



wwPDB EM Validation Summary Report ⓘ

Jun 10, 2026 – 04:15 pm BST

PDB ID : 9SQ5 / pdb_00009sq5
EMDB ID : EMD-55107
Title : Cryo-EM structure of the DDB1deltaB-CRBN-Pomalidomide complex bound to IKZF1(ZF1-ZF2-Helix)
Authors : Galli, P.; Kater, L.; Kempf, G.; Cavadini, S.; Thoma, N.H.
Deposited on : 2025-09-19
Resolution : 3.68 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
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

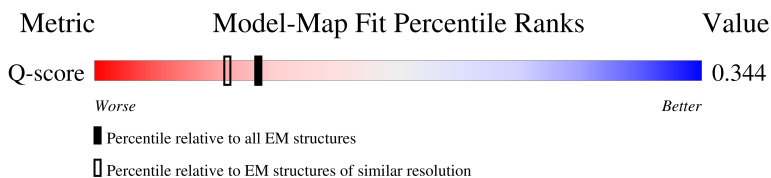
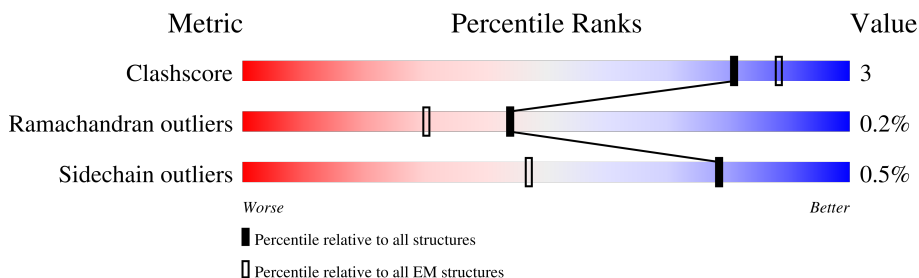
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.68 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11376 (3.18 - 4.18)

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

Mol	Chain	Length	Quality of chain
1	A	864	 89% 6% 5%
2	B	466	 73% 23%
3	C	111	 7% 23% 77%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9531 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 damage-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	824	6470	4095	1091	1249	35	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q16531
A	-26	GLY	-	expression tag	UNP Q16531
A	-25	SER	-	expression tag	UNP Q16531
A	-24	SER	-	expression tag	UNP Q16531
A	-23	HIS	-	expression tag	UNP Q16531
A	-22	HIS	-	expression tag	UNP Q16531
A	-21	HIS	-	expression tag	UNP Q16531
A	-20	HIS	-	expression tag	UNP Q16531
A	-19	HIS	-	expression tag	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	SER	-	expression tag	UNP Q16531
A	-16	ALA	-	expression tag	UNP Q16531
A	-15	ALA	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	ILE	-	expression tag	UNP Q16531
A	-12	VAL	-	expression tag	UNP Q16531
A	-11	MET	-	expression tag	UNP Q16531
A	-10	VAL	-	expression tag	UNP Q16531
A	-9	ASP	-	expression tag	UNP Q16531
A	-8	ALA	-	expression tag	UNP Q16531
A	-7	TYR	-	expression tag	UNP Q16531
A	-6	LYS	-	expression tag	UNP Q16531
A	-5	PRO	-	expression tag	UNP Q16531
A	-4	THR	-	expression tag	UNP Q16531
A	-3	LYS	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	359	Total	C	N	O	S	0	0
			2897	1849	496	529	23		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-23	MET	-	initiating methionine	UNP Q96SW2
B	-22	GLY	-	expression tag	UNP Q96SW2
B	-21	SER	-	expression tag	UNP Q96SW2
B	-20	SER	-	expression tag	UNP Q96SW2
B	-19	HIS	-	expression tag	UNP Q96SW2
B	-18	HIS	-	expression tag	UNP Q96SW2
B	-17	HIS	-	expression tag	UNP Q96SW2
B	-16	HIS	-	expression tag	UNP Q96SW2
B	-15	HIS	-	expression tag	UNP Q96SW2
B	-14	HIS	-	expression tag	UNP Q96SW2
B	-13	SER	-	expression tag	UNP Q96SW2
B	-12	ALA	-	expression tag	UNP Q96SW2
B	-11	VAL	-	expression tag	UNP Q96SW2
B	-10	ASP	-	expression tag	UNP Q96SW2
B	-9	GLU	-	expression tag	UNP Q96SW2
B	-8	ASN	-	expression tag	UNP Q96SW2
B	-7	LEU	-	expression tag	UNP Q96SW2
B	-6	TYR	-	expression tag	UNP Q96SW2
B	-5	PHE	-	expression tag	UNP Q96SW2
B	-4	GLN	-	expression tag	UNP Q96SW2
B	-3	GLY	-	expression tag	UNP Q96SW2
B	-2	GLY	-	expression tag	UNP Q96SW2
B	-1	GLY	-	expression tag	UNP Q96SW2
B	0	ARG	-	expression tag	UNP Q96SW2

- Molecule 3 is a protein called Isoform Ik7 of DNA-binding protein Ikaros.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	26	Total	C	N	O	S	0	0
			142	84	30	26	2		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	91	MET	-	initiating methionine	UNP Q13422
C	92	ASP	-	expression tag	UNP Q13422
C	93	TRP	-	expression tag	UNP Q13422
C	94	SER	-	expression tag	UNP Q13422
C	95	HIS	-	expression tag	UNP Q13422
C	96	PRO	-	expression tag	UNP Q13422
C	97	GLN	-	expression tag	UNP Q13422
C	98	PHE	-	expression tag	UNP Q13422
C	99	GLU	-	expression tag	UNP Q13422
C	100	LYS	-	expression tag	UNP Q13422
C	101	SER	-	expression tag	UNP Q13422
C	102	ALA	-	expression tag	UNP Q13422
C	103	VAL	-	expression tag	UNP Q13422
C	104	MET	-	expression tag	UNP Q13422
C	105	SER	-	expression tag	UNP Q13422
C	106	GLY	-	expression tag	UNP Q13422
C	107	LEU	-	expression tag	UNP Q13422
C	108	ASN	-	expression tag	UNP Q13422
C	109	ASP	-	expression tag	UNP Q13422
C	110	ILE	-	expression tag	UNP Q13422
C	111	PHE	-	expression tag	UNP Q13422
C	112	GLU	-	expression tag	UNP Q13422
C	113	ALA	-	expression tag	UNP Q13422
C	114	GLN	-	expression tag	UNP Q13422
C	115	LYS	-	expression tag	UNP Q13422
C	116	ILE	-	expression tag	UNP Q13422
C	117	GLU	-	expression tag	UNP Q13422
C	118	TRP	-	expression tag	UNP Q13422
C	119	HIS	-	expression tag	UNP Q13422
C	120	GLU	-	expression tag	UNP Q13422
C	121	GLY	-	expression tag	UNP Q13422
C	122	GLY	-	expression tag	UNP Q13422
C	123	GLY	-	expression tag	UNP Q13422
C	124	GLY	-	expression tag	UNP Q13422
C	125	SER	-	expression tag	UNP Q13422
C	126	GLY	-	expression tag	UNP Q13422
C	127	GLY	-	expression tag	UNP Q13422

Continued on next page...

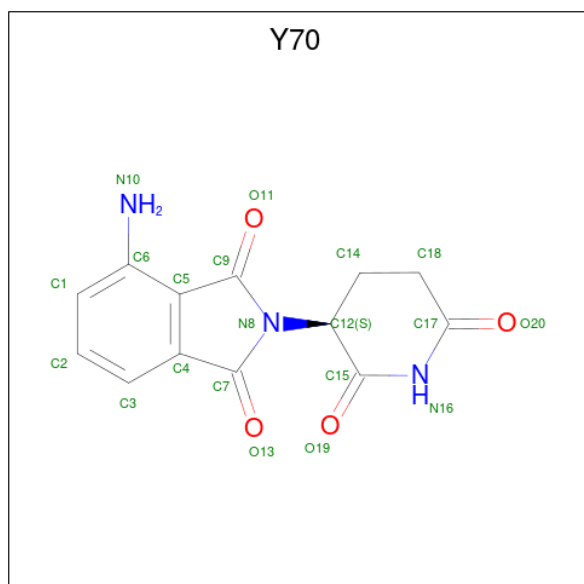
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	128	GLY	-	expression tag	UNP Q13422
C	129	GLY	-	expression tag	UNP Q13422
C	130	ASP	-	expression tag	UNP Q13422
C	131	GLU	-	expression tag	UNP Q13422
C	132	ASN	-	expression tag	UNP Q13422
C	133	LEU	-	expression tag	UNP Q13422
C	134	TYR	-	expression tag	UNP Q13422
C	135	PHE	-	expression tag	UNP Q13422
C	136	GLN	-	expression tag	UNP Q13422
C	137	GLY	-	expression tag	UNP Q13422
C	138	GLY	-	expression tag	UNP Q13422
C	139	GLY	-	expression tag	UNP Q13422
C	140	ARG	-	expression tag	UNP Q13422

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Zn 1 1	0
4	C	1	Total Zn 1 1	0

- Molecule 5 is S-Pomalidomide (CCD ID: Y70) (formula: C₁₃H₁₁N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	20	13	3	4	0

K157	L160	S168	GLY	GLU	LYS	PRO	PHE	LYS	CYS	HIS	LEU	CYS	ASN	TYR	ALA	CYS	ARG	ARG	ARG	ASP	ALA	LEU	THR	GLY	HIS	LEU	ARG	THR	HIS	SER	VAL	ILE	LYS	GLU	GLU
------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102811	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)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.758	Depositor
Minimum map value	-0.340	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.128	Depositor
Map size (Å)	324.48, 324.48, 324.48	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.845, 0.845, 0.845	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, Y70

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/6587	0.48	0/8909
2	B	0.22	0/2966	0.37	0/4023
3	C	0.20	0/144	0.49	0/198
All	All	0.35	0/9697	0.45	0/13130

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	TRP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6470	0	6433	35	0
2	B	2897	0	2886	14	0
3	C	142	0	75	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	20	0	11	1	0
All	All	9531	0	9405	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 49 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HH21	1:A:54:GLU:HG2	1.44	0.83
2:B:391:CYS:HB3	2:B:394:CYS:SG	2.22	0.79
2:B:391:CYS:CB	2:B:394:CYS:SG	2.81	0.66
1:A:938:MET:SD	1:A:938:MET:N	2.69	0.65
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.79	0.65

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	820/864 (95%)	778 (95%)	40 (5%)	2 (0%)	43	71
2	B	355/466 (76%)	342 (96%)	13 (4%)	0	100	100
3	C	24/111 (22%)	23 (96%)	1 (4%)	0	100	100
All	All	1199/1441 (83%)	1143 (95%)	54 (4%)	2 (0%)	44	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	855	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	719/749 (96%)	716 (100%)	3 (0%)	84	81
2	B	323/417 (78%)	321 (99%)	2 (1%)	78	79
3	C	5/89 (6%)	5 (100%)	0	100	100
All	All	1047/1255 (83%)	1042 (100%)	5 (0%)	78	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ASP
1	A	208	LYS
1	A	209	GLN
2	B	47	ILE
2	B	326	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	727	GLN
1	A	907	ASN
2	B	390	GLN
1	A	991	HIS
1	A	255	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
5	Y70	B	502	-	22,22,22	1.03	2 (9%)	31,33,33	1.48	5 (16%)

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
5	Y70	B	502	-	-	0/4/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	Y70	C5-C9	-2.31	1.45	1.49
5	B	502	Y70	C5-C6	-2.25	1.39	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	Y70	C15-C12-N8	-5.04	104.48	109.08
5	B	502	Y70	C18-C14-C12	2.67	114.79	109.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	Y70	C14-C12-C15	2.63	116.12	111.61
5	B	502	Y70	C1-C6-C5	-2.42	115.02	118.29
5	B	502	Y70	C2-C3-C4	-2.24	115.59	119.81

There are no chirality outliers.

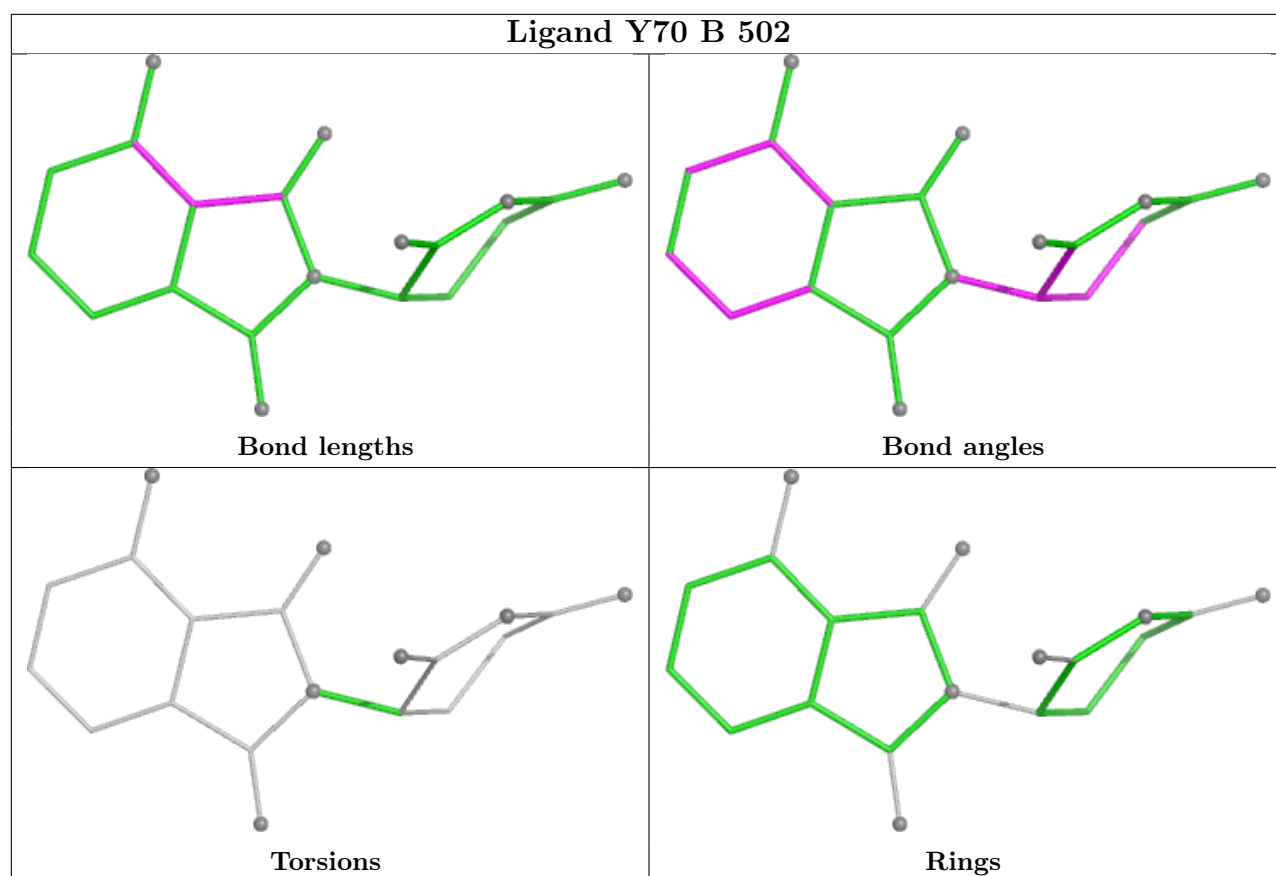
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	Y70	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

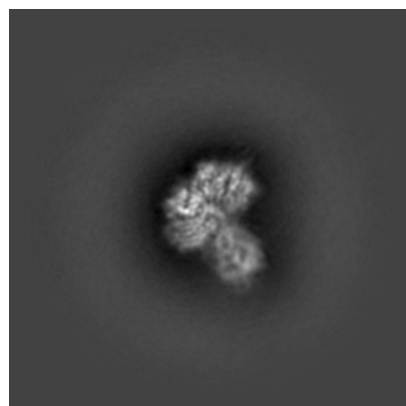
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55107. These allow visual inspection of the internal detail of the map and identification of artifacts.

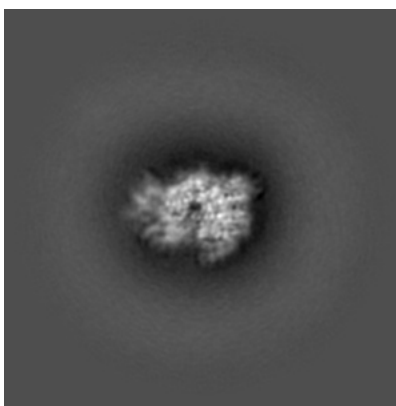
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

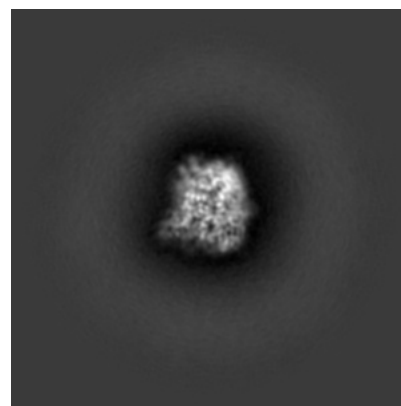
6.1.1 Primary map



X

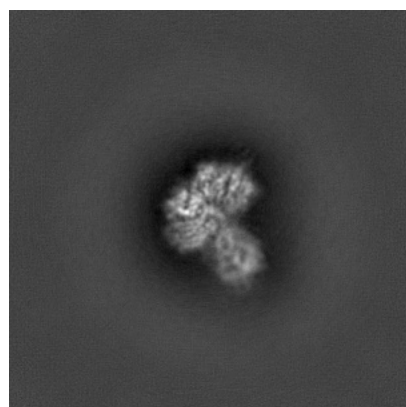


Y

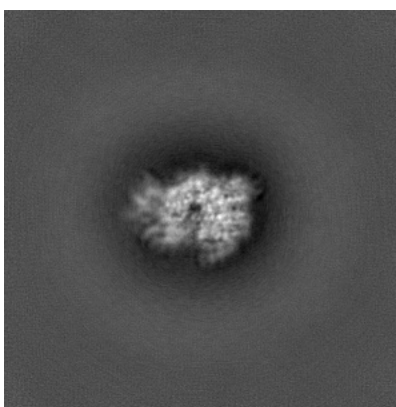


Z

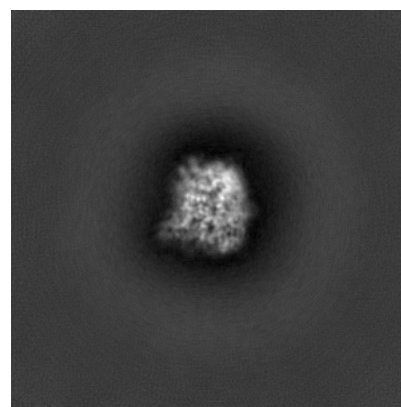
6.1.2 Raw map



X



Y

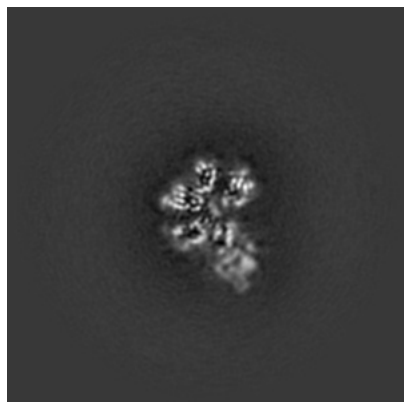


Z

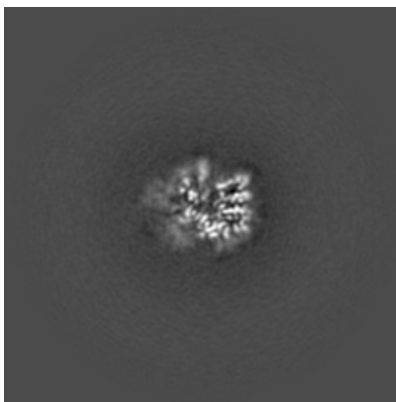
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

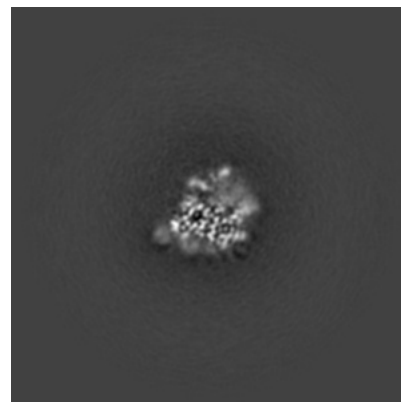
6.2.1 Primary map



X Index: 192

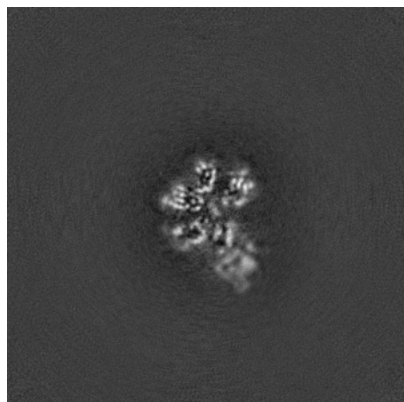


Y Index: 192

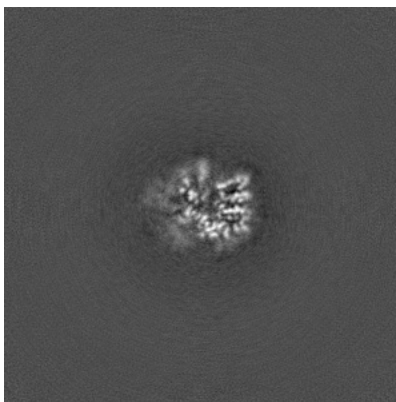


Z Index: 192

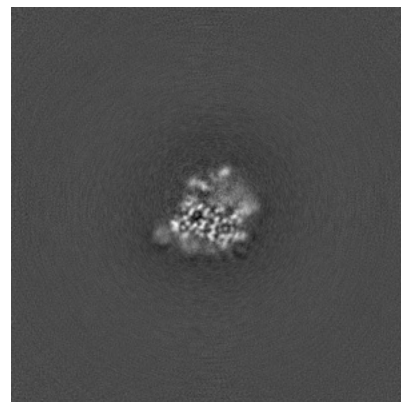
6.2.2 Raw map



X Index: 192



Y Index: 192

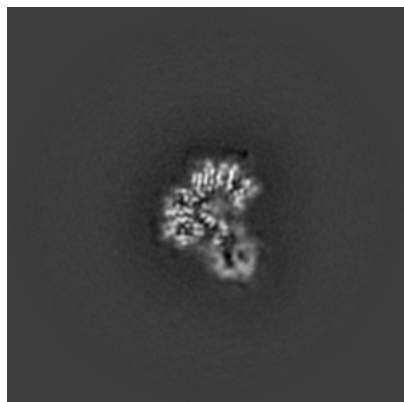


Z Index: 192

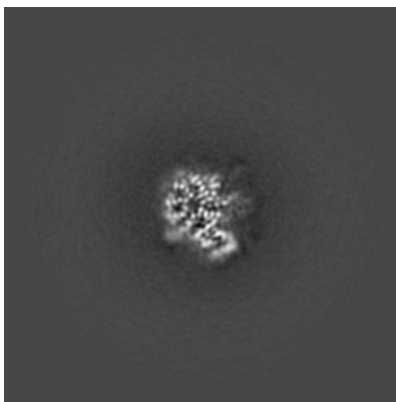
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

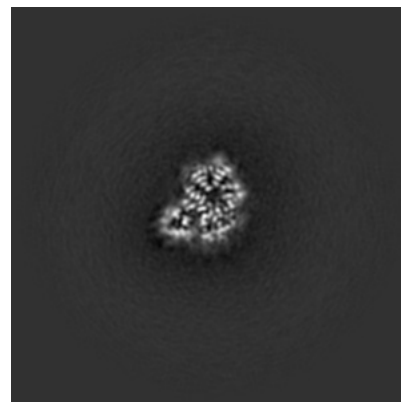
6.3.1 Primary map



X Index: 201

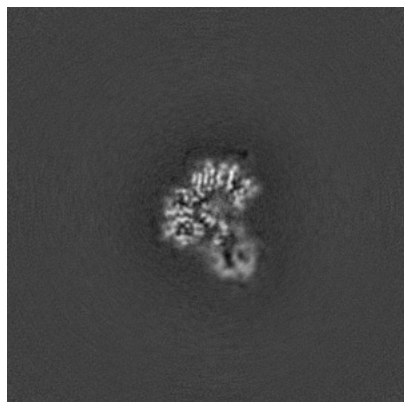


Y Index: 177

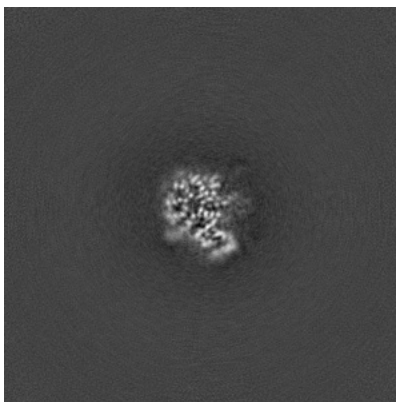


Z Index: 206

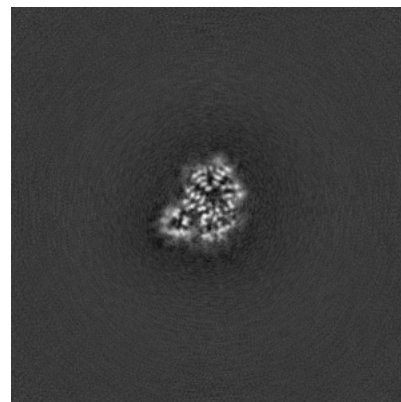
6.3.2 Raw map



X Index: 201



Y Index: 177

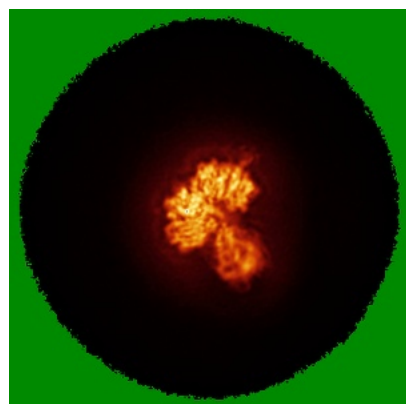


Z Index: 206

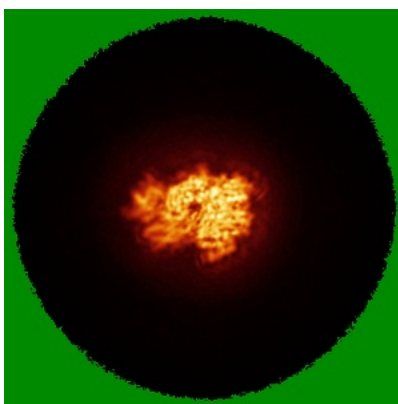
The images above show the largest variance slices of the map in three orthogonal directions.

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

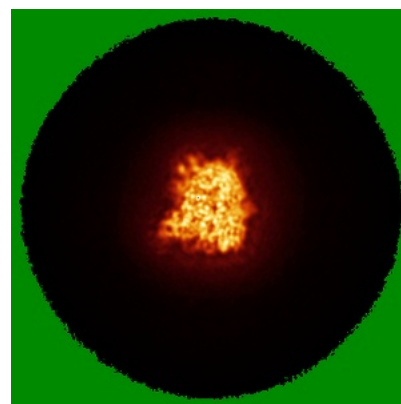
6.4.1 Primary map



X

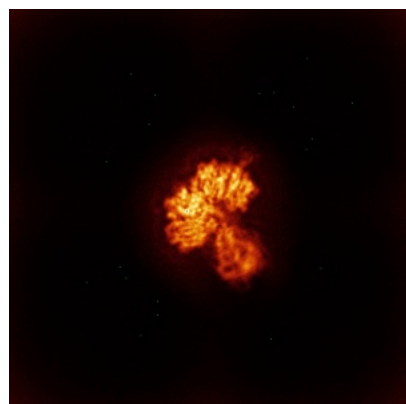


Y

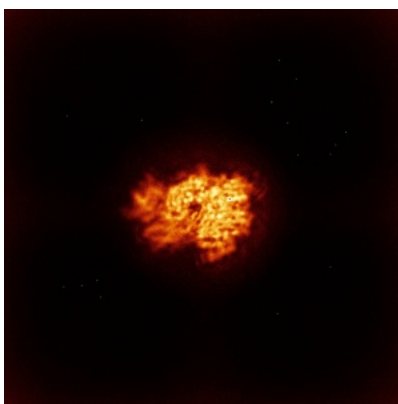


Z

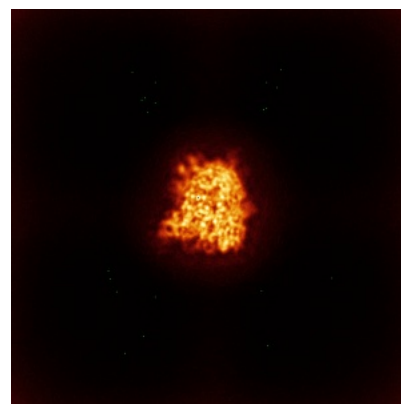
6.4.2 Raw map



X



Y

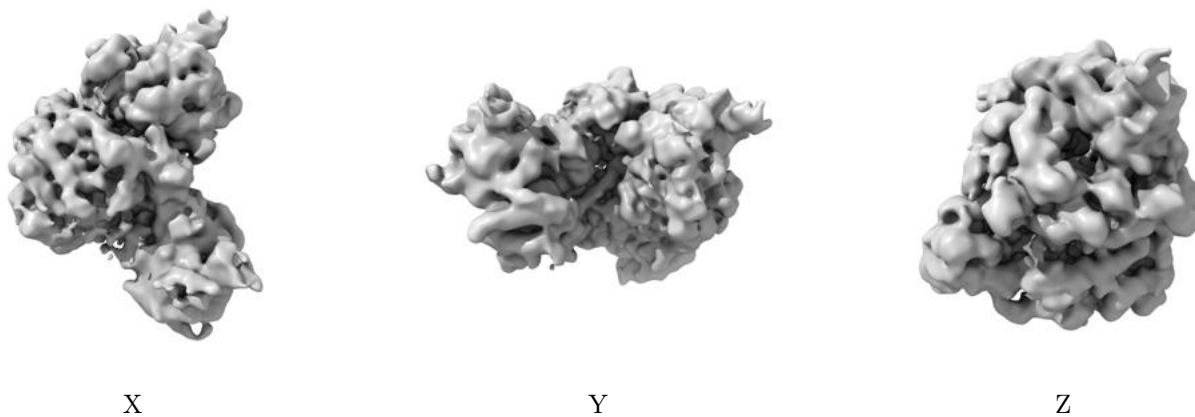


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

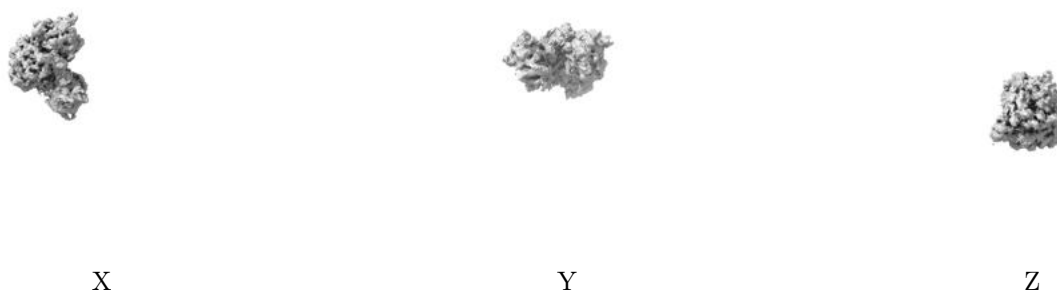
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.128. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

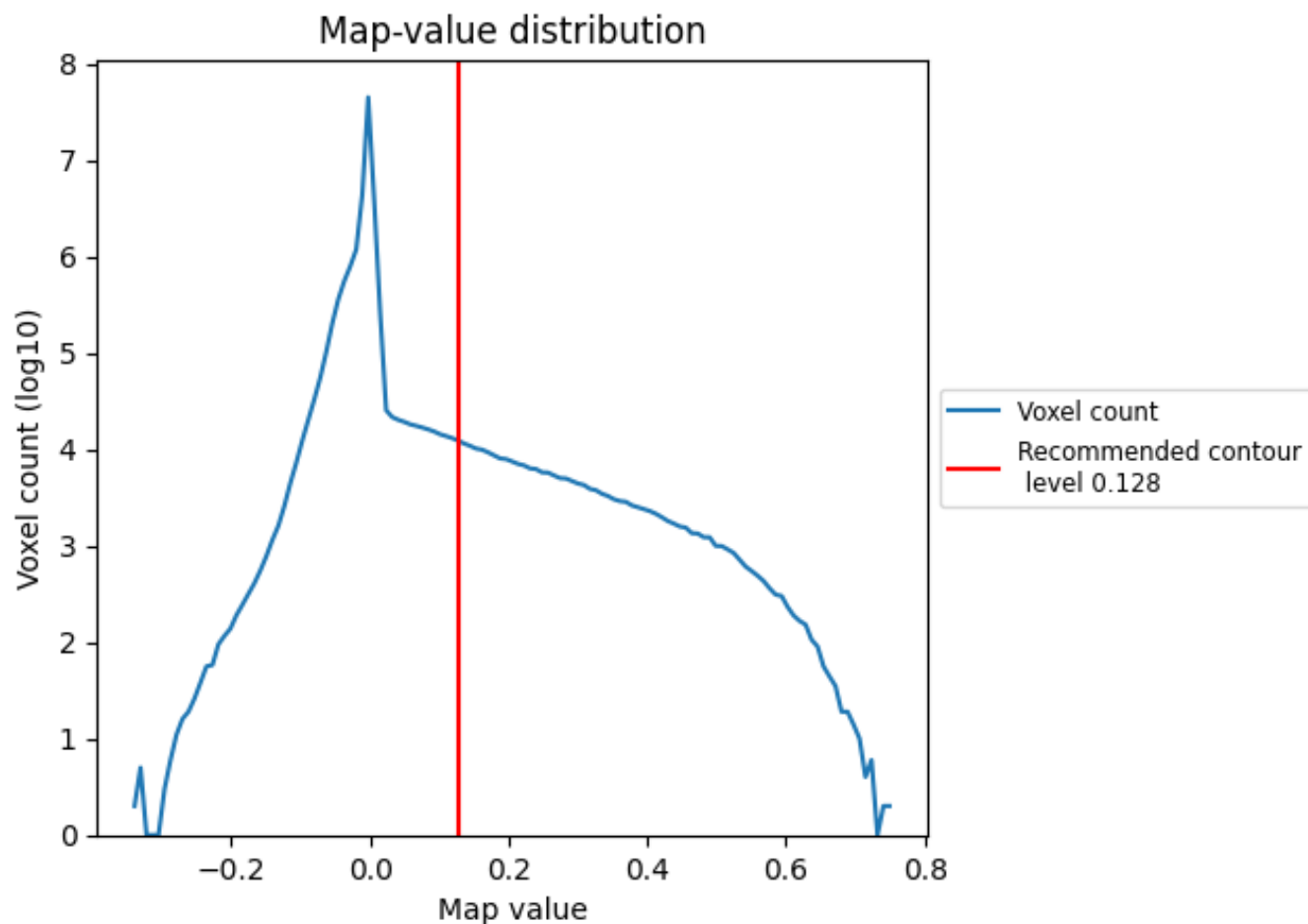
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

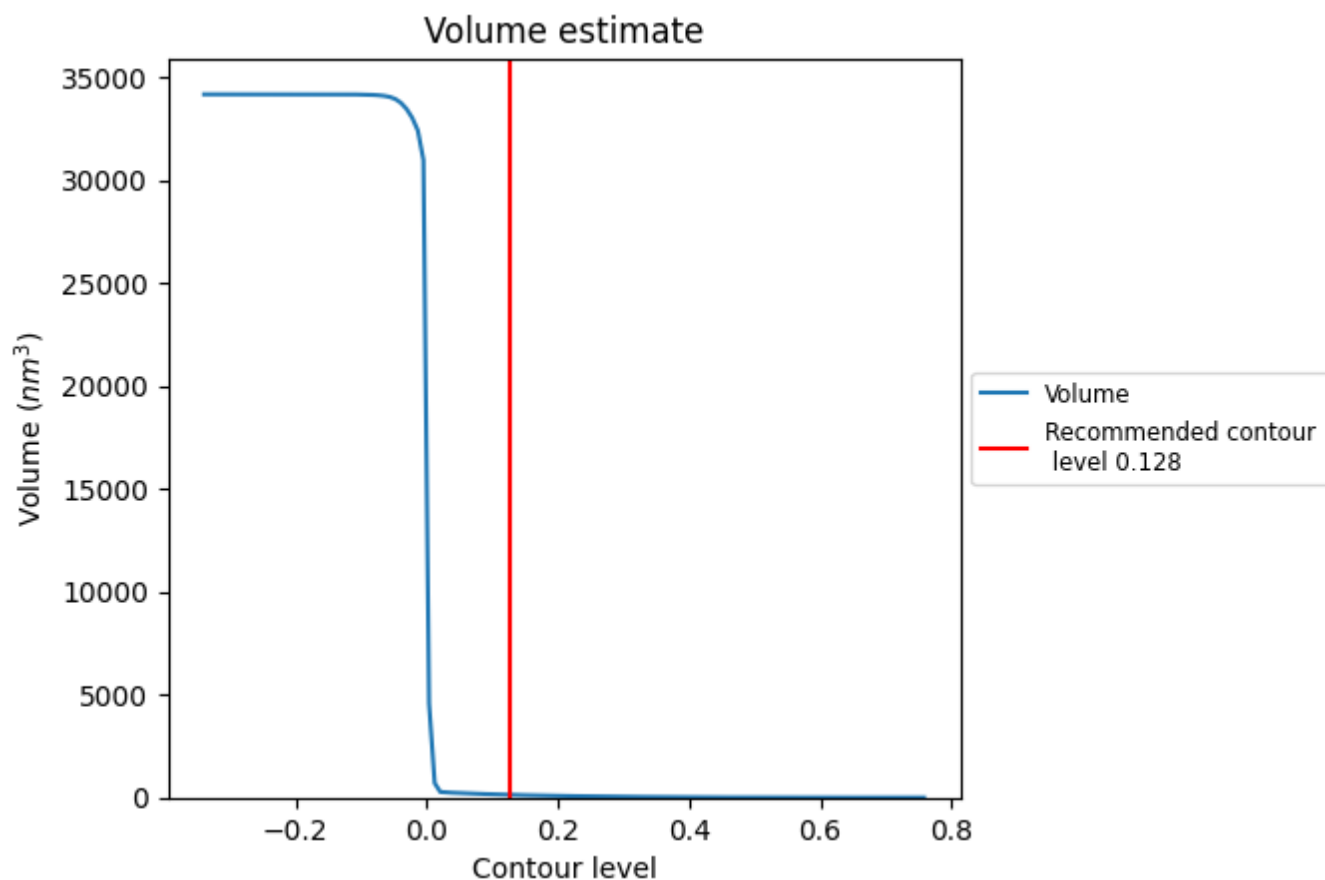
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

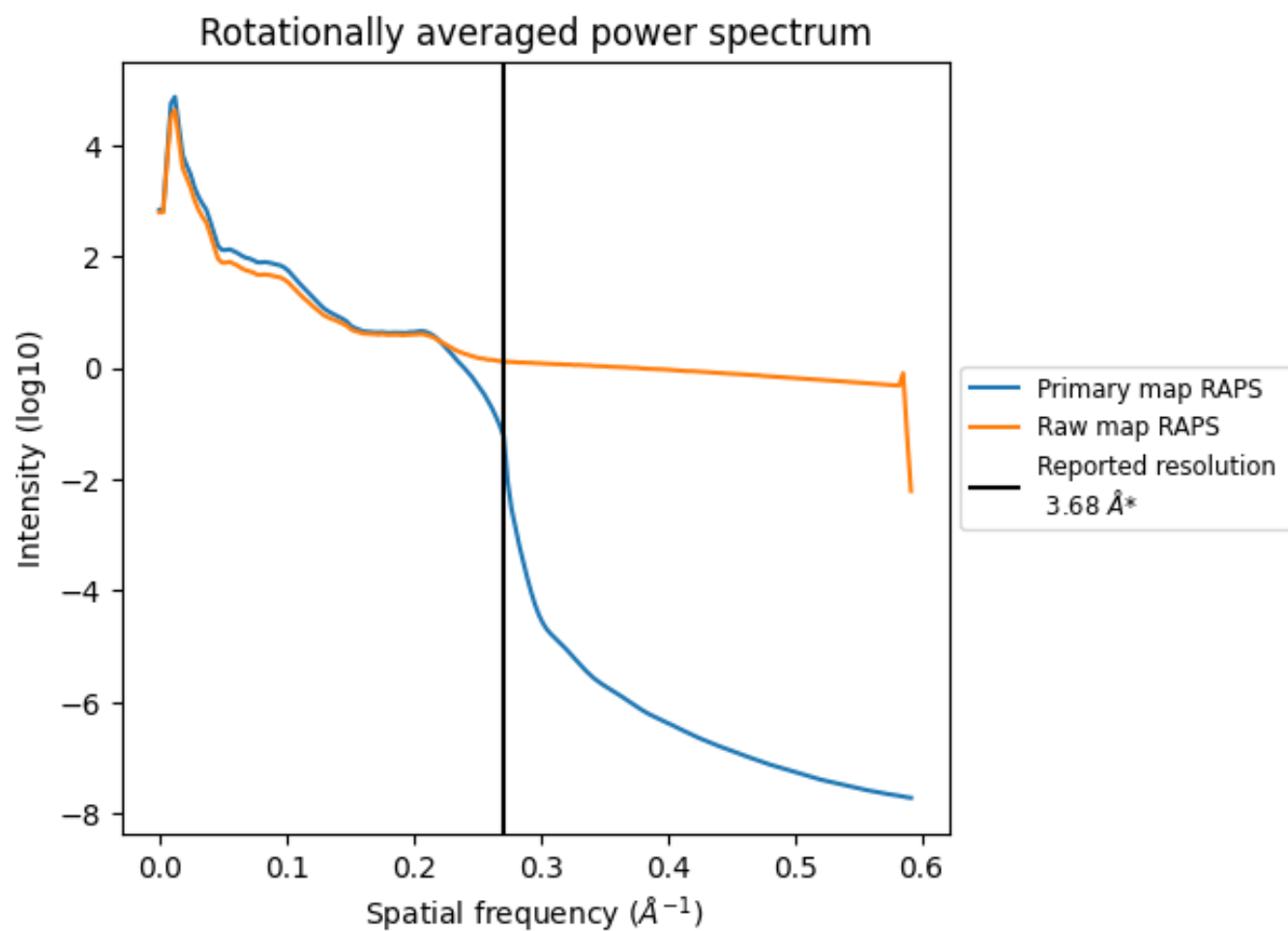
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm^3 ; this corresponds to an approximate mass of 119 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

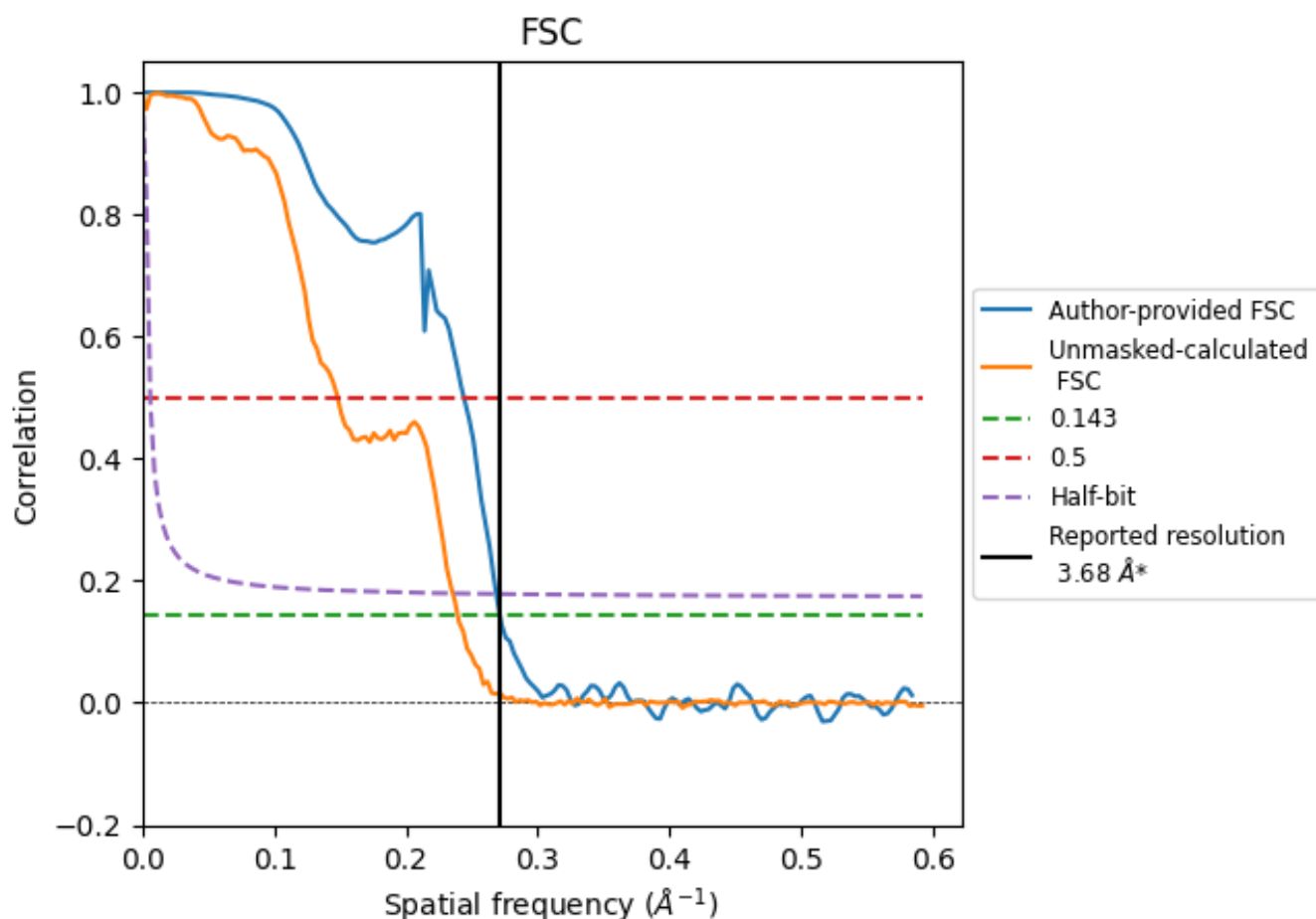


*Reported resolution corresponds to spatial frequency of 0.272 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.272 \AA^{-1}

8.2 Resolution estimates [i](#)

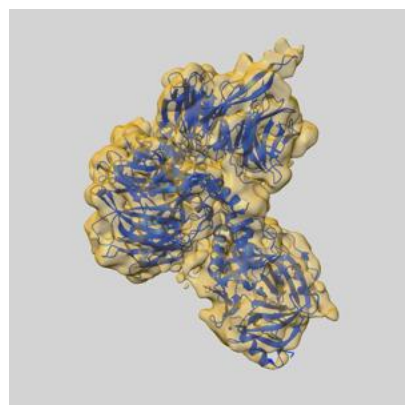
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.10	3.72
Unmasked-calculated*	4.18	6.74	4.24

*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 4.18 differs from the reported value 3.68 by more than 10 %

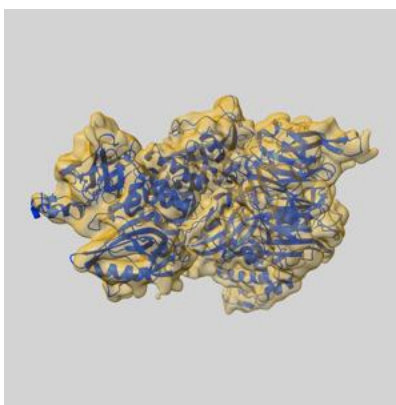
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55107 and PDB model 9SQ5. Per-residue inclusion information can be found in section [3](#) on page [8](#).

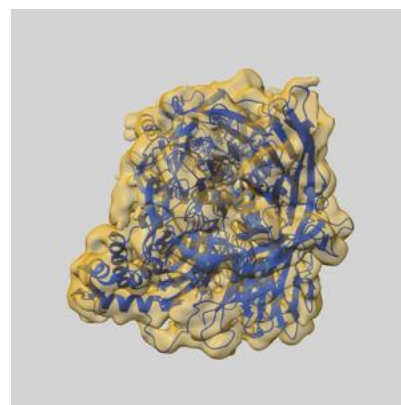
9.1 Map-model overlay [i](#)



X



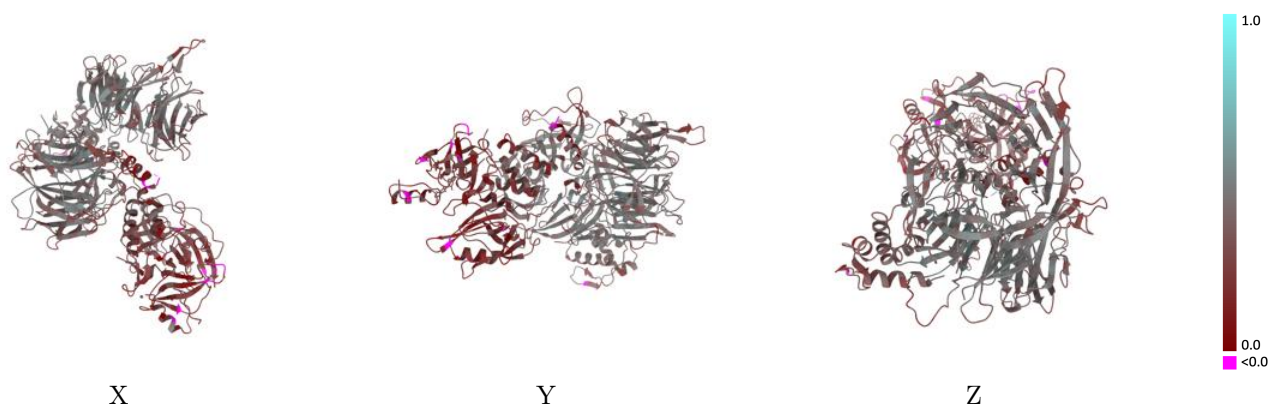
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.128 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



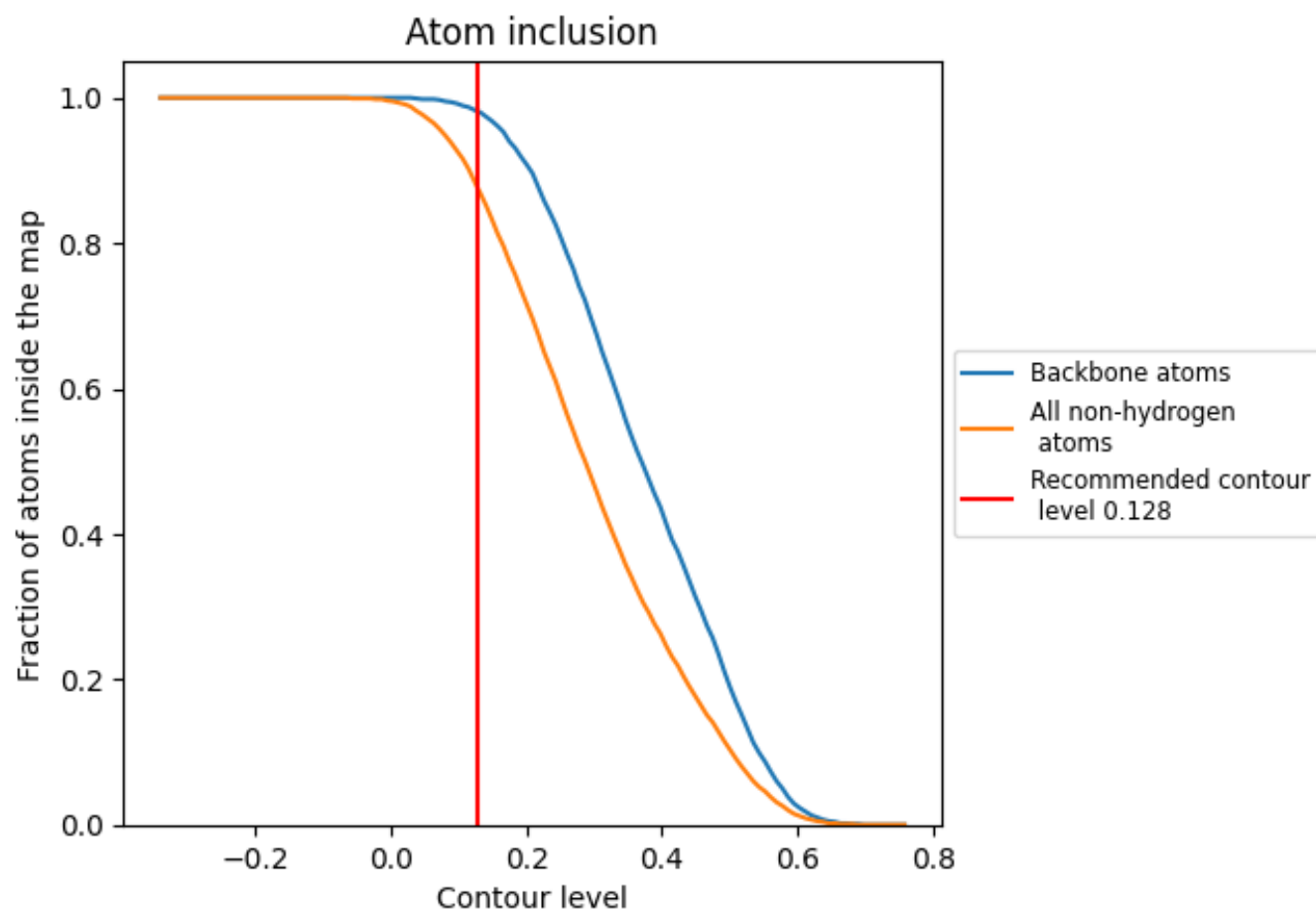
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.128).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.128) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8760	<div></div> 0.3440
A	<div></div> 0.9120	<div></div> 0.3970
B	<div></div> 0.8080	<div></div> 0.2350
C	<div></div> 0.6570	<div></div> 0.1840

