



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 03:30 AM JST

PDB ID : 7BSU / pdb_00007bsu
EMDB ID : EMD-30167
Title : Cryo-EM structure of a human ATP11C-CDC50A flippase in PtdSer-bound E2BeF state
Authors : Abe, K.; Nishizawa, T.; Nakanishi, H.
Deposited on : 2020-03-31
Resolution : 3.20 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

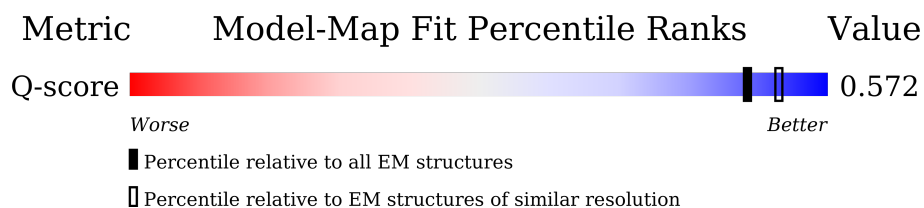
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9407 atoms, of which 82 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 ATP11C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	814	Total	C	N	O	S	0	0
			6587	4300	1059	1195	33		

- Molecule 2 is a protein called Cell cycle control protein 50A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	324	Total	C	N	O	S	0	0
			2613	1696	439	466	12		

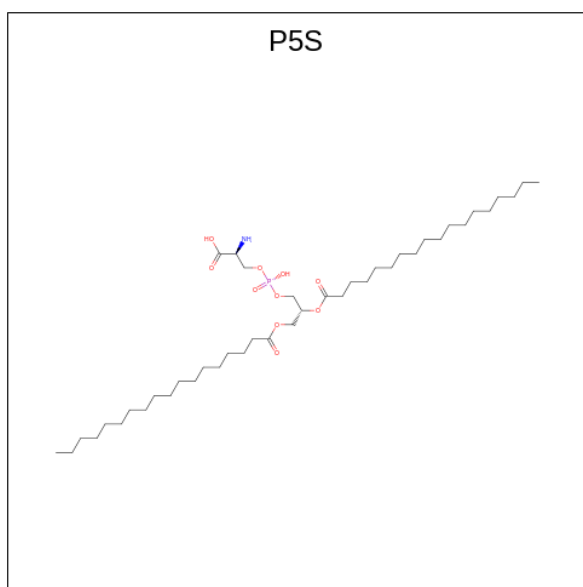
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	175	MET	ALA	engineered mutation	UNP Q9NV96
C	190	GLN	ASN	engineered mutation	UNP Q9NV96
C	292	TRP	SER	engineered mutation	UNP Q9NV96

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

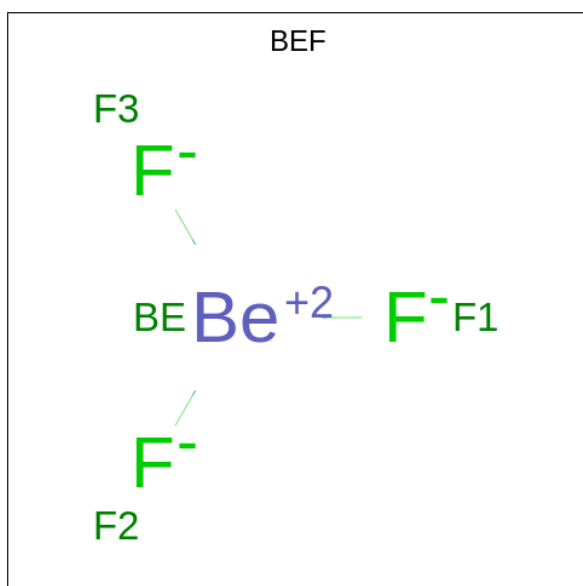
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	

- Molecule 4 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P) (labeled as "Ligand of Interest" by depositor).



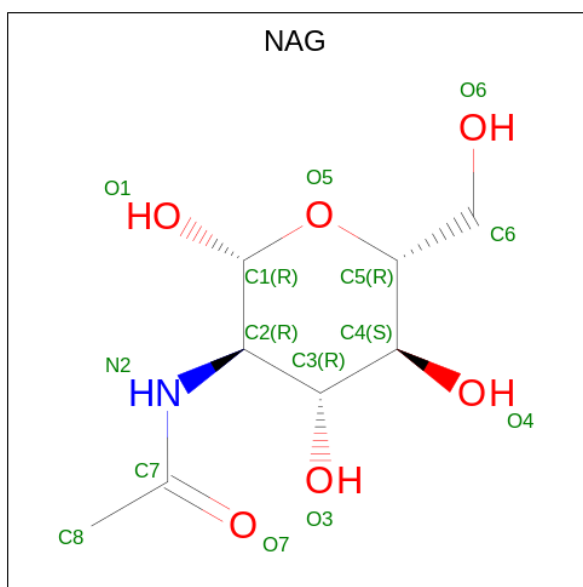
Mol	Chain	Residues	Atoms					AltConf	
4	A	1	Total	C	H	N	O	P	0
			136	42	82	1	10	1	

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



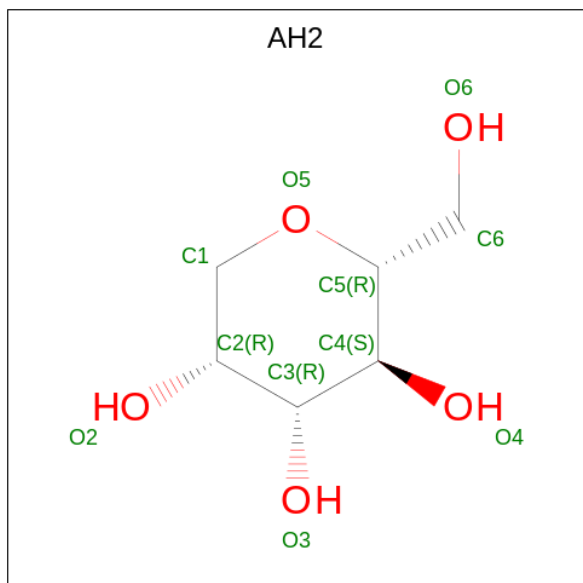
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Be	F	0
			4	1	3	

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			13	8	1	4	

- Molecule 7 is 1-deoxy-alpha-D-mannopyranose (CCD ID: AH2) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	C	O	0
			11	6	5	

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, Not provided	
Number of particles used	500000	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0158	Depositor
Map size (Å)	215.8, 215.8, 215.8	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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 8 ligands modelled in this entry, 1 is 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	NAG	C	404	2	14,14,15	0.35	0	17,19,21	0.77	0
6	NAG	C	401	-	14,14,15	0.33	0	17,19,21	0.74	0
6	NAG	C	402	-	14,14,15	0.32	0	17,19,21	0.89	0
5	BEF	A	1102	1	0,3,3	-	-	-	-	-
7	AH2	C	403	-	11,11,11	0.27	0	15,15,15	0.78	0
4	P5S	A	1101	-	52,53,53	0.91	2 (3%)	56,60,60	0.99	3 (5%)
6	NAG	C	405	-	13,13,15	0.35	0	14,17,21	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	404	2	-	1/6/23/26	0/1/1/1
6	NAG	C	401	-	-	4/6/23/26	0/1/1/1
6	NAG	C	402	-	-	4/6/23/26	0/1/1/1
7	AH2	C	403	-	-	1/2/19/19	0/1/1/1
4	P5S	A	1101	-	-	19/59/59/59	-
6	NAG	C	405	-	-	3/6/19/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	P5S	O19-C17	4.20	1.45	1.33
4	A	1101	P5S	O37-C38	4.05	1.45	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	P5S	O37-C38-C39	3.80	119.70	111.50
4	A	1101	P5S	O19-C17-C20	2.32	119.20	111.91
4	A	1101	P5S	OXT-C-O	-2.12	119.27	124.09

There are no chirality outliers.

All (32) torsion outliers are listed below:

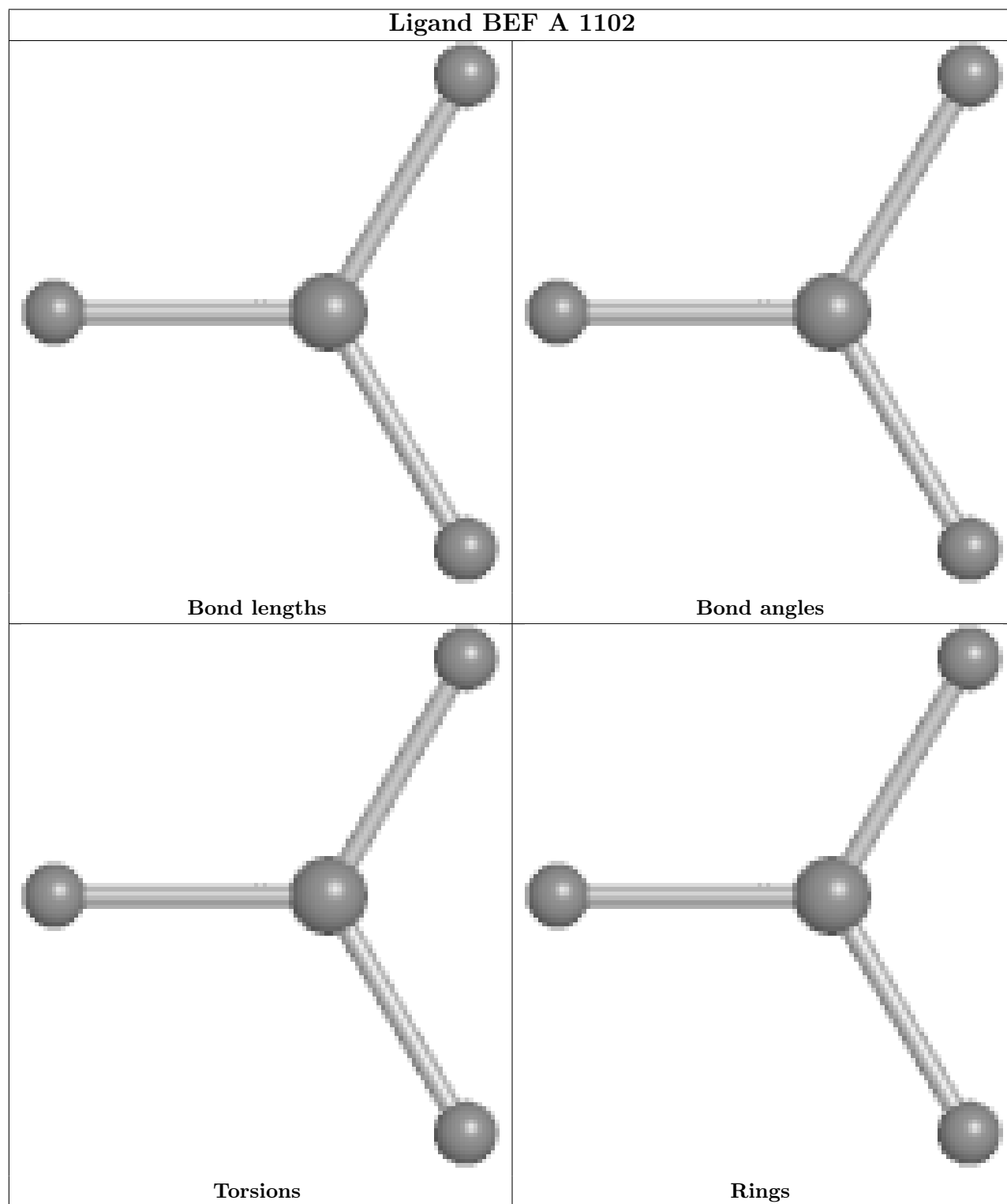
Mol	Chain	Res	Type	Atoms
4	A	1101	P5S	O-C-CA-CB
4	A	1101	P5S	OXT-C-CA-CB
6	C	401	NAG	C8-C7-N2-C2
6	C	401	NAG	O7-C7-N2-C2
6	C	402	NAG	C1-C2-N2-C7
6	C	402	NAG	C8-C7-N2-C2
6	C	402	NAG	O7-C7-N2-C2
6	C	405	NAG	C8-C7-N2-C2
6	C	405	NAG	O7-C7-N2-C2
4	A	1101	P5S	C25-C26-C27-C28
4	A	1101	P5S	C41-C42-C43-C44
6	C	404	NAG	O5-C5-C6-O6
7	C	403	AH2	O5-C5-C6-O6
4	A	1101	P5S	C40-C41-C42-C43
6	C	401	NAG	O5-C5-C6-O6
4	A	1101	P5S	C50-C51-C52-C53
4	A	1101	P5S	C52-C53-C54-C55
6	C	402	NAG	O5-C5-C6-O6
4	A	1101	P5S	C26-C27-C28-C29
4	A	1101	P5S	C39-C38-O37-C2
4	A	1101	P5S	O-C-CA-N
4	A	1101	P5S	O47-C38-O37-C2
4	A	1101	P5S	O19-C1-C2-C3
4	A	1101	P5S	O19-C1-C2-O37
4	A	1101	P5S	N-CA-CB-OG
4	A	1101	P5S	C43-C44-C45-C46
6	C	405	NAG	C3-C2-N2-C7
4	A	1101	P5S	C21-C22-C23-C24
4	A	1101	P5S	OXT-C-CA-N
6	C	401	NAG	C3-C2-N2-C7
4	A	1101	P5S	CB-OG-P12-O13
4	A	1101	P5S	C22-C23-C24-C25

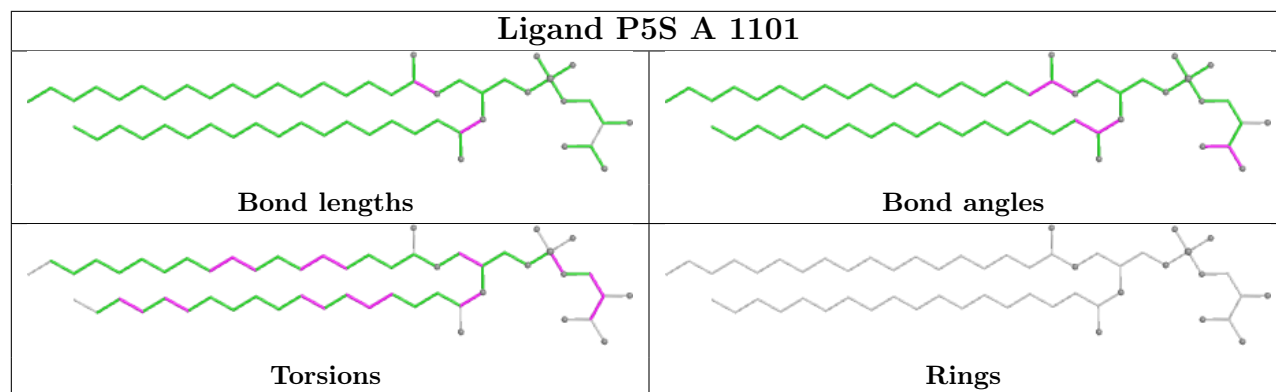
There are no ring outliers.

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.

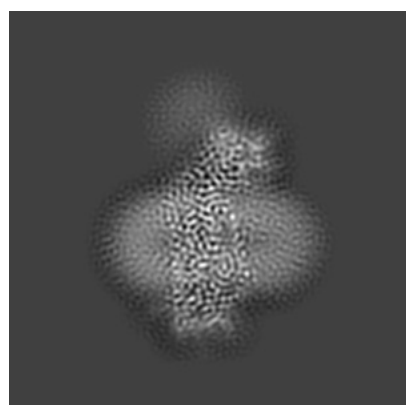
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30167. These allow visual inspection of the internal detail of the map and identification of artifacts.

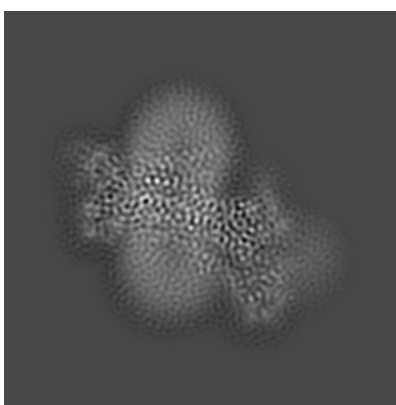
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

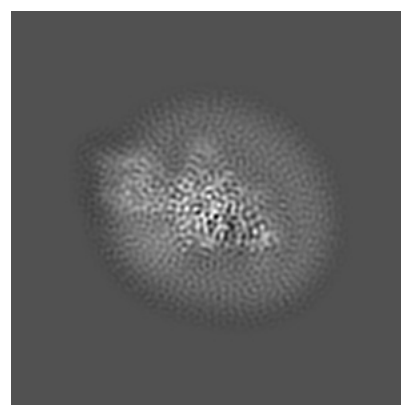
5.1.1 Primary map



X



Y

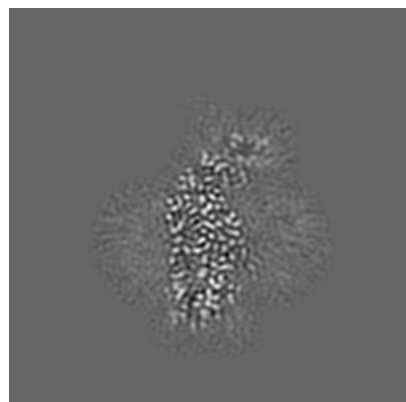


Z

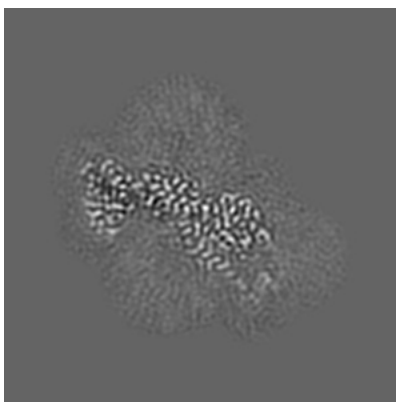
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

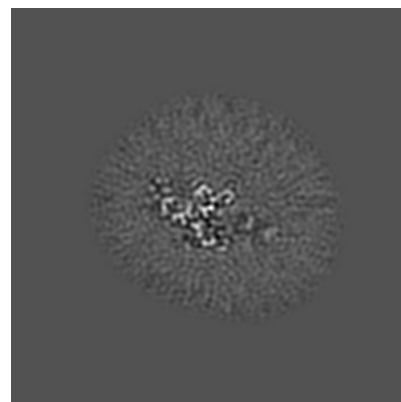
5.2.1 Primary map



X Index: 130



Y Index: 130

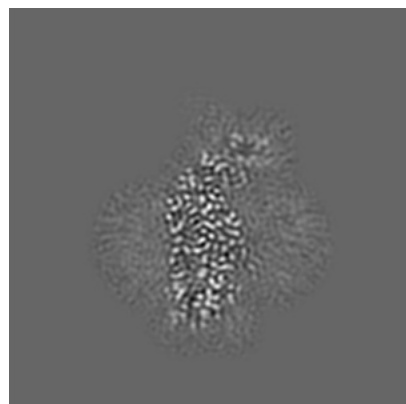


Z Index: 130

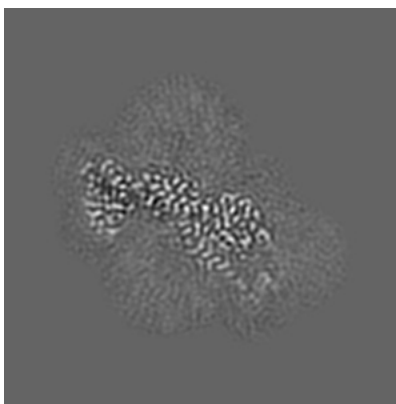
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

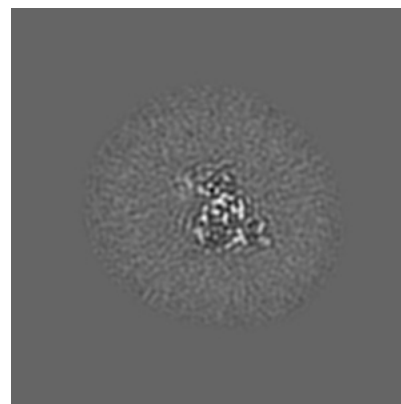
5.3.1 Primary map



X Index: 130



Y Index: 130

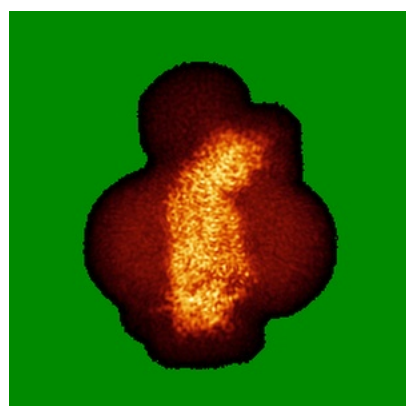


Z Index: 99

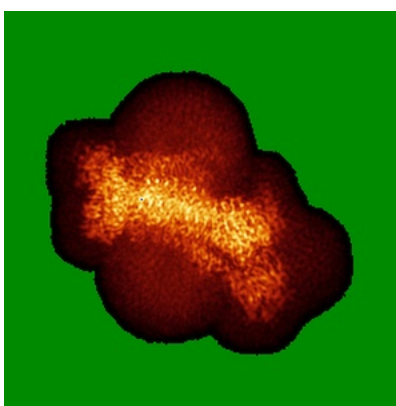
The images above show the largest variance slices of the map in three orthogonal directions.

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

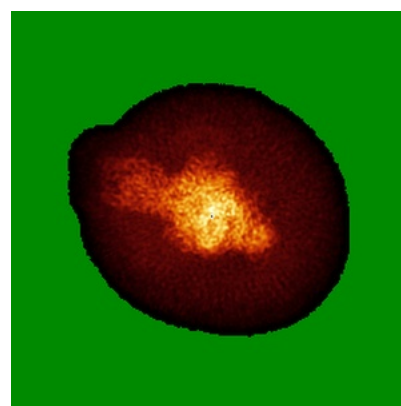
5.4.1 Primary map



X



Y

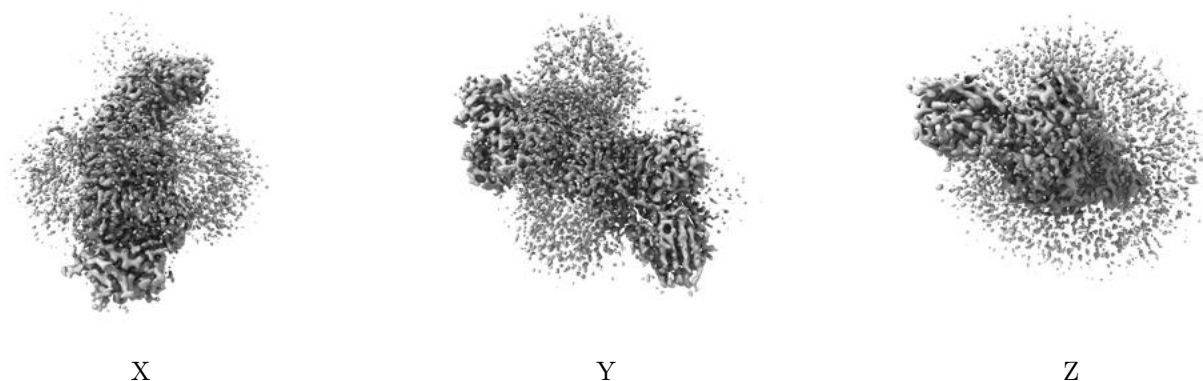


Z

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 0.0158. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

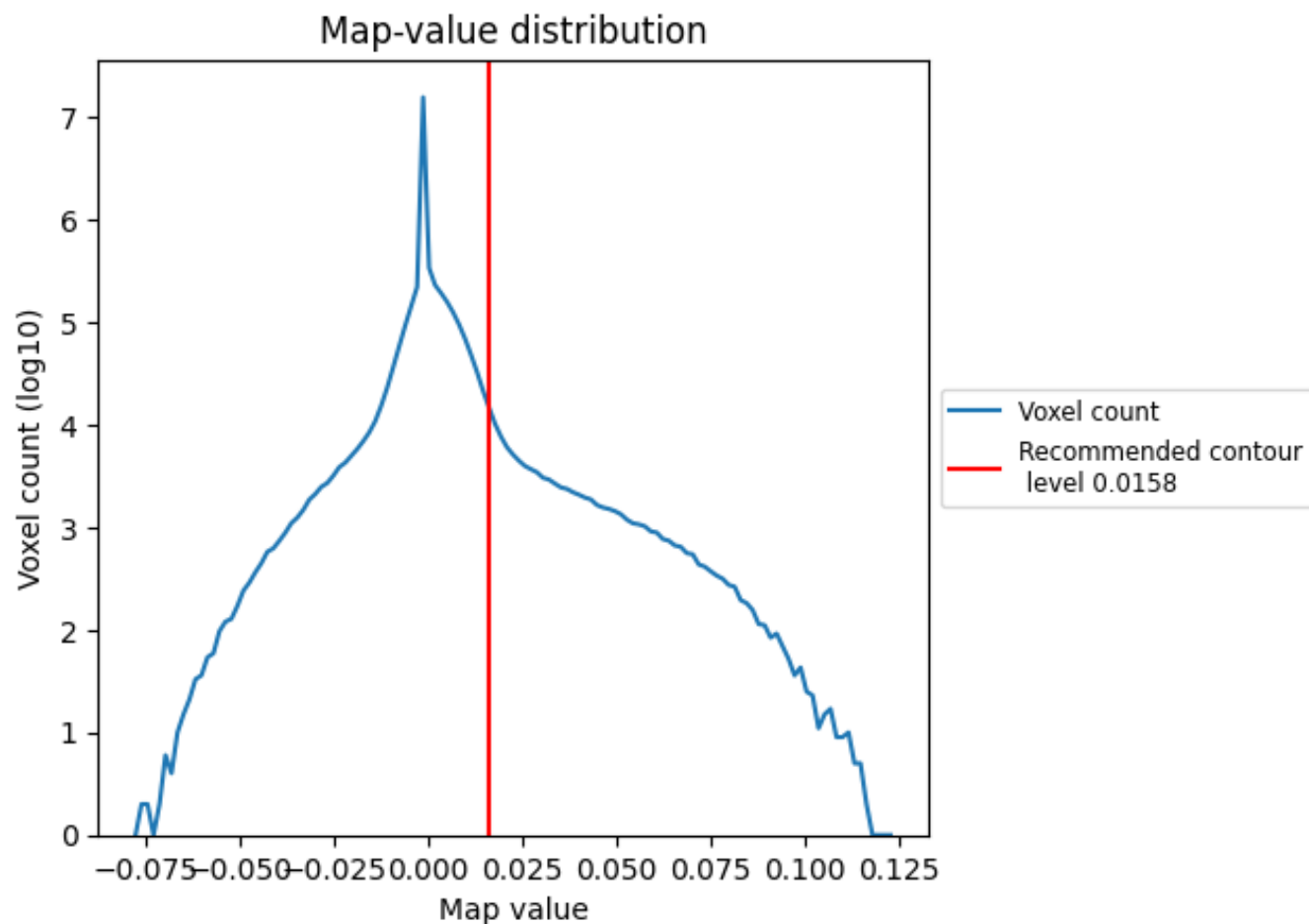
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

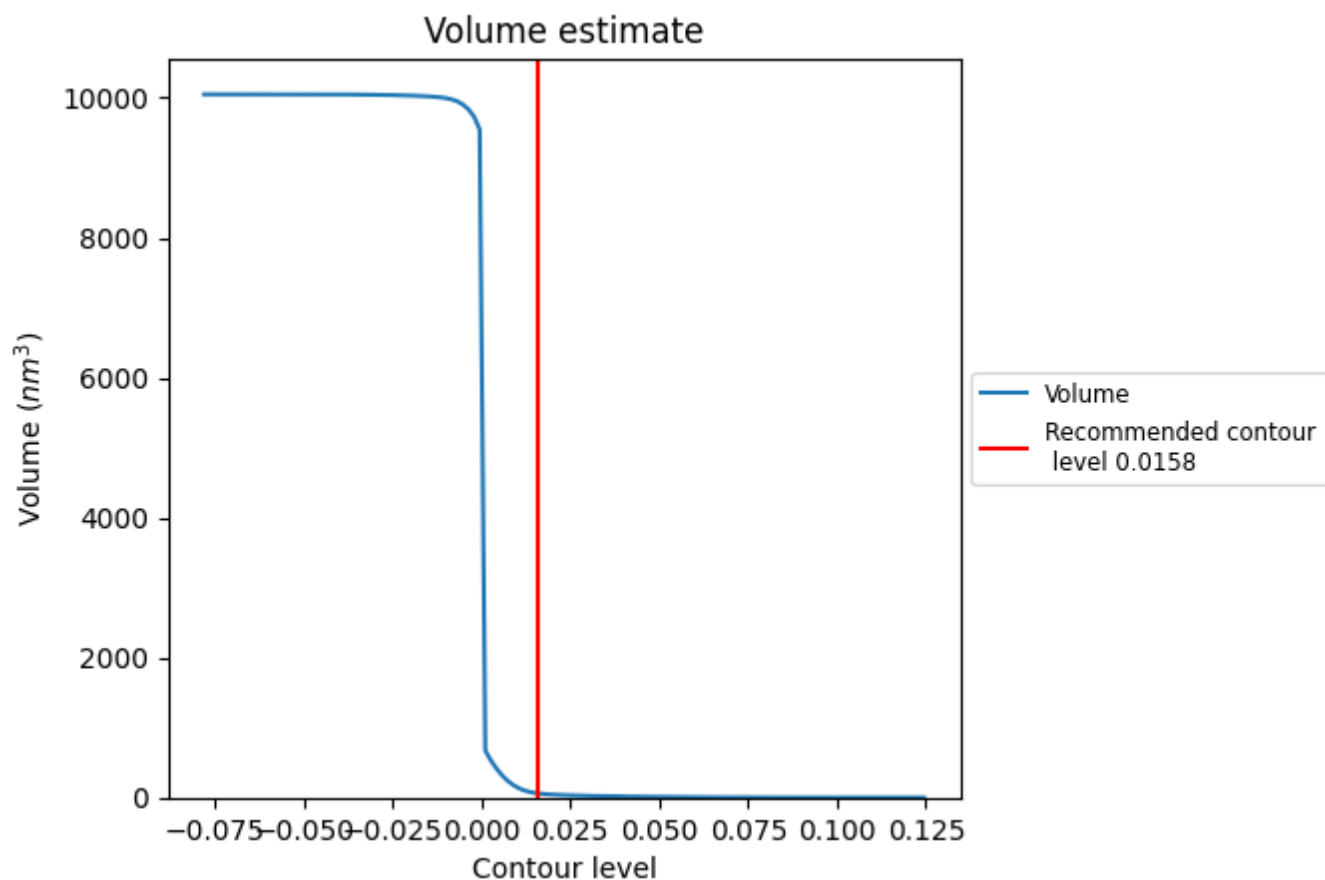
This section contains the results of statistical analysis of the map.

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.

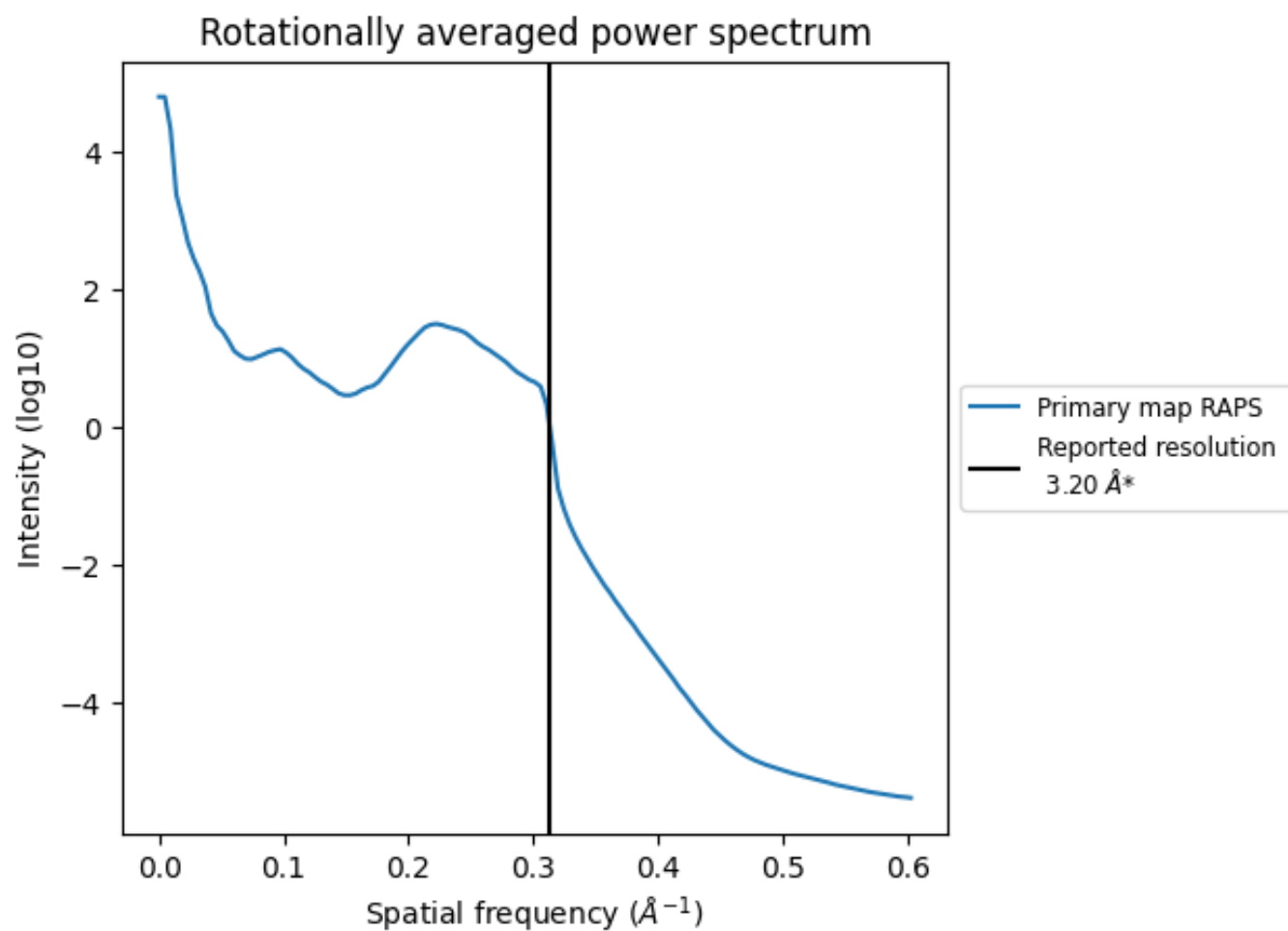
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 61 nm³; this corresponds to an approximate mass of 55 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 0.312 Å⁻¹

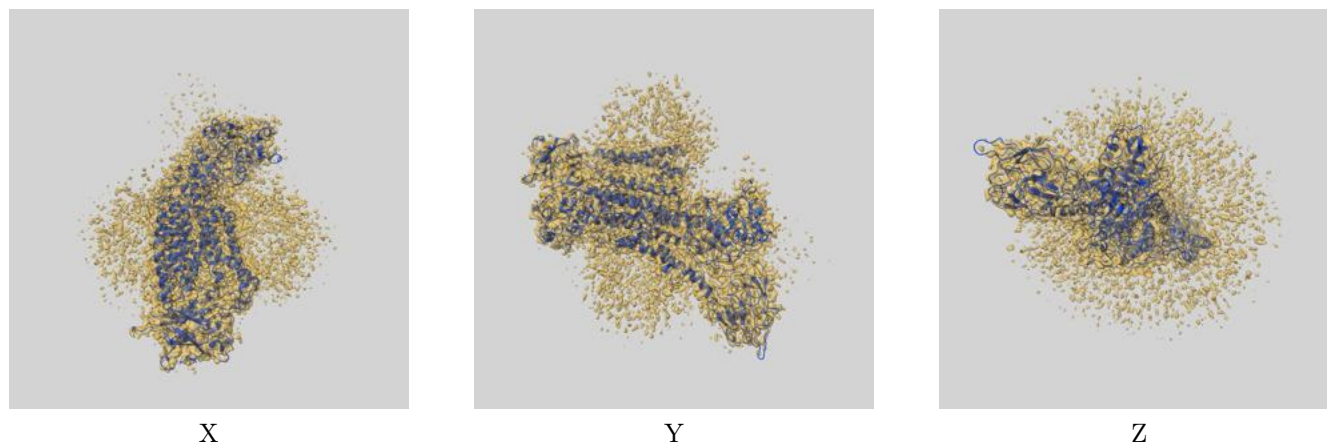
7 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

8 Map-model fit [i](#)

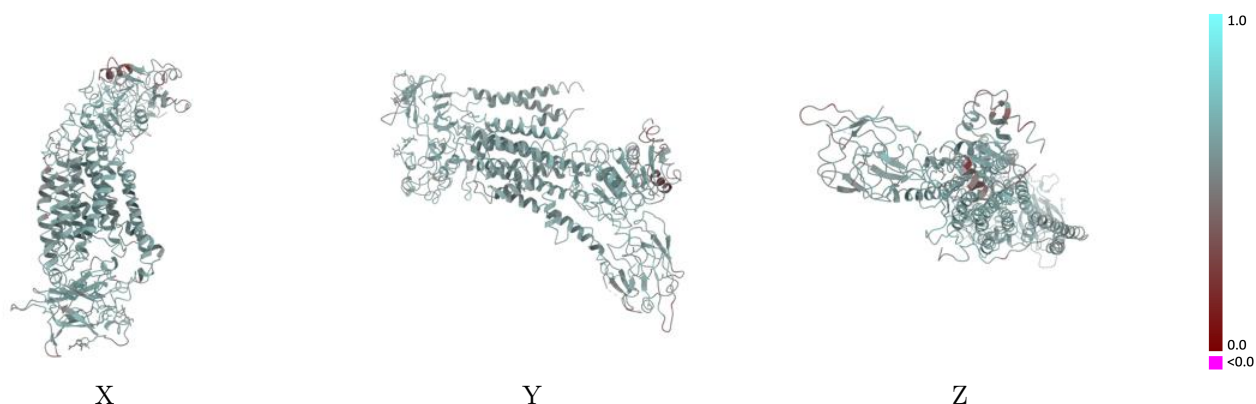
This section contains information regarding the fit between EMDB map EMD-30167 and PDB model 7BSU. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)



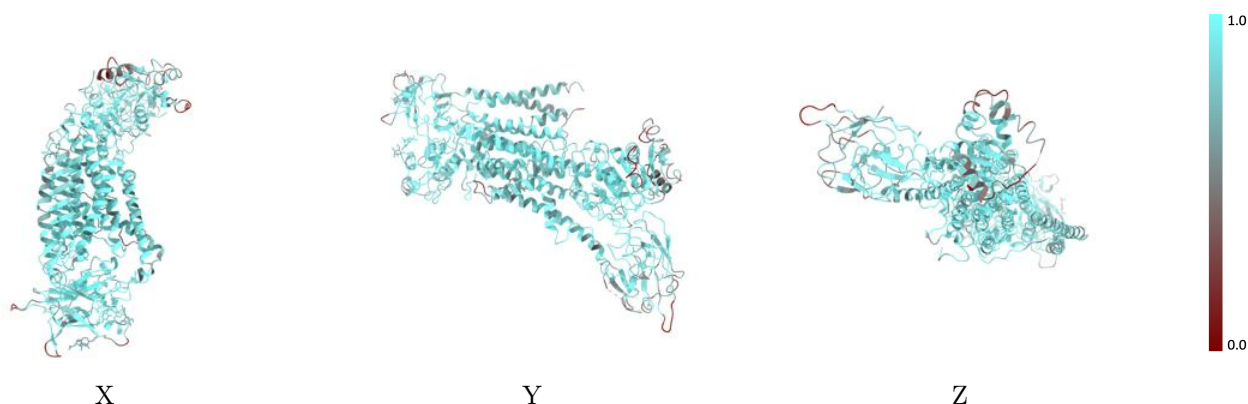
The images above show the 3D surface view of the map at the recommended contour level 0.0158 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



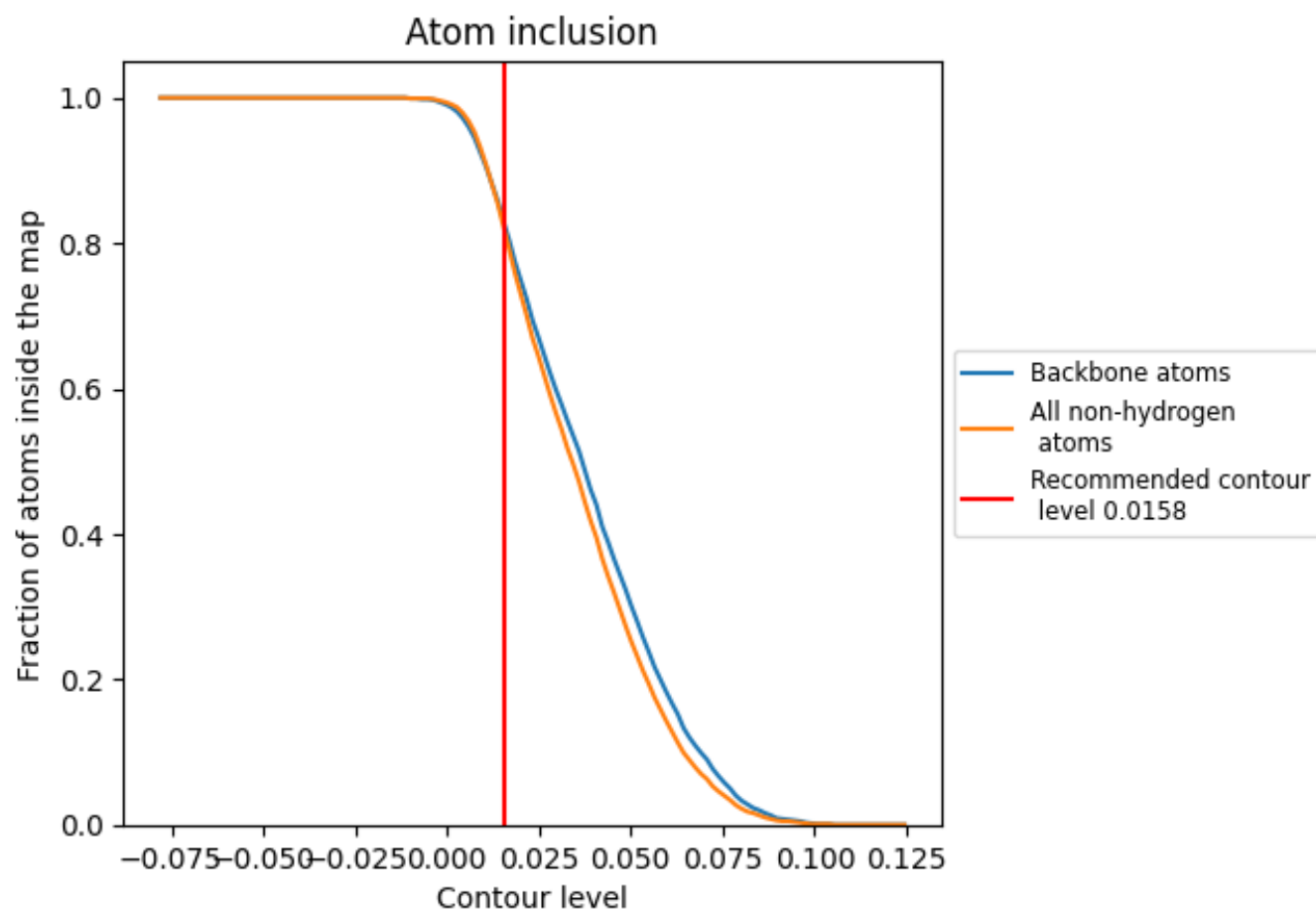
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0158).

8.4 Atom inclusion [i](#)



At the recommended contour level, 82% 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 (0.0158) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8150	0.5720
A	0.8150	0.5740
C	0.8200	0.5690

