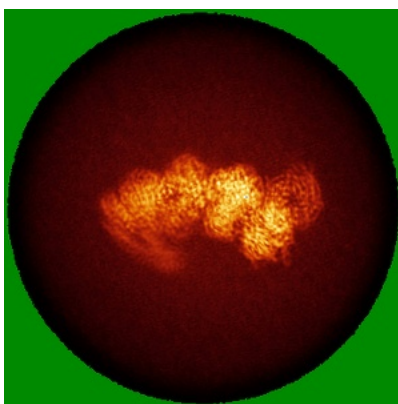
The images above show the largest variance slices of the map in three orthogonal directions.

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

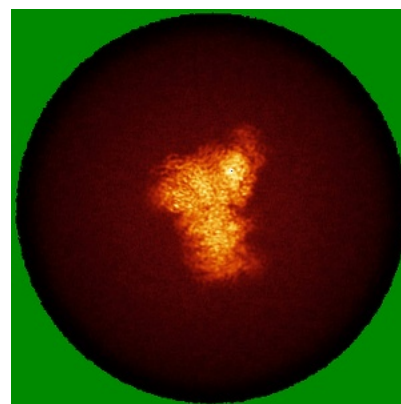
6.4.1 Primary map



X

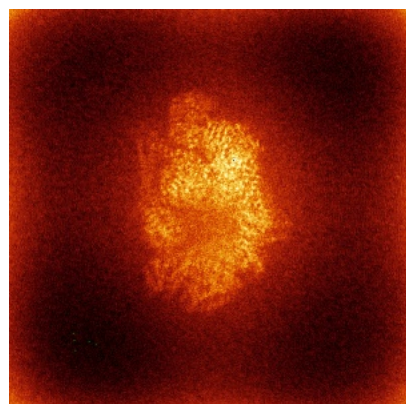


Y

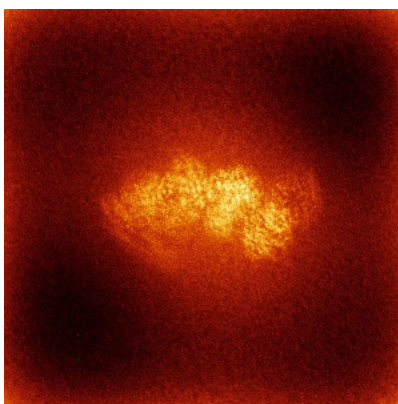


Z

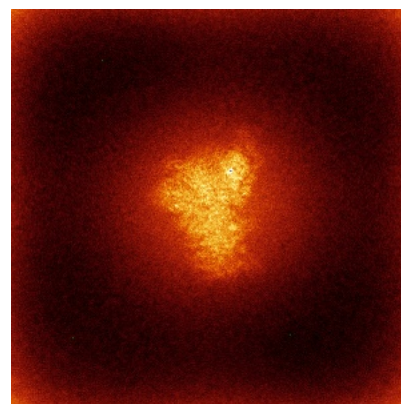
6.4.2 Raw map



X



Y

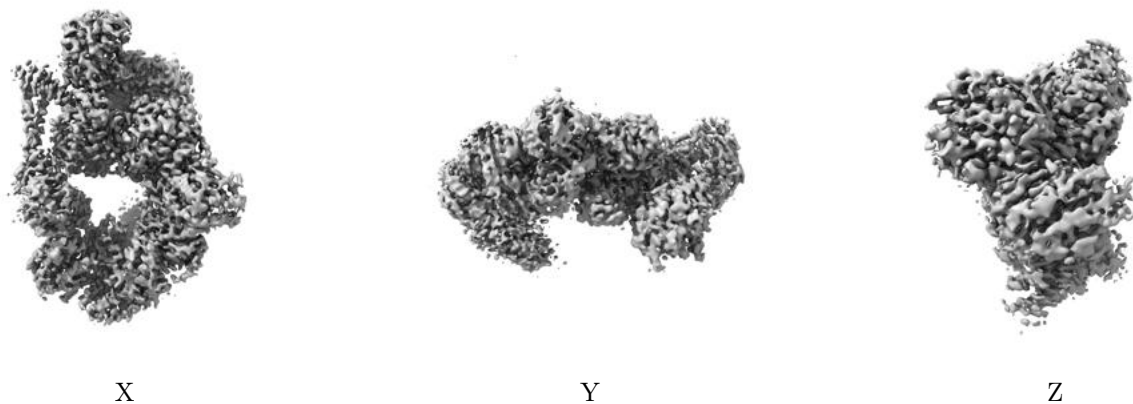


Z

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.

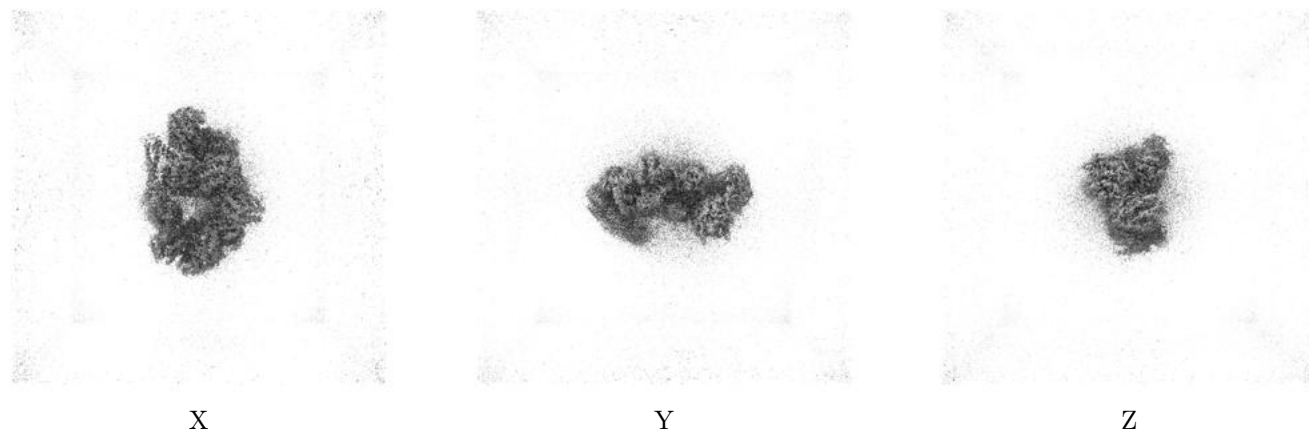
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. 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.

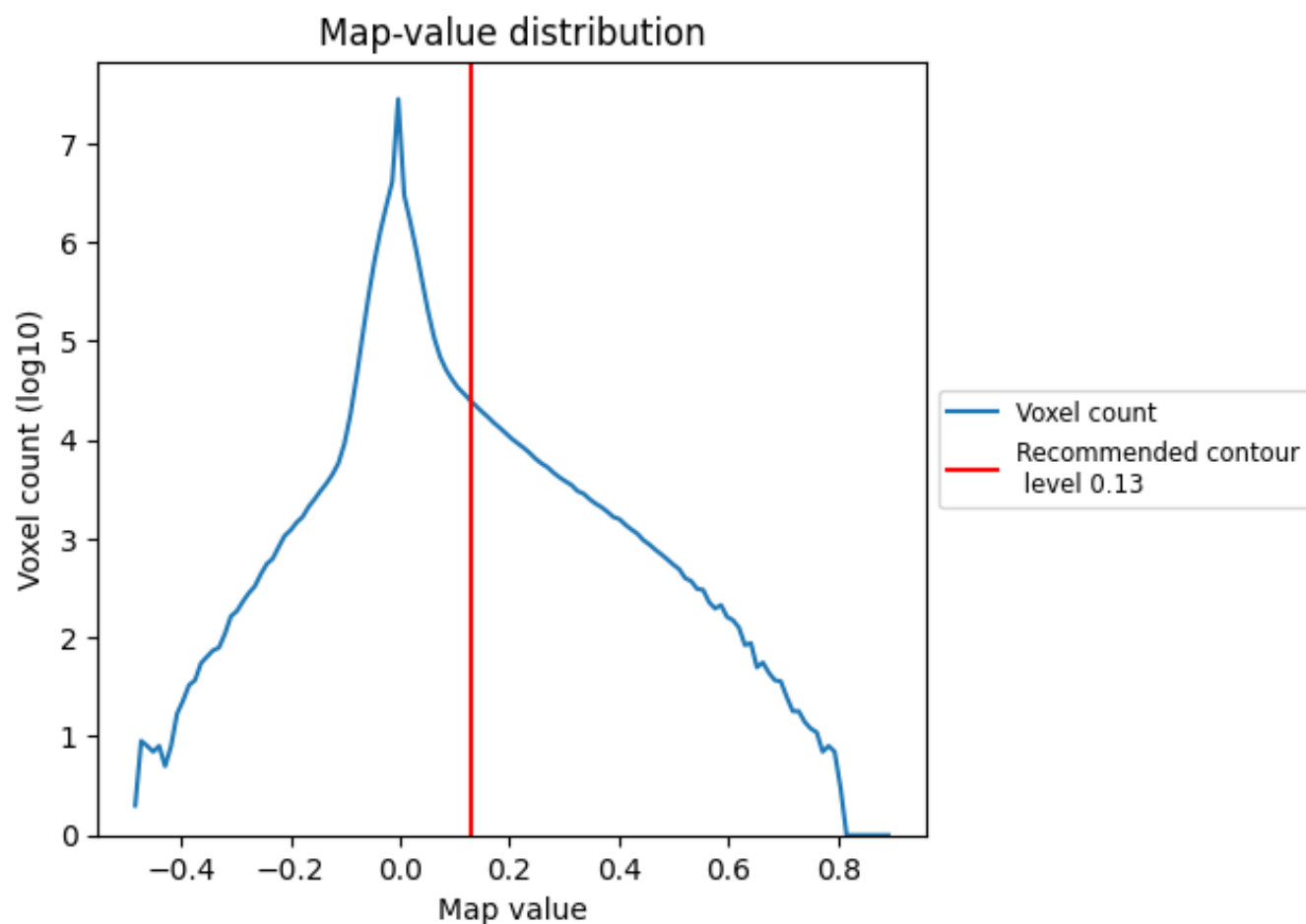
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

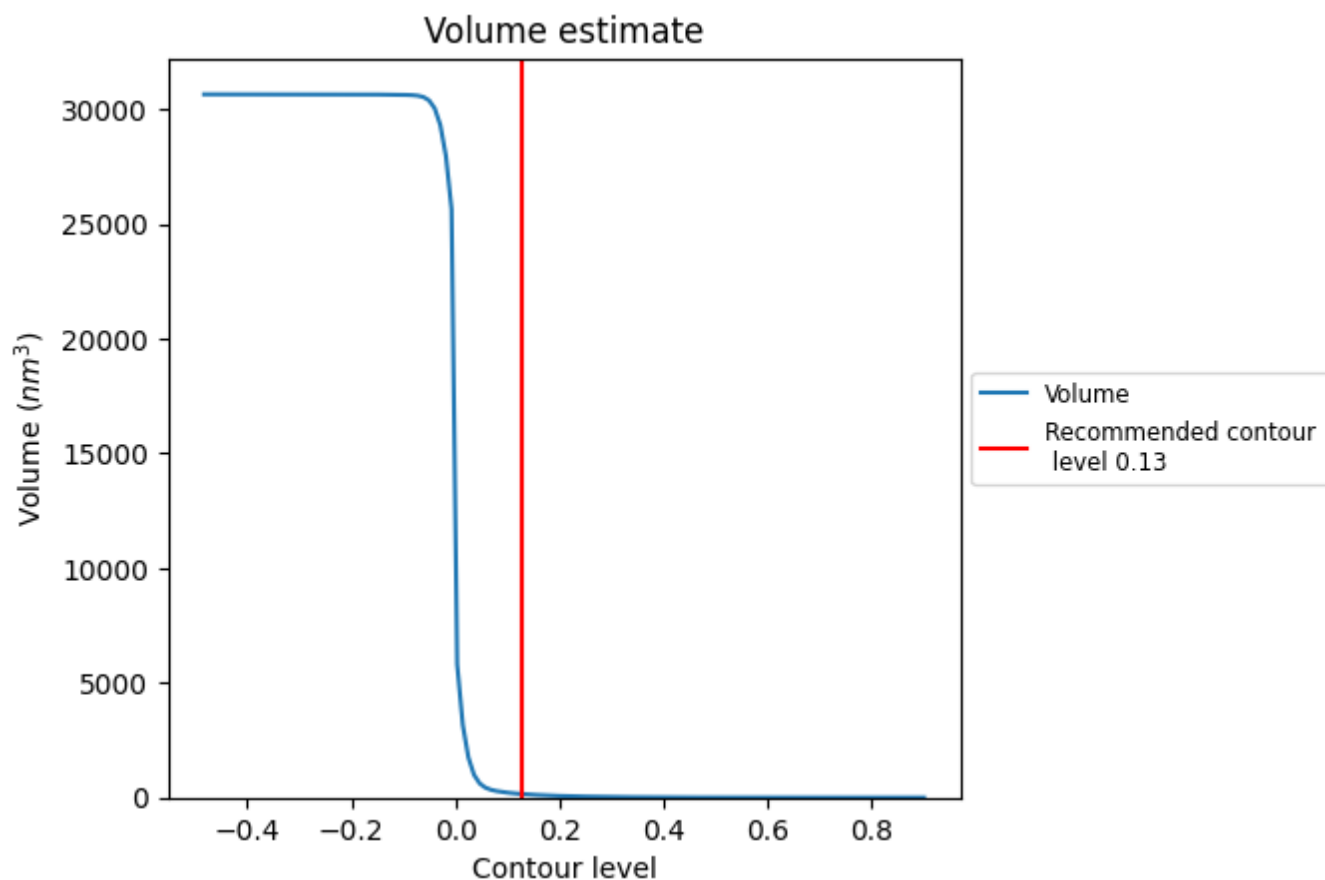
This section contains the results of statistical analysis of the map.

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.

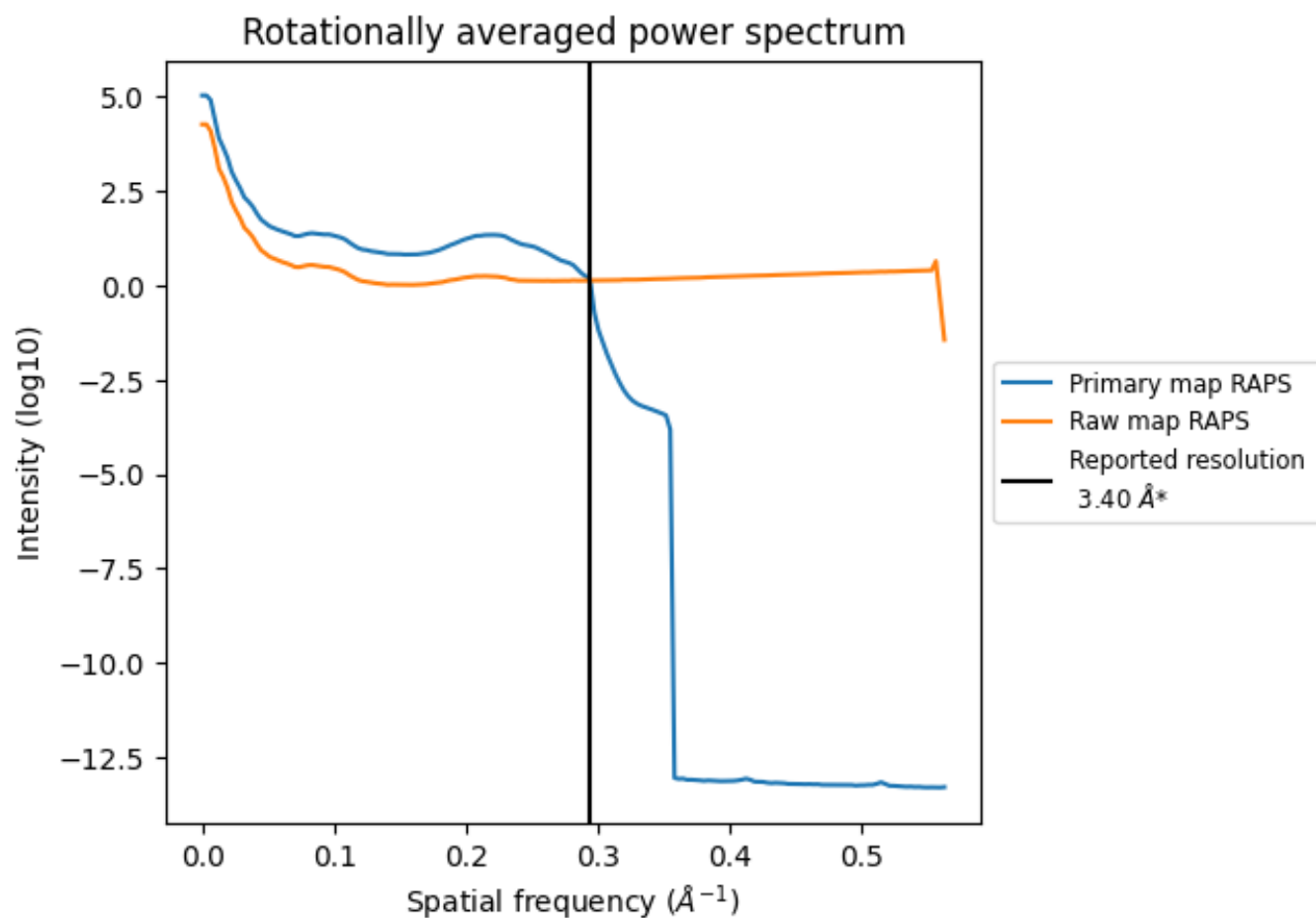
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm^3 ; this corresponds to an approximate mass of 138 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 ⓘ

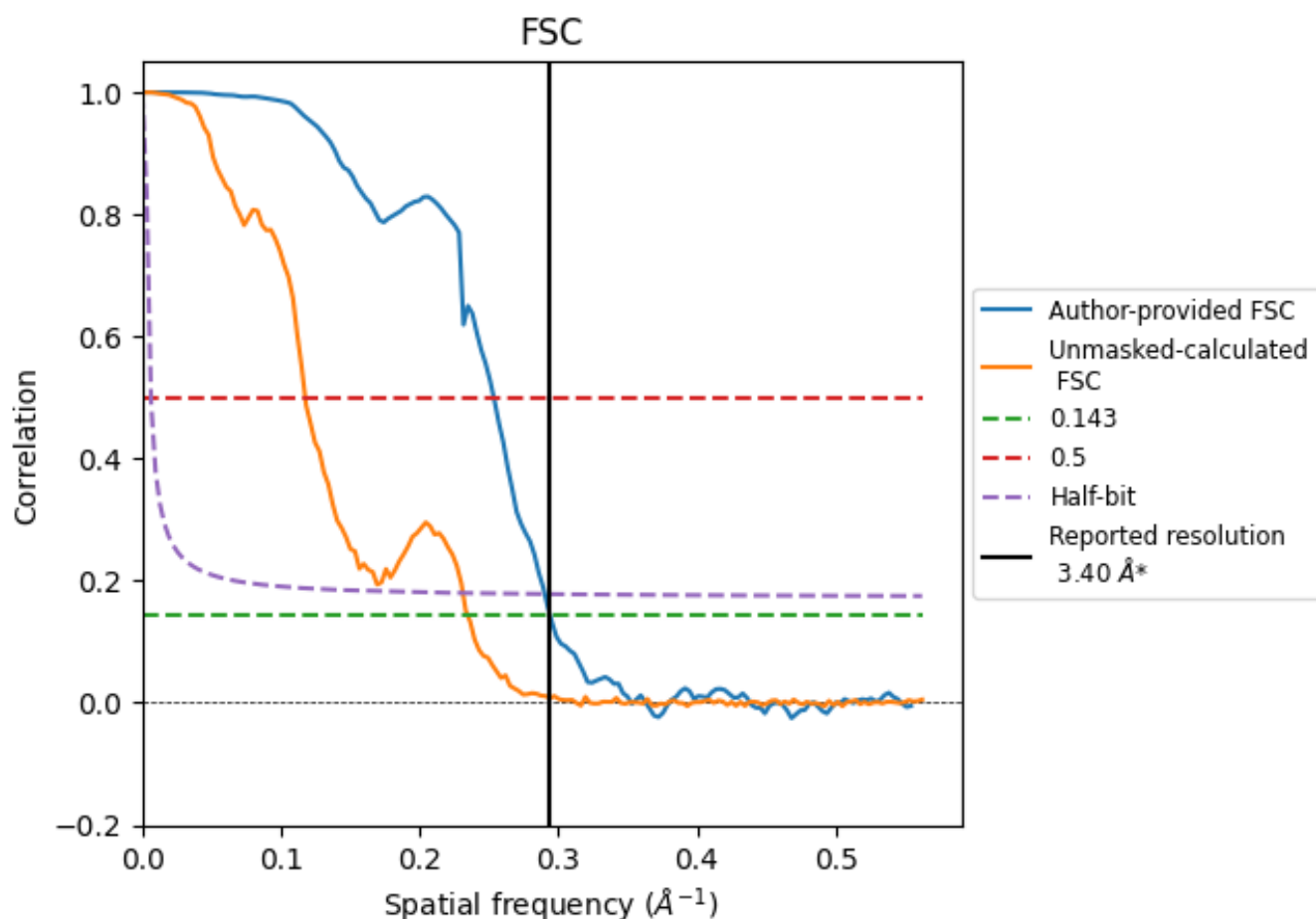


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

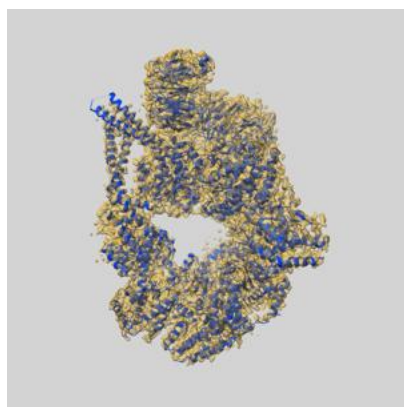
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.94	3.44
Unmasked-calculated*	4.26	8.50	4.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.26 differs from the reported value 3.4 by more than 10 %

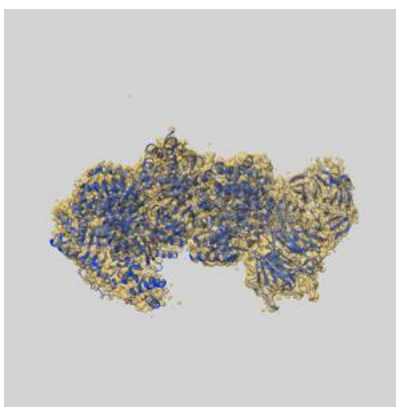
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46975 and PDB model 9DLE. Per-residue inclusion information can be found in section [3](#) on page [6](#).

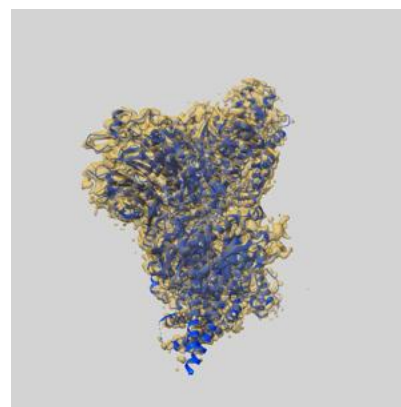
9.1 Map-model overlay [i](#)



X



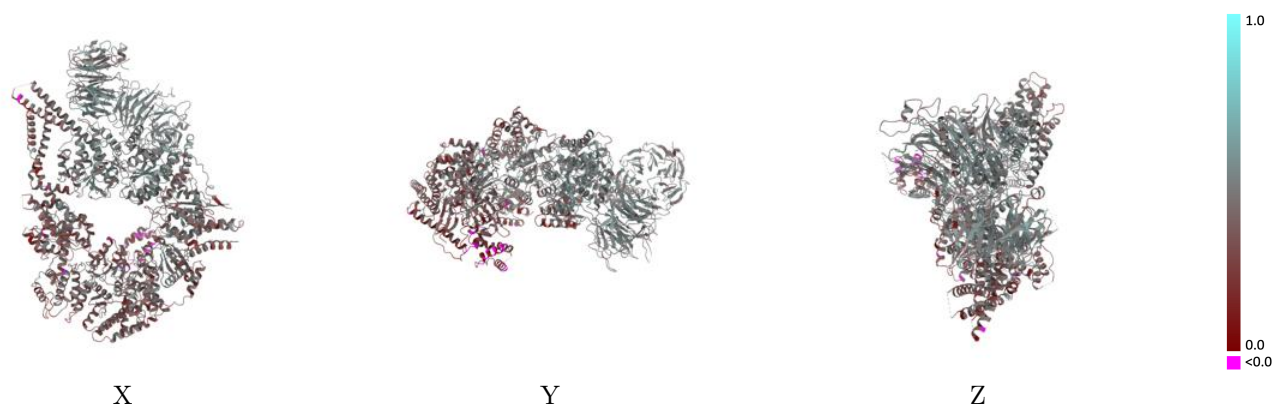
Y



Z

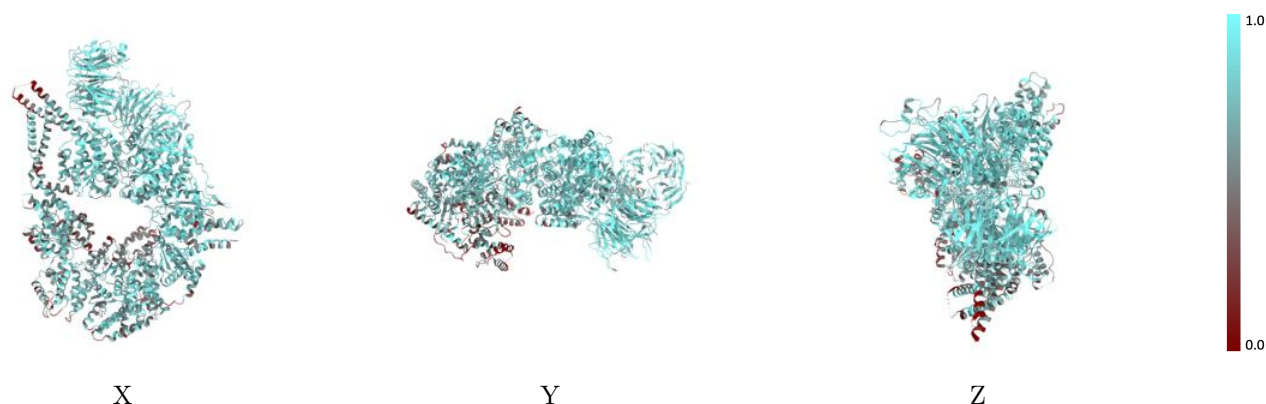
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



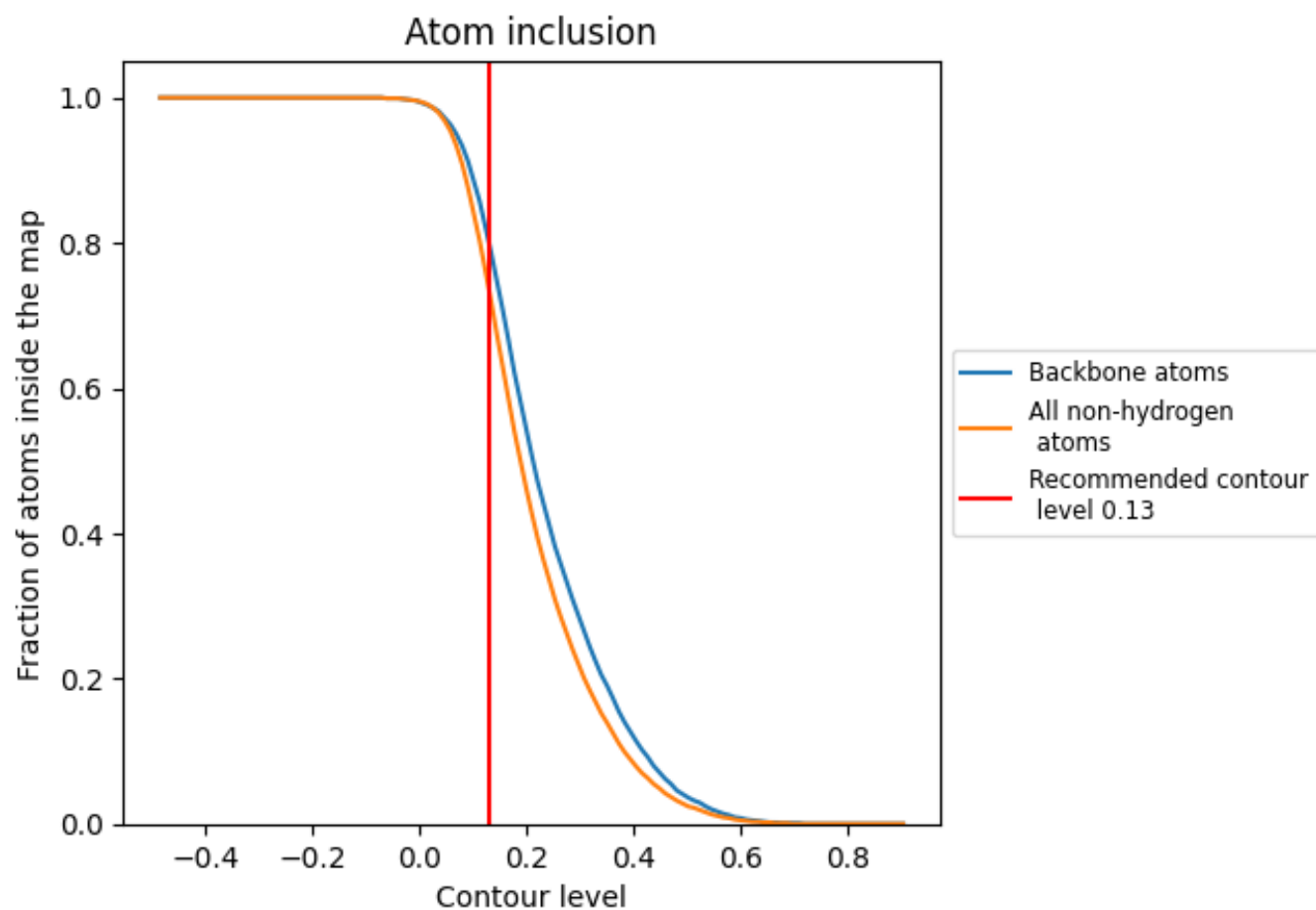
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7350	<div></div> 0.4230
A	<div></div> 0.7100	<div></div> 0.4050
B	<div></div> 0.8100	<div></div> 0.4880
C	<div></div> 0.8380	<div></div> 0.4920

