



wwPDB EM Validation Summary Report ⓘ

May 29, 2025 – 04:46 PM EDT

PDB ID : 9DI3 / pdb_00009di3
EMDB ID : EMD-46897
Title : CryoEM structures of yeast cytoplasmic dynein in the presence of ATP and Lis1.
Authors : Kendrick, A.A.; Leschziner, A.E.
Deposited on : 2024-09-05
Resolution : 4.10 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

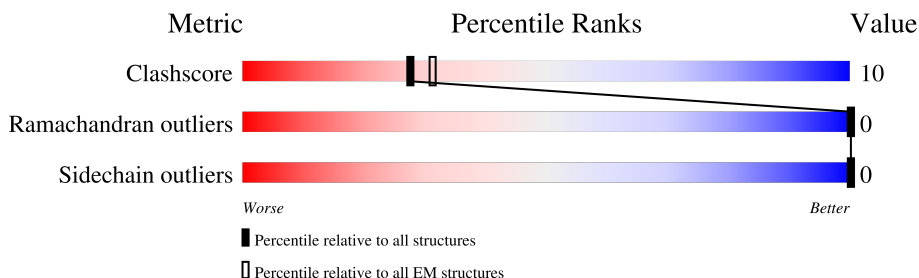
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2875	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17694 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	2282	Total	C	N	O	S	0	0
			17582	11303	2945	3256	78		

There are 14 discrepancies between the modelled and reference sequences:

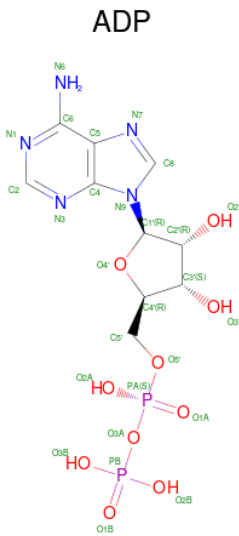
Chain	Residue	Modelled	Actual	Comment	Reference
A	1218	GLY	-	expression tag	UNP P36022
A	1575	PHE	LEU	conflict	UNP P36022
A	1578	SER	PHE	conflict	UNP P36022
A	1668	GLU	GLN	conflict	UNP P36022
A	1777	VAL	ILE	conflict	UNP P36022
A	1984	VAL	ILE	conflict	UNP P36022
A	2936	VAL	ILE	conflict	UNP P36022
A	3266	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).



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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

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



D4019	H3858	K3722	K3541	S3467	K3378	VAL
M4020	V3859	L3726	Q3542	R3468	K3378	LYS
L4021	E3860	L3726	R3543	E3469	E3381	S3298
I4023	GLU	P3734	K3544	A3473	C3382	L3299
V4027	THR	T3737	R3545	GLY	G3383	T3300
R4028	LYS	VAL	E3546	ASN	L3384	F3301
L4029	ALA	ASP	D3547	ARG	N3387	E3302
L4076	E3867	THR	I3549	V3477	D3388	K3303
Q4077	K3741	K3741	K3550	E3480	Y3389	E3304
V4081	Y3756	Y3756	L3551	I3481	F3390	K3305
E4091	M3875	I3757	N3552	G3482	L3391	W3306
MET	L3879	L3760	T3553	D3483	E3392	L3307
	P3885	N3761	E3554	H3484	N3393	N3308
	L3888	V3769	R3555	E3485	S3400	T3309
	R3894	D3770	R3556	V3486	Q3401	T3310
	F3916	V3777	L3557	D3487	D3402	K3311
	THR	N3783	L3558	V3488	A3403	Q3312
	GLY	N3784	L3559	S3489	V3404	F3313
	LYS	F3785	K3560	K3493	P3405	K3315
	I3920	F3786	N3561	F3495	L3407	T3316
	L3931	T3787	E3562	C3499	D3408	S3317
	W3934	S3790	K3563	D3500	D3409	Q3318
	F3935	E3791	K3564	P3501	P3410	E3319
	T3940	D3793	R3565	SER	M3414	K3323
	T3943	I3801	R3566	ASP	V3417	S3327
	V3946	L3811	L3567	I3505	I3418	I3329
	G3949	L3812	L3568	P3506	Y3422	Y3330
	K3952	L3813	E3569	I3507	G3423	F3334
	K3953	P3815	L3570	R3612	N3424	L3337
	Y3954	L3816	N3571	V3513	K3425	N3338
	Y3955	L3822	N3572	R3514	S3430	E3339
	F3963	L3829	S3573	H3517	F3431	R3340
	A3964	S3832	GLN	F3518	LEU	E3341
	H3988	K3833	GLY	V3519	GLU	R3342
	I3989	L3834	ASN	T3520	GLU	L3349
	I3992	W3838	ASP	N3521	G3435	L3353
	V3993	T3688	GLU	K3523	K3438	L3354
	D4003	A3689	LEU	S3524	V3449	A3357
	V4014	L3690	THR	I3525	Q3453	N3363
		L3693	VAL	F3530	E3456	Y3364
		F3694	THR	D3531	F3457	R3365
		K3695	LEU	T3532	ASP	F3366
		M3696	ASN	L3533	P3460	I3367
		C3704	LYS	L3534	I3461	D3368
		F3708	K3592	T3535	I3462	Y3369
			E3593	E3536	S3463	W3371
			A3594	E3537	R3464	T3372
			M3595	N3538		L3373
			N3596			D3374
			I3597			
			E3598			
			K3599			
			K3600			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68450	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.3	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.193	Depositor
Minimum map value	-0.695	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	408.31998, 408.31998, 408.31998	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.16	0/17919	0.36	0/24280

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	17582	0	16934	330	0
2	A	31	0	12	4	0
3	A	81	0	36	5	0
All	All	17694	0	16982	330	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 10.

The worst 5 of 330 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:1714:GLN:HB3	1:A:1727:LEU:HD21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2294:LEU:HB3	1:A:2317:LEU:HD13	1.73	0.69
1:A:1733:LYS:HB2	1:A:1750:SER:HB3	1.75	0.69
1:A:2391:VAL:HG21	1:A:2430:ASN:HB2	1.77	0.66
1:A:1846:CYS:SG	1:A:1847:PHE:N	2.69	0.65

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	2232/2875 (78%)	2149 (96%)	83 (4%)	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	1835/2631 (70%)	1835 (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	2463	ASN
1	A	3761	ASN
1	A	2634	ASN
1	A	3856	HIS
1	A	3338	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	4103	-	24,29,29	0.89	0	29,45,45	1.21	2 (6%)
3	ADP	A	4104	-	24,29,29	0.84	0	29,45,45	1.27	2 (6%)
3	ADP	A	4102	-	24,29,29	0.80	0	29,45,45	1.32	4 (13%)
2	ATP	A	4101	-	28,33,33	0.94	2 (7%)	34,52,52	0.66	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	4103	-	-	2/12/32/32	0/3/3/3
3	ADP	A	4104	-	-	4/12/32/32	0/3/3/3
3	ADP	A	4102	-	-	3/12/32/32	0/3/3/3
2	ATP	A	4101	-	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4101	ATP	PB-O3B	-2.73	1.56	1.59
2	A	4101	ATP	PA-O3A	-2.02	1.57	1.59

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4103	ADP	N3-C2-N1	-3.79	123.53	128.67
3	A	4104	ADP	N3-C2-N1	-3.70	123.65	128.67
3	A	4102	ADP	N3-C2-N1	-3.51	123.91	128.67
3	A	4102	ADP	O4'-C1'-N9	2.69	112.31	108.75
3	A	4103	ADP	C4-C5-N7	-2.50	106.69	109.34

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4101	ATP	C5'-O5'-PA-O2A
2	A	4101	ATP	C5'-O5'-PA-O3A
3	A	4102	ADP	C5'-O5'-PA-O1A
3	A	4102	ADP	O4'-C4'-C5'-O5'
3	A	4102	ADP	C3'-C4'-C5'-O5'

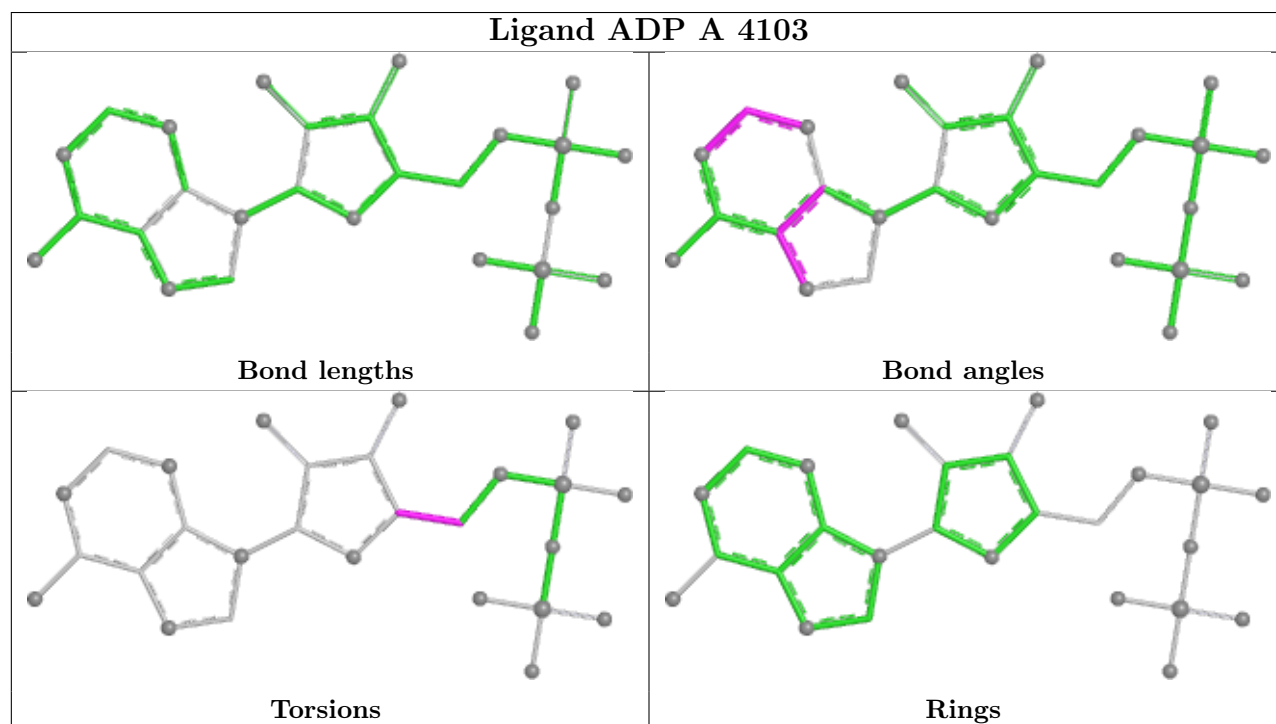
There are no ring outliers.

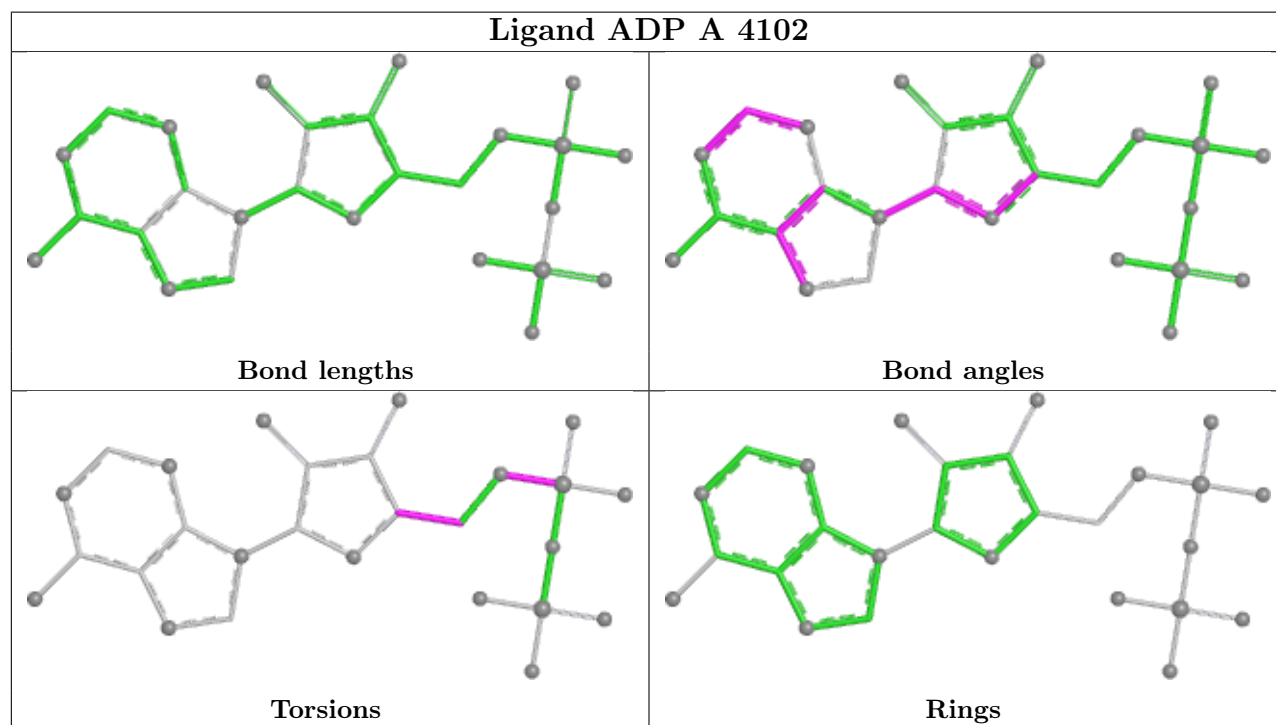
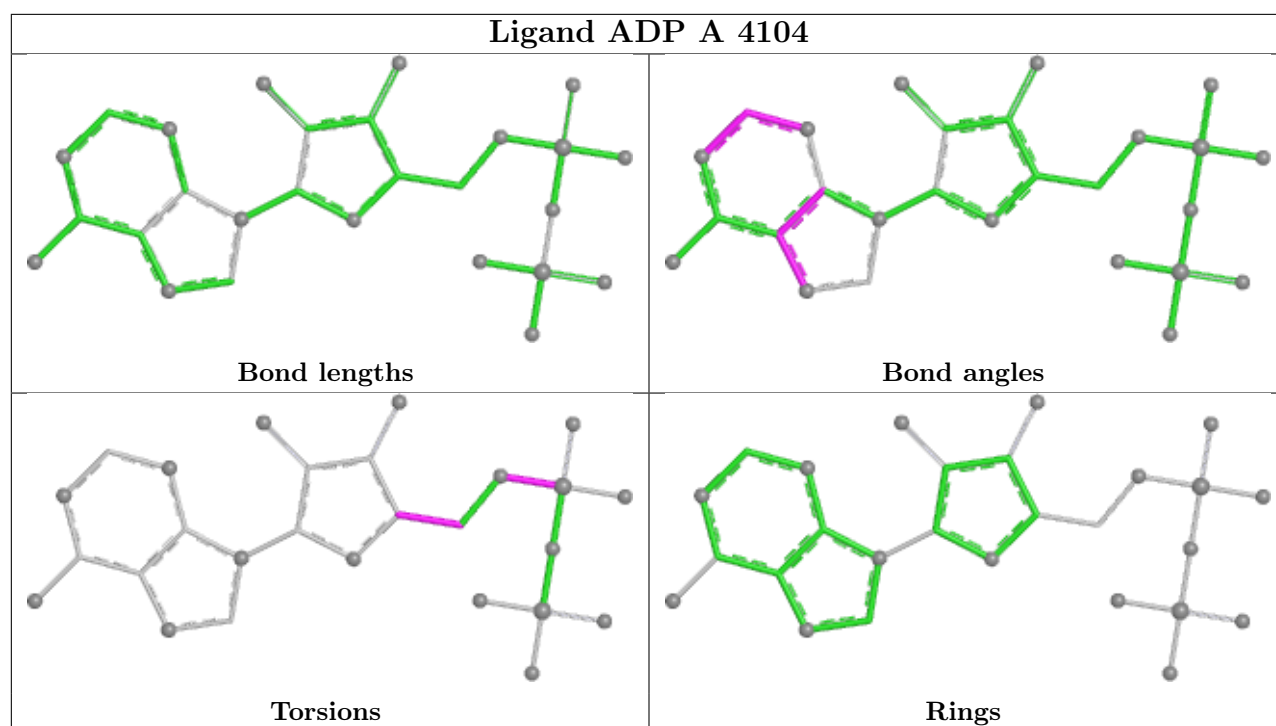
3 monomers are involved in 9 short contacts:

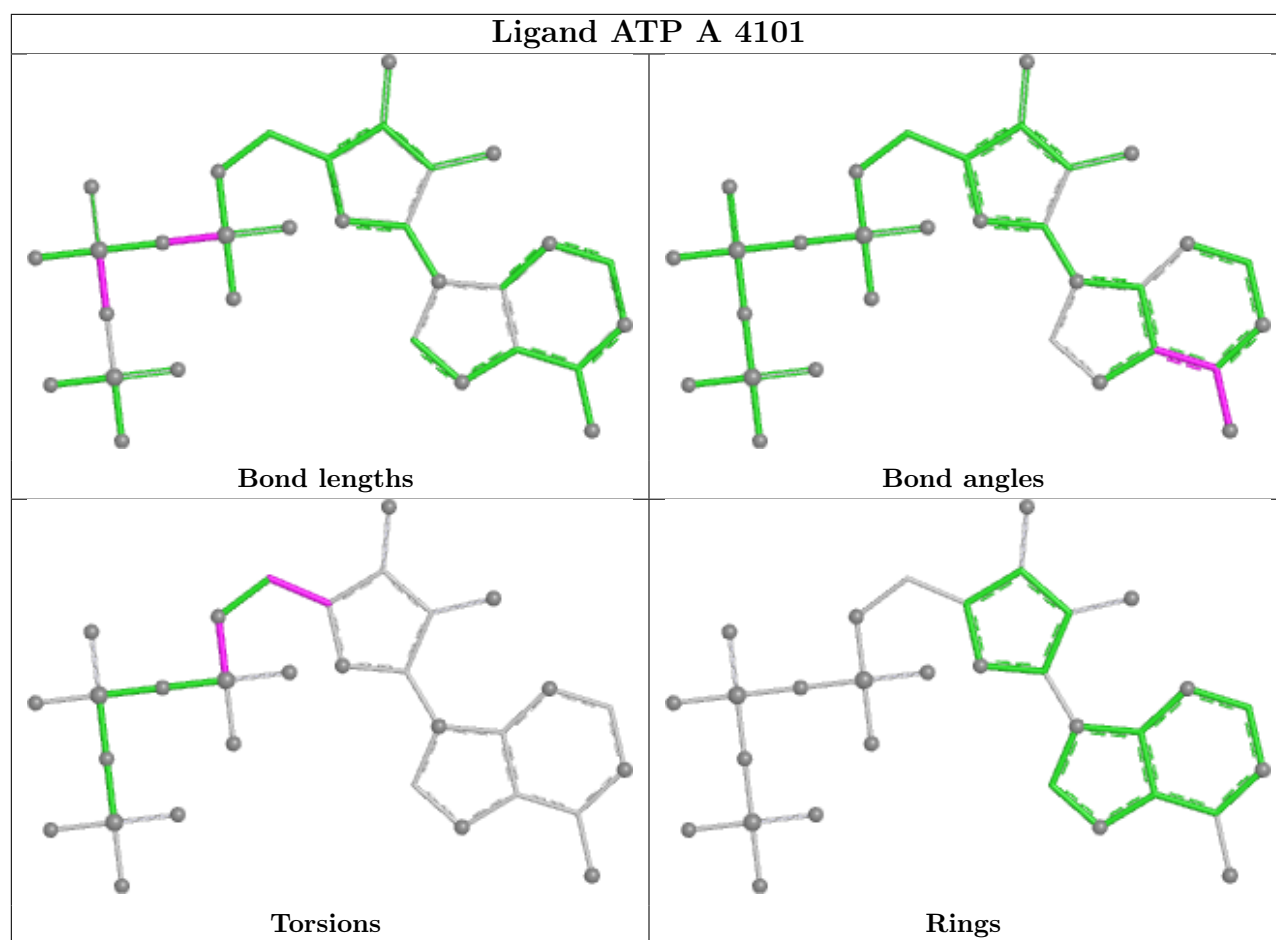
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4103	ADP	1	0
3	A	4102	ADP	4	0
2	A	4101	ATP	4	0

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.

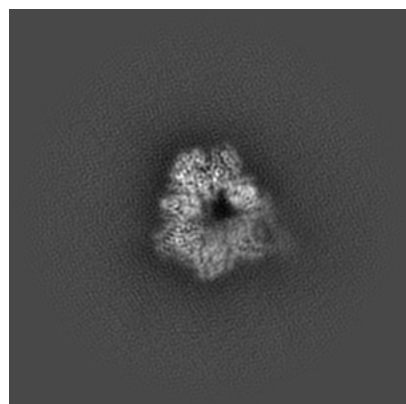
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46897. These allow visual inspection of the internal detail of the map and identification of artifacts.

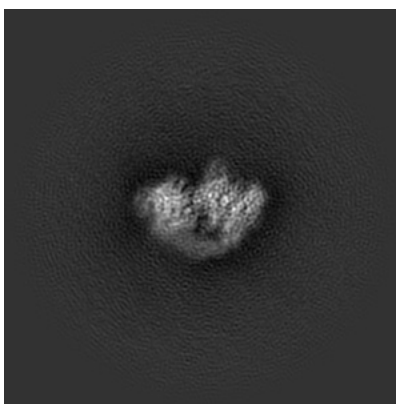
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

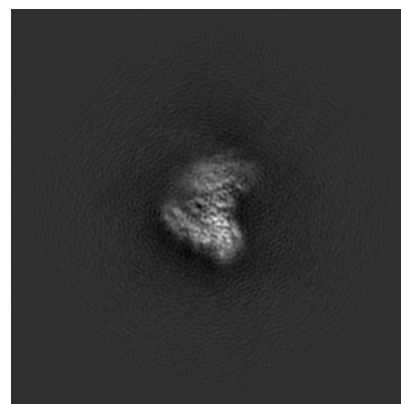
6.1.1 Primary map



X

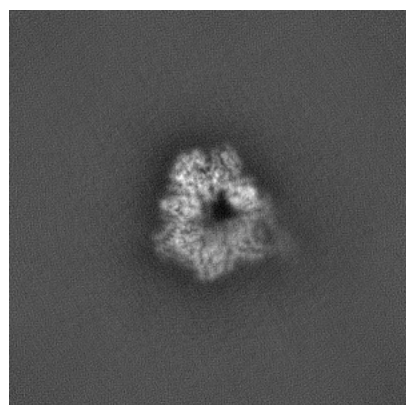


Y

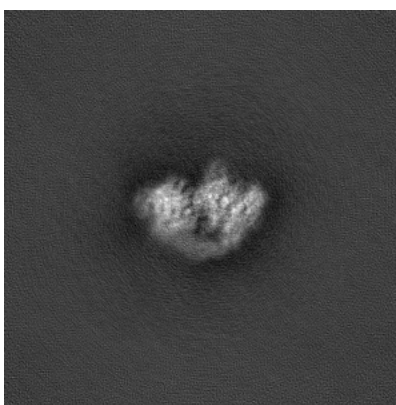


Z

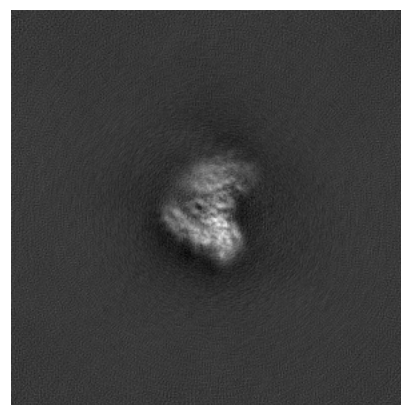
6.1.2 Raw map



X



Y

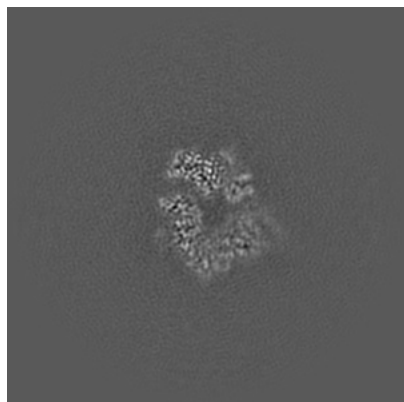


Z

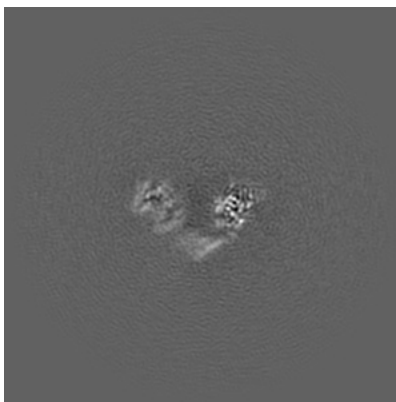
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

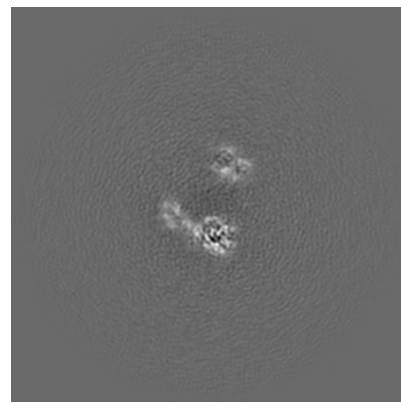
6.2.1 Primary map



X Index: 176

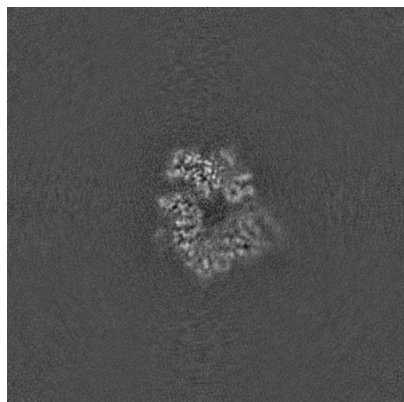


Y Index: 176

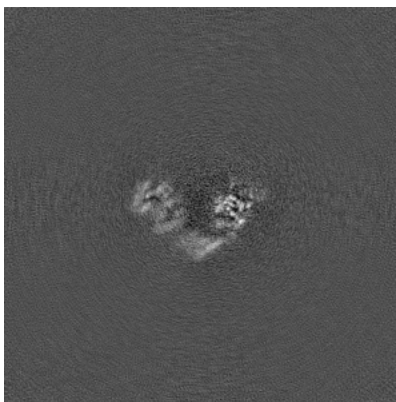


Z Index: 176

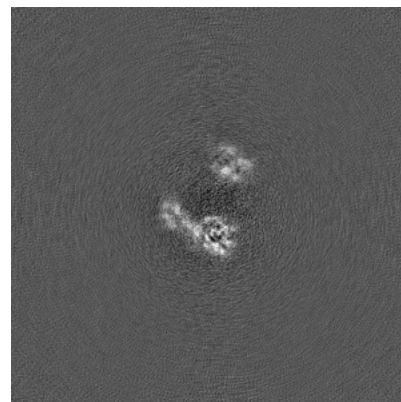
6.2.2 Raw map



X Index: 176



Y Index: 176

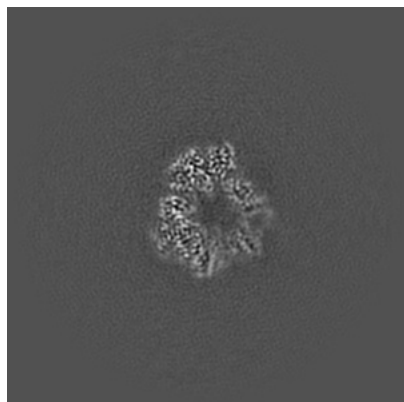


Z Index: 176

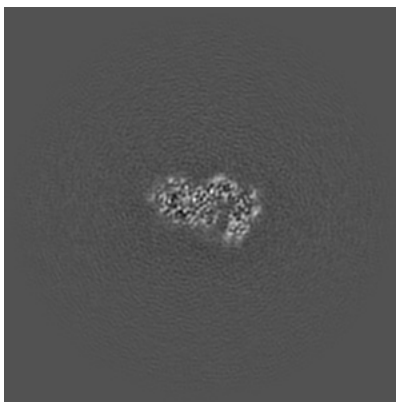
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

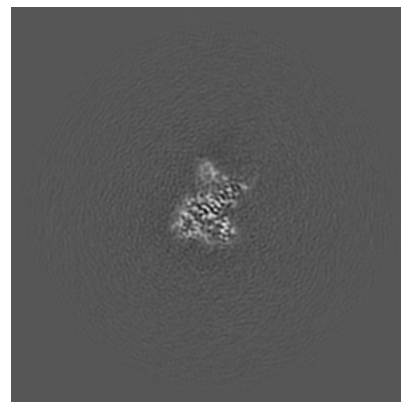
6.3.1 Primary map



X Index: 183

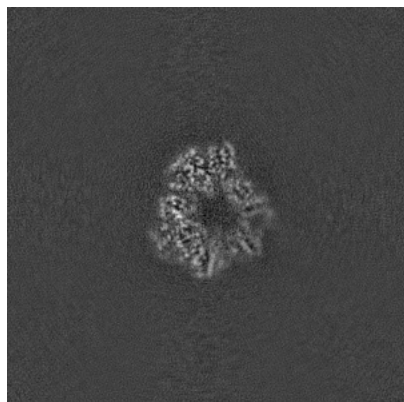


Y Index: 153

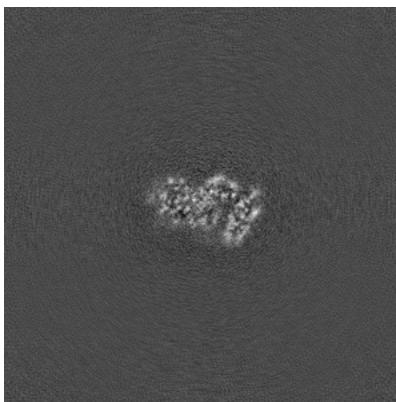


Z Index: 201

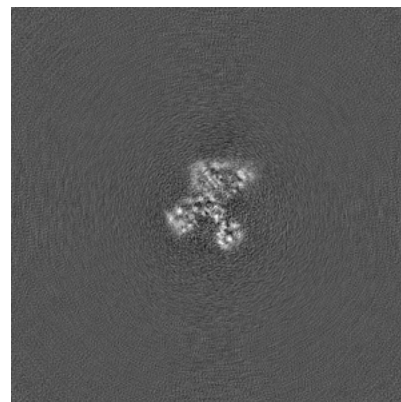
6.3.2 Raw map



X Index: 183



Y Index: 154

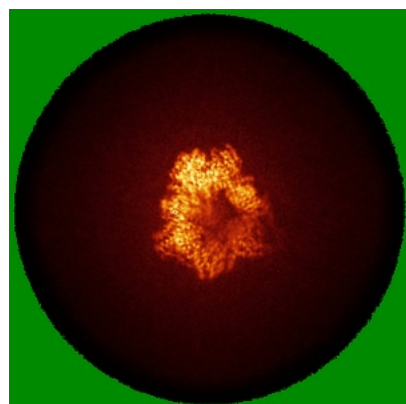


Z Index: 194

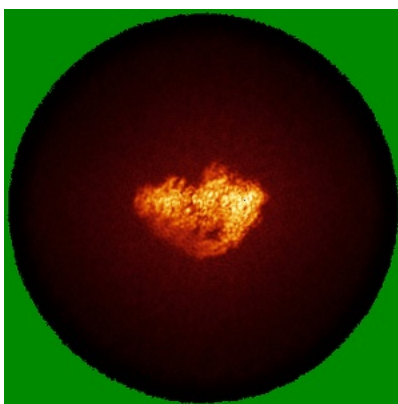
The images above show the largest variance slices of the map in three orthogonal directions.

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

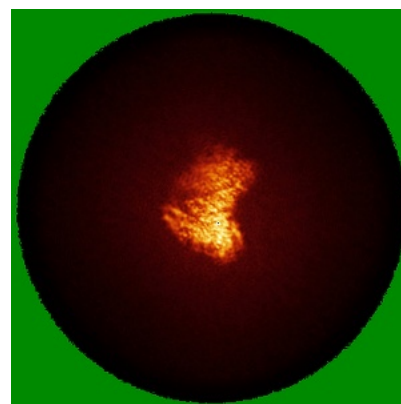
6.4.1 Primary map



X

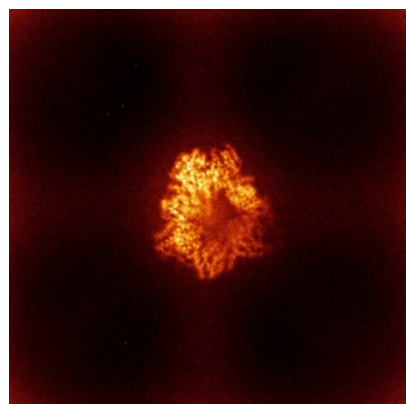


Y

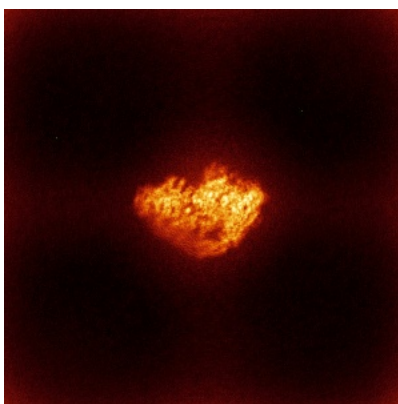


Z

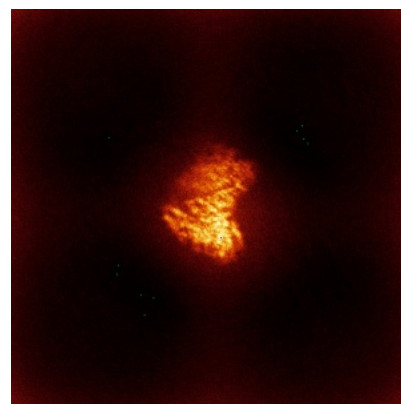
6.4.2 Raw map



X



Y

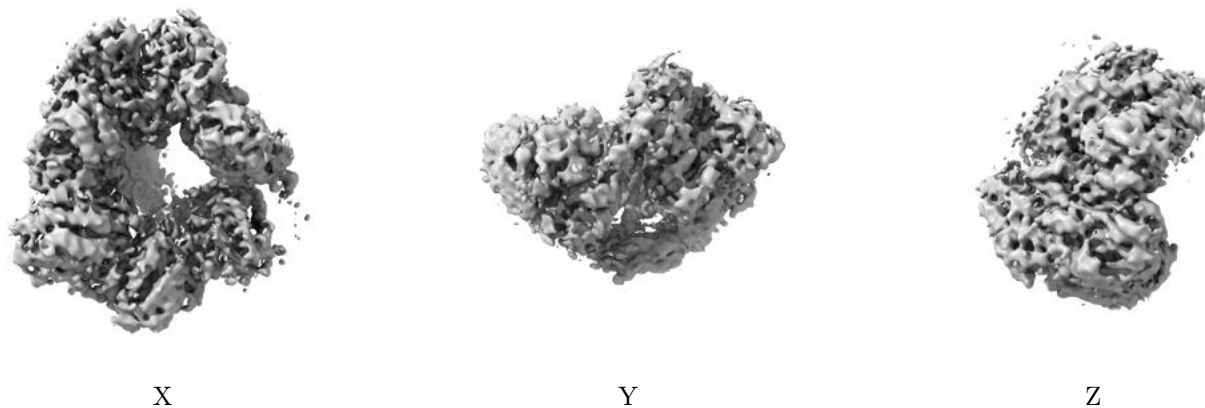


Z

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.

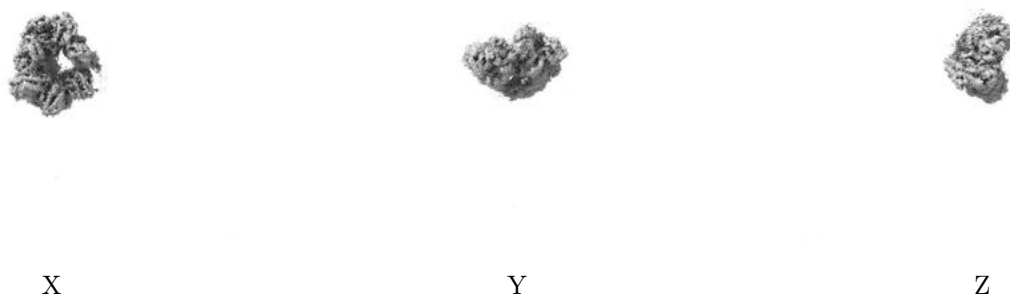
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. 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.

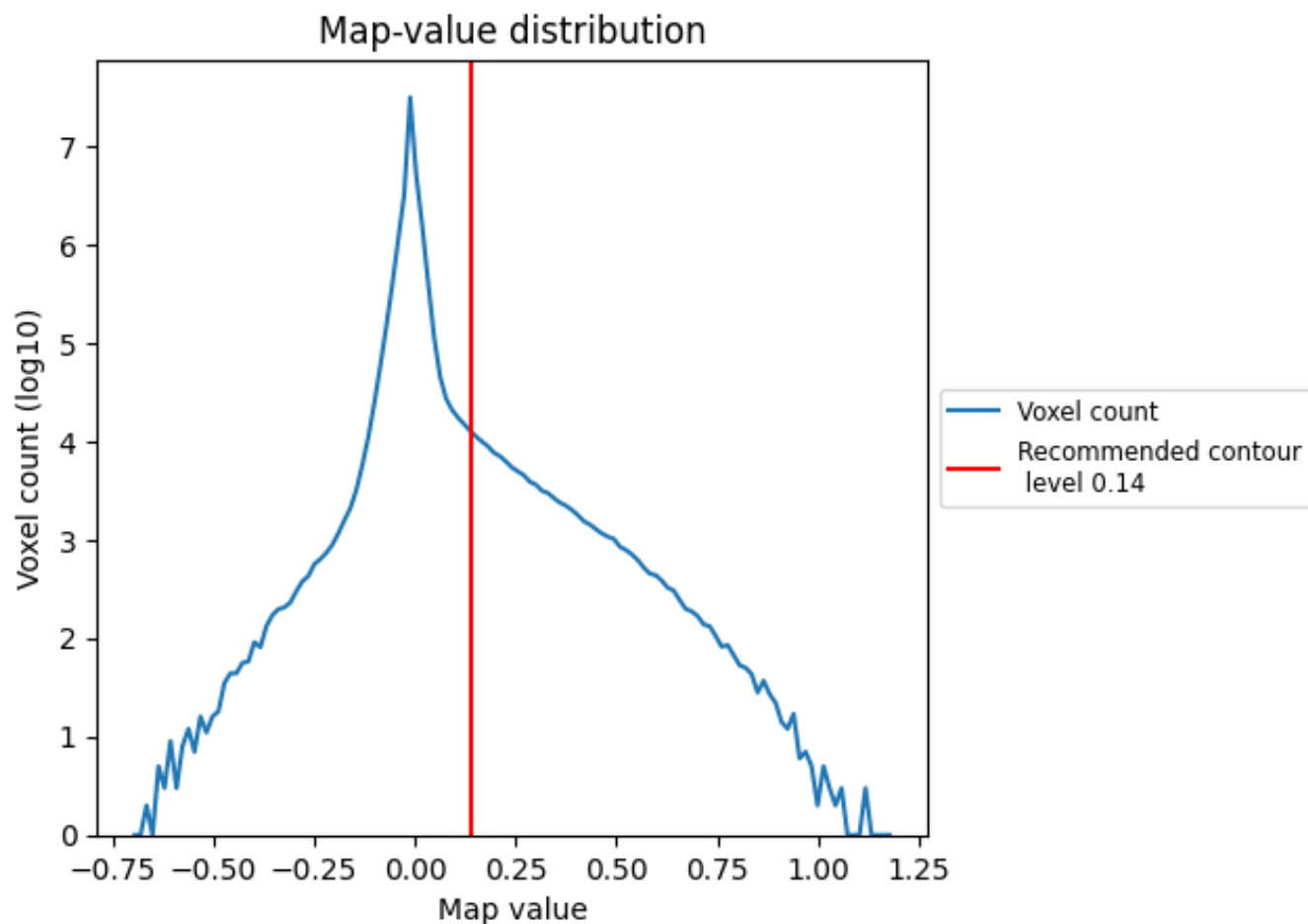
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

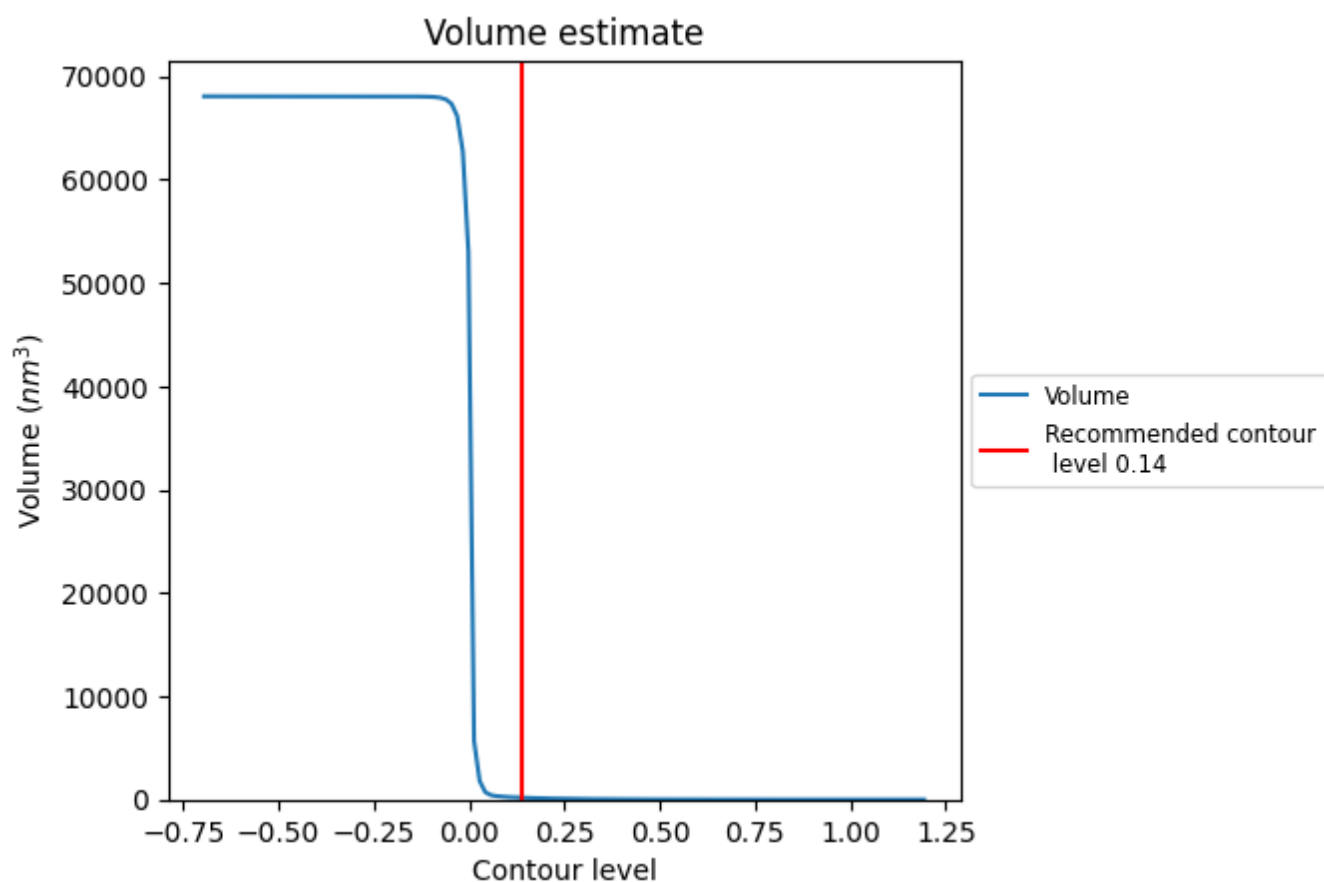
This section contains the results of statistical analysis of the map.

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.

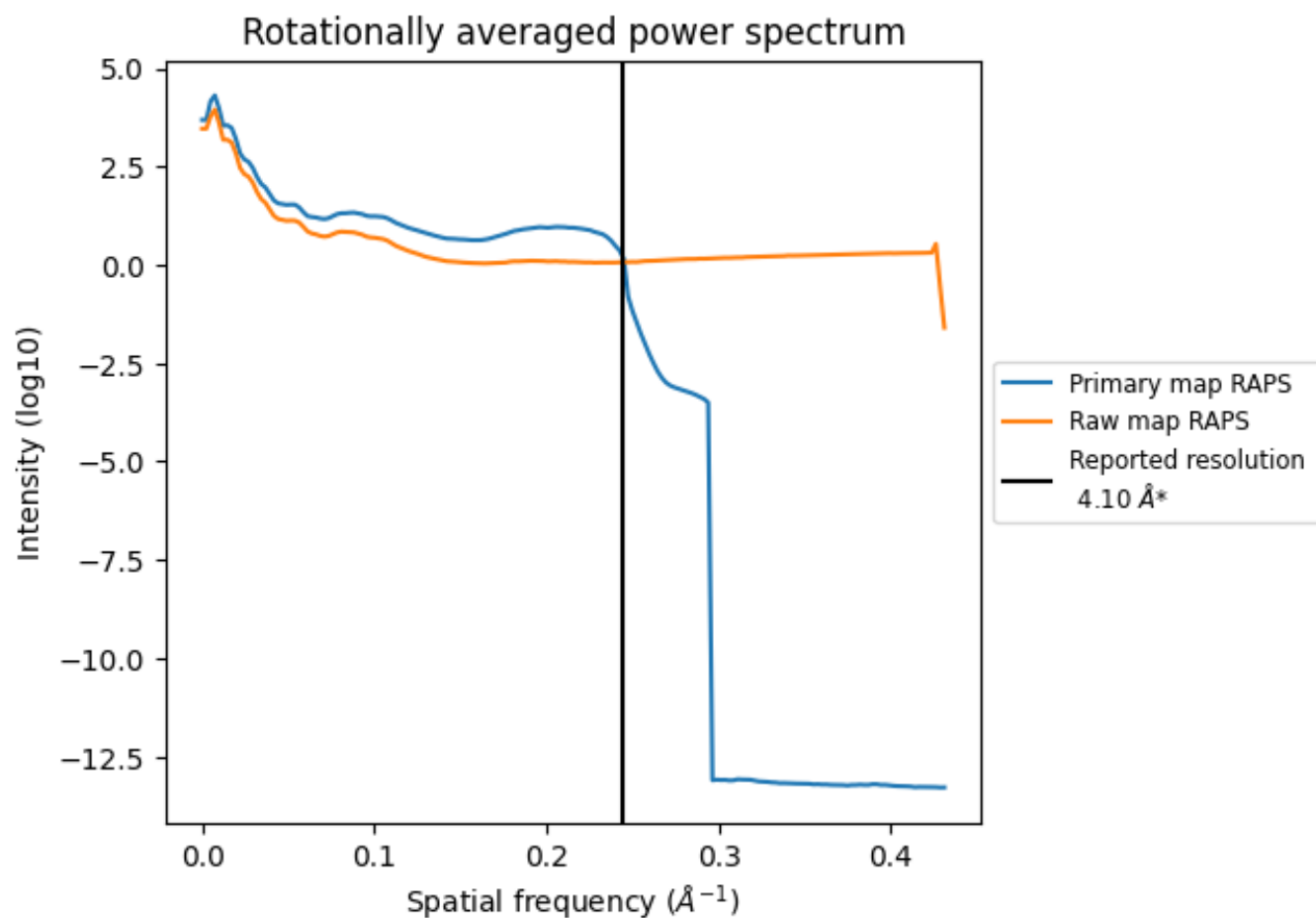
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm³; this corresponds to an approximate mass of 163 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 ⓘ

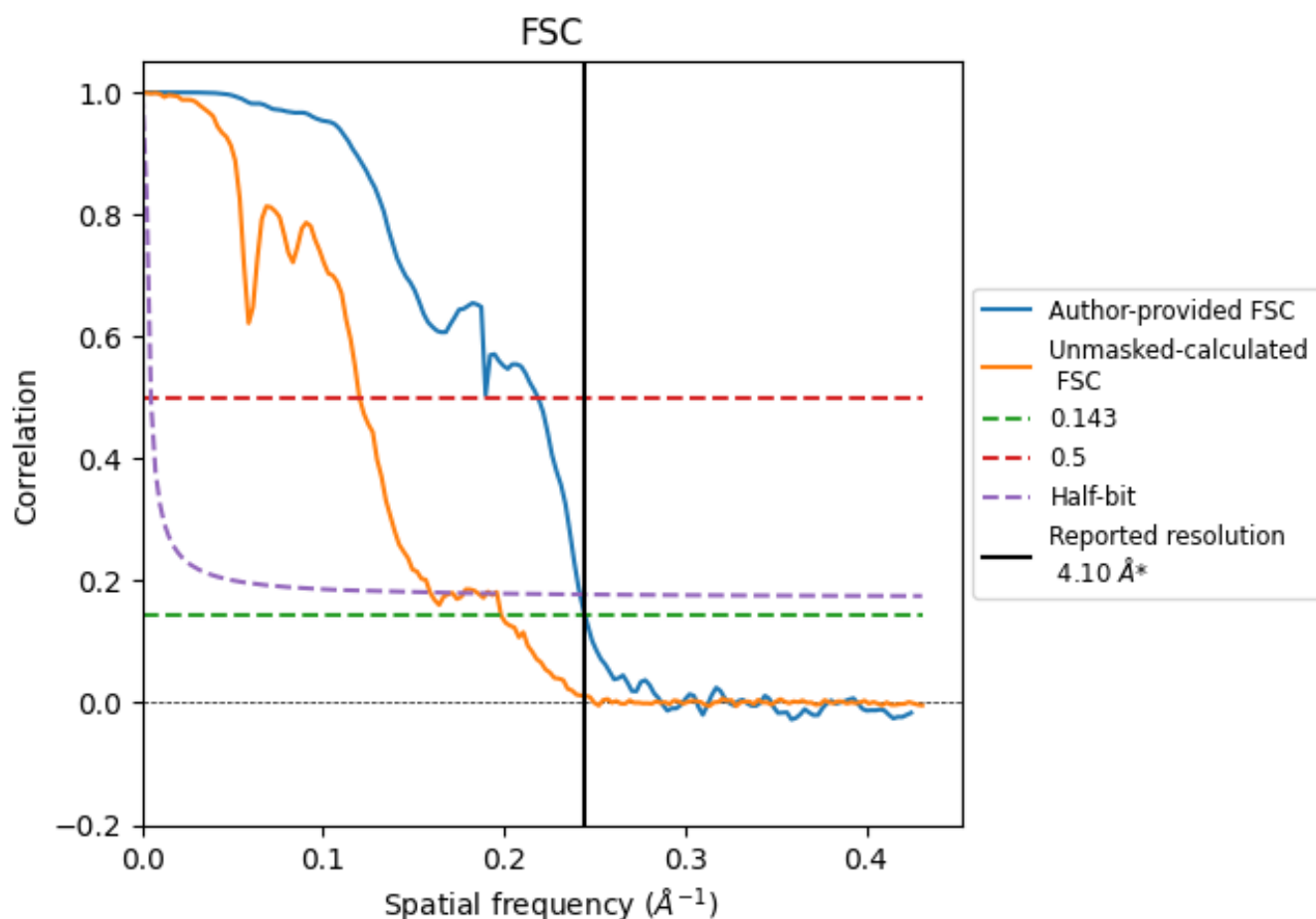


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 \AA^{-1}

8.2 Resolution estimates [i](#)

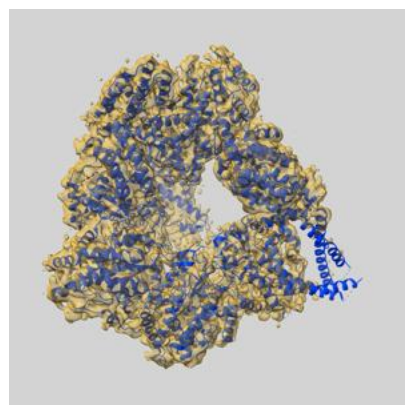
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.09	4.57	4.13
Unmasked-calculated*	5.04	8.33	6.29

*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 5.04 differs from the reported value 4.1 by more than 10 %

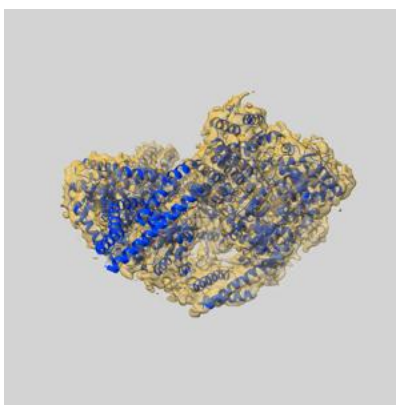
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46897 and PDB model 9DI3. Per-residue inclusion information can be found in section 3 on page 6.

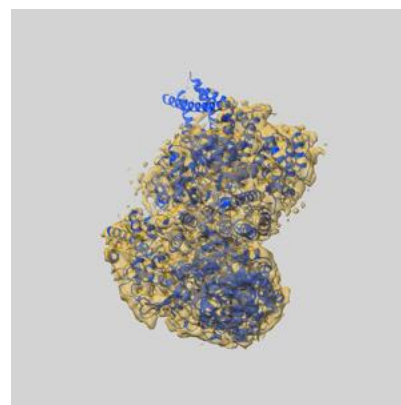
9.1 Map-model overlay [i](#)



X



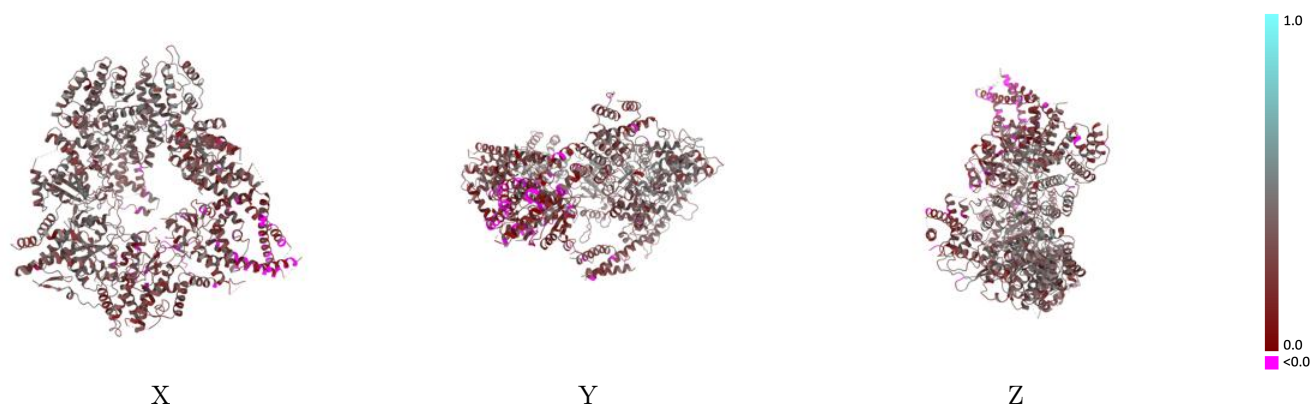
Y



Z

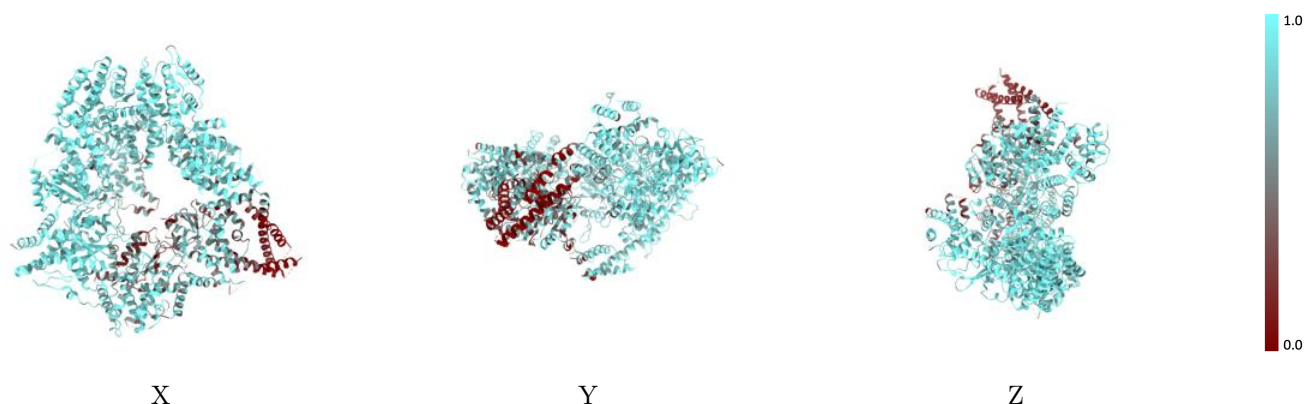
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



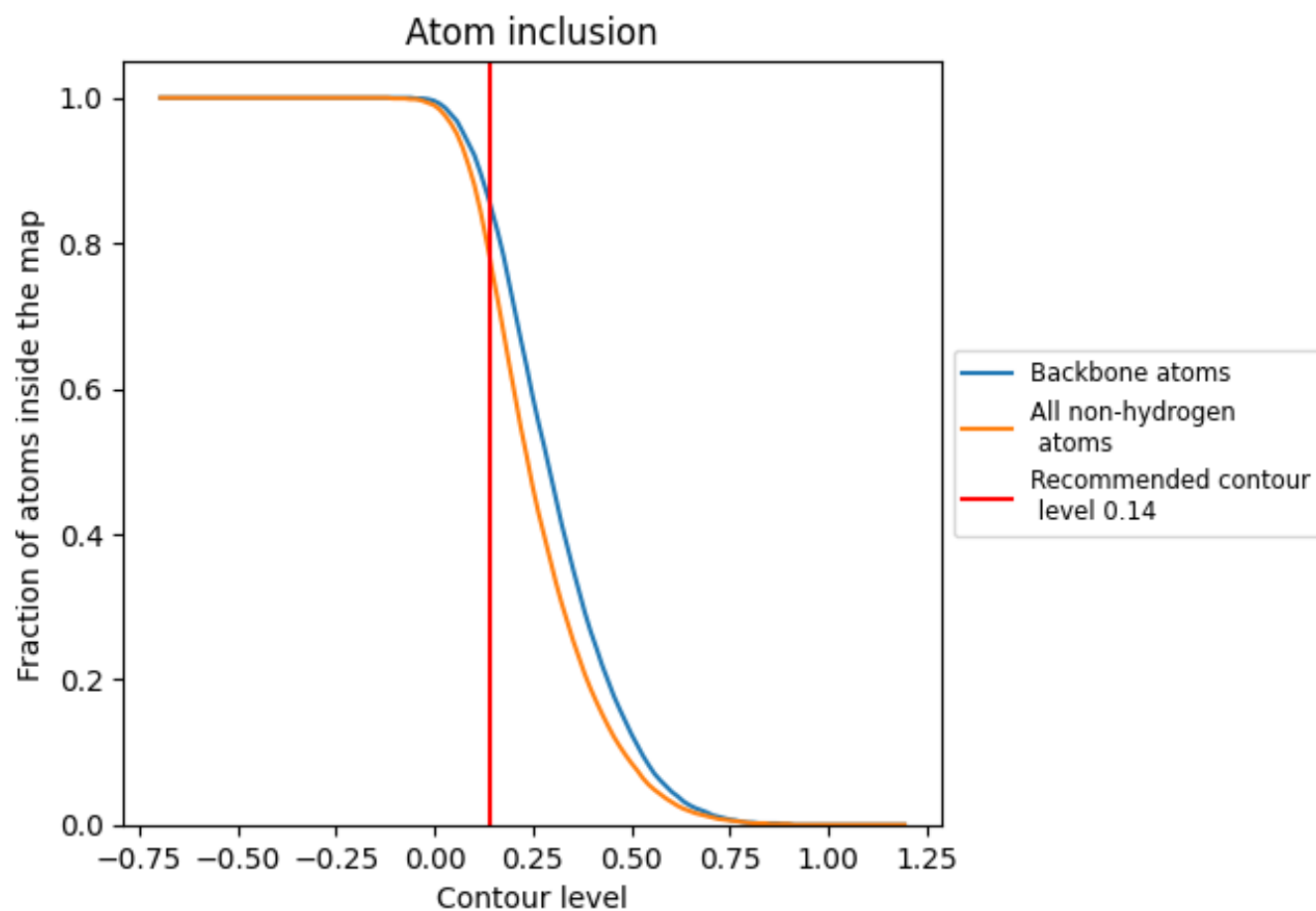
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7820	<div></div> 0.3180
A	<div></div> 0.7820	<div></div> 0.3180

