Full wwPDB EM Validation Report

May 22, 2025 – 06:32 PM EDT

PDB ID	:	9MOD / pdb_00009mod
EMDB ID	:	EMD-48456
Title	:	Structure of native murine cardiac thin filament variant I79N in troponin T at pCa=5.8 in Ca2+-free tilted state (upper strand)
Authors	:	Risi, C.M.; Galkin, V.E.
Deposited on	:	2024-12-25
Resolution	:	5.70 Å(reported)
Based on initial models	:	8UWX, 7KO4, 7UTL, 8DD0

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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	FAILED
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 (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 28813 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 Actin, alpha cardiac muscle 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	B	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	C	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	D	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	E	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	F	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		
1	G	371	Total	C	N	O	S	0	0
			2898	1836	489	553	20		

- Molecule 2 is a protein called Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	160	Total	C	N	O	S	0	0
			1273	787	195	278	13		

- Molecule 3 is a protein called Troponin I, cardiac muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	170	Total	C	N	O	S	0	0
			1389	855	266	261	7		

- Molecule 4 is a protein called Isoform 6 of Troponin T, cardiac muscle.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	74	Total	C	N	O	0	0
			643	401	123	119		

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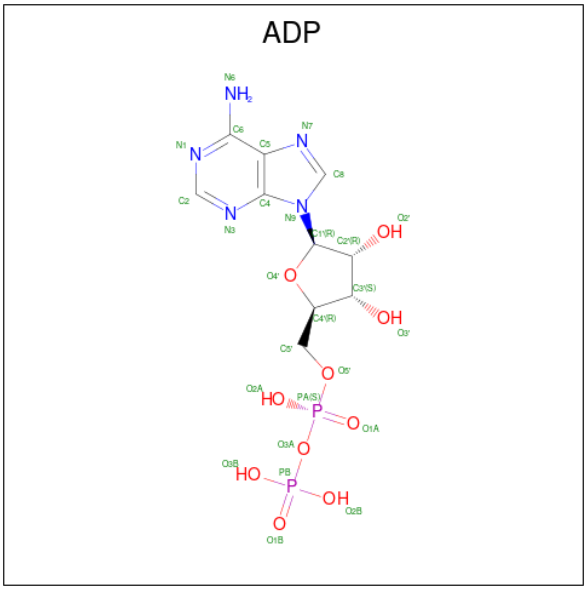
Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	66	Total	C	N	O	S	0	0
			586	349	123	113	1		

- Molecule 5 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	221	Total	C	N	O	S	0	0
			1783	1091	302	386	4		
5	M	221	Total	C	N	O	S	0	0
			1783	1091	302	386	4		
5	N	55	Total	C	N	O	S	0	0
			437	266	77	91	3		
5	O	55	Total	C	N	O	S	0	0
			437	266	77	91	3		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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Mol	Chain	Residues	Atoms					AltConf
6	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	
7	C	1	Total	Mg	0
			1	1	
7	D	1	Total	Mg	0
			1	1	
7	E	1	Total	Mg	0
			1	1	
7	F	1	Total	Mg	0
			1	1	
7	G	1	Total	Mg	0
			1	1	

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

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48557	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	9.444	Depositor
Minimum map value	-3.123	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.276	Depositor
Recommended contour level	0.515	Depositor
Map size (Å)	439.344, 439.344, 439.344	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.356, 1.356, 1.356	Depositor

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no oligosaccharides in this entry.

4.6 Ligand geometry

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
6	ADP	B	401	7	24,29,29	0.83	0	29,45,45	1.18	2 (6%)
6	ADP	E	401	7	24,29,29	0.86	0	29,45,45	1.19	2 (6%)
6	ADP	C	401	7	24,29,29	0.85	0	29,45,45	1.16	2 (6%)
6	ADP	D	401	7	24,29,29	0.82	0	29,45,45	1.18	2 (6%)
6	ADP	F	401	7	24,29,29	0.82	0	29,45,45	1.17	2 (6%)
6	ADP	A	401	7	24,29,29	0.82	0	29,45,45	1.19	2 (6%)
6	ADP	G	401	7	24,29,29	0.86	0	29,45,45	1.16	2 (6%)

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
6	ADP	B	401	7	-	3/12/32/32	0/3/3/3
6	ADP	E	401	7	-	3/12/32/32	0/3/3/3
6	ADP	C	401	7	-	3/12/32/32	0/3/3/3
6	ADP	D	401	7	-	3/12/32/32	0/3/3/3
6	ADP	F	401	7	-	3/12/32/32	0/3/3/3
6	ADP	A	401	7	-	3/12/32/32	0/3/3/3
6	ADP	G	401	7	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	401	ADP	N3-C2-N1	-3.21	124.31	128.67
6	B	401	ADP	N3-C2-N1	-3.11	124.45	128.67
6	A	401	ADP	N3-C2-N1	-3.10	124.47	128.67
6	G	401	ADP	N3-C2-N1	-3.09	124.47	128.67
6	D	401	ADP	N3-C2-N1	-3.08	124.49	128.67
6	C	401	ADP	N3-C2-N1	-3.06	124.52	128.67
6	F	401	ADP	N3-C2-N1	-3.03	124.56	128.67
6	A	401	ADP	C4-C5-N7	-2.49	106.71	109.34
6	B	401	ADP	C4-C5-N7	-2.49	106.71	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	401	ADP	C4-C5-N7	-2.48	106.72	109.34
6	E	401	ADP	C4-C5-N7	-2.39	106.81	109.34
6	F	401	ADP	C4-C5-N7	-2.30	106.90	109.34
6	G	401	ADP	C4-C5-N7	-2.27	106.94	109.34
6	C	401	ADP	C4-C5-N7	-2.25	106.95	109.34

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	ADP	C5'-O5'-PA-O1A
6	A	401	ADP	C5'-O5'-PA-O2A
6	A	401	ADP	C5'-O5'-PA-O3A
6	B	401	ADP	C5'-O5'-PA-O1A
6	B	401	ADP	C5'-O5'-PA-O2A
6	B	401	ADP	C5'-O5'-PA-O3A
6	C	401	ADP	C5'-O5'-PA-O1A
6	C	401	ADP	C5'-O5'-PA-O2A
6	C	401	ADP	C5'-O5'-PA-O3A
6	D	401	ADP	C5'-O5'-PA-O1A
6	D	401	ADP	C5'-O5'-PA-O2A
6	D	401	ADP	C5'-O5'-PA-O3A
6	E	401	ADP	C5'-O5'-PA-O1A
6	E	401	ADP	C5'-O5'-PA-O2A
6	E	401	ADP	C5'-O5'-PA-O3A
6	F	401	ADP	C5'-O5'-PA-O1A
6	F	401	ADP	C5'-O5'-PA-O2A
6	F	401	ADP	C5'-O5'-PA-O3A
6	G	401	ADP	C5'-O5'-PA-O1A
6	G	401	ADP	C5'-O5'-PA-O2A
6	G	401	ADP	C5'-O5'-PA-O3A

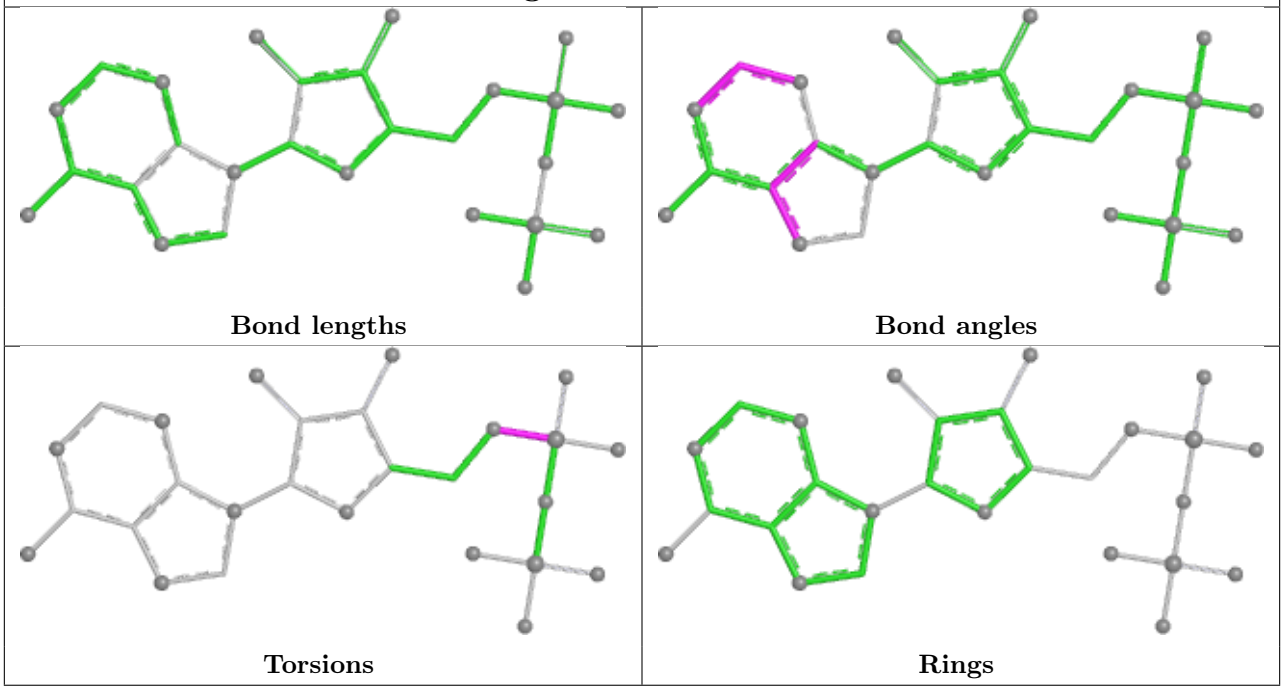
There are no ring outliers.

No monomer is involved in short contacts.

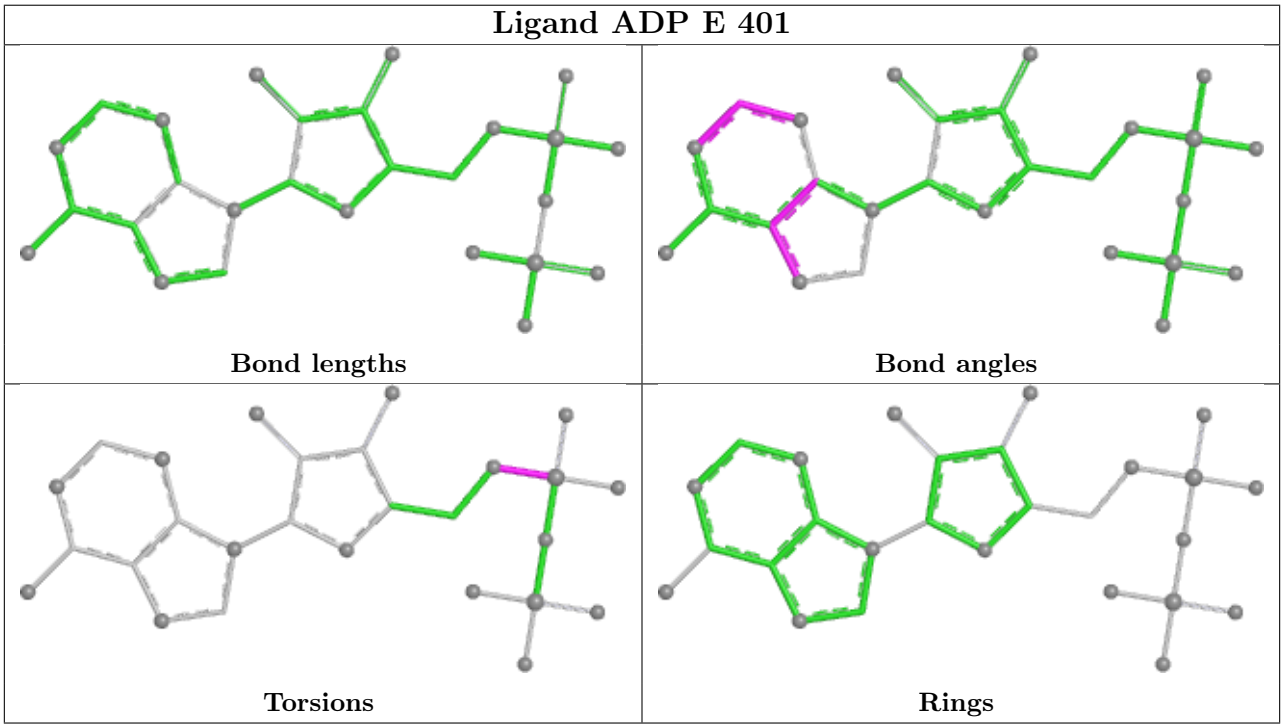
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

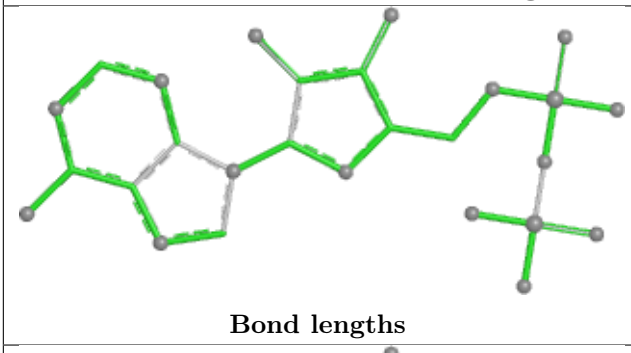
Ligand ADP B 401



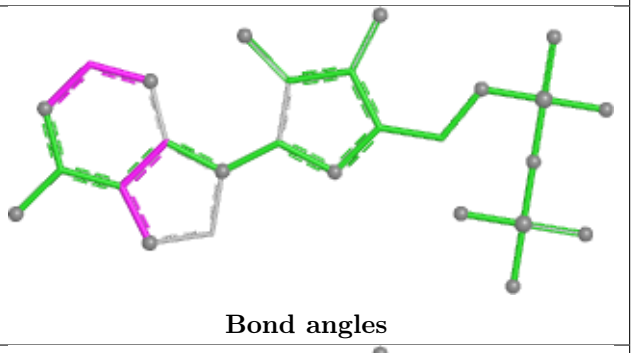
Ligand ADP E 401



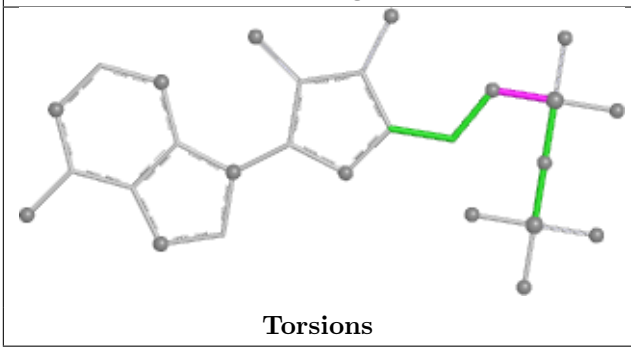
Ligand ADP C 401



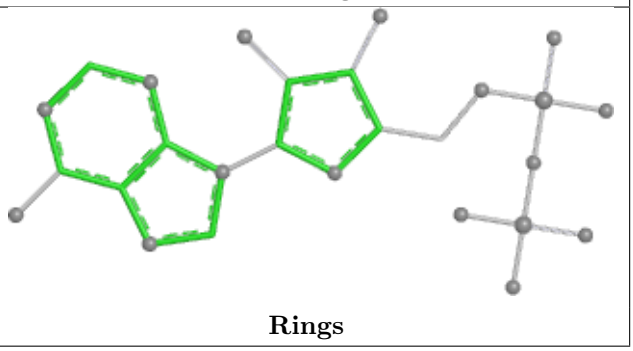
Bond lengths



Bond angles

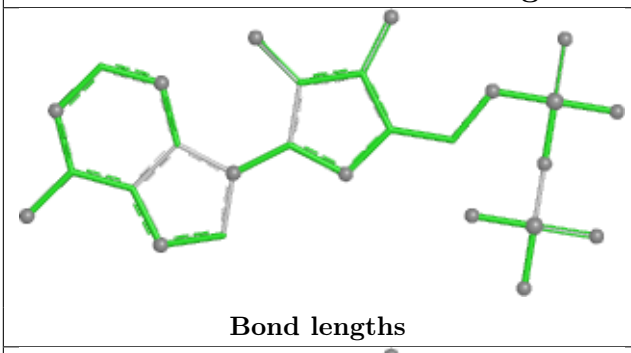


Torsions

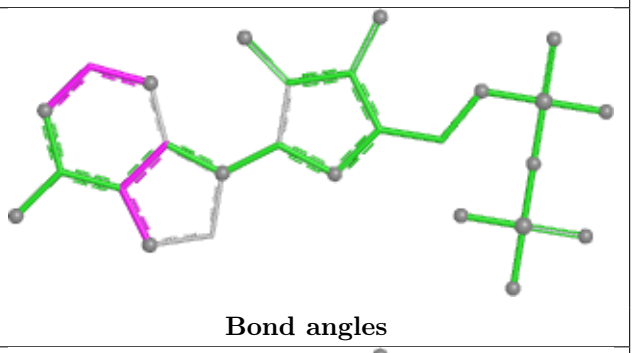


Rings

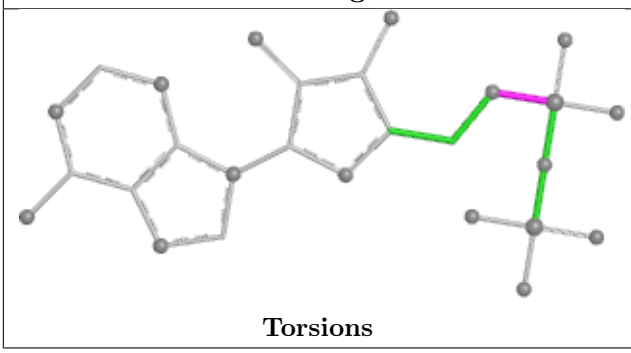
Ligand ADP D 401



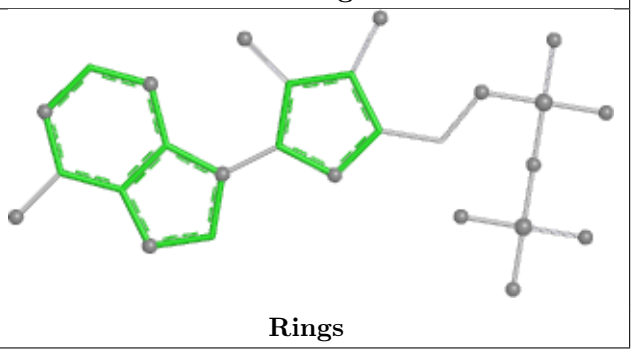
Bond lengths



Bond angles

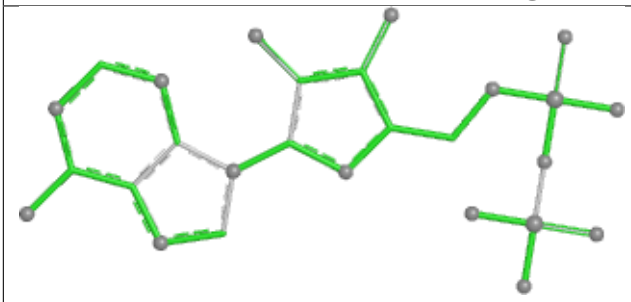


Torsions

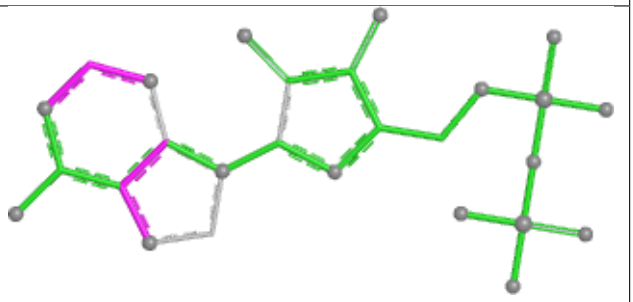


Rings

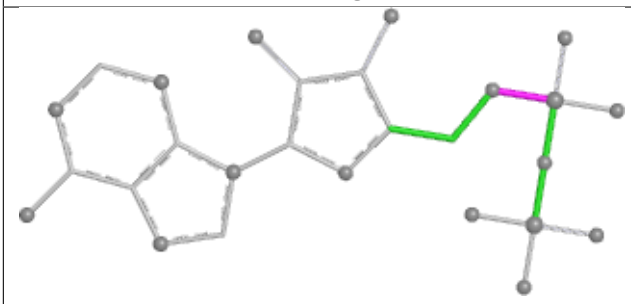
Ligand ADP F 401



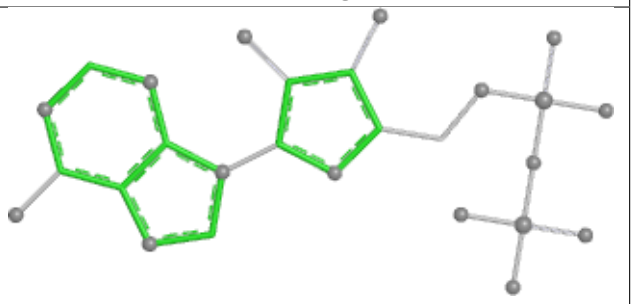
Bond lengths



Bond angles

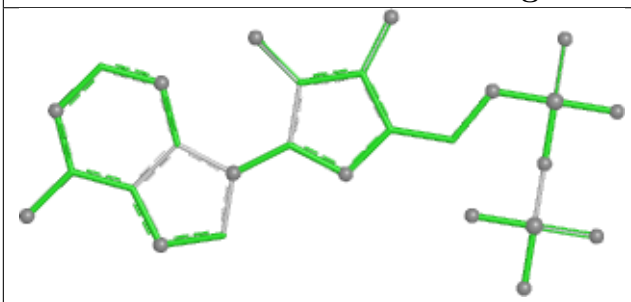


Torsions

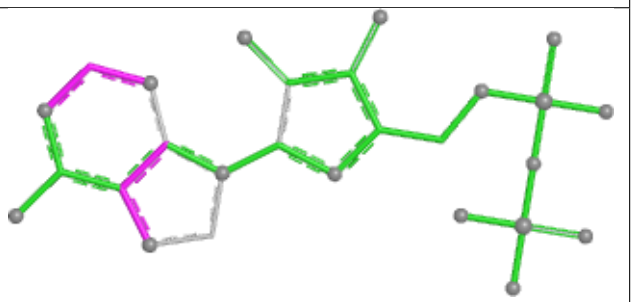


Rings

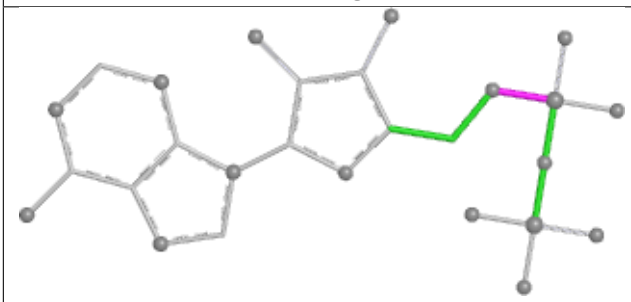
Ligand ADP A 401



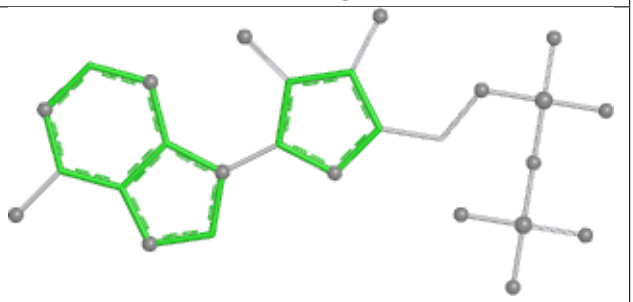
Bond lengths



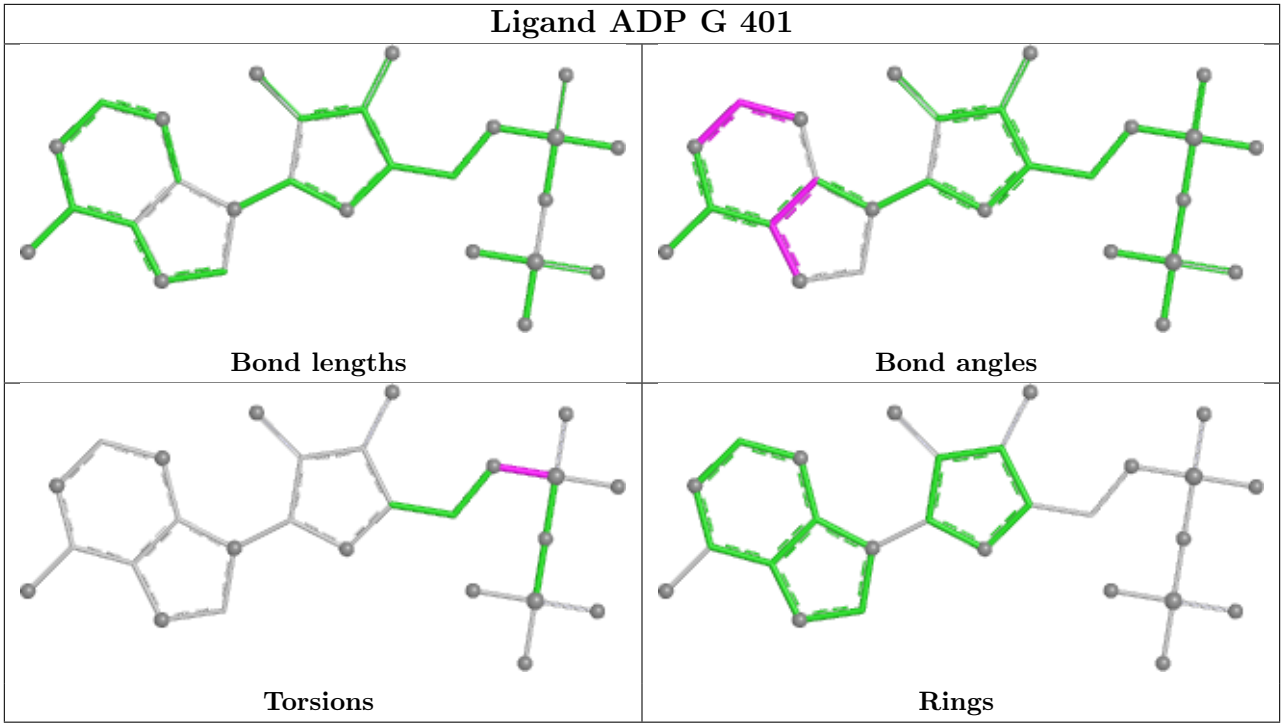
Bond angles



Torsions



Rings



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

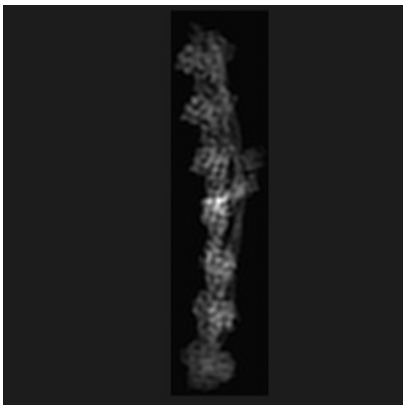
5 Map visualisation

This section contains visualisations of the EMDB entry EMD-48456. These allow visual inspection of the internal detail of the map and identification of artifacts.

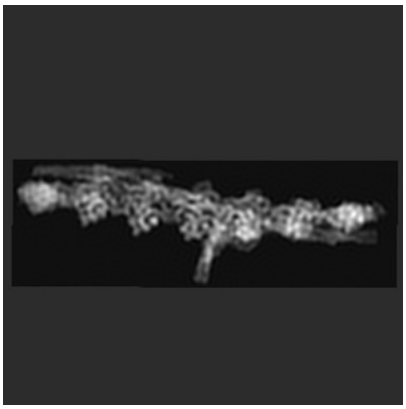
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections

5.1.1 Primary map



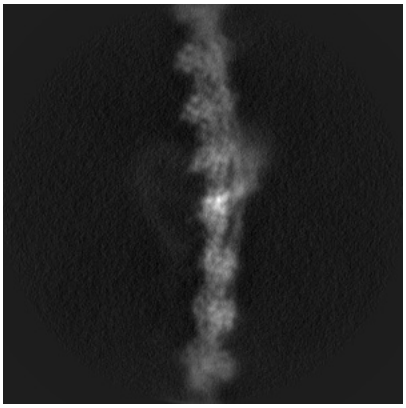
X



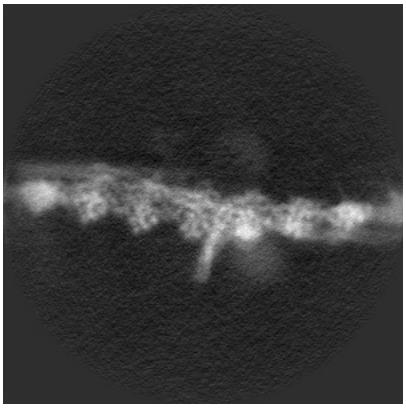
Y

Z

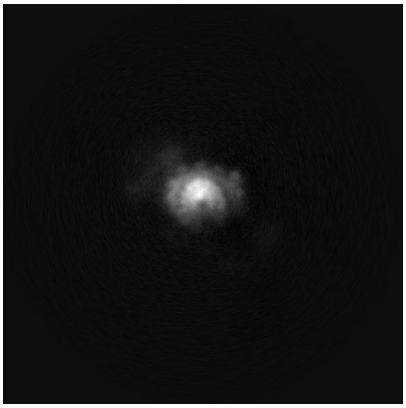
5.1.2 Raw map



X



Y



Z

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

5.2 Central slices (i)

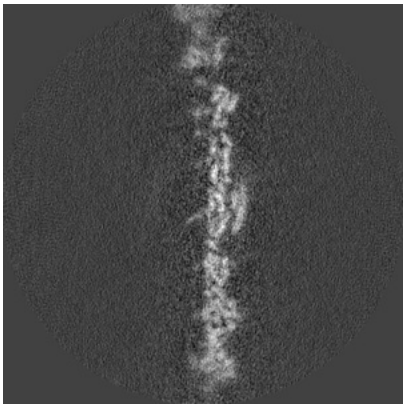
5.2.1 Primary map

X Index: 162

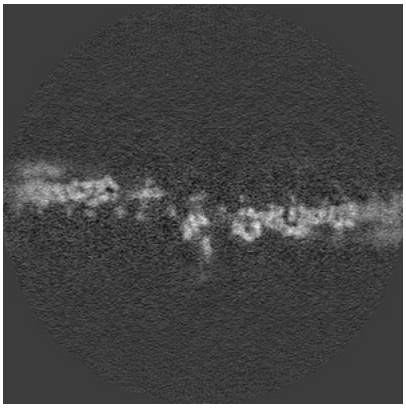
Y Index: 162

Z Index: 162

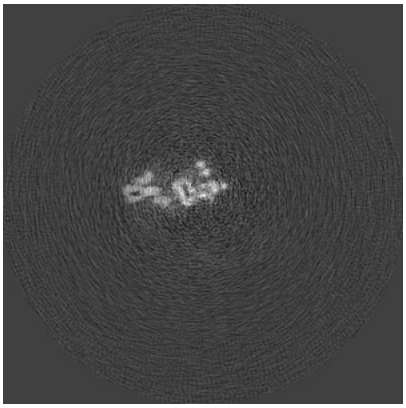
5.2.2 Raw map



X Index: 162



Y Index: 162



Z Index: 162

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

5.3 Largest variance slices (i)

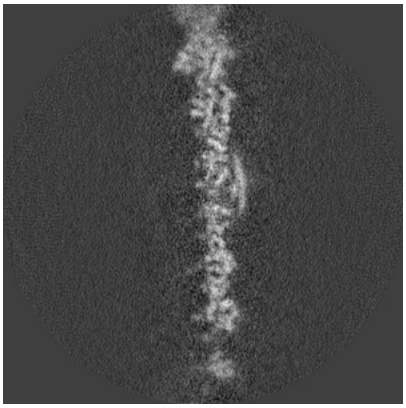
5.3.1 Primary map

X Index: 157

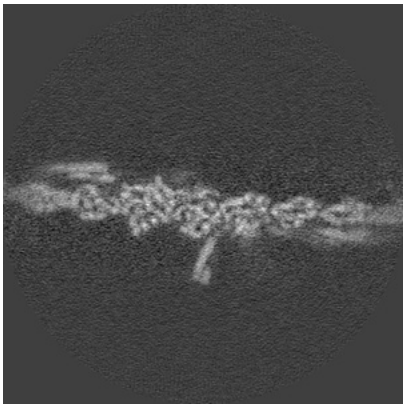
Y Index: 173

Z Index: 165

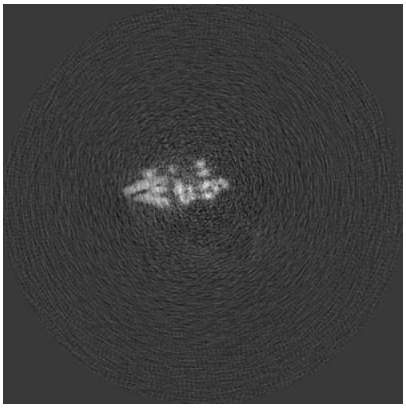
5.3.2 Raw map



X Index: 157



Y Index: 172

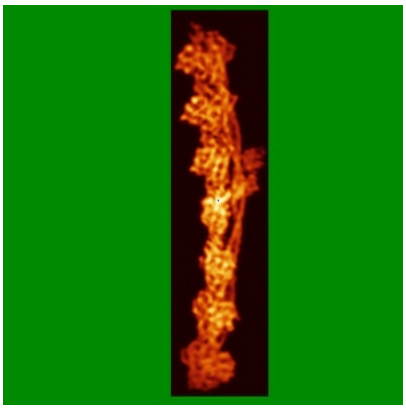


Z Index: 165

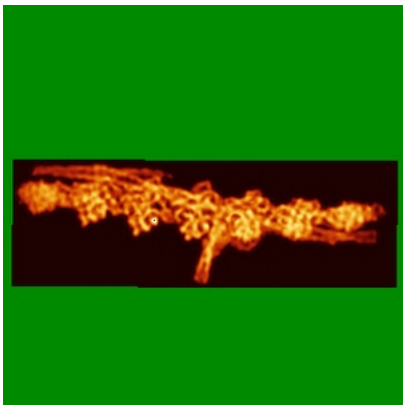
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) (i)

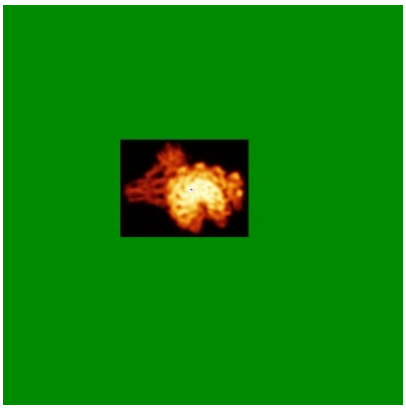
5.4.1 Primary map



X

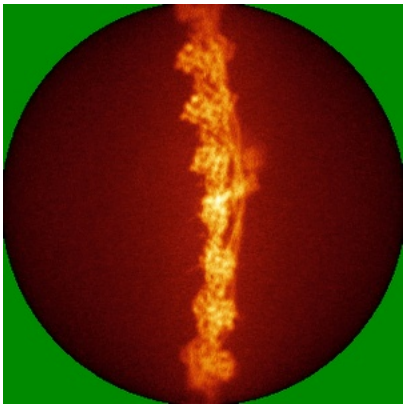


Y

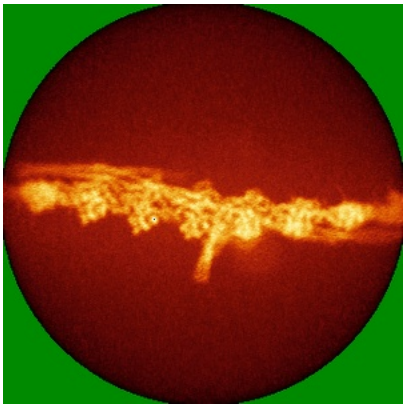


Z

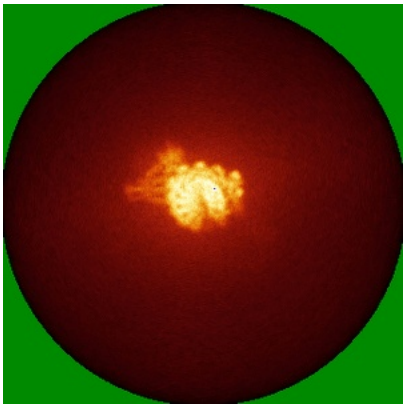
5.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.515. 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

X Y Z

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.

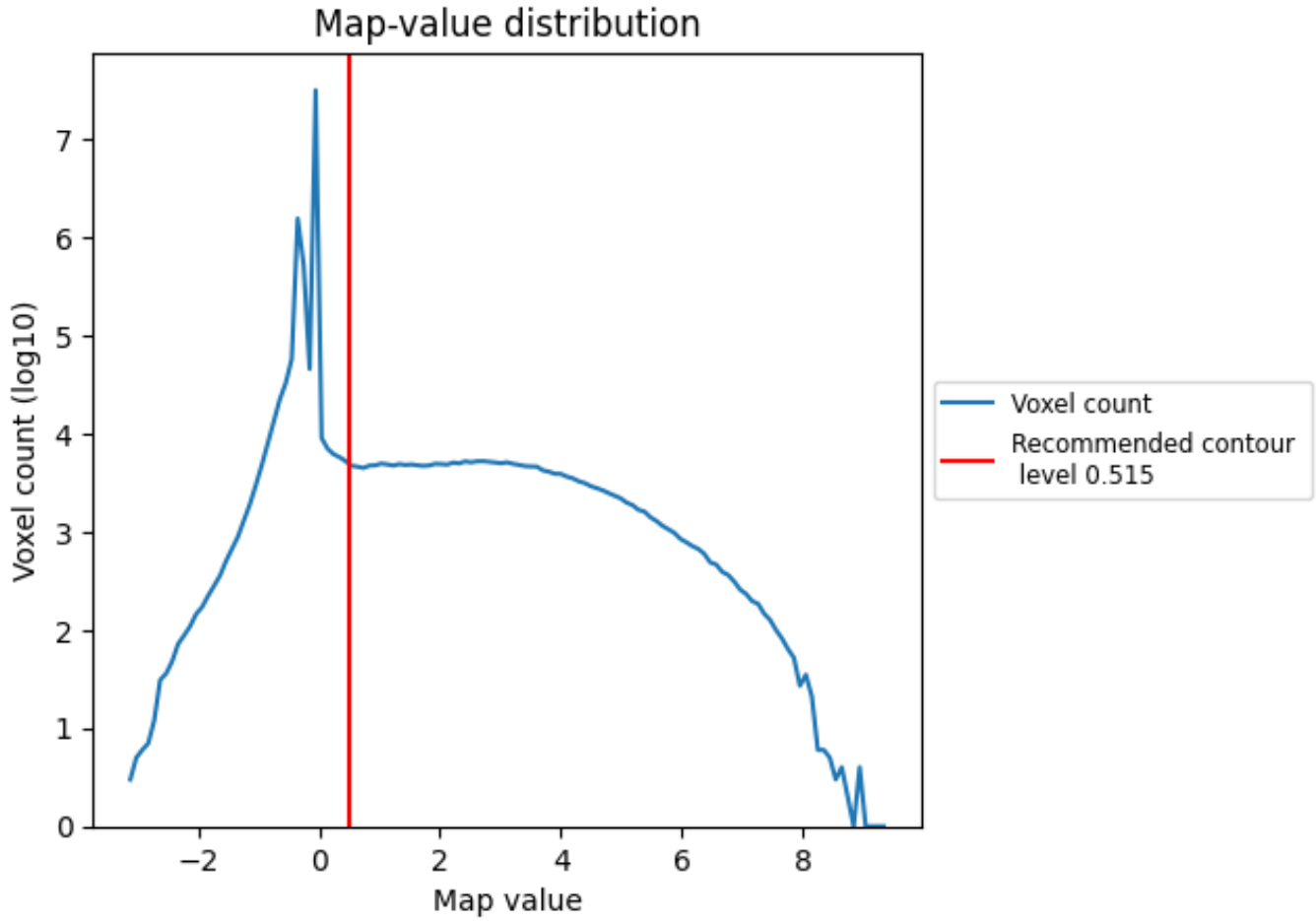
5.6 Mask visualisation (i)

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

6 Map analysis

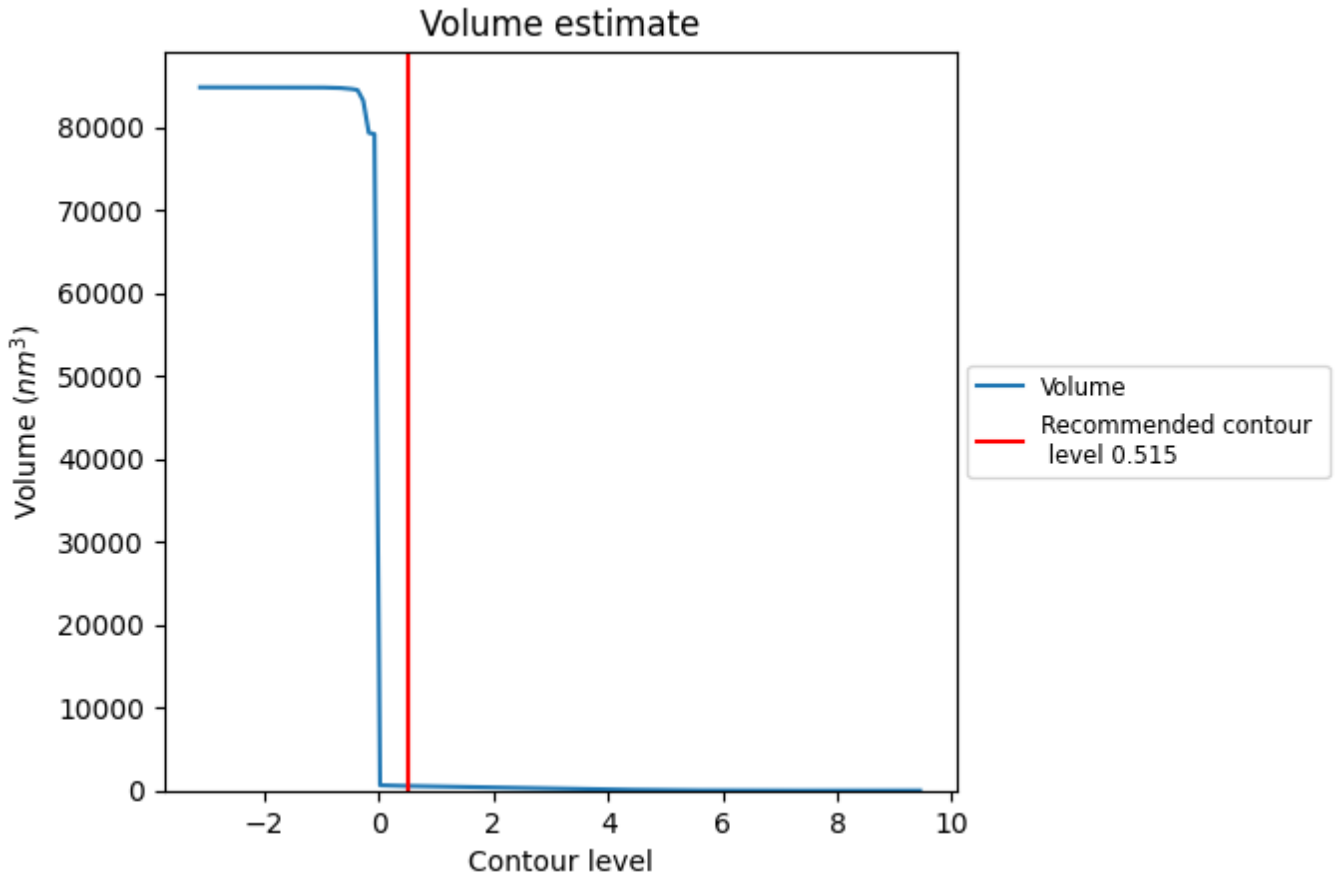
This section contains the results of statistical analysis of the map.

6.1 Map-value distribution



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.

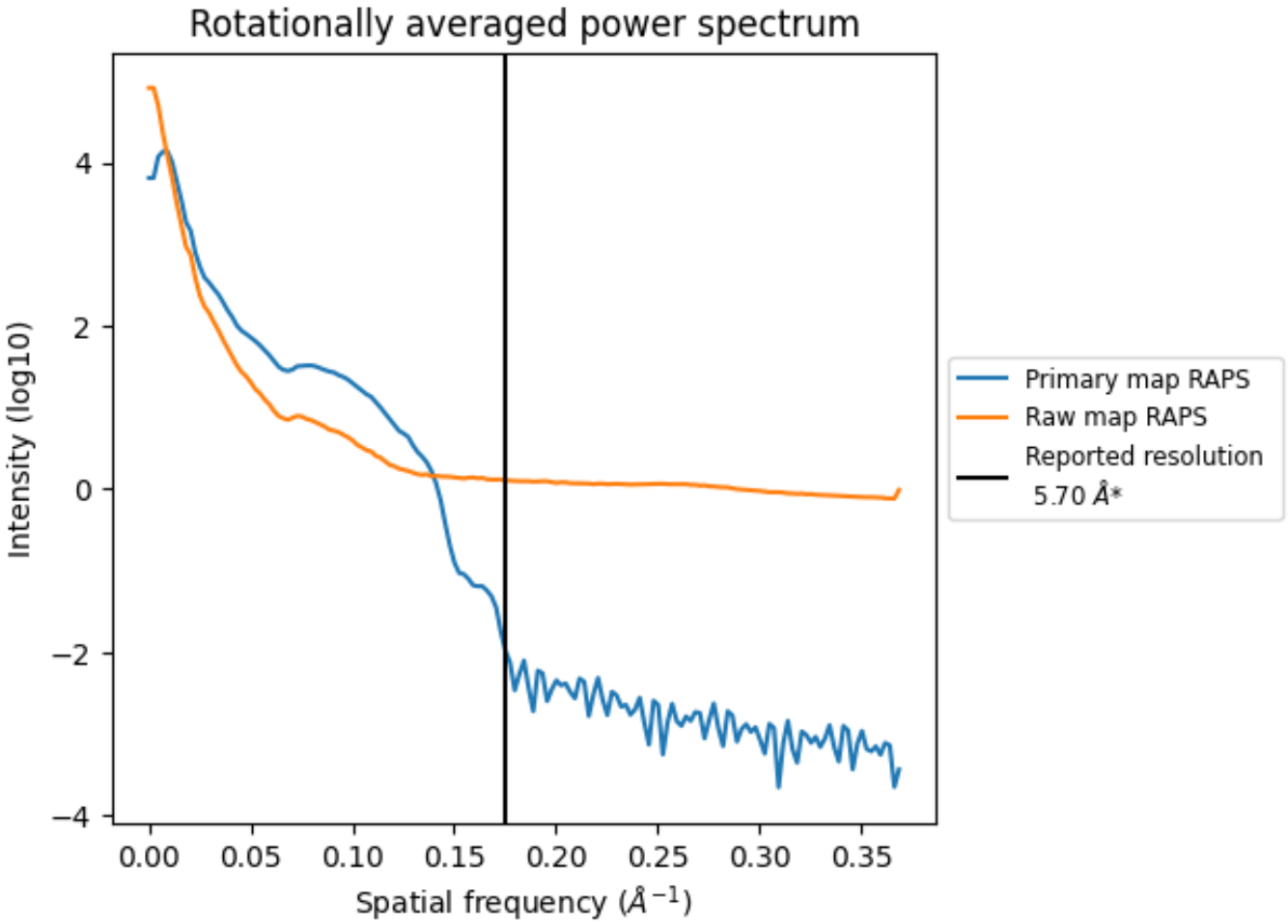
6.2 Volume estimate



The volume at the recommended contour level is 554 nm^3; this corresponds to an approximate mass of 501 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 (i)

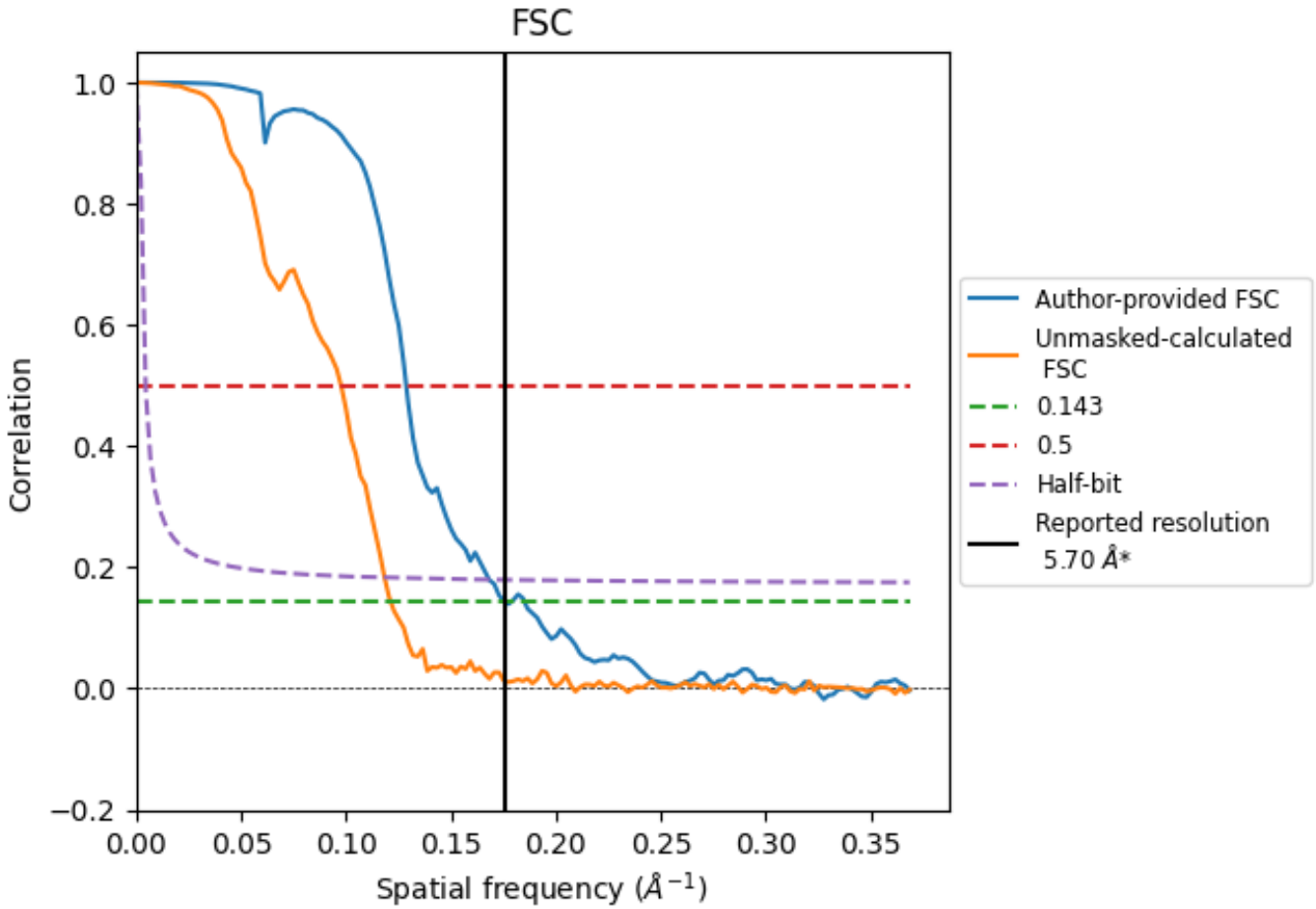


*Reported resolution corresponds to spatial frequency of 0.175 Å^{-1}

7 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.175 Å^{-1}

7.2 Resolution estimates (i)

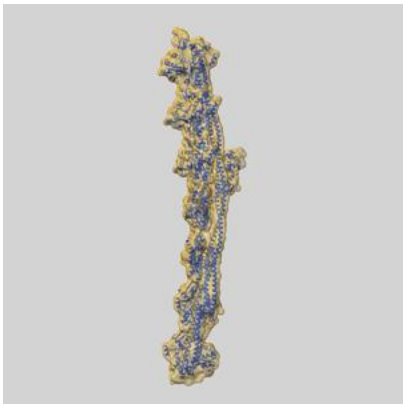
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	5.69	7.76	5.94
Unmasked-calculated*	8.24	10.24	8.45

*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 8.24 differs from the reported value 5.7 by more than 10 %

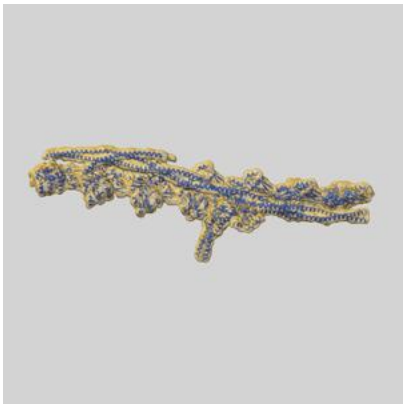
8 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48456 and PDB model 9MOD. Per-residue inclusion information can be found in section ?? on page ??.

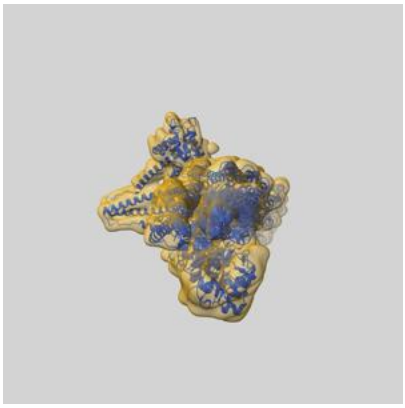
8.1 Map-model overlay



X



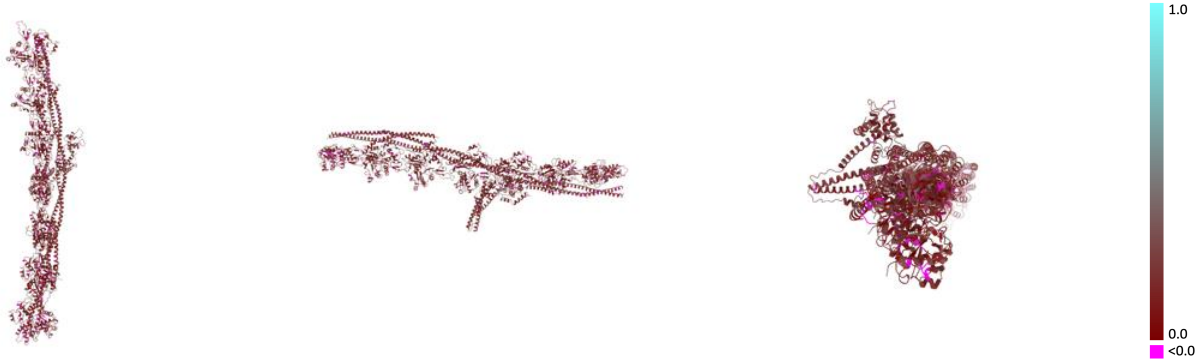
Y



Z

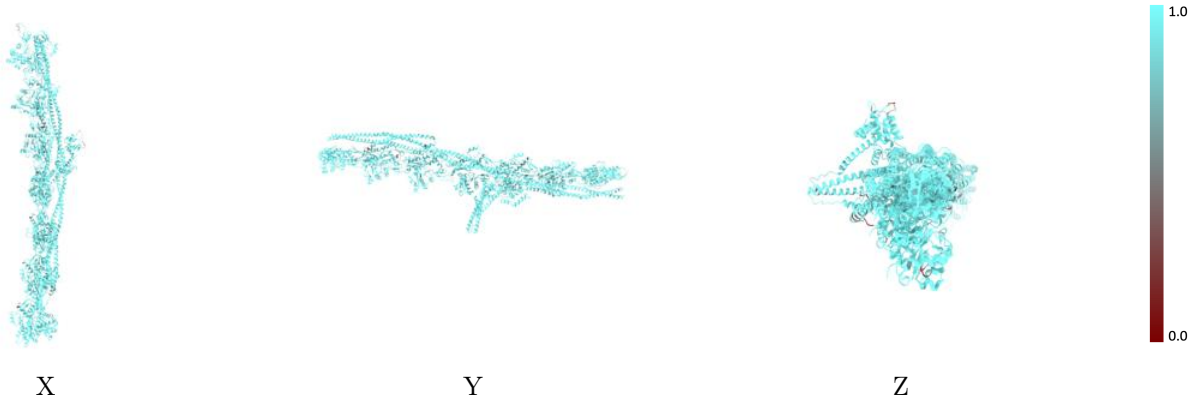
The images above show the 3D surface view of the map at the recommended contour level 0.515 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

8.2 Q-score mapped to coordinate model



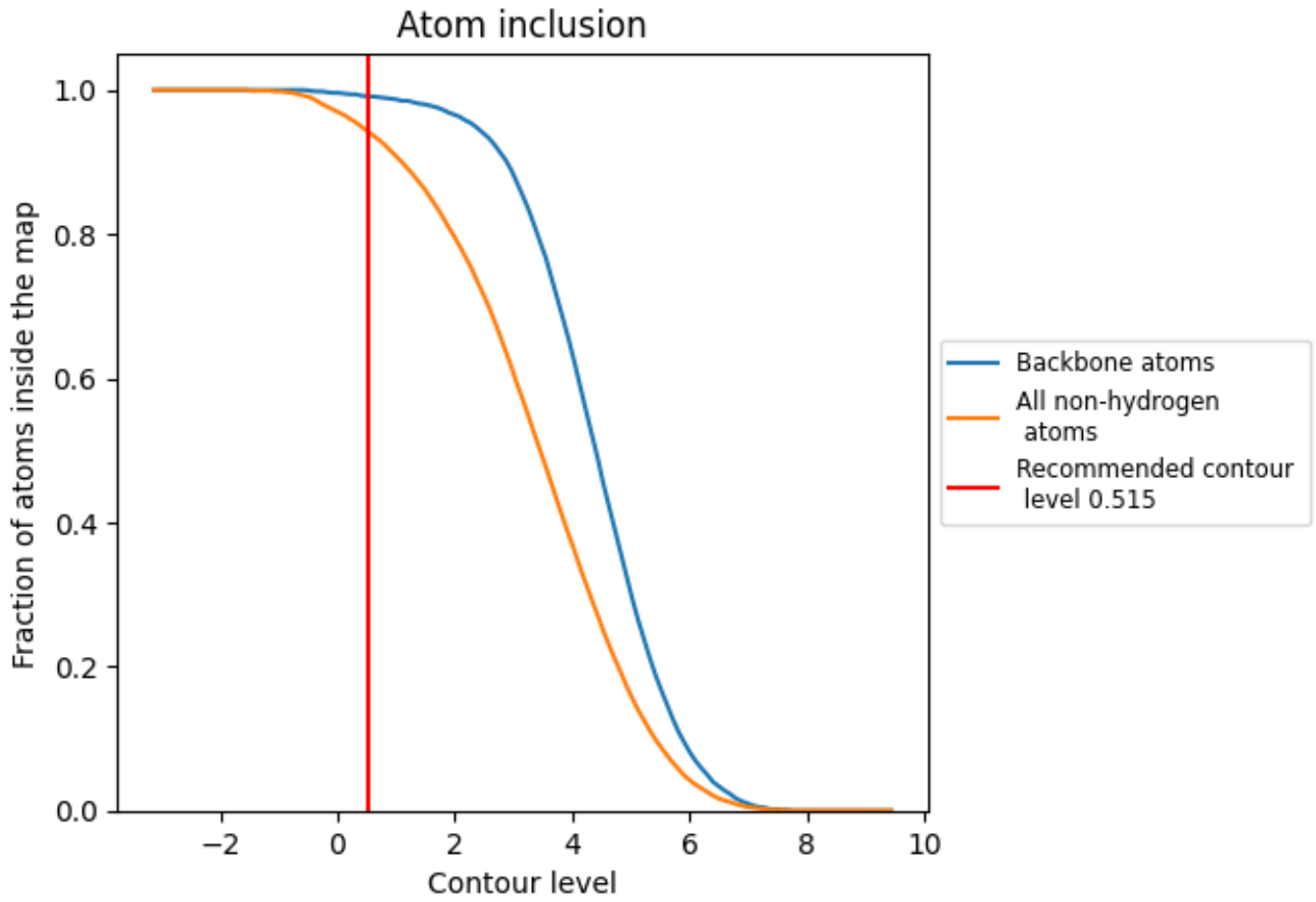
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 Atom inclusion mapped to coordinate model



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 (0.515).

8.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.515) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9430	0.1770
A	0.9690	0.1590
B	0.9510	0.1730
C	0.9430	0.1720
D	0.9390	0.1710
E	0.9350	0.1710
F	0.9410	0.1710
G	0.9560	0.1690
H	0.9600	0.2280
I	0.8910	0.1930
J	0.9790	0.2200
K	0.8570	0.1460
L	0.9400	0.1940
M	0.9470	0.1980
N	0.9450	0.1660
O	0.8750	0.1720