



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 02:53 AM UTC

PDB ID : 9DKE / pdb_00009dke
EMDB ID : EMD-46954
Title : CryoEM structures of yeast cytoplasmic dynein in the presence of ATP and Lis1.
Authors : Kendrick, A.A.; Leschziner, A.E.
Deposited on : 2024-09-08
Resolution : 3.60 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

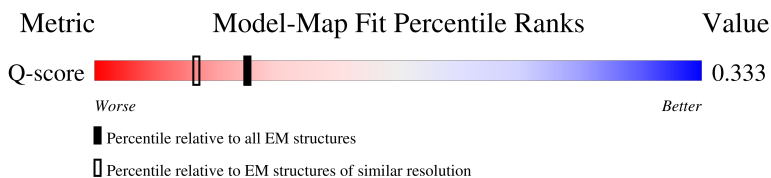
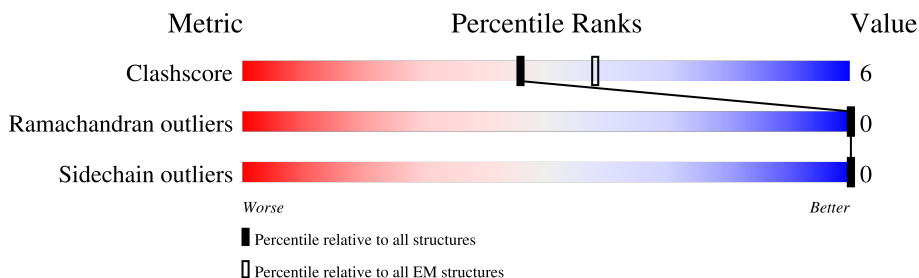
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17457 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.

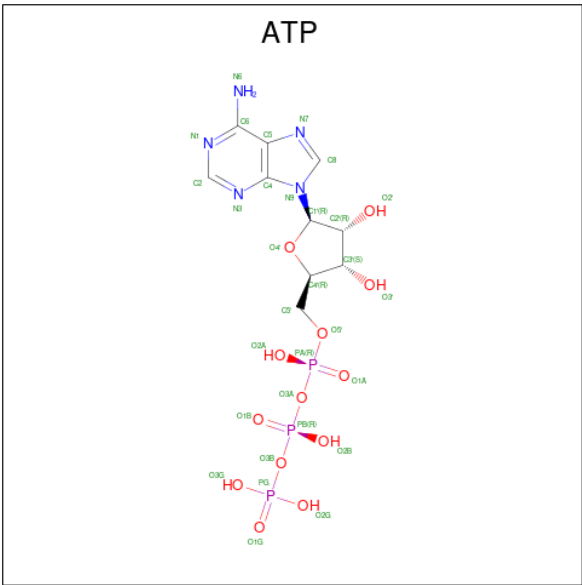
- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2291	Total	C	N	O	S	0	0
			17344	11142	2888	3245	69		

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 ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



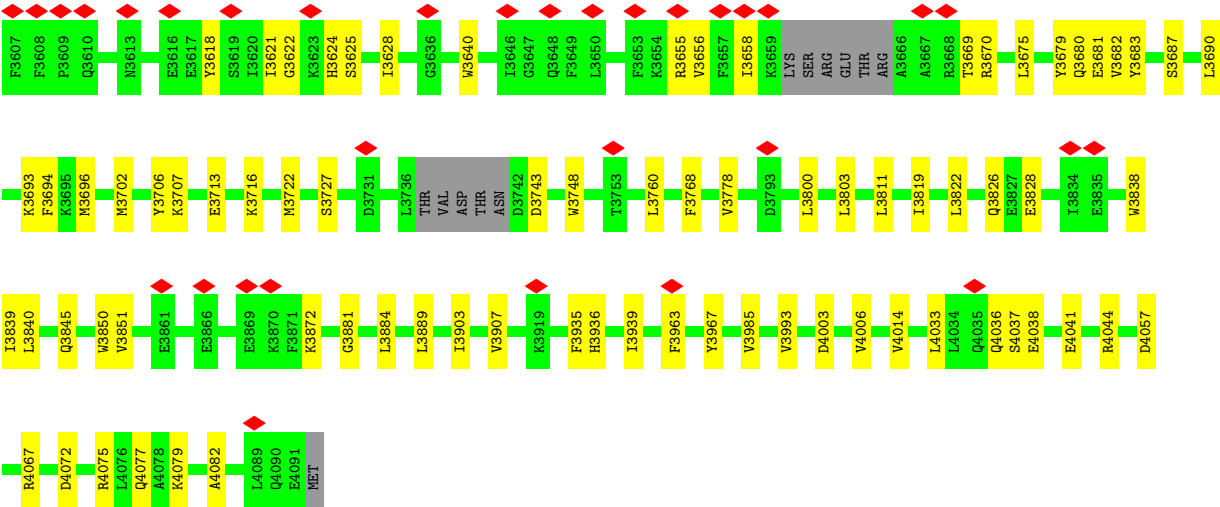
Continued from previous page...

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

D3547	L3465	I3329	ASN	SER	ASN	VAL	LEU	G3020	S2905	T2764	R2642	N2501	L2380	S2254
L3548	A3473	Y3330	ARG	ILE	ARG	CYS	LYS	L3021	N2910	G2765	S2643	L2506	I2385	D2255
I3549	G3482	E3331	VAL	VAL	SER	ALA	VAL	E3022	R2911	K2766	R2654	R2507	I2396	S2256
K3550	GLY	Y3332	SER	VAL	LYS	ILE	GLN	K3023	L2914	L2786	D2658	K2517	E2401	M2259
L3551	ASN	F3333	LYS	SER	ALA	GLY	GLU	L3024	Q2927	HIS	D2659	K2520	K2402	T2263
K3552	R3476	F3334	GLN	GLN	CYS	TYR	ASP	N3025	W2928	HIS	L2660	E2521	I2403	T2266
T3553	L3337	L3337	LYS	LYS	GLY	GLN	ILE	N3026	Q2928	SER	L2661	K2522	D2406	L2272
E3554	R3342	R3342	TYR	SER	PRO	PHE	ASP	E3027	D2934	ASN	VAL	H2530	L2408	L2273
Y3555	G3483	G3483	LEU	LEU	TRP	ASN	ARG	S3028	V2935	GLY	K2664	L2530	N2409	L2274
L3556	D3487	L3346	ILE	ILE	TRP	ARG	GLU	V3029	W2936	VAL	K2667	A2534	S2410	L2275
K3557	VAL	L3349	ARG	ARG	VAL	ASP	VAL	K3030	D2937	LYS	N2667	L2534	K2411	L2276
L3558	SER	K3350	VAL	VAL	ALA	GLN	MET	V3031	W2938	ASN	D2678	P2537	L2415	L2277
L3559	G3484	K3351	GLN	GLN	GLN	PHE	LYS	N3032	T2944	E2810	Q2684	H2537	L2408	L2278
K3560	L3353	L3353	ALA	ALA	ILE	ILE	ILE	E3033	E2947	D2818	Q2688	T2539	N2428	L2279
N3561	G3354	G3354	ASN	PHE	ASN	ARG	GLN	L3034	V2948	E2819	N2688	D2540	N2429	G2277
E3562	L3484	L3361	LYS	LYS	LYS	ASP	ASP	ASN	N2949	S2820	N2688	P2541	N2430	K2282
K3563	F3495	V3362	THR	THR	VAL	VAL	GLU	LEU	K2950	L2823	N2700	GLY	Y2438	K2283
K3564	F3496	N3363	MET	MET	VAL	ASP	PRO	SER	E2951	E2824	L2700	P2544	Y2438	L2290
L3565	P3501	V3364	ASN	ASN	GLY	ILE	THR	LYS	F2954	F2827	S2701	P2545	G2442	L2304
K3566	S3502	Y3369	VAL	VAL	ASP	ASN	LEU	SER	T2955	L2828	L2702	M2546	F2445	D2307
L3567	GLY	L3370	ALA	ALA	PRO	VAL	ALA	THR	E2956	E2829	D2703	R2549	D2448	T2314
E3568	D3504	T3372	ASN	ASN	LEU	TYR	GLY	LEU	Q2959	T2833	L2712	R2552	THR	Y2324
K3569	I3507	T3372	ASN	ASN	LEU	ASP	GLY	THR	R2962	D2839	L2713	I2556	THR	G2328
L3570	R3512	N3377	GLN	GLN	GLY	THR	VAL	LYS	K2962	L2840	L2716	L2557	GLU	D2329
N3571	V3513	F3377	LYS	LYS	THR	THR	GLY	GLU	T2968	E2717	E2717	Y2558	H2453	L2344
SER	H3517	K3386	ARG	ARG	ILE	ILE	ILE	GLU	VAL	S2737	M2732	Y2560	THR	T2345
GLN	T3520	E3392	ILE	ILE	MET	LYS	LYS	ALA	VAL	H2741	V2733	K2604	GLY	PHE
ASN	N3521	N3393	GLY	GLY	GLY	LYS	LYS	ARG	N2985	R2744	I2734	L2616	LYS	GLY
MET	K3522	L3408	THR	THR	GLU	GLN	GLN	THR	P2986	L2745	H2735	L2616	GLY	ASP
LEU	E3523	L3408	LEU	LEU	ILE	ILE	ILE	LEU	K2987	I2745	E2756	R2620	THR	ASP
GLU	S3524	K3414	LEU	LEU	ARG	ARG	THR	ASP	VAL	K2851	R2748	E2621	SER	GLN
ASP	I3525	V3417	LYS	LYS	LYS	LYS	LYS	LYS	VAL	N2854	A2748	L2622	GLN	LEU
E3582	R3528	I3418	THR	THR	THR	TYR	ILE	ASN	N2985	L2863	V2752	Q2753	LEU	S2354
L3583	I3529	S3419	LYS	LYS	LYS	MET	ARG	LEU	P2986	L2867	Q2753	T2623	GLU	D2355
K3584	F3530	N3420	ALA	ALA	ALA	GLU	SER	GLU	R2987	L2868	G2754	R2624	N2490	Y2356
V3585	D3531	T3426	LEU	LEU	LEU	GLY	VAL	ARG	Q2990	L2868	H2755	L2625	K2483	L2361
L3586	I3532	L3429	LEU	LEU	LEU	GLY	VAL	LYS	V3000	D2868	R2757	V2626	L2494	ALA
T3587	T3533	S3430	LEU	LEU	ALA	ASP	PRO	GLN	K3006	L2868	M2758	L2626	ASP	LYS
N3588	L3534	E3434	ALA	ALA	ALA	SER	PRO	ASN	Q3008	H2886	L2758	Q2637	LYS	ASN
K3589	T3535	V3449	ALA	ALA	ALA	ASP	PRO	GLY	E3012	V2887	L2759	R2637	TYR	ASP
L3590	E3536	Y3450	GLY	GLY	GLY	GLY	GLY	GLY	K3015	F2888	Q2760	Q2639	GLY	K2365
K3591	E3537	I3451	THR	THR	THR	THR	THR	THR	F3016	F2889	S2761	T2640	SER	L2366
K3592	E3540	Q3453	GLN	GLN	GLN	GLN	GLN	GLN	N3017	N2897	R2763	L2641	Q2500	
E3593	M3541	F3457	ASP	ASP	ASP	TYR	VAL	ALA	N3018	S2900				
K3594	Q3542		LEU	LEU	LEU	GLY	MET	THR	N3019					
L3595	K3543		THR	THR	THR	THR	THR	THR						
K3596	K3544		THR	THR	THR	THR	THR	THR						
I3597	R3545		THR	THR	THR	THR	THR	THR						
E3598	E3546		THR	THR	THR	THR	THR	THR						
K3599			THR	THR	THR	THR	THR	THR						
K3600			THR	THR	THR	THR	THR	THR						
L3601			THR	THR	THR	THR	THR	THR						
S3602			THR	THR	THR	THR	THR	THR						
E3603			THR	THR	THR	THR	THR	THR						
S3604			THR	THR	THR	THR	THR	THR						
E3605			THR	THR	THR	THR	THR	THR						
E3606			THR	THR	THR	THR	THR	THR						



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94448	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	0.655	Depositor
Minimum map value	-0.392	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	312.928, 312.928, 312.928	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: MG, 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	0/17665	0.40	0/23983

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	17344	0	16350	210	0
2	A	31	0	10	3	0
3	A	81	0	36	5	0
4	A	1	0	0	0	0
All	All	17457	0	16396	211	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 211 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:2282:ASN:HB3	1:A:2552:ARG:HG3	1.59	0.84
1:A:2489:ILE:HG23	1:A:2546:MET:HE1	1.75	0.67
1:A:1645:PHE:HB2	1:A:1697:LYS:HG2	1.78	0.65
1:A:3935:PHE:HB2	1:A:4014:VAL:HG11	1.79	0.65
1:A:3537:GLU:HB2	1:A:3670:ARG:HH12	1.63	0.64

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	2229/2875 (78%)	2175 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1758/2631 (67%)	1758 (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 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2264	ASN
1	A	3685	GLN
1	A	2481	ASN
1	A	3845	GLN
1	A	3517	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ATP	A	4101	-	32,33,33	0.36	0	48,52,52	0.36	0
3	ADP	A	4104	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
3	ADP	A	4102	-	28,29,29	1.42	4 (14%)	43,45,45	1.77	7 (16%)
3	ADP	A	4103	4	28,29,29	1.43	4 (14%)	43,45,45	1.94	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
2	ATP	A	4101	-	-	8/22/38/38	0/3/3/3
3	ADP	A	4104	-	-	4/16/32/32	0/3/3/3
3	ADP	A	4102	-	-	5/16/32/32	0/3/3/3
3	ADP	A	4103	4	-	7/16/32/32	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)
3	A	4103	ADP	C5-C4	4.85	1.47	1.39
3	A	4102	ADP	C5-C4	4.74	1.47	1.39
3	A	4104	ADP	C5-C4	4.65	1.47	1.39
3	A	4103	ADP	C5-C6	2.68	1.48	1.41
3	A	4104	ADP	C5-C6	2.60	1.48	1.41

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4103	ADP	C5-C4-N3	-6.71	117.47	126.72
3	A	4102	ADP	C5-C4-N3	-6.02	118.43	126.72
3	A	4104	ADP	C5-C4-N3	-5.86	118.65	126.72
3	A	4103	ADP	N3-C4-N9	5.45	136.43	127.17
3	A	4104	ADP	N3-C4-N9	4.70	135.16	127.17

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

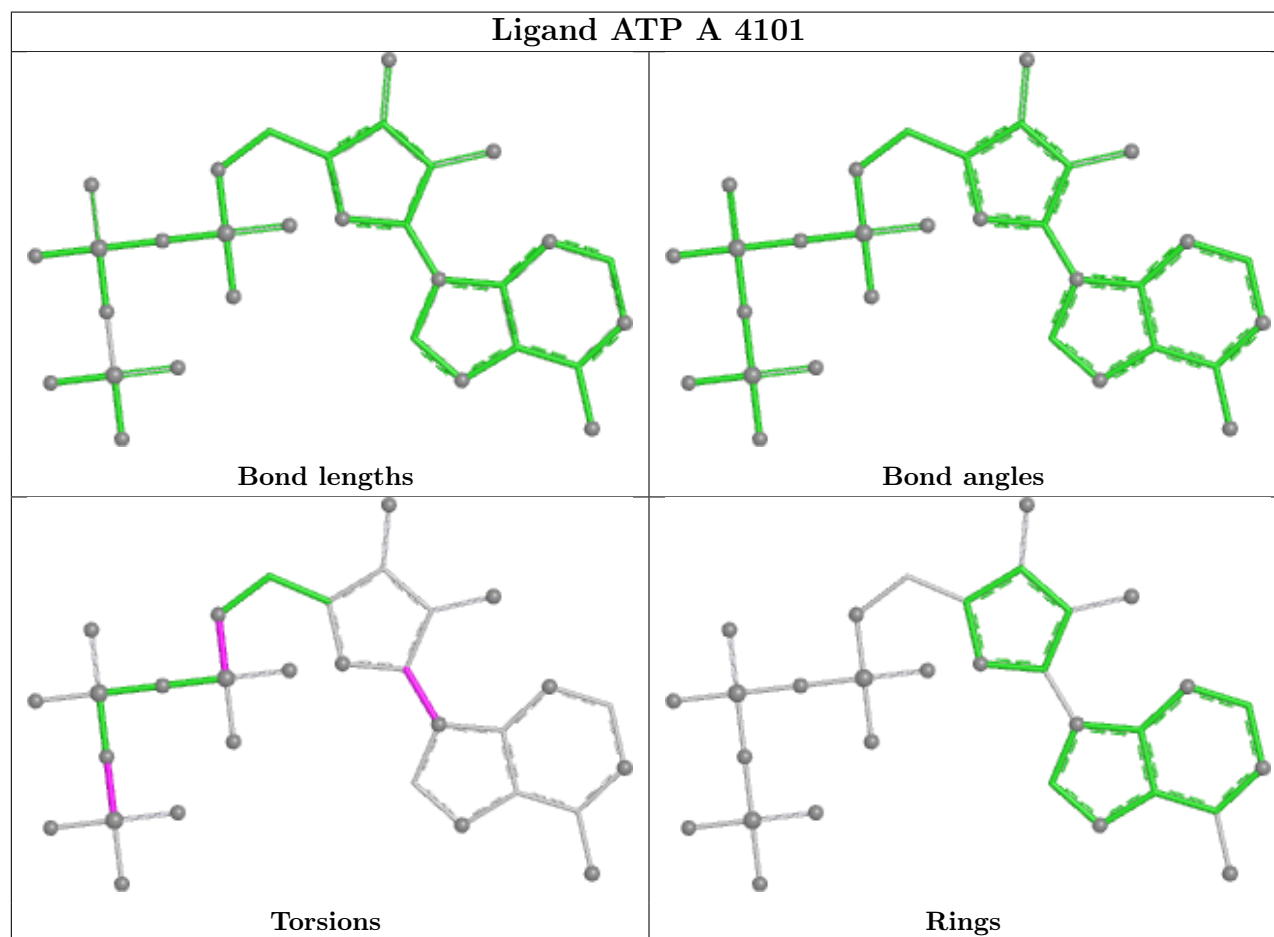
Mol	Chain	Res	Type	Atoms
2	A	4101	ATP	C5'-O5'-PA-O1A
2	A	4101	ATP	C5'-O5'-PA-O2A
2	A	4101	ATP	C5'-O5'-PA-O3A
3	A	4102	ADP	C5'-O5'-PA-O3A
3	A	4103	ADP	C5'-O5'-PA-O1A

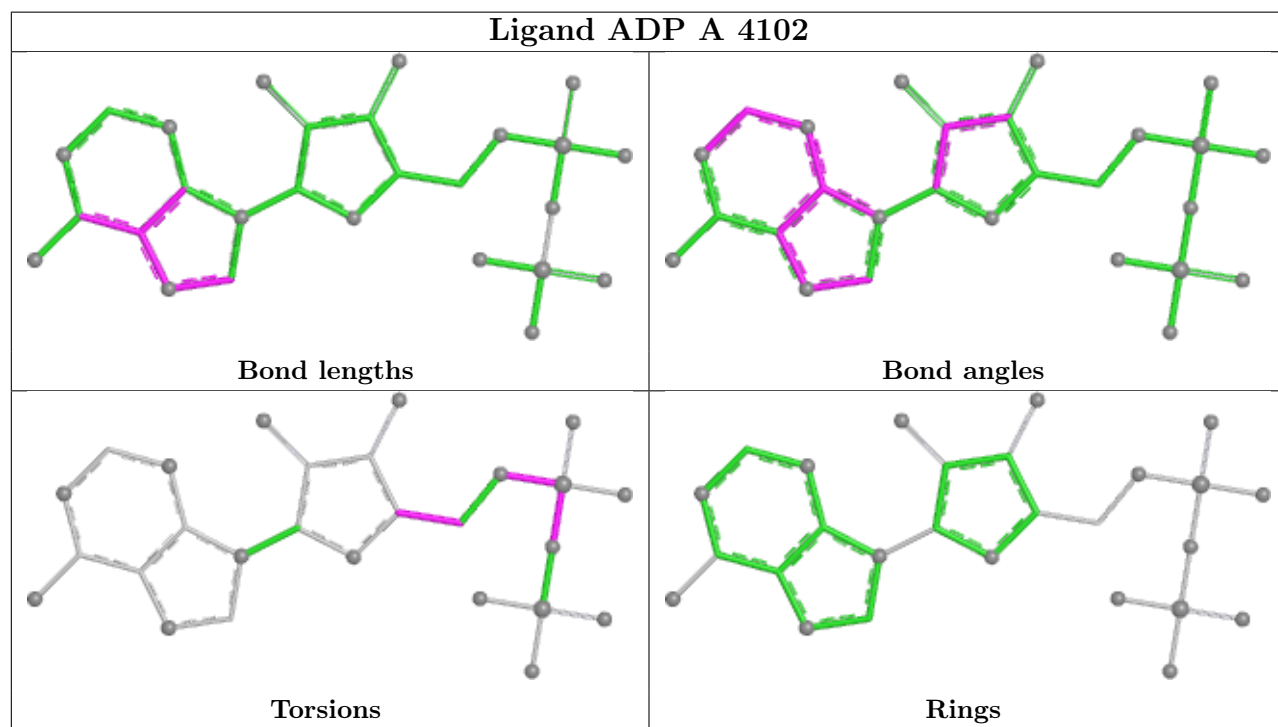
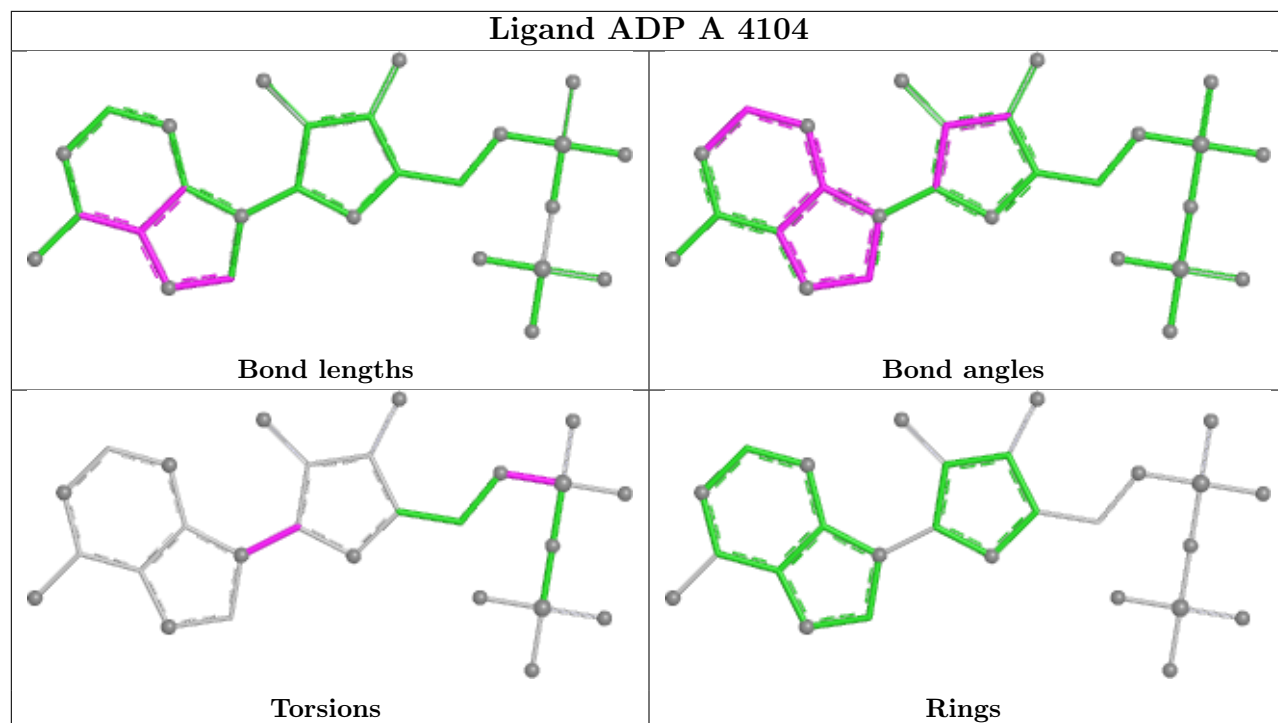
There are no ring outliers.

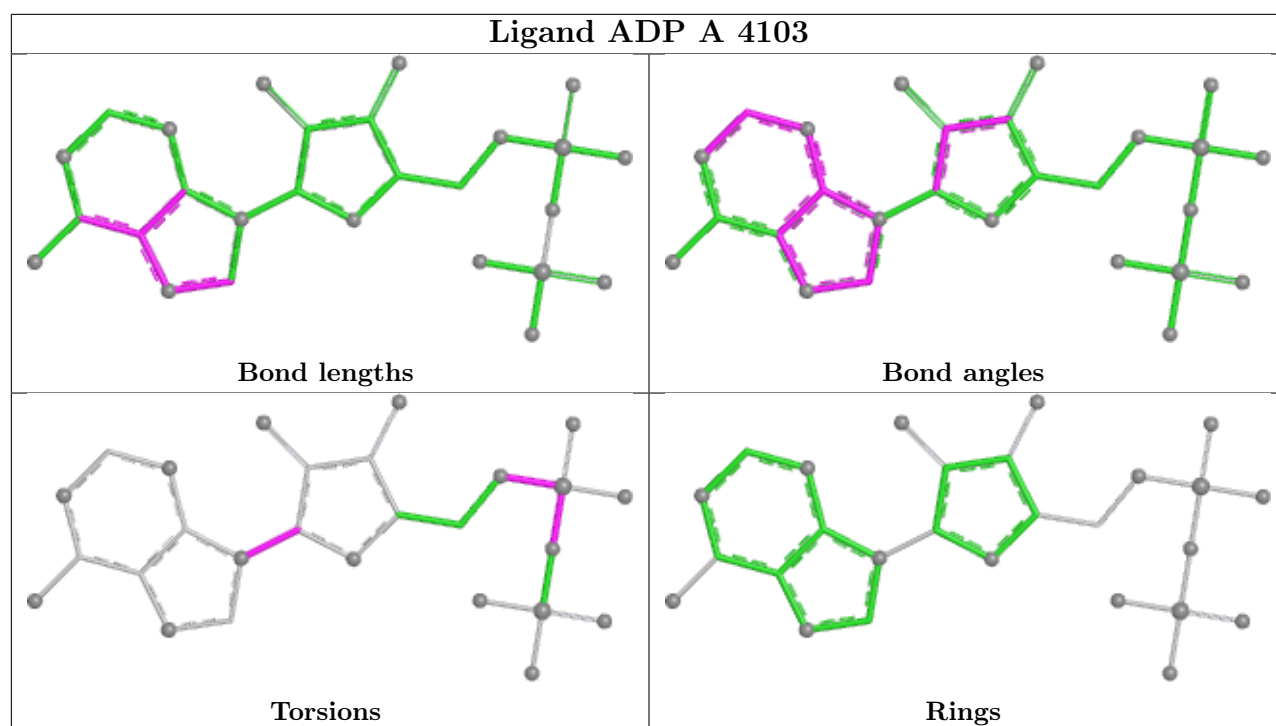
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4101	ATP	3	0
3	A	4104	ADP	2	0
3	A	4102	ADP	2	0
3	A	4103	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.

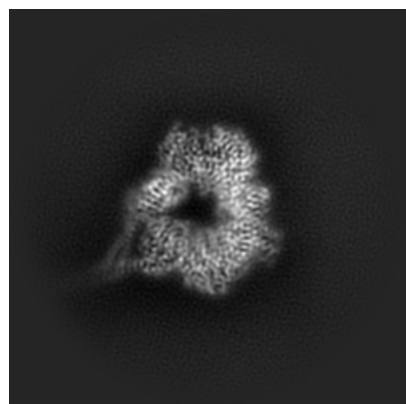
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46954. These allow visual inspection of the internal detail of the map and identification of artifacts.

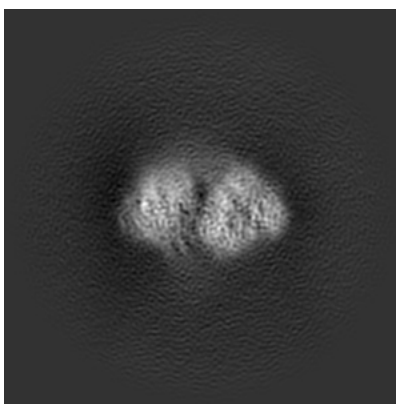
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

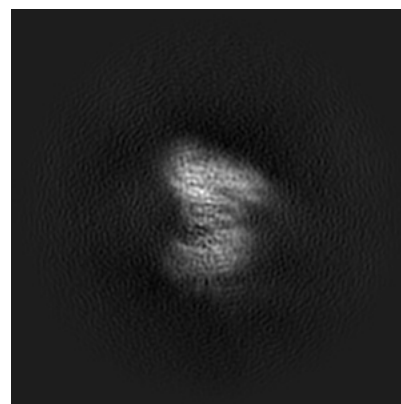
6.1.1 Primary map



X

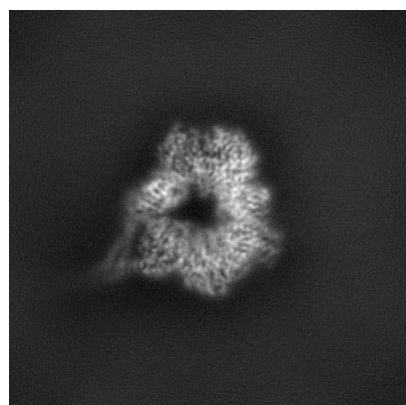


Y

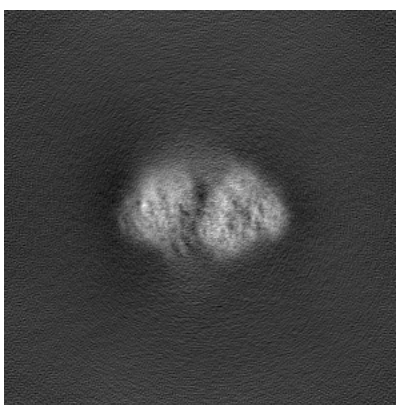


Z

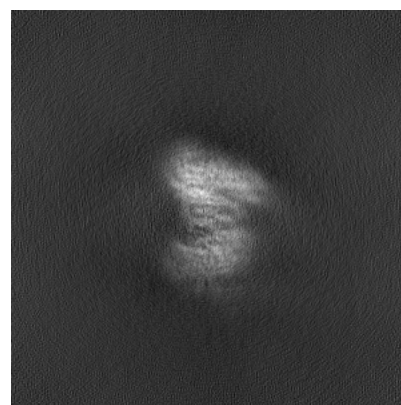
6.1.2 Raw map



X



Y

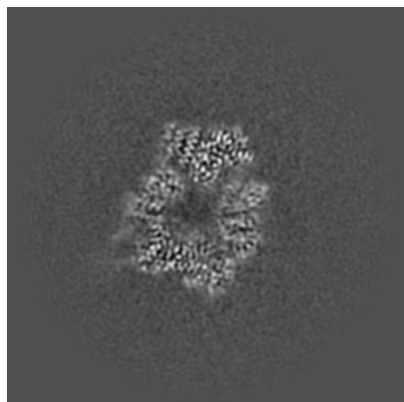


Z

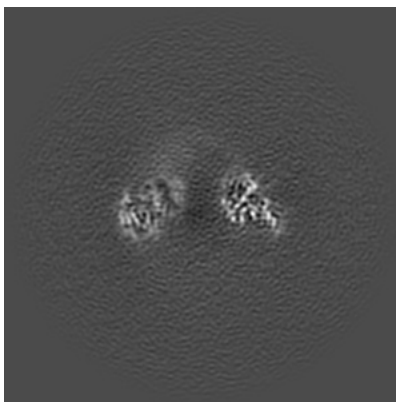
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

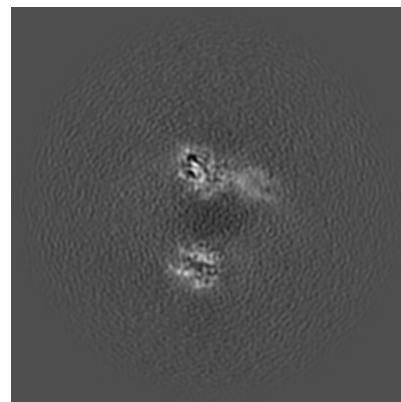
6.2.1 Primary map



X Index: 176

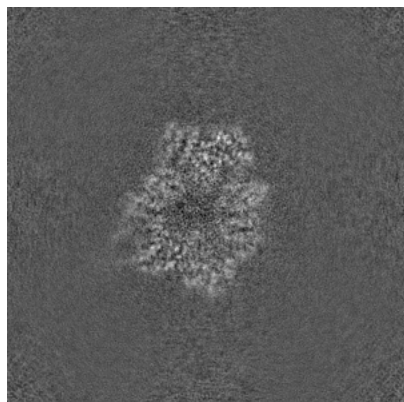


Y Index: 176

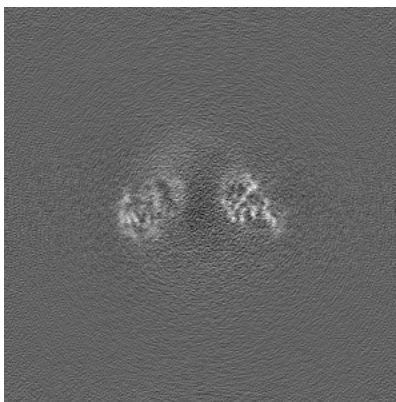


Z Index: 176

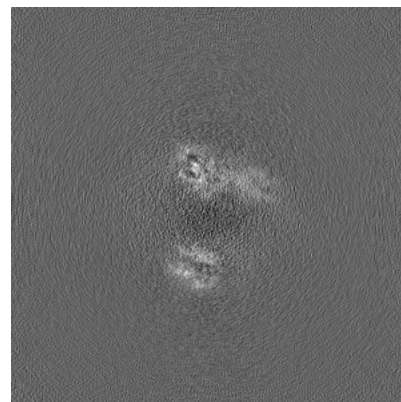
6.2.2 Raw map



X Index: 176



Y Index: 176

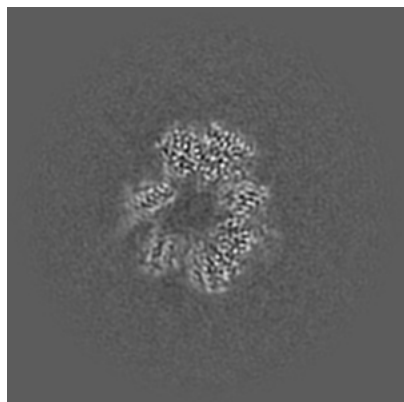


Z Index: 176

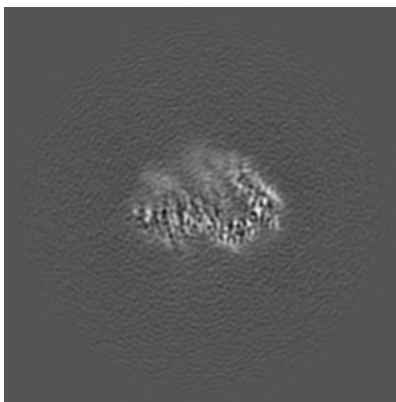
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

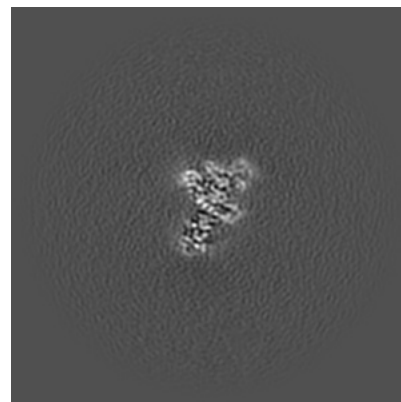
6.3.1 Primary map



X Index: 166

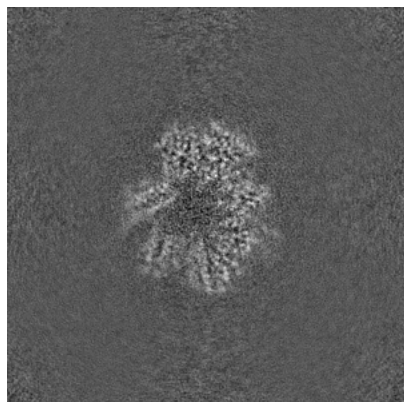


Y Index: 199

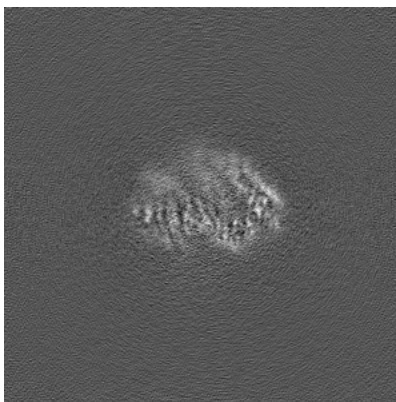


Z Index: 218

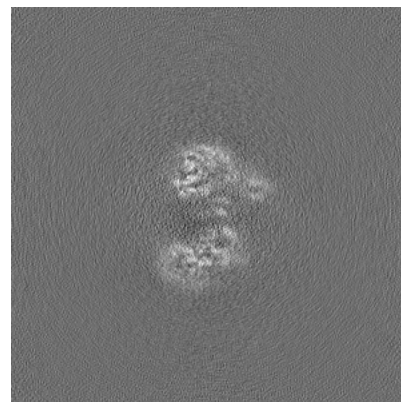
6.3.2 Raw map



X Index: 166



Y Index: 199

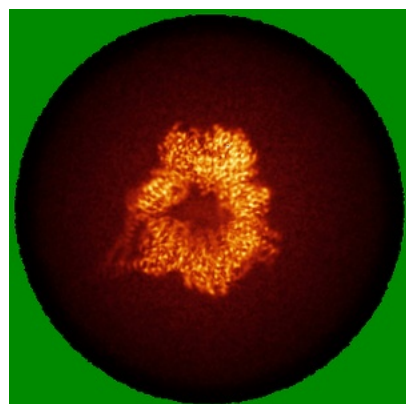


Z Index: 189

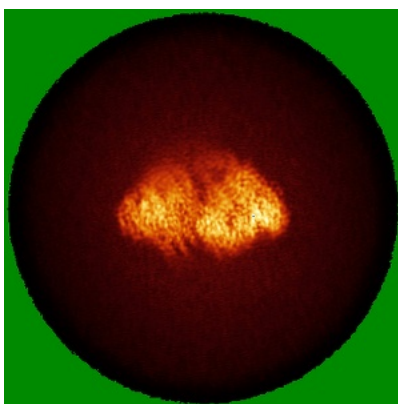
The images above show the largest variance slices of the map in three orthogonal directions.

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

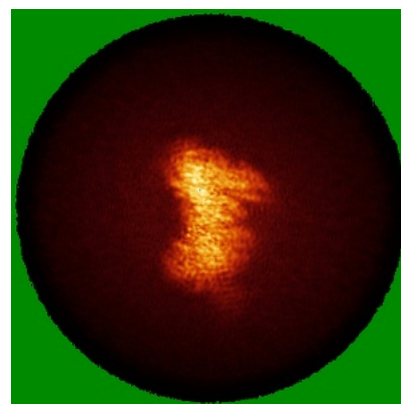
6.4.1 Primary map



X

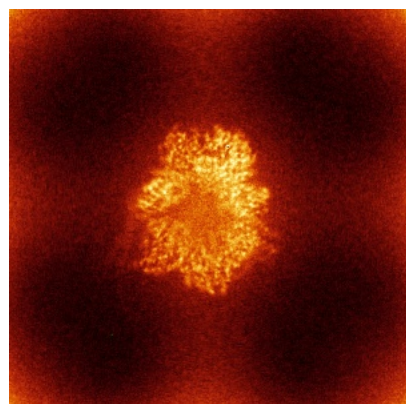


Y

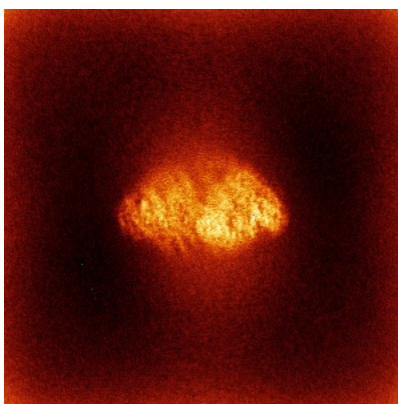


Z

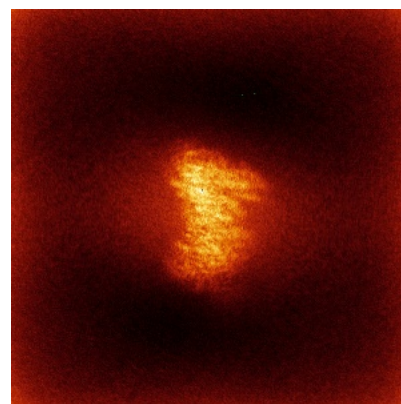
6.4.2 Raw map



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.

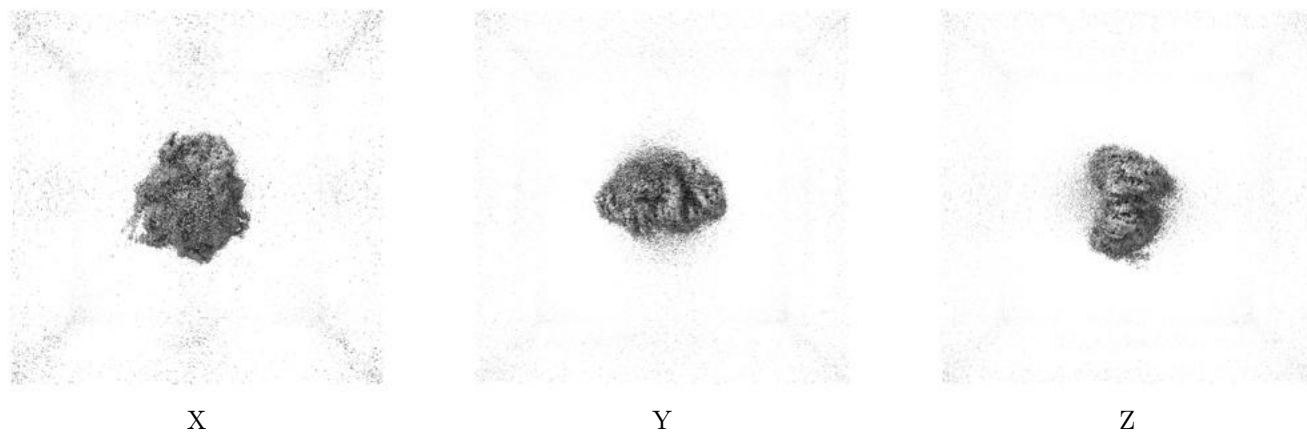
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

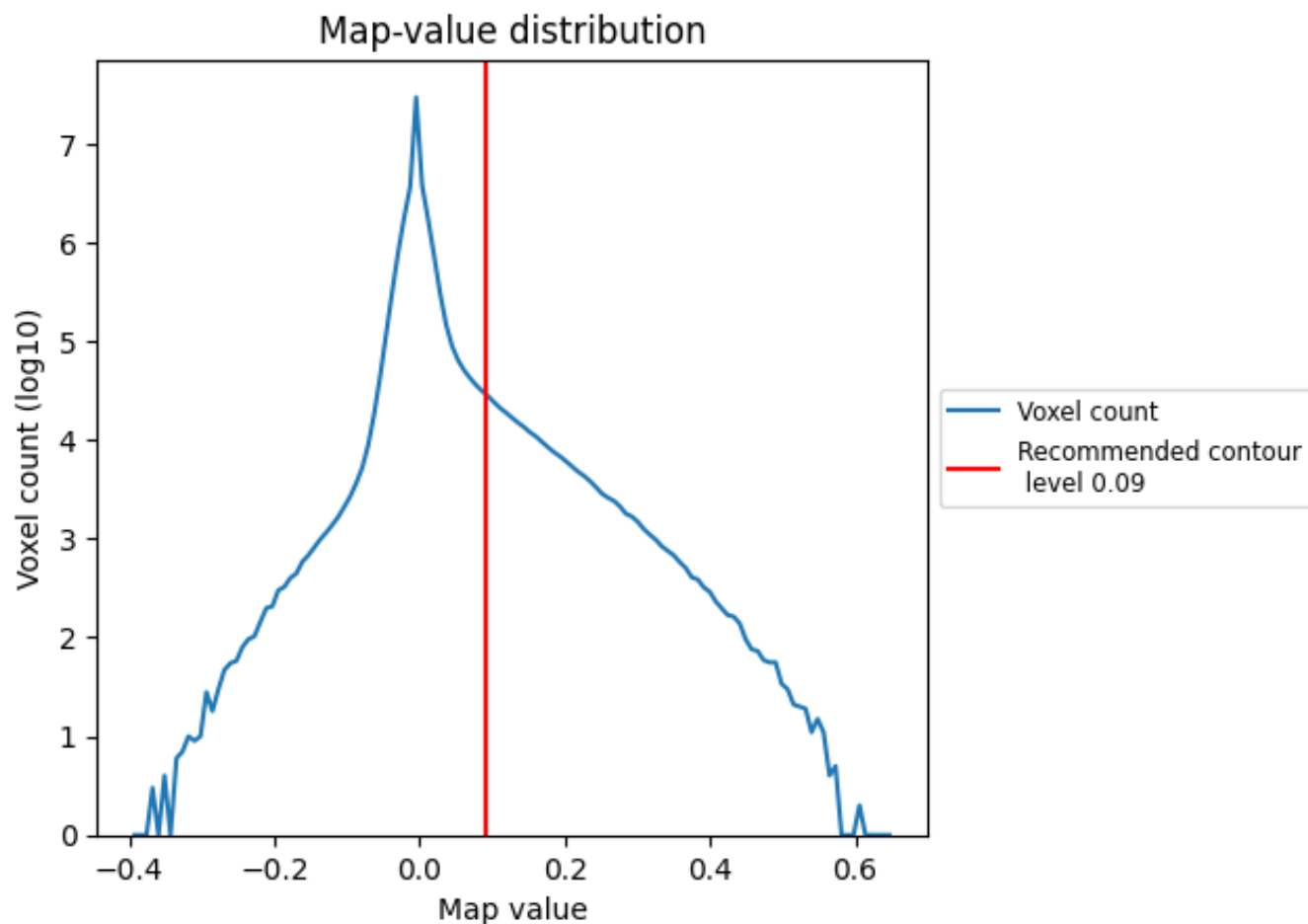
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

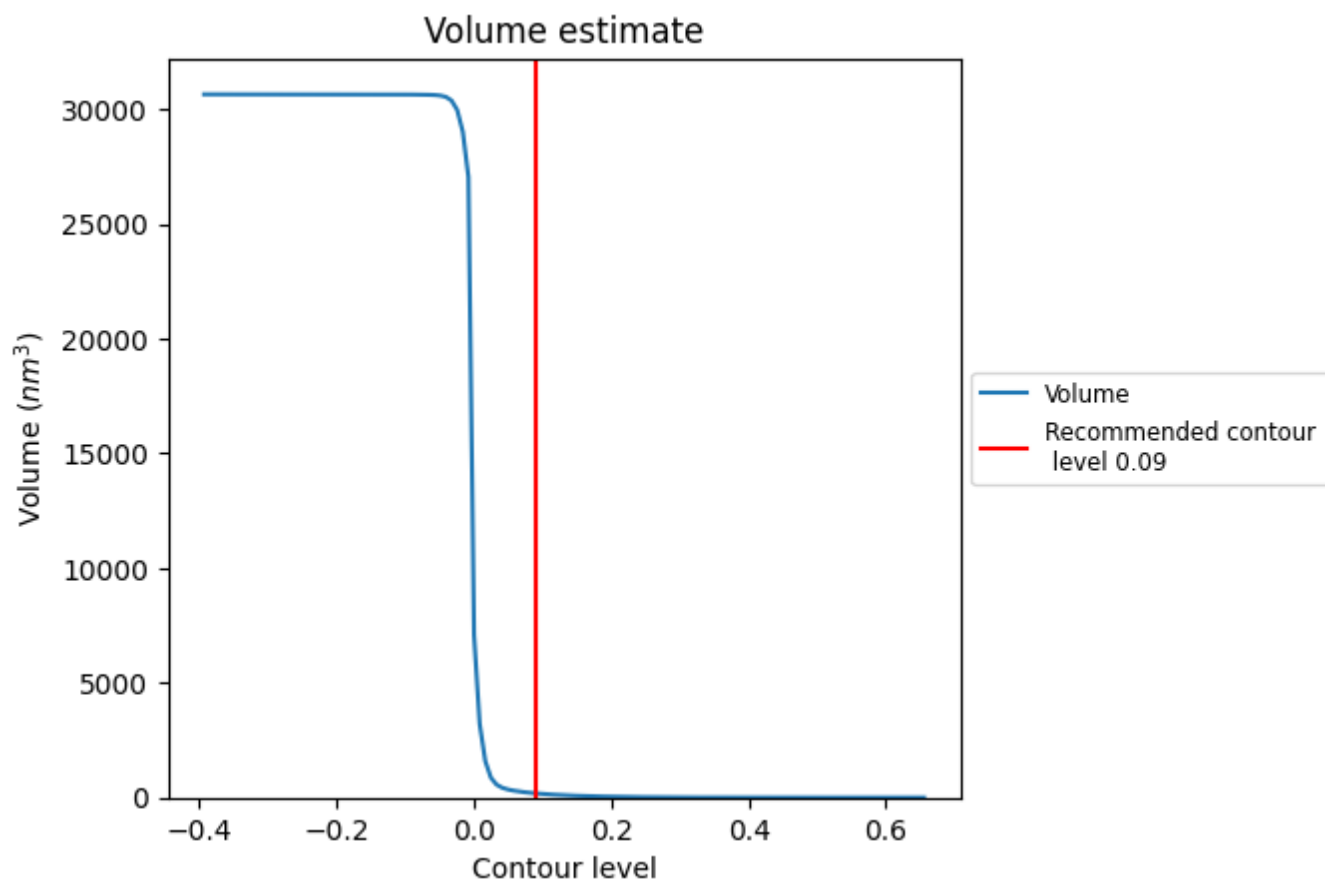
This section contains the results of statistical analysis of the map.

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.

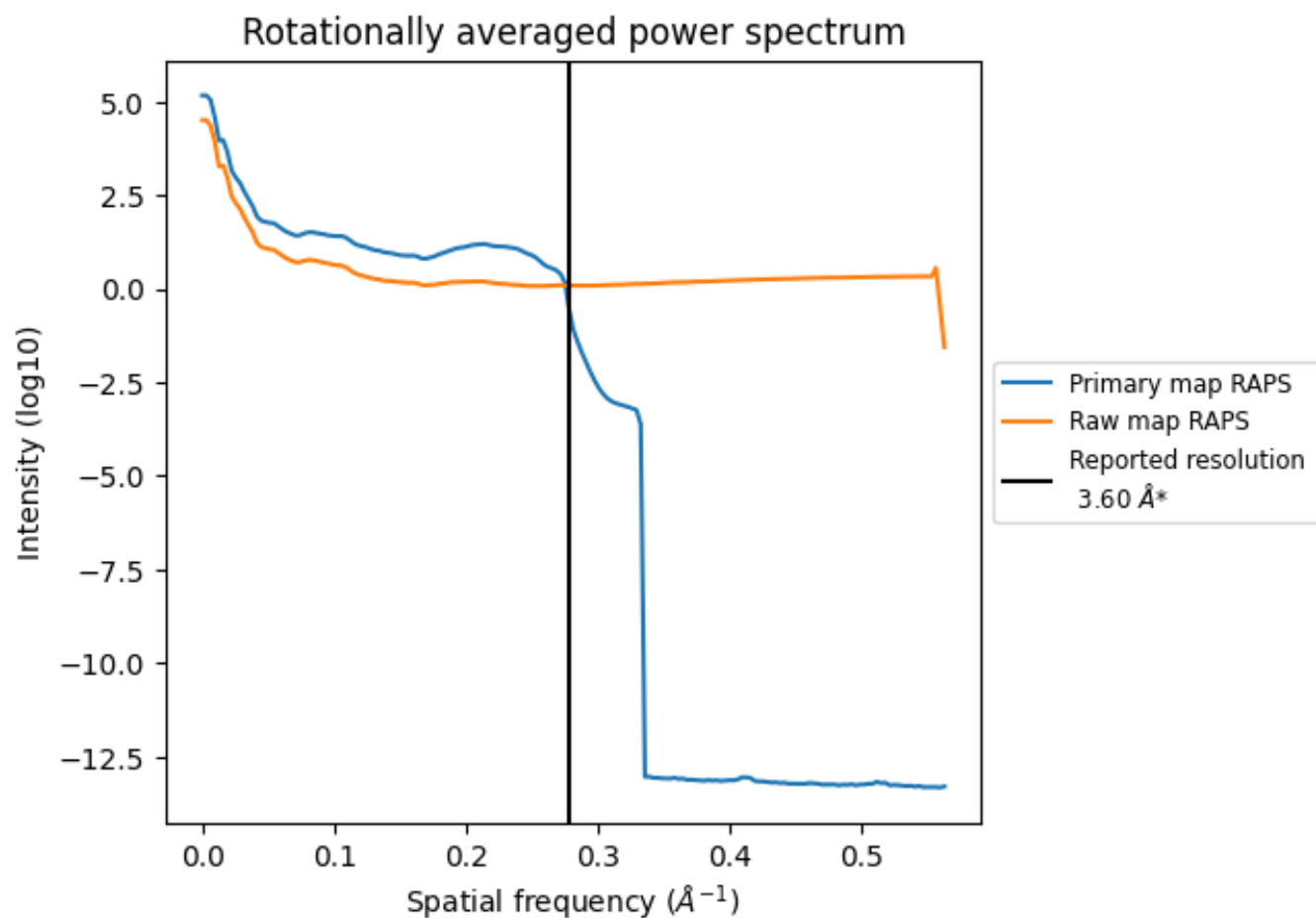
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 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 ⓘ

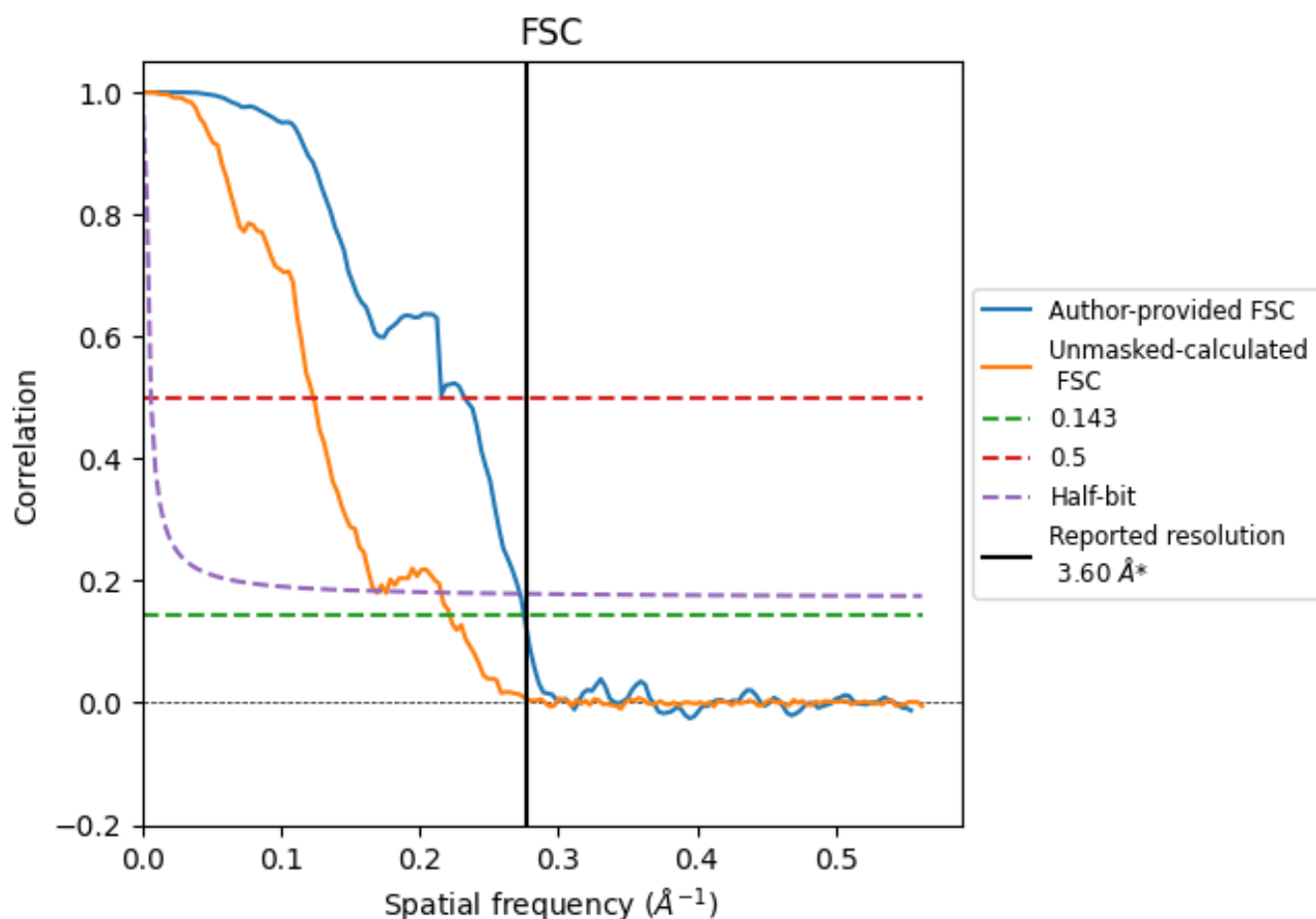


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

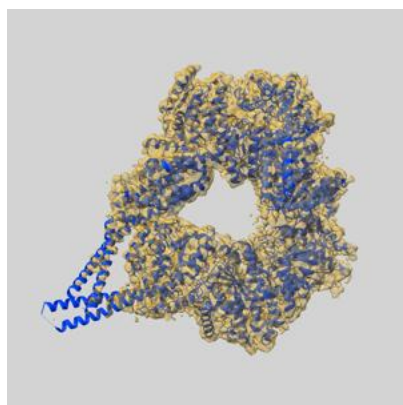
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.63	4.30	3.67
Unmasked-calculated*	4.51	8.10	5.94

*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 4.51 differs from the reported value 3.6 by more than 10 %

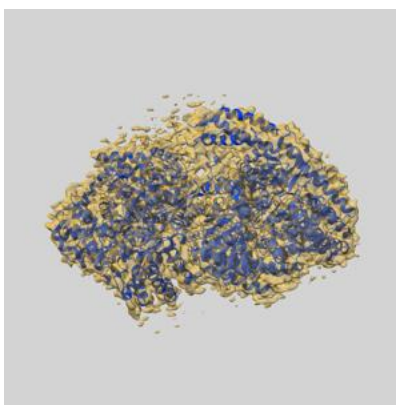
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46954 and PDB model 9DKE. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

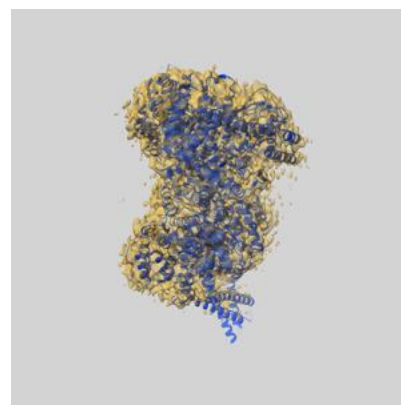
9.1 Map-model overlay [i](#)



X



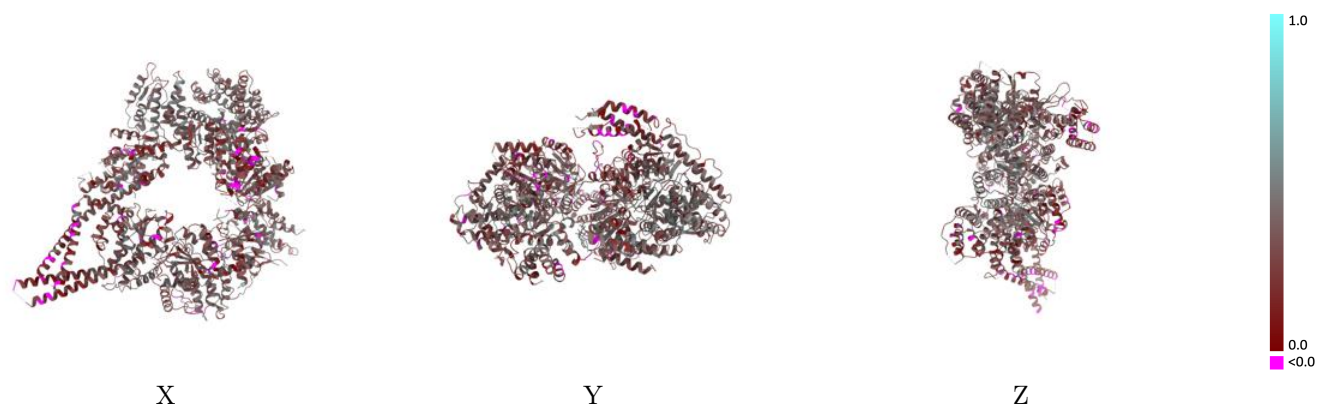
Y



Z

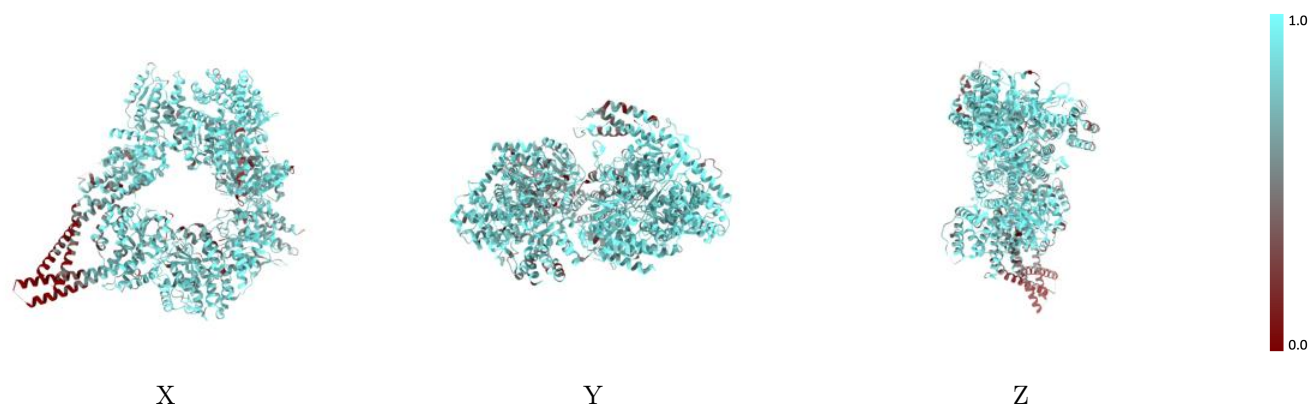
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



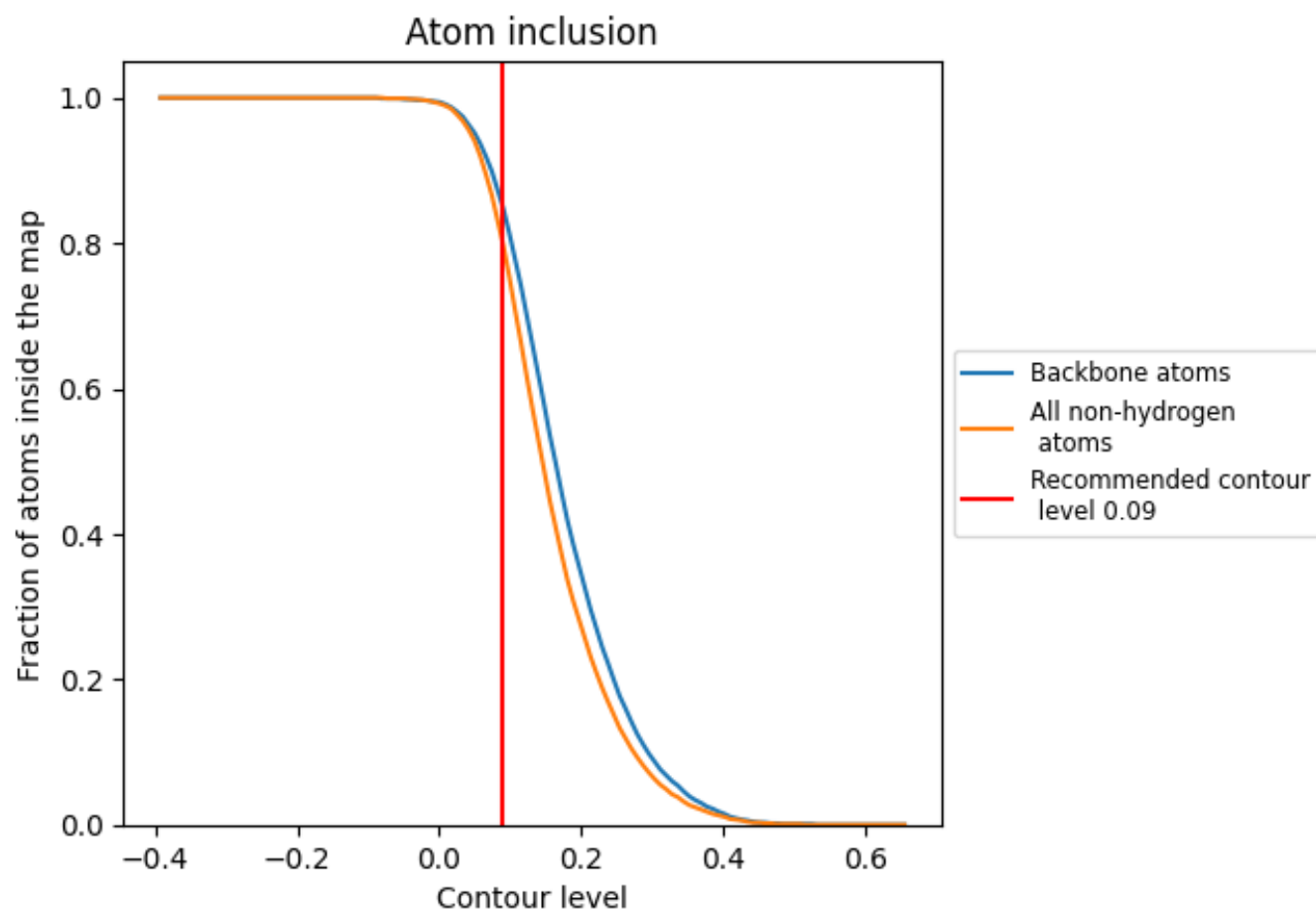
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.3330
A	0.7980	0.3330

