



## Full wwPDB EM Validation Report ⓘ

Sep 8, 2025 – 01:42 pm BST

PDB ID : 9FMG / pdb\_00009fmg  
EMDB ID : EMD-50553  
Title : Methylthio-alkane reductase complex  
Authors : Lago-Maciel, A.; Zarzycki, J.; Prinz, S.; Reif-Trauttmansdorff, T.; Rebelein, J.G.  
Deposited on : 2024-06-06  
Resolution : 2.71 Å(reported)  
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev126  
Mogul : 1.8.4, CSD as541be (2020)  
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) : 2.45.1

# 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 2.71 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

There are 9 unique types of molecules in this entry. The entry contains 13763 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 Nitrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	467	Total	C	N	O	S	0	0
			3643	2304	651	675	13		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	512	TRP	-	expression tag	UNP Q2RW97
A	513	SER	-	expression tag	UNP Q2RW97
A	514	HIS	-	expression tag	UNP Q2RW97
A	515	PRO	-	expression tag	UNP Q2RW97
A	516	GLN	-	expression tag	UNP Q2RW97
A	517	PHE	-	expression tag	UNP Q2RW97
A	518	GLU	-	expression tag	UNP Q2RW97
A	519	LYS	-	expression tag	UNP Q2RW97

- Molecule 2 is a protein called Nitrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	445	Total	C	N	O	S	0	0
			3447	2216	579	646	6		
2	C	313	Total	C	N	O		0	0
			2481	1606	414	461			

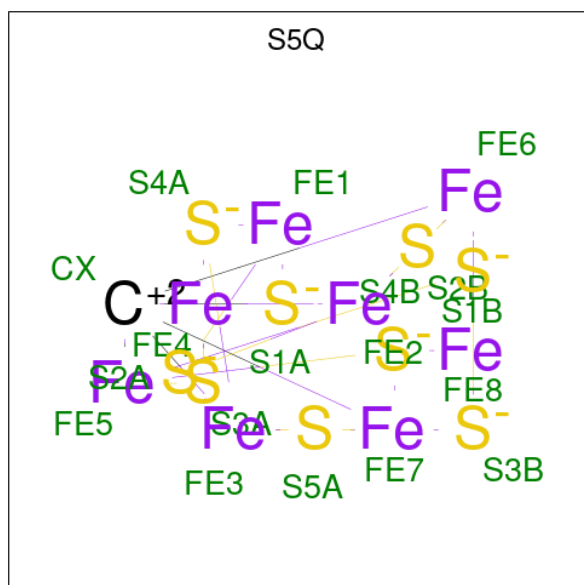
- Molecule 3 is a protein called Nitrogenase iron protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	269	Total	C	N	O	S	0	0
			2022	1275	345	396	6		
3	E	274	Total	C	N	O	S	0	0
			2065	1299	354	406	6		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	MET	-	initiating methionine	UNP Q2RW96
D	-4	HIS	-	expression tag	UNP Q2RW96
D	-3	HIS	-	expression tag	UNP Q2RW96
D	-2	HIS	-	expression tag	UNP Q2RW96
D	-1	HIS	-	expression tag	UNP Q2RW96
D	0	HIS	-	expression tag	UNP Q2RW96
D	1	HIS	-	expression tag	UNP Q2RW96
E	-5	MET	-	initiating methionine	UNP Q2RW96
E	-4	HIS	-	expression tag	UNP Q2RW96
E	-3	HIS	-	expression tag	UNP Q2RW96
E	-2	HIS	-	expression tag	UNP Q2RW96
E	-1	HIS	-	expression tag	UNP Q2RW96
E	0	HIS	-	expression tag	UNP Q2RW96
E	1	HIS	-	expression tag	UNP Q2RW96

- Molecule 4 is FeFe cofactor (CCD ID: S5Q) (formula:  $\text{CFe}_8\text{S}_9$ ) (labeled as "Ligand of Interest" by depositor).



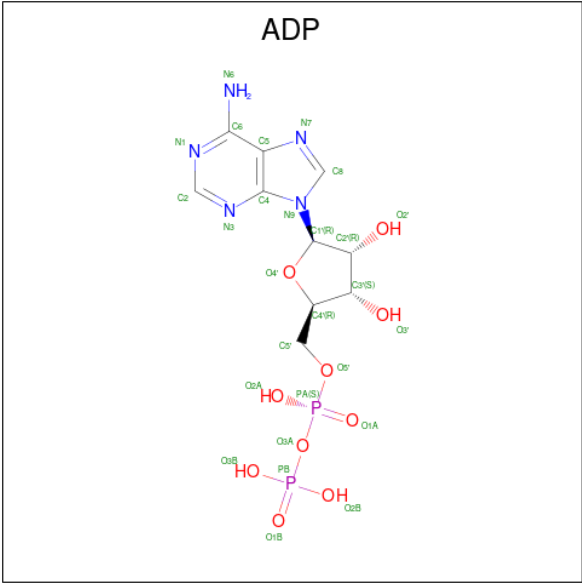
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	Fe	S	0
			18	1	8	9	

- Molecule 5 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula:  $\text{Fe}_8\text{S}_7$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	Fe	S	0
			15	8	7	

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

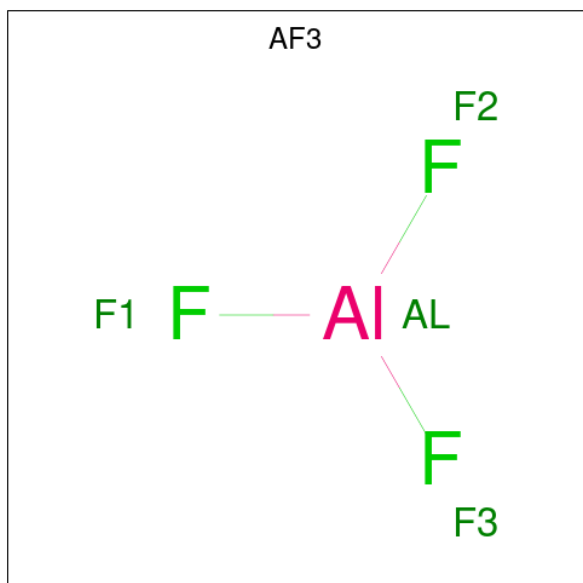


Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

Mol	Chain	Residues	Atoms		AltConf
7	D	1	Total	Mg	0
			1	1	
7	E	1	Total	Mg	0
			1	1	

- Molecule 8 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula:  $\text{AlF}_3$ ).



Mol	Chain	Residues	Atoms			AltConf
8	D	1	Total	Al	F	0
			4	1	3	
8	E	1	Total	Al	F	0
			4	1	3	

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
9	D	1	8	4	4	0

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

### 3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	116370	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	40.230	Depositor
Minimum map value	-19.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.75	Depositor
Map size (Å)	318.06, 318.06, 318.06	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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](#)

Of 9 ligands modelled in this entry, 2 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
8	AF3	E	303	-	0,3,3	-	-	-		
6	ADP	E	301	7	24,29,29	0.88	0	29,45,45	0.86	0
8	AF3	D	303	-	0,3,3	-	-	-		
9	SF4	D	304	3	0,12,12	-	-	-		
5	CLF	B	501	2,1	0,24,24	-	-	-		
6	ADP	D	301	7	24,29,29	0.87	0	29,45,45	0.76	1 (3%)
4	S5Q	A	601	1	18,30,30	2.63	9 (50%)	-		

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	SF4	D	304	3	-	-	0/6/5/5
6	ADP	D	301	7	-	4/12/32/32	0/3/3/3
6	ADP	E	301	7	-	4/12/32/32	0/3/3/3
5	CLF	B	501	2,1	-	-	0/12/10/10

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	S5Q	S4B-FE5	-4.66	2.20	2.32
4	A	601	S5Q	S4B-FE7	-4.49	2.21	2.32
4	A	601	S5Q	S3B-FE6	-4.41	2.21	2.32
4	A	601	S5Q	S1B-FE6	-3.89	2.22	2.32
4	A	601	S5Q	S1B-FE5	-3.23	2.24	2.32
4	A	601	S5Q	S2B-FE6	-3.01	2.17	2.24
4	A	601	S5Q	S3B-FE7	-2.75	2.25	2.32
4	A	601	S5Q	S1A-FE2	-2.56	2.26	2.32
4	A	601	S5Q	S2A-FE2	-2.17	2.27	2.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	301	ADP	N3-C2-N1	-2.38	124.95	128.68

There are no chirality outliers.

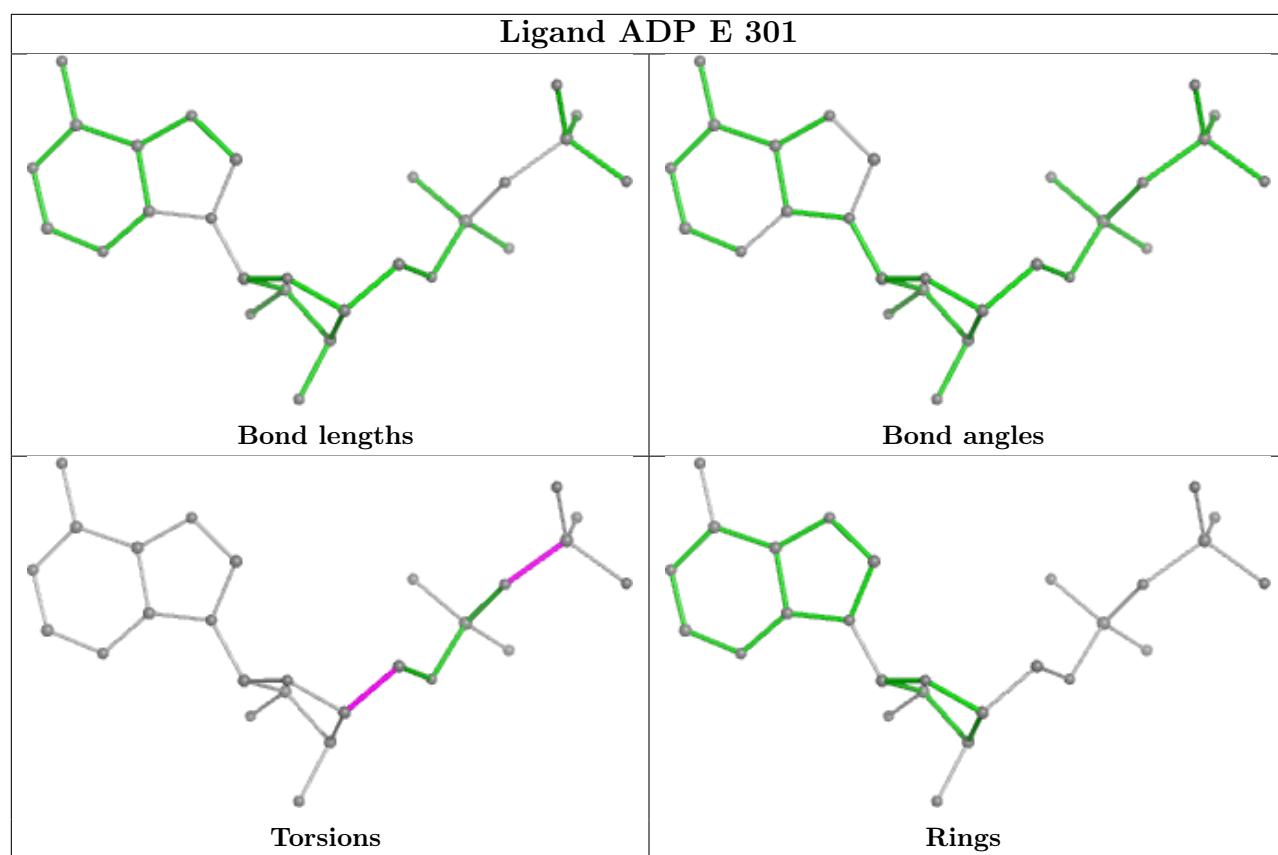
All (8) torsion outliers are listed below:

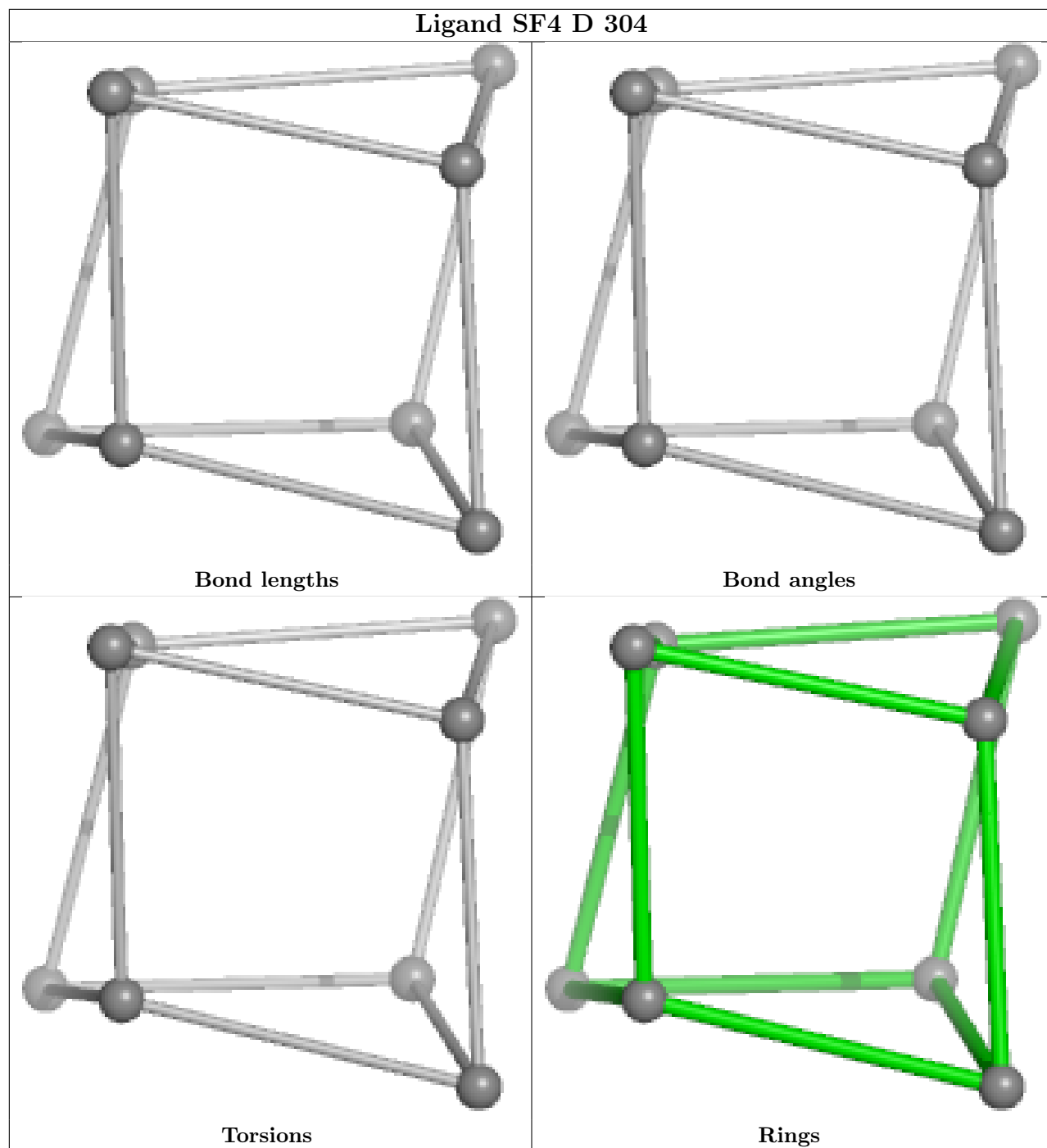
Mol	Chain	Res	Type	Atoms
6	D	301	ADP	PA-O3A-PB-O2B
6	D	301	ADP	O4'-C4'-C5'-O5'
6	E	301	ADP	O4'-C4'-C5'-O5'
6	E	301	ADP	C3'-C4'-C5'-O5'
6	E	301	ADP	PA-O3A-PB-O1B
6	E	301	ADP	PA-O3A-PB-O2B
6	D	301	ADP	C3'-C4'-C5'-O5'
6	D	301	ADP	PA-O3A-PB-O1B

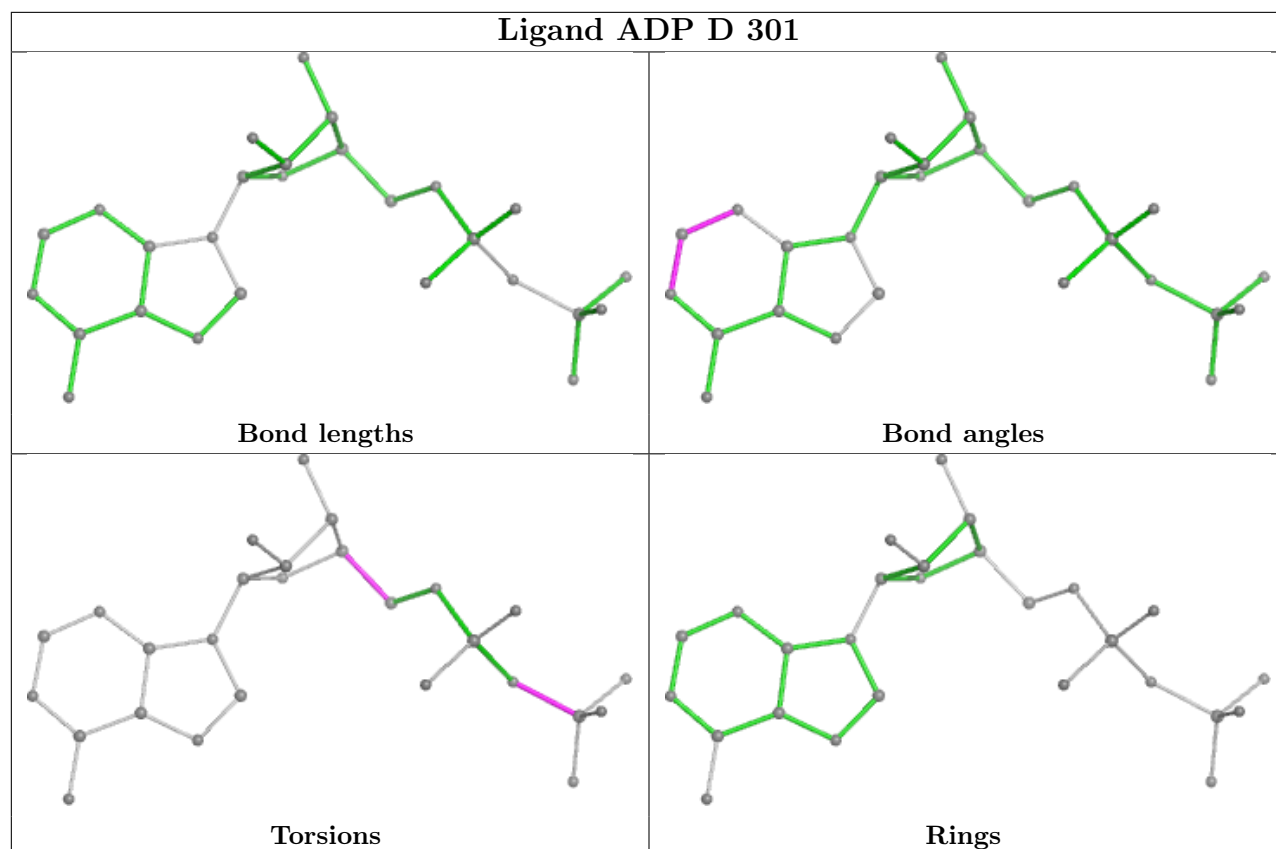
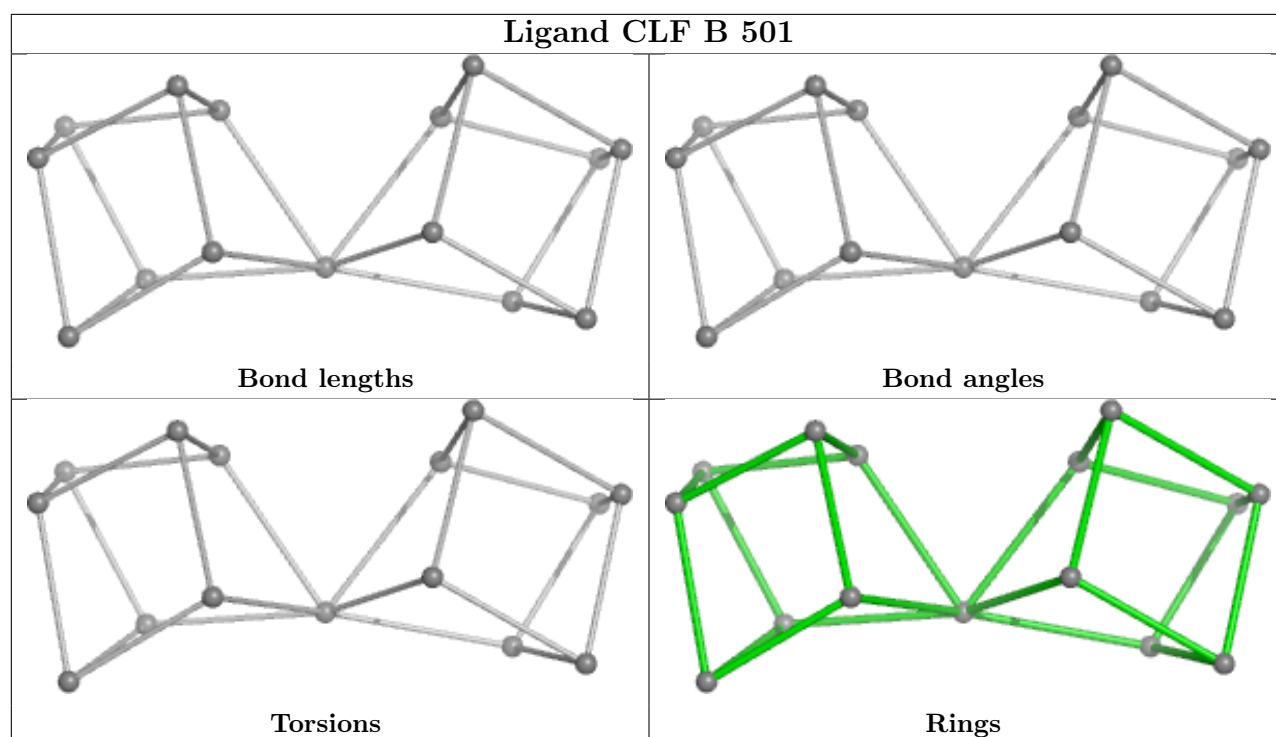
There are no ring outliers.

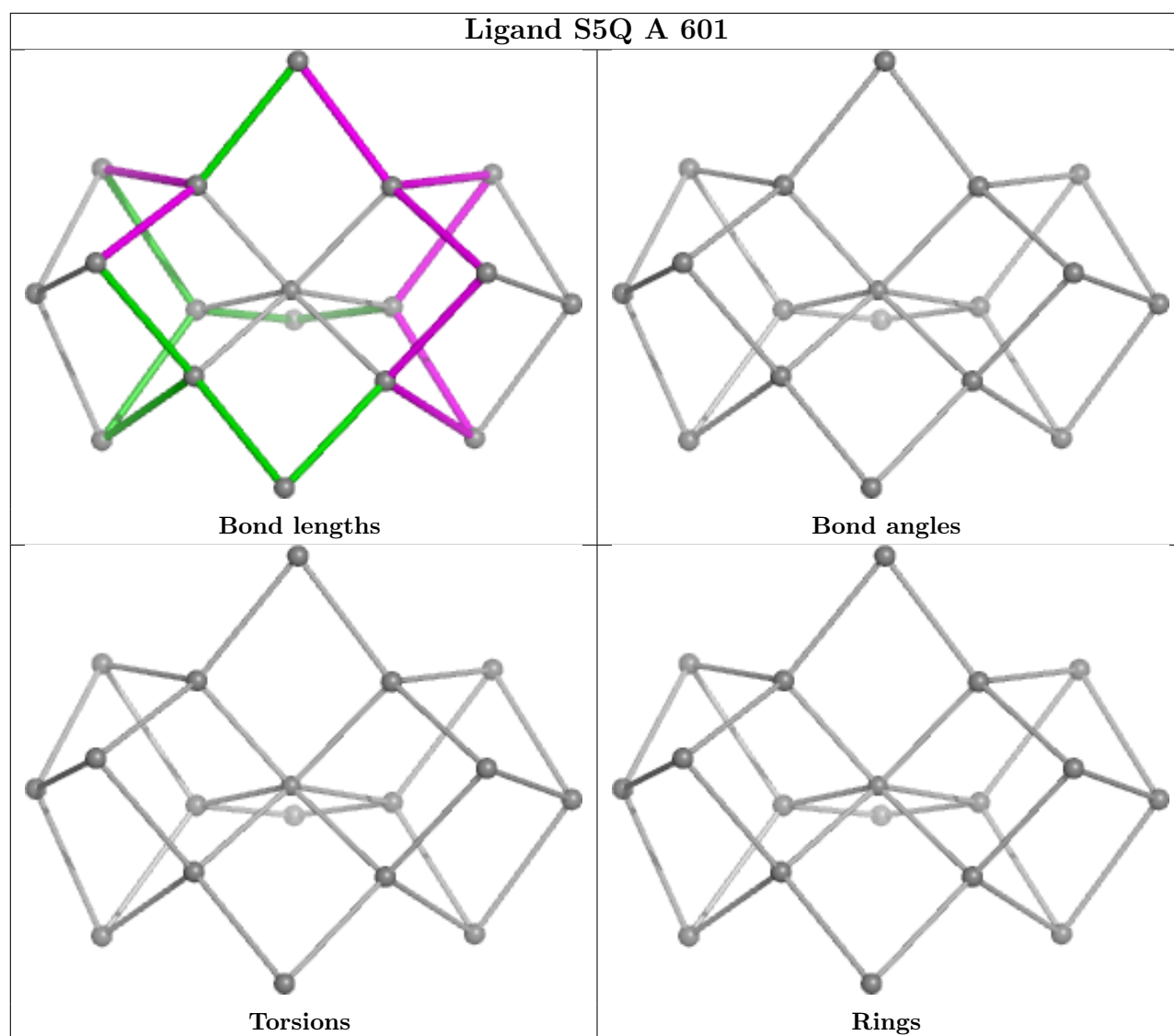
No monomer is involved in short contacts.

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 [i](#)

There are no chain breaks in this entry.

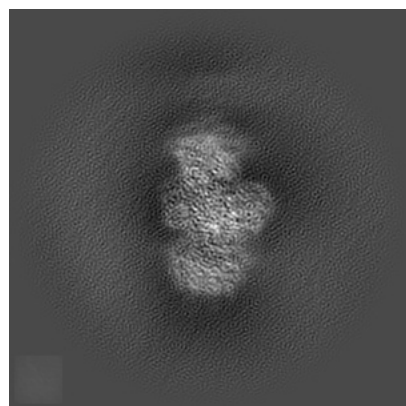
## 5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50553. These allow visual inspection of the internal detail of the map and identification of artifacts.

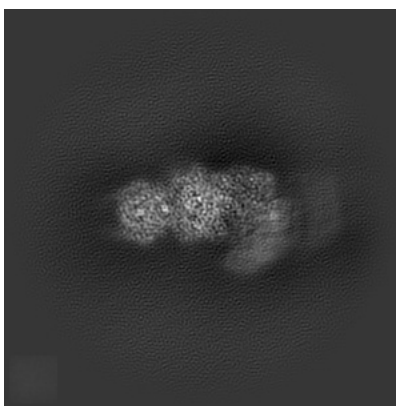
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 5.1 Orthogonal projections [i](#)

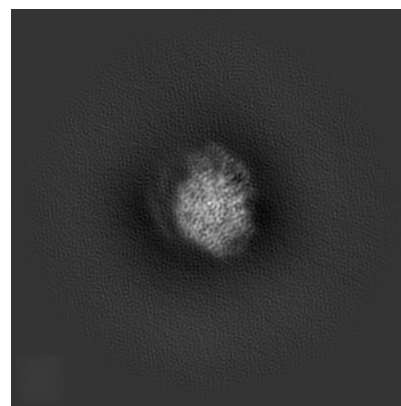
#### 5.1.1 Primary map



X

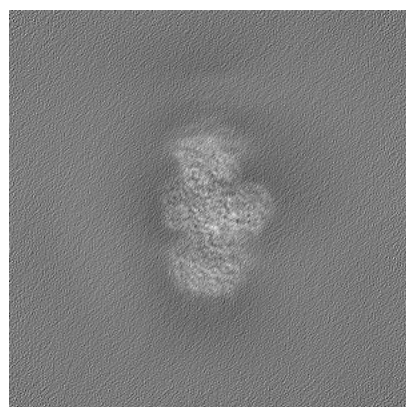


Y

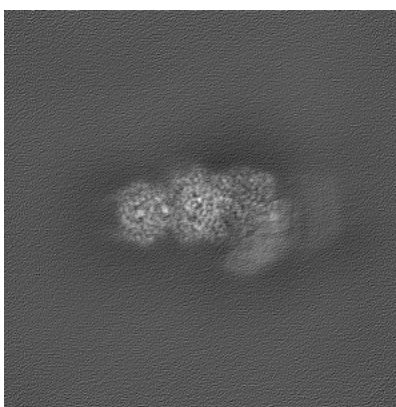


Z

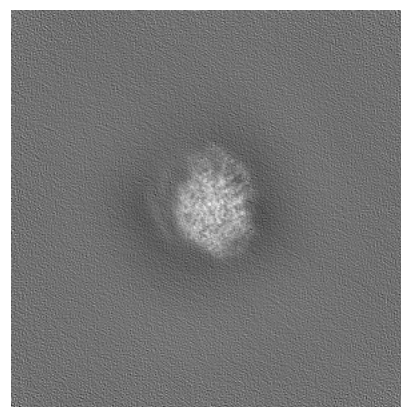
#### 5.1.2 Raw map



X



Y



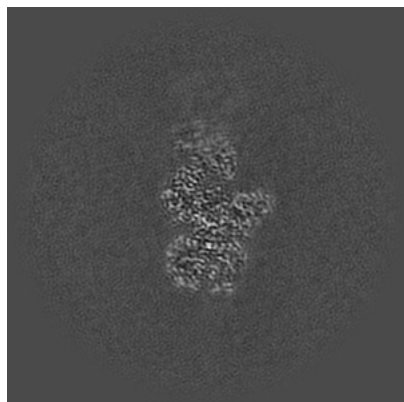
Z

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

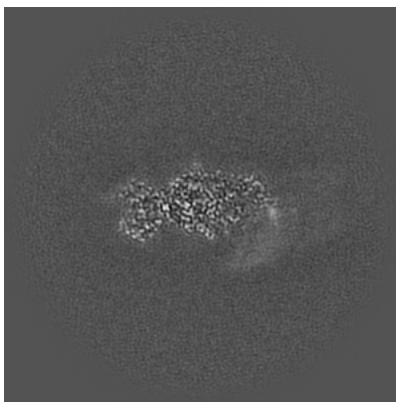


## 5.2 Central slices [i](#)

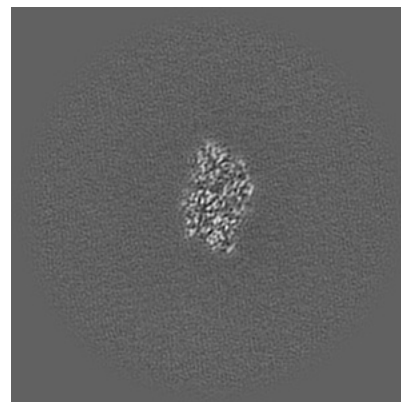
### 5.2.1 Primary map



X Index: 190

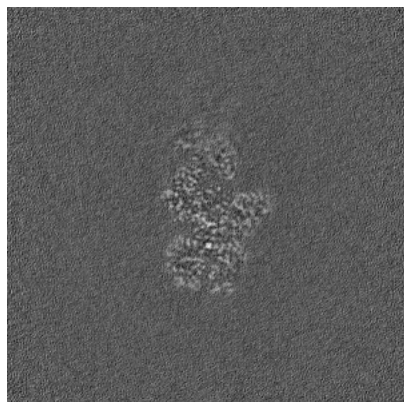


Y Index: 190

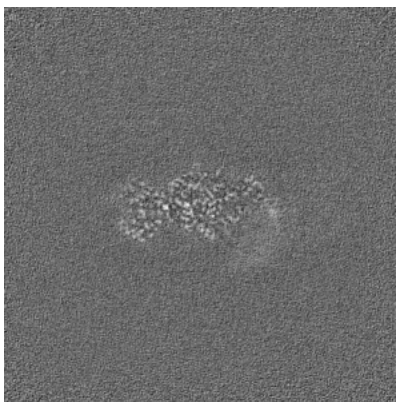


Z Index: 190

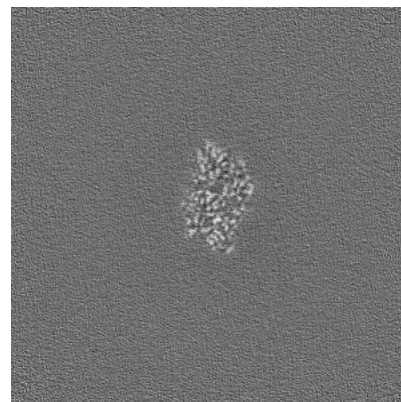
### 5.2.2 Raw map



X Index: 190



Y Index: 190

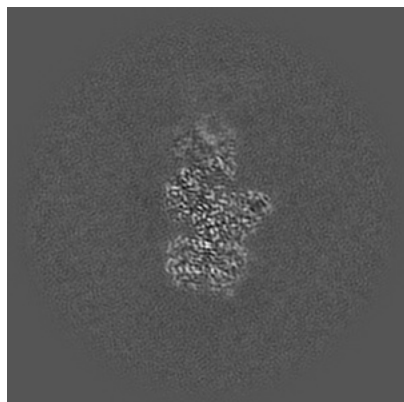


Z Index: 190

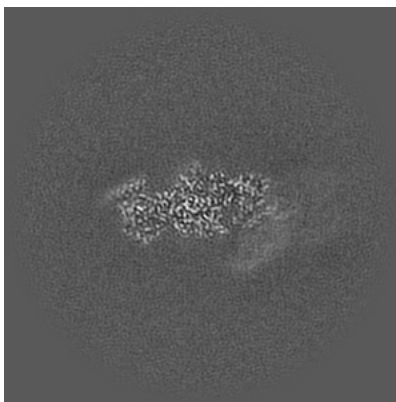
The images above show central slices of the map in three orthogonal directions.

## 5.3 Largest variance slices [i](#)

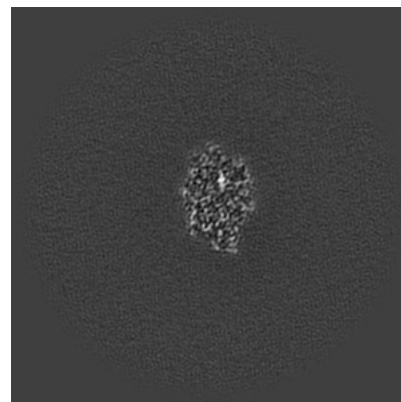
### 5.3.1 Primary map



X Index: 188

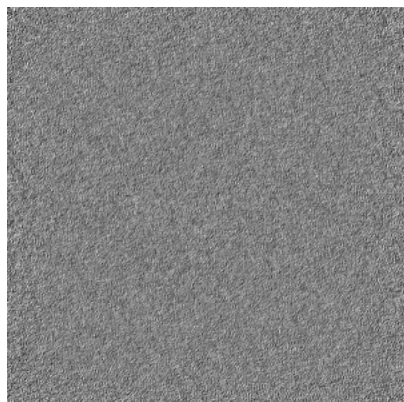


Y Index: 195

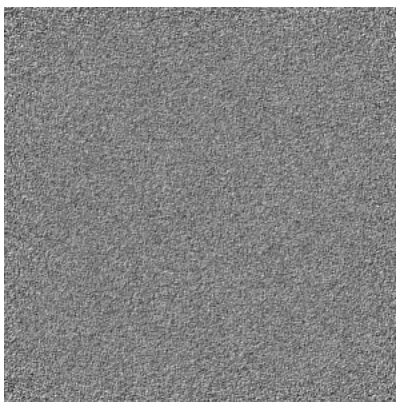


Z Index: 185

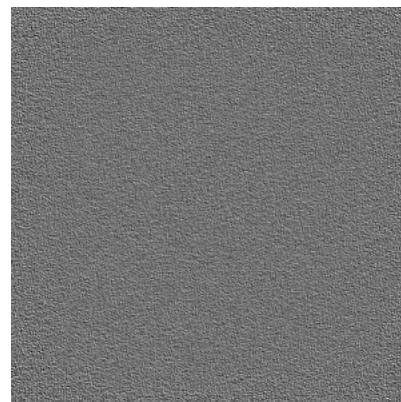
### 5.3.2 Raw map



X Index: 0



Y Index: 0

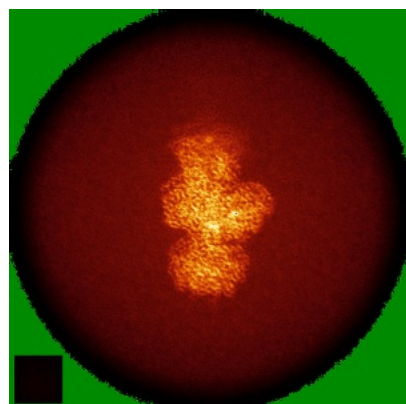


Z Index: 379

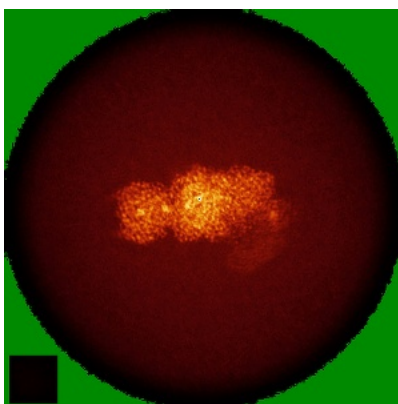
The images above show the largest variance slices of the map in three orthogonal directions.

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

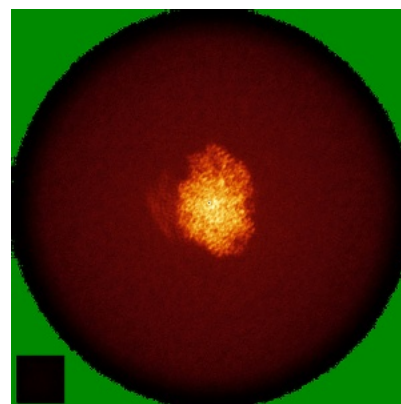
### 5.4.1 Primary map



X

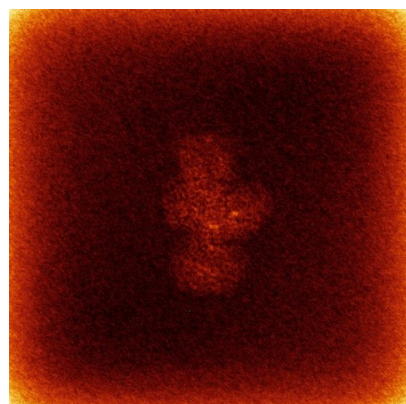


Y

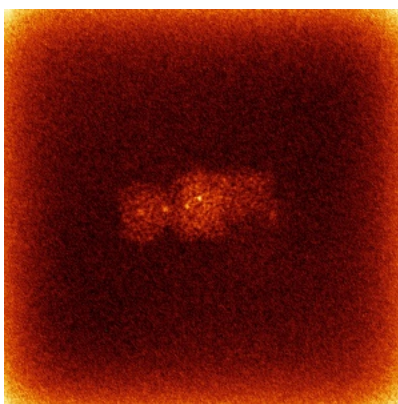


Z

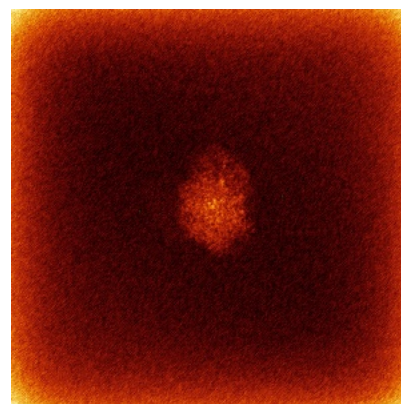
### 5.4.2 Raw map



X



Y



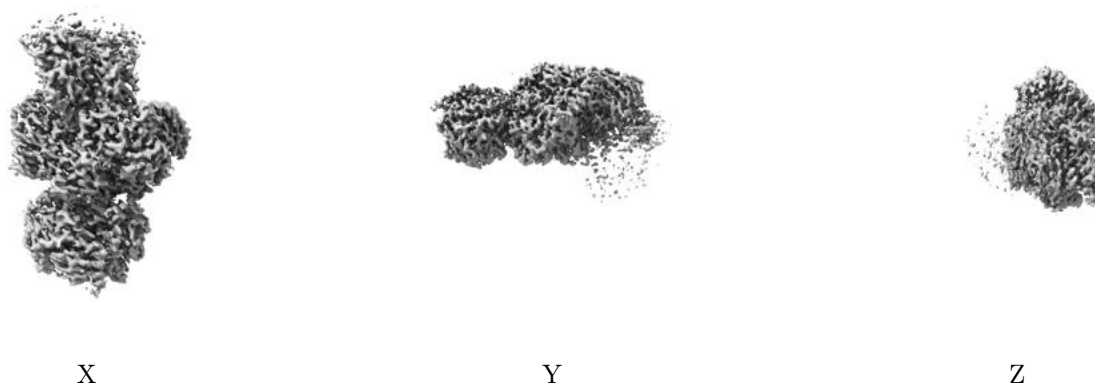
Z

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.



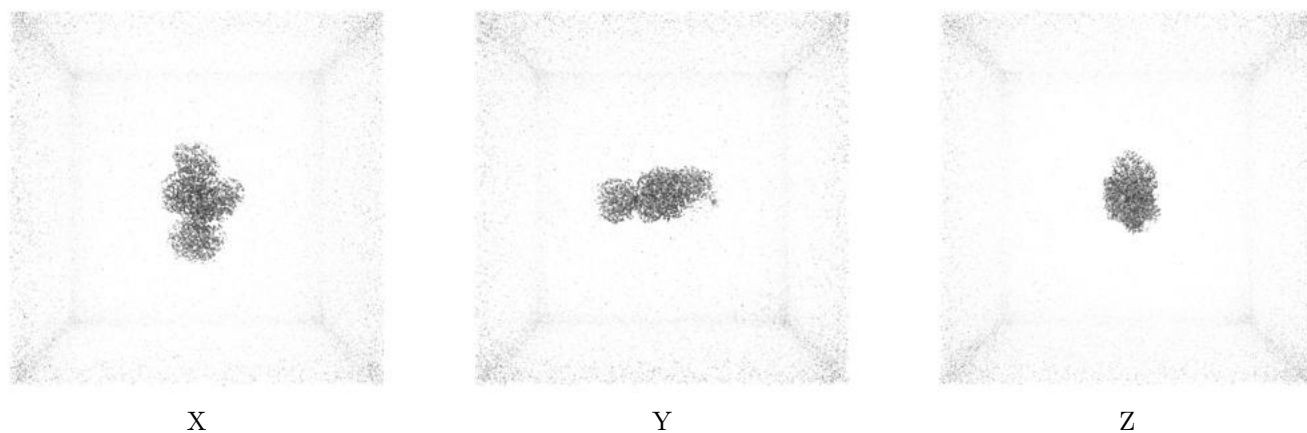
## 5.5 Orthogonal surface views [i](#)

### 5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.75. 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.

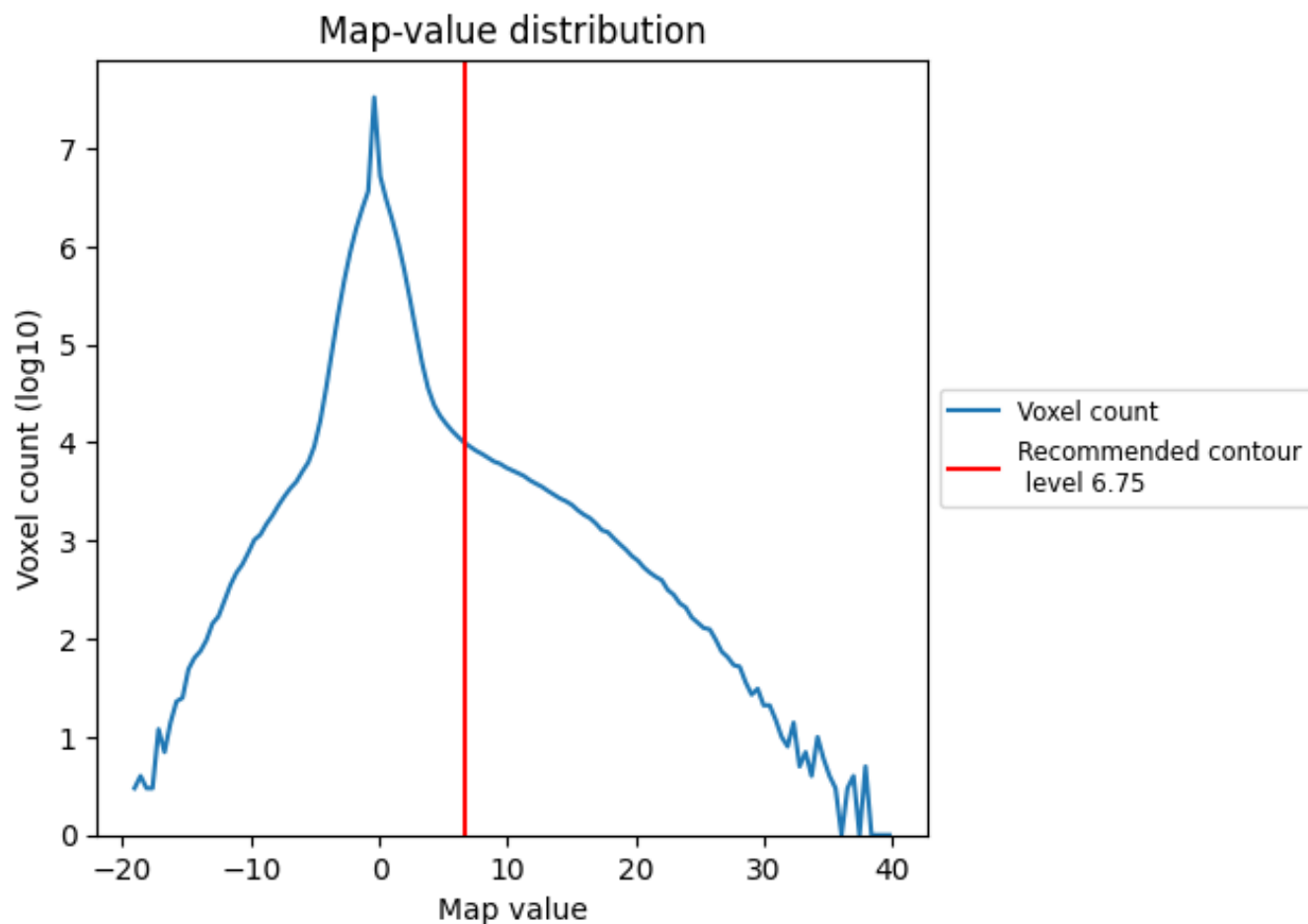
## 5.6 Mask visualisation [i](#)

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

## 6 Map analysis [i](#)

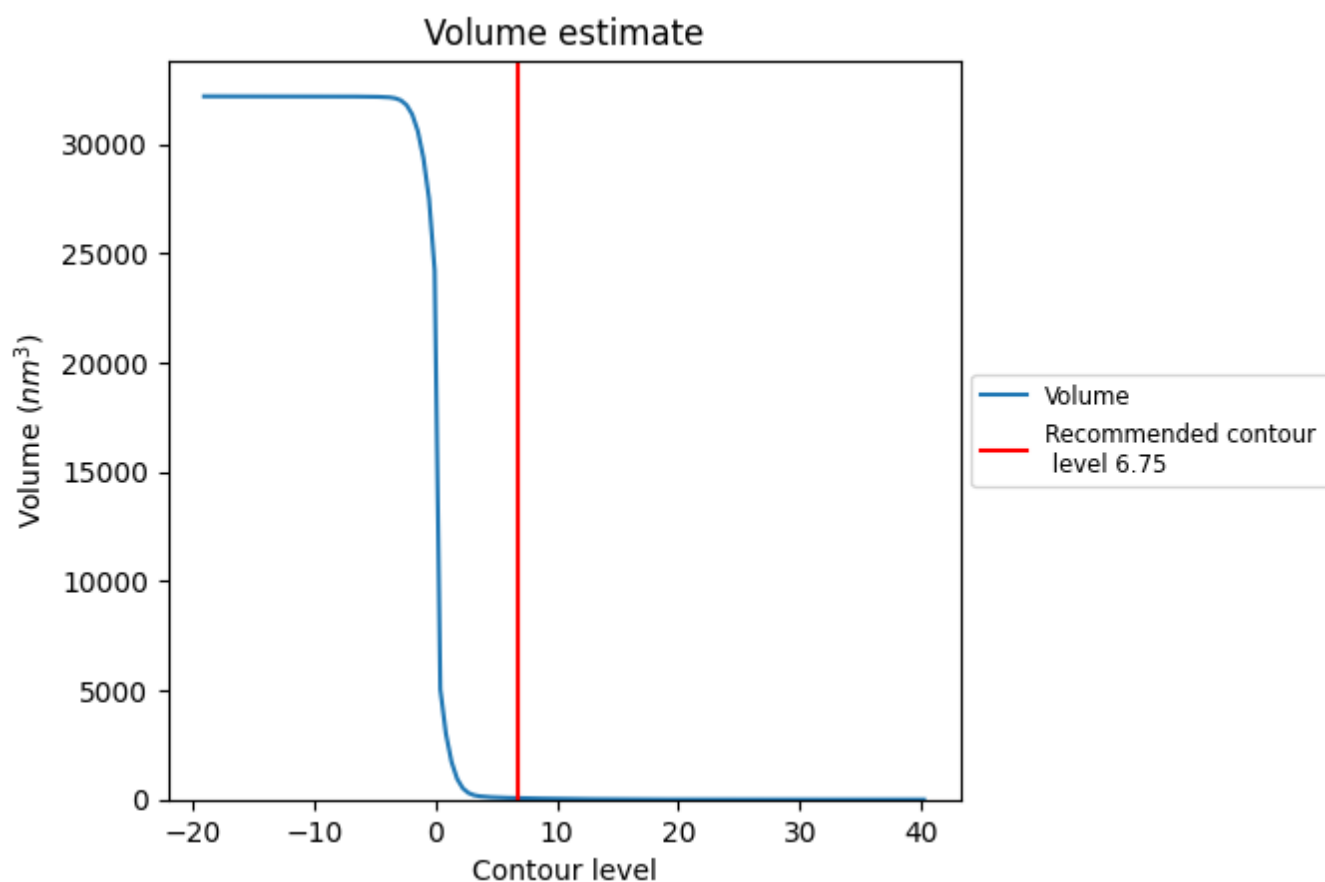
This section contains the results of statistical analysis of the map.

### 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.

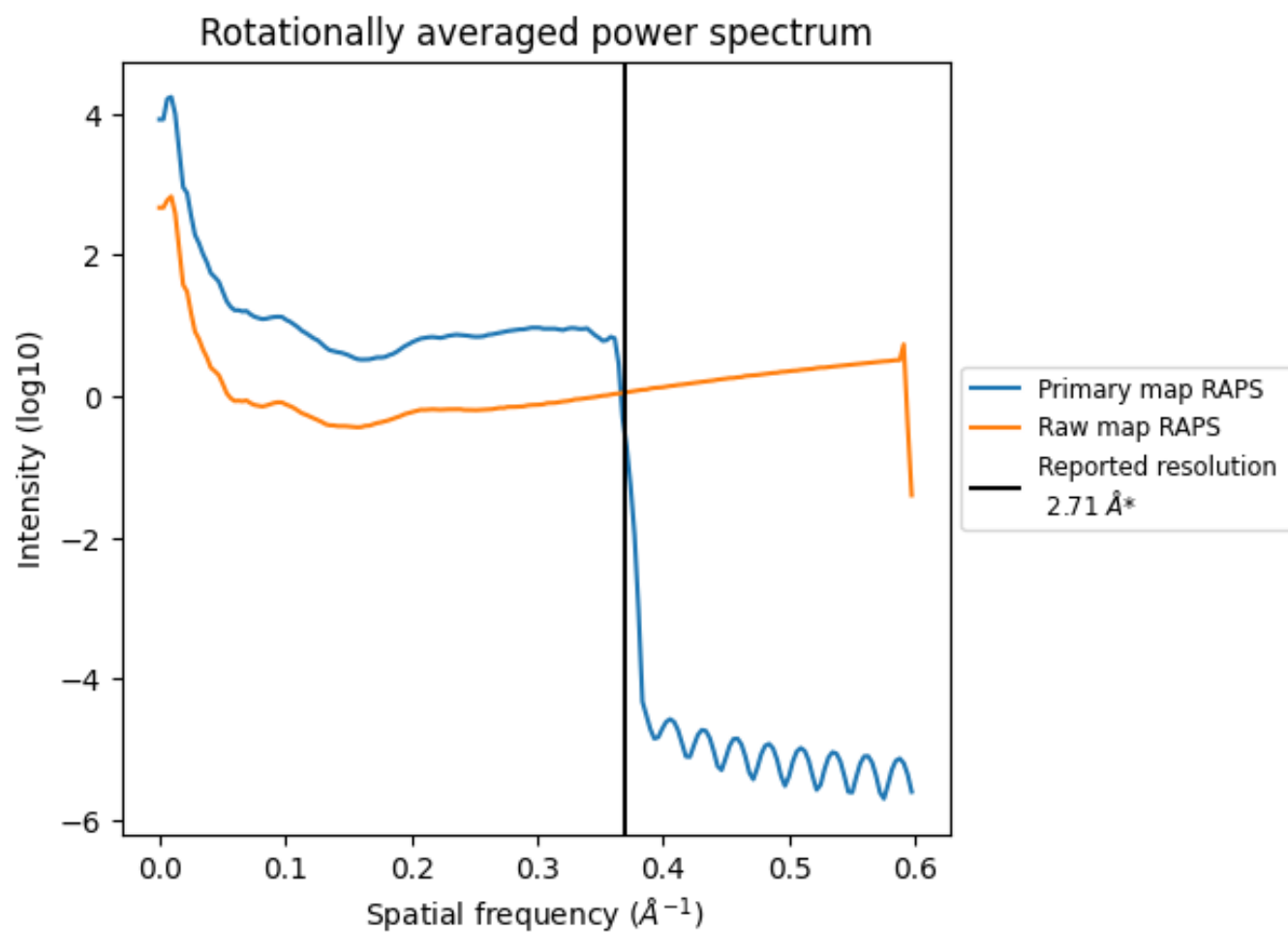
## 6.2 Volume estimate [i](#)



The volume at the recommended contour level is 67  $\text{nm}^3$ ; this corresponds to an approximate mass of 61 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 ⓘ

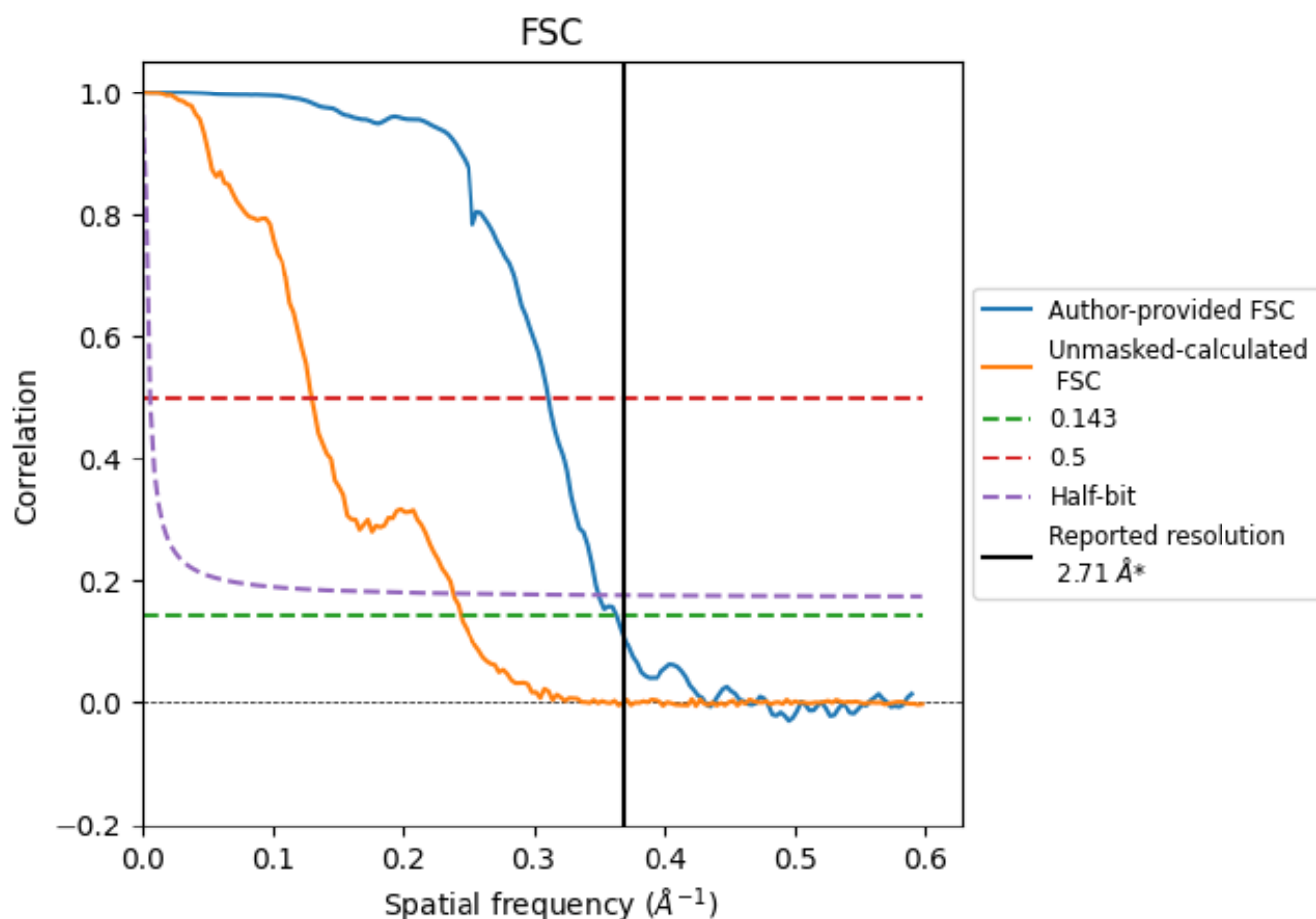


\*Reported resolution corresponds to spatial frequency of 0.369  $\text{\AA}^{-1}$

## 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  $0.369 \text{ \AA}^{-1}$



## 7.2 Resolution estimates [i](#)

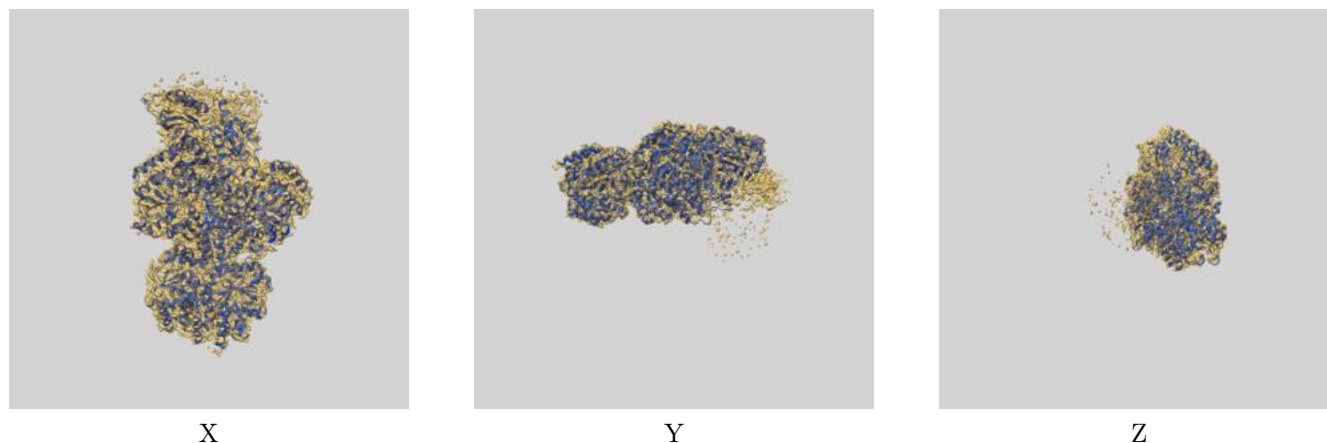
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	2.75	3.21	2.86
Unmasked-calculated*	4.10	7.69	4.20

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.10 differs from the reported value 2.71 by more than 10 %

## 8 Map-model fit [i](#)

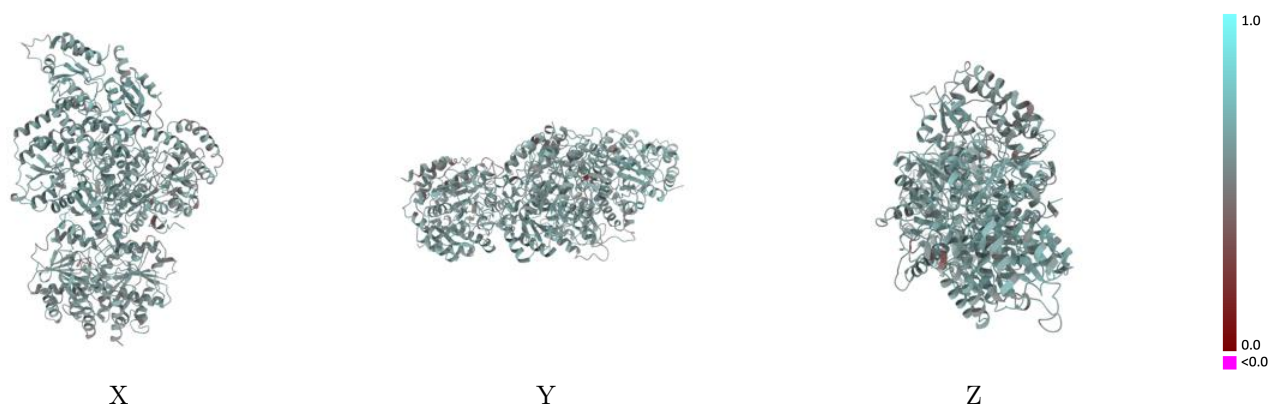
This section contains information regarding the fit between EMDB map EMD-50553 and PDB model 9FMG. Per-residue inclusion information can be found in section ?? on page ??.

### 8.1 Map-model overlay [i](#)



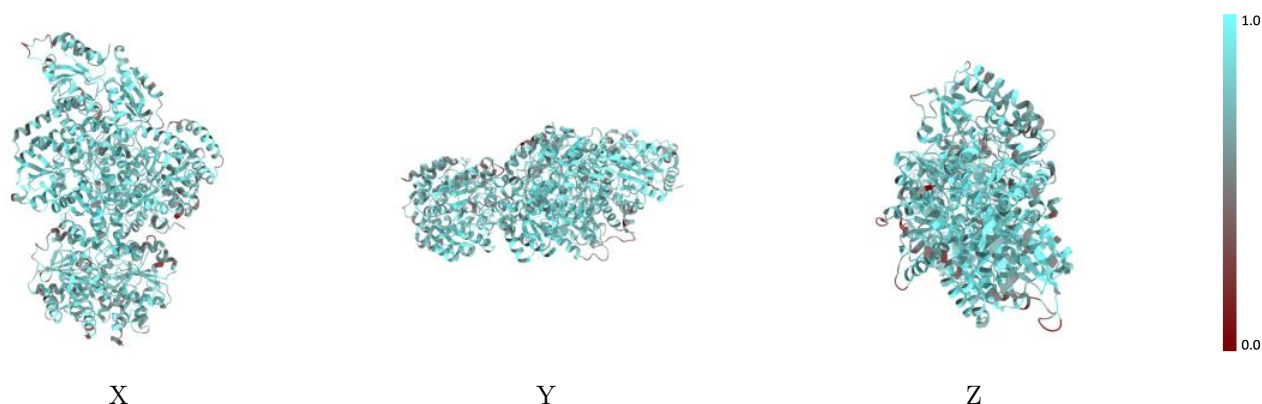
The images above show the 3D surface view of the map at the recommended contour level 6.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



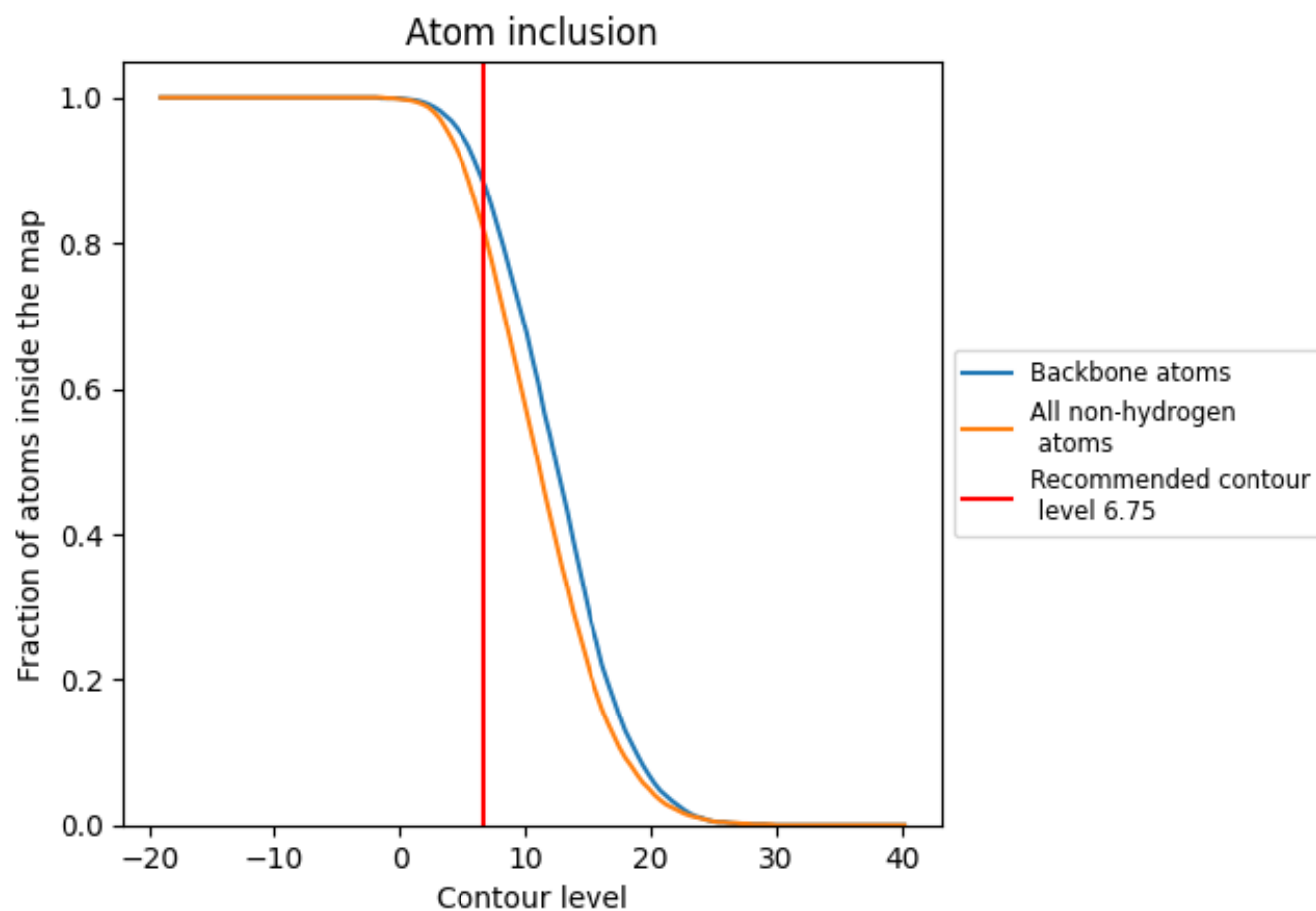
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.75).

## 8.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (6.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8150	<div><div></div></div> 0.5850
A	<div><div></div></div> 0.8180	<div><div></div></div> 0.5800
B	<div><div></div></div> 0.8450	<div><div></div></div> 0.5970
C	<div><div></div></div> 0.8120	<div><div></div></div> 0.6020
D	<div><div></div></div> 0.7850	<div><div></div></div> 0.5610
E	<div><div></div></div> 0.7940	<div><div></div></div> 0.5750

