



wwPDB EM Validation Summary Report ⓘ

Aug 23, 2026 – 12:16 AM JST

PDB ID : 27QA / pdb_000027qa
EMDB ID : EMD-81337
Title : Dictyostelium discoideum cytoplasmic dynein motor domain in the presence of ADP (Apo state 1)
Authors : Shimo-Kon, R.; Tokita, H.; Imai, H.; Maeshima, T.; Kon, T.
Deposited on : 2026-06-09
Resolution : 2.76 Å(reported)
Based on initial model : 3VKG

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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

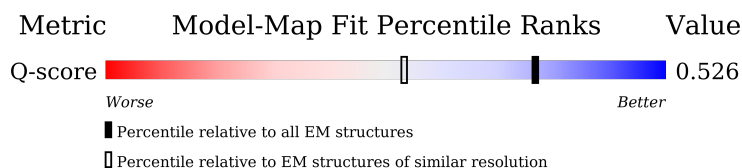
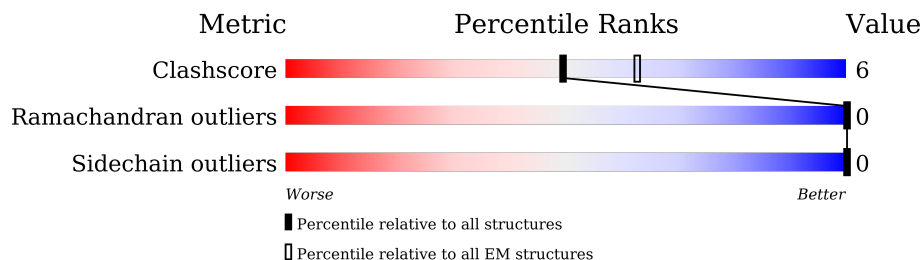
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.76 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	10642 (2.26 - 3.26)

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	3367	9% 77% 14% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24612 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.

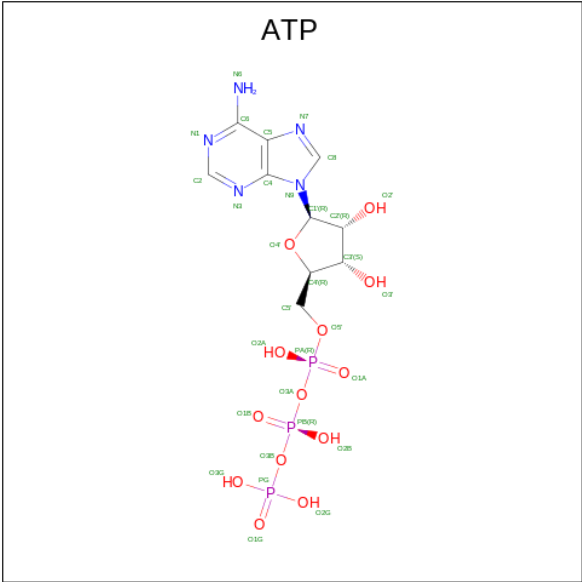
- Molecule 1 is a protein called Dynein heavy chain, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3046	Total	C	N	O	S	0	0
			24526	15649	4181	4599	97		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1364	MET	-	initiating methionine	UNP P34036
A	1365	THR	-	expression tag	UNP P34036
A	1366	ARG	-	expression tag	UNP P34036
A	1367	HIS	-	expression tag	UNP P34036
A	1368	HIS	-	expression tag	UNP P34036
A	1369	HIS	-	expression tag	UNP P34036
A	1370	HIS	-	expression tag	UNP P34036
A	1371	HIS	-	expression tag	UNP P34036
A	1372	HIS	-	expression tag	UNP P34036
A	1373	GLY	-	expression tag	UNP P34036
A	1374	GLY	-	expression tag	UNP P34036
A	1375	GLY	-	expression tag	UNP P34036
A	1376	ASP	-	expression tag	UNP P34036
A	1377	TYR	-	expression tag	UNP P34036
A	1378	LYS	-	expression tag	UNP P34036
A	1379	ASP	-	expression tag	UNP P34036
A	1380	ASP	-	expression tag	UNP P34036
A	1381	ASP	-	expression tag	UNP P34036
A	1382	ASP	-	expression tag	UNP P34036
A	1383	LYS	-	expression tag	UNP P34036
A	1384	GLY	-	expression tag	UNP P34036
A	1385	GLY	-	expression tag	UNP P34036
A	1386	GLY	-	expression tag	UNP P34036
A	1387	LYS	-	expression tag	UNP P34036

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

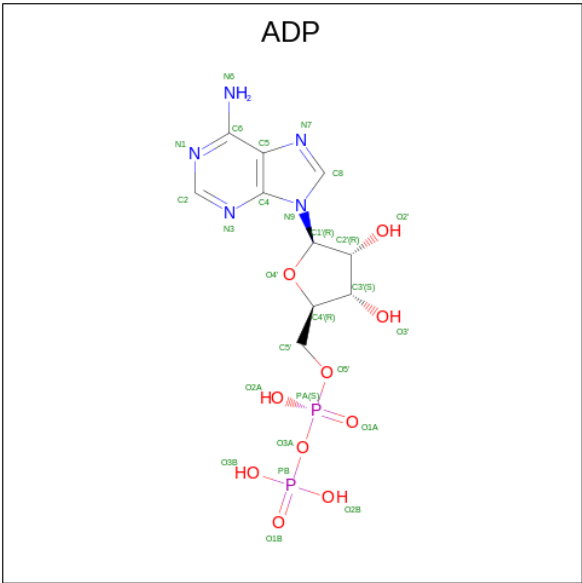


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (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	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Dynein heavy chain, cytoplasmic



Y4157	L3923	Q3794	W3617	ILE	ARG	CYS	ASP	L3289	D3124	R2969	V2767	R2685	A2490
P4169	D3932	R3806	P3635	THR	ALA	LEU	VAL	K3290	S3125	Y2980	G2771	R2680	G2491
I4175	L3940	K3818	S3639	LYS	LYS	GLY	ASN	L3292	E3126	L2990	S27716	H2667	Q2495
A4178	L3943	L3819	D3655	GLY	ALA	LYS	GLY	R3293	E3127	V3004	T2779	H2669	K2496
G4182	Q3820	G3821	E3656	LYS	LYS	LYS	ALA	D3294	L3128	A3012	L2783	L2672	V2515
T4183	F3823	F3822	L3657	THR	VAL	GLN	GLN	T3295	E3129	L3014	D2784	L2684	H2524
W4184	L3824	L3823	E3660	LEU	LYS	TRP	VAL	A3297	L3130	L3015	Q2787	T2686	L2534
W4185	Q3825	Q3824	N3661	ARG	ALA	ASP	ALA	Q3298	K3131	Q3018	F2788	T2687	R2543
L4186	L3827	L3826	R3670	THR	THR	ILE	TYR	V3299	F3145	V3042	P2812	L2684	S2544
L4187	R3828	R3827	D3676	GLN	ALA	ASP	ALA	K3300	N3148	N3043	L2924	T2687	T2544
I4190	L3830	L3829	A3681	LYS	THR	LYS	ALA	D3301	P3149	N3043	L2699	D2693	V2546
L4197	L3833	L3832	L3685	THR	THR	ILE	GLY	Q3303	D3153	N3044	M2836	F2694	N2547
W4198	E3831	E3830	R3713	GLY	THR	MET	GLY	V3304	P3162	N3045	L2699	L2554	H2555
Q4199	E3832	E3831	F3714	ASP	THR	PRO	GLU	S3305	N3166	Y3046	A2946	S2556	S2556
L4200	L3836	L3835	V3723	ILE	ILE	ILE	ILE	A3307	L3170	D3053	E2855	D2557	D2557
K4202	S3839	S3838	D3727	LYS	LYS	SER	ILE	Q3309	T3189	D3054	L2709	F2558	F2558
K4203	Q3840	Q3839	P3728	ILE	PRO	ILE	GLU	N3310	L3192	G3063	Y2872	P2562	P2562
H4205	L3842	L3841	L3730	ARG	LEU	ASN	GLN	E3312	G3213	L3079	P2876	T2713	E2563
L4011	Q3844	Q3843	N3735	GLY	GLY	THR	VAL	L3313	N3214	E3080	S2880	F2714	W2564
L4012	L3846	L3845	L3746	VAL	VAL	LYS	SER	D3314	L3215	S3081	R2884	D2715	L2581
Q4016	D3847	D3846	D3751	THR	GLY	MET	THR	VAL	R3224	S3082	I2890	E2719	L2581
L4020	Q3752	Q3751	Q3752	ILE	GLN	MET	ILE	ASN	V3227	F3083	K2721	Y2720	S2584
K4045	L3753	L3752	L3753	LYS	LEU	THR	LYS	GLY	L3231	L3084	R2722	T2723	F2596
D4051	V3754	V3753	V3754	ASN	GLY	MET	LYS	GLN	L3234	E3085	P2724	T2723	T2597
M4079	P3758	P3757	P3758	ALA	ASN	ARG	ASP	ASN	L3234	R3086	S2725	T2723	Q2598
I4083	F3765	F3764	F3765	LEU	GLY	GLY	ILE	GLN	E3101	L3091	Q2726	T2602	A2601
S3853	T3766	T3765	T3766	LYS	LYS	ILE	ILE	LYS	G3102	E3101	E2922	T2603	L2600
T3854	R3767	R3766	R3767	THR	LEU	THR	SER	GLN	E3103	L2935	L2730	P2606	P2606
L3855	D3768	D3767	D3768	GLY	GLN	LYS	SER	VAL	F3104	K2936	R2731	A2607	A2607
E3856	A3771	A3770	A3771	ASP	ASP	THR	THR	ASP	T3106	H2937	T2733	W2608	W2608
K3860	S3779	S3778	S3779	LEU	ILE	GLY	PRO	GLN	A3107	V2941	Q2734	S2616	S2616
E3864	R3780	R3779	R3780	ALA	THR	PHO	ALA	ALA	H3110	N2942	G2736	W2627	W2627
V3882	V3781	V3780	V3781	ILE	THR	PHE	GLY	VAL	C3112	L2943	K2737	E2637	E2637
N3887	F3786	F3785	F3786	THR	ALA	ASP	ASP	THR	K3113	D2944	P2749	K2640	K2640
C3893	T3787	T3786	T3787	LYS	LEU	THR	LYS	LYS	E3114	P2949	T2756	V2641	V2641
S3904	S3792	S3791	S3792	GLY	GLY	GLY	MET	GLY	T3115	Q2757	Q2757	A2642	A2642
Q3905	F3598	F3597	F3598	VAL	VAL	VAL	ALA	ASP	A3116	K2958	V2759	V2647	V2647
Y3909	Y3601	Y3600	Y3601	ASN	SER	ASN	VAL	ARG	Q3117	D2959	F2762	V2651	V2651
F3916	Q3607	Q3606	Q3607	LEU	LEU	LEU	LEU	GLY	R3118	N3119	M2766	D2652	D2652
I3919	R3610	R3609	R3610	LEU	LEU	LEU	VAL	GLN	L3122	L3123			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1347494	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF parameters were estimated using Patch CTF estimation in cryoSPARC and further refined by global and local CTF refinement.	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.194	Depositor
Minimum map value	-1.356	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	261.9, 261.9, 261.9	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87299997, 0.87299997, 0.87299997	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	0.16	0/25047	0.30	0/33929

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	24526	0	24587	279	0
2	A	31	0	12	0	0
3	A	1	0	0	0	0
4	A	54	0	24	0	0
All	All	24612	0	24623	279	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 279 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:2440:ASP:HB2	1:A:2443:GLU:HG2	1.53	0.89
1:A:3292:LEU:HB3	1:A:3571:ARG:HH22	1.36	0.89
1:A:3788:VAL:O	1:A:3792:SER:OG	1.96	0.83
1:A:4190:ILE:HB	1:A:4197:LEU:HD21	1.61	0.81
1:A:2642:ALA:HB3	1:A:2884:ARG:HG3	1.66	0.75

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	3036/3367 (90%)	2975 (98%)	61 (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	2749/3028 (91%)	2749 (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 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4040	ASN
1	A	4073	GLN
1	A	4247	ASN
1	A	2717	HIS
1	A	2661	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	5004	-	27,29,29	0.53	0	42,45,45	0.55	0
4	ADP	A	5003	-	27,29,29	0.50	0	42,45,45	0.43	0
2	ATP	A	5001	3	29,33,33	0.57	0	44,52,52	0.54	0

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	5004	-	-	3/16/32/32	0/3/3/3
4	ADP	A	5003	-	-	5/16/32/32	0/3/3/3
2	ATP	A	5001	3	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

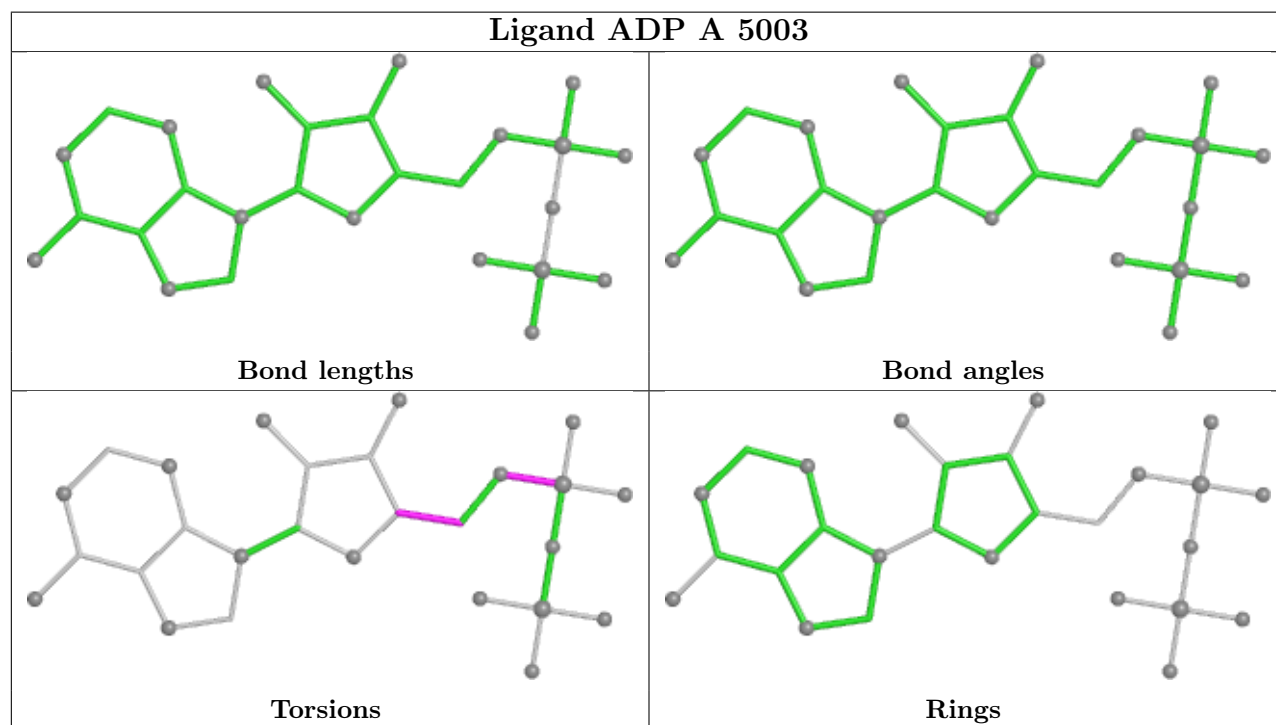
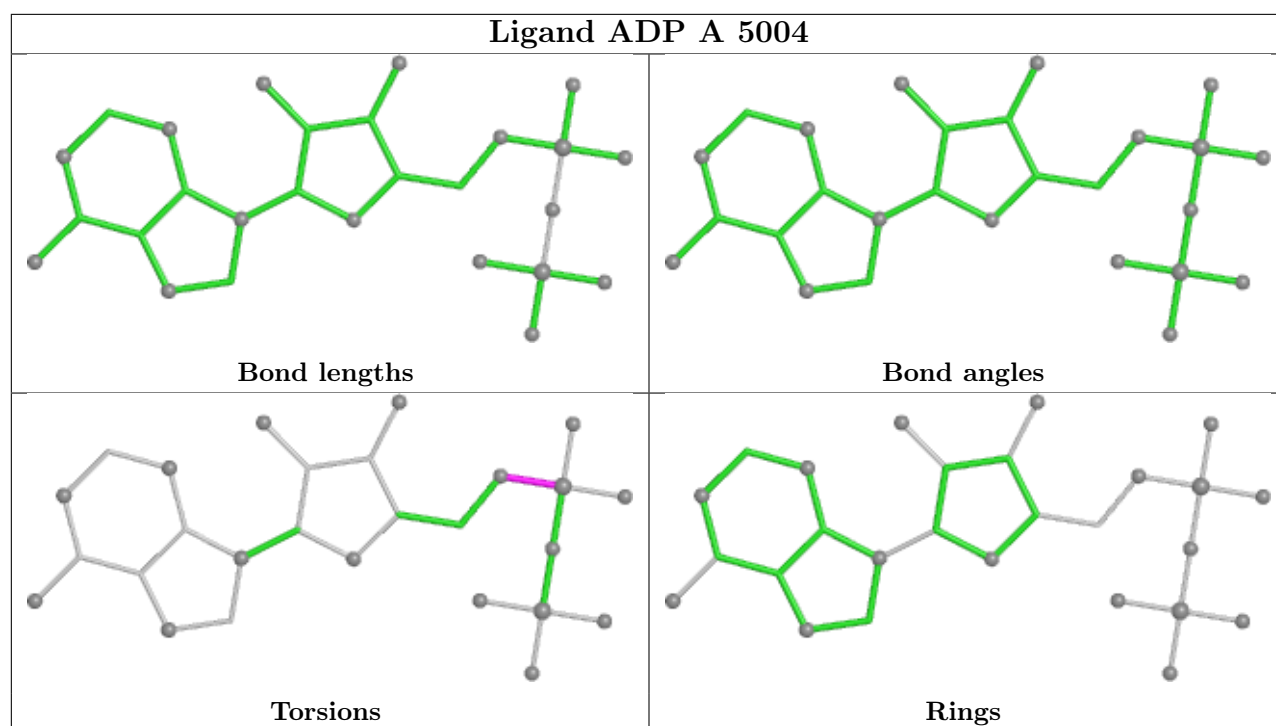
5 of 10 torsion outliers are listed below:

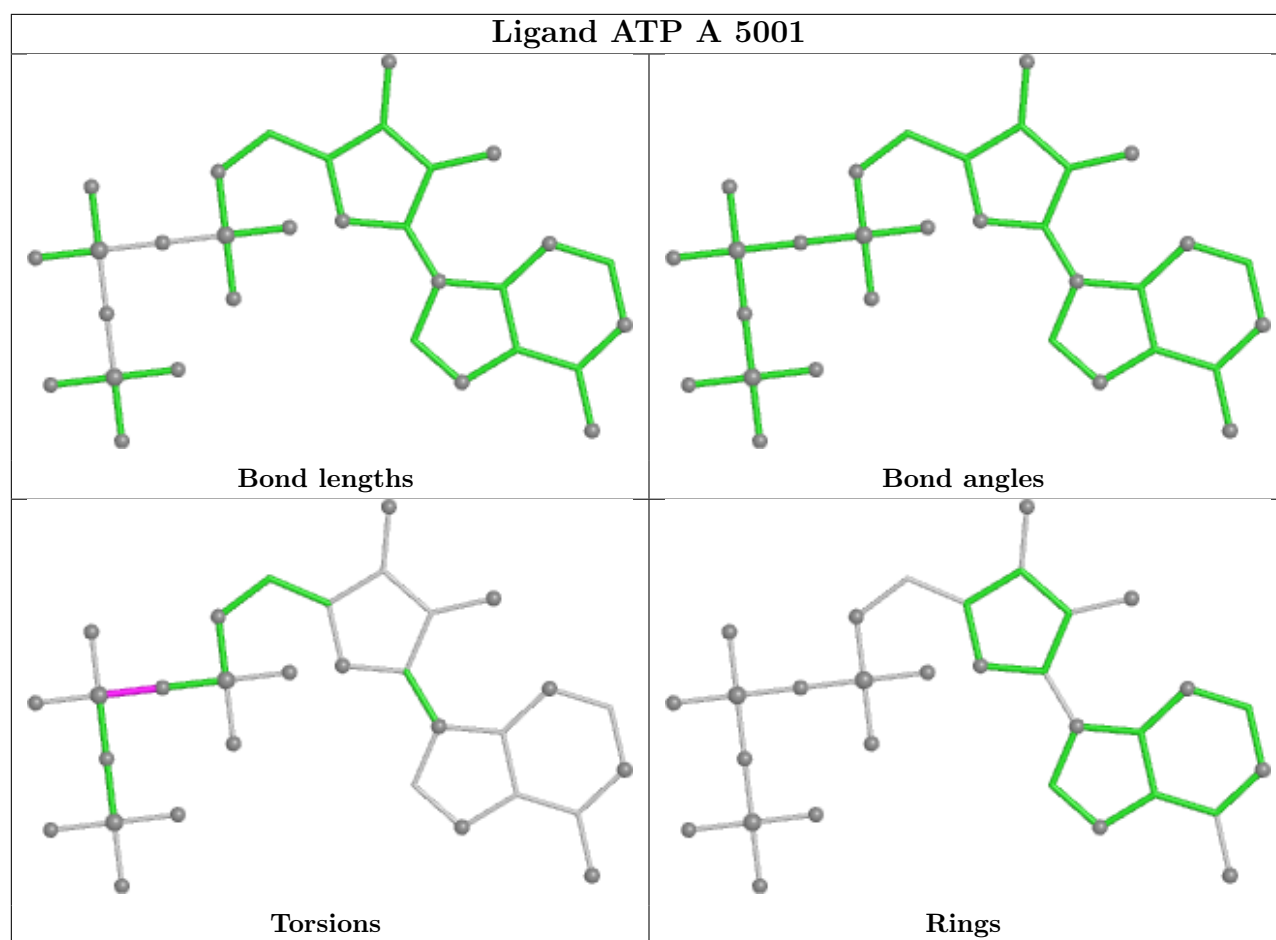
Mol	Chain	Res	Type	Atoms
4	A	5003	ADP	C5'-O5'-PA-O1A
4	A	5004	ADP	C5'-O5'-PA-O2A
4	A	5003	ADP	O4'-C4'-C5'-O5'
4	A	5003	ADP	C5'-O5'-PA-O3A
4	A	5004	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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.

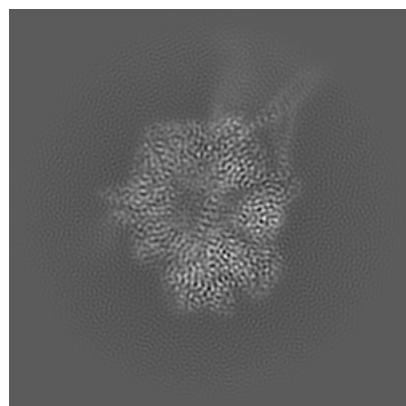
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-81337. These allow visual inspection of the internal detail of the map and identification of artifacts.

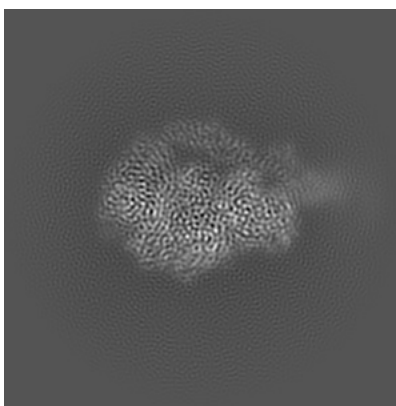
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

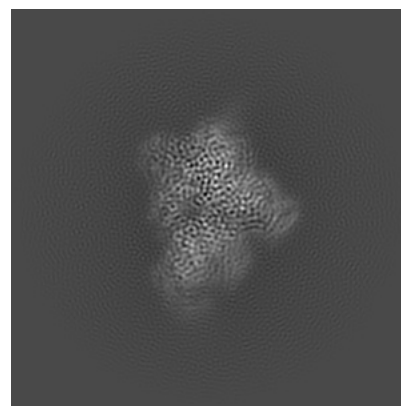
6.1.1 Primary map



X

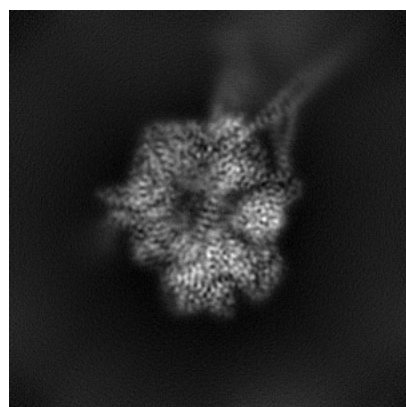


Y

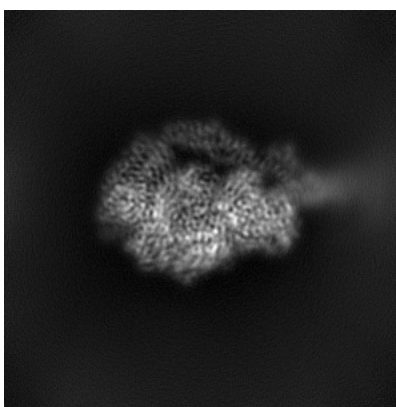


Z

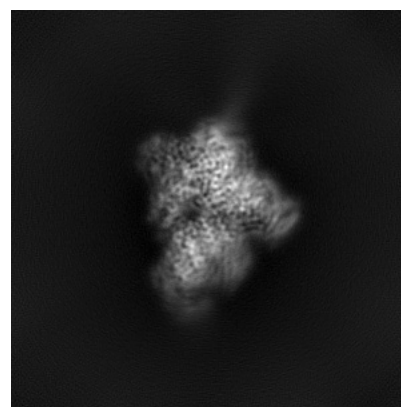
6.1.2 Raw map



X



Y

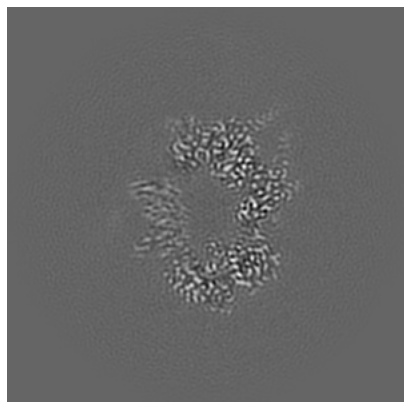


Z

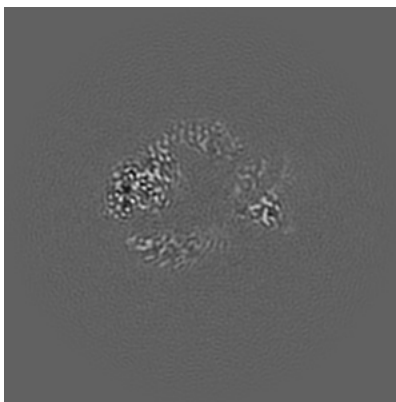
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

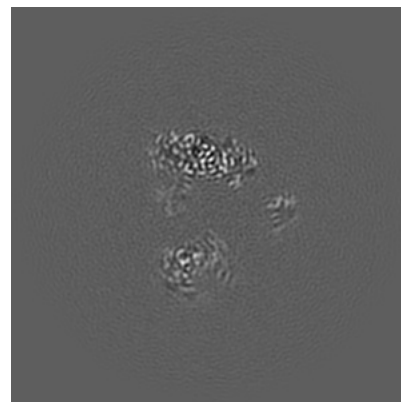
6.2.1 Primary map



X Index: 150

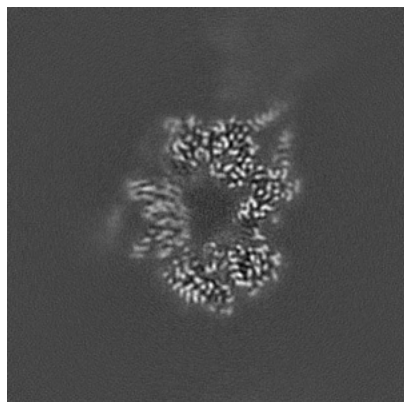


Y Index: 150

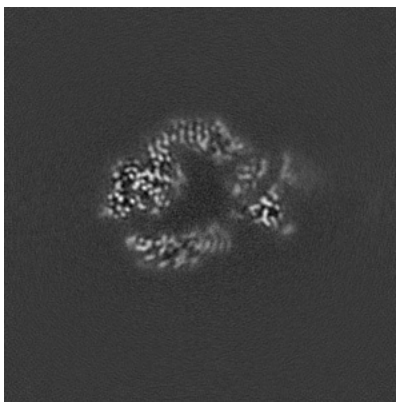


Z Index: 150

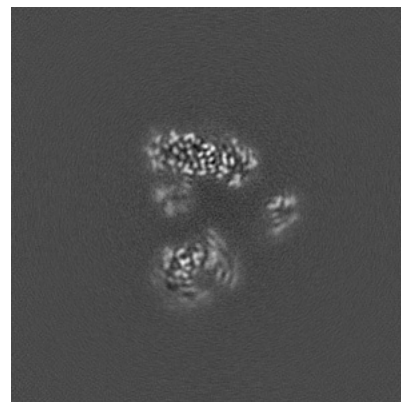
6.2.2 Raw map



X Index: 150



Y Index: 150

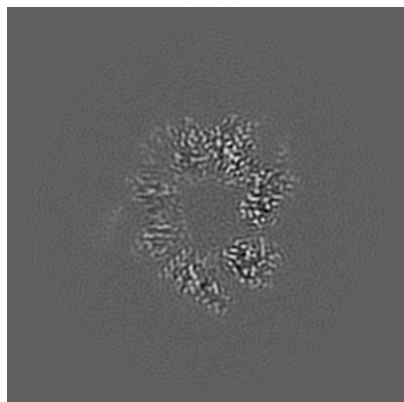


Z Index: 150

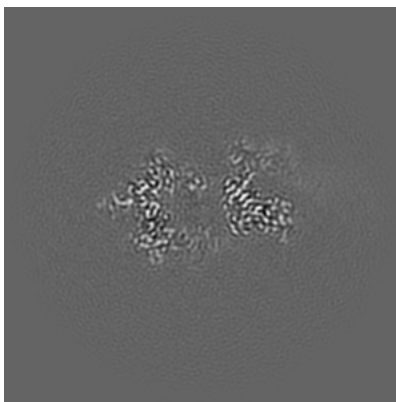
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

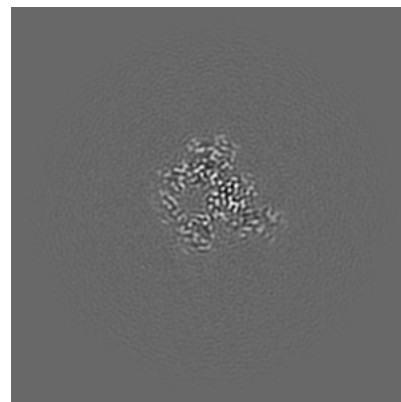
6.3.1 Primary map



X Index: 145

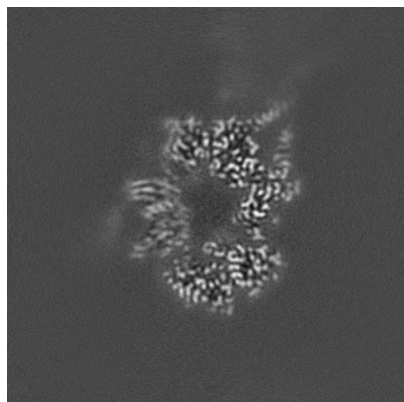


Y Index: 167

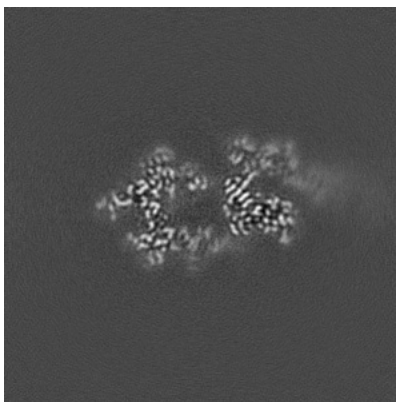


Z Index: 104

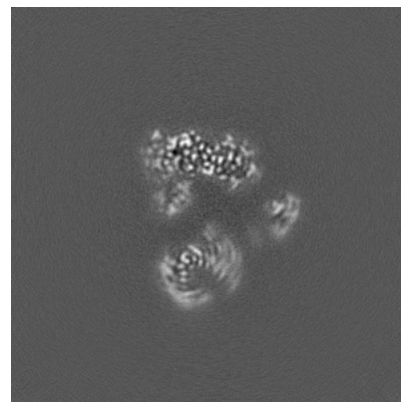
6.3.2 Raw map



X Index: 151



Y Index: 167

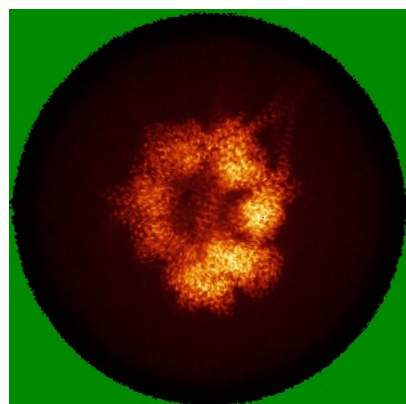


Z Index: 146

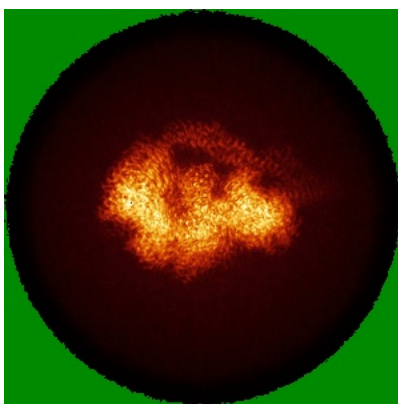
The images above show the largest variance slices of the map in three orthogonal directions.

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

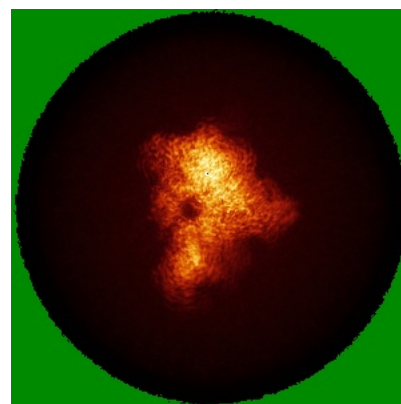
6.4.1 Primary map



X

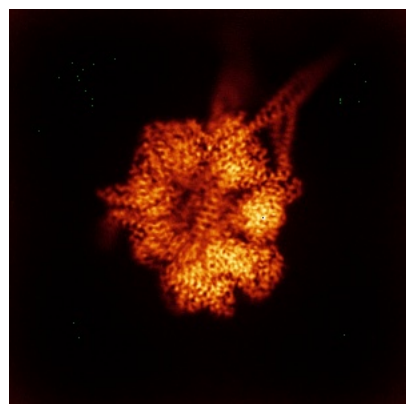


Y

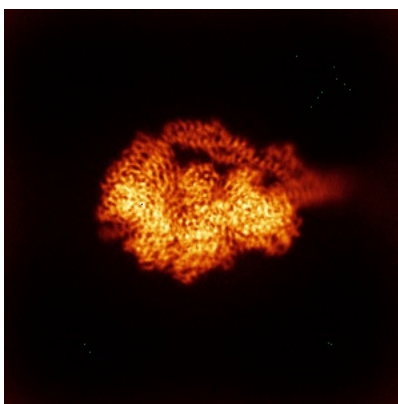


Z

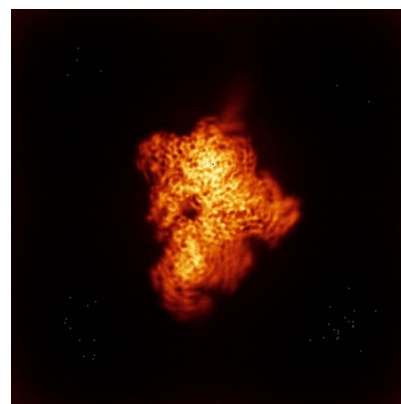
6.4.2 Raw map



X



Y

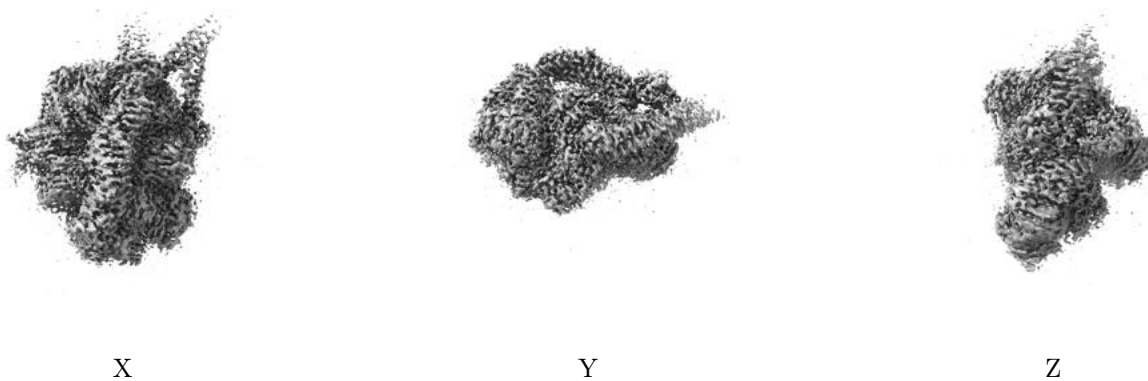


Z

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.

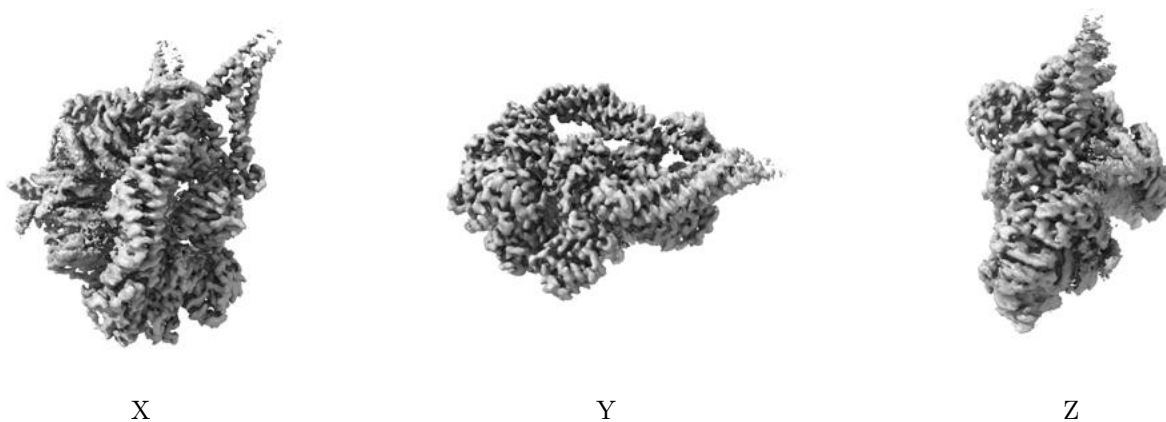
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

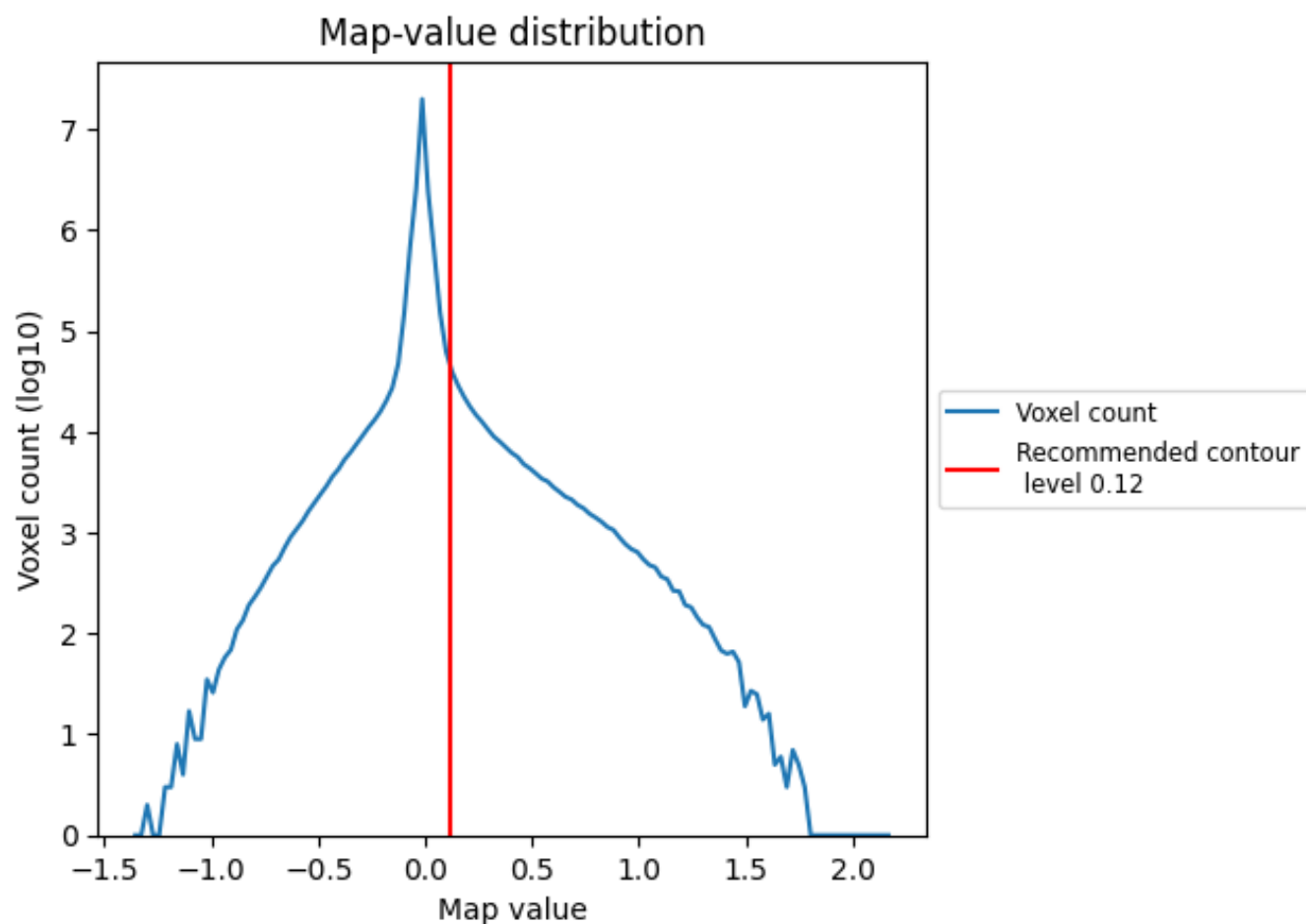
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

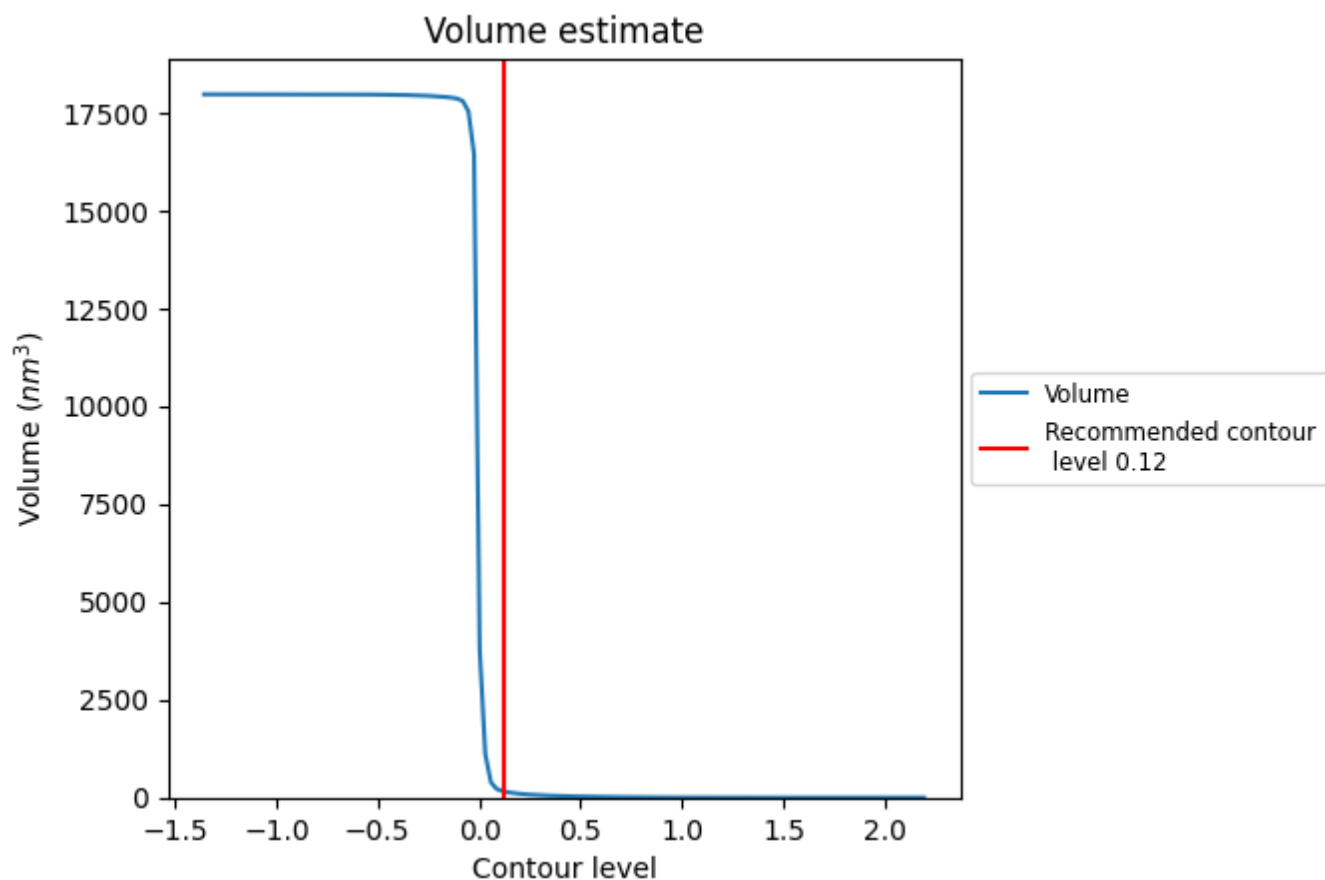
This section contains the results of statistical analysis of the map.

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.

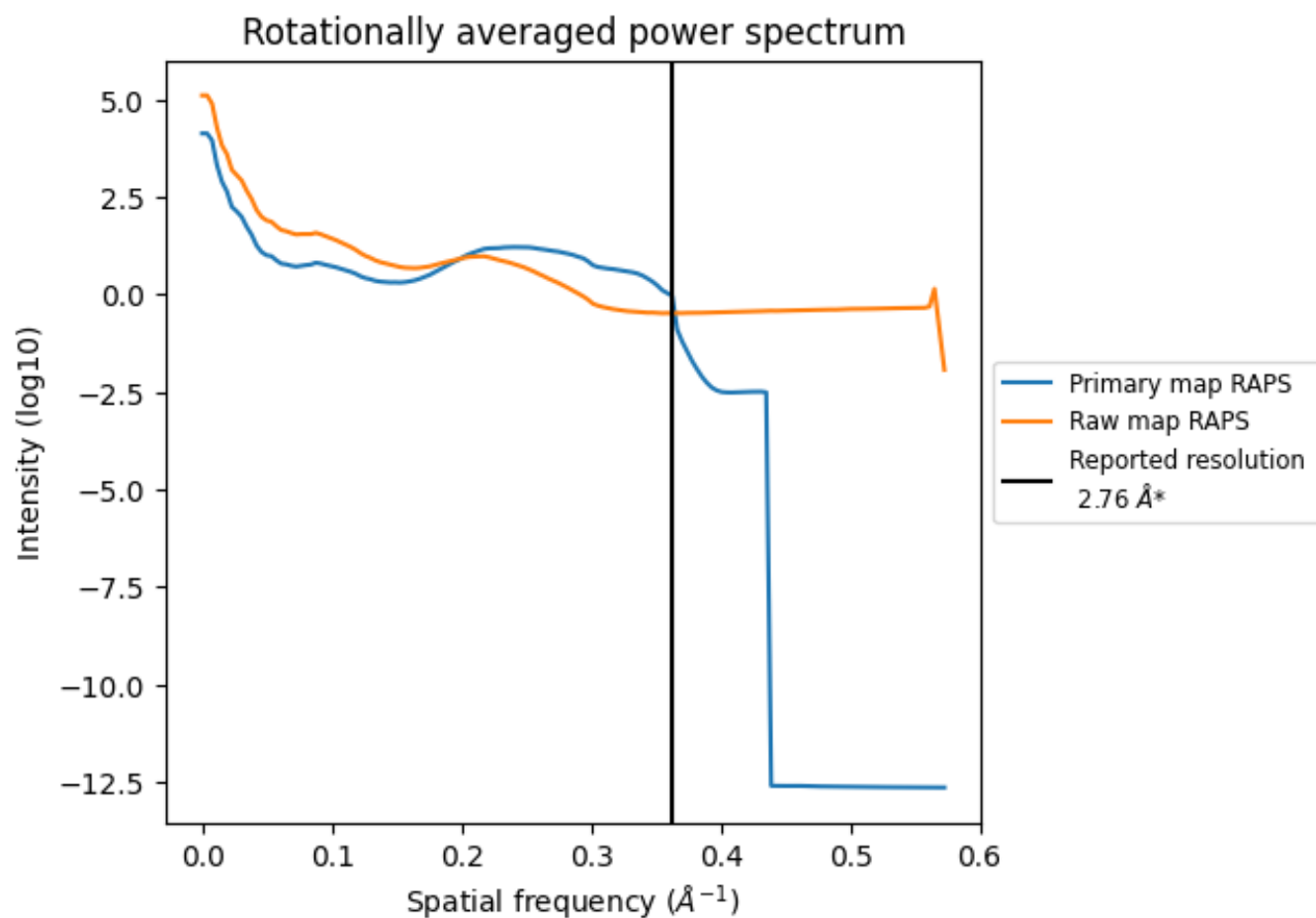
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 160 nm³; this corresponds to an approximate mass of 144 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 ⓘ

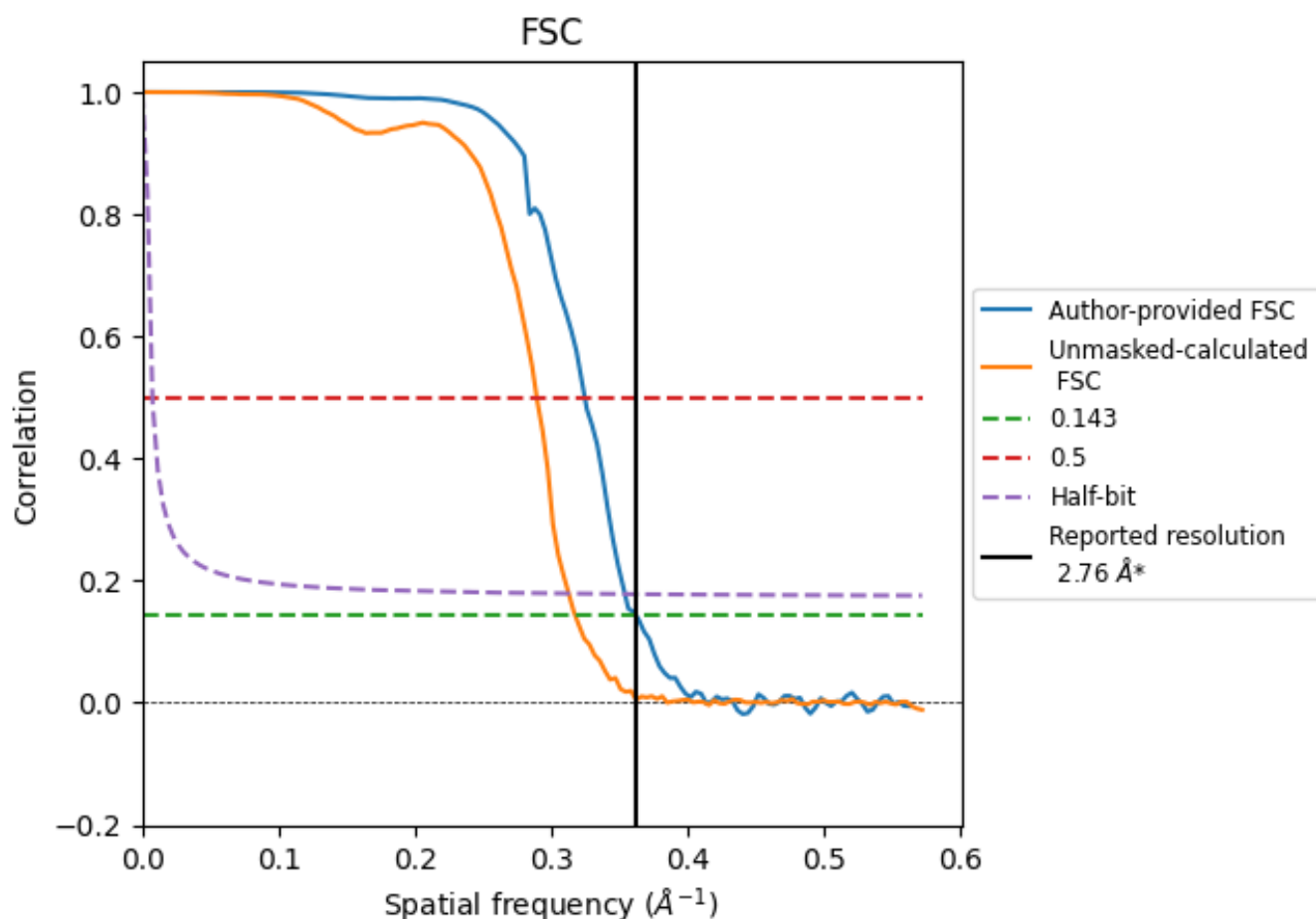


*Reported resolution corresponds to spatial frequency of 0.362 $\text{\AA}^{-1}$

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 0.362 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

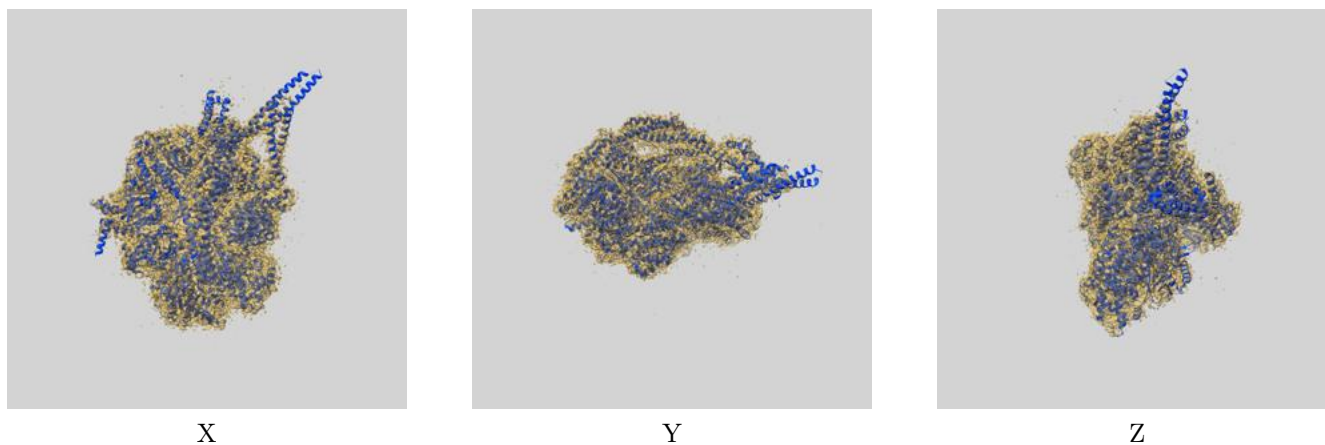
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.76	-	-
Author-provided FSC curve	2.76	3.08	2.82
Unmasked-calculated*	3.14	3.45	3.19

*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 3.14 differs from the reported value 2.76 by more than 10 %

9 Map-model fit [i](#)

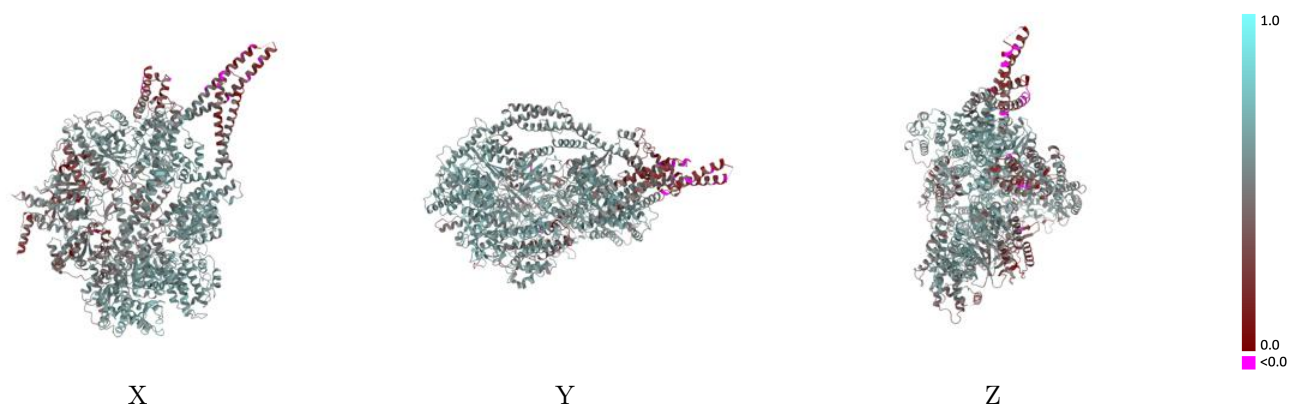
This section contains information regarding the fit between EMDB map EMD-81337 and PDB model 27QA. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



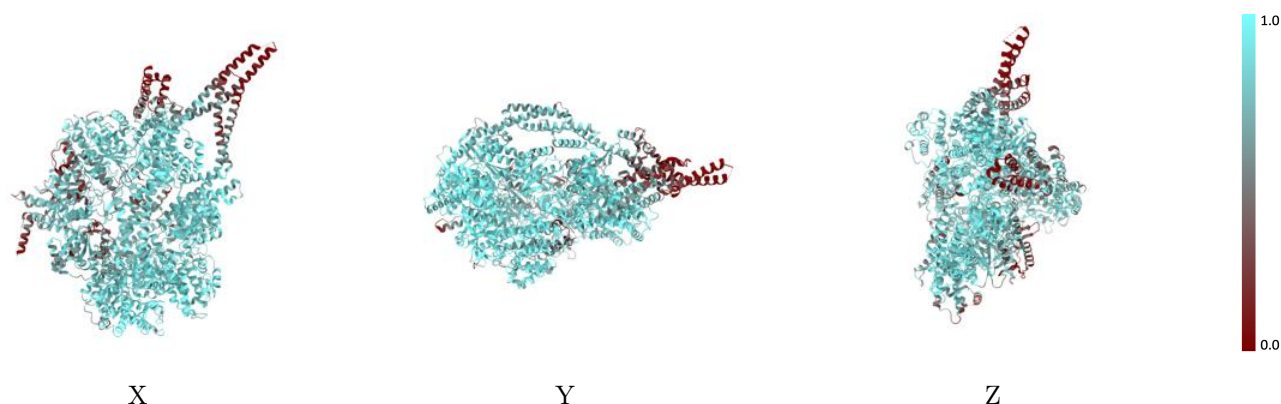
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



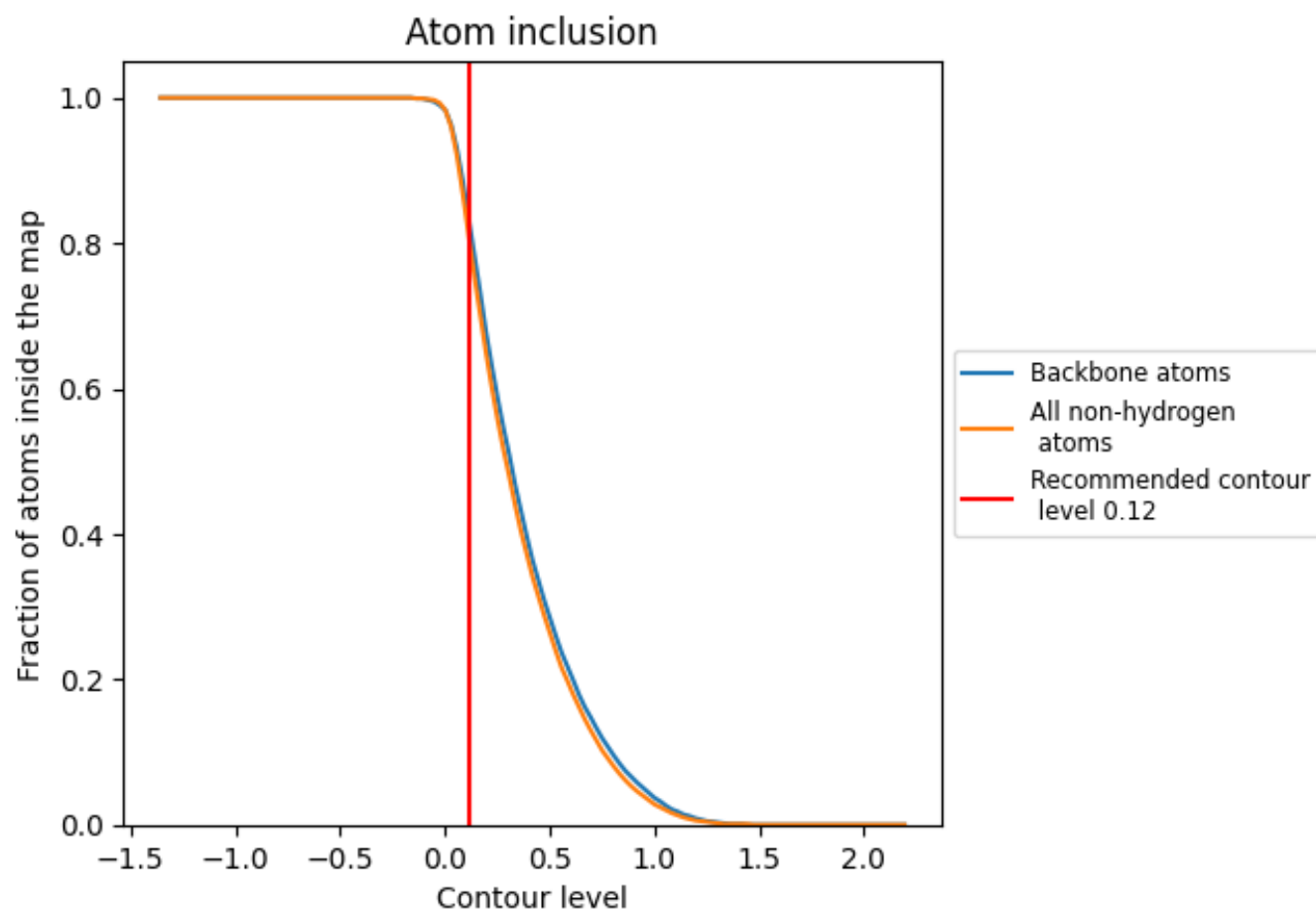
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.5260
A	0.7990	0.5260

