



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 03:20 PM UTC

PDB ID : 6F0L / pdb_00006f0l
EMDB ID : EMD-3960
Title : S. cerevisiae MCM double hexamer bound to duplex DNA
Authors : Abid Ali, F.; Pye, V.E.; Douglas, M.E.; Locke, J.; Nans, A.; Diffley, J.F.X.; Costa, A.
Deposited on : 2017-11-20
Resolution : 4.77 Å(reported)

This is a Full wwPDB EM Validation 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 : **FAILED**
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

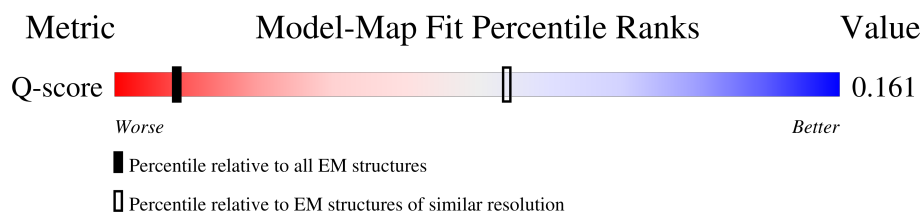
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.77 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	456 (6.43 - 7.41)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 61818 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	603	Total	C	N	O	S	0	0
			4714	2974	842	881	17		
1	A	603	Total	C	N	O	S	0	0
			4714	2974	842	881	17		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	596	Total	C	N	O	S	0	0
			4670	2941	834	882	13		
2	B	596	Total	C	N	O	S	0	0
			4670	2941	834	882	13		

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	642	Total	C	N	O	S	0	0
			5083	3194	878	983	28		
3	C	642	Total	C	N	O	S	0	0
			5083	3194	878	983	28		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	634	Total	C	N	O	S	0	0
			4975	3121	855	974	25		
4	D	634	Total	C	N	O	S	0	0
			4975	3121	855	974	25		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	615	Total	C	N	O	S	0	0
			4731	2979	837	895	20		
5	E	615	Total	C	N	O	S	0	0
			4731	2979	837	895	20		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	687	Total	C	N	O	S	0	0
			5411	3408	938	1035	30		
6	F	687	Total	C	N	O	S	0	0
			5411	3408	938	1035	30		

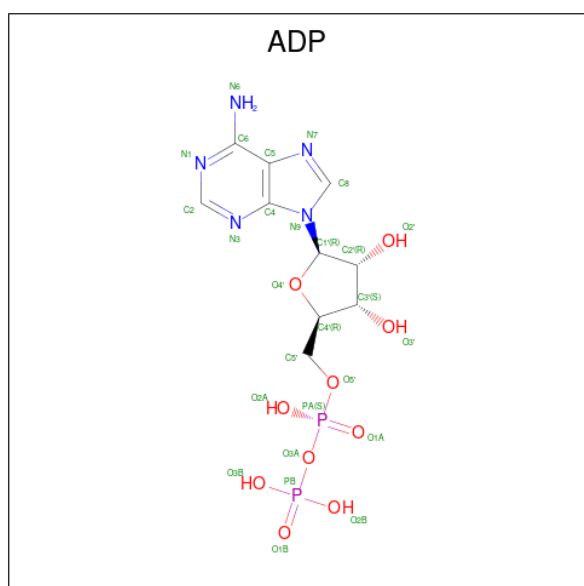
- Molecule 7 is a DNA chain called DNA (62-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	62	Total	C	N	O	P	0	0
			1270	604	233	371	62		

- Molecule 8 is a DNA chain called DNA (62-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	62	Total	C	N	O	P	0	0
			1272	605	232	373	62		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
9	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	5	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

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3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	52319	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.543	Depositor
Minimum map value	-0.721	Depositor
Average map value	0.040	Depositor
Map value standard deviation	0.175	Depositor
Recommended contour level	0.68	Depositor
Map size ($\text{\AA}$)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.38, 1.38, 1.38	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 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
9	ADP	B	1001	-	28,29,29	1.42	4 (14%)	43,45,45	1.97	9 (20%)
9	ADP	3	1001	-	28,29,29	1.43	4 (14%)	43,45,45	1.96	9 (20%)
9	ADP	D	1001	-	28,29,29	1.36	3 (10%)	43,45,45	2.02	8 (18%)
9	ADP	5	1001	-	28,29,29	1.37	3 (10%)	43,45,45	2.02	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
9	ADP	B	1001	-	-	3/16/32/32	0/3/3/3
9	ADP	3	1001	-	-	3/16/32/32	0/3/3/3
9	ADP	D	1001	-	-	8/16/32/32	0/3/3/3
9	ADP	5	1001	-	-	8/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	5	1001	ADP	C5-C4	4.63	1.47	1.39
9	D	1001	ADP	C5-C4	4.62	1.47	1.39
9	B	1001	ADP	C5-C4	4.56	1.47	1.39
9	3	1001	ADP	C5-C4	4.55	1.47	1.39
9	3	1001	ADP	C5-N7	-2.89	1.33	1.39
9	5	1001	ADP	C5-N7	-2.88	1.33	1.39
9	D	1001	ADP	C5-N7	-2.87	1.33	1.39
9	B	1001	ADP	C5-N7	-2.86	1.33	1.39
9	3	1001	ADP	C5-C6	2.41	1.47	1.41
9	B	1001	ADP	C5-C6	2.41	1.47	1.41
9	5	1001	ADP	C5-C6	2.38	1.47	1.41
9	D	1001	ADP	C5-C6	2.38	1.47	1.41
9	3	1001	ADP	PA-O3A	2.18	1.61	1.59
9	B	1001	ADP	PA-O3A	2.12	1.61	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	1001	ADP	C5-C4-N3	-7.17	116.84	126.72
9	5	1001	ADP	C5-C4-N3	-7.17	116.85	126.72
9	B	1001	ADP	C5-C4-N3	-6.79	117.37	126.72
9	3	1001	ADP	C5-C4-N3	-6.74	117.43	126.72
9	D	1001	ADP	N3-C4-N9	5.76	136.97	127.17
9	5	1001	ADP	N3-C4-N9	5.76	136.96	127.17
9	B	1001	ADP	N3-C4-N9	5.45	136.44	127.17
9	3	1001	ADP	N3-C4-N9	5.44	136.42	127.17
9	B	1001	ADP	C2-N3-C4	4.09	121.83	111.83
9	D	1001	ADP	C2-N3-C4	4.07	121.78	111.83
9	3	1001	ADP	C2-N3-C4	4.07	121.77	111.83
9	5	1001	ADP	C2-N3-C4	4.05	121.73	111.83
9	B	1001	ADP	N3-C2-N1	-3.33	123.54	128.58
9	3	1001	ADP	N3-C2-N1	-3.32	123.56	128.58
9	B	1001	ADP	C4-C5-N7	-3.11	107.03	110.58
9	D	1001	ADP	N3-C2-N1	-3.08	123.92	128.58
9	5	1001	ADP	N3-C2-N1	-3.07	123.94	128.58
9	3	1001	ADP	C4-C5-N7	-3.05	107.09	110.58
9	5	1001	ADP	C4-C5-N7	-2.96	107.20	110.58
9	D	1001	ADP	C4-C5-N7	-2.95	107.21	110.58
9	3	1001	ADP	C3'-C2'-C1'	2.48	106.16	101.46
9	B	1001	ADP	C3'-C2'-C1'	2.47	106.14	101.46
9	D	1001	ADP	C3'-C2'-C1'	2.38	105.97	101.46
9	5	1001	ADP	C3'-C2'-C1'	2.38	105.97	101.46
9	B	1001	ADP	C5-N7-C8	2.32	107.10	103.45
9	3	1001	ADP	C5-N7-C8	2.30	107.07	103.45
9	D	1001	ADP	C5-N7-C8	2.19	106.89	103.45
9	5	1001	ADP	C5-N7-C8	2.18	106.88	103.45
9	B	1001	ADP	O2A-PA-O3A	2.12	113.01	107.27
9	3	1001	ADP	O2A-PA-O3A	2.12	113.00	107.27
9	B	1001	ADP	C2'-C3'-C4'	2.11	106.69	102.61
9	3	1001	ADP	C2'-C3'-C4'	2.10	106.67	102.61
9	D	1001	ADP	C1'-N9-C8	-2.06	122.53	127.09
9	5	1001	ADP	C1'-N9-C8	-2.05	122.55	127.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	3	1001	ADP	C5'-O5'-PA-O1A
9	3	1001	ADP	C5'-O5'-PA-O2A
9	3	1001	ADP	C5'-O5'-PA-O3A
9	5	1001	ADP	C5'-O5'-PA-O1A

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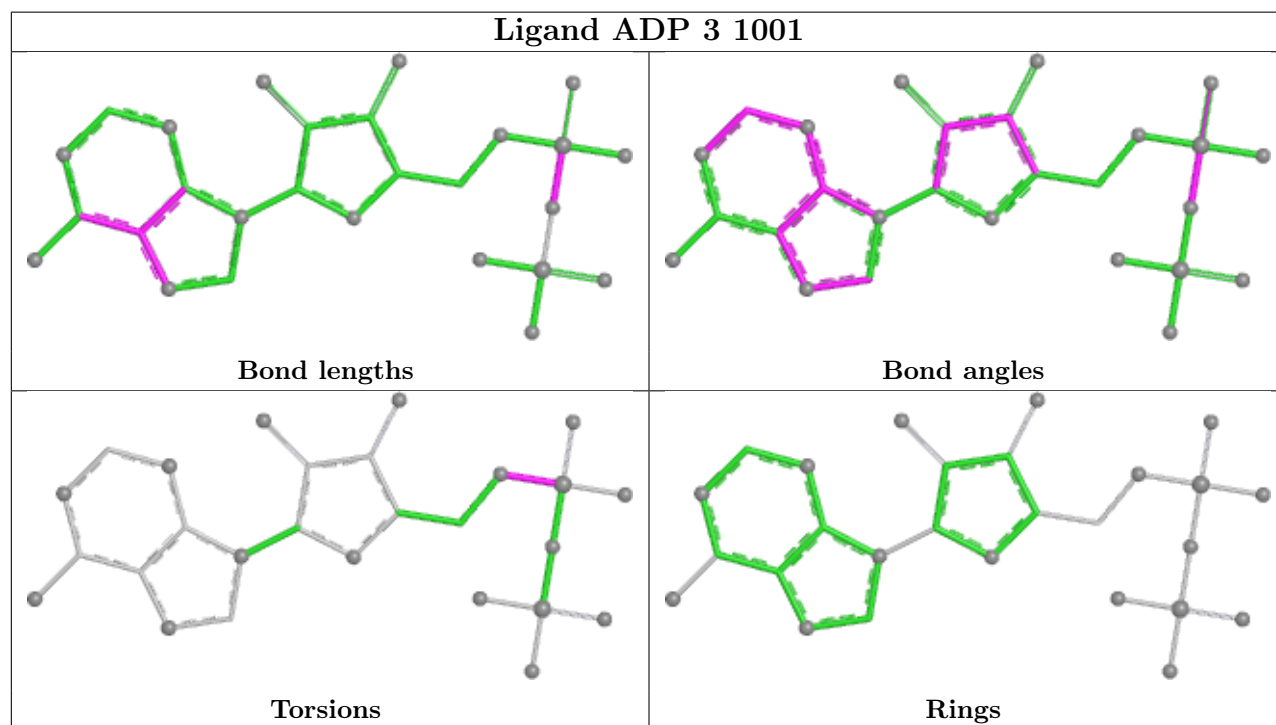
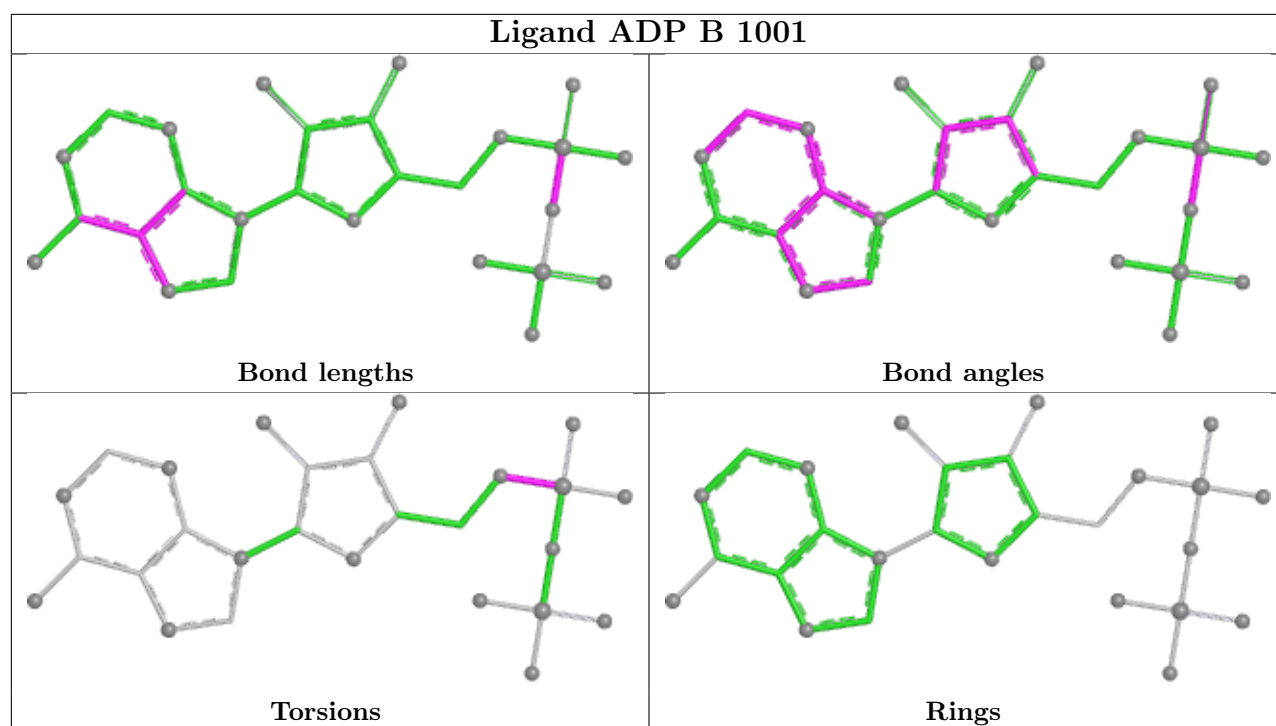
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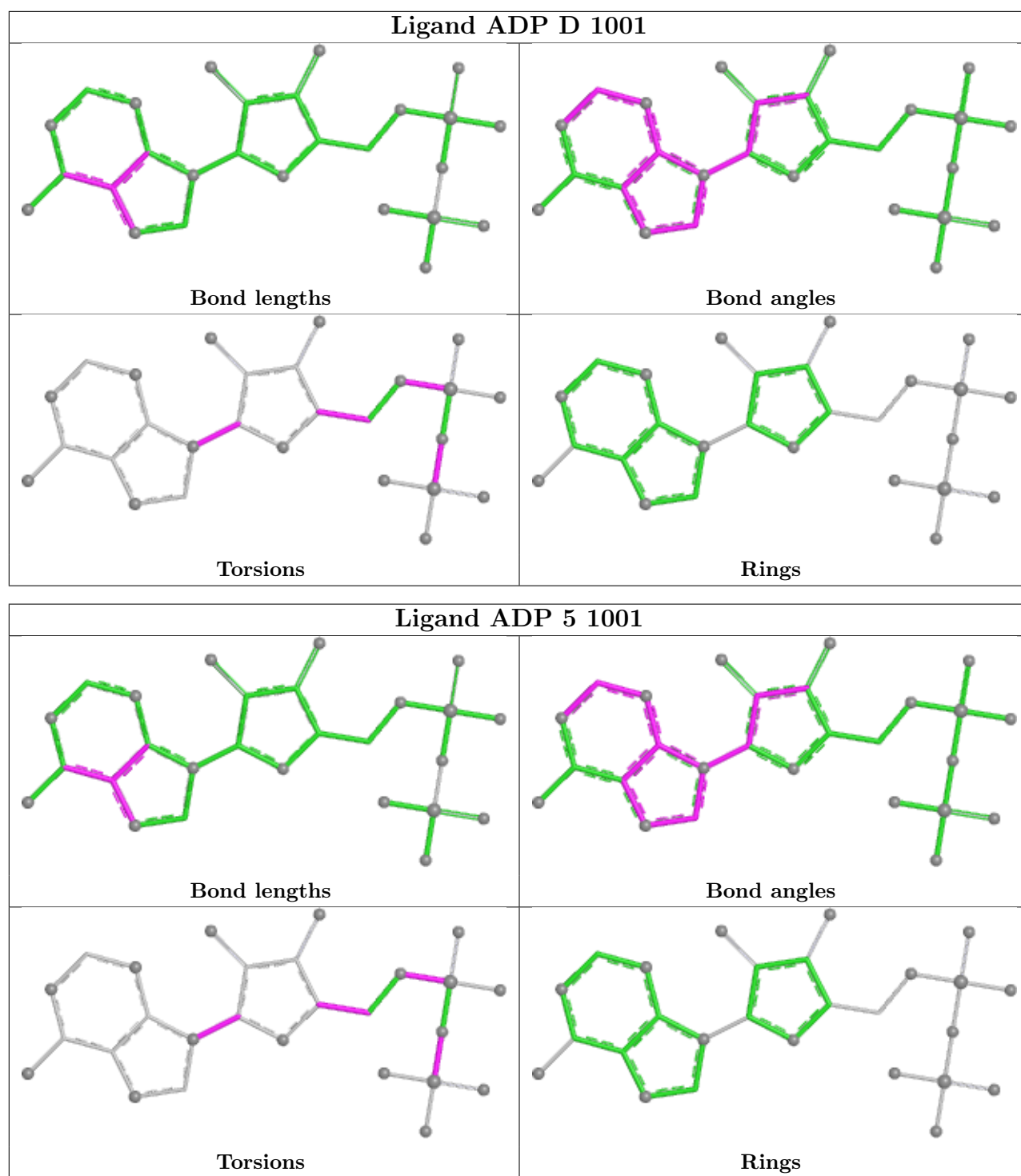
Mol	Chain	Res	Type	Atoms
9	5	1001	ADP	C5'-O5'-PA-O2A
9	5	1001	ADP	C5'-O5'-PA-O3A
9	B	1001	ADP	C5'-O5'-PA-O1A
9	B	1001	ADP	C5'-O5'-PA-O2A
9	B	1001	ADP	C5'-O5'-PA-O3A
9	D	1001	ADP	C5'-O5'-PA-O1A
9	D	1001	ADP	C5'-O5'-PA-O2A
9	D	1001	ADP	C5'-O5'-PA-O3A
9	5	1001	ADP	PA-O3A-PB-O1B
9	D	1001	ADP	PA-O3A-PB-O1B
9	5	1001	ADP	C3'-C4'-C5'-O5'
9	D	1001	ADP	C3'-C4'-C5'-O5'
9	5	1001	ADP	PA-O3A-PB-O2B
9	5	1001	ADP	PA-O3A-PB-O3B
9	D	1001	ADP	PA-O3A-PB-O2B
9	D	1001	ADP	PA-O3A-PB-O3B
9	5	1001	ADP	C2'-C1'-N9-C8
9	D	1001	ADP	C2'-C1'-N9-C8

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.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	X	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	34:DT	O3'	35:DG	P	3.37
1	X	24:DC	O3'	25:DA	P	1.89
1	X	23:DG	O3'	24:DC	P	1.88

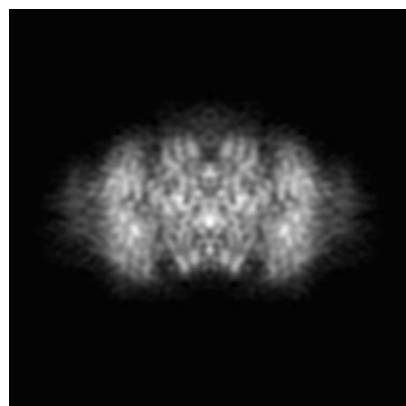
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3960. These allow visual inspection of the internal detail of the map and identification of artifacts.

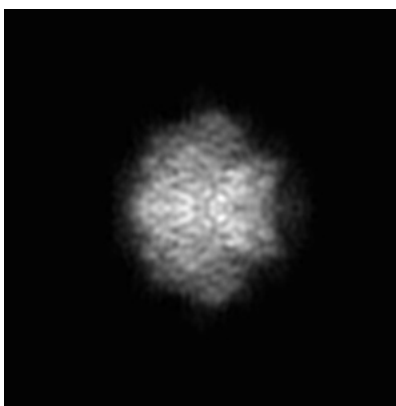
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

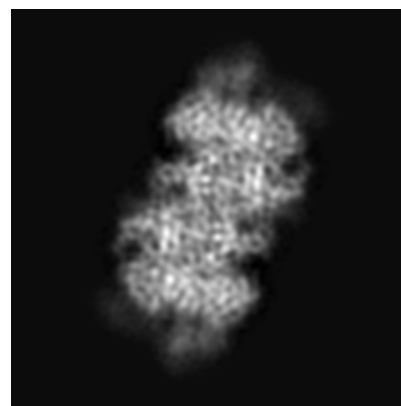
5.1.1 Primary map



X

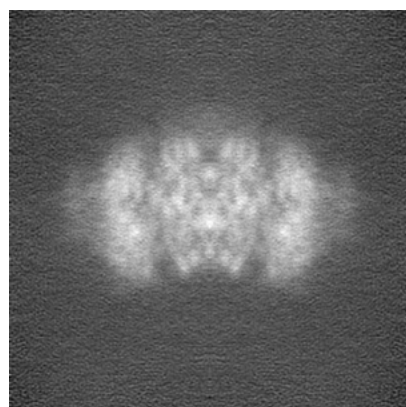


Y

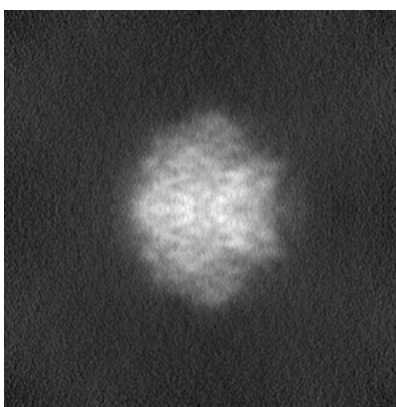


Z

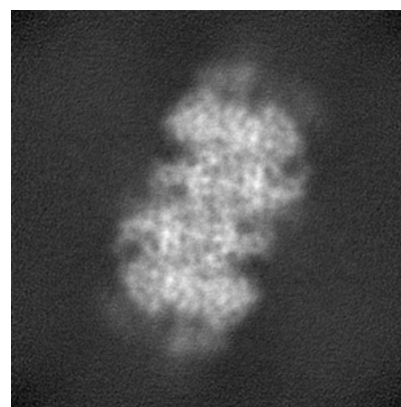
5.1.2 Raw map



X



Y



Z

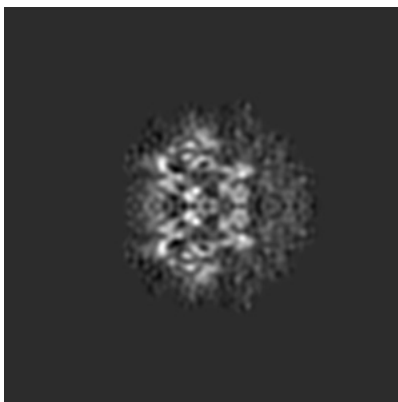
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

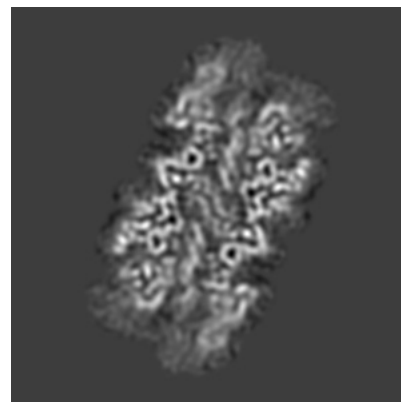
5.2.1 Primary map



X Index: 128

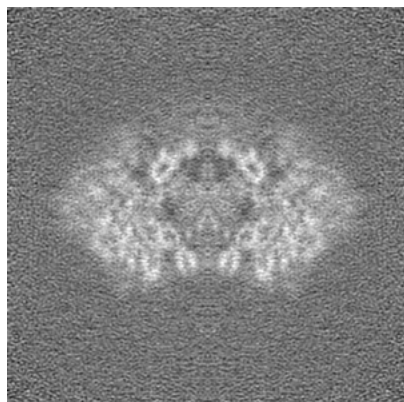


Y Index: 128

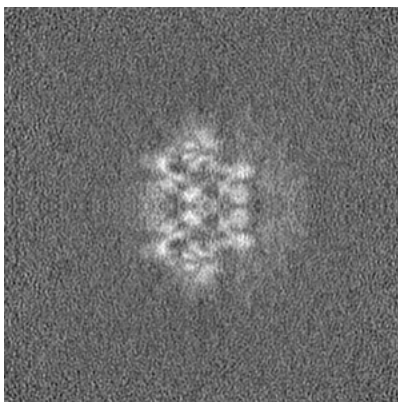


Z Index: 128

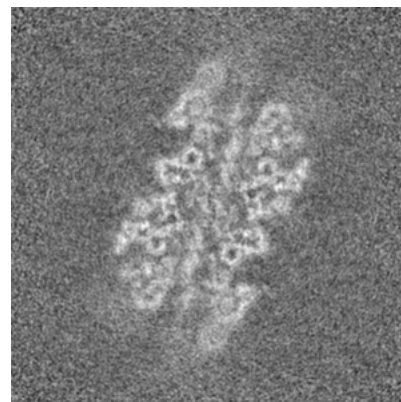
5.2.2 Raw map



X Index: 128



Y Index: 128

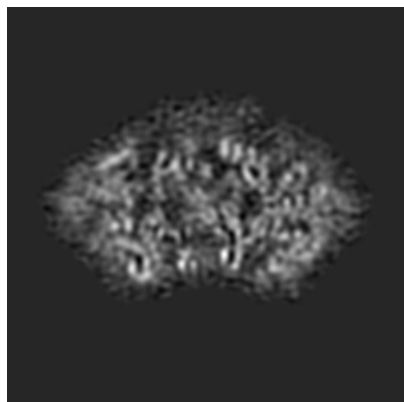


Z Index: 128

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

5.3 Largest variance slices [i](#)

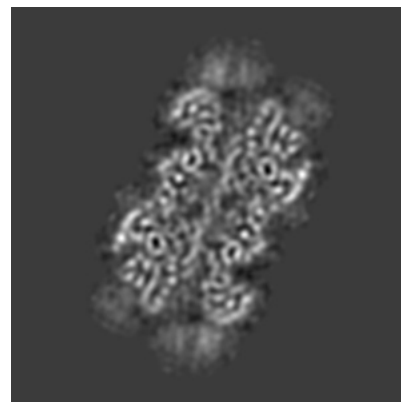
5.3.1 Primary map



X Index: 125

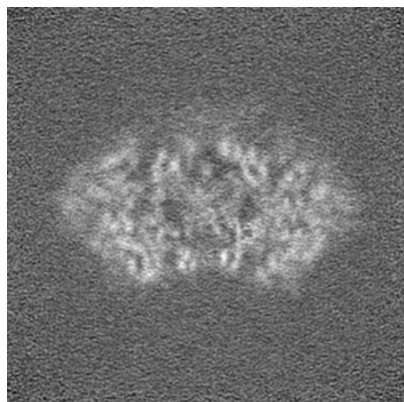


Y Index: 110

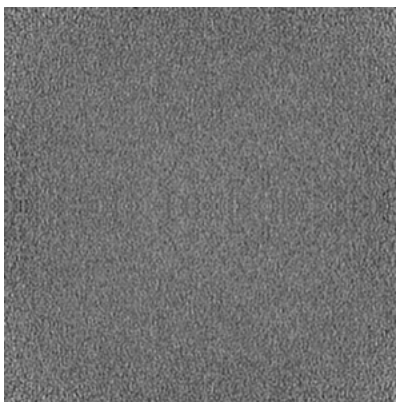


Z Index: 132

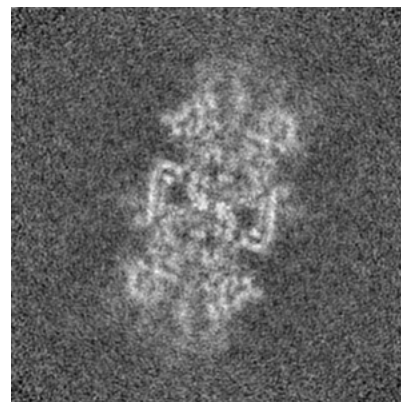
5.3.2 Raw map



X Index: 126



Y Index: 0

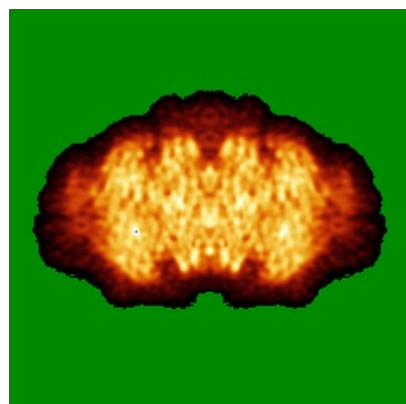


Z Index: 119

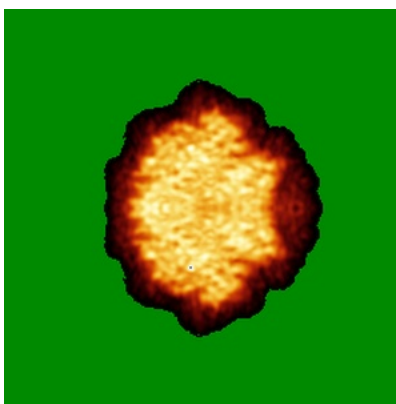
The images above show the largest variance slices of the map in three orthogonal directions.

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

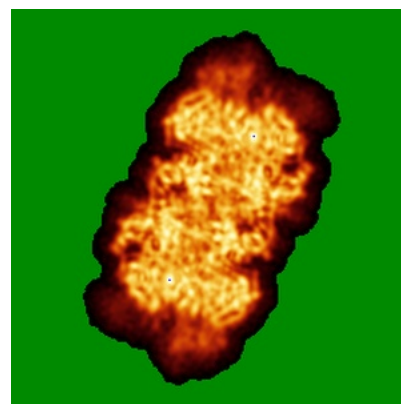
5.4.1 Primary map



X

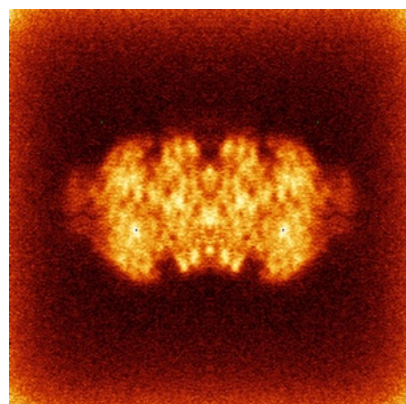


Y

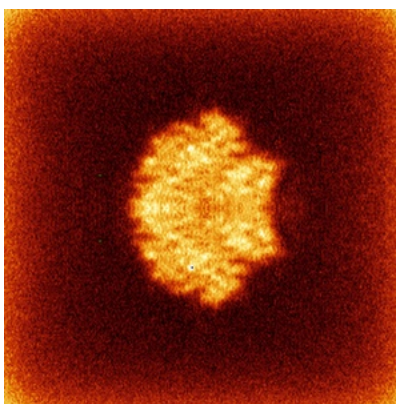


Z

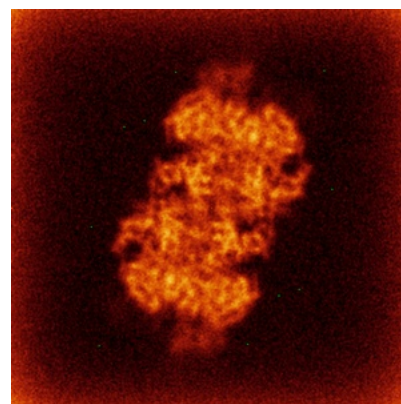
5.4.2 Raw map



X



Y

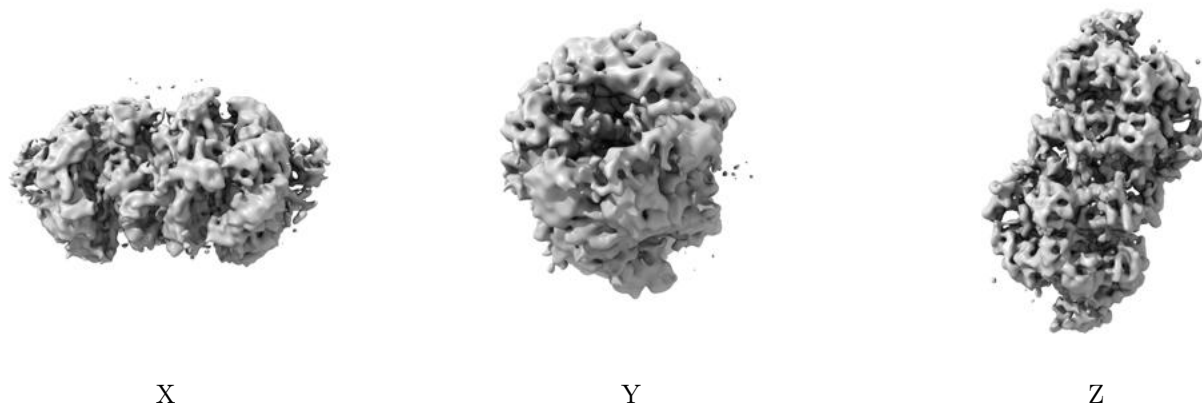


Z

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.

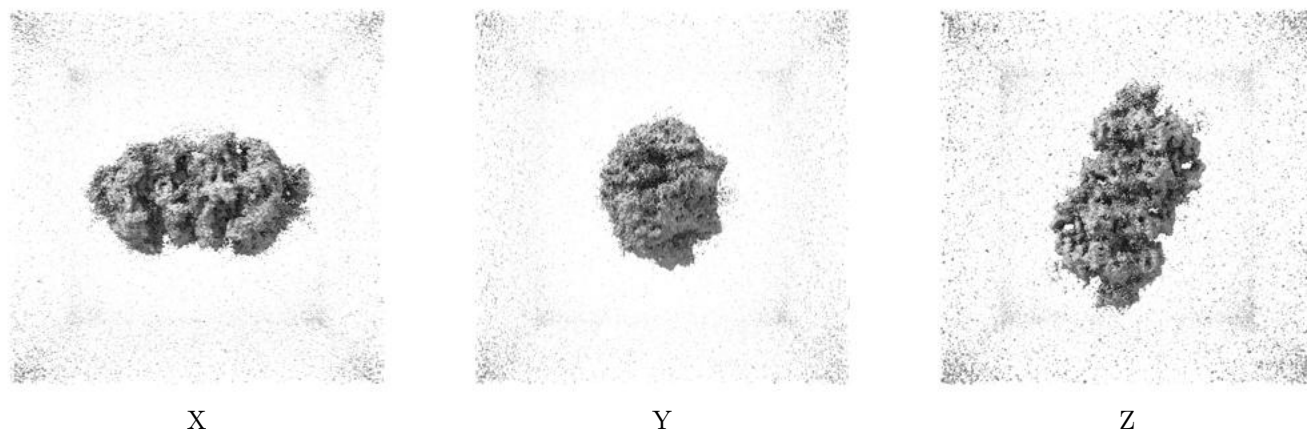
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.68. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

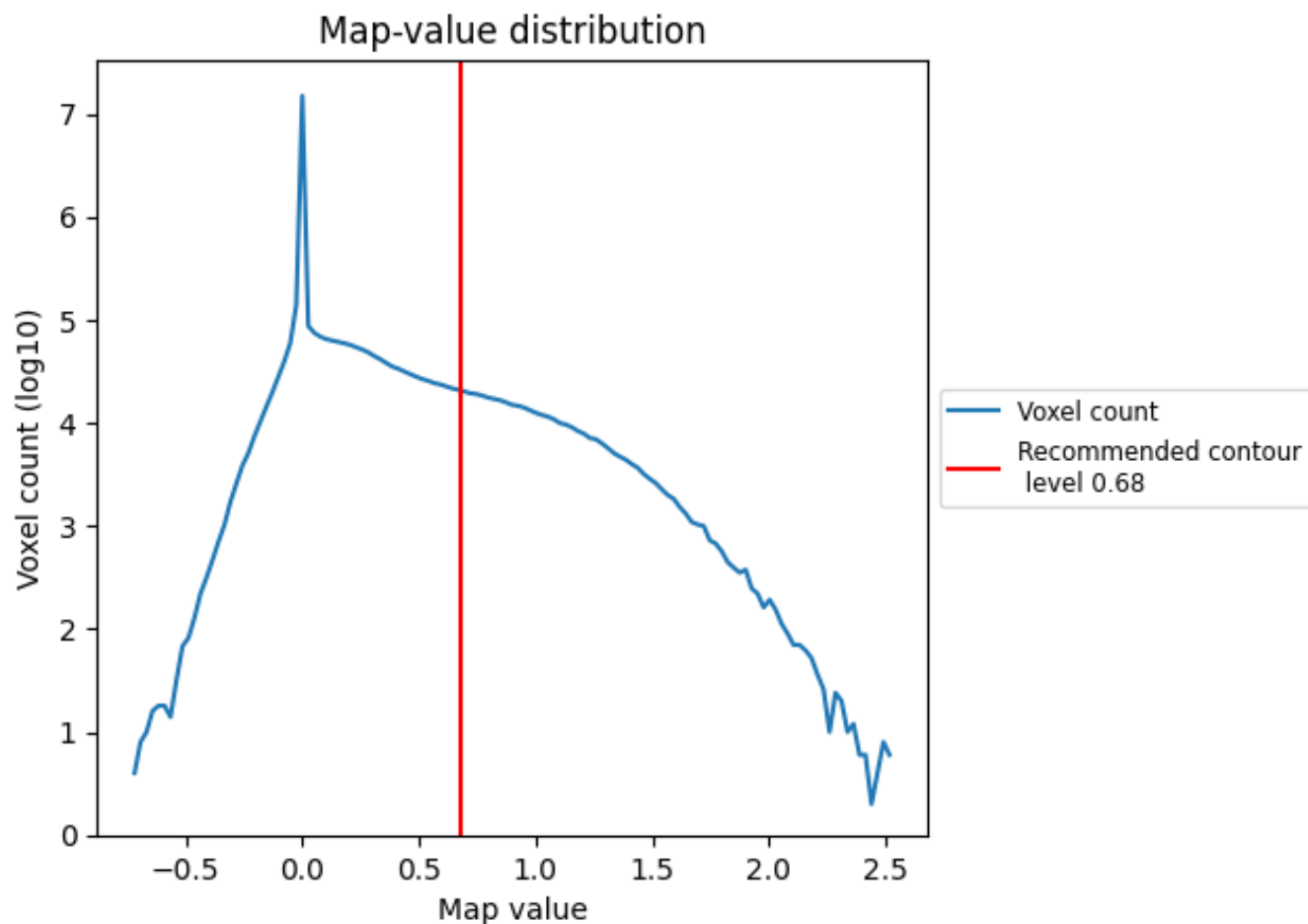
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

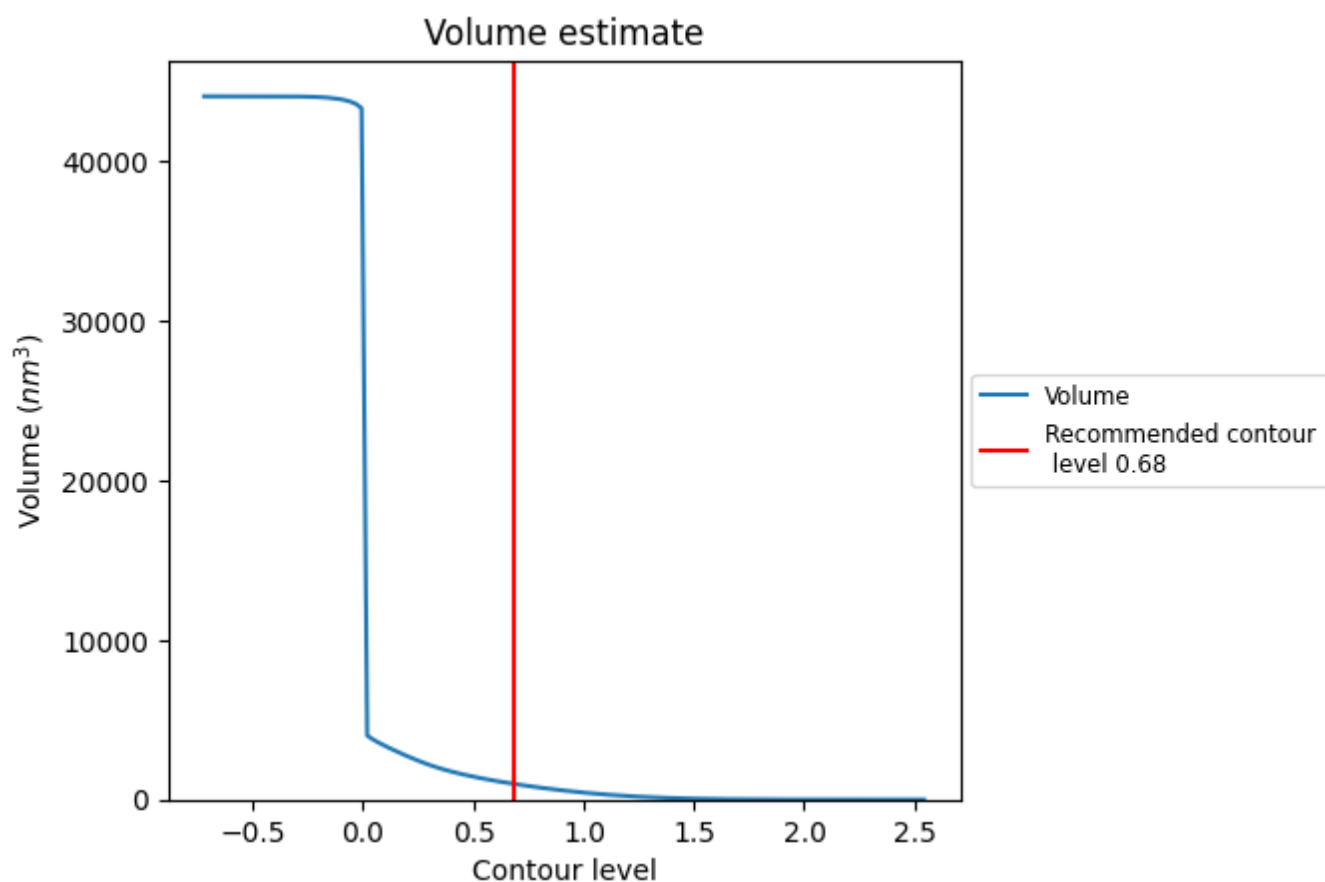
This section contains the results of statistical analysis of the map.

6.1 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.

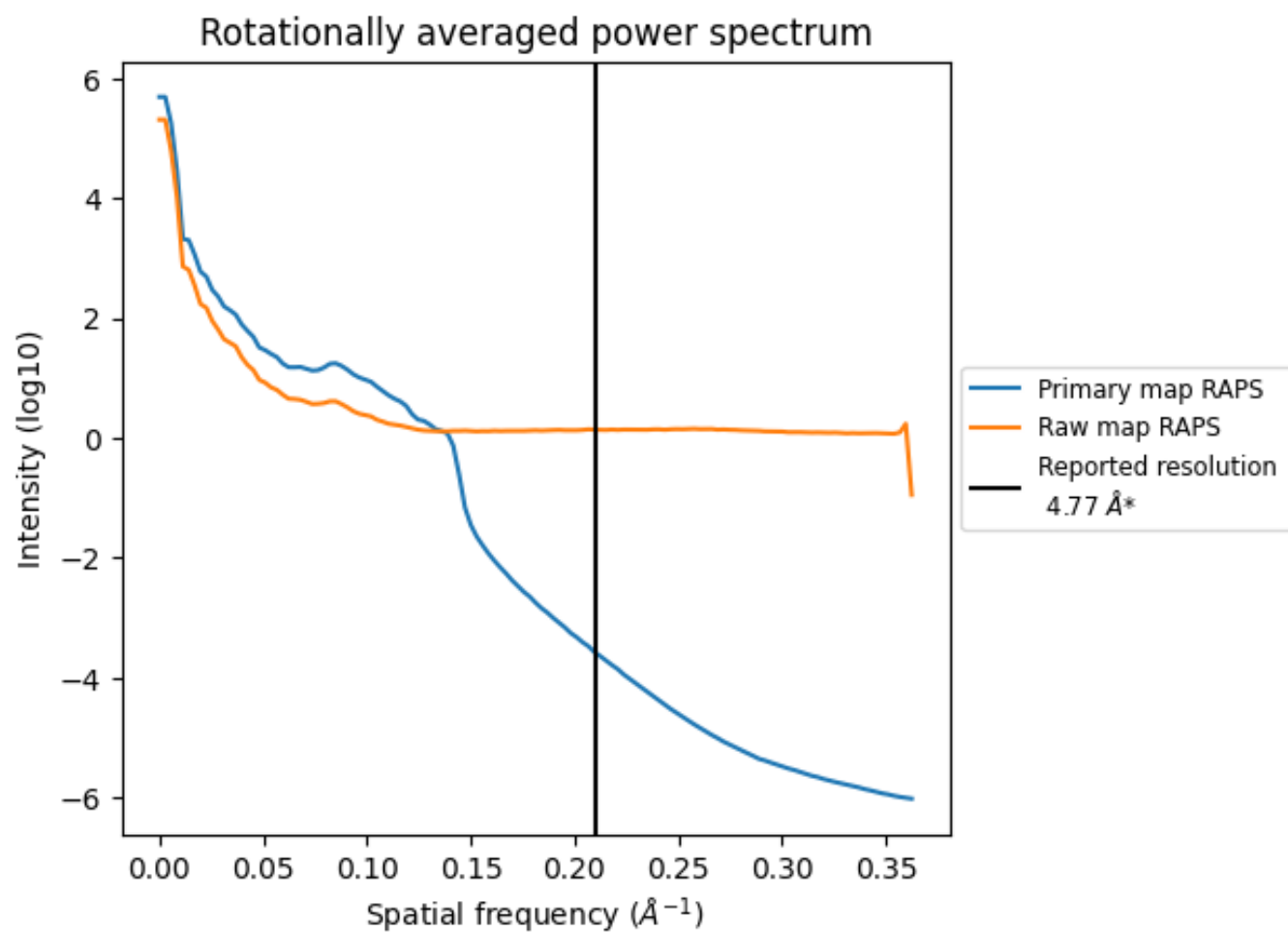
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 991 nm³; this corresponds to an approximate mass of 895 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.

6.3 Rotationally averaged power spectrum ⓘ

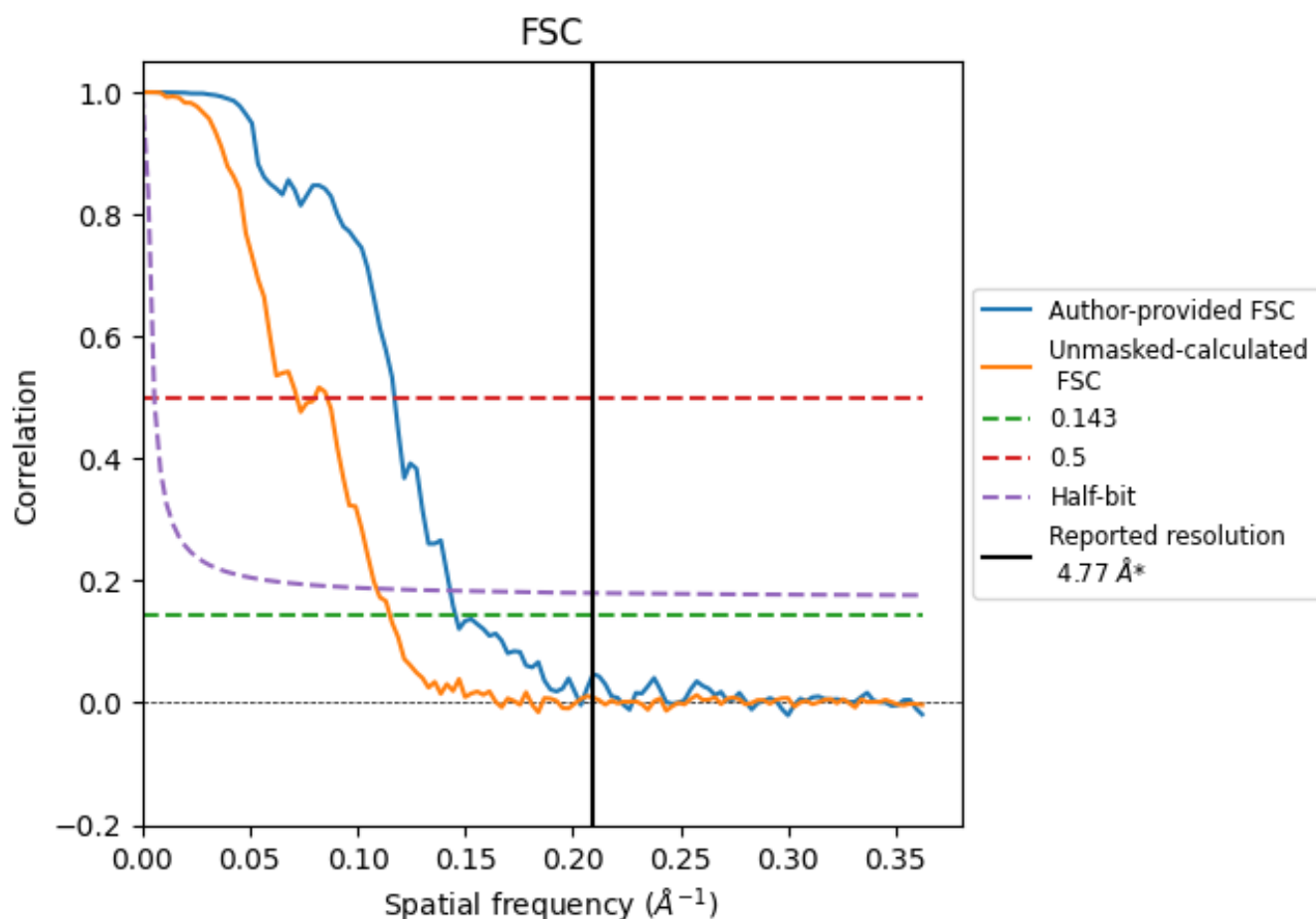


*Reported resolution corresponds to spatial frequency of 0.210 $\text{\AA}^{-1}$

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.210 $\text{\AA}^{-1}$

7.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.77	-	-
Author-provided FSC curve	6.87	8.54	6.99
Unmasked-calculated*	8.69	13.93	9.18

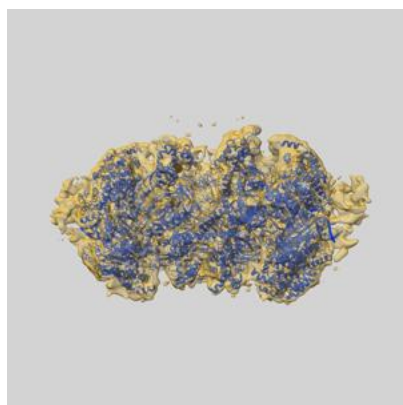
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.87 differs from the reported value 4.77 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.69 differs from the reported value 4.77 by more than 10 %

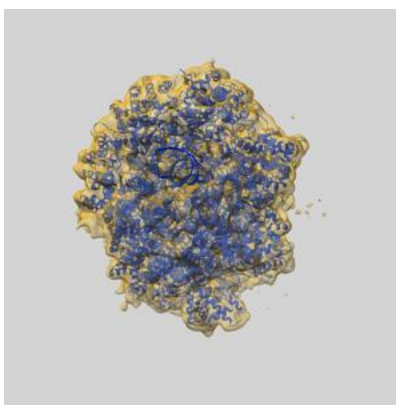
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3960 and PDB model 6F0L. Per-residue inclusion information can be found in section ?? on page ??.

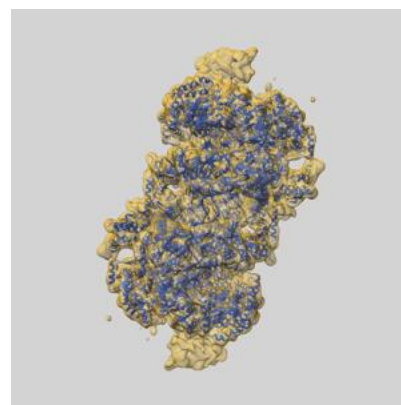
8.1 Map-model overlay [i](#)



X



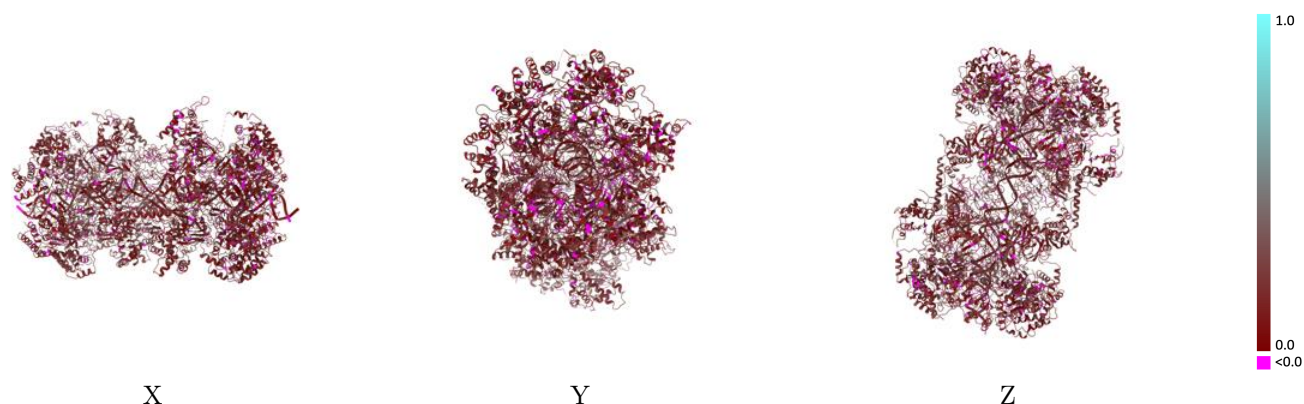
Y



Z

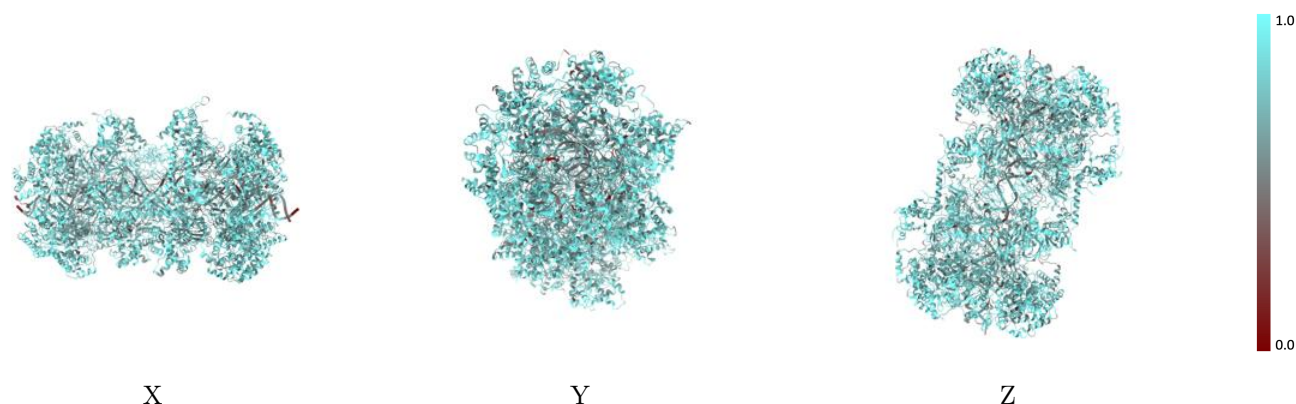
The images above show the 3D surface view of the map at the recommended contour level 0.68 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



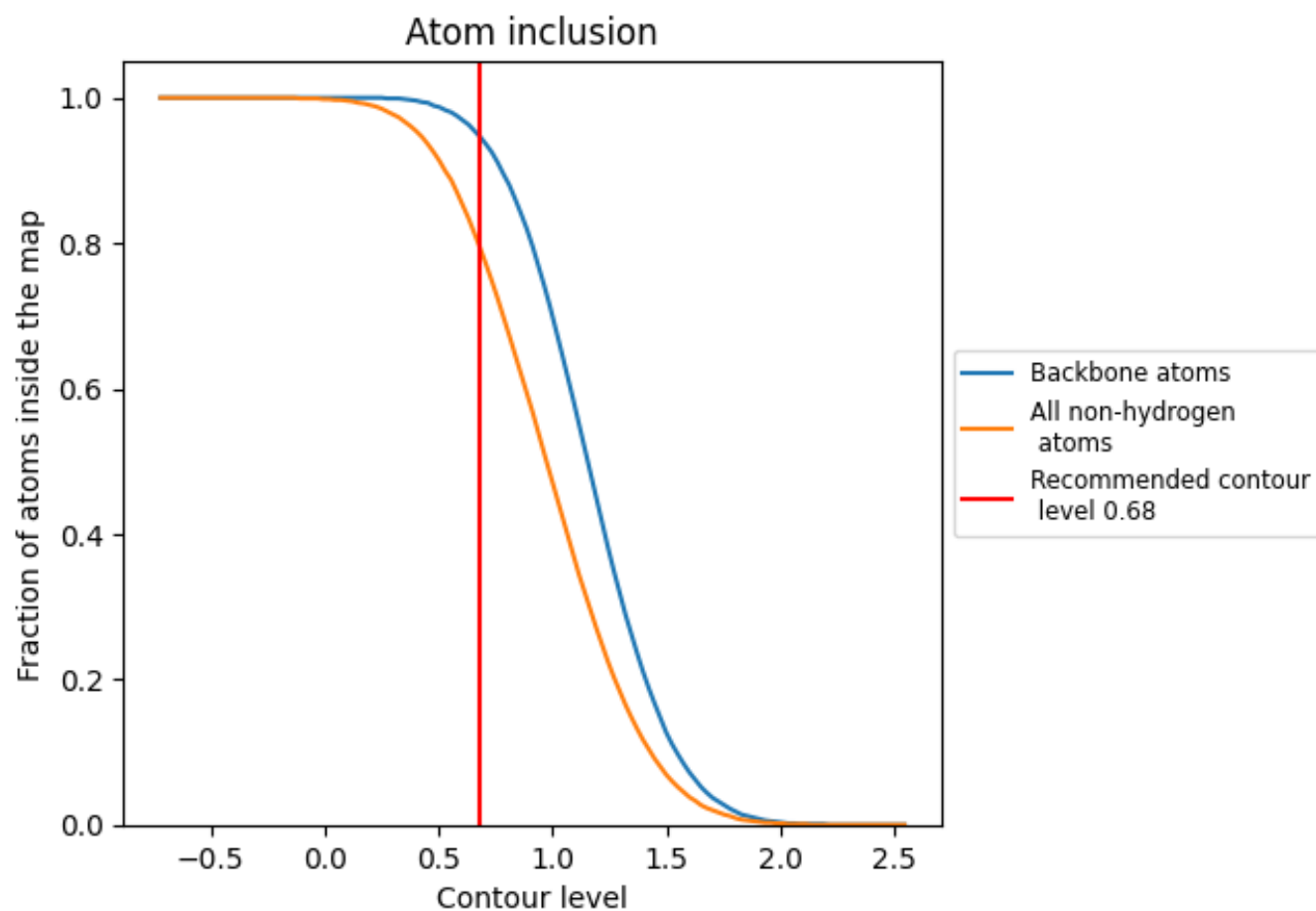
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.68).

8.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.68) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7950	 0.1610
2	 0.8190	 0.1700
3	 0.8000	 0.1680
4	 0.8130	 0.1650
5	 0.8050	 0.1620
6	 0.8140	 0.1650
7	 0.8020	 0.1700
A	 0.8010	 0.1540
B	 0.7930	 0.1650
C	 0.8010	 0.1510
D	 0.7910	 0.1550
E	 0.7920	 0.1470
F	 0.7960	 0.1630
X	 0.6270	 0.1490
Y	 0.6290	 0.1520

